



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 06:03 PM EST

PDB ID : 1S5L
Title : Architecture of the photosynthetic oxygen evolving center
Authors : Ferreira, K.N.; Iverson, T.M.; Maghlaoui, K.; Barber, J.; Iwata, S.
Deposited on : 2004-01-21
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

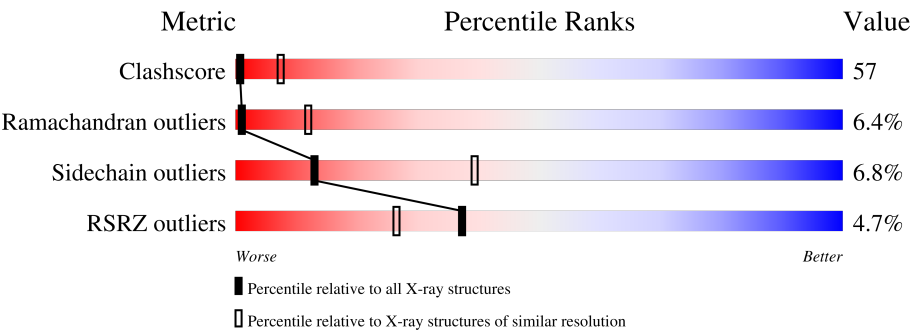
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div><div>4%</div><div>28%</div><div>57%</div><div>11%</div><div></div></div>
1	a	344	<div><div>4%</div><div>84%</div><div>12%</div><div></div></div>
2	B	510	<div><div>6%</div><div>30%</div><div>56%</div><div>6%</div><div>7%</div></div>
2	b	510	<div><div>4%</div><div>84%</div><div>9%</div><div>7%</div></div>
3	C	473	<div><div>4%</div><div>22%</div><div>57%</div><div>9%</div><div>11%</div></div>
3	c	473	<div><div>5%</div><div>79%</div><div>9%</div><div>11%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	246	
13	o	246	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	50	
17	x	50	
18	N	37	
18	n	37	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	348	X	-	-	-
23	CLA	A	349	X	-	-	-
23	CLA	A	350	X	-	-	-
23	CLA	A	352	X	-	-	-
23	CLA	B	511	X	-	-	-
23	CLA	B	512	X	-	-	-
23	CLA	B	513	X	-	-	-
23	CLA	B	514	X	-	-	-
23	CLA	B	515	X	-	-	-
23	CLA	B	516	X	-	-	-
23	CLA	B	517	X	-	-	-
23	CLA	B	518	X	-	-	-
23	CLA	B	519	X	-	-	-
23	CLA	B	520	X	-	-	-
23	CLA	B	521	X	-	-	-
23	CLA	B	522	X	-	-	-
23	CLA	B	523	X	-	-	-
23	CLA	B	524	X	-	X	-
23	CLA	B	525	X	-	-	-
23	CLA	B	527	X	-	-	-
23	CLA	C	474	X	-	-	-
23	CLA	C	475	X	-	-	-
23	CLA	C	476	X	-	-	-
23	CLA	C	477	X	-	-	-
23	CLA	C	478	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	479	X	-	-	-
23	CLA	C	480	X	-	-	-
23	CLA	C	481	X	-	-	-
23	CLA	C	482	X	-	-	-
23	CLA	C	483	X	-	-	-
23	CLA	C	484	X	-	-	-
23	CLA	C	485	X	-	-	-
23	CLA	C	486	X	-	-	-
23	CLA	C	487	X	-	-	-
23	CLA	D	354	X	-	-	-
23	CLA	D	356	X	-	-	-
23	CLA	a	2348	X	-	-	-
23	CLA	a	2349	X	-	-	-
23	CLA	a	2351	X	-	-	-
23	CLA	b	2511	X	-	-	-
23	CLA	b	2512	X	-	-	-
23	CLA	b	2513	X	-	-	-
23	CLA	b	2514	X	-	-	-
23	CLA	b	2515	X	-	-	-
23	CLA	b	2516	X	-	-	-
23	CLA	b	2517	X	-	-	-
23	CLA	b	2518	X	-	-	-
23	CLA	b	2519	X	-	-	-
23	CLA	b	2520	X	-	-	-
23	CLA	b	2521	X	-	-	-
23	CLA	b	2522	X	-	-	-
23	CLA	b	2523	X	-	-	-
23	CLA	b	2524	X	-	-	-
23	CLA	b	2525	X	-	-	-
23	CLA	b	2526	X	-	-	-
23	CLA	c	2474	X	-	-	-
23	CLA	c	2475	X	-	-	-
23	CLA	c	2476	X	-	-	-
23	CLA	c	2477	X	-	-	-
23	CLA	c	2478	X	-	-	-
23	CLA	c	2479	X	-	-	-
23	CLA	c	2480	X	-	-	-
23	CLA	c	2481	X	-	-	-
23	CLA	c	2482	X	-	-	-
23	CLA	c	2483	X	-	-	-
23	CLA	c	2484	X	-	-	-
23	CLA	c	2485	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	2486	X	-	-	-
23	CLA	c	2487	X	-	-	-
23	CLA	d	2354	X	-	-	-
23	CLA	d	2355	X	-	-	-
23	CLA	d	2357	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2616	1714	430	457	15			

- Molecule 2 is a protein called photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			
2	b	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			
3	c	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	insertion	UNP Q8DIF8
C	2	LYS	-	insertion	UNP Q8DIF8
C	3	THR	-	insertion	UNP Q8DIF8
C	4	LEU	-	insertion	UNP Q8DIF8
C	5	SER	-	insertion	UNP Q8DIF8
C	6	SER	-	insertion	UNP Q8DIF8
C	7	GLN	-	insertion	UNP Q8DIF8
C	8	LYS	-	insertion	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ARG	-	insertion	UNP Q8DIF8
C	10	TYR	-	insertion	UNP Q8DIF8
C	11	SER	-	insertion	UNP Q8DIF8
C	12	PRO	-	insertion	UNP Q8DIF8
C	13	VAL	-	insertion	UNP Q8DIF8
c	2001	MET	-	insertion	UNP Q8DIF8
c	2002	LYS	-	insertion	UNP Q8DIF8
c	2003	THR	-	insertion	UNP Q8DIF8
c	2004	LEU	-	insertion	UNP Q8DIF8
c	2005	SER	-	insertion	UNP Q8DIF8
c	2006	SER	-	insertion	UNP Q8DIF8
c	2007	GLN	-	insertion	UNP Q8DIF8
c	2008	LYS	-	insertion	UNP Q8DIF8
c	2009	ARG	-	insertion	UNP Q8DIF8
c	2010	TYR	-	insertion	UNP Q8DIF8
c	2011	SER	-	insertion	UNP Q8DIF8
c	2012	PRO	-	insertion	UNP Q8DIF8
c	2013	VAL	-	insertion	UNP Q8DIF8

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			
4	d	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			

- Molecule 5 is a protein called Cytochrome b559 alpha subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			624	411	99	114			
5	e	76	Total	C	N	O	0	0	0
			624	411	99	114			

- Molecule 6 is a protein called Cytochrome b559 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called photosystem II PsbH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			
7	h	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			

- Molecule 8 is a protein called Photosystem II reaction center I protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- Molecule 9 is a protein called Photosystem II reaction center J protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center L protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			
12	m	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			
13	o	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			

- Molecule 14 is a protein called photosystem II PsbT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			
14	t	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	105	Total	C	N	O		0	0	0
			827	521	137	169				
15	u	105	Total	C	N	O		0	0	0
			827	521	137	169				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called photosystem II PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O	0	0	0
			296	197	47	52			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	x	40	Total	C	N	O	0	0	0
			296	197	47	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	insertion	UNP Q9F1R6
X	2	ILE	-	insertion	UNP Q9F1R6
X	3	GLN	-	insertion	UNP Q9F1R6
X	4	SER	-	insertion	UNP Q9F1R6
X	5	ALA	-	insertion	UNP Q9F1R6
X	6	SER	-	insertion	UNP Q9F1R6
X	7	SER	-	insertion	UNP Q9F1R6
X	8	LEU	-	insertion	UNP Q9F1R6
X	9	LEU	-	insertion	UNP Q9F1R6
X	10	LEU	-	insertion	UNP Q9F1R6
x	2001	MET	-	insertion	UNP Q9F1R6
x	2002	ILE	-	insertion	UNP Q9F1R6
x	2003	GLN	-	insertion	UNP Q9F1R6
x	2004	SER	-	insertion	UNP Q9F1R6
x	2005	ALA	-	insertion	UNP Q9F1R6
x	2006	SER	-	insertion	UNP Q9F1R6
x	2007	SER	-	insertion	UNP Q9F1R6
x	2008	LEU	-	insertion	UNP Q9F1R6
x	2009	LEU	-	insertion	UNP Q9F1R6
x	2010	LEU	-	insertion	UNP Q9F1R6

- Molecule 18 is a protein called Photosystem II PsbN protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	37	Total	C	N	O	0	0	0
			186	111	37	38			
18	n	37	Total	C	N	O	0	0	0
			186	111	37	38			

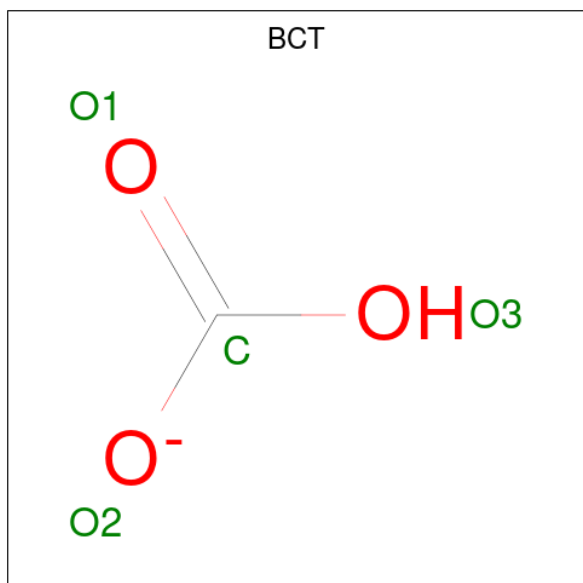
- Molecule 19 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			
19	z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe).

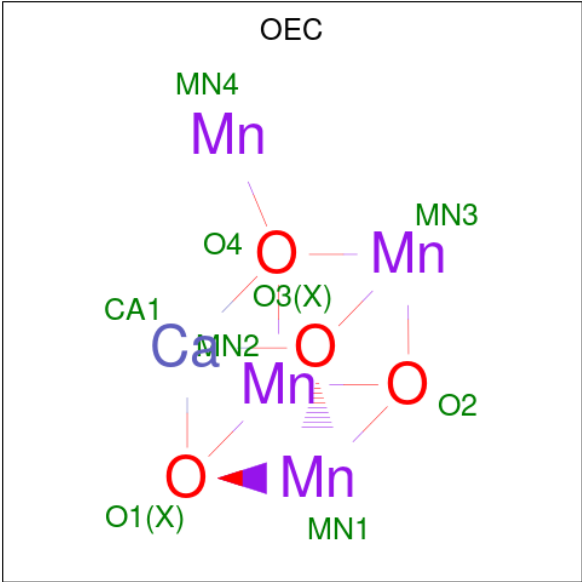
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



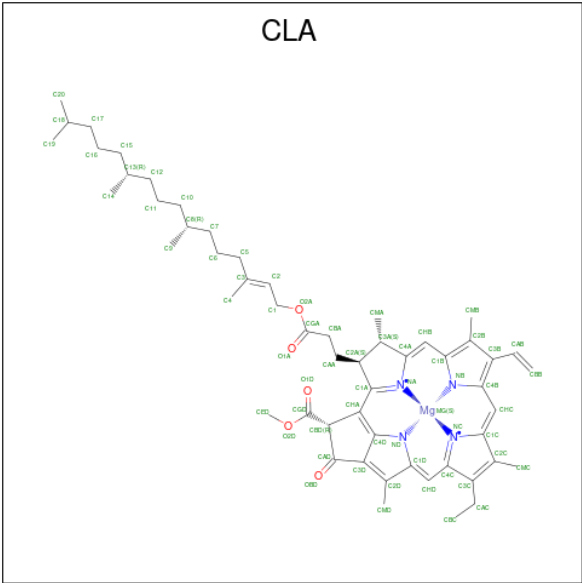
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	1	3		
21	D	1	Total	C	O	0	0
			4	1	3		
21	a	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	Ca	Mn	O	0	0
			9	1	4	4		
22	a	1	Total	Ca	Mn	O	0	0
			9	1	4	4		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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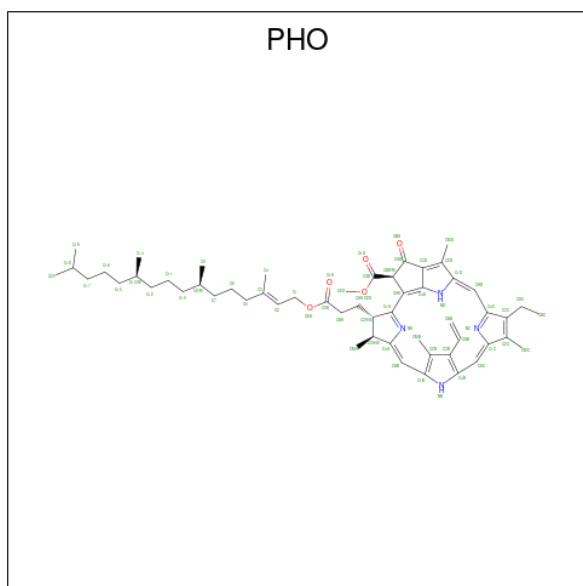
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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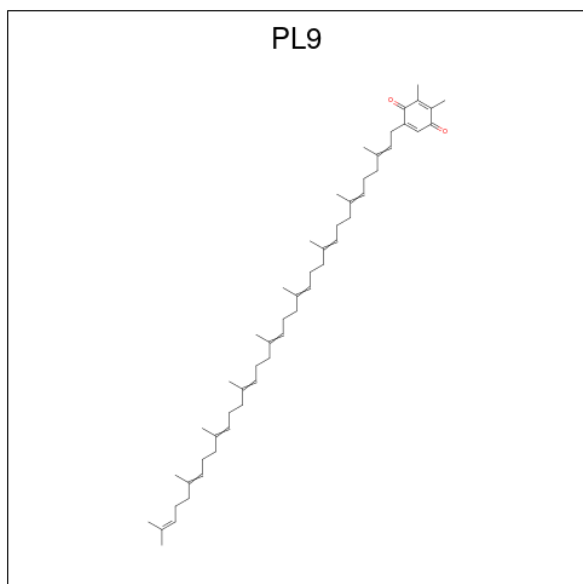
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



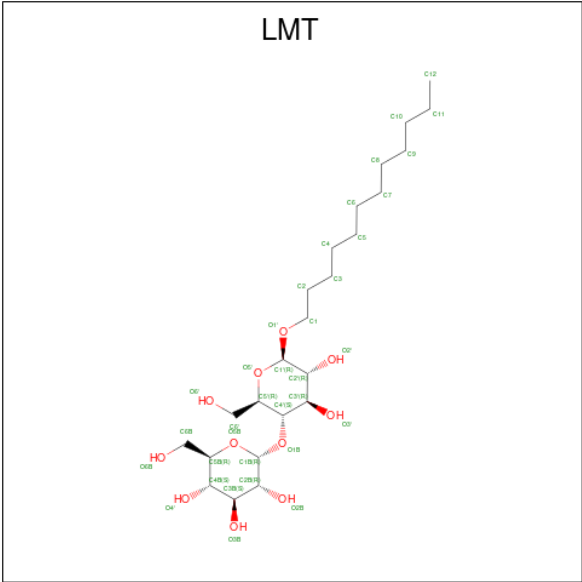
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



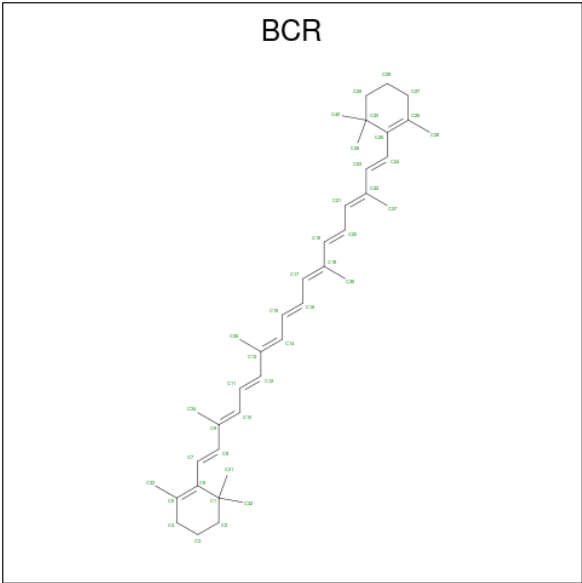
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			45	43	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			45	43	2		

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	B	1	Total	C	O	0
			35	24	11	
26	d	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



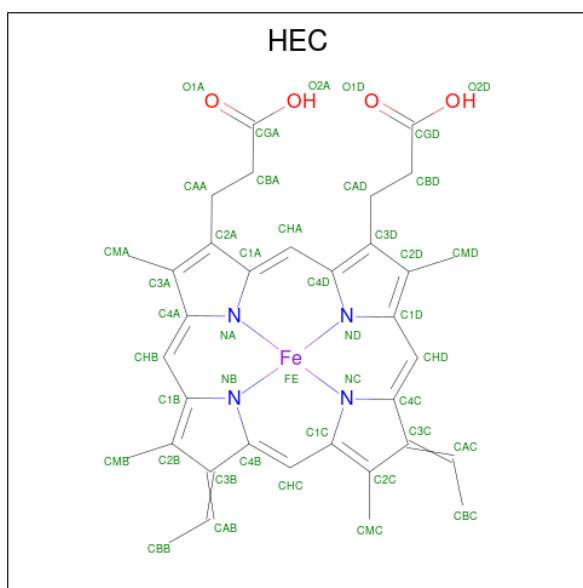
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	C		0
			40	40		
27	B	1	Total	C		0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	F	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

- Molecule 28 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).

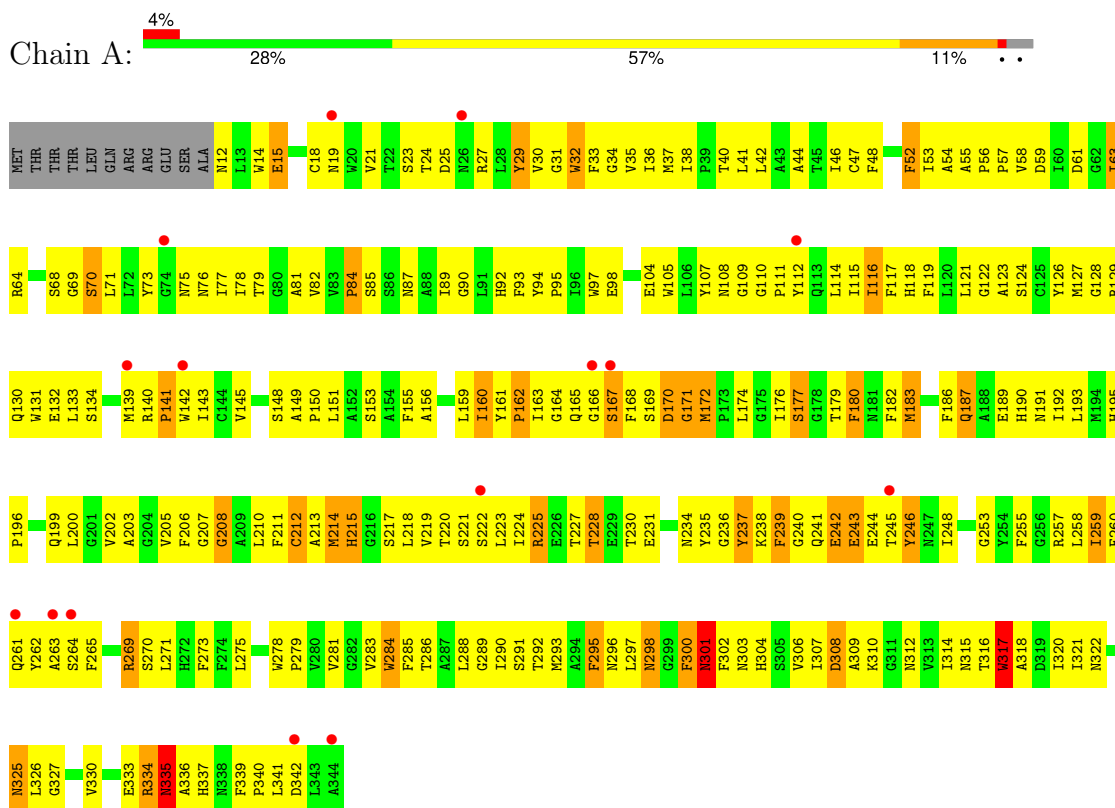


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

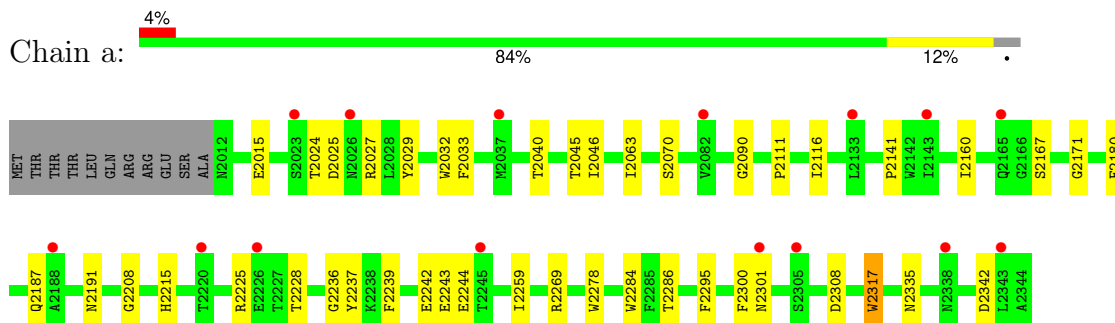
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem Q(B) protein

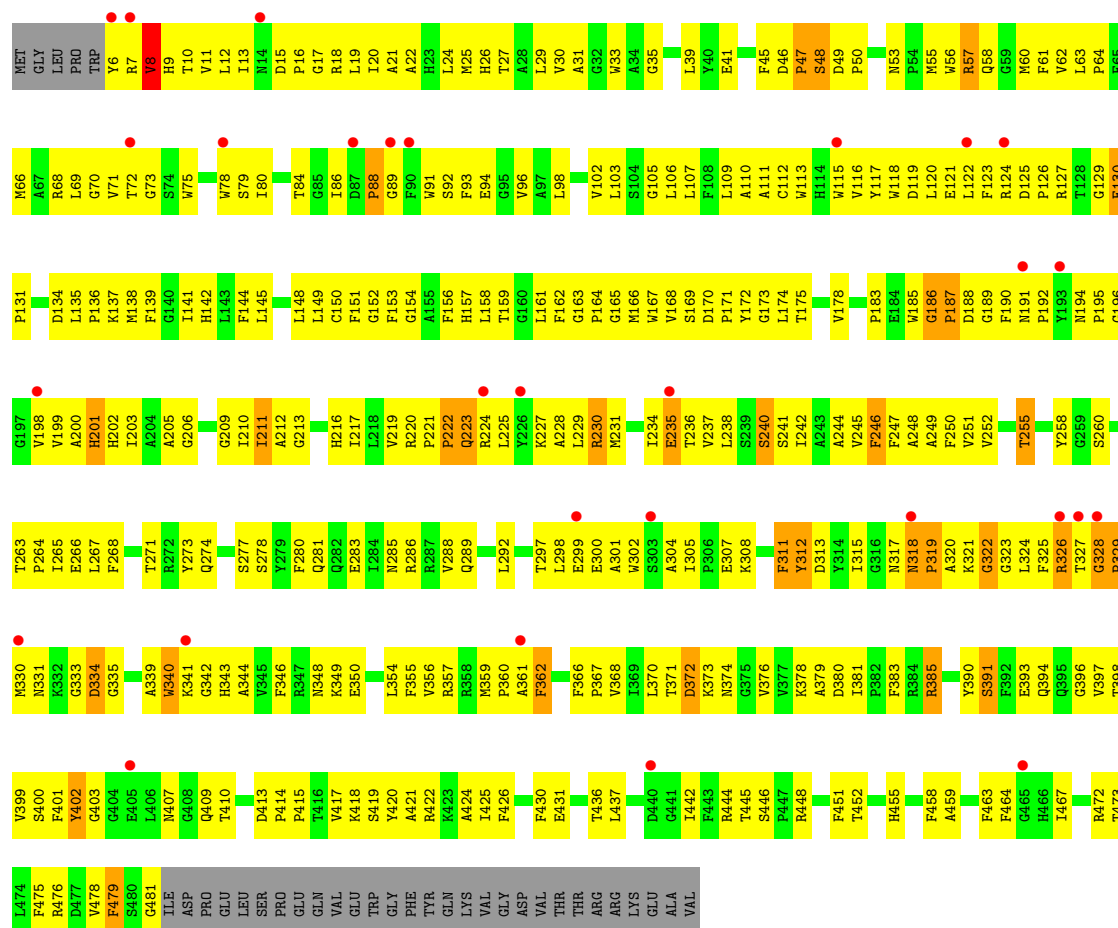


- Molecule 1: Photosystem Q(B) protein




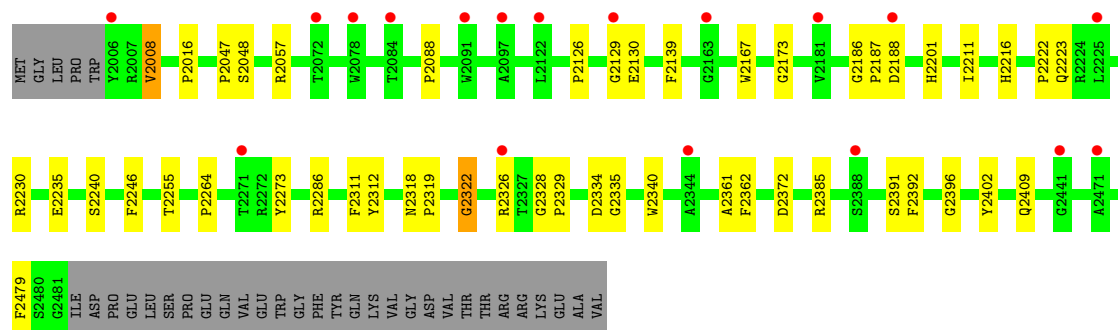
- Molecule 2: photosystem II core light harvesting protein

Chain B: 



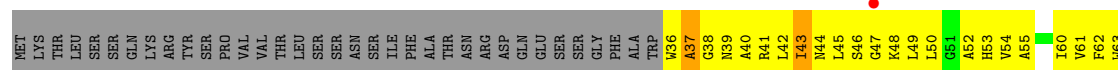
• Molecule 2: photosystem II core light harvesting protein

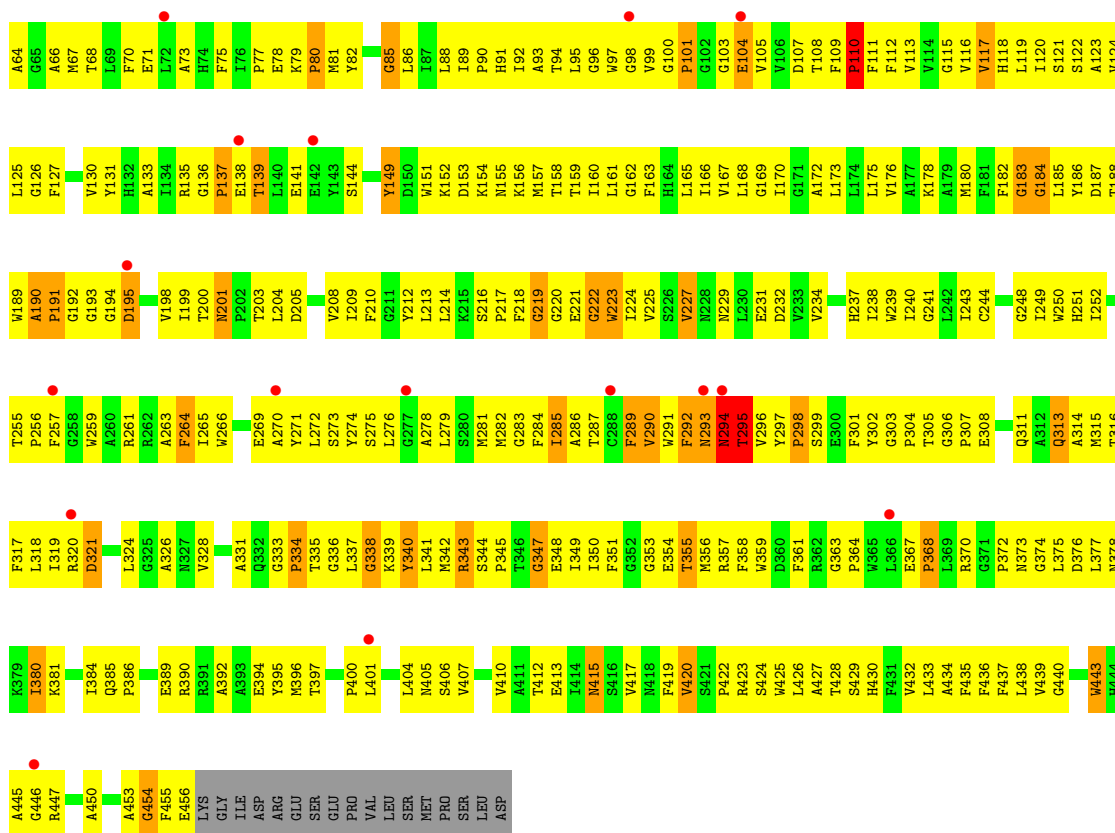
Chain b: 



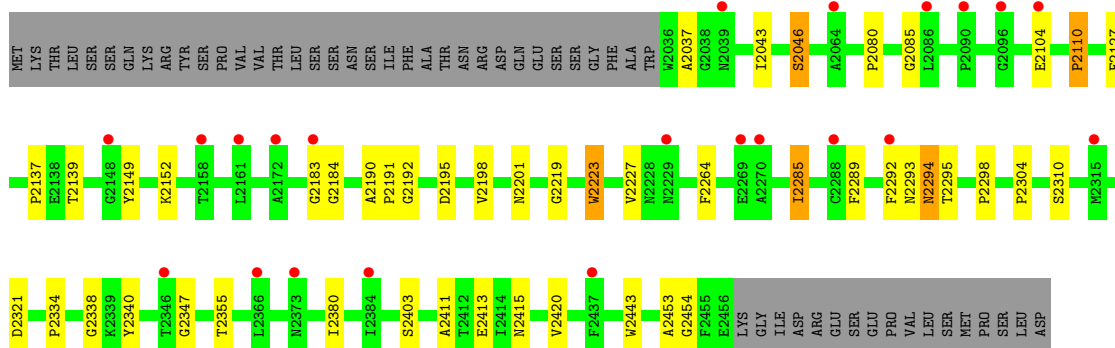
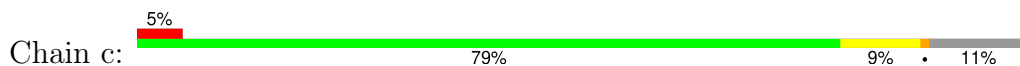
• Molecule 3: photosystem II CP43 protein

Chain C: 

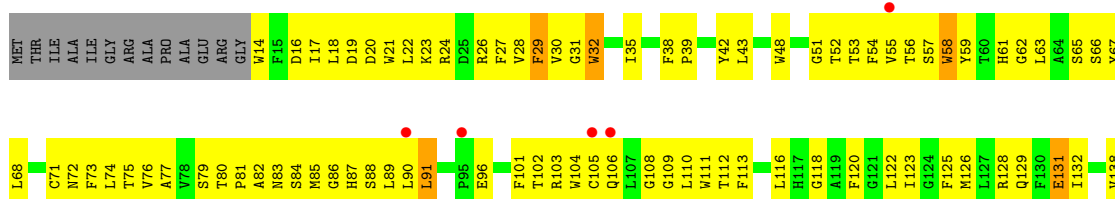


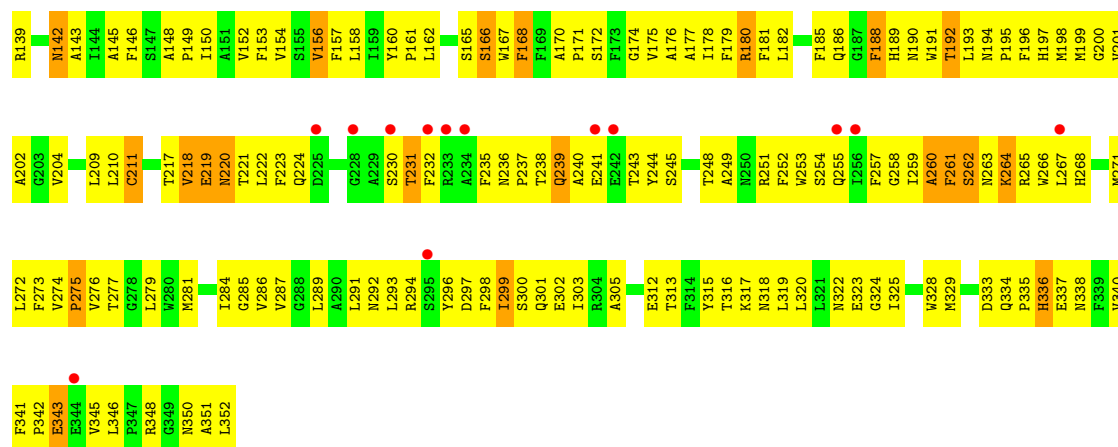


• Molecule 3: photosystem II CP43 protein

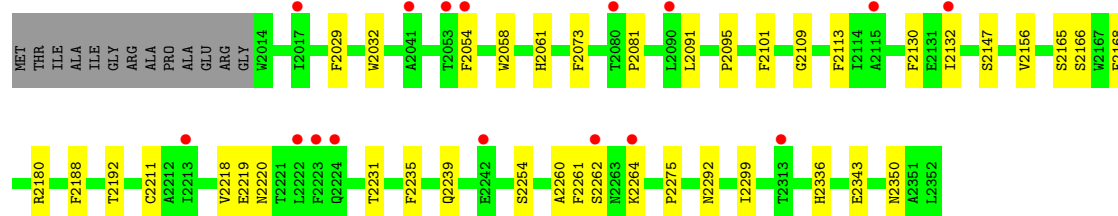
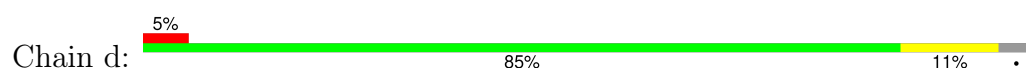


• Molecule 4: photosystem II reaction center D2 protein

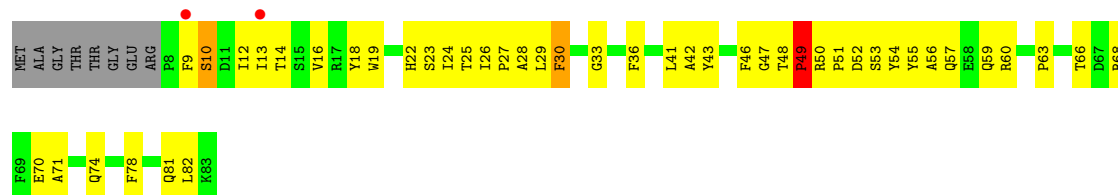




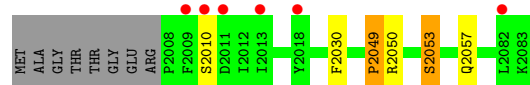
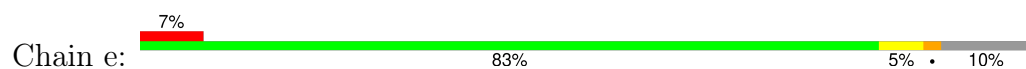
- Molecule 4: photosystem II reaction center D2 protein



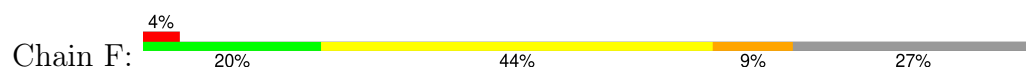
- Molecule 5: Cytochrome b559 alpha subunit



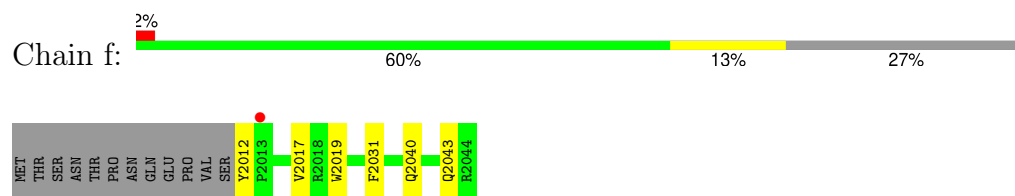
- Molecule 5: Cytochrome b559 alpha subunit



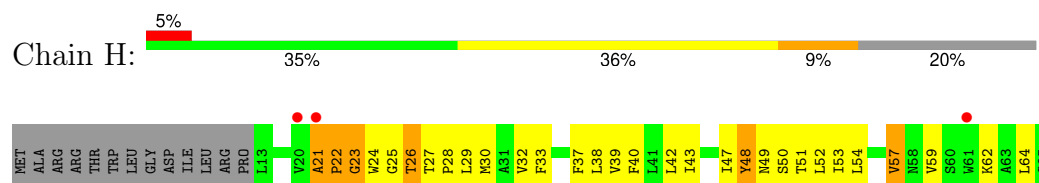
- Molecule 6: Cytochrome b559 beta subunit



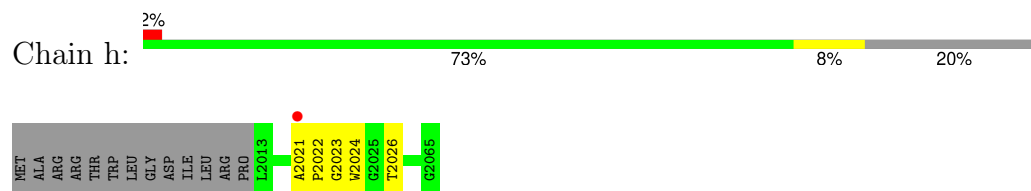
- Molecule 6: Cytochrome b559 beta subunit



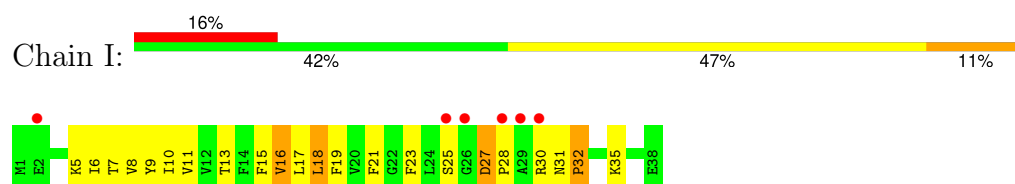
- Molecule 7: photosystem II PsbH protein



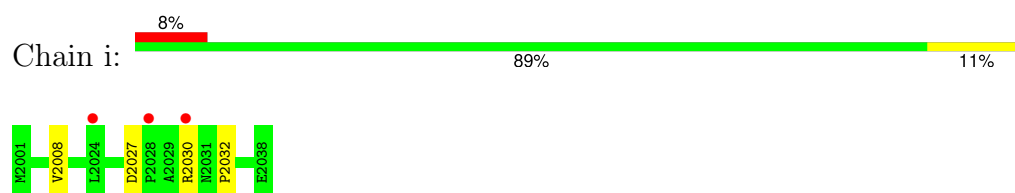
- Molecule 7: photosystem II PsbH protein



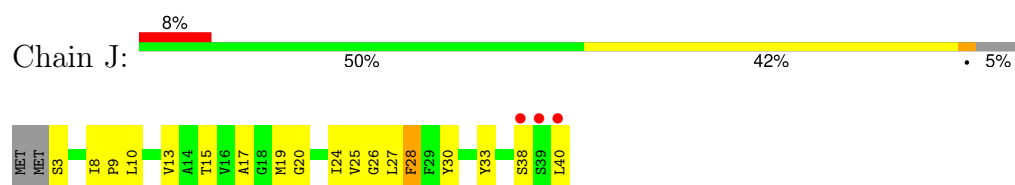
- Molecule 8: Photosystem II reaction center I protein



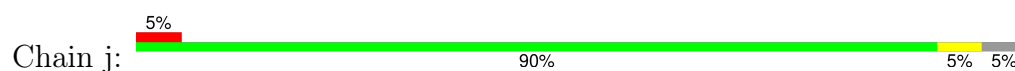
- Molecule 8: Photosystem II reaction center I protein



- Molecule 9: Photosystem II reaction center J protein

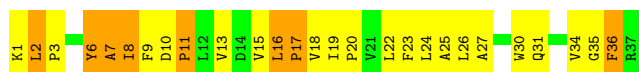
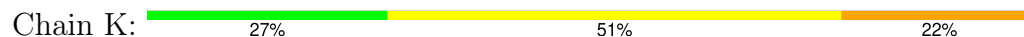


- Molecule 9: Photosystem II reaction center J protein

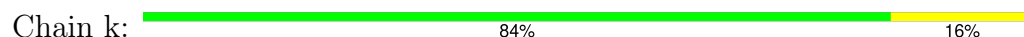




- Molecule 10: Photosystem II reaction center protein K



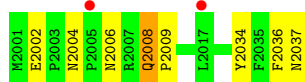
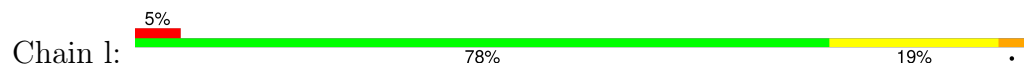
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center L protein



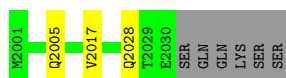
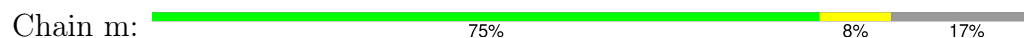
- Molecule 11: Photosystem II reaction center L protein



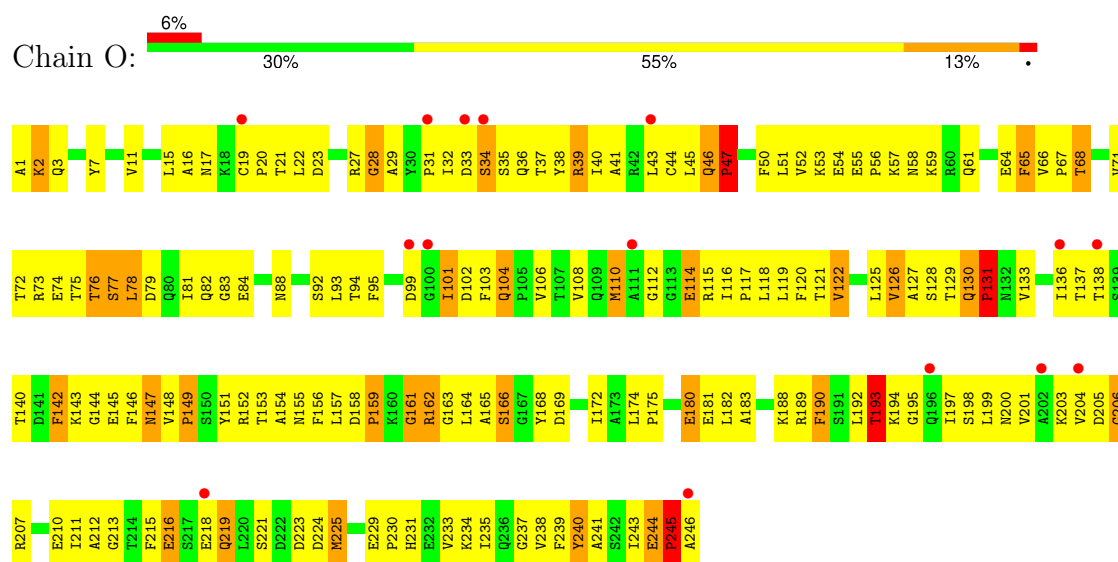
- Molecule 12: Photosystem II reaction center M protein



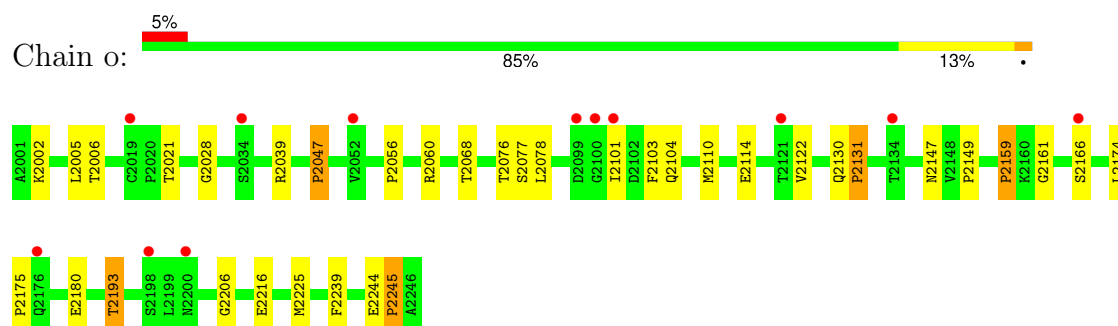
- Molecule 12: Photosystem II reaction center M protein



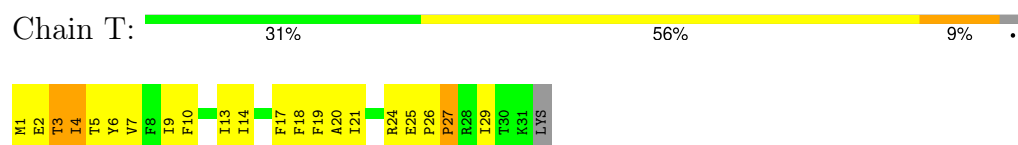
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



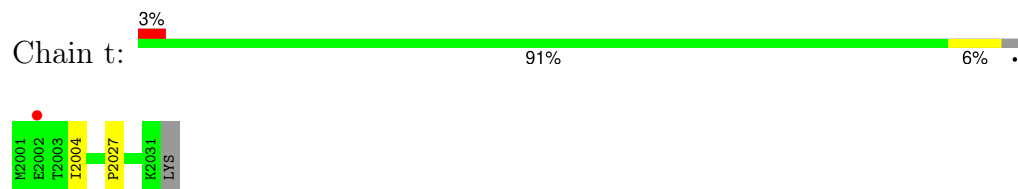
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



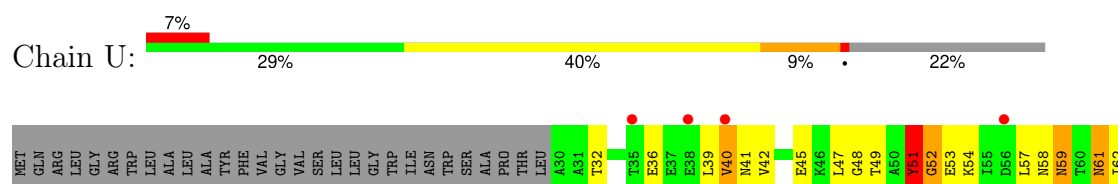
• Molecule 14: photosystem II PsbT protein

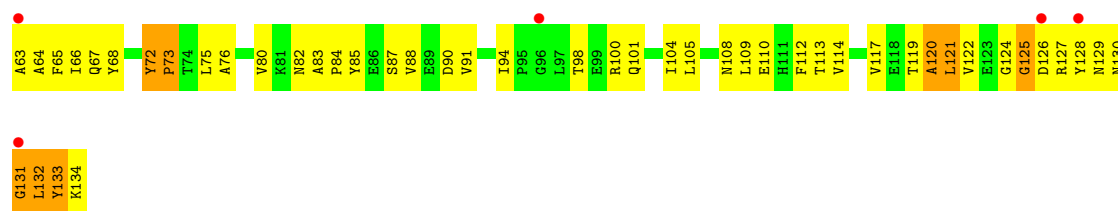


• Molecule 14: photosystem II PsbT protein

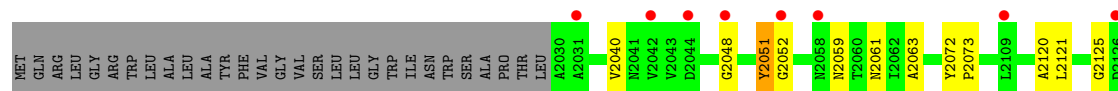


• Molecule 15: Photosystem II 12 kDa extrinsic protein

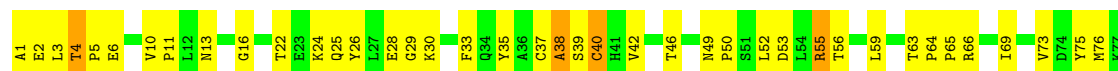




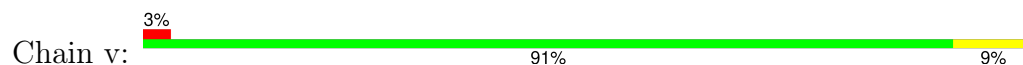
• Molecule 15: Photosystem II 12 kDa extrinsic protein



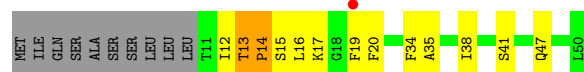
• Molecule 16: Cytochrome c-550



• Molecule 16: Cytochrome c-550



• Molecule 17: photosystem II PsbX protein

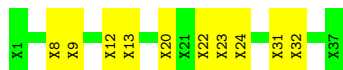


• Molecule 17: photosystem II PsbX protein

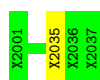




- Molecule 18: Photosystem II PsbN protein



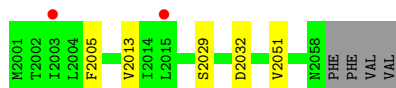
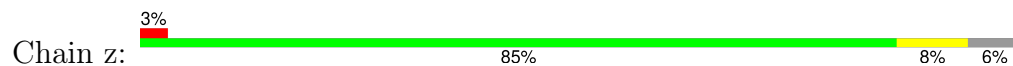
- Molecule 18: Photosystem II PsbN protein



- Molecule 19: Photosystem II reaction center Z protein



- Molecule 19: Photosystem II reaction center Z protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 228.85Å 309.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 85.2 (20.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.342 0.309 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	45945	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FE, CLA, OEC, PL9, BCR, BCT, PHO, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/2702	0.85	2/3685 (0.1%)
1	a	0.62	0/2701	0.83	2/3685 (0.1%)
2	B	0.57	0/3870	0.80	3/5271 (0.1%)
2	b	0.56	0/3870	0.80	4/5271 (0.1%)
3	C	0.60	0/3361	0.81	3/4579 (0.1%)
3	c	0.57	0/3361	0.80	3/4579 (0.1%)
4	D	0.62	0/2797	0.82	1/3813 (0.0%)
4	d	0.62	0/2797	0.83	2/3813 (0.1%)
5	E	0.59	0/643	0.89	1/876 (0.1%)
5	e	0.61	0/643	0.87	1/876 (0.1%)
6	F	0.74	0/278	0.84	0/379
6	f	0.68	0/278	0.84	0/379
7	H	0.58	0/419	0.81	0/570
7	h	0.60	0/419	0.81	0/570
8	I	0.63	0/319	0.73	0/429
8	i	0.61	0/319	0.73	0/429
9	J	0.60	0/278	0.80	0/376
9	j	0.62	0/278	0.84	0/376
10	K	0.66	0/303	0.92	0/416
10	k	0.63	0/303	0.86	0/416
11	L	0.74	1/311 (0.3%)	0.87	0/422
11	l	0.73	1/311 (0.3%)	0.91	0/422
12	M	0.63	0/237	0.77	0/324
12	m	0.70	0/237	0.80	0/324
13	O	0.67	0/1919	0.97	4/2601 (0.2%)
13	o	0.68	0/1919	0.96	3/2601 (0.1%)
14	T	0.71	0/274	0.78	0/370
14	t	0.74	0/274	0.80	0/370
15	U	0.68	0/838	0.91	1/1137 (0.1%)
15	u	0.62	0/838	0.87	0/1137
16	V	0.62	0/1085	0.78	0/1473
16	v	0.56	0/1085	0.77	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.57	0/299	0.72	0/403
17	x	0.61	0/299	0.75	0/403
19	Z	0.54	0/451	0.74	0/617
19	z	0.54	0/451	0.72	0/617
All	All	0.61	2/40767 (0.0%)	0.83	30/55482 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	b	0	1
11	l	0	1
13	O	0	1
15	U	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	2037	ASN	C-OXT	5.21	1.33	1.23
11	L	37	ASN	C-OXT	5.18	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2171	GLY	N-CA-C	-7.28	94.91	113.10
1	A	171	GLY	N-CA-C	-7.27	94.93	113.10
13	O	131	PRO	N-CA-C	6.48	128.95	112.10
1	a	2236	GLY	N-CA-C	6.41	129.12	113.10
4	D	231	THR	N-CA-C	-6.30	93.98	111.00
1	A	236	GLY	N-CA-C	6.29	128.83	113.10
4	d	2231	THR	N-CA-C	-6.18	94.30	111.00
13	o	2131	PRO	N-CA-C	6.08	127.89	112.10
2	B	129	GLY	N-CA-C	-5.90	98.35	113.10
2	b	2129	GLY	N-CA-C	-5.73	98.78	113.10
15	U	121	LEU	CA-CB-CG	-5.67	102.25	115.30
13	o	2193	THR	N-CA-C	5.46	125.75	111.00
13	o	2002	LYS	N-CA-C	5.42	125.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	2335	GLY	N-CA-C	-5.40	99.60	113.10
13	O	193	THR	N-CA-C	5.36	125.47	111.00
3	C	222	GLY	N-CA-C	-5.31	99.83	113.10
2	b	2329	PRO	N-CA-C	-5.25	98.46	112.10
2	B	329	PRO	N-CA-C	-5.23	98.49	112.10
3	c	2294	ASN	N-CA-C	-5.23	96.88	111.00
5	e	2053	SER	N-CA-C	5.22	125.10	111.00
2	B	335	GLY	N-CA-C	-5.19	100.13	113.10
13	O	23	ASP	N-CA-C	5.18	125.00	111.00
3	c	2223	TRP	CA-CB-CG	5.17	123.53	113.70
4	d	2054	PHE	N-CA-C	5.17	124.96	111.00
3	C	347	GLY	N-CA-C	5.12	125.91	113.10
3	C	294	ASN	N-CA-C	-5.11	97.19	111.00
13	O	2	LYS	N-CA-C	5.11	124.80	111.00
2	b	2322	GLY	N-CA-C	5.10	125.84	113.10
3	c	2347	GLY	N-CA-C	5.08	125.80	113.10
5	E	53	SER	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain
2	B	273	TYR	Sidechain
13	O	240	TYR	Sidechain
15	U	133	TYR	Sidechain
15	U	51	TYR	Sidechain
2	b	2273	TYR	Sidechain
11	l	2034	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	451	0
1	a	2616	0	2514	0	0
2	B	3739	0	3613	450	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3739	0	3613	0	0
3	C	3253	0	3192	532	0
3	c	3253	0	3192	0	0
4	D	2702	0	2605	412	0
4	d	2702	0	2605	0	0
5	E	624	0	613	96	0
5	e	624	0	613	0	0
6	F	269	0	277	45	0
6	f	269	0	277	0	0
7	H	409	0	424	52	0
7	h	409	0	424	0	0
8	I	312	0	329	25	0
8	i	312	0	326	0	0
9	J	272	0	279	43	0
9	j	272	0	279	0	0
10	K	293	0	308	57	0
10	k	293	0	305	0	0
11	L	304	0	316	49	0
11	l	304	0	313	0	0
12	M	234	0	255	32	0
12	m	234	0	252	0	0
13	O	1888	0	1867	274	6
13	o	1888	0	1864	0	0
14	T	265	0	275	41	0
14	t	265	0	272	0	0
15	U	827	0	819	121	0
15	u	827	0	819	0	0
16	V	1064	0	1075	123	0
16	v	1064	0	1070	0	0
17	X	296	0	328	14	0
17	x	296	0	328	0	0
18	N	186	0	40	10	0
18	n	186	0	40	0	6
19	Z	442	0	480	61	0
19	z	442	0	477	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	4	0	0	0	0
21	D	4	0	0	0	0
21	a	4	0	0	0	0
21	d	4	0	0	0	0
22	A	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	9	0	0	0	0
23	A	260	0	288	29	0
23	B	1040	0	1152	116	0
23	C	910	0	1008	104	0
23	D	130	0	144	18	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	910	0	1008	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	8	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	45	0	61	8	0
25	D	45	0	61	5	0
25	a	45	0	61	0	0
25	d	45	0	61	0	0
26	B	35	0	46	0	0
26	d	35	0	46	0	0
27	B	80	0	112	16	0
27	C	80	0	112	23	0
27	F	40	0	56	3	0
27	J	40	0	56	2	0
27	K	40	0	56	13	0
27	b	80	0	112	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	j	40	0	56	0	0
27	k	40	0	56	0	0
28	E	43	0	32	19	0
28	V	43	0	32	8	0
28	e	43	0	32	0	0
28	v	43	0	31	0	0
All	All	45945	0	45919	2601	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (2601) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:138:HEC:C2B	28:V:138:HEC:CMB	1.74	1.58
28:V:138:HEC:C2C	28:V:138:HEC:CMC	1.75	1.57
16:V:37:CYS:SG	28:V:138:HEC:HAB	1.57	1.44
5:E:12:ILE:CG2	5:E:18:TYR:HB2	1.44	1.43
5:E:12:ILE:HD12	28:E:84:HEC:O2D	1.31	1.25
6:F:40:GLN:NE2	9:J:27:LEU:HG	1.52	1.24
5:E:12:ILE:HG22	5:E:18:TYR:CB	1.71	1.21
13:O:40:ILE:HG12	13:O:84:GLU:OE1	1.07	1.19
2:B:75:TRP:H	2:B:94:GLU:HG3	1.07	1.18
3:C:158:THR:HG22	3:C:251:HIS:HB3	1.23	1.17
5:E:14:THR:HG22	9:J:8:ILE:HB	1.24	1.16
3:C:158:THR:CG2	3:C:251:HIS:HB3	1.75	1.16
6:F:39:MET:O	6:F:42:ILE:HG22	1.47	1.14
2:B:326:ARG:CD	2:B:327:THR:H	1.61	1.14
5:E:12:ILE:CD1	28:E:84:HEC:O2D	1.96	1.12
13:O:122:VAL:HA	13:O:146:PHE:CE2	1.85	1.12
3:C:308:GLU:HG2	3:C:361:PHE:CE1	1.85	1.10
5:E:60:ARG:HH22	16:V:129:LYS:HE3	1.05	1.10
3:C:455:PHE:HE1	4:D:224:GLN:HA	1.07	1.10
3:C:138:GLU:HG2	3:C:139:THR:H	1.09	1.09
13:O:146:PHE:HB2	13:O:195:GLY:HA3	1.10	1.09
4:D:298:PHE:HA	11:L:37:ASN:HD21	0.93	1.09
4:D:298:PHE:HA	11:L:37:ASN:ND2	1.67	1.09
5:E:14:THR:CG2	9:J:8:ILE:HB	1.83	1.08
1:A:186:PHE:HD2	1:A:192:ILE:HD11	1.05	1.08
3:C:344:SER:HB3	3:C:350:ILE:HD11	1.34	1.08
13:O:130:GLN:HB3	13:O:131:PRO:CD	1.83	1.08
3:C:223:TRP:CD1	3:C:224:ILE:HG13	1.90	1.07
5:E:12:ILE:HG22	5:E:18:TYR:HB2	1.10	1.07
15:U:57:LEU:HD21	15:U:112:PHE:HD2	1.02	1.07
16:V:37:CYS:SG	28:V:138:HEC:CAB	2.41	1.07
5:E:10:SER:HA	5:E:13:ILE:HD12	1.37	1.07
1:A:150:PRO:HB2	23:A:348:CLA:H62	1.38	1.06
15:U:59:ASN:HD22	15:U:59:ASN:N	1.33	1.06
5:E:14:THR:CG2	9:J:8:ILE:HD12	1.85	1.06
13:O:121:THR:HG21	13:O:148:VAL:HG22	1.37	1.06
13:O:40:ILE:CG1	13:O:84:GLU:OE1	2.04	1.05
2:B:326:ARG:HD2	2:B:327:THR:H	0.88	1.05
5:E:60:ARG:NH2	16:V:129:LYS:HE3	1.71	1.05
13:O:47:PRO:HG3	13:O:76:THR:HG21	1.36	1.04
3:C:223:TRP:HD1	3:C:224:ILE:HG13	1.19	1.04
2:B:57:ARG:HD3	2:B:331:ASN:HD21	1.17	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:57:LEU:HD21	15:U:112:PHE:CD2	1.93	1.03
2:B:47:PRO:HB3	2:B:78:TRP:CD1	1.94	1.02
2:B:138:MET:HG2	23:B:522:CLA:HBC2	1.37	1.02
3:C:294:ASN:HD22	3:C:294:ASN:N	1.52	1.02
5:E:14:THR:HG21	9:J:8:ILE:CD1	1.89	1.02
2:B:326:ARG:HD2	2:B:327:THR:N	1.74	1.01
5:E:14:THR:HG21	9:J:8:ILE:HD12	1.38	1.01
3:C:77:PRO:HA	3:C:104:GLU:OE2	1.59	1.00
13:O:81:ILE:HG22	13:O:82:GLN:H	1.24	1.00
1:A:186:PHE:CD2	1:A:192:ILE:HD11	1.95	1.00
3:C:62:PHE:CZ	10:K:19:ILE:HD11	1.95	1.00
4:D:336:HIS:H	4:D:336:HIS:CD2	1.78	1.00
15:U:132:LEU:HD23	15:U:132:LEU:H	1.20	1.00
3:C:104:GLU:HG2	3:C:105:VAL:HG23	1.40	0.99
6:F:40:GLN:OE1	9:J:28:PHE:HA	1.61	0.99
13:O:130:GLN:CB	13:O:131:PRO:HD2	1.91	0.99
5:E:12:ILE:CG2	5:E:18:TYR:CB	2.35	0.99
13:O:106:VAL:HG13	13:O:117:PRO:HG3	1.43	0.99
2:B:222:PRO:HB3	7:H:25:GLY:HA2	1.43	0.98
13:O:193:THR:HG22	13:O:194:LYS:H	1.27	0.98
13:O:39:ARG:HB3	13:O:245:PRO:HG3	1.42	0.98
3:C:343:ARG:HD2	3:C:343:ARG:C	1.84	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.46	0.97
3:C:158:THR:HG22	3:C:251:HIS:CB	1.95	0.97
3:C:455:PHE:CE1	4:D:224:GLN:HA	1.97	0.97
4:D:198:MET:HE1	11:L:30:LEU:HD11	1.46	0.97
3:C:320:ARG:NE	15:U:128:TYR:CE2	2.33	0.96
13:O:47:PRO:HA	13:O:237:GLY:HA3	1.47	0.95
2:B:130:GLU:HG2	2:B:131:PRO:HD3	1.48	0.95
19:Z:19:MET:O	19:Z:23:VAL:HG23	1.65	0.95
23:C:478:CLA:H62	23:C:485:CLA:H12	1.48	0.95
4:D:158:LEU:O	4:D:162:LEU:HG	1.66	0.95
2:B:326:ARG:HH11	2:B:327:THR:CB	1.80	0.95
2:B:475:PHE:HB3	2:B:478:VAL:HB	1.46	0.95
4:D:88:SER:HB3	5:E:68:ARG:HH21	1.29	0.95
15:U:59:ASN:N	15:U:59:ASN:ND2	2.05	0.95
13:O:130:GLN:HB3	13:O:131:PRO:HD2	0.96	0.94
3:C:42:LEU:HG	23:C:486:CLA:HED1	1.49	0.94
23:B:521:CLA:HAB	23:B:527:CLA:HED1	1.47	0.94
5:E:14:THR:HG21	9:J:8:ILE:CG1	1.95	0.94
13:O:81:ILE:HG22	13:O:82:GLN:N	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:TYR:OH	12:M:21:PHE:HZ	1.48	0.93
3:C:326:ALA:HB2	15:U:127:ARG:HD2	1.50	0.93
16:V:133:GLY:O	16:V:137:TYR:HB2	1.69	0.93
15:U:72:TYR:CD2	15:U:73:PRO:N	2.36	0.93
3:C:71:GLU:OE1	3:C:86:LEU:HB3	1.69	0.93
1:A:225:ARG:HB3	2:B:481:GLY:C	1.88	0.93
3:C:320:ARG:HE	15:U:128:TYR:HE2	1.08	0.93
15:U:59:ASN:HD22	15:U:59:ASN:H	0.99	0.93
3:C:271:TYR:HA	3:C:274:TYR:CD1	2.04	0.93
13:O:44:CYS:HB3	13:O:240:TYR:HB3	1.51	0.93
3:C:157:MET:HE2	3:C:160:ILE:HD12	1.50	0.92
3:C:308:GLU:OE2	3:C:361:PHE:HZ	1.52	0.92
4:D:319:LEU:HA	4:D:322:ASN:HD22	1.34	0.92
4:D:52:THR:HG22	4:D:67:TYR:HE1	1.35	0.91
3:C:344:SER:HB3	3:C:350:ILE:CD1	1.99	0.91
3:C:62:PHE:HZ	10:K:19:ILE:HD11	1.32	0.91
6:F:40:GLN:HE22	9:J:27:LEU:C	1.74	0.91
27:C:488:BCR:H312	19:Z:9:LEU:HD11	1.50	0.91
1:A:237:TYR:CZ	1:A:245:THR:HG23	2.06	0.90
2:B:57:ARG:HD3	2:B:331:ASN:ND2	1.85	0.90
4:D:68:LEU:HA	6:F:39:MET:HE1	1.52	0.90
1:A:317:TRP:HA	4:D:63:LEU:HD13	1.54	0.90
13:O:43:LEU:HD12	13:O:240:TYR:O	1.72	0.90
2:B:56:TRP:CZ3	2:B:266:GLU:HA	2.07	0.90
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.54	0.89
1:A:300:PHE:HB3	1:A:302:PHE:HE1	1.36	0.89
3:C:138:GLU:HG2	3:C:139:THR:N	1.87	0.89
5:E:12:ILE:HG21	5:E:18:TYR:HB2	1.53	0.89
5:E:14:THR:HG22	9:J:8:ILE:CB	2.02	0.89
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.51	0.89
2:B:318:ASN:HD22	2:B:319:PRO:N	1.70	0.89
16:V:4:THR:HG22	16:V:5:PRO:HD2	1.53	0.89
13:O:104:GLN:OE1	13:O:104:GLN:N	2.05	0.89
3:C:43:ILE:HG13	3:C:44:ASN:H	1.36	0.89
16:V:46:THR:HG22	16:V:49:ASN:H	1.38	0.89
1:A:307:ILE:CG1	1:A:314:ILE:HD11	2.03	0.88
1:A:89:ILE:HG12	13:O:73:ARG:NH2	1.88	0.88
1:A:239:PHE:HZ	4:D:223:PHE:HZ	1.22	0.88
2:B:56:TRP:HZ3	2:B:266:GLU:HA	1.38	0.88
3:C:55:ALA:HB1	27:C:488:BCR:H373	1.55	0.88
19:Z:33:TRP:HE3	19:Z:37:LYS:HD3	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:GLY:HA2	2:B:325:PHE:CE1	2.08	0.88
1:A:334:ARG:HH11	4:D:320:LEU:HD11	1.38	0.88
1:A:286:THR:HG22	23:A:348:CLA:O1D	1.73	0.88
4:D:71:CYS:HB2	4:D:76:VAL:HG23	1.55	0.87
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.38	0.87
3:C:116:VAL:HG13	27:C:488:BCR:H332	1.57	0.87
3:C:307:PRO:HB3	3:C:358:PHE:CD2	2.09	0.87
13:O:146:PHE:HB2	13:O:195:GLY:CA	2.01	0.87
13:O:164:LEU:HD23	15:U:42:VAL:HG13	1.56	0.87
3:C:305:THR:HA	3:C:423:ARG:NH1	1.90	0.87
13:O:163:GLY:HA2	13:O:188:LYS:HG3	1.57	0.87
4:D:198:MET:CE	11:L:30:LEU:HD11	2.03	0.87
13:O:155:ASN:HD22	15:U:129:ASN:ND2	1.72	0.87
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.56	0.87
1:A:230:THR:HG22	1:A:231:GLU:H	1.39	0.87
13:O:140:THR:HB	13:O:201:VAL:H	1.40	0.87
13:O:146:PHE:CB	13:O:195:GLY:HA3	2.01	0.86
19:Z:51:VAL:HG12	19:Z:52:LEU:HD23	1.53	0.86
3:C:285:ILE:HA	23:C:487:CLA:HMB2	1.56	0.86
2:B:326:ARG:HD3	27:B:529:BCR:H402	1.56	0.86
11:L:7:ARG:C	11:L:9:PRO:HD3	1.96	0.86
2:B:9:HIS:HB2	23:B:523:CLA:HBA2	1.55	0.86
13:O:155:ASN:ND2	15:U:129:ASN:ND2	2.23	0.86
5:E:60:ARG:HH22	16:V:129:LYS:CE	1.87	0.86
13:O:140:THR:HG21	13:O:201:VAL:O	1.74	0.86
1:A:57:PRO:HG2	13:O:115:ARG:NH1	1.91	0.86
5:E:14:THR:CG2	9:J:8:ILE:CB	2.53	0.86
3:C:269:GLU:OE2	3:C:447:ARG:HG2	1.75	0.86
1:A:214:MET:HA	1:A:214:MET:CE	2.05	0.86
16:V:75:TYR:HE2	16:V:80:THR:H	1.22	0.86
2:B:120:LEU:HD23	2:B:130:GLU:HA	1.58	0.85
7:H:39:VAL:O	7:H:43:ILE:HG13	1.76	0.85
1:A:142:TRP:NE1	3:C:443:TRP:CH2	2.45	0.85
11:L:31:PHE:HB3	11:L:35:PHE:HE1	1.40	0.85
2:B:280:PHE:CE1	2:B:312:TYR:HB3	2.12	0.85
16:V:55:ARG:HH21	16:V:131:GLY:HA3	1.39	0.85
1:A:223:LEU:HD22	1:A:245:THR:HG22	1.57	0.85
3:C:305:THR:H	3:C:308:GLU:HG3	1.41	0.85
1:A:29:TYR:HD2	1:A:133:LEU:CD1	1.90	0.85
1:A:307:ILE:HG13	1:A:314:ILE:HD11	1.58	0.85
23:B:518:CLA:H141	23:B:524:CLA:HMA2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:197:HIS:O	4:D:201:VAL:HG23	1.76	0.85
2:B:122:LEU:HD12	23:B:525:CLA:HMA2	1.57	0.85
13:O:47:PRO:HG3	13:O:76:THR:CG2	2.06	0.85
12:M:19:SER:O	12:M:23:ILE:HG12	1.77	0.84
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.12	0.84
3:C:257:PHE:O	3:C:261:ARG:HG3	1.77	0.84
3:C:282:MET:HA	3:C:285:ILE:HG13	1.57	0.84
4:D:90:LEU:HD11	4:D:96:GLU:OE1	1.78	0.84
13:O:126:VAL:O	13:O:144:GLY:HA3	1.78	0.84
2:B:318:ASN:HD22	2:B:318:ASN:C	1.79	0.84
13:O:43:LEU:CD1	13:O:241:ALA:HB2	2.08	0.84
2:B:357:ARG:HH22	4:D:337:GLU:HB3	1.41	0.83
2:B:339:ALA:HB3	2:B:430:PHE:HD1	1.43	0.83
2:B:322:GLY:HA2	2:B:325:PHE:CD1	2.13	0.83
1:A:334:ARG:NH1	4:D:320:LEU:HD11	1.93	0.83
1:A:221:SER:HA	4:D:139:ARG:HB2	1.60	0.83
1:A:243:GLU:HA	4:D:240:ALA:HB1	1.58	0.83
3:C:294:ASN:N	3:C:294:ASN:ND2	2.21	0.83
5:E:14:THR:CG2	9:J:8:ILE:CG1	2.56	0.83
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.43	0.83
23:B:512:CLA:H191	23:B:520:CLA:H151	1.61	0.83
3:C:279:LEU:HB3	23:C:481:CLA:HBC1	1.59	0.83
2:B:339:ALA:HB3	2:B:430:PHE:CD1	2.14	0.82
10:K:25:ALA:HB1	27:K:50:BCR:H19C	1.60	0.82
3:C:55:ALA:HB1	27:C:488:BCR:C37	2.09	0.82
4:D:174:GLY:O	4:D:178:ILE:HG12	1.80	0.82
23:A:350:CLA:HED1	4:D:175:VAL:HG13	1.61	0.82
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.14	0.82
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.14	0.82
2:B:212:ALA:HB2	23:B:511:CLA:HMC3	1.62	0.82
4:D:195:PRO:HA	4:D:198:MET:HE2	1.59	0.82
5:E:12:ILE:HD12	28:E:84:HEC:CGD	2.09	0.82
1:A:306:VAL:HG22	1:A:307:ILE:H	1.42	0.82
1:A:330:VAL:CG1	4:D:348:ARG:HG3	2.10	0.82
3:C:203:THR:HG22	3:C:208:VAL:HG11	1.62	0.82
4:D:195:PRO:HA	4:D:198:MET:CE	2.09	0.82
15:U:91:VAL:O	15:U:94:ILE:HG13	1.80	0.82
16:V:80:THR:HG23	16:V:84:GLY:HA2	1.62	0.81
4:D:71:CYS:HB2	4:D:76:VAL:CG2	2.09	0.81
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.62	0.81
1:A:301:ASN:HD21	3:C:407:VAL:CG2	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:PHE:HD2	3:C:292:PHE:N	1.78	0.81
4:D:102:THR:HG22	4:D:106:GLN:HE21	1.43	0.81
16:V:56:THR:HA	16:V:59:LEU:HD12	1.60	0.81
2:B:413:ASP:HB3	2:B:415:PRO:HD2	1.60	0.81
13:O:95:PHE:CB	13:O:127:ALA:HB3	2.10	0.81
1:A:92:HIS:HD2	3:C:219:GLY:HA3	1.44	0.81
1:A:326:LEU:HD13	3:C:412:THR:HG21	1.60	0.81
13:O:39:ARG:CB	13:O:245:PRO:HG3	2.10	0.81
13:O:81:ILE:CG2	13:O:82:GLN:H	1.94	0.81
13:O:40:ILE:HG22	13:O:41:ALA:H	1.46	0.81
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.62	0.81
13:O:40:ILE:HG12	13:O:84:GLU:CD	2.02	0.81
2:B:222:PRO:HB3	7:H:25:GLY:CA	2.11	0.80
2:B:248:ALA:HA	23:B:517:CLA:H42	1.62	0.80
3:C:295:THR:O	3:C:298:PRO:HD3	1.79	0.80
2:B:170:ASP:OD1	2:B:175:THR:HG22	1.81	0.80
3:C:199:ILE:HD12	3:C:234:VAL:HG21	1.62	0.80
9:J:40:LEU:HD23	16:V:30:LYS:HE2	1.61	0.80
3:C:120:ILE:O	3:C:124:VAL:HG23	1.82	0.80
3:C:212:TYR:O	3:C:223:TRP:HB2	1.81	0.80
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.62	0.80
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.17	0.80
2:B:302:TRP:O	2:B:341:LYS:HE3	1.81	0.80
3:C:126:GLY:O	3:C:130:VAL:HG23	1.80	0.80
2:B:75:TRP:N	2:B:94:GLU:HG3	1.93	0.80
2:B:136:PRO:HD3	2:B:231:MET:HE1	1.64	0.80
2:B:478:VAL:HG11	4:D:139:ARG:HA	1.64	0.80
3:C:308:GLU:HG2	3:C:361:PHE:HE1	1.42	0.80
4:D:138:VAL:HG12	4:D:139:ARG:N	1.97	0.80
4:D:190:ASN:HB2	4:D:296:TYR:HD1	1.44	0.80
19:Z:8:ALA:O	19:Z:11:ALA:HB3	1.82	0.80
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.64	0.80
1:A:29:TYR:C	1:A:29:TYR:HD1	1.85	0.79
1:A:246:TYR:CE1	1:A:248:ILE:HG12	2.17	0.79
3:C:405:ASN:HB2	3:C:407:VAL:HG23	1.62	0.79
11:L:12:LEU:HD11	11:L:16:SER:HB3	1.64	0.79
13:O:122:VAL:HA	13:O:146:PHE:HE2	1.47	0.79
16:V:4:THR:HG22	16:V:5:PRO:CD	2.12	0.79
4:D:336:HIS:H	4:D:336:HIS:HD2	1.28	0.79
1:A:210:LEU:HD12	1:A:210:LEU:O	1.82	0.79
3:C:334:PRO:HA	13:O:153:THR:HB	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:ALA:HB2	5:E:82:LEU:HD23	1.62	0.79
23:B:512:CLA:H193	23:B:523:CLA:H102	1.62	0.79
3:C:292:PHE:N	3:C:292:PHE:CD2	2.50	0.79
15:U:132:LEU:HD23	15:U:132:LEU:N	1.96	0.79
5:E:14:THR:CG2	9:J:8:ILE:CD1	2.54	0.79
3:C:285:ILE:HA	23:C:487:CLA:CMB	2.11	0.79
3:C:264:PHE:N	3:C:264:PHE:HD2	1.81	0.79
16:V:79:PRO:HB2	16:V:88:ILE:CG1	2.13	0.79
1:A:14:TRP:CZ3	1:A:18:CYS:SG	2.76	0.79
1:A:239:PHE:HZ	4:D:223:PHE:CZ	2.01	0.79
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.65	0.79
1:A:296:ASN:CG	3:C:401:LEU:HD23	2.04	0.78
3:C:273:SER:HB3	3:C:445:ALA:HB2	1.66	0.78
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.18	0.78
2:B:264:PRO:HG3	2:B:267:LEU:HD12	1.64	0.78
13:O:140:THR:HB	13:O:201:VAL:HG23	1.64	0.78
10:K:16:LEU:HB3	10:K:17:PRO:CD	2.13	0.78
13:O:75:THR:HG22	13:O:103:PHE:HD2	1.47	0.78
8:I:27:ASP:HB2	8:I:28:PRO:CD	2.13	0.78
1:A:239:PHE:CE1	4:D:245:SER:HA	2.19	0.78
1:A:253:GLY:O	1:A:257:ARG:HG2	1.83	0.78
23:A:350:CLA:H121	25:A:353:PL9:H162	1.66	0.78
2:B:221:PRO:HG3	2:B:225:LEU:HD12	1.64	0.78
4:D:236:ASN:OD1	4:D:239:GLN:HB2	1.83	0.78
1:A:301:ASN:ND2	3:C:407:VAL:HG21	1.99	0.78
3:C:86:LEU:HD13	3:C:89:ILE:HD12	1.64	0.78
5:E:22:HIS:HA	5:E:25:THR:HB	1.64	0.77
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.18	0.77
3:C:347:GLY:HA3	13:O:17:ASN:OD1	1.85	0.77
4:D:298:PHE:CA	11:L:37:ASN:HD21	1.87	0.77
2:B:145:LEU:HD13	23:B:522:CLA:HMB1	1.65	0.77
4:D:176:ALA:HA	4:D:179:PHE:HD1	1.48	0.77
6:F:36:ILE:HA	6:F:39:MET:HG3	1.67	0.77
10:K:2:LEU:N	10:K:3:PRO:HD3	1.98	0.77
23:B:522:CLA:H171	23:B:525:CLA:CMD	2.14	0.77
5:E:12:ILE:HG22	5:E:18:TYR:CG	2.20	0.77
3:C:320:ARG:HH12	16:V:50:PRO:HD2	1.46	0.77
2:B:327:THR:HG22	2:B:329:PRO:HD3	1.67	0.77
2:B:478:VAL:CG1	4:D:139:ARG:HA	2.15	0.77
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.67	0.77
1:A:63:ILE:HD11	1:A:336:ALA:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:79:PRO:HB2	16:V:88:ILE:HG12	1.67	0.77
3:C:320:ARG:NH1	16:V:50:PRO:HD2	1.99	0.77
1:A:306:VAL:HG22	1:A:307:ILE:N	1.99	0.76
2:B:326:ARG:CD	2:B:327:THR:N	2.41	0.76
25:D:357:PL9:H38	14:T:18:PHE:HB2	1.66	0.76
2:B:326:ARG:NH1	2:B:327:THR:OG1	2.17	0.76
2:B:113:TRP:HB3	23:B:525:CLA:HED1	1.67	0.76
8:I:7:THR:O	8:I:11:VAL:HG23	1.85	0.76
1:A:295:PHE:HB3	3:C:291:TRP:CZ3	2.20	0.76
1:A:301:ASN:HD21	3:C:407:VAL:HG21	1.48	0.76
2:B:142:HIS:CE1	23:B:524:CLA:H142	2.21	0.76
4:D:323:GLU:HG2	13:O:168:TYR:OH	1.86	0.76
1:A:142:TRP:HE1	3:C:443:TRP:HH2	1.33	0.76
1:A:29:TYR:HD1	1:A:30:VAL:N	1.83	0.76
3:C:175:LEU:HD11	23:C:479:CLA:HED3	1.67	0.76
1:A:87:ASN:HD21	3:C:357:ARG:HH11	1.32	0.76
5:E:12:ILE:CD1	28:E:84:HEC:O1A	2.34	0.76
9:J:15:THR:HA	27:K:50:BCR:H372	1.67	0.76
2:B:326:ARG:HH11	2:B:327:THR:HB	1.48	0.75
23:B:522:CLA:H171	23:B:525:CLA:HMD3	1.68	0.75
1:A:141:PRO:HG2	3:C:443:TRP:HZ3	1.52	0.75
1:A:148:SER:HB2	1:A:284:TRP:HH2	1.50	0.75
2:B:118:TRP:CZ2	11:L:3:PRO:HB3	2.21	0.75
1:A:172:MET:HE2	23:A:349:CLA:HMC3	1.69	0.75
23:C:479:CLA:H92	23:C:479:CLA:HAB	1.69	0.75
4:D:31:GLY:HA3	4:D:131:GLU:OE1	1.86	0.75
2:B:305:ILE:O	2:B:305:ILE:HG13	1.86	0.75
3:C:264:PHE:N	3:C:264:PHE:CD2	2.54	0.75
1:A:56:PRO:HA	1:A:73:TYR:CE1	2.22	0.75
1:A:57:PRO:HB3	1:A:68:SER:HB3	1.68	0.75
2:B:25:MET:HB3	27:B:529:BCR:H332	1.69	0.75
13:O:7:TYR:O	13:O:11:VAL:HG23	1.86	0.75
1:A:159:LEU:HD21	23:C:487:CLA:HBD	1.69	0.75
4:D:336:HIS:CD2	4:D:336:HIS:N	2.52	0.75
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.68	0.74
3:C:98:GLY:O	3:C:99:VAL:HG23	1.86	0.74
2:B:187:PRO:O	2:B:190:PHE:N	2.20	0.74
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.69	0.74
4:D:88:SER:CB	5:E:68:ARG:HH21	1.98	0.74
3:C:285:ILE:HG21	23:C:479:CLA:H51	1.69	0.74
3:C:374:GLY:HA2	13:O:7:TYR:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ASP:OD1	4:D:23:LYS:HD2	1.87	0.74
11:L:4:ASN:N	11:L:5:PRO:HD3	2.03	0.74
2:B:172:TYR:CE2	2:B:283:GLU:HB2	2.23	0.74
3:C:293:ASN:C	3:C:294:ASN:HD22	1.89	0.74
2:B:112:CYS:O	2:B:116:VAL:HG23	1.87	0.74
3:C:308:GLU:HG2	3:C:361:PHE:CZ	2.22	0.74
3:C:363:GLY:O	3:C:367:GLU:HG2	1.87	0.74
1:A:29:TYR:C	1:A:29:TYR:CD1	2.59	0.74
3:C:229:ASN:HB3	3:C:232:ASP:OD1	1.88	0.74
4:D:68:LEU:CA	6:F:39:MET:HE1	2.18	0.74
4:D:235:PHE:HA	4:D:239:GLN:OE1	1.86	0.74
5:E:9:PHE:O	5:E:10:SER:HB3	1.85	0.74
5:E:43:TYR:CD2	5:E:50:ARG:HG2	2.22	0.74
2:B:63:LEU:HD11	2:B:93:PHE:CE1	2.22	0.74
3:C:350:ILE:HG12	3:C:359:TRP:HB2	1.70	0.74
4:D:51:GLY:HA2	4:D:55:VAL:HG23	1.69	0.74
4:D:71:CYS:HB3	4:D:75:THR:HB	1.68	0.74
5:E:19:TRP:HZ2	9:J:13:VAL:HG22	1.50	0.74
1:A:78:ILE:HD11	11:L:34:TYR:CE1	2.23	0.74
3:C:41:ARG:HB2	23:C:486:CLA:HED3	1.69	0.74
3:C:61:VAL:HG22	23:C:480:CLA:HAC2	1.70	0.74
3:C:227:VAL:HG23	3:C:294:ASN:HB3	1.68	0.74
3:C:320:ARG:NE	15:U:128:TYR:HE2	1.79	0.74
4:D:152:VAL:O	4:D:156:VAL:HG23	1.88	0.74
10:K:19:ILE:HA	10:K:22:LEU:HD12	1.70	0.74
3:C:101:PRO:N	3:C:195:ASP:HB3	2.03	0.73
13:O:43:LEU:HD13	13:O:241:ALA:HB2	1.69	0.73
10:K:2:LEU:H	10:K:3:PRO:HD3	1.51	0.73
2:B:27:THR:O	23:B:518:CLA:HBC1	1.88	0.73
3:C:138:GLU:CG	3:C:139:THR:H	1.96	0.73
4:D:267:LEU:O	4:D:271:MET:HG3	1.87	0.73
1:A:317:TRP:HA	4:D:63:LEU:CD1	2.19	0.73
2:B:357:ARG:NH2	4:D:337:GLU:HB3	2.04	0.73
2:B:368:VAL:HA	2:B:425:ILE:HD11	1.69	0.73
4:D:56:THR:HB	5:E:48:THR:HG23	1.71	0.73
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.69	0.73
3:C:248:GLY:O	3:C:252:ILE:HG13	1.89	0.73
14:T:18:PHE:HD2	14:T:19:PHE:CD1	2.07	0.73
3:C:123:ALA:HB1	19:Z:47:TRP:HH2	1.53	0.73
13:O:50:PHE:HZ	13:O:76:THR:HG23	1.54	0.72
1:A:334:ARG:HH12	13:O:159:PRO:HA	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:HB3	14:T:2:GLU:OE2	1.90	0.72
2:B:246:PHE:HE1	2:B:463:PHE:HB2	1.53	0.72
4:D:238:THR:O	4:D:240:ALA:N	2.20	0.72
1:A:69:GLY:HA2	1:A:75:ASN:OD1	1.90	0.72
2:B:66:MET:O	2:B:71:VAL:HG23	1.89	0.72
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.71	0.72
19:Z:41:PHE:HD1	19:Z:41:PHE:H	1.35	0.72
1:A:182:PHE:O	1:A:186:PHE:HB2	1.88	0.72
2:B:172:TYR:CZ	2:B:283:GLU:HB2	2.25	0.72
2:B:400:SER:OG	2:B:410:THR:HG23	1.88	0.72
3:C:271:TYR:HA	3:C:274:TYR:HD1	1.50	0.72
2:B:340:TRP:CZ3	2:B:342:GLY:HA3	2.24	0.72
4:D:194:ASN:O	4:D:198:MET:HG3	1.88	0.72
4:D:235:PHE:CD1	4:D:236:ASN:N	2.57	0.72
13:O:162:ARG:O	13:O:162:ARG:HG2	1.90	0.72
3:C:42:LEU:CG	23:C:486:CLA:HED1	2.18	0.72
4:D:319:LEU:HA	4:D:322:ASN:ND2	2.04	0.72
15:U:132:LEU:H	15:U:132:LEU:CD2	1.96	0.72
3:C:42:LEU:HD13	23:C:486:CLA:HMA3	1.70	0.72
8:I:15:PHE:HA	8:I:18:LEU:HG	1.72	0.72
15:U:83:ALA:HA	15:U:85:TYR:CE2	2.25	0.72
23:C:477:CLA:CMD	23:C:485:CLA:HAB	2.19	0.72
5:E:14:THR:HG21	9:J:8:ILE:HG13	1.71	0.72
13:O:201:VAL:HG13	13:O:211:ILE:HG23	1.71	0.72
13:O:223:ASP:HB3	13:O:230:PRO:HG3	1.71	0.72
2:B:68:ARG:HH12	23:B:516:CLA:HED1	1.54	0.71
23:B:518:CLA:C14	23:B:524:CLA:HMA2	2.20	0.71
12:M:18:PRO:O	12:M:22:LEU:HG	1.89	0.71
1:A:29:TYR:CD2	1:A:133:LEU:CD1	2.72	0.71
1:A:326:LEU:CD1	3:C:412:THR:HG21	2.20	0.71
23:B:520:CLA:HBC3	23:B:523:CLA:H41	1.72	0.71
3:C:99:VAL:HG22	3:C:104:GLU:O	1.90	0.71
3:C:343:ARG:HA	3:C:348:GLU:O	1.90	0.71
2:B:248:ALA:O	2:B:252:VAL:HG23	1.89	0.71
1:A:239:PHE:CZ	4:D:223:PHE:HZ	2.08	0.71
13:O:40:ILE:HG22	13:O:41:ALA:N	2.04	0.71
1:A:63:ILE:HD11	1:A:336:ALA:CB	2.20	0.71
2:B:17:GLY:O	2:B:20:ILE:HG22	1.89	0.71
3:C:385:GLN:OE1	3:C:386:PRO:HD2	1.91	0.71
3:C:437:PHE:HA	23:C:483:CLA:CMC	2.19	0.71
1:A:330:VAL:HG11	4:D:348:ARG:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HB3	2:B:78:TRP:HD1	1.51	0.71
2:B:397:VAL:HG12	2:B:398:THR:N	2.05	0.71
3:C:43:ILE:HG13	3:C:44:ASN:N	2.06	0.71
1:A:309:ALA:O	16:V:3:LEU:N	2.24	0.71
2:B:318:ASN:C	2:B:318:ASN:ND2	2.44	0.71
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.72	0.71
4:D:244:TYR:OH	4:D:264:LYS:NZ	2.21	0.71
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.71	0.71
1:A:29:TYR:HE1	1:A:31:GLY:CA	2.03	0.71
1:A:243:GLU:CA	4:D:240:ALA:HB1	2.21	0.71
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.54	0.71
4:D:190:ASN:CB	4:D:296:TYR:HD1	2.04	0.71
4:D:262:SER:O	4:D:263:ASN:ND2	2.24	0.71
1:A:159:LEU:HG	1:A:163:ILE:HD11	1.73	0.71
2:B:339:ALA:HB2	2:B:431:GLU:H	1.56	0.71
3:C:345:PRO:O	13:O:74:GLU:HB2	1.90	0.71
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.23	0.71
2:B:321:LYS:CE	2:B:325:PHE:HZ	2.04	0.71
2:B:348:ASN:OD1	2:B:349:LYS:N	2.17	0.71
15:U:73:PRO:HB2	16:V:83:ASP:OD2	1.91	0.71
1:A:89:ILE:HG21	1:A:94:TYR:HB2	1.73	0.70
13:O:71:VAL:HG21	13:O:108:VAL:HG23	1.71	0.70
1:A:214:MET:HA	1:A:214:MET:HE2	1.71	0.70
1:A:307:ILE:O	1:A:309:ALA:N	2.23	0.70
4:D:221:THR:O	4:D:221:THR:HG22	1.90	0.70
13:O:17:ASN:O	13:O:46:GLN:HG3	1.91	0.70
1:A:214:MET:HE1	4:D:142:ASN:OD1	1.91	0.70
3:C:350:ILE:HG21	3:C:359:TRP:HB3	1.73	0.70
13:O:164:LEU:O	13:O:165:ALA:HB3	1.89	0.70
3:C:343:ARG:C	3:C:343:ARG:CD	2.59	0.70
4:D:16:ASP:O	4:D:19:ASP:HB3	1.90	0.70
1:A:159:LEU:HD11	23:C:487:CLA:OBD	1.92	0.70
5:E:52:ASP:O	16:V:1:ALA:HB3	1.90	0.70
10:K:15:VAL:HG11	18:N:13:UNK:CB	2.21	0.70
13:O:155:ASN:ND2	15:U:129:ASN:HD22	1.88	0.70
13:O:211:ILE:HB	13:O:241:ALA:HB3	1.73	0.70
1:A:142:TRP:NE1	3:C:443:TRP:HH2	1.89	0.70
3:C:450:ALA:HA	3:C:454:GLY:HA3	1.73	0.70
6:F:31:PHE:HD2	6:F:31:PHE:O	1.74	0.70
3:C:42:LEU:CD1	23:C:486:CLA:HMA3	2.21	0.70
1:A:75:ASN:ND2	1:A:79:THR:HG21	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:59:VAL:O	7:H:59:VAL:HG12	1.91	0.70
12:M:15:VAL:HG12	12:M:16:LEU:HD23	1.73	0.70
2:B:414:PRO:HG2	2:B:415:PRO:HD3	1.72	0.70
4:D:68:LEU:HA	6:F:39:MET:CE	2.19	0.70
1:A:317:TRP:CA	4:D:63:LEU:HD13	2.22	0.70
4:D:90:LEU:CD1	4:D:96:GLU:HB3	2.21	0.70
3:C:121:SER:O	3:C:125:LEU:HG	1.91	0.69
4:D:18:LEU:O	4:D:22:LEU:HB3	1.92	0.69
4:D:118:GLY:HA3	24:D:355:PHO:H71	1.72	0.69
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.22	0.69
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.26	0.69
2:B:397:VAL:HG12	2:B:398:THR:H	1.56	0.69
3:C:123:ALA:CB	19:Z:47:TRP:HH2	2.04	0.69
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.74	0.69
16:V:37:CYS:O	16:V:39:SER:N	2.26	0.69
2:B:41:GLU:OE1	2:B:63:LEU:HB2	1.91	0.69
3:C:305:THR:HA	3:C:423:ARG:HH11	1.56	0.69
13:O:118:LEU:CD1	13:O:233:VAL:HG11	2.23	0.69
16:V:75:TYR:CD2	16:V:79:PRO:HA	2.26	0.69
1:A:235:TYR:HA	4:D:265:ARG:NH2	2.06	0.69
2:B:324:LEU:CD1	11:L:34:TYR:HB3	2.22	0.69
10:K:30:TRP:CE3	10:K:31:GLN:NE2	2.60	0.69
1:A:219:VAL:HG11	4:D:268:HIS:CG	2.28	0.69
1:A:320:ILE:HG22	1:A:320:ILE:O	1.93	0.69
4:D:87:HIS:NE2	4:D:166:SER:HA	2.08	0.69
4:D:90:LEU:HD11	4:D:96:GLU:CD	2.13	0.69
4:D:186:GLN:HB2	23:D:354:CLA:HBC1	1.73	0.69
16:V:133:GLY:O	16:V:137:TYR:CB	2.41	0.69
1:A:161:TYR:HB3	1:A:162:PRO:CD	2.21	0.69
13:O:28:GLY:HA3	13:O:137:THR:HG22	1.73	0.69
1:A:281:VAL:O	1:A:281:VAL:HG12	1.91	0.69
2:B:30:VAL:HG12	23:B:518:CLA:HHD	1.73	0.69
3:C:176:VAL:O	3:C:180:MET:HG2	1.93	0.69
3:C:343:ARG:HD2	3:C:343:ARG:O	1.92	0.69
3:C:319:ILE:HD13	3:C:389:GLU:HG2	1.74	0.69
13:O:47:PRO:CG	13:O:76:THR:HG21	2.20	0.69
13:O:75:THR:HG22	13:O:103:PHE:CD2	2.28	0.69
2:B:57:ARG:HH11	2:B:57:ARG:CG	2.06	0.69
2:B:268:PHE:HB2	2:B:448:ARG:HE	1.56	0.69
23:B:519:CLA:HMD1	23:B:524:CLA:HAB	1.75	0.69
13:O:211:ILE:HG22	13:O:212:ALA:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:HD2	1:A:133:LEU:HD13	1.59	0.68
2:B:57:ARG:HH11	2:B:57:ARG:HG3	1.56	0.68
3:C:158:THR:HG23	3:C:251:HIS:HB3	1.74	0.68
4:D:138:VAL:HG12	4:D:139:ARG:H	1.55	0.68
13:O:140:THR:CB	13:O:201:VAL:H	2.06	0.68
15:U:62:ILE:HG23	15:U:76:ALA:HB1	1.74	0.68
1:A:76:ASN:HD21	4:D:298:PHE:HE2	1.39	0.68
1:A:301:ASN:OD1	3:C:407:VAL:HG21	1.94	0.68
3:C:203:THR:CG2	3:C:208:VAL:HG11	2.23	0.68
13:O:22:LEU:O	13:O:203:LYS:HD3	1.94	0.68
3:C:116:VAL:HG21	27:C:489:BCR:H323	1.75	0.68
4:D:53:THR:HA	4:D:67:TYR:CD1	2.29	0.68
1:A:81:ALA:HB3	1:A:174:LEU:O	1.93	0.68
2:B:145:LEU:HD13	23:B:522:CLA:CMB	2.23	0.68
3:C:443:TRP:CE3	3:C:443:TRP:HA	2.28	0.68
4:D:261:PHE:HA	14:T:24:ARG:HH22	1.59	0.68
13:O:163:GLY:HA3	13:O:188:LYS:HE2	1.76	0.68
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.29	0.68
2:B:105:GLY:HA2	27:B:528:BCR:H383	1.75	0.68
3:C:156:LYS:O	3:C:160:ILE:HG13	1.93	0.68
23:C:475:CLA:HBD	27:J:53:BCR:HC21	1.76	0.68
25:D:357:PL9:H261	14:T:21:ILE:HD11	1.74	0.68
2:B:86:ILE:O	2:B:88:PRO:HD3	1.93	0.68
1:A:61:ASP:HA	1:A:87:ASN:HB2	1.75	0.68
2:B:6:TYR:HH	12:M:21:PHE:HZ	0.74	0.68
2:B:124:ARG:HG2	2:B:125:ASP:N	2.07	0.68
3:C:275:SER:HB3	23:C:485:CLA:HAA1	1.76	0.68
4:D:80:THR:HG21	4:D:167:TRP:O	1.94	0.68
2:B:383:PHE:O	13:O:166:SER:HA	1.93	0.68
9:J:9:PRO:O	9:J:10:LEU:HD23	1.94	0.68
10:K:34:VAL:O	10:K:34:VAL:HG12	1.93	0.68
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.74	0.68
27:C:488:BCR:H341	27:K:50:BCR:HC31	1.76	0.67
7:H:57:VAL:O	7:H:57:VAL:CG1	2.41	0.67
5:E:33:GLY:HA2	6:F:31:PHE:CE2	2.29	0.67
7:H:53:ILE:HG23	17:X:13:THR:OG1	1.94	0.67
2:B:113:TRP:O	2:B:117:TYR:HB2	1.94	0.67
3:C:149:TYR:CD2	3:C:156:LYS:HG3	2.29	0.67
3:C:308:GLU:OE2	3:C:361:PHE:CZ	2.43	0.67
2:B:86:ILE:O	2:B:86:ILE:HG22	1.94	0.67
3:C:108:THR:HG21	10:K:2:LEU:HG	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:GLY:C	4:D:87:HIS:HD2	1.98	0.67
24:A:351:PHO:NC	4:D:209:LEU:HD12	2.09	0.67
2:B:326:ARG:NH1	2:B:327:THR:CB	2.56	0.67
3:C:141:GLU:HB3	3:C:144:SER:OG	1.93	0.67
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.76	0.67
3:C:305:THR:CA	3:C:423:ARG:NH1	2.57	0.67
19:Z:48:ILE:O	19:Z:52:LEU:HG	1.95	0.67
1:A:206:PHE:HE1	23:A:348:CLA:HMB1	1.57	0.67
2:B:266:GLU:O	2:B:266:GLU:HG2	1.93	0.67
3:C:141:GLU:HB2	3:C:144:SER:HB2	1.75	0.67
3:C:282:MET:HA	3:C:285:ILE:CG1	2.24	0.67
4:D:108:GLY:O	4:D:110:LEU:N	2.27	0.67
1:A:75:ASN:ND2	1:A:79:THR:CG2	2.57	0.67
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.09	0.67
2:B:135:LEU:HB2	2:B:231:MET:HE3	1.77	0.67
13:O:104:GLN:N	13:O:104:GLN:CD	2.46	0.67
13:O:168:TYR:CE1	13:O:172:ILE:HD11	2.29	0.67
2:B:162:PHE:HB3	23:B:515:CLA:HMD3	1.75	0.67
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.24	0.67
5:E:26:ILE:CG1	5:E:27:PRO:HD3	2.25	0.67
13:O:125:LEU:HD12	13:O:145:GLU:O	1.93	0.67
2:B:324:LEU:HD12	11:L:34:TYR:HB3	1.77	0.67
2:B:414:PRO:CD	2:B:415:PRO:HD3	2.24	0.67
3:C:291:TRP:HB3	3:C:292:PHE:CD2	2.29	0.67
3:C:419:PHE:O	3:C:420:VAL:HG23	1.95	0.67
13:O:243:ILE:O	13:O:244:GLU:HB2	1.95	0.67
1:A:141:PRO:HG3	3:C:446:GLY:O	1.94	0.67
28:E:84:HEC:HAC	6:F:26:ALA:HB1	1.75	0.67
6:F:40:GLN:HE21	9:J:27:LEU:HG	1.55	0.67
3:C:131:TYR:HE1	3:C:135:ARG:HD3	1.60	0.66
4:D:29:PHE:C	4:D:29:PHE:CD2	2.67	0.66
13:O:164:LEU:H	13:O:188:LYS:HE2	1.60	0.66
1:A:180:PHE:CE2	4:D:192:THR:HG22	2.31	0.66
1:A:290:ILE:HD11	23:A:348:CLA:CGD	2.25	0.66
14:T:3:THR:O	14:T:5:THR:N	2.28	0.66
23:A:348:CLA:H192	25:D:357:PL9:H252	1.77	0.66
2:B:380:ASP:OD1	2:B:390:TYR:HB2	1.95	0.66
1:A:222:SER:O	1:A:246:TYR:HB2	1.96	0.66
1:A:255:PHE:HD2	1:A:264:SER:HA	1.60	0.66
3:C:37:ALA:HA	23:C:483:CLA:O1A	1.95	0.66
13:O:140:THR:CG2	13:O:201:VAL:HB	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:164:LEU:CD2	15:U:42:VAL:HG13	2.25	0.66
2:B:58:GLN:O	2:B:329:PRO:CB	2.43	0.66
3:C:450:ALA:HB1	3:C:455:PHE:O	1.96	0.66
13:O:102:ASP:OD2	13:O:119:LEU:HD11	1.96	0.66
16:V:78:ASN:HB2	16:V:96:ARG:HH11	1.60	0.66
15:U:39:LEU:O	15:U:41:ASN:N	2.28	0.66
2:B:58:GLN:O	2:B:329:PRO:HB2	1.94	0.66
3:C:269:GLU:CD	3:C:447:ARG:HG2	2.16	0.66
5:E:12:ILE:HD13	28:E:84:HEC:O1A	1.95	0.66
2:B:6:TYR:OH	23:B:520:CLA:HMD3	1.96	0.66
3:C:443:TRP:HA	3:C:443:TRP:HE3	1.61	0.66
5:E:19:TRP:CZ2	9:J:13:VAL:HG22	2.30	0.66
15:U:88:VAL:HG22	15:U:114:VAL:HG23	1.78	0.66
19:Z:7:LEU:O	19:Z:11:ALA:HB2	1.95	0.66
4:D:189:HIS:ND1	4:D:294:ARG:NE	2.43	0.66
13:O:118:LEU:HD13	13:O:233:VAL:HG11	1.78	0.66
2:B:92:SER:O	2:B:96:VAL:HG23	1.96	0.65
3:C:208:VAL:HG13	3:C:209:ILE:N	2.10	0.65
3:C:380:ILE:HG22	3:C:381:LYS:N	2.10	0.65
1:A:119:PHE:O	1:A:123:ALA:HB2	1.96	0.65
4:D:14:TRP:HA	4:D:17:ILE:HD12	1.78	0.65
8:I:18:LEU:N	8:I:18:LEU:HD23	2.10	0.65
1:A:29:TYR:CE1	1:A:31:GLY:N	2.63	0.65
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.30	0.65
13:O:224:ASP:C	13:O:225:MET:HG2	2.16	0.65
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.31	0.65
2:B:84:THR:O	2:B:84:THR:HG22	1.95	0.65
3:C:108:THR:HG23	10:K:2:LEU:HD23	1.79	0.65
3:C:320:ARG:HH12	16:V:50:PRO:CD	2.10	0.65
13:O:158:ASP:HB2	13:O:159:PRO:HD2	1.78	0.65
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.27	0.65
4:D:210:LEU:HD13	4:D:271:MET:HG2	1.79	0.65
7:H:27:THR:N	7:H:28:PRO:HD2	2.10	0.65
13:O:27:ARG:HG3	13:O:29:ALA:HB3	1.77	0.65
1:A:29:TYR:HE1	1:A:31:GLY:N	1.95	0.65
3:C:249:ILE:HA	3:C:252:ILE:HD12	1.78	0.65
15:U:72:TYR:HD2	15:U:73:PRO:N	1.93	0.65
13:O:128:SER:O	13:O:142:PHE:HA	1.96	0.65
2:B:414:PRO:CG	2:B:415:PRO:HD3	2.26	0.65
3:C:285:ILE:HG23	23:C:487:CLA:HMB1	1.78	0.65
8:I:17:LEU:O	8:I:21:PHE:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:PHE:CZ	2:B:312:TYR:HB3	2.32	0.65
4:D:28:VAL:HB	6:F:17:VAL:HG13	1.79	0.65
1:A:97:TRP:HZ3	8:I:8:VAL:HG21	1.62	0.65
1:A:221:SER:HB3	4:D:138:VAL:HG12	1.78	0.65
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.11	0.65
3:C:61:VAL:HG22	23:C:480:CLA:CAC	2.25	0.65
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.79	0.65
10:K:25:ALA:HB1	27:K:50:BCR:C19	2.27	0.65
13:O:152:ARG:NH1	13:O:156:PHE:CZ	2.65	0.65
2:B:238:LEU:O	2:B:242:ILE:HG13	1.97	0.64
23:B:520:CLA:H161	12:M:17:VAL:HG11	1.79	0.64
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.78	0.64
7:H:49:ASN:OD1	7:H:49:ASN:O	2.15	0.64
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.78	0.64
3:C:293:ASN:OD1	3:C:297:TYR:O	2.15	0.64
1:A:183:MET:HE2	23:A:349:CLA:HMD3	1.79	0.64
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.79	0.64
4:D:52:THR:HG22	4:D:67:TYR:CE1	2.26	0.64
9:J:15:THR:HA	27:K:50:BCR:C37	2.27	0.64
15:U:132:LEU:N	15:U:132:LEU:CD2	2.57	0.64
1:A:285:PHE:O	1:A:288:LEU:HB2	1.97	0.64
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.29	0.64
23:B:513:CLA:H91	23:B:516:CLA:HAA1	1.77	0.64
23:B:520:CLA:H161	12:M:17:VAL:CG1	2.27	0.64
6:F:40:GLN:NE2	9:J:27:LEU:CG	2.46	0.64
1:A:221:SER:HB3	4:D:138:VAL:CG1	2.27	0.64
6:F:25:LEU:O	6:F:28:PRO:HD2	1.98	0.64
10:K:9:PHE:O	10:K:13:VAL:HG23	1.96	0.64
11:L:2:GLU:N	11:L:3:PRO:CD	2.61	0.64
13:O:20:PRO:HB2	13:O:240:TYR:CE1	2.33	0.64
13:O:66:VAL:HG13	13:O:67:PRO:HD2	1.80	0.64
2:B:478:VAL:HG12	4:D:139:ARG:HG2	1.80	0.64
3:C:42:LEU:HG	23:C:486:CLA:CED	2.24	0.64
3:C:319:ILE:CD1	3:C:389:GLU:HG2	2.28	0.64
4:D:57:SER:OG	4:D:65:SER:HB2	1.98	0.64
5:E:59:GLN:HE21	5:E:81:GLN:NE2	1.96	0.64
2:B:130:GLU:HG2	2:B:131:PRO:CD	2.26	0.64
2:B:138:MET:CG	23:B:522:CLA:HBC2	2.20	0.64
2:B:271:THR:OG1	2:B:274:GLN:HG3	1.97	0.64
15:U:39:LEU:C	15:U:41:ASN:H	2.01	0.64
1:A:310:LYS:HB3	1:A:312:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:2:LEU:N	10:K:3:PRO:CD	2.60	0.64
2:B:73:GLY:O	2:B:92:SER:HB2	1.98	0.64
3:C:162:GLY:O	3:C:165:LEU:HB2	1.95	0.64
1:A:159:LEU:HG	1:A:163:ILE:CD1	2.28	0.63
8:I:27:ASP:HB2	8:I:28:PRO:HD3	1.80	0.63
1:A:281:VAL:HA	1:A:284:TRP:CD1	2.33	0.63
3:C:305:THR:CA	3:C:423:ARG:HH12	2.11	0.63
3:C:348:GLU:OE1	3:C:348:GLU:N	2.31	0.63
4:D:263:ASN:O	4:D:265:ARG:N	2.31	0.63
2:B:221:PRO:HB3	2:B:225:LEU:HB2	1.78	0.63
3:C:426:LEU:O	3:C:430:HIS:HB2	1.98	0.63
13:O:39:ARG:CA	13:O:245:PRO:HG3	2.28	0.63
13:O:155:ASN:HD22	15:U:129:ASN:HD21	1.42	0.63
13:O:238:VAL:HG12	13:O:239:PHE:N	2.12	0.63
2:B:221:PRO:CG	2:B:225:LEU:HD12	2.29	0.63
2:B:326:ARG:NH1	2:B:327:THR:HB	2.13	0.63
3:C:78:GLU:H	3:C:104:GLU:CD	2.01	0.63
1:A:29:TYR:HD2	1:A:133:LEU:HD12	1.63	0.63
4:D:39:PRO:O	4:D:43:LEU:HG	1.99	0.63
1:A:63:ILE:HG23	3:C:335:THR:CG2	2.28	0.63
1:A:206:PHE:HE1	23:A:348:CLA:CMB	2.11	0.63
3:C:160:ILE:O	3:C:163:PHE:HB2	1.98	0.63
8:I:19:PHE:CZ	8:I:23:PHE:HE1	2.16	0.63
19:Z:46:LEU:O	19:Z:50:LEU:HG	1.99	0.63
3:C:321:ASP:OD1	3:C:321:ASP:N	2.31	0.63
4:D:52:THR:HG23	4:D:76:VAL:HG12	1.81	0.63
4:D:222:LEU:HA	4:D:243:THR:O	1.98	0.63
4:D:253:TRP:HA	4:D:253:TRP:CE3	2.33	0.63
8:I:25:SER:HB2	8:I:28:PRO:HD2	1.80	0.63
16:V:75:TYR:HE2	16:V:80:THR:N	1.95	0.63
1:A:59:ASP:OD2	1:A:63:ILE:O	2.17	0.63
2:B:327:THR:OG1	27:B:529:BCR:H401	1.99	0.63
4:D:42:TYR:CZ	6:F:24:THR:HG23	2.33	0.63
15:U:113:THR:HG22	15:U:114:VAL:N	2.13	0.63
3:C:119:LEU:O	3:C:122:SER:OG	2.17	0.62
4:D:298:PHE:CA	11:L:37:ASN:ND2	2.54	0.62
12:M:8:LEU:HD22	14:T:1:MET:CE	2.29	0.62
1:A:261:GLN:HG3	1:A:262:TYR:N	2.13	0.62
1:A:322:ASN:OD1	3:C:412:THR:HG23	1.99	0.62
3:C:120:ILE:HG21	27:C:489:BCR:H353	1.81	0.62
3:C:370:ARG:HD3	3:C:375:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:489:BCR:H312	19:Z:55:GLY:HA2	1.81	0.62
5:E:12:ILE:HD11	28:E:84:HEC:O1A	1.99	0.62
16:V:102:PRO:HA	16:V:105:ARG:HG3	1.81	0.62
1:A:161:TYR:CE1	1:A:186:PHE:HE1	2.17	0.62
23:A:350:CLA:HED1	4:D:175:VAL:CG1	2.29	0.62
2:B:106:LEU:HD22	23:B:522:CLA:H143	1.80	0.62
2:B:234:ILE:O	2:B:236:THR:N	2.32	0.62
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.67	0.62
2:B:225:LEU:HD13	2:B:231:MET:SD	2.38	0.62
23:B:520:CLA:HAA2	23:B:520:CLA:HBD	1.81	0.62
3:C:70:PHE:O	3:C:73:ALA:HB3	1.99	0.62
4:D:56:THR:HG23	4:D:56:THR:O	1.98	0.62
1:A:180:PHE:HE2	4:D:192:THR:O	1.82	0.62
1:A:239:PHE:HE1	4:D:245:SER:HA	1.61	0.62
1:A:309:ALA:HB1	16:V:1:ALA:O	2.00	0.62
10:K:15:VAL:HG21	18:N:9:UNK:O	1.99	0.62
13:O:162:ARG:O	13:O:162:ARG:CG	2.48	0.62
19:Z:37:LYS:O	19:Z:41:PHE:CD1	2.52	0.62
2:B:323:GLY:HA2	4:D:293:LEU:HG	1.81	0.62
3:C:216:SER:O	3:C:221:GLU:O	2.18	0.62
3:C:320:ARG:NH1	16:V:49:ASN:HA	2.15	0.62
4:D:186:GLN:HA	4:D:186:GLN:NE2	2.14	0.62
10:K:10:ASP:HB3	10:K:11:PRO:HD3	1.81	0.62
13:O:168:TYR:CD1	13:O:172:ILE:HD11	2.35	0.62
1:A:180:PHE:HD1	1:A:180:PHE:H	1.47	0.62
5:E:12:ILE:HD13	28:E:84:HEC:CGA	2.30	0.62
13:O:11:VAL:HG12	13:O:11:VAL:O	2.00	0.62
15:U:57:LEU:CD2	15:U:112:PHE:HD2	1.95	0.62
2:B:29:LEU:HB3	27:B:528:BCR:H351	1.82	0.62
2:B:69:LEU:HD12	23:B:518:CLA:HBA2	1.82	0.62
27:B:528:BCR:HC8	27:B:528:BCR:H331	1.82	0.62
3:C:120:ILE:CG2	27:C:489:BCR:H353	2.30	0.62
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.81	0.62
4:D:180:ARG:C	4:D:180:ARG:HD3	2.21	0.62
5:E:56:ALA:O	5:E:57:GLN:C	2.37	0.62
16:V:129:LYS:CE	16:V:135:VAL:HG23	2.30	0.62
1:A:237:TYR:CE2	1:A:245:THR:HA	2.35	0.61
23:B:524:CLA:H13	23:B:524:CLA:OBD	2.00	0.61
5:E:9:PHE:O	5:E:10:SER:CB	2.47	0.61
7:H:53:ILE:HG23	17:X:13:THR:HG1	1.65	0.61
19:Z:44:SER:O	19:Z:48:ILE:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:GLY:HA2	3:C:41:ARG:HE	1.64	0.61
3:C:103:GLY:O	3:C:104:GLU:C	2.39	0.61
3:C:405:ASN:HB2	3:C:407:VAL:CG2	2.30	0.61
4:D:91:LEU:N	4:D:91:LEU:HD23	2.14	0.61
13:O:53:LYS:HE2	13:O:234:LYS:HB2	1.82	0.61
3:C:225:VAL:HB	23:C:487:CLA:HMC3	1.81	0.61
27:C:489:BCR:H341	19:Z:51:VAL:HG13	1.82	0.61
1:A:89:ILE:HD12	1:A:108:ASN:HB3	1.83	0.61
5:E:12:ILE:CG1	28:E:84:HEC:O2D	2.47	0.61
13:O:50:PHE:HZ	13:O:76:THR:CG2	2.13	0.61
15:U:59:ASN:ND2	15:U:59:ASN:H	1.80	0.61
16:V:76:MET:HE3	16:V:115:ILE:HG21	1.83	0.61
4:D:108:GLY:C	4:D:110:LEU:H	2.02	0.61
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.31	0.61
13:O:102:ASP:O	13:O:103:PHE:CD1	2.53	0.61
13:O:163:GLY:CA	13:O:188:LYS:HE2	2.30	0.61
14:T:4:ILE:HG13	14:T:5:THR:N	2.15	0.61
1:A:114:LEU:CD1	1:A:118:HIS:CE1	2.84	0.61
2:B:135:LEU:HD23	2:B:138:MET:SD	2.40	0.61
3:C:285:ILE:HG12	23:C:487:CLA:HMB2	1.82	0.61
27:C:489:BCR:C34	19:Z:51:VAL:HG13	2.31	0.61
13:O:94:THR:HA	13:O:127:ALA:O	2.01	0.61
1:A:296:ASN:OD1	3:C:401:LEU:HD23	2.00	0.61
3:C:265:ILE:HG22	3:C:266:TRP:H	1.66	0.61
3:C:282:MET:HA	3:C:285:ILE:HB	1.83	0.61
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.81	0.61
13:O:40:ILE:CG2	13:O:41:ALA:H	2.14	0.61
1:A:301:ASN:CG	3:C:407:VAL:HG21	2.19	0.61
2:B:271:THR:HG22	2:B:448:ARG:NH1	2.15	0.61
15:U:82:ASN:O	15:U:85:TYR:HE2	1.84	0.61
1:A:149:ALA:HA	1:A:284:TRP:CZ3	2.36	0.61
3:C:36:TRP:O	3:C:38:GLY:N	2.31	0.61
3:C:227:VAL:HG23	3:C:227:VAL:O	2.00	0.61
4:D:22:LEU:HD21	4:D:32:TRP:CE3	2.35	0.61
4:D:157:PHE:O	4:D:158:LEU:HD23	2.00	0.61
4:D:171:PRO:HG3	4:D:181:PHE:CE1	2.36	0.61
13:O:92:SER:HB2	13:O:129:THR:O	2.01	0.61
15:U:127:ARG:O	15:U:128:TYR:HD1	1.82	0.61
1:A:224:ILE:HG21	1:A:227:THR:OG1	2.01	0.61
1:A:306:VAL:CG2	1:A:307:ILE:H	2.13	0.61
3:C:39:ASN:HA	3:C:42:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:333:GLY:O	3:C:335:THR:N	2.34	0.61
4:D:18:LEU:HA	17:X:41:SER:OG	2.01	0.61
13:O:112:GLY:C	13:O:114:GLU:H	2.03	0.61
13:O:137:THR:O	13:O:140:THR:HG23	2.01	0.61
1:A:180:PHE:CD2	4:D:192:THR:HB	2.37	0.60
1:A:322:ASN:O	1:A:326:LEU:HB2	2.00	0.60
3:C:272:LEU:O	3:C:276:LEU:HB2	2.00	0.60
4:D:83:ASN:ND2	4:D:83:ASN:O	2.34	0.60
13:O:95:PHE:HB2	13:O:127:ALA:HB3	1.81	0.60
1:A:187:GLN:HG3	1:A:193:LEU:HG	1.83	0.60
2:B:57:ARG:NH1	2:B:57:ARG:CG	2.64	0.60
2:B:98:LEU:O	2:B:102:VAL:HG23	2.01	0.60
13:O:28:GLY:HA3	13:O:137:THR:CG2	2.30	0.60
2:B:321:LYS:HE3	2:B:325:PHE:HZ	1.66	0.60
3:C:433:LEU:O	3:C:437:PHE:HB2	2.02	0.60
23:C:486:CLA:H61	27:C:488:BCR:H393	1.83	0.60
1:A:279:PRO:HG2	4:D:211:CYS:HB3	1.81	0.60
2:B:7:ARG:HA	23:B:523:CLA:O1A	2.01	0.60
4:D:253:TRP:HA	4:D:253:TRP:HE3	1.67	0.60
10:K:6:TYR:O	10:K:8:ILE:N	2.34	0.60
1:A:223:LEU:HD22	1:A:245:THR:CG2	2.30	0.60
2:B:399:VAL:HG23	2:B:417:VAL:HG13	1.83	0.60
3:C:95:LEU:HD21	23:C:479:CLA:OBD	2.01	0.60
3:C:275:SER:CB	23:C:485:CLA:HAA1	2.30	0.60
4:D:77:ALA:CB	4:D:174:GLY:HA3	2.31	0.60
4:D:138:VAL:CG1	4:D:139:ARG:N	2.65	0.60
4:D:188:PHE:N	4:D:188:PHE:CD1	2.69	0.60
4:D:196:PHE:HD1	4:D:285:GLY:HA2	1.66	0.60
11:L:23:LEU:O	11:L:27:LEU:HB2	2.01	0.60
1:A:261:GLN:HG3	1:A:262:TYR:H	1.66	0.60
2:B:123:PHE:CG	2:B:123:PHE:O	2.54	0.60
2:B:142:HIS:ND1	23:B:524:CLA:H142	2.16	0.60
2:B:229:LEU:O	2:B:230:ARG:C	2.40	0.60
3:C:78:GLU:OE1	3:C:78:GLU:HA	2.01	0.60
3:C:95:LEU:HA	3:C:185:LEU:HD12	1.84	0.60
23:C:486:CLA:H42	10:K:30:TRP:NE1	2.17	0.60
7:H:30:MET:O	7:H:33:PHE:N	2.35	0.60
13:O:95:PHE:HB3	13:O:127:ALA:CB	2.31	0.60
1:A:321:ILE:O	1:A:325:ASN:ND2	2.34	0.60
2:B:191:ASN:HB2	2:B:192:PRO:HD2	1.83	0.60
23:C:474:CLA:H8	23:C:477:CLA:H143	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.83	0.60
13:O:88:ASN:ND2	13:O:92:SER:OG	2.34	0.60
1:A:104:GLU:OE2	13:O:73:ARG:HD3	2.02	0.60
2:B:372:ASP:OD2	2:B:376:VAL:HG23	2.02	0.60
2:B:321:LYS:CE	2:B:325:PHE:CZ	2.84	0.60
3:C:297:TYR:CD2	3:C:302:TYR:HE1	2.19	0.60
4:D:261:PHE:HD1	4:D:266:TRP:CD1	2.19	0.60
11:L:8:GLN:N	11:L:9:PRO:HD3	2.17	0.60
16:V:38:ALA:O	16:V:42:VAL:HG23	2.01	0.60
17:X:12:ILE:HG22	17:X:16:LEU:HD13	1.82	0.60
2:B:355:PHE:CE1	2:B:373:LYS:HB3	2.36	0.60
4:D:58:TRP:HA	4:D:62:GLY:H	1.67	0.60
5:E:12:ILE:HG23	5:E:18:TYR:HB2	1.70	0.60
5:E:59:GLN:HE21	5:E:81:GLN:HE22	1.50	0.60
7:H:28:PRO:O	7:H:32:VAL:HG23	2.02	0.60
11:L:1:MET:C	11:L:3:PRO:HD2	2.23	0.60
11:L:36:PHE:O	12:M:3:VAL:HG23	2.01	0.60
3:C:62:PHE:CZ	10:K:19:ILE:CD1	2.81	0.59
3:C:240:ILE:HG22	3:C:244:CYS:SG	2.42	0.59
5:E:26:ILE:HG12	5:E:27:PRO:HD3	1.84	0.59
16:V:118:HIS:CD2	16:V:122:GLU:OE1	2.55	0.59
1:A:57:PRO:HG2	13:O:115:ARG:HH11	1.67	0.59
1:A:281:VAL:O	1:A:281:VAL:CG1	2.50	0.59
2:B:190:PHE:CE1	23:B:527:CLA:HED3	2.38	0.59
2:B:235:GLU:HB3	2:B:473:THR:OG1	2.02	0.59
13:O:27:ARG:C	13:O:29:ALA:H	2.04	0.59
16:V:76:MET:HE3	28:V:138:HEC:HMB1	1.82	0.59
3:C:169:GLY:O	3:C:173:LEU:HG	2.02	0.59
3:C:349:ILE:C	3:C:350:ILE:HG13	2.22	0.59
4:D:101:PHE:CE2	4:D:105:CYS:SG	2.95	0.59
10:K:6:TYR:O	10:K:7:ALA:C	2.41	0.59
13:O:194:LYS:HG3	13:O:194:LYS:O	2.01	0.59
1:A:281:VAL:HG22	1:A:284:TRP:HD1	1.67	0.59
2:B:171:PRO:CG	7:H:62:LYS:HA	2.33	0.59
3:C:299:SER:HB2	3:C:303:GLY:O	2.02	0.59
23:C:486:CLA:H172	19:Z:23:VAL:HG21	1.84	0.59
6:F:40:GLN:HE22	9:J:27:LEU:HG	1.58	0.59
16:V:69:ILE:O	16:V:73:VAL:HG23	2.01	0.59
2:B:12:LEU:HD11	2:B:18:ARG:C	2.23	0.59
3:C:141:GLU:HB2	3:C:144:SER:CB	2.32	0.59
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:233:VAL:HG12	13:O:234:LYS:N	2.17	0.59
2:B:380:ASP:OD1	2:B:390:TYR:CB	2.50	0.59
16:V:117:GLY:O	16:V:121:VAL:HG23	2.03	0.59
3:C:223:TRP:CD1	3:C:224:ILE:N	2.71	0.59
4:D:66:SER:HA	4:D:76:VAL:HG13	1.85	0.59
16:V:55:ARG:HG3	16:V:56:THR:N	2.16	0.59
2:B:174:LEU:HG	2:B:174:LEU:O	2.01	0.59
2:B:302:TRP:O	2:B:305:ILE:HG12	2.02	0.59
1:A:265:PHE:HB2	1:A:271:LEU:HD21	1.85	0.59
2:B:321:LYS:HE2	2:B:325:PHE:CZ	2.37	0.59
3:C:374:GLY:HA2	13:O:7:TYR:HE1	1.65	0.59
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.37	0.59
4:D:235:PHE:CG	4:D:236:ASN:N	2.70	0.59
7:H:53:ILE:HG22	17:X:15:SER:HB2	1.85	0.59
13:O:164:LEU:O	13:O:165:ALA:CB	2.51	0.59
15:U:32:THR:O	15:U:36:GLU:HG3	2.03	0.59
19:Z:47:TRP:CD1	19:Z:47:TRP:C	2.76	0.59
2:B:225:LEU:O	2:B:231:MET:HG2	2.03	0.59
2:B:301:ALA:O	2:B:304:ALA:HB3	2.02	0.59
3:C:284:PHE:HD1	3:C:434:ALA:HB1	1.66	0.59
3:C:429:SER:O	3:C:432:VAL:HB	2.03	0.59
3:C:437:PHE:HA	23:C:483:CLA:HMC3	1.84	0.59
10:K:15:VAL:O	10:K:15:VAL:HG12	2.02	0.59
3:C:239:TRP:O	3:C:243:ILE:HG13	2.03	0.58
5:E:30:PHE:O	5:E:30:PHE:HD2	1.84	0.58
2:B:46:ASP:HB3	2:B:58:GLN:OE1	2.03	0.58
2:B:136:PRO:HD3	2:B:231:MET:CE	2.32	0.58
2:B:171:PRO:HG3	7:H:62:LYS:HA	1.86	0.58
2:B:223:GLN:HG3	2:B:227:LYS:HE3	1.85	0.58
2:B:340:TRP:N	2:B:340:TRP:CD1	2.71	0.58
4:D:88:SER:OG	5:E:68:ARG:NE	2.36	0.58
1:A:29:TYR:CD2	1:A:133:LEU:HD12	2.37	0.58
1:A:307:ILE:HG13	1:A:314:ILE:CD1	2.30	0.58
2:B:234:ILE:HG21	23:B:513:CLA:HAC1	1.85	0.58
3:C:62:PHE:CE1	3:C:119:LEU:HD11	2.39	0.58
4:D:27:PHE:HB3	6:F:17:VAL:HG11	1.84	0.58
8:I:19:PHE:CE1	8:I:23:PHE:HE1	2.21	0.58
13:O:156:PHE:O	13:O:188:LYS:NZ	2.36	0.58
13:O:221:SER:OG	13:O:231:HIS:N	2.36	0.58
1:A:210:LEU:HD13	24:D:355:PHO:ND	2.18	0.58
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:PRO:O	3:C:78:GLU:HB2	2.03	0.58
3:C:266:TRP:HA	3:C:271:TYR:HE2	1.68	0.58
4:D:32:TRP:N	4:D:131:GLU:OE2	2.35	0.58
1:A:98:GLU:O	1:A:98:GLU:HG3	2.02	0.58
3:C:71:GLU:HB3	3:C:89:ILE:HD11	1.85	0.58
3:C:293:ASN:OD1	3:C:423:ARG:NH2	2.37	0.58
3:C:373:ASN:OD1	13:O:16:ALA:HA	2.03	0.58
4:D:29:PHE:HE2	4:D:31:GLY:CA	2.16	0.58
4:D:267:LEU:O	4:D:271:MET:HE2	2.03	0.58
16:V:63:THR:HB	16:V:83:ASP:O	2.03	0.58
27:B:529:BCR:H311	27:B:529:BCR:H342	1.86	0.58
3:C:113:VAL:O	3:C:117:VAL:HG23	2.03	0.58
3:C:271:TYR:HA	3:C:274:TYR:CE1	2.39	0.58
13:O:215:PHE:O	13:O:216:GLU:HB2	2.02	0.58
2:B:150:CYS:HB2	23:B:517:CLA:HMC3	1.84	0.58
4:D:35:ILE:O	4:D:39:PRO:HD2	2.03	0.58
13:O:40:ILE:HG23	13:O:84:GLU:OE2	2.04	0.58
13:O:215:PHE:HB3	13:O:237:GLY:H	1.69	0.58
1:A:334:ARG:HH11	4:D:320:LEU:CD1	2.13	0.58
3:C:63:TRP:CE2	3:C:67:MET:HG3	2.39	0.58
23:C:477:CLA:H142	23:C:477:CLA:H101	1.84	0.58
17:X:34:PHE:O	17:X:38:ILE:HG13	2.04	0.58
3:C:243:ILE:O	23:C:474:CLA:HMC1	2.03	0.58
13:O:39:ARG:HA	13:O:245:PRO:HG3	1.85	0.58
14:T:3:THR:O	14:T:6:TYR:N	2.33	0.58
16:V:75:TYR:CE2	16:V:79:PRO:HA	2.39	0.58
1:A:14:TRP:HH2	8:I:25:SER:HB3	1.68	0.58
23:B:521:CLA:CAB	23:B:527:CLA:HED1	2.27	0.58
3:C:63:TRP:CZ2	3:C:67:MET:HG3	2.39	0.58
3:C:123:ALA:HB1	19:Z:47:TRP:CH2	2.37	0.58
1:A:78:ILE:O	1:A:177:SER:HB2	2.03	0.57
1:A:228:THR:HG22	1:A:228:THR:O	2.04	0.57
23:B:520:CLA:HAA2	23:B:520:CLA:CB D	2.33	0.57
3:C:188:THR:HG22	3:C:188:THR:O	2.03	0.57
4:D:28:VAL:H	6:F:17:VAL:HG11	1.69	0.57
11:L:27:LEU:HD23	12:M:14:PHE:CE2	2.39	0.57
13:O:53:LYS:HG2	13:O:65:PHE:CD2	2.39	0.57
16:V:76:MET:O	16:V:94:SER:HA	2.04	0.57
23:B:518:CLA:H142	23:B:524:CLA:HBA1	1.86	0.57
3:C:94:THR:C	3:C:96:GLY:H	2.07	0.57
3:C:286:ALA:O	3:C:289:PHE:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:O	3:C:308:GLU:HB2	2.04	0.57
3:C:344:SER:O	3:C:347:GLY:N	2.32	0.57
3:C:436:PHE:O	3:C:439:VAL:HB	2.04	0.57
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.39	0.57
6:F:14:ILE:O	6:F:14:ILE:HG13	2.03	0.57
8:I:5:LYS:O	8:I:9:TYR:HD1	1.86	0.57
10:K:11:PRO:HB3	18:N:9:UNK:CB	2.34	0.57
13:O:200:ASN:O	13:O:213:GLY:HA3	2.04	0.57
13:O:215:PHE:HB3	13:O:237:GLY:N	2.19	0.57
16:V:38:ALA:O	16:V:42:VAL:CG2	2.52	0.57
1:A:89:ILE:HD13	1:A:94:TYR:CG	2.39	0.57
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.19	0.57
1:A:141:PRO:HG3	3:C:446:GLY:C	2.24	0.57
1:A:218:LEU:CD2	4:D:142:ASN:HD22	2.16	0.57
1:A:286:THR:CG2	23:A:348:CLA:O1D	2.50	0.57
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.86	0.57
3:C:318:LEU:HD22	3:C:328:VAL:HG21	1.87	0.57
10:K:24:LEU:O	10:K:27:ALA:HB3	2.04	0.57
12:M:8:LEU:HD22	14:T:1:MET:HE3	1.85	0.57
19:Z:12:LEU:HD12	19:Z:12:LEU:O	2.04	0.57
1:A:15:GLU:O	1:A:19:ASN:ND2	2.38	0.57
1:A:69:GLY:O	1:A:81:ALA:HA	2.04	0.57
1:A:142:TRP:CD1	3:C:443:TRP:CH2	2.92	0.57
1:A:161:TYR:CE2	1:A:165:GLN:HG3	2.40	0.57
1:A:263:ALA:HB1	25:A:353:PL9:H151	1.86	0.57
1:A:341:LEU:HD21	15:U:134:LYS:NZ	2.19	0.57
2:B:192:PRO:HG3	7:H:48:TYR:CE1	2.40	0.57
3:C:291:TRP:HB3	3:C:292:PHE:CE2	2.39	0.57
4:D:72:ASN:OD1	4:D:74:LEU:HB2	2.03	0.57
14:T:9:ILE:O	14:T:9:ILE:HG22	2.05	0.57
15:U:75:LEU:HD21	15:U:101:GLN:HE21	1.69	0.57
1:A:142:TRP:HB2	4:D:220:ASN:HB2	1.86	0.57
3:C:155:ASN:HB3	3:C:255:THR:OG1	2.05	0.57
4:D:261:PHE:CD1	4:D:266:TRP:CD1	2.93	0.57
14:T:24:ARG:HG2	14:T:25:GLU:N	2.19	0.57
1:A:143:ILE:HD13	4:D:253:TRP:CH2	2.40	0.57
2:B:45:PHE:CE2	2:B:78:TRP:CZ2	2.92	0.57
2:B:479:PHE:HD2	2:B:479:PHE:C	2.07	0.57
23:B:524:CLA:O1A	23:B:524:CLA:H2	2.04	0.57
4:D:68:LEU:N	6:F:39:MET:HE1	2.20	0.57
4:D:122:LEU:HD21	23:D:354:CLA:C9	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.03	0.57
1:A:316:THR:O	1:A:318:ALA:N	2.37	0.57
2:B:247:PHE:CE1	23:B:521:CLA:H72	2.40	0.57
2:B:250:PHE:CD1	2:B:459:ALA:HB1	2.40	0.57
2:B:414:PRO:N	2:B:415:PRO:CD	2.67	0.57
2:B:479:PHE:C	2:B:479:PHE:CD2	2.78	0.57
4:D:110:LEU:O	4:D:113:PHE:HB3	2.05	0.57
4:D:168:PHE:HD2	4:D:168:PHE:C	2.08	0.57
3:C:42:LEU:CD2	23:C:486:CLA:HED1	2.35	0.57
3:C:284:PHE:O	3:C:285:ILE:C	2.42	0.57
3:C:292:PHE:HE1	23:C:487:CLA:HBC3	1.69	0.57
16:V:22:THR:H	16:V:25:GLN:NE2	2.03	0.57
1:A:335:ASN:C	1:A:335:ASN:HD22	2.08	0.57
2:B:414:PRO:N	2:B:415:PRO:HD3	2.20	0.57
3:C:282:MET:CA	3:C:285:ILE:HG13	2.32	0.57
13:O:78:LEU:O	13:O:79:ASP:OD1	2.23	0.57
2:B:10:THR:O	2:B:13:ILE:HG22	2.04	0.57
3:C:155:ASN:OD1	3:C:156:LYS:HG2	2.04	0.57
4:D:29:PHE:C	4:D:29:PHE:HD2	2.08	0.57
4:D:52:THR:O	4:D:67:TYR:HD1	1.88	0.57
4:D:86:GLY:C	4:D:87:HIS:CD2	2.78	0.57
13:O:39:ARG:HA	13:O:245:PRO:CB	2.35	0.57
13:O:102:ASP:O	13:O:103:PHE:HD1	1.85	0.57
15:U:40:VAL:O	15:U:40:VAL:HG12	2.05	0.57
1:A:29:TYR:CD1	1:A:30:VAL:N	2.69	0.56
2:B:414:PRO:O	2:B:418:LYS:HG3	2.04	0.56
3:C:141:GLU:CB	3:C:144:SER:OG	2.53	0.56
3:C:314:ALA:HB3	3:C:351:PHE:CD1	2.40	0.56
3:C:326:ALA:CB	15:U:127:ARG:HD2	2.31	0.56
3:C:412:THR:HG22	16:V:136:TYR:HE2	1.69	0.56
3:C:417:VAL:HG21	16:V:42:VAL:HG22	1.86	0.56
13:O:53:LYS:CE	13:O:234:LYS:HB2	2.35	0.56
13:O:66:VAL:CG1	13:O:67:PRO:HD2	2.35	0.56
17:X:12:ILE:HA	17:X:16:LEU:HD12	1.87	0.56
1:A:52:PHE:CE1	1:A:81:ALA:HB2	2.40	0.56
1:A:114:LEU:HD11	1:A:118:HIS:CE1	2.39	0.56
1:A:214:MET:HA	1:A:214:MET:HE3	1.83	0.56
1:A:237:TYR:CD1	1:A:237:TYR:N	2.73	0.56
2:B:348:ASN:CG	2:B:349:LYS:H	2.07	0.56
23:B:512:CLA:H203	23:B:523:CLA:H192	1.87	0.56
4:D:138:VAL:CG1	4:D:139:ARG:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:GLN:HA	4:D:186:GLN:HE21	1.69	0.56
4:D:329:MET:HG2	4:D:329:MET:O	2.05	0.56
28:E:84:HEC:HMC2	6:F:27:VAL:HA	1.87	0.56
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.87	0.56
2:B:458:PHE:CE1	23:B:516:CLA:HBB1	2.41	0.56
23:B:511:CLA:HMD1	7:H:26:THR:HB	1.86	0.56
3:C:88:LEU:O	3:C:91:HIS:HB2	2.05	0.56
3:C:229:ASN:OD1	3:C:231:GLU:HG3	2.05	0.56
3:C:324:LEU:HD21	15:U:72:TYR:OH	2.05	0.56
23:C:476:CLA:H12	23:C:483:CLA:H2	1.86	0.56
4:D:261:PHE:HA	14:T:24:ARG:NH2	2.20	0.56
7:H:53:ILE:HG23	7:H:53:ILE:O	2.04	0.56
11:L:7:ARG:O	11:L:9:PRO:HD3	2.05	0.56
13:O:149:PRO:HA	13:O:192:LEU:HD12	1.86	0.56
3:C:281:MET:O	3:C:284:PHE:HB2	2.05	0.56
4:D:231:THR:HG22	4:D:232:PHE:N	2.20	0.56
13:O:43:LEU:HD12	13:O:241:ALA:HB2	1.87	0.56
1:A:110:GLY:O	1:A:111:PRO:C	2.43	0.56
1:A:133:LEU:HD23	4:D:252:PHE:CD1	2.41	0.56
1:A:195:HIS:O	1:A:199:GLN:HG3	2.06	0.56
2:B:372:ASP:OD2	2:B:374:ASN:HB2	2.03	0.56
3:C:284:PHE:CD1	3:C:434:ALA:HB1	2.41	0.56
14:T:24:ARG:HG2	14:T:25:GLU:H	1.70	0.56
16:V:129:LYS:NZ	16:V:135:VAL:CG2	2.69	0.56
1:A:114:LEU:CD1	1:A:118:HIS:HE1	2.19	0.56
1:A:330:VAL:HG13	4:D:348:ARG:HG3	1.87	0.56
2:B:394:GLN:NE2	15:U:52:GLY:HA3	2.21	0.56
3:C:350:ILE:CG2	3:C:359:TRP:HB3	2.35	0.56
4:D:87:HIS:CD2	4:D:166:SER:HA	2.41	0.56
11:L:12:LEU:HD11	11:L:16:SER:CB	2.34	0.56
13:O:192:LEU:HD22	15:U:119:THR:HG23	1.88	0.56
1:A:93:PHE:CZ	23:A:352:CLA:HBA1	2.41	0.56
2:B:371:THR:HG22	2:B:372:ASP:O	2.05	0.56
3:C:279:LEU:HB3	23:C:481:CLA:CBC	2.35	0.56
7:H:47:ILE:HG12	7:H:52:LEU:HD23	1.87	0.56
16:V:22:THR:H	16:V:25:GLN:HE21	1.52	0.56
2:B:41:GLU:HG2	2:B:60:MET:SD	2.45	0.56
4:D:32:TRP:CE3	4:D:32:TRP:HA	2.41	0.56
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.36	0.56
1:A:281:VAL:HG22	1:A:284:TRP:CD1	2.41	0.56
3:C:61:VAL:HG11	3:C:121:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:84:HEC:C4A	6:F:19:TRP:HH2	2.18	0.56
10:K:16:LEU:HB3	10:K:17:PRO:HD3	1.88	0.56
1:A:95:PRO:HD2	1:A:98:GLU:HB3	1.87	0.56
1:A:205:VAL:HG12	4:D:204:VAL:HG12	1.87	0.56
23:B:519:CLA:H142	23:D:356:CLA:H42	1.88	0.56
4:D:87:HIS:CD2	4:D:87:HIS:N	2.73	0.56
5:E:59:GLN:NE2	5:E:81:GLN:NE2	2.54	0.56
13:O:32:ILE:C	13:O:34:SER:H	2.10	0.56
13:O:118:LEU:CD1	13:O:233:VAL:HG21	2.35	0.56
16:V:75:TYR:HE1	28:V:138:HEC:C2A	2.19	0.56
1:A:316:THR:O	1:A:317:TRP:C	2.43	0.55
4:D:168:PHE:C	4:D:168:PHE:CD2	2.79	0.55
10:K:30:TRP:CZ3	10:K:31:GLN:NE2	2.74	0.55
1:A:159:LEU:CG	1:A:163:ILE:HD11	2.36	0.55
3:C:101:PRO:CA	3:C:195:ASP:HB3	2.36	0.55
3:C:331:ALA:O	3:C:338:GLY:HA2	2.05	0.55
4:D:257:PHE:CZ	25:D:357:PL9:H253	2.41	0.55
4:D:302:GLU:O	4:D:305:ALA:HB3	2.06	0.55
11:L:2:GLU:N	11:L:3:PRO:HD2	2.21	0.55
1:A:221:SER:CA	4:D:139:ARG:HB2	2.33	0.55
3:C:173:LEU:HA	3:C:176:VAL:HG23	1.88	0.55
4:D:118:GLY:CA	24:D:355:PHO:H71	2.37	0.55
1:A:139:MET:HE2	4:D:248:THR:CG2	2.36	0.55
1:A:142:TRP:HH2	1:A:273:PHE:HE1	1.54	0.55
3:C:342:MET:HE3	3:C:353:GLY:H	1.70	0.55
1:A:12:ASN:O	1:A:15:GLU:HG3	2.06	0.55
2:B:326:ARG:HD3	27:B:529:BCR:C40	2.31	0.55
2:B:418:LYS:HZ1	15:U:45:GLU:CD	2.10	0.55
23:B:511:CLA:HBC3	7:H:33:PHE:CD2	2.42	0.55
3:C:285:ILE:HG12	23:C:487:CLA:CMB	2.37	0.55
3:C:294:ASN:O	3:C:296:VAL:N	2.40	0.55
4:D:59:TYR:HE1	5:E:49:PRO:HG2	1.72	0.55
4:D:198:MET:HE1	11:L:30:LEU:CD1	2.30	0.55
13:O:68:THR:HA	13:O:110:MET:HE1	1.87	0.55
16:V:55:ARG:O	16:V:59:LEU:HG	2.07	0.55
1:A:297:LEU:HD22	3:C:428:THR:HG21	1.87	0.55
1:A:325:ASN:HD22	1:A:325:ASN:N	2.05	0.55
2:B:12:LEU:HG	2:B:19:LEU:HB2	1.87	0.55
13:O:153:THR:HG22	13:O:154:ALA:N	2.22	0.55
15:U:88:VAL:CG2	15:U:114:VAL:HG23	2.36	0.55
1:A:224:ILE:O	1:A:224:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:TYR:N	2:B:6:TYR:CD2	2.75	0.55
2:B:12:LEU:HD21	2:B:19:LEU:HA	1.88	0.55
3:C:187:ASP:O	3:C:194:GLY:O	2.25	0.55
7:H:21:ALA:HB3	7:H:22:PRO:CD	2.37	0.55
13:O:19:CYS:HB3	13:O:240:TYR:HB2	1.89	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.88	0.55
1:A:301:ASN:HD21	3:C:407:VAL:HG23	1.71	0.55
2:B:47:PRO:HA	2:B:78:TRP:HE1	1.72	0.55
3:C:98:GLY:O	3:C:105:VAL:HG13	2.07	0.55
3:C:116:VAL:HG13	27:C:488:BCR:C33	2.33	0.55
3:C:158:THR:O	3:C:161:LEU:HB3	2.07	0.55
3:C:447:ARG:HG3	3:C:447:ARG:O	2.06	0.55
23:C:478:CLA:C9	23:C:482:CLA:HAA1	2.36	0.55
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.41	0.55
13:O:32:ILE:C	13:O:34:SER:N	2.59	0.55
1:A:180:PHE:CD2	4:D:192:THR:CG2	2.90	0.55
1:A:224:ILE:HD11	1:A:243:GLU:HG3	1.89	0.55
2:B:356:VAL:HG23	2:B:370:LEU:HD23	1.89	0.55
23:C:478:CLA:H162	23:C:482:CLA:HMD2	1.89	0.55
4:D:29:PHE:HE2	4:D:31:GLY:HA3	1.72	0.55
15:U:57:LEU:HD11	15:U:112:PHE:HB3	1.89	0.55
2:B:153:PHE:N	23:B:515:CLA:HMC3	2.22	0.55
2:B:327:THR:C	2:B:329:PRO:HD3	2.27	0.55
12:M:17:VAL:HG12	12:M:18:PRO:N	2.22	0.55
15:U:124:GLY:O	15:U:125:GLY:C	2.46	0.55
16:V:66:ARG:HH11	16:V:66:ARG:HG3	1.72	0.55
1:A:14:TRP:CH2	8:I:25:SER:HB3	2.42	0.54
1:A:291:SER:O	1:A:295:PHE:CE1	2.59	0.54
2:B:231:MET:HE2	2:B:231:MET:O	2.07	0.54
2:B:342:GLY:HA2	2:B:403:GLY:HA3	1.89	0.54
3:C:90:PRO:HB2	3:C:302:TYR:HE2	1.72	0.54
2:B:302:TRP:CZ3	2:B:343:HIS:HB2	2.43	0.54
3:C:182:PHE:O	3:C:184:GLY:N	2.41	0.54
4:D:71:CYS:HB3	4:D:75:THR:CB	2.38	0.54
10:K:19:ILE:HG13	10:K:20:PRO:HD3	1.89	0.54
13:O:211:ILE:CG2	13:O:212:ALA:N	2.70	0.54
15:U:51:TYR:O	15:U:53:GLU:N	2.40	0.54
1:A:97:TRP:CE3	8:I:5:LYS:HA	2.43	0.54
1:A:142:TRP:N	4:D:220:ASN:OD1	2.40	0.54
1:A:334:ARG:O	1:A:335:ASN:ND2	2.40	0.54
2:B:6:TYR:OH	12:M:21:PHE:CZ	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:THR:O	2:B:159:THR:HG22	2.07	0.54
2:B:212:ALA:CB	23:B:511:CLA:HMC3	2.36	0.54
2:B:458:PHE:CD1	23:B:516:CLA:HMC3	2.42	0.54
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
4:D:30:VAL:HG22	4:D:38:PHE:HE1	1.71	0.54
10:K:9:PHE:O	10:K:10:ASP:C	2.44	0.54
13:O:22:LEU:O	13:O:203:LYS:CD	2.55	0.54
16:V:92:HIS:ND1	16:V:93:PRO:HD2	2.22	0.54
19:Z:17:PHE:O	19:Z:21:ILE:HG13	2.06	0.54
1:A:278:TRP:HE1	23:A:350:CLA:H42	1.73	0.54
1:A:303:ASN:C	1:A:304:HIS:HD1	2.10	0.54
2:B:15:ASP:C	2:B:15:ASP:OD1	2.45	0.54
2:B:45:PHE:HE1	2:B:55:MET:HA	1.72	0.54
2:B:372:ASP:CG	2:B:373:LYS:N	2.60	0.54
3:C:36:TRP:C	3:C:38:GLY:H	2.10	0.54
3:C:199:ILE:CD1	3:C:234:VAL:HG21	2.33	0.54
3:C:200:THR:C	3:C:201:ASN:HD22	2.10	0.54
4:D:90:LEU:HD13	4:D:96:GLU:HB3	1.87	0.54
13:O:140:THR:HG21	13:O:201:VAL:HB	1.88	0.54
13:O:243:ILE:HG22	13:O:244:GLU:N	2.22	0.54
2:B:321:LYS:HE2	2:B:325:PHE:HZ	1.71	0.54
1:A:63:ILE:HG23	3:C:335:THR:HG21	1.89	0.54
1:A:133:LEU:HD21	4:D:252:PHE:HA	1.90	0.54
1:A:180:PHE:HD2	4:D:192:THR:HB	1.72	0.54
1:A:302:PHE:N	1:A:302:PHE:CD1	2.75	0.54
2:B:225:LEU:C	2:B:231:MET:HG2	2.28	0.54
2:B:371:THR:HG22	2:B:372:ASP:N	2.23	0.54
2:B:402:TYR:N	2:B:402:TYR:HD1	2.06	0.54
3:C:88:LEU:O	3:C:91:HIS:N	2.40	0.54
4:D:29:PHE:HD2	4:D:29:PHE:O	1.91	0.54
1:A:258:LEU:O	4:D:128:ARG:NH2	2.40	0.54
2:B:110:ALA:O	2:B:113:TRP:N	2.37	0.54
4:D:52:THR:O	4:D:76:VAL:HG11	2.08	0.54
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.43	0.54
4:D:336:HIS:HD2	4:D:336:HIS:N	1.99	0.54
6:F:19:TRP:CH2	6:F:23:HIS:NE2	2.76	0.54
19:Z:37:LYS:O	19:Z:41:PHE:HD1	1.90	0.54
1:A:89:ILE:CG2	1:A:94:TYR:HB2	2.38	0.54
1:A:243:GLU:HA	4:D:240:ALA:CB	2.34	0.54
2:B:134:ASP:OD2	2:B:220:ARG:NH2	2.40	0.54
2:B:183:PRO:HD3	2:B:199:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:489:BCR:C31	19:Z:55:GLY:HA2	2.37	0.54
4:D:182:LEU:HA	23:D:354:CLA:HMD2	1.90	0.54
4:D:221:THR:O	4:D:221:THR:CG2	2.56	0.54
4:D:281:MET:O	4:D:284:ILE:N	2.40	0.54
13:O:193:THR:HG22	13:O:194:LYS:N	2.11	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.76	0.54
1:A:320:ILE:O	1:A:320:ILE:CG2	2.55	0.54
2:B:153:PHE:O	2:B:158:LEU:HG	2.07	0.54
3:C:285:ILE:O	23:C:487:CLA:HBB1	2.07	0.54
4:D:83:ASN:HB3	4:D:336:HIS:ND1	2.23	0.54
7:H:57:VAL:O	7:H:57:VAL:HG12	2.07	0.54
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.07	0.54
1:A:114:LEU:HD12	1:A:118:HIS:CE1	2.43	0.54
23:A:349:CLA:H51	24:A:351:PHO:HMB3	1.89	0.54
3:C:151:TRP:C	3:C:153:ASP:H	2.10	0.54
4:D:156:VAL:CG1	4:D:171:PRO:HG2	2.38	0.54
15:U:72:TYR:HD2	15:U:73:PRO:CD	2.20	0.54
2:B:21:ALA:O	2:B:24:LEU:HB2	2.08	0.53
2:B:209:GLY:HA3	23:B:518:CLA:H201	1.90	0.53
4:D:152:VAL:HG13	23:D:354:CLA:CED	2.38	0.53
3:C:324:LEU:HD12	15:U:128:TYR:CZ	2.43	0.53
3:C:417:VAL:HG22	16:V:38:ALA:HB1	1.90	0.53
4:D:96:GLU:CD	5:E:68:ARG:O	2.46	0.53
4:D:319:LEU:CA	4:D:322:ASN:HD22	2.14	0.53
5:E:68:ARG:HH12	7:H:50:SER:HB3	1.72	0.53
13:O:152:ARG:HD2	13:O:156:PHE:CD2	2.43	0.53
15:U:73:PRO:HG2	16:V:83:ASP:CG	2.28	0.53
16:V:22:THR:N	16:V:25:GLN:HE21	2.06	0.53
19:Z:36:SER:HA	19:Z:39:LEU:HD12	1.89	0.53
2:B:6:TYR:CE1	2:B:8:VAL:HG21	2.42	0.53
2:B:137:LYS:O	2:B:141:ILE:HG12	2.09	0.53
23:B:513:CLA:H18	23:B:524:CLA:CGA	2.38	0.53
23:B:518:CLA:C14	23:B:524:CLA:HBA1	2.38	0.53
3:C:55:ALA:HB1	27:C:488:BCR:H371	1.90	0.53
3:C:88:LEU:HD22	23:C:480:CLA:CGD	2.39	0.53
3:C:437:PHE:HA	23:C:483:CLA:HMC1	1.90	0.53
4:D:179:PHE:HA	4:D:182:LEU:CD1	2.38	0.53
4:D:195:PRO:O	4:D:198:MET:HB2	2.09	0.53
13:O:133:VAL:O	13:O:133:VAL:HG12	2.07	0.53
1:A:213:ALA:O	1:A:217:SER:HB2	2.08	0.53
1:A:292:THR:HG23	3:C:428:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:CG2	23:B:524:CLA:H193	2.38	0.53
3:C:165:LEU:HD21	23:C:474:CLA:CBB	2.38	0.53
3:C:316:THR:HG21	3:C:396:MET:HE1	1.91	0.53
4:D:83:ASN:CB	4:D:336:HIS:HD1	2.22	0.53
4:D:201:VAL:O	4:D:201:VAL:HG12	2.09	0.53
13:O:79:ASP:HA	13:O:101:ILE:HG21	1.91	0.53
2:B:174:LEU:HD22	2:B:308:LYS:HZ2	1.74	0.53
2:B:321:LYS:HE3	2:B:325:PHE:CZ	2.43	0.53
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.91	0.53
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.89	0.53
3:C:318:LEU:HD22	3:C:328:VAL:CG2	2.38	0.53
23:C:477:CLA:HMD1	23:C:485:CLA:HAB	1.91	0.53
15:U:75:LEU:HD21	15:U:101:GLN:NE2	2.24	0.53
2:B:313:ASP:O	2:B:313:ASP:OD1	2.26	0.53
3:C:176:VAL:HG13	3:C:234:VAL:HG13	1.91	0.53
5:E:26:ILE:HG13	5:E:27:PRO:HD3	1.89	0.53
16:V:40:CYS:SG	28:V:138:HEC:CAC	2.97	0.53
2:B:308:LYS:HE2	2:B:312:TYR:CE2	2.43	0.53
3:C:291:TRP:O	3:C:305:THR:HG23	2.08	0.53
3:C:384:ILE:HG23	3:C:384:ILE:O	2.06	0.53
15:U:72:TYR:CG	15:U:73:PRO:N	2.74	0.53
16:V:100:ILE:C	16:V:102:PRO:HD3	2.29	0.53
16:V:122:GLU:HB3	16:V:123:PRO:CD	2.39	0.53
1:A:29:TYR:HE1	1:A:31:GLY:HA3	1.73	0.53
1:A:31:GLY:O	1:A:34:GLY:N	2.38	0.53
1:A:306:VAL:CG2	1:A:307:ILE:N	2.69	0.53
2:B:62:VAL:HG11	23:B:518:CLA:HED3	1.91	0.53
2:B:263:THR:HG22	2:B:263:THR:O	2.09	0.53
2:B:340:TRP:CE3	2:B:342:GLY:HA3	2.44	0.53
2:B:381:ILE:HG22	2:B:381:ILE:O	2.09	0.53
2:B:479:PHE:O	4:D:139:ARG:NH2	2.29	0.53
14:T:10:PHE:CE2	14:T:14:ILE:HD11	2.43	0.53
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.33	0.53
16:V:52:LEU:HD23	28:V:138:HEC:HAD2	1.90	0.53
1:A:307:ILE:C	1:A:309:ALA:N	2.62	0.53
16:V:78:ASN:ND2	16:V:87:GLU:OE2	2.42	0.53
1:A:23:SER:OG	1:A:24:THR:N	2.41	0.53
2:B:236:THR:O	2:B:240:SER:HB3	2.09	0.53
2:B:458:PHE:CG	23:B:516:CLA:HMC3	2.44	0.53
3:C:112:PHE:O	3:C:116:VAL:HG23	2.09	0.53
6:F:30:ILE:O	6:F:30:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:110:MET:H	13:O:110:MET:HE2	1.73	0.53
1:A:63:ILE:CD1	1:A:336:ALA:HB2	2.38	0.52
2:B:344:ALA:HB2	2:B:401:PHE:HE1	1.74	0.52
2:B:421:ALA:O	2:B:424:ALA:HB3	2.08	0.52
3:C:222:GLY:O	3:C:223:TRP:C	2.47	0.52
10:K:16:LEU:HB3	10:K:17:PRO:HD2	1.90	0.52
19:Z:37:LYS:HA	19:Z:40:ILE:HD12	1.91	0.52
1:A:217:SER:OG	4:D:142:ASN:HA	2.09	0.52
3:C:292:PHE:CE1	23:C:487:CLA:HBC3	2.43	0.52
4:D:108:GLY:C	4:D:110:LEU:N	2.60	0.52
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.44	0.52
5:E:48:THR:O	5:E:49:PRO:O	2.27	0.52
7:H:22:PRO:O	7:H:23:GLY:O	2.26	0.52
1:A:189:GLU:CD	22:A:347:OEC:O1	2.37	0.52
1:A:218:LEU:HD23	4:D:142:ASN:HD22	1.74	0.52
1:A:223:LEU:O	1:A:225:ARG:HG3	2.09	0.52
2:B:46:ASP:OD1	2:B:48:SER:OG	2.19	0.52
2:B:103:LEU:HD21	23:B:518:CLA:HMC3	1.91	0.52
2:B:328:GLY:HA3	23:B:514:CLA:O1A	2.10	0.52
14:T:18:PHE:HD2	14:T:19:PHE:HD1	1.56	0.52
1:A:246:TYR:HE1	1:A:248:ILE:HG12	1.74	0.52
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.52
3:C:201:ASN:O	3:C:201:ASN:ND2	2.41	0.52
4:D:83:ASN:OD1	4:D:336:HIS:ND1	2.39	0.52
23:D:356:CLA:H12	7:H:42:LEU:HD21	1.91	0.52
5:E:43:TYR:O	5:E:47:GLY:N	2.42	0.52
10:K:19:ILE:CG1	10:K:20:PRO:HD3	2.39	0.52
1:A:52:PHE:CD2	1:A:52:PHE:O	2.63	0.52
2:B:62:VAL:CG1	23:B:518:CLA:HED3	2.40	0.52
4:D:268:HIS:O	4:D:271:MET:HB2	2.10	0.52
7:H:51:THR:HG22	7:H:51:THR:O	2.10	0.52
13:O:201:VAL:CG1	13:O:211:ILE:HG23	2.37	0.52
1:A:53:ILE:O	1:A:53:ILE:HG22	2.10	0.52
1:A:295:PHE:CD1	1:A:295:PHE:N	2.76	0.52
2:B:110:ALA:O	2:B:111:ALA:C	2.46	0.52
4:D:87:HIS:HA	4:D:167:TRP:NE1	2.25	0.52
1:A:303:ASN:O	1:A:304:HIS:ND1	2.40	0.52
2:B:110:ALA:HA	23:B:522:CLA:H203	1.90	0.52
2:B:247:PHE:O	2:B:251:VAL:HG23	2.09	0.52
23:B:520:CLA:H201	12:M:18:PRO:HB3	1.92	0.52
3:C:122:SER:O	27:C:488:BCR:H363	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:VAL:CG2	23:C:482:CLA:HMB2	2.39	0.52
3:C:278:ALA:O	3:C:282:MET:HG3	2.09	0.52
4:D:286:VAL:HG21	23:D:354:CLA:HED2	1.92	0.52
8:I:31:ASN:CG	8:I:31:ASN:O	2.48	0.52
19:Z:5:PHE:CZ	19:Z:54:VAL:HG13	2.45	0.52
1:A:153:SER:OG	23:A:348:CLA:HED1	2.09	0.52
3:C:264:PHE:CZ	23:C:474:CLA:CGA	2.92	0.52
3:C:289:PHE:O	3:C:289:PHE:HD2	1.92	0.52
4:D:83:ASN:HB3	4:D:336:HIS:HD1	1.75	0.52
4:D:122:LEU:HD21	23:D:354:CLA:H92	1.92	0.52
13:O:38:TYR:O	13:O:245:PRO:HB2	2.09	0.52
13:O:52:VAL:HG11	13:O:116:ILE:HD13	1.91	0.52
13:O:122:VAL:HA	13:O:146:PHE:CD2	2.43	0.52
14:T:18:PHE:CD2	14:T:19:PHE:CD1	2.95	0.52
15:U:62:ILE:O	15:U:64:ALA:N	2.42	0.52
3:C:131:TYR:HE1	3:C:135:ARG:CD	2.23	0.52
3:C:316:THR:HG21	3:C:396:MET:CE	2.39	0.52
8:I:32:PRO:HG2	8:I:35:LYS:O	2.09	0.52
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.45	0.52
1:A:260:PHE:O	1:A:263:ALA:HB3	2.09	0.52
1:A:340:PRO:O	4:D:352:LEU:HD23	2.10	0.52
3:C:350:ILE:HG22	3:C:351:PHE:O	2.10	0.52
13:O:17:ASN:ND2	13:O:77:SER:OG	2.43	0.52
13:O:233:VAL:CG1	13:O:234:LYS:N	2.72	0.52
16:V:79:PRO:HG3	16:V:88:ILE:C	2.30	0.52
1:A:337:HIS:CE1	4:D:352:LEU:HD12	2.44	0.51
2:B:451:PHE:CD1	2:B:451:PHE:C	2.84	0.51
23:B:521:CLA:H112	23:D:356:CLA:H92	1.92	0.51
3:C:390:ARG:NH1	16:V:100:ILE:CG2	2.73	0.51
23:C:486:CLA:H42	10:K:30:TRP:HE1	1.74	0.51
2:B:393:GLU:OE1	2:B:393:GLU:N	2.43	0.51
3:C:340:TYR:CD1	3:C:340:TYR:N	2.77	0.51
7:H:21:ALA:CB	7:H:22:PRO:CD	2.87	0.51
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.68	0.51
3:C:138:GLU:O	3:C:139:THR:HB	2.09	0.51
3:C:354:GLU:C	3:C:356:MET:H	2.13	0.51
4:D:318:ASN:O	4:D:322:ASN:ND2	2.44	0.51
7:H:37:PHE:O	7:H:40:PHE:HB3	2.11	0.51
12:M:5:GLN:HG3	12:M:5:GLN:O	2.10	0.51
13:O:93:LEU:O	13:O:128:SER:HA	2.11	0.51
1:A:307:ILE:HG22	1:A:309:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:VAL:HG12	2:B:169:SER:N	2.24	0.51
2:B:246:PHE:CD2	2:B:246:PHE:C	2.83	0.51
2:B:250:PHE:CE1	2:B:459:ALA:HB1	2.45	0.51
4:D:220:ASN:O	4:D:220:ASN:ND2	2.44	0.51
11:L:27:LEU:HD23	12:M:14:PHE:HE2	1.75	0.51
1:A:70:SER:O	1:A:75:ASN:HB2	2.10	0.51
1:A:131:TRP:O	1:A:134:SER:HB2	2.10	0.51
2:B:164:PRO:HB3	23:B:515:CLA:HED2	1.93	0.51
3:C:68:THR:HB	3:C:115:GLY:HA2	1.93	0.51
4:D:80:THR:HG22	4:D:81:PRO:HD2	1.92	0.51
4:D:90:LEU:HD11	4:D:96:GLU:HB3	1.90	0.51
13:O:1:ALA:O	13:O:2:LYS:HB2	2.10	0.51
13:O:164:LEU:HG	13:O:188:LYS:HB2	1.93	0.51
16:V:63:THR:CG2	16:V:83:ASP:O	2.59	0.51
1:A:162:PRO:HG3	1:A:171:GLY:HA2	1.93	0.51
2:B:318:ASN:O	2:B:320:ALA:N	2.43	0.51
23:B:519:CLA:HMD1	23:B:524:CLA:CAB	2.40	0.51
3:C:105:VAL:HG12	3:C:107:ASP:O	2.10	0.51
3:C:343:ARG:HB3	13:O:78:LEU:CD1	2.40	0.51
4:D:258:GLY:O	14:T:21:ILE:HG23	2.10	0.51
5:E:26:ILE:HA	5:E:29:LEU:HD12	1.93	0.51
5:E:68:ARG:HH12	7:H:50:SER:CB	2.24	0.51
13:O:152:ARG:HD2	13:O:156:PHE:CE2	2.46	0.51
1:A:333:GLU:OE1	3:C:354:GLU:OE2	2.29	0.51
2:B:308:LYS:HE2	2:B:312:TYR:CZ	2.46	0.51
2:B:340:TRP:CZ3	2:B:342:GLY:CA	2.92	0.51
23:B:521:CLA:H172	23:D:356:CLA:H72	1.92	0.51
3:C:166:ILE:O	3:C:170:ILE:HG13	2.10	0.51
4:D:58:TRP:HB3	4:D:63:LEU:O	2.10	0.51
6:F:36:ILE:CA	6:F:39:MET:HG3	2.40	0.51
13:O:188:LYS:HD2	13:O:225:MET:HG3	1.93	0.51
16:V:64:PRO:HD2	16:V:66:ARG:HH22	1.76	0.51
19:Z:41:PHE:CD1	19:Z:41:PHE:N	2.73	0.51
1:A:176:ILE:O	1:A:179:THR:HB	2.11	0.51
2:B:452:THR:HG22	4:D:291:LEU:HD11	1.92	0.51
4:D:175:VAL:HG12	4:D:179:PHE:HE1	1.76	0.51
14:T:3:THR:O	14:T:4:ILE:C	2.48	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
1:A:116:ILE:HG22	1:A:117:PHE:N	2.25	0.51
3:C:318:LEU:HD21	3:C:340:TYR:CB	2.40	0.51
3:C:343:ARG:NH1	3:C:345:PRO:HD3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:THR:O	4:D:67:TYR:CD1	2.64	0.51
4:D:261:PHE:CD2	14:T:24:ARG:NH2	2.79	0.51
4:D:298:PHE:O	4:D:299:ILE:C	2.49	0.51
13:O:27:ARG:O	13:O:29:ALA:N	2.44	0.51
16:V:30:LYS:HG2	16:V:118:HIS:CD2	2.46	0.51
19:Z:23:VAL:O	19:Z:27:TYR:CD1	2.64	0.51
2:B:62:VAL:HG13	23:B:518:CLA:O1D	2.11	0.51
2:B:321:LYS:NZ	4:D:297:ASP:OD2	2.42	0.51
2:B:402:TYR:N	2:B:402:TYR:CD1	2.78	0.51
4:D:71:CYS:HB2	4:D:76:VAL:HG22	1.89	0.51
4:D:82:ALA:H	4:D:85:MET:CE	2.24	0.51
4:D:199:MET:O	4:D:202:ALA:HB3	2.11	0.51
11:L:4:ASN:N	11:L:5:PRO:CD	2.72	0.51
14:T:20:ALA:O	14:T:24:ARG:HB2	2.11	0.51
1:A:126:TYR:O	1:A:130:GLN:HG3	2.11	0.50
1:A:210:LEU:HD13	24:D:355:PHO:C1D	2.40	0.50
23:A:348:CLA:CAB	23:A:350:CLA:HMD2	2.41	0.50
2:B:420:TYR:O	2:B:424:ALA:N	2.44	0.50
3:C:37:ALA:HA	23:C:483:CLA:HBA1	1.92	0.50
4:D:54:PHE:HB3	5:E:46:PHE:CD1	2.46	0.50
16:V:33:PHE:CD2	16:V:37:CYS:SG	3.04	0.50
16:V:133:GLY:O	16:V:137:TYR:CA	2.59	0.50
1:A:57:PRO:CB	1:A:68:SER:HB3	2.37	0.50
1:A:316:THR:HB	4:D:75:THR:CG2	2.40	0.50
1:A:317:TRP:N	4:D:63:LEU:HD13	2.26	0.50
2:B:340:TRP:CH2	2:B:342:GLY:HA3	2.45	0.50
3:C:123:ALA:CB	19:Z:47:TRP:CH2	2.91	0.50
3:C:301:PHE:CD2	3:C:301:PHE:N	2.79	0.50
1:A:183:MET:CE	23:A:349:CLA:HMD3	2.41	0.50
1:A:316:THR:HB	4:D:75:THR:HG21	1.93	0.50
3:C:305:THR:H	3:C:308:GLU:CG	2.19	0.50
3:C:420:VAL:HG12	3:C:425:TRP:CD1	2.46	0.50
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.46	0.50
13:O:54:GLU:OE1	13:O:231:HIS:CD2	2.64	0.50
16:V:64:PRO:O	16:V:66:ARG:NH1	2.44	0.50
1:A:177:SER:O	1:A:180:PHE:HB2	2.12	0.50
1:A:237:TYR:CE2	1:A:245:THR:HG23	2.46	0.50
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.94	0.50
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.42	0.50
2:B:418:LYS:NZ	15:U:45:GLU:OE2	2.45	0.50
3:C:377:LEU:HD21	13:O:99:ASP:CG	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:41:ALA:N	13:O:83:GLY:O	2.43	0.50
13:O:121:THR:HG21	13:O:148:VAL:CG2	2.26	0.50
15:U:42:VAL:HG12	15:U:45:GLU:H	1.76	0.50
15:U:85:TYR:N	15:U:85:TYR:CD2	2.75	0.50
1:A:148:SER:HB2	1:A:284:TRP:CH2	2.37	0.50
1:A:200:LEU:O	1:A:203:ALA:HB3	2.11	0.50
1:A:278:TRP:CB	1:A:279:PRO:HD3	2.35	0.50
1:A:334:ARG:NH1	13:O:159:PRO:HA	2.25	0.50
3:C:183:GLY:O	3:C:184:GLY:O	2.30	0.50
3:C:350:ILE:HG22	3:C:351:PHE:N	2.27	0.50
6:F:31:PHE:HD2	6:F:31:PHE:C	2.15	0.50
8:I:6:ILE:O	8:I:10:ILE:HG13	2.11	0.50
1:A:78:ILE:HD13	11:L:34:TYR:OH	2.10	0.50
1:A:180:PHE:N	1:A:180:PHE:CD1	2.77	0.50
1:A:237:TYR:CD2	1:A:241:GLN:OE1	2.65	0.50
6:F:40:GLN:OE1	9:J:28:PHE:CD2	2.65	0.50
13:O:120:PHE:HE1	13:O:235:ILE:HG21	1.77	0.50
15:U:54:LYS:HD2	15:U:113:THR:OG1	2.11	0.50
15:U:105:LEU:O	15:U:109:LEU:N	2.41	0.50
15:U:108:ASN:O	15:U:109:LEU:C	2.50	0.50
1:A:24:THR:CB	4:D:251:ARG:NH2	2.74	0.50
1:A:95:PRO:HG2	1:A:98:GLU:CB	2.41	0.50
2:B:29:LEU:HD11	27:B:529:BCR:H331	1.94	0.50
2:B:136:PRO:CD	2:B:231:MET:HE1	2.40	0.50
2:B:240:SER:OG	2:B:241:SER:N	2.44	0.50
3:C:287:THR:O	3:C:290:VAL:HB	2.11	0.50
3:C:302:TYR:O	3:C:422:PRO:HD2	2.12	0.50
23:C:487:CLA:HBC2	23:C:487:CLA:HHD	1.94	0.50
4:D:200:GLY:O	4:D:204:VAL:HG23	2.11	0.50
4:D:222:LEU:HD22	4:D:243:THR:HB	1.93	0.50
4:D:261:PHE:HD2	14:T:24:ARG:NH2	2.10	0.50
11:L:6:ASN:HD22	11:L:6:ASN:H	1.59	0.50
13:O:168:TYR:CZ	13:O:172:ILE:HD11	2.46	0.50
16:V:37:CYS:O	16:V:38:ALA:C	2.50	0.50
16:V:75:TYR:CE2	16:V:80:THR:N	2.70	0.50
19:Z:5:PHE:CE2	19:Z:54:VAL:HG13	2.47	0.50
1:A:320:ILE:HG21	4:D:333:ASP:OD2	2.12	0.50
2:B:206:GLY:O	2:B:210:ILE:HG13	2.11	0.50
6:F:40:GLN:OE1	9:J:28:PHE:HD2	1.95	0.50
13:O:54:GLU:CD	13:O:231:HIS:CE1	2.85	0.50
1:A:89:ILE:HD13	1:A:94:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:O	1:A:153:SER:HB3	2.12	0.50
1:A:300:PHE:CB	1:A:302:PHE:HE1	2.16	0.50
4:D:24:ARG:HB3	4:D:26:ARG:HE	1.77	0.50
13:O:39:ARG:HA	13:O:245:PRO:HB3	1.92	0.50
13:O:238:VAL:CG1	13:O:239:PHE:N	2.75	0.50
15:U:72:TYR:HD2	15:U:73:PRO:HG3	1.77	0.50
15:U:84:PRO:C	15:U:85:TYR:CD2	2.85	0.50
2:B:205:ALA:O	23:B:518:CLA:H191	2.12	0.49
3:C:98:GLY:O	3:C:99:VAL:CG2	2.58	0.49
23:C:487:CLA:H102	23:C:487:CLA:H51	1.94	0.49
4:D:198:MET:HE3	11:L:30:LEU:HD11	1.90	0.49
13:O:189:ARG:NE	15:U:39:LEU:HD23	2.27	0.49
1:A:183:MET:HB3	23:A:348:CLA:HBC2	1.94	0.49
23:A:348:CLA:HBB1	23:D:354:CLA:NC	2.27	0.49
2:B:244:ALA:O	2:B:247:PHE:HB3	2.11	0.49
3:C:91:HIS:O	3:C:94:THR:HB	2.11	0.49
23:C:486:CLA:H192	19:Z:19:MET:HG2	1.94	0.49
6:F:31:PHE:C	6:F:31:PHE:CD2	2.83	0.49
7:H:24:TRP:CE3	7:H:24:TRP:HA	2.46	0.49
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.94	0.49
1:A:308:ASP:O	1:A:309:ALA:C	2.50	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
2:B:194:ASN:C	2:B:196:GLY:N	2.66	0.49
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.42	0.49
3:C:88:LEU:O	3:C:89:ILE:C	2.50	0.49
3:C:278:ALA:HB1	23:C:479:CLA:H142	1.94	0.49
3:C:345:PRO:HB3	13:O:73:ARG:CZ	2.41	0.49
3:C:349:ILE:O	3:C:350:ILE:HG13	2.13	0.49
4:D:56:THR:O	4:D:56:THR:CG2	2.60	0.49
16:V:33:PHE:HD2	16:V:37:CYS:SG	2.34	0.49
1:A:215:HIS:HA	25:A:353:PL9:O1	2.12	0.49
2:B:297:THR:O	2:B:298:LEU:C	2.48	0.49
2:B:472:ARG:NE	2:B:479:PHE:HE1	2.11	0.49
3:C:149:TYR:CG	3:C:156:LYS:HG3	2.47	0.49
3:C:291:TRP:HB3	3:C:292:PHE:HD2	1.74	0.49
3:C:337:LEU:HA	13:O:104:GLN:HE21	1.75	0.49
5:E:26:ILE:HG13	5:E:27:PRO:CD	2.42	0.49
13:O:118:LEU:CD2	13:O:233:VAL:HG21	2.43	0.49
16:V:63:THR:HB	16:V:83:ASP:C	2.32	0.49
2:B:12:LEU:CD2	2:B:19:LEU:HD12	2.43	0.49
2:B:260:SER:H	2:B:263:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.12	0.49
3:C:450:ALA:HA	3:C:454:GLY:CA	2.42	0.49
5:E:48:THR:O	5:E:48:THR:HG22	2.13	0.49
27:K:50:BCR:H333	19:Z:17:PHE:HA	1.94	0.49
1:A:75:ASN:HD22	1:A:79:THR:HG21	1.77	0.49
2:B:61:PHE:O	2:B:64:PRO:HD2	2.12	0.49
3:C:138:GLU:CG	3:C:139:THR:N	2.61	0.49
3:C:285:ILE:CA	23:C:487:CLA:HMB2	2.35	0.49
3:C:286:ALA:HA	3:C:289:PHE:HB3	1.95	0.49
1:A:166:GLY:O	1:A:167:SER:HB3	2.13	0.49
2:B:234:ILE:HG23	23:B:513:CLA:HMD2	1.95	0.49
2:B:311:PHE:O	2:B:313:ASP:N	2.45	0.49
2:B:326:ARG:HG2	12:M:4:ASN:HD22	1.78	0.49
2:B:451:PHE:CZ	2:B:455:HIS:ND1	2.80	0.49
3:C:52:ALA:HB1	23:C:486:CLA:HMB3	1.95	0.49
3:C:66:ALA:HB1	10:K:17:PRO:HB3	1.95	0.49
3:C:297:TYR:O	3:C:298:PRO:C	2.51	0.49
6:F:17:VAL:O	6:F:18:ARG:C	2.50	0.49
11:L:12:LEU:CD1	11:L:16:SER:HB3	2.39	0.49
13:O:50:PHE:O	13:O:68:THR:OG1	2.31	0.49
13:O:65:PHE:N	13:O:65:PHE:CD1	2.81	0.49
15:U:75:LEU:CD2	15:U:101:GLN:HE21	2.25	0.49
1:A:124:SER:O	1:A:127:MET:HB3	2.12	0.49
2:B:45:PHE:CE2	2:B:46:ASP:O	2.66	0.49
2:B:156:PHE:HA	2:B:161:LEU:HB2	1.93	0.49
2:B:397:VAL:CG1	2:B:398:THR:N	2.76	0.49
2:B:422:ARG:NH2	13:O:169:ASP:HB3	2.28	0.49
3:C:99:VAL:CG1	3:C:100:GLY:N	2.74	0.49
3:C:109:PHE:CZ	27:C:489:BCR:HC32	2.47	0.49
4:D:188:PHE:N	4:D:188:PHE:HD1	2.10	0.49
4:D:195:PRO:CA	4:D:198:MET:HE2	2.38	0.49
5:E:12:ILE:HD12	28:E:84:HEC:CBD	2.42	0.49
5:E:63:PRO:HB3	5:E:78:PHE:CD2	2.47	0.49
2:B:6:TYR:CE1	2:B:8:VAL:CG2	2.96	0.49
2:B:24:LEU:HD12	2:B:111:ALA:HA	1.93	0.49
2:B:78:TRP:HZ3	2:B:93:PHE:CE1	2.30	0.49
2:B:305:ILE:O	2:B:341:LYS:HD2	2.12	0.49
2:B:326:ARG:HG2	12:M:4:ASN:ND2	2.27	0.49
4:D:18:LEU:HD12	17:X:41:SER:OG	2.12	0.49
8:I:27:ASP:OD1	8:I:27:ASP:N	2.46	0.49
16:V:128:ASP:HB3	16:V:134:LYS:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:53:VAL:O	19:Z:57:LEU:HG	2.13	0.49
1:A:243:GLU:N	4:D:240:ALA:HB1	2.28	0.49
1:A:255:PHE:CE2	25:A:353:PL9:H152	2.48	0.49
1:A:301:ASN:CG	1:A:301:ASN:O	2.51	0.49
2:B:360:PRO:C	2:B:362:PHE:H	2.16	0.49
3:C:71:GLU:C	3:C:73:ALA:H	2.15	0.49
3:C:97:TRP:HA	3:C:97:TRP:CE3	2.48	0.49
3:C:296:VAL:O	3:C:298:PRO:HD2	2.13	0.49
3:C:304:PRO:HB3	3:C:395:TYR:CG	2.48	0.49
4:D:20:ASP:O	4:D:21:TRP:C	2.50	0.49
6:F:43:GLN:HG2	6:F:44:ARG:HG2	1.94	0.49
11:L:10:VAL:O	12:M:28:GLN:NE2	2.46	0.49
12:M:9:ILE:O	12:M:13:LEU:HG	2.13	0.49
15:U:47:LEU:C	15:U:49:THR:H	2.16	0.49
2:B:31:ALA:N	23:B:518:CLA:HBC3	2.28	0.48
2:B:62:VAL:O	2:B:63:LEU:C	2.51	0.48
4:D:158:LEU:O	4:D:161:PRO:HD2	2.13	0.48
4:D:196:PHE:HD1	4:D:285:GLY:CA	2.25	0.48
4:D:315:TYR:CE2	4:D:319:LEU:HD11	2.48	0.48
7:H:23:GLY:C	7:H:25:GLY:N	2.66	0.48
13:O:38:TYR:O	13:O:245:PRO:CG	2.61	0.48
2:B:475:PHE:O	2:B:476:ARG:C	2.51	0.48
23:B:512:CLA:H2A	23:B:512:CLA:O2A	2.13	0.48
3:C:186:TYR:C	3:C:186:TYR:CD2	2.86	0.48
3:C:282:MET:O	3:C:285:ILE:HB	2.13	0.48
23:C:486:CLA:CHB	27:C:488:BCR:H402	2.43	0.48
4:D:333:ASP:O	4:D:333:ASP:OD1	2.31	0.48
9:J:24:ILE:O	9:J:27:LEU:HB3	2.12	0.48
1:A:89:ILE:CG1	13:O:73:ARG:NH2	2.71	0.48
1:A:107:TYR:HD1	13:O:115:ARG:CZ	2.26	0.48
1:A:200:LEU:HD13	1:A:285:PHE:HD1	1.75	0.48
1:A:242:GLU:O	4:D:241:GLU:HA	2.12	0.48
2:B:84:THR:O	2:B:84:THR:CG2	2.61	0.48
3:C:153:ASP:OD1	3:C:155:ASN:OD1	2.30	0.48
3:C:208:VAL:CG1	3:C:209:ILE:N	2.77	0.48
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.48	0.48
4:D:112:THR:HG22	4:D:116:LEU:CD1	2.43	0.48
4:D:236:ASN:HB2	4:D:237:PRO:HD2	1.96	0.48
6:F:22:VAL:O	6:F:26:ALA:HB3	2.13	0.48
6:F:39:MET:O	6:F:41:PHE:N	2.46	0.48
15:U:72:TYR:HD2	15:U:73:PRO:CG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:CE2	1:A:278:TRP:CD1	3.02	0.48
1:A:307:ILE:C	1:A:309:ALA:H	2.16	0.48
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.43	0.48
3:C:71:GLU:C	3:C:73:ALA:N	2.67	0.48
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.43	0.48
3:C:316:THR:OG1	3:C:392:ALA:HB1	2.14	0.48
3:C:320:ARG:HH11	16:V:49:ASN:HA	1.78	0.48
3:C:347:GLY:O	13:O:16:ALA:HB3	2.13	0.48
4:D:84:SER:HB2	5:E:66:THR:O	2.13	0.48
4:D:154:VAL:HG13	4:D:158:LEU:HD12	1.94	0.48
4:D:343:GLU:OE2	16:V:134:LYS:NZ	2.40	0.48
10:K:19:ILE:HD12	27:K:50:BCR:H342	1.95	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CA	2.96	0.48
15:U:76:ALA:O	15:U:80:VAL:HG23	2.14	0.48
16:V:133:GLY:O	16:V:137:TYR:N	2.47	0.48
2:B:57:ARG:HA	2:B:330:MET:HG3	1.96	0.48
23:B:519:CLA:C14	23:D:356:CLA:H11	2.43	0.48
3:C:40:ALA:O	3:C:43:ILE:HG23	2.12	0.48
3:C:109:PHE:O	3:C:111:PHE:N	2.47	0.48
3:C:293:ASN:CG	3:C:423:ARG:NH2	2.67	0.48
13:O:45:LEU:HD11	13:O:215:PHE:CE1	2.48	0.48
1:A:129:ARG:NH2	4:D:255:GLN:O	2.46	0.48
1:A:224:ILE:CG2	1:A:227:THR:OG1	2.61	0.48
1:A:259:ILE:HD13	25:A:353:PL9:H172	1.95	0.48
2:B:302:TRP:C	2:B:304:ALA:H	2.17	0.48
3:C:367:GLU:O	3:C:370:ARG:N	2.37	0.48
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.96	0.48
23:C:479:CLA:HAB	23:C:479:CLA:C9	2.41	0.48
15:U:61:ASN:CB	15:U:126:ASP:O	2.62	0.48
16:V:13:ASN:C	16:V:13:ASN:OD1	2.51	0.48
16:V:33:PHE:CD2	16:V:37:CYS:HB2	2.48	0.48
1:A:180:PHE:HE2	4:D:192:THR:C	2.17	0.48
1:A:284:TRP:HA	1:A:284:TRP:CE3	2.49	0.48
2:B:71:VAL:O	2:B:93:PHE:HE2	1.96	0.48
2:B:360:PRO:O	2:B:362:PHE:N	2.46	0.48
2:B:372:ASP:HB3	2:B:376:VAL:HB	1.95	0.48
4:D:129:GLN:HE21	4:D:142:ASN:HB3	1.78	0.48
6:F:20:VAL:O	6:F:21:ALA:C	2.52	0.48
7:H:29:LEU:O	7:H:33:PHE:HD1	1.96	0.48
15:U:65:PHE:HD1	15:U:76:ALA:HB1	1.78	0.48
16:V:46:THR:HG22	16:V:49:ASN:N	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:63:THR:O	16:V:80:THR:HG21	2.14	0.48
1:A:119:PHE:O	1:A:123:ALA:CB	2.62	0.48
1:A:150:PRO:O	1:A:153:SER:N	2.47	0.48
1:A:278:TRP:CE3	1:A:278:TRP:HA	2.48	0.48
2:B:63:LEU:HB3	2:B:64:PRO:CD	2.38	0.48
2:B:91:TRP:CB	23:B:515:CLA:H43	2.44	0.48
2:B:199:VAL:O	2:B:203:ILE:HG13	2.13	0.48
3:C:289:PHE:CE2	3:C:294:ASN:OD1	2.67	0.48
3:C:294:ASN:O	3:C:295:THR:C	2.50	0.48
3:C:372:PRO:O	3:C:373:ASN:HB2	2.14	0.48
10:K:26:LEU:HD21	18:N:20:UNK:CB	2.43	0.48
13:O:32:ILE:O	13:O:35:SER:N	2.45	0.48
13:O:71:VAL:CG2	13:O:108:VAL:HG23	2.39	0.48
13:O:161:GLY:O	13:O:168:TYR:N	2.43	0.48
15:U:61:ASN:HB3	15:U:126:ASP:O	2.14	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CD	2.96	0.48
3:C:282:MET:HA	3:C:285:ILE:CB	2.44	0.48
3:C:282:MET:HE2	23:C:479:CLA:H41	1.95	0.48
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.48	0.48
8:I:27:ASP:HB2	8:I:28:PRO:HD2	1.94	0.48
8:I:31:ASN:O	8:I:31:ASN:OD1	2.31	0.48
13:O:45:LEU:HB3	13:O:79:ASP:HB2	1.96	0.48
13:O:137:THR:HG23	13:O:138:THR:N	2.29	0.48
15:U:47:LEU:O	15:U:49:THR:N	2.46	0.48
1:A:238:LYS:O	1:A:240:GLY:N	2.47	0.48
1:A:242:GLU:O	1:A:244:GLU:N	2.47	0.48
1:A:307:ILE:HD13	5:E:54:TYR:HB2	1.95	0.48
2:B:57:ARG:NH2	2:B:334:ASP:OD2	2.45	0.48
2:B:235:GLU:OE1	2:B:235:GLU:HA	2.14	0.48
2:B:237:VAL:HG22	23:B:524:CLA:HBC2	1.96	0.48
2:B:385:ARG:HG3	13:O:165:ALA:HA	1.95	0.48
3:C:64:ALA:HB3	3:C:118:HIS:HB3	1.95	0.48
3:C:305:THR:N	3:C:308:GLU:HG3	2.21	0.48
4:D:152:VAL:CG1	23:D:354:CLA:H43	2.44	0.48
6:F:27:VAL:N	6:F:28:PRO:CD	2.77	0.48
15:U:66:ILE:O	15:U:66:ILE:HG22	2.13	0.48
16:V:25:GLN:O	16:V:26:TYR:C	2.52	0.48
1:A:104:GLU:HG2	1:A:105:TRP:N	2.29	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
1:A:284:TRP:HA	1:A:284:TRP:HE3	1.79	0.47
2:B:12:LEU:HG	2:B:19:LEU:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:LEU:O	2:B:151:PHE:HB3	2.13	0.47
2:B:328:GLY:HA2	2:B:444:ARG:HD3	1.95	0.47
3:C:208:VAL:HG13	3:C:209:ILE:H	1.79	0.47
3:C:370:ARG:HD3	3:C:375:LEU:HD23	1.94	0.47
4:D:90:LEU:HD11	4:D:96:GLU:CB	2.44	0.47
4:D:191:TRP:HE1	4:D:197:HIS:CD2	2.31	0.47
10:K:35:GLY:O	10:K:36:PHE:HB2	2.13	0.47
13:O:46:GLN:O	13:O:238:VAL:O	2.31	0.47
16:V:79:PRO:HG3	16:V:89:ALA:N	2.29	0.47
1:A:75:ASN:HD21	4:D:313:THR:HG21	1.79	0.47
1:A:205:VAL:CG1	4:D:204:VAL:HG12	2.44	0.47
2:B:247:PHE:HE1	23:B:521:CLA:H72	1.77	0.47
2:B:326:ARG:C	27:B:529:BCR:H292	2.34	0.47
2:B:394:GLN:CD	15:U:52:GLY:HA3	2.34	0.47
3:C:339:LYS:HB2	3:C:340:TYR:CE1	2.49	0.47
3:C:376:ASP:OD1	3:C:378:ASN:HB2	2.14	0.47
4:D:83:ASN:CB	4:D:336:HIS:ND1	2.77	0.47
4:D:178:ILE:O	4:D:182:LEU:HG	2.14	0.47
4:D:243:THR:O	4:D:243:THR:HG22	2.13	0.47
13:O:164:LEU:N	13:O:188:LYS:HE2	2.29	0.47
1:A:42:LEU:O	1:A:46:ILE:HG12	2.14	0.47
1:A:283:VAL:O	1:A:284:TRP:C	2.52	0.47
23:A:348:CLA:H191	14:T:17:PHE:CZ	2.49	0.47
4:D:80:THR:CG2	4:D:168:PHE:HA	2.43	0.47
4:D:348:ARG:NH1	15:U:133:TYR:CE1	2.82	0.47
13:O:193:THR:CG2	13:O:194:LYS:H	2.05	0.47
15:U:61:ASN:HB3	15:U:130:ASN:ND2	2.28	0.47
16:V:53:ASP:OD1	16:V:55:ARG:HB3	2.14	0.47
1:A:225:ARG:CB	2:B:481:GLY:C	2.72	0.47
1:A:301:ASN:HB2	1:A:303:ASN:HD21	1.79	0.47
2:B:198:VAL:O	2:B:201:HIS:HB3	2.14	0.47
3:C:199:ILE:HD12	3:C:234:VAL:CG2	2.39	0.47
4:D:337:GLU:O	4:D:338:ASN:HB2	2.14	0.47
6:F:19:TRP:CZ3	6:F:23:HIS:CE1	3.03	0.47
17:X:12:ILE:HG13	17:X:12:ILE:O	2.15	0.47
19:Z:19:MET:HE1	19:Z:43:GLY:HA3	1.97	0.47
1:A:161:TYR:CE1	1:A:186:PHE:CE1	3.00	0.47
1:A:180:PHE:CE2	4:D:192:THR:CG2	2.97	0.47
1:A:202:VAL:HG21	23:A:350:CLA:OBD	2.15	0.47
2:B:264:PRO:HG2	2:B:267:LEU:HB2	1.96	0.47
23:B:514:CLA:H202	11:L:27:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:LEU:HD21	23:C:474:CLA:H171	1.97	0.47
3:C:249:ILE:O	3:C:252:ILE:HB	2.15	0.47
3:C:392:ALA:O	3:C:396:MET:HB3	2.15	0.47
23:C:478:CLA:H91	23:C:482:CLA:HAA1	1.96	0.47
5:E:74:GLN:O	5:E:78:PHE:CD1	2.67	0.47
13:O:27:ARG:C	13:O:29:ALA:N	2.68	0.47
13:O:81:ILE:CG2	13:O:82:GLN:N	2.52	0.47
15:U:58:ASN:C	15:U:59:ASN:HD22	2.08	0.47
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.14	0.47
1:A:44:ALA:CB	24:A:351:PHO:H91	2.44	0.47
1:A:139:MET:HE2	4:D:248:THR:HG21	1.96	0.47
1:A:315:ASN:HB2	4:D:63:LEU:HD23	1.95	0.47
2:B:464:PHE:HD2	23:B:523:CLA:HAC2	1.79	0.47
3:C:154:LYS:O	3:C:158:THR:OG1	2.15	0.47
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.97	0.47
7:H:24:TRP:HA	7:H:24:TRP:HE3	1.78	0.47
13:O:211:ILE:HG22	13:O:212:ALA:H	1.79	0.47
15:U:73:PRO:HG2	16:V:83:ASP:OD1	2.13	0.47
15:U:112:PHE:N	15:U:112:PHE:CD1	2.82	0.47
1:A:52:PHE:CD1	1:A:81:ALA:HB2	2.50	0.47
1:A:143:ILE:HG21	4:D:253:TRP:HH2	1.80	0.47
2:B:124:ARG:CG	2:B:125:ASP:N	2.76	0.47
2:B:252:VAL:O	2:B:255:THR:HB	2.15	0.47
23:B:519:CLA:CBB	4:D:123:ILE:HG12	2.44	0.47
3:C:79:LYS:O	3:C:80:PRO:C	2.53	0.47
23:C:476:CLA:HED3	23:C:483:CLA:H71	1.96	0.47
4:D:71:CYS:HB3	4:D:75:THR:CG2	2.45	0.47
4:D:291:LEU:O	4:D:293:LEU:N	2.48	0.47
7:H:54:LEU:HB2	7:H:57:VAL:HB	1.97	0.47
10:K:31:GLN:HB3	10:K:36:PHE:HD2	1.80	0.47
12:M:21:PHE:CD2	12:M:22:LEU:HD23	2.50	0.47
13:O:39:ARG:HA	13:O:245:PRO:CG	2.44	0.47
13:O:118:LEU:HD13	13:O:233:VAL:HG21	1.96	0.47
13:O:147:ASN:HD22	13:O:147:ASN:HA	1.43	0.47
15:U:66:ILE:HG23	16:V:82:TYR:CE2	2.49	0.47
17:X:13:THR:O	17:X:15:SER:N	2.47	0.47
1:A:210:LEU:HD12	1:A:210:LEU:C	2.36	0.47
1:A:261:GLN:CG	1:A:262:TYR:H	2.28	0.47
2:B:11:VAL:HG13	11:L:6:ASN:CB	2.45	0.47
2:B:187:PRO:HA	2:B:190:PHE:HB2	1.95	0.47
3:C:39:ASN:HB2	23:C:483:CLA:HBA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:TRP:CZ3	3:C:178:LYS:HE3	2.50	0.47
3:C:227:VAL:HG23	3:C:294:ASN:CB	2.42	0.47
4:D:153:PHE:CZ	24:D:355:PHO:H92	2.50	0.47
5:E:23:SER:O	5:E:27:PRO:HG2	2.15	0.47
1:A:186:PHE:CD2	1:A:192:ILE:CD1	2.85	0.47
1:A:271:LEU:O	1:A:275:LEU:HG	2.15	0.47
2:B:153:PHE:O	2:B:157:HIS:HB3	2.14	0.47
2:B:250:PHE:HB3	23:B:521:CLA:H142	1.96	0.47
3:C:305:THR:O	3:C:306:GLY:C	2.52	0.47
3:C:320:ARG:HG2	15:U:128:TYR:HE2	1.80	0.47
3:C:343:ARG:HB3	13:O:78:LEU:HD12	1.97	0.47
23:C:476:CLA:HBD	23:C:486:CLA:CBB	2.45	0.47
5:E:14:THR:CB	9:J:8:ILE:HD12	2.43	0.47
9:J:27:LEU:O	9:J:30:TYR:N	2.48	0.47
13:O:158:ASP:CB	13:O:159:PRO:CD	2.92	0.47
15:U:72:TYR:CB	15:U:73:PRO:CD	2.91	0.47
18:N:31:UNK:HA	19:Z:30:PRO:CG	2.45	0.47
19:Z:37:LYS:O	19:Z:41:PHE:CE1	2.68	0.47
1:A:291:SER:O	1:A:295:PHE:HE1	1.98	0.47
2:B:26:HIS:HB2	23:B:513:CLA:HMB2	1.96	0.47
2:B:224:ARG:O	2:B:228:ALA:HB3	2.15	0.47
2:B:340:TRP:HH2	2:B:401:PHE:CD1	2.33	0.47
2:B:390:TYR:O	2:B:391:SER:O	2.33	0.47
4:D:52:THR:HG23	4:D:76:VAL:CG1	2.44	0.47
4:D:83:ASN:CG	4:D:336:HIS:HD1	2.16	0.47
5:E:70:GLU:O	5:E:71:ALA:C	2.52	0.47
7:H:27:THR:N	7:H:28:PRO:CD	2.78	0.47
13:O:54:GLU:OE1	13:O:231:HIS:NE2	2.48	0.47
13:O:152:ARG:HD2	13:O:156:PHE:CG	2.50	0.47
13:O:210:GLU:OE1	13:O:210:GLU:HA	2.15	0.47
1:A:36:ILE:HD13	23:C:487:CLA:H141	1.97	0.46
2:B:45:PHE:CE2	2:B:78:TRP:HZ2	2.32	0.46
2:B:183:PRO:HB2	2:B:200:ALA:HB2	1.96	0.46
2:B:401:PHE:HZ	2:B:420:TYR:CD2	2.34	0.46
2:B:467:ILE:HD13	4:D:126:MET:CE	2.45	0.46
23:B:519:CLA:HBB2	4:D:123:ILE:HG12	1.97	0.46
3:C:337:LEU:HA	13:O:104:GLN:NE2	2.29	0.46
4:D:188:PHE:HD1	4:D:188:PHE:H	1.63	0.46
7:H:21:ALA:HB3	7:H:22:PRO:HD2	1.97	0.46
13:O:122:VAL:O	13:O:122:VAL:HG12	2.15	0.46
16:V:126:LEU:O	16:V:129:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG22	1:A:231:GLU:N	2.18	0.46
1:A:288:LEU:O	1:A:289:GLY:C	2.54	0.46
2:B:25:MET:HB3	27:B:529:BCR:C33	2.42	0.46
2:B:119:ASP:HB3	2:B:121:GLU:HG3	1.97	0.46
2:B:234:ILE:O	2:B:235:GLU:C	2.53	0.46
3:C:292:PHE:HD2	3:C:292:PHE:H	1.56	0.46
3:C:412:THR:HG22	3:C:412:THR:O	2.14	0.46
23:C:480:CLA:H42	23:C:481:CLA:HBD	1.98	0.46
11:L:12:LEU:CD1	11:L:16:SER:CB	2.93	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.97	0.46
13:O:180:GLU:HG3	13:O:181:GLU:H	1.80	0.46
1:A:31:GLY:O	1:A:33:PHE:N	2.48	0.46
27:B:529:BCR:H371	27:B:529:BCR:H393	1.97	0.46
23:C:477:CLA:HMD3	23:C:485:CLA:HAB	1.96	0.46
13:O:32:ILE:O	13:O:34:SER:N	2.48	0.46
13:O:114:GLU:OE2	13:O:231:HIS:NE2	2.47	0.46
1:A:211:PHE:HE2	1:A:278:TRP:CD1	2.33	0.46
2:B:297:THR:O	2:B:300:GLU:N	2.49	0.46
23:B:518:CLA:H61	23:B:518:CLA:H41	1.79	0.46
3:C:93:ALA:HB3	3:C:301:PHE:CE1	2.51	0.46
3:C:108:THR:CG2	10:K:2:LEU:HD23	2.44	0.46
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.50	0.46
4:D:72:ASN:OD1	4:D:74:LEU:CB	2.63	0.46
4:D:325:ILE:O	4:D:329:MET:HB3	2.14	0.46
9:J:19:MET:SD	27:K:50:BCR:H361	2.55	0.46
15:U:100:ARG:HG3	15:U:104:ILE:HD11	1.98	0.46
1:A:33:PHE:CD1	1:A:128:GLY:C	2.89	0.46
2:B:163:GLY:O	2:B:165:GLY:N	2.46	0.46
2:B:185:TRP:O	2:B:186:GLY:O	2.33	0.46
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.15	0.46
3:C:200:THR:O	3:C:201:ASN:ND2	2.32	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD1	2.38	0.46
27:K:50:BCR:HC42	19:Z:17:PHE:CD1	2.49	0.46
13:O:137:THR:CG2	13:O:138:THR:N	2.77	0.46
16:V:33:PHE:CD2	16:V:37:CYS:CB	2.99	0.46
1:A:75:ASN:ND2	1:A:79:THR:HG22	2.31	0.46
1:A:261:GLN:CG	1:A:262:TYR:N	2.78	0.46
3:C:71:GLU:O	3:C:75:PHE:HB2	2.15	0.46
3:C:73:ALA:O	10:K:1:LYS:HA	2.14	0.46
3:C:100:GLY:O	3:C:101:PRO:C	2.53	0.46
3:C:281:MET:O	3:C:285:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:347:GLY:O	13:O:16:ALA:CB	2.64	0.46
13:O:46:GLN:HE21	13:O:46:GLN:HB3	1.50	0.46
1:A:312:ASN:HB3	5:E:55:TYR:CE1	2.51	0.46
2:B:53:ASN:ND2	2:B:58:GLN:OE1	2.49	0.46
2:B:307:GLU:O	2:B:308:LYS:C	2.48	0.46
3:C:293:ASN:N	3:C:293:ASN:HD22	2.12	0.46
3:C:335:THR:HG22	3:C:335:THR:O	2.16	0.46
4:D:110:LEU:O	4:D:113:PHE:N	2.49	0.46
4:D:238:THR:C	4:D:240:ALA:N	2.68	0.46
4:D:267:LEU:C	4:D:271:MET:HE2	2.35	0.46
10:K:10:ASP:N	10:K:11:PRO:CD	2.79	0.46
2:B:55:MET:HE1	2:B:80:ILE:HD13	1.97	0.46
2:B:222:PRO:CB	7:H:25:GLY:HA2	2.30	0.46
2:B:234:ILE:HG13	23:B:524:CLA:H191	1.97	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.46
3:C:99:VAL:HG12	3:C:100:GLY:O	2.15	0.46
3:C:286:ALA:HA	3:C:289:PHE:CB	2.46	0.46
4:D:87:HIS:HE1	4:D:162:LEU:HA	1.80	0.46
4:D:165:SER:O	4:D:166:SER:HB3	2.16	0.46
4:D:329:MET:O	4:D:333:ASP:HB2	2.15	0.46
13:O:40:ILE:CG2	13:O:41:ALA:N	2.72	0.46
13:O:238:VAL:HG12	13:O:239:PHE:H	1.78	0.46
16:V:81:THR:O	16:V:83:ASP:N	2.49	0.46
1:A:109:GLY:O	1:A:110:GLY:C	2.53	0.46
1:A:141:PRO:HG2	3:C:443:TRP:CZ3	2.41	0.46
1:A:218:LEU:CD2	4:D:142:ASN:ND2	2.79	0.46
2:B:19:LEU:HD21	23:B:524:CLA:H192	1.97	0.46
3:C:95:LEU:HD11	23:C:480:CLA:HBA2	1.97	0.46
3:C:406:SER:OG	23:C:475:CLA:O1A	2.34	0.46
11:L:28:ALA:O	11:L:29:LEU:C	2.53	0.46
13:O:40:ILE:O	13:O:243:ILE:HG23	2.16	0.46
13:O:152:ARG:NH1	13:O:156:PHE:CE2	2.84	0.46
14:T:7:VAL:O	14:T:10:PHE:HB3	2.16	0.46
16:V:78:ASN:HB2	16:V:96:ARG:NH1	2.28	0.46
19:Z:48:ILE:O	19:Z:48:ILE:HG12	2.15	0.46
2:B:346:PHE:O	2:B:354:LEU:HB2	2.16	0.46
3:C:48:LYS:NZ	23:C:486:CLA:HBA1	2.31	0.46
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.98	0.46
5:E:43:TYR:CE2	5:E:50:ARG:HG2	2.51	0.46
28:E:84:HEC:HMC2	6:F:27:VAL:HG22	1.98	0.46
11:L:24:ILE:HD13	12:M:18:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:28:GLY:HA2	13:O:204:VAL:HB	1.96	0.46
15:U:39:LEU:C	15:U:41:ASN:N	2.68	0.46
1:A:159:LEU:CD2	1:A:163:ILE:HD11	2.46	0.45
2:B:280:PHE:O	2:B:281:GLN:C	2.55	0.45
2:B:479:PHE:C	2:B:481:GLY:N	2.69	0.45
3:C:210:PHE:O	3:C:213:LEU:HB2	2.16	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG23	2.31	0.45
7:H:53:ILE:HG22	17:X:15:SER:CB	2.45	0.45
13:O:53:LYS:HB3	13:O:64:GLU:O	2.16	0.45
13:O:136:ILE:HG22	13:O:204:VAL:HG21	1.98	0.45
18:N:22:UNK:C	18:N:24:UNK:N	2.75	0.45
1:A:112:TYR:CZ	1:A:116:ILE:HD11	2.51	0.45
1:A:169:SER:O	1:A:170:ASP:HB2	2.16	0.45
1:A:172:MET:HE2	23:A:349:CLA:CMC	2.44	0.45
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.99	0.45
1:A:320:ILE:HD13	4:D:333:ASP:HA	1.98	0.45
2:B:19:LEU:HD21	23:B:524:CLA:C19	2.46	0.45
2:B:249:ALA:CB	2:B:459:ALA:HB2	2.47	0.45
23:B:521:CLA:HAB	23:B:527:CLA:CED	2.31	0.45
3:C:285:ILE:HD12	23:C:479:CLA:H71	1.98	0.45
3:C:341:LEU:HD22	3:C:349:ILE:HG22	1.97	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG21	2.32	0.45
28:E:84:HEC:C4A	6:F:19:TRP:CH2	2.99	0.45
16:V:66:ARG:HG3	16:V:66:ARG:NH1	2.31	0.45
1:A:155:PHE:O	1:A:159:LEU:N	2.41	0.45
2:B:171:PRO:HD3	7:H:64:LEU:HD11	1.98	0.45
27:B:529:BCR:H361	27:B:529:BCR:H20C	1.66	0.45
3:C:151:TRP:C	3:C:153:ASP:N	2.70	0.45
4:D:65:SER:OG	4:D:77:ALA:O	2.31	0.45
11:L:37:ASN:ND2	11:L:37:ASN:OXT	2.50	0.45
14:T:17:PHE:O	14:T:18:PHE:C	2.55	0.45
15:U:72:TYR:O	15:U:76:ALA:HB3	2.16	0.45
19:Z:51:VAL:HG12	19:Z:52:LEU:CD2	2.36	0.45
1:A:14:TRP:CH2	1:A:18:CYS:SG	3.09	0.45
1:A:117:PHE:O	1:A:121:LEU:HG	2.16	0.45
23:A:350:CLA:H121	25:A:353:PL9:C16	2.43	0.45
2:B:194:ASN:O	2:B:196:GLY:N	2.50	0.45
3:C:169:GLY:O	3:C:173:LEU:CD1	2.65	0.45
27:C:488:BCR:C21	10:K:23:PHE:HE2	2.29	0.45
16:V:30:LYS:HG2	16:V:118:HIS:NE2	2.32	0.45
19:Z:2:THR:O	19:Z:6:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:O	1:A:52:PHE:HD2	1.98	0.45
1:A:63:ILE:HD11	1:A:336:ALA:HB1	1.99	0.45
1:A:303:ASN:HB2	3:C:415:ASN:OD1	2.16	0.45
2:B:219:VAL:HG12	2:B:220:ARG:N	2.32	0.45
3:C:178:LYS:CG	3:C:178:LYS:O	2.64	0.45
3:C:313:GLN:O	3:C:317:PHE:HD1	2.00	0.45
3:C:435:PHE:O	3:C:436:PHE:C	2.55	0.45
3:C:456:GLU:C	4:D:230:SER:CB	2.85	0.45
4:D:279:LEU:N	4:D:279:LEU:HD23	2.32	0.45
13:O:110:MET:H	13:O:110:MET:CE	2.28	0.45
15:U:100:ARG:O	15:U:101:GLN:C	2.55	0.45
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.49	0.45
2:B:12:LEU:HG	2:B:19:LEU:HD13	1.97	0.45
2:B:113:TRP:HB3	23:B:525:CLA:CED	2.41	0.45
2:B:422:ARG:H	2:B:422:ARG:HG3	1.57	0.45
3:C:229:ASN:HD21	3:C:231:GLU:HB2	1.82	0.45
3:C:336:GLY:O	13:O:104:GLN:HG2	2.17	0.45
23:C:477:CLA:HAA2	23:C:477:CLA:HBD	1.97	0.45
4:D:231:THR:HG22	4:D:232:PHE:H	1.81	0.45
5:E:25:THR:HG23	28:E:84:HEC:HAB	1.98	0.45
8:I:5:LYS:HG3	8:I:9:TYR:HE1	1.82	0.45
10:K:9:PHE:HE2	19:Z:13:VAL:HG21	1.81	0.45
13:O:38:TYR:O	13:O:245:PRO:CB	2.65	0.45
14:T:18:PHE:HD2	14:T:19:PHE:CE1	2.35	0.45
14:T:29:ILE:O	14:T:29:ILE:HG22	2.16	0.45
16:V:111:ASP:O	16:V:115:ILE:HG13	2.16	0.45
1:A:224:ILE:HD11	1:A:243:GLU:CG	2.47	0.45
1:A:289:GLY:O	1:A:293:MET:HG3	2.16	0.45
1:A:300:PHE:CD2	3:C:404:LEU:HB2	2.52	0.45
2:B:152:GLY:C	23:B:515:CLA:HMC3	2.37	0.45
2:B:194:ASN:C	2:B:196:GLY:H	2.20	0.45
3:C:297:TYR:CG	3:C:302:TYR:HE1	2.35	0.45
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.97	0.45
12:M:8:LEU:HD22	14:T:1:MET:HE1	1.98	0.45
15:U:58:ASN:HB2	15:U:59:ASN:ND2	2.32	0.45
19:Z:19:MET:CE	19:Z:43:GLY:HA3	2.47	0.45
1:A:193:LEU:HB3	4:D:179:PHE:CD2	2.52	0.45
2:B:135:LEU:O	2:B:138:MET:N	2.50	0.45
2:B:315:ILE:HD13	2:B:359:MET:CE	2.47	0.45
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.99	0.45
3:C:63:TRP:CZ3	3:C:88:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:O	3:C:81:MET:C	2.53	0.45
3:C:276:LEU:HD23	3:C:440:GLY:O	2.17	0.45
4:D:129:GLN:NE2	4:D:142:ASN:HB3	2.32	0.45
15:U:113:THR:CG2	15:U:114:VAL:N	2.78	0.45
2:B:271:THR:HG22	2:B:448:ARG:HH11	1.82	0.45
2:B:302:TRP:CH2	2:B:343:HIS:CG	3.05	0.45
2:B:302:TRP:CE3	2:B:343:HIS:HB2	2.52	0.45
2:B:451:PHE:CD1	2:B:451:PHE:O	2.69	0.45
27:B:529:BCR:H403	12:M:6:LEU:HD12	1.99	0.45
3:C:294:ASN:C	3:C:296:VAL:N	2.70	0.45
3:C:395:TYR:O	3:C:396:MET:C	2.55	0.45
4:D:19:ASP:O	4:D:23:LYS:HG3	2.16	0.45
13:O:163:GLY:HA3	13:O:188:LYS:CE	2.45	0.45
14:T:26:PRO:HA	14:T:27:PRO:HD3	1.83	0.45
16:V:5:PRO:O	16:V:6:GLU:C	2.55	0.45
1:A:38:ILE:O	1:A:42:LEU:HG	2.17	0.45
1:A:87:ASN:HD21	3:C:357:ARG:NH1	2.08	0.45
1:A:161:TYR:O	1:A:162:PRO:C	2.54	0.45
1:A:235:TYR:HA	4:D:265:ARG:HH22	1.77	0.45
1:A:307:ILE:HG12	1:A:314:ILE:HD11	1.92	0.45
2:B:156:PHE:HB2	23:B:515:CLA:HAC1	1.99	0.45
3:C:205:ASP:O	3:C:208:VAL:HG12	2.17	0.45
16:V:64:PRO:HB2	16:V:65:PRO:HD2	1.98	0.45
19:Z:33:TRP:CE3	19:Z:37:LYS:HD3	2.30	0.45
1:A:192:ILE:O	1:A:193:LEU:C	2.55	0.44
1:A:295:PHE:HB3	3:C:291:TRP:CH2	2.53	0.44
2:B:234:ILE:O	2:B:237:VAL:N	2.43	0.44
2:B:258:TYR:N	2:B:258:TYR:CD2	2.85	0.44
3:C:105:VAL:CG1	3:C:107:ASP:O	2.65	0.44
3:C:339:LYS:NZ	15:U:125:GLY:HA3	2.32	0.44
5:E:25:THR:O	5:E:28:ALA:HB3	2.16	0.44
5:E:56:ALA:CB	5:E:82:LEU:HD23	2.38	0.44
9:J:8:ILE:HA	9:J:9:PRO:HD3	1.82	0.44
13:O:140:THR:HG22	13:O:201:VAL:HB	1.98	0.44
16:V:25:GLN:O	16:V:28:GLU:N	2.51	0.44
1:A:95:PRO:CG	1:A:98:GLU:HB2	2.48	0.44
1:A:224:ILE:HG13	1:A:245:THR:O	2.18	0.44
23:A:350:CLA:HMA1	24:D:355:PHO:C20	2.47	0.44
3:C:435:PHE:O	3:C:438:LEU:N	2.48	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
4:D:89:LEU:CB	4:D:91:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:SER:HA	5:E:13:ILE:CD1	2.27	0.44
8:I:7:THR:HA	8:I:10:ILE:HD12	1.98	0.44
13:O:68:THR:HA	13:O:110:MET:CE	2.47	0.44
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.83	0.44
1:A:29:TYR:CE1	1:A:31:GLY:CA	2.93	0.44
2:B:190:PHE:CE1	23:B:527:CLA:CED	3.01	0.44
3:C:296:VAL:HG21	23:C:479:CLA:HMA2	1.99	0.44
3:C:376:ASP:OD1	3:C:378:ASN:N	2.50	0.44
4:D:68:LEU:HD23	5:E:48:THR:HB	1.99	0.44
4:D:156:VAL:O	4:D:161:PRO:HD3	2.17	0.44
4:D:281:MET:HE1	4:D:284:ILE:HD12	1.99	0.44
4:D:300:SER:N	11:L:37:ASN:OD1	2.51	0.44
10:K:27:ALA:O	10:K:31:GLN:HG2	2.18	0.44
13:O:153:THR:CG2	13:O:154:ALA:N	2.81	0.44
13:O:211:ILE:CG2	13:O:212:ALA:H	2.29	0.44
2:B:31:ALA:HB2	23:B:518:CLA:CBC	2.47	0.44
2:B:436:THR:O	2:B:437:LEU:HD23	2.17	0.44
3:C:136:GLY:HA2	3:C:137:PRO:HD3	1.77	0.44
3:C:220:GLY:H	23:C:487:CLA:HBC1	1.82	0.44
3:C:311:GLN:NE2	3:C:355:THR:O	2.50	0.44
4:D:91:LEU:N	4:D:91:LEU:CD2	2.73	0.44
4:D:102:THR:HG23	5:E:46:PHE:C	2.38	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
13:O:55:GLU:HG2	13:O:64:GLU:HG3	2.00	0.44
13:O:218:GLU:HG3	13:O:233:VAL:O	2.17	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HA	1.98	0.44
1:A:104:GLU:O	1:A:105:TRP:C	2.56	0.44
1:A:238:LYS:O	1:A:239:PHE:C	2.55	0.44
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.52	0.44
2:B:370:LEU:HD12	2:B:379:ALA:HB3	1.99	0.44
2:B:397:VAL:CG1	2:B:398:THR:H	2.28	0.44
2:B:478:VAL:O	2:B:481:GLY:N	2.47	0.44
3:C:50:LEU:HD23	23:C:482:CLA:HMD3	2.00	0.44
3:C:286:ALA:O	3:C:290:VAL:N	2.49	0.44
4:D:88:SER:CB	5:E:68:ARG:NH2	2.74	0.44
4:D:296:TYR:CG	4:D:296:TYR:O	2.70	0.44
9:J:25:VAL:O	9:J:26:GLY:C	2.54	0.44
13:O:55:GLU:HB3	13:O:61:GLN:NE2	2.32	0.44
14:T:13:ILE:HG22	14:T:13:ILE:O	2.17	0.44
16:V:79:PRO:HG3	16:V:89:ALA:HA	1.99	0.44
16:V:92:HIS:CE1	16:V:93:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TRP:CZ3	8:I:8:VAL:HG21	2.49	0.44
1:A:230:THR:CG2	1:A:231:GLU:H	2.20	0.44
1:A:269:ARG:HD3	1:A:270:SER:N	2.32	0.44
1:A:330:VAL:HG12	4:D:348:ARG:HA	2.00	0.44
2:B:12:LEU:HD21	2:B:22:ALA:CB	2.48	0.44
3:C:85:GLY:C	3:C:86:LEU:HD23	2.37	0.44
3:C:270:ALA:O	3:C:274:TYR:CE1	2.71	0.44
3:C:287:THR:HG23	3:C:427:ALA:HA	1.99	0.44
4:D:42:TYR:CZ	6:F:24:THR:CG2	3.00	0.44
4:D:158:LEU:C	4:D:161:PRO:HD2	2.37	0.44
11:L:24:ILE:HD11	12:M:18:PRO:HB2	2.00	0.44
15:U:133:TYR:O	15:U:134:LYS:OXT	2.36	0.44
19:Z:39:LEU:H	19:Z:39:LEU:HG	1.39	0.44
1:A:78:ILE:CD1	11:L:34:TYR:CE1	2.99	0.44
1:A:107:TYR:HD1	13:O:115:ARG:NH1	2.16	0.44
1:A:149:ALA:CA	1:A:284:TRP:CZ3	3.00	0.44
1:A:213:ALA:O	1:A:217:SER:CB	2.65	0.44
2:B:350:GLU:OE1	2:B:350:GLU:N	2.50	0.44
3:C:93:ALA:CB	3:C:301:PHE:CE1	3.01	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HB3	2.52	0.44
3:C:217:PRO:HA	3:C:222:GLY:HA2	2.00	0.44
23:C:476:CLA:H61	23:C:483:CLA:H72	1.99	0.44
4:D:57:SER:CB	4:D:79:SER:HB2	2.48	0.44
10:K:6:TYR:N	10:K:6:TYR:CD1	2.86	0.44
15:U:62:ILE:CG2	15:U:76:ALA:HB1	2.47	0.44
19:Z:5:PHE:HD2	19:Z:5:PHE:O	2.01	0.44
1:A:315:ASN:O	4:D:63:LEU:HD22	2.16	0.44
3:C:201:ASN:O	3:C:201:ASN:CG	2.57	0.44
4:D:28:VAL:O	4:D:28:VAL:HG12	2.17	0.44
4:D:350:ASN:HD22	4:D:351:ALA:N	2.16	0.44
4:D:350:ASN:ND2	4:D:351:ALA:N	2.65	0.44
13:O:33:ASP:O	13:O:36:GLN:HB2	2.17	0.44
1:A:54:ALA:O	1:A:55:ALA:C	2.55	0.44
25:A:353:PL9:H23	25:A:353:PL9:H271	1.42	0.44
2:B:200:ALA:C	23:B:521:CLA:HBB1	2.38	0.44
23:B:519:CLA:H142	23:D:356:CLA:H11	1.99	0.44
3:C:89:ILE:HB	3:C:90:PRO:CD	2.44	0.44
3:C:157:MET:HE2	3:C:160:ILE:CD1	2.34	0.44
3:C:274:TYR:HB3	23:C:485:CLA:C3B	2.48	0.44
3:C:299:SER:O	3:C:303:GLY:O	2.36	0.44
3:C:317:PHE:O	3:C:321:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:PHE:O	4:D:102:THR:C	2.56	0.44
4:D:110:LEU:O	4:D:111:TRP:C	2.55	0.44
4:D:146:PHE:O	4:D:149:PRO:HD2	2.18	0.44
4:D:161:PRO:HG3	4:D:170:ALA:CB	2.46	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
5:E:68:ARG:NH1	7:H:50:SER:O	2.50	0.44
13:O:31:PRO:HB2	13:O:33:ASP:H	1.83	0.44
13:O:190:PHE:CE1	15:U:120:ALA:HA	2.53	0.44
15:U:75:LEU:CD2	15:U:101:GLN:NE2	2.81	0.44
1:A:41:LEU:HD13	24:A:351:PHO:C2	2.48	0.43
1:A:187:GLN:HE21	1:A:187:GLN:HB3	1.50	0.43
1:A:326:LEU:HD13	3:C:412:THR:CG2	2.39	0.43
1:A:341:LEU:HD21	15:U:134:LYS:HZ2	1.81	0.43
2:B:264:PRO:HD2	2:B:268:PHE:HE1	1.83	0.43
2:B:360:PRO:C	2:B:362:PHE:N	2.71	0.43
3:C:243:ILE:HG22	23:C:474:CLA:HMC1	2.00	0.43
5:E:33:GLY:O	5:E:36:PHE:N	2.48	0.43
6:F:40:GLN:NE2	9:J:27:LEU:O	2.48	0.43
15:U:47:LEU:HB3	15:U:51:TYR:HD1	1.83	0.43
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.18	0.43
2:B:234:ILE:HG21	23:B:524:CLA:H193	2.00	0.43
3:C:189:TRP:O	3:C:190:ALA:O	2.36	0.43
3:C:350:ILE:CG2	3:C:351:PHE:N	2.81	0.43
4:D:101:PHE:O	4:D:104:TRP:N	2.52	0.43
12:M:16:LEU:O	12:M:17:VAL:C	2.53	0.43
13:O:32:ILE:HA	13:O:133:VAL:HG11	2.00	0.43
13:O:182:LEU:O	13:O:183:ALA:C	2.55	0.43
15:U:88:VAL:HG12	15:U:109:LEU:CD1	2.48	0.43
16:V:134:LYS:C	16:V:137:TYR:H	2.22	0.43
1:A:160:ILE:H	1:A:160:ILE:HG13	1.66	0.43
2:B:18:ARG:NH1	2:B:115:TRP:O	2.50	0.43
2:B:91:TRP:HB3	23:B:515:CLA:H43	2.00	0.43
2:B:156:PHE:CD1	2:B:156:PHE:N	2.86	0.43
2:B:418:LYS:O	2:B:419:SER:C	2.55	0.43
3:C:48:LYS:HD3	3:C:133:ALA:O	2.18	0.43
3:C:187:ASP:OD1	3:C:189:TRP:N	2.51	0.43
4:D:178:ILE:O	4:D:181:PHE:HB3	2.19	0.43
5:E:55:TYR:O	16:V:1:ALA:HB2	2.17	0.43
7:H:59:VAL:O	7:H:59:VAL:CG1	2.64	0.43
13:O:243:ILE:CG2	13:O:244:GLU:N	2.81	0.43
16:V:35:TYR:CD2	16:V:35:TYR:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:O	1:A:160:ILE:C	2.56	0.43
2:B:302:TRP:C	2:B:304:ALA:N	2.71	0.43
3:C:191:PRO:O	3:C:193:GLY:N	2.48	0.43
3:C:394:GLU:O	3:C:397:THR:HB	2.18	0.43
5:E:22:HIS:C	5:E:24:ILE:N	2.70	0.43
5:E:24:ILE:O	5:E:24:ILE:HG22	2.18	0.43
5:E:30:PHE:C	5:E:30:PHE:CD2	2.91	0.43
7:H:57:VAL:O	7:H:57:VAL:HG13	2.17	0.43
10:K:9:PHE:N	10:K:9:PHE:CD1	2.86	0.43
12:M:20:VAL:O	12:M:21:PHE:C	2.55	0.43
13:O:57:LYS:HG3	13:O:57:LYS:O	2.18	0.43
1:A:162:PRO:CG	1:A:171:GLY:HA2	2.48	0.43
1:A:339:PHE:CE1	3:C:314:ALA:HA	2.53	0.43
2:B:479:PHE:C	2:B:481:GLY:H	2.21	0.43
3:C:94:THR:C	3:C:96:GLY:N	2.71	0.43
3:C:155:ASN:O	3:C:159:THR:OG1	2.27	0.43
3:C:167:VAL:CG1	23:C:482:CLA:H11	2.48	0.43
3:C:223:TRP:HD1	3:C:224:ILE:N	2.14	0.43
4:D:181:PHE:O	4:D:182:LEU:C	2.57	0.43
4:D:189:HIS:CE1	4:D:294:ARG:HH21	2.36	0.43
4:D:218:VAL:O	4:D:220:ASN:N	2.52	0.43
4:D:273:PHE:O	4:D:277:THR:HB	2.17	0.43
23:D:356:CLA:H12	7:H:42:LEU:CD2	2.48	0.43
13:O:34:SER:C	13:O:36:GLN:N	2.69	0.43
13:O:34:SER:O	13:O:35:SER:C	2.57	0.43
19:Z:13:VAL:HG13	19:Z:17:PHE:CE1	2.54	0.43
19:Z:42:LEU:O	19:Z:46:LEU:HB2	2.18	0.43
2:B:63:LEU:HD12	2:B:63:LEU:HA	1.87	0.43
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.84	0.43
2:B:234:ILE:HG23	23:B:524:CLA:H193	2.01	0.43
2:B:311:PHE:C	2:B:313:ASP:N	2.71	0.43
2:B:354:LEU:CD2	2:B:378:LYS:HG3	2.48	0.43
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.18	0.43
4:D:195:PRO:HA	4:D:198:MET:HE3	1.95	0.43
4:D:195:PRO:O	4:D:199:MET:HG3	2.19	0.43
6:F:32:PHE:CE1	27:F:48:BCR:H14C	2.54	0.43
1:A:295:PHE:O	3:C:291:TRP:CH2	2.72	0.43
23:A:350:CLA:HMD3	4:D:182:LEU:HD11	2.01	0.43
2:B:252:VAL:HG22	23:B:517:CLA:O1A	2.19	0.43
2:B:297:THR:HB	2:B:299:GLU:OE1	2.18	0.43
2:B:327:THR:O	2:B:329:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.33	0.43
4:D:22:LEU:CD2	4:D:32:TRP:CE3	3.01	0.43
10:K:31:GLN:HB3	10:K:36:PHE:CD2	2.54	0.43
16:V:22:THR:N	16:V:25:GLN:NE2	2.65	0.43
1:A:234:ASN:C	4:D:265:ARG:HH12	2.22	0.43
1:A:290:ILE:HD11	23:A:348:CLA:OBD	2.19	0.43
1:A:301:ASN:HD22	1:A:301:ASN:N	2.16	0.43
23:A:350:CLA:HMA1	24:D:355:PHO:H201	2.00	0.43
2:B:265:ILE:C	2:B:267:LEU:H	2.22	0.43
3:C:256:PRO:HA	23:C:474:CLA:HED3	2.01	0.43
3:C:355:THR:O	3:C:355:THR:OG1	2.37	0.43
3:C:377:LEU:HD21	13:O:99:ASP:OD2	2.18	0.43
10:K:34:VAL:O	10:K:34:VAL:CG1	2.64	0.43
11:L:6:ASN:HD22	11:L:6:ASN:N	2.15	0.43
13:O:58:ASN:O	13:O:59:LYS:HB2	2.19	0.43
13:O:126:VAL:O	13:O:126:VAL:HG12	2.18	0.43
14:T:1:MET:C	14:T:3:THR:N	2.68	0.43
14:T:10:PHE:HE2	14:T:14:ILE:HD11	1.83	0.43
19:Z:7:LEU:O	19:Z:11:ALA:CB	2.63	0.43
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.53	0.43
1:A:196:PRO:HA	1:A:199:GLN:HB2	2.01	0.43
2:B:88:PRO:O	2:B:89:GLY:C	2.57	0.43
2:B:135:LEU:N	2:B:136:PRO:HD2	2.33	0.43
2:B:149:LEU:O	2:B:150:CYS:C	2.56	0.43
2:B:237:VAL:CG2	23:B:524:CLA:HBC2	2.49	0.43
4:D:21:TRP:O	4:D:26:ARG:NH2	2.40	0.43
7:H:49:ASN:O	7:H:49:ASN:CG	2.57	0.43
16:V:112:LEU:HD23	16:V:112:LEU:HA	1.80	0.43
1:A:89:ILE:HD13	1:A:94:TYR:CD1	2.54	0.43
1:A:104:GLU:O	1:A:107:TYR:N	2.41	0.43
1:A:168:PHE:O	1:A:169:SER:C	2.57	0.43
2:B:6:TYR:HE1	2:B:8:VAL:HG21	1.83	0.43
23:C:484:CLA:C4B	27:C:489:BCR:H393	2.48	0.43
4:D:55:VAL:O	4:D:65:SER:HB3	2.18	0.43
4:D:204:VAL:HG21	23:D:354:CLA:HMA1	2.01	0.43
4:D:328:TRP:CE2	4:D:346:LEU:HD13	2.54	0.43
5:E:33:GLY:O	5:E:36:PHE:HB3	2.18	0.43
5:E:48:THR:O	5:E:49:PRO:C	2.57	0.43
10:K:8:ILE:H	10:K:8:ILE:HG13	1.68	0.43
13:O:152:ARG:HD2	13:O:156:PHE:CZ	2.54	0.43
15:U:87:SER:HB3	15:U:90:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:35:TYR:CD2	16:V:35:TYR:C	2.92	0.43
16:V:100:ILE:O	16:V:102:PRO:HD3	2.19	0.43
2:B:368:VAL:HG22	2:B:425:ILE:HD12	2.01	0.42
23:B:522:CLA:H171	23:B:525:CLA:HMD1	1.99	0.42
3:C:274:TYR:CE2	23:C:477:CLA:HED3	2.53	0.42
10:K:10:ASP:O	10:K:11:PRO:C	2.58	0.42
11:L:6:ASN:OD1	11:L:8:GLN:HG2	2.19	0.42
13:O:33:ASP:O	13:O:37:THR:N	2.50	0.42
15:U:58:ASN:C	15:U:59:ASN:ND2	2.70	0.42
16:V:79:PRO:CB	16:V:88:ILE:HG12	2.44	0.42
16:V:104:MET:HE3	16:V:107:LEU:HD12	2.00	0.42
18:N:31:UNK:HA	19:Z:30:PRO:HG2	2.01	0.42
1:A:150:PRO:O	1:A:151:LEU:C	2.55	0.42
2:B:323:GLY:N	4:D:294:ARG:O	2.49	0.42
2:B:331:ASN:C	2:B:333:GLY:H	2.21	0.42
3:C:116:VAL:HG11	27:C:489:BCR:H321	2.00	0.42
3:C:276:LEU:HD13	23:C:483:CLA:HBB1	2.01	0.42
4:D:221:THR:HG22	4:D:245:SER:H	1.84	0.42
4:D:350:ASN:O	4:D:351:ALA:HB3	2.19	0.42
28:E:84:HEC:O1D	6:F:18:ARG:NE	2.48	0.42
9:J:3:SER:N	18:N:32:UNK:CB	2.82	0.42
10:K:30:TRP:HE3	10:K:31:GLN:HE21	1.65	0.42
13:O:43:LEU:HD11	13:O:239:PHE:CD1	2.53	0.42
13:O:54:GLU:OE1	13:O:114:GLU:OE1	2.37	0.42
13:O:122:VAL:O	13:O:125:LEU:HB2	2.19	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.02	0.42
1:A:142:TRP:HH2	1:A:273:PHE:CE1	2.34	0.42
1:A:307:ILE:HG22	1:A:309:ALA:HB3	2.00	0.42
2:B:327:THR:O	2:B:329:PRO:N	2.53	0.42
3:C:108:THR:HG21	10:K:2:LEU:CG	2.47	0.42
3:C:204:LEU:HD12	3:C:239:TRP:HE1	1.84	0.42
3:C:315:MET:O	3:C:319:ILE:HG13	2.18	0.42
4:D:170:ALA:O	4:D:171:PRO:C	2.56	0.42
4:D:316:THR:O	4:D:317:LYS:C	2.58	0.42
5:E:14:THR:HG22	9:J:8:ILE:CD1	2.44	0.42
5:E:14:THR:HG22	9:J:8:ILE:HD12	1.88	0.42
5:E:30:PHE:HD2	5:E:30:PHE:C	2.23	0.42
13:O:104:GLN:HB3	13:O:151:TYR:HE1	1.85	0.42
15:U:51:TYR:HB3	15:U:52:GLY:H	1.34	0.42
15:U:130:ASN:O	15:U:131:GLY:C	2.57	0.42
1:A:57:PRO:CA	1:A:68:SER:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:O	13:O:152:ARG:NH2	2.50	0.42
1:A:77:ILE:HD11	14:T:6:TYR:CD2	2.54	0.42
1:A:139:MET:CE	4:D:248:THR:CG2	2.97	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.01	0.42
23:B:524:CLA:O1D	23:B:524:CLA:H93	2.20	0.42
3:C:81:MET:HE2	3:C:90:PRO:HG3	2.02	0.42
3:C:139:THR:O	3:C:139:THR:HG23	2.19	0.42
3:C:159:THR:HA	3:C:252:ILE:HA	2.01	0.42
3:C:168:LEU:HD21	23:C:478:CLA:H72	2.02	0.42
3:C:213:LEU:HD11	23:C:474:CLA:H171	2.01	0.42
3:C:324:LEU:HD23	3:C:324:LEU:HA	1.77	0.42
3:C:443:TRP:CE3	3:C:443:TRP:CA	3.00	0.42
4:D:126:MET:SD	4:D:143:ALA:O	2.77	0.42
4:D:273:PHE:O	4:D:277:THR:CB	2.67	0.42
8:I:13:THR:O	8:I:16:VAL:HB	2.19	0.42
13:O:229:GLU:HA	13:O:230:PRO:HD3	1.91	0.42
16:V:37:CYS:HB2	16:V:38:ALA:H	1.71	0.42
17:X:17:LYS:O	17:X:20:PHE:N	2.52	0.42
1:A:55:ALA:HA	1:A:56:PRO:HD3	1.92	0.42
1:A:297:LEU:CD2	3:C:428:THR:HG21	2.50	0.42
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.49	0.42
2:B:49:ASP:HA	2:B:50:PRO:HD3	1.87	0.42
2:B:168:VAL:CG1	2:B:169:SER:N	2.83	0.42
2:B:245:VAL:HG22	23:B:513:CLA:H172	2.02	0.42
3:C:48:LYS:HZ2	23:C:486:CLA:HBA1	1.83	0.42
3:C:97:TRP:CE3	3:C:178:LYS:CE	3.02	0.42
4:D:20:ASP:O	4:D:24:ARG:N	2.52	0.42
4:D:249:ALA:O	4:D:252:PHE:HB3	2.20	0.42
6:F:32:PHE:CD1	27:F:48:BCR:H14C	2.54	0.42
9:J:15:THR:CA	27:K:50:BCR:H372	2.45	0.42
15:U:108:ASN:O	15:U:110:GLU:N	2.53	0.42
1:A:31:GLY:HA3	1:A:132:GLU:OE2	2.19	0.42
1:A:76:ASN:CB	14:T:2:GLU:OE2	2.64	0.42
1:A:142:TRP:CH2	1:A:273:PHE:HE1	2.35	0.42
1:A:180:PHE:CE2	4:D:192:THR:O	2.68	0.42
2:B:35:GLY:O	2:B:39:LEU:HG	2.19	0.42
2:B:277:SER:O	2:B:278:SER:C	2.57	0.42
3:C:37:ALA:O	3:C:38:GLY:C	2.57	0.42
9:J:15:THR:HG23	27:K:50:BCR:H372	2.01	0.42
10:K:16:LEU:O	10:K:18:VAL:N	2.52	0.42
19:Z:47:TRP:HE1	19:Z:51:VAL:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:O	1:A:164:GLY:N	2.46	0.42
2:B:106:LEU:HB3	23:B:522:CLA:H121	2.02	0.42
2:B:340:TRP:CE3	2:B:342:GLY:CA	3.02	0.42
23:B:511:CLA:H102	7:H:37:PHE:CD1	2.55	0.42
23:B:523:CLA:HAA2	23:B:523:CLA:HBD	2.01	0.42
3:C:38:GLY:HA3	23:C:486:CLA:C1D	2.50	0.42
4:D:116:LEU:O	4:D:120:PHE:HD1	2.03	0.42
4:D:146:PHE:O	4:D:150:ILE:HG13	2.20	0.42
7:H:51:THR:O	7:H:51:THR:CG2	2.68	0.42
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.02	0.42
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.42
16:V:29:GLY:HA3	16:V:118:HIS:HB2	2.02	0.42
1:A:63:ILE:HG23	3:C:335:THR:HG23	1.99	0.42
1:A:73:TYR:N	1:A:73:TYR:CD2	2.88	0.42
1:A:142:TRP:O	1:A:145:VAL:N	2.49	0.42
1:A:339:PHE:HB3	3:C:313:GLN:OE1	2.19	0.42
2:B:366:PHE:HA	2:B:367:PRO:HD3	1.71	0.42
2:B:399:VAL:CG2	2:B:417:VAL:HG13	2.49	0.42
2:B:451:PHE:CZ	2:B:455:HIS:CE1	3.08	0.42
2:B:463:PHE:CZ	2:B:467:ILE:HD11	2.54	0.42
3:C:60:ILE:O	23:C:480:CLA:HMD3	2.20	0.42
3:C:210:PHE:O	3:C:214:LEU:HG	2.20	0.42
23:C:475:CLA:H51	27:J:53:BCR:H342	2.01	0.42
4:D:30:VAL:HG22	4:D:38:PHE:CE1	2.53	0.42
4:D:80:THR:CG2	4:D:81:PRO:HD2	2.49	0.42
4:D:186:GLN:NE2	4:D:192:THR:OG1	2.53	0.42
4:D:281:MET:O	4:D:284:ILE:HB	2.19	0.42
9:J:17:ALA:O	9:J:20:GLY:N	2.53	0.42
9:J:19:MET:HG2	27:K:50:BCR:H361	2.01	0.42
9:J:30:TYR:O	9:J:33:TYR:HB2	2.20	0.42
11:L:36:PHE:C	12:M:3:VAL:HG23	2.40	0.42
15:U:67:GLN:O	15:U:68:TYR:CD2	2.73	0.42
16:V:81:THR:HB	16:V:83:ASP:OD1	2.19	0.42
1:A:21:VAL:HG13	1:A:30:VAL:O	2.19	0.42
1:A:327:GLY:HA3	4:D:324:GLY:O	2.20	0.42
2:B:56:TRP:HH2	2:B:312:TYR:HE2	1.67	0.42
2:B:223:GLN:HG2	2:B:227:LYS:HG3	2.01	0.42
2:B:325:PHE:O	2:B:328:GLY:N	2.52	0.42
23:B:512:CLA:OBD	23:B:520:CLA:HHC	2.20	0.42
23:B:516:CLA:H111	23:B:522:CLA:H42	2.00	0.42
3:C:173:LEU:HA	3:C:176:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:TRP:HZ3	23:C:474:CLA:O2A	2.03	0.42
3:C:289:PHE:CD1	23:C:487:CLA:HBB2	2.55	0.42
3:C:307:PRO:O	3:C:308:GLU:C	2.57	0.42
3:C:425:TRP:CE2	23:C:475:CLA:HBA2	2.54	0.42
4:D:43:LEU:HD22	27:F:48:BCR:H323	2.02	0.42
5:E:25:THR:HG21	28:E:84:HEC:C4B	2.50	0.42
5:E:68:ARG:NH1	7:H:50:SER:HB3	2.34	0.42
13:O:198:SER:O	13:O:199:LEU:HD23	2.20	0.42
14:T:18:PHE:CD2	14:T:19:PHE:CE1	3.08	0.42
19:Z:9:LEU:HD12	19:Z:9:LEU:HA	1.83	0.42
1:A:214:MET:HG2	25:A:353:PL9:HC8	2.02	0.42
1:A:315:ASN:C	4:D:63:LEU:HD22	2.39	0.42
2:B:19:LEU:HD23	23:B:524:CLA:H201	2.02	0.42
2:B:72:THR:HG22	2:B:79:SER:HB2	2.02	0.42
2:B:264:PRO:O	2:B:448:ARG:NH2	2.52	0.42
3:C:172:ALA:N	23:C:479:CLA:HAC1	2.35	0.42
4:D:67:TYR:C	6:F:39:MET:HE1	2.40	0.42
4:D:90:LEU:HD11	4:D:96:GLU:CG	2.49	0.42
4:D:103:ARG:C	4:D:105:CYS:N	2.72	0.42
4:D:291:LEU:C	4:D:293:LEU:N	2.73	0.42
25:D:357:PL9:H38	14:T:18:PHE:CB	2.44	0.42
7:H:47:ILE:CG1	7:H:52:LEU:HD23	2.50	0.42
13:O:142:PHE:O	13:O:143:LYS:HG2	2.19	0.42
1:A:89:ILE:HG21	1:A:94:TYR:CB	2.46	0.41
1:A:141:PRO:O	3:C:443:TRP:CZ3	2.73	0.41
1:A:220:THR:O	1:A:223:LEU:HG	2.20	0.41
1:A:291:SER:O	1:A:295:PHE:CD1	2.73	0.41
3:C:273:SER:CB	3:C:445:ALA:HB2	2.44	0.41
3:C:339:LYS:HE2	15:U:129:ASN:OD1	2.19	0.41
4:D:48:TRP:CE3	24:D:355:PHO:H161	2.55	0.41
4:D:189:HIS:CE1	4:D:294:ARG:HE	2.38	0.41
4:D:301:GLN:O	4:D:302:GLU:C	2.58	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41
10:K:16:LEU:CB	10:K:17:PRO:CD	2.85	0.41
13:O:75:THR:O	13:O:76:THR:C	2.57	0.41
13:O:101:ILE:HG22	13:O:102:ASP:N	2.35	0.41
13:O:118:LEU:HD22	13:O:233:VAL:HG21	2.01	0.41
2:B:145:LEU:CD1	23:B:522:CLA:HAB	2.49	0.41
23:B:516:CLA:HAA2	23:B:516:CLA:HBD	2.02	0.41
3:C:49:LEU:O	3:C:52:ALA:N	2.53	0.41
3:C:199:ILE:HG22	3:C:200:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:339:LYS:HB2	3:C:340:TYR:CD1	2.54	0.41
23:C:474:CLA:HBB2	23:C:485:CLA:HED1	2.01	0.41
5:E:41:LEU:O	5:E:42:ALA:C	2.59	0.41
9:J:19:MET:CG	27:K:50:BCR:H361	2.50	0.41
13:O:197:ILE:HG12	13:O:198:SER:N	2.35	0.41
13:O:207:ARG:O	13:O:210:GLU:OE2	2.38	0.41
14:T:9:ILE:O	14:T:9:ILE:CG2	2.68	0.41
16:V:129:LYS:NZ	16:V:135:VAL:HG23	2.35	0.41
19:Z:52:LEU:O	19:Z:56:VAL:HG23	2.21	0.41
1:A:143:ILE:HD12	4:D:252:PHE:CE2	2.56	0.41
1:A:337:HIS:ND1	4:D:352:LEU:HD12	2.35	0.41
2:B:46:ASP:HA	2:B:47:PRO:HD3	1.68	0.41
2:B:175:THR:O	2:B:175:THR:HG23	2.21	0.41
2:B:235:GLU:O	2:B:238:LEU:HB3	2.21	0.41
2:B:372:ASP:OD1	2:B:373:LYS:N	2.53	0.41
3:C:78:GLU:HG3	16:V:105:ARG:NH1	2.35	0.41
3:C:89:ILE:O	3:C:92:ILE:N	2.53	0.41
3:C:195:ASP:N	3:C:195:ASP:OD1	2.53	0.41
3:C:412:THR:HG22	16:V:136:TYR:CE2	2.52	0.41
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.37	0.41
8:I:27:ASP:CB	8:I:28:PRO:CD	2.88	0.41
11:L:14:ARG:HA	12:M:26:TYR:CE1	2.55	0.41
11:L:31:PHE:O	11:L:32:SER:C	2.57	0.41
15:U:62:ILE:HG12	15:U:80:VAL:HG21	2.02	0.41
16:V:22:THR:OG1	16:V:25:GLN:HG3	2.20	0.41
16:V:63:THR:HG21	16:V:83:ASP:O	2.19	0.41
17:X:34:PHE:O	17:X:35:ALA:C	2.58	0.41
1:A:160:ILE:HG21	1:A:291:SER:OG	2.20	0.41
1:A:339:PHE:CB	3:C:313:GLN:OE1	2.68	0.41
3:C:218:PHE:O	3:C:219:GLY:C	2.58	0.41
3:C:320:ARG:NE	15:U:128:TYR:CZ	2.77	0.41
23:C:474:CLA:H122	23:C:485:CLA:H13	2.03	0.41
4:D:199:MET:O	4:D:202:ALA:N	2.51	0.41
4:D:259:ILE:O	4:D:260:ALA:HB2	2.20	0.41
15:U:84:PRO:C	15:U:85:TYR:HD2	2.22	0.41
1:A:140:ARG:HB2	4:D:220:ASN:CG	2.41	0.41
1:A:210:LEU:O	1:A:214:MET:HB2	2.20	0.41
1:A:307:ILE:O	1:A:308:ASP:C	2.58	0.41
2:B:265:ILE:O	2:B:267:LEU:N	2.54	0.41
2:B:288:VAL:O	2:B:292:LEU:HB2	2.21	0.41
2:B:467:ILE:HD13	4:D:126:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:GLY:C	3:C:99:VAL:HG23	2.41	0.41
3:C:222:GLY:O	3:C:223:TRP:O	2.38	0.41
3:C:321:ASP:CG	15:U:128:TYR:CD2	2.94	0.41
4:D:29:PHE:CD2	4:D:29:PHE:O	2.72	0.41
4:D:342:PRO:HG2	4:D:345:VAL:CG2	2.51	0.41
10:K:6:TYR:HD1	10:K:6:TYR:H	1.67	0.41
14:T:27:PRO:HG2	14:T:27:PRO:O	2.21	0.41
16:V:79:PRO:CB	16:V:88:ILE:CG1	2.93	0.41
18:N:22:UNK:O	18:N:23:UNK:C	2.68	0.41
19:Z:47:TRP:CD1	19:Z:51:VAL:HG23	2.55	0.41
1:A:58:VAL:HG13	1:A:107:TYR:O	2.21	0.41
1:A:207:GLY:HA3	1:A:278:TRP:CD1	2.56	0.41
2:B:308:LYS:HE2	2:B:312:TYR:OH	2.20	0.41
3:C:90:PRO:CB	3:C:302:TYR:HE2	2.33	0.41
3:C:190:ALA:HA	3:C:191:PRO:HA	1.49	0.41
3:C:320:ARG:HG2	15:U:128:TYR:CE2	2.56	0.41
3:C:343:ARG:HD3	3:C:344:SER:C	2.40	0.41
7:H:22:PRO:HG2	7:H:23:GLY:H	1.85	0.41
7:H:43:ILE:HG12	17:X:19:PHE:CZ	2.56	0.41
13:O:76:THR:HB	13:O:77:SER:H	1.29	0.41
13:O:157:LEU:HD23	13:O:157:LEU:HA	1.79	0.41
14:T:14:ILE:O	14:T:17:PHE:HB2	2.21	0.41
1:A:95:PRO:HG2	1:A:98:GLU:HB2	2.02	0.41
1:A:149:ALA:HA	1:A:284:TRP:CE3	2.56	0.41
1:A:159:LEU:HD21	1:A:163:ILE:HD11	2.03	0.41
2:B:339:ALA:HB1	2:B:340:TRP:HD1	1.86	0.41
23:B:513:CLA:H18	23:B:524:CLA:O1A	2.20	0.41
3:C:45:LEU:O	3:C:47:GLY:N	2.54	0.41
3:C:54:VAL:O	3:C:54:VAL:HG12	2.21	0.41
3:C:82:TYR:CD1	3:C:82:TYR:C	2.94	0.41
3:C:281:MET:C	3:C:285:ILE:HG13	2.41	0.41
3:C:395:TYR:N	3:C:395:TYR:CD2	2.87	0.41
3:C:443:TRP:CD1	23:C:483:CLA:HMD3	2.56	0.41
4:D:217:THR:OG1	4:D:253:TRP:HZ2	2.03	0.41
4:D:322:ASN:O	4:D:325:ILE:N	2.53	0.41
13:O:71:VAL:HG21	13:O:108:VAL:CG2	2.46	0.41
19:Z:31:GLN:O	19:Z:32:ASP:C	2.59	0.41
1:A:40:THR:CG2	1:A:118:HIS:O	2.69	0.41
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.21	0.41
1:A:208:GLY:O	1:A:212:CYS:HB2	2.20	0.41
1:A:341:LEU:HD21	15:U:134:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HD11	2:B:19:LEU:N	2.36	0.41
2:B:135:LEU:HB2	2:B:231:MET:CE	2.47	0.41
2:B:288:VAL:O	2:B:292:LEU:CB	2.68	0.41
2:B:315:ILE:HD13	2:B:359:MET:HE2	2.02	0.41
2:B:385:ARG:HG3	13:O:165:ALA:C	2.41	0.41
3:C:53:HIS:ND1	23:C:478:CLA:H141	2.35	0.41
3:C:175:LEU:HD23	3:C:237:HIS:CD2	2.55	0.41
3:C:273:SER:HB2	23:C:477:CLA:HED1	2.02	0.41
3:C:275:SER:OG	23:C:485:CLA:HAA1	2.21	0.41
4:D:58:TRP:HA	4:D:62:GLY:N	2.32	0.41
4:D:218:VAL:O	4:D:219:GLU:C	2.59	0.41
5:E:19:TRP:HZ2	9:J:13:VAL:CG2	2.27	0.41
13:O:15:LEU:O	13:O:16:ALA:C	2.59	0.41
13:O:118:LEU:HD22	13:O:221:SER:HA	2.01	0.41
15:U:57:LEU:HA	15:U:57:LEU:HD23	1.78	0.41
15:U:113:THR:HG22	15:U:114:VAL:H	1.82	0.41
1:A:24:THR:OG1	4:D:251:ARG:NH2	2.53	0.41
1:A:41:LEU:HD21	1:A:122:GLY:C	2.40	0.41
1:A:180:PHE:HD1	1:A:180:PHE:N	2.12	0.41
1:A:309:ALA:HB1	16:V:2:GLU:HA	2.03	0.41
2:B:9:HIS:HE1	23:B:512:CLA:HED1	1.86	0.41
2:B:12:LEU:HG	2:B:19:LEU:CB	2.51	0.41
2:B:33:TRP:HE1	23:B:514:CLA:HBC2	1.86	0.41
2:B:187:PRO:O	2:B:189:GLY:N	2.53	0.41
2:B:340:TRP:CZ3	2:B:407:ASN:HB3	2.55	0.41
2:B:472:ARG:O	2:B:472:ARG:HG2	2.19	0.41
23:B:514:CLA:H61	23:B:514:CLA:H41	1.93	0.41
23:B:520:CLA:H51	27:B:529:BCR:H313	2.02	0.41
3:C:62:PHE:CD2	10:K:20:PRO:HG3	2.56	0.41
3:C:101:PRO:HA	3:C:195:ASP:HB3	2.02	0.41
3:C:172:ALA:N	23:C:479:CLA:CAC	2.84	0.41
3:C:249:ILE:HG13	3:C:250:TRP:N	2.36	0.41
3:C:263:ALA:HB3	3:C:264:PHE:CD2	2.55	0.41
3:C:290:VAL:HG12	3:C:291:TRP:N	2.35	0.41
27:C:488:BCR:C20	10:K:23:PHE:HE2	2.33	0.41
4:D:51:GLY:HA2	4:D:55:VAL:CG2	2.46	0.41
4:D:125:PHE:CD2	4:D:125:PHE:O	2.74	0.41
4:D:156:VAL:HG23	23:D:354:CLA:HED1	2.03	0.41
7:H:29:LEU:HA	7:H:29:LEU:HD12	1.79	0.41
9:J:25:VAL:O	9:J:28:PHE:N	2.54	0.41
13:O:205:ASP:O	13:O:206:GLY:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:224:ASP:O	13:O:224:ASP:OD1	2.38	0.41
15:U:65:PHE:CD1	15:U:76:ALA:CB	3.04	0.41
15:U:100:ARG:O	15:U:104:ILE:HG13	2.21	0.41
19:Z:47:TRP:NE1	19:Z:51:VAL:HG23	2.36	0.41
1:A:225:ARG:HG3	1:A:225:ARG:H	1.19	0.41
1:A:325:ASN:HD22	1:A:325:ASN:H	1.69	0.41
2:B:9:HIS:CE1	23:B:512:CLA:HED1	2.55	0.41
2:B:135:LEU:O	2:B:137:LYS:N	2.54	0.41
2:B:166:MET:CE	2:B:195:PRO:HB3	2.51	0.41
2:B:201:HIS:CD2	2:B:202:HIS:N	2.89	0.41
2:B:265:ILE:HG21	2:B:312:TYR:CE1	2.55	0.41
23:B:516:CLA:H61	23:B:516:CLA:H41	1.94	0.41
3:C:81:MET:HE1	3:C:90:PRO:N	2.35	0.41
4:D:32:TRP:HA	4:D:32:TRP:HE3	1.82	0.41
4:D:341:PHE:HA	4:D:342:PRO:HD2	1.73	0.41
1:A:32:TRP:HA	1:A:35:VAL:CG2	2.51	0.40
1:A:53:ILE:O	1:A:53:ILE:CG2	2.69	0.40
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.65	0.40
2:B:12:LEU:HD23	2:B:19:LEU:HD12	2.02	0.40
2:B:47:PRO:HA	2:B:78:TRP:NE1	2.36	0.40
2:B:91:TRP:CD1	23:B:515:CLA:H51	2.55	0.40
2:B:211:ILE:HG22	2:B:212:ALA:N	2.36	0.40
2:B:249:ALA:HB3	2:B:459:ALA:HB2	2.02	0.40
2:B:271:THR:CG2	2:B:448:ARG:NH1	2.82	0.40
2:B:321:LYS:CG	2:B:322:GLY:N	2.84	0.40
2:B:325:PHE:CZ	4:D:297:ASP:OD2	2.74	0.40
2:B:445:THR:HG22	2:B:446:SER:N	2.35	0.40
3:C:291:TRP:HZ3	3:C:424:SER:HA	1.86	0.40
4:D:303:ILE:HD13	12:M:2:GLU:OE1	2.21	0.40
5:E:50:ARG:HB3	5:E:51:PRO:HD2	2.03	0.40
7:H:38:LEU:HA	7:H:38:LEU:HD23	1.87	0.40
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.72	0.40
13:O:152:ARG:HD2	13:O:156:PHE:CD1	2.56	0.40
13:O:238:VAL:CG1	13:O:239:PHE:H	2.33	0.40
14:T:3:THR:C	14:T:5:THR:N	2.74	0.40
15:U:61:ASN:HB3	15:U:130:ASN:HD22	1.85	0.40
18:N:8:UNK:O	18:N:12:UNK:N	2.54	0.40
19:Z:13:VAL:HG13	19:Z:17:PHE:HE1	1.86	0.40
1:A:40:THR:HG22	1:A:41:LEU:N	2.36	0.40
1:A:41:LEU:HD21	1:A:122:GLY:HA3	2.04	0.40
1:A:131:TRP:O	1:A:134:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD13	24:A:351:PHO:H143	2.02	0.40
1:A:183:MET:HA	23:A:348:CLA:HMD2	2.03	0.40
2:B:109:LEU:O	2:B:113:TRP:HE3	2.03	0.40
2:B:124:ARG:HG3	23:B:525:CLA:H43	2.03	0.40
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.95	0.40
2:B:327:THR:N	27:B:529:BCR:H292	2.36	0.40
3:C:42:LEU:O	3:C:43:ILE:C	2.59	0.40
3:C:297:TYR:HB3	3:C:302:TYR:HD1	1.86	0.40
3:C:305:THR:CB	3:C:308:GLU:HG3	2.51	0.40
23:C:479:CLA:CMD	23:C:481:CLA:H111	2.52	0.40
4:D:287:VAL:HG12	4:D:287:VAL:O	2.20	0.40
15:U:65:PHE:HD1	15:U:76:ALA:CB	2.34	0.40
1:A:52:PHE:CD1	1:A:81:ALA:CB	3.04	0.40
1:A:110:GLY:O	1:A:112:TYR:N	2.54	0.40
1:A:239:PHE:C	1:A:241:GLN:N	2.73	0.40
2:B:122:LEU:HB3	2:B:123:PHE:H	1.63	0.40
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.86	0.40
3:C:176:VAL:HG11	3:C:238:ILE:HG12	2.04	0.40
3:C:271:TYR:N	3:C:271:TYR:CD2	2.90	0.40
3:C:308:GLU:CG	3:C:361:PHE:CZ	2.98	0.40
3:C:425:TRP:NE1	23:C:475:CLA:HBA2	2.36	0.40
27:C:489:BCR:H342	19:Z:51:VAL:HG13	2.03	0.40
4:D:68:LEU:HA	4:D:68:LEU:HD12	1.84	0.40
10:K:19:ILE:O	10:K:23:PHE:HD1	2.05	0.40
13:O:137:THR:O	13:O:140:THR:CG2	2.67	0.40
13:O:168:TYR:CE1	13:O:172:ILE:CD1	3.01	0.40
15:U:108:ASN:C	15:U:112:PHE:HE1	2.25	0.40
1:A:44:ALA:HB1	24:A:351:PHO:H91	2.02	0.40
1:A:48:PHE:HB2	1:A:115:ILE:HD13	2.03	0.40
1:A:255:PHE:CD2	1:A:264:SER:HA	2.47	0.40
1:A:301:ASN:OD1	3:C:407:VAL:HG11	2.20	0.40
2:B:258:TYR:N	2:B:258:TYR:HD2	2.19	0.40
2:B:333:GLY:HA2	2:B:442:ILE:O	2.22	0.40
3:C:112:PHE:HE2	10:K:6:TYR:CZ	2.39	0.40
3:C:189:TRP:O	3:C:190:ALA:C	2.59	0.40
3:C:240:ILE:HG13	23:C:479:CLA:HBB1	2.03	0.40
4:D:66:SER:O	4:D:71:CYS:SG	2.74	0.40
5:E:12:ILE:HB	28:E:84:HEC:HAD2	2.02	0.40
11:L:36:PHE:CE2	12:M:8:LEU:N	2.90	0.40
13:O:27:ARG:HG3	13:O:29:ALA:CB	2.48	0.40
13:O:201:VAL:HG11	13:O:204:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:10:VAL:HA	16:V:11:PRO:HD3	1.98	0.40
16:V:24:LYS:HE2	16:V:28:GLU:OE2	2.21	0.40
16:V:63:THR:CB	16:V:83:ASP:O	2.67	0.40
16:V:75:TYR:HD2	16:V:79:PRO:HA	1.82	0.40
16:V:81:THR:O	16:V:84:GLY:N	2.54	0.40
1:A:46:ILE:O	1:A:47:CYS:C	2.59	0.40
1:A:243:GLU:O	1:A:244:GLU:HB2	2.22	0.40
2:B:225:LEU:HD23	2:B:229:LEU:HD12	2.03	0.40
2:B:346:PHE:CE2	2:B:399:VAL:HG22	2.57	0.40
3:C:162:GLY:HA3	3:C:248:GLY:O	2.21	0.40
3:C:343:ARG:CB	13:O:78:LEU:CD1	2.99	0.40
4:D:190:ASN:ND2	4:D:193:LEU:CD1	2.85	0.40
23:D:356:CLA:H112	23:D:356:CLA:H151	1.92	0.40
5:E:25:THR:HG21	28:E:84:HEC:C3B	2.51	0.40
13:O:72:THR:HG22	13:O:75:THR:OG1	2.21	0.40
13:O:120:PHE:HA	13:O:219:GLN:HE22	1.86	0.40
19:Z:9:LEU:C	19:Z:11:ALA:N	2.73	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:246:ALA:C	18:n:2035:UNK:O[2_555]	1.76	0.44
13:O:246:ALA:N	18:n:2035:UNK:O[2_555]	1.97	0.23
13:O:246:ALA:O	18:n:2035:UNK:O[2_555]	2.07	0.13
13:O:246:ALA:O	18:n:2035:UNK:CB[2_555]	2.15	0.05
13:O:246:ALA:N	18:n:2035:UNK:C[2_555]	2.17	0.03
13:O:246:ALA:CA	18:n:2035:UNK:O[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	251 (76%)	58 (18%)	22 (7%)	1	11
1	a	331/344 (96%)	253 (76%)	56 (17%)	22 (7%)	1	11
2	B	474/510 (93%)	367 (77%)	84 (18%)	23 (5%)	2	16
2	b	474/510 (93%)	367 (77%)	83 (18%)	24 (5%)	1	16
3	C	419/473 (89%)	326 (78%)	60 (14%)	33 (8%)	1	8
3	c	419/473 (89%)	326 (78%)	62 (15%)	31 (7%)	1	9
4	D	337/352 (96%)	274 (81%)	49 (14%)	14 (4%)	2	19
4	d	337/352 (96%)	270 (80%)	51 (15%)	16 (5%)	2	17
5	E	74/84 (88%)	62 (84%)	10 (14%)	2 (3%)	4	28
5	e	74/84 (88%)	57 (77%)	14 (19%)	3 (4%)	2	20
6	F	31/45 (69%)	23 (74%)	5 (16%)	3 (10%)	0	6
6	f	31/45 (69%)	22 (71%)	6 (19%)	3 (10%)	0	6
7	H	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	1	13
7	h	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	1	13
8	I	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	4	27
8	i	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	1	14
9	J	36/40 (90%)	32 (89%)	3 (8%)	1 (3%)	4	27
9	j	36/40 (90%)	30 (83%)	4 (11%)	2 (6%)	1	14
10	K	35/37 (95%)	27 (77%)	2 (6%)	6 (17%)	0	2
10	k	35/37 (95%)	26 (74%)	3 (9%)	6 (17%)	0	2
11	L	35/37 (95%)	28 (80%)	3 (9%)	4 (11%)	0	5
11	l	35/37 (95%)	27 (77%)	5 (14%)	3 (9%)	0	7
12	M	28/36 (78%)	22 (79%)	5 (18%)	1 (4%)	3	22
12	m	28/36 (78%)	22 (79%)	4 (14%)	2 (7%)	1	10
13	O	244/246 (99%)	180 (74%)	44 (18%)	20 (8%)	1	8
13	o	244/246 (99%)	179 (73%)	45 (18%)	20 (8%)	1	8
14	T	29/32 (91%)	23 (79%)	3 (10%)	3 (10%)	0	6
14	t	29/32 (91%)	22 (76%)	5 (17%)	2 (7%)	1	10
15	U	103/134 (77%)	78 (76%)	14 (14%)	11 (11%)	0	5
15	u	103/134 (77%)	81 (79%)	11 (11%)	11 (11%)	0	5
16	V	135/137 (98%)	111 (82%)	16 (12%)	8 (6%)	1	13
16	v	135/137 (98%)	106 (78%)	22 (16%)	7 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	38/50 (76%)	36 (95%)	1 (3%)	1 (3%)	4	28
17	x	38/50 (76%)	35 (92%)	2 (5%)	1 (3%)	4	28
19	Z	56/62 (90%)	39 (70%)	15 (27%)	2 (4%)	3	22
19	z	56/62 (90%)	40 (71%)	13 (23%)	3 (5%)	1	14
All	All	4984/5446 (92%)	3864 (78%)	801 (16%)	319 (6%)	1	12

All (319) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLY
1	A	228	THR
1	A	242	GLU
1	A	308	ASP
2	B	88	PRO
2	B	126	PRO
2	B	173	GLY
2	B	235	GLU
2	B	326	ARG
2	B	391	SER
3	C	37	ALA
3	C	104	GLU
3	C	137	PRO
3	C	184	GLY
3	C	190	ALA
3	C	192	GLY
3	C	227	VAL
3	C	285	ILE
4	D	218	VAL
4	D	264	LYS
5	E	49	PRO
6	F	17	VAL
7	H	21	ALA
10	K	7	ALA
10	K	8	ILE
11	L	8	GLN
11	L	9	PRO
13	O	76	THR
13	O	77	SER
13	O	101	ILE
13	O	130	GLN
13	O	245	PRO

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Mol	Chain	Res	Type
15	U	40	VAL
15	U	52	GLY
15	U	72	TYR
16	V	38	ALA
17	X	14	PRO
1	a	2090	GLY
1	a	2141	PRO
1	a	2228	THR
2	b	2088	PRO
2	b	2126	PRO
2	b	2173	GLY
2	b	2235	GLU
2	b	2326	ARG
2	b	2391	SER
3	c	2037	ALA
3	c	2104	GLU
3	c	2184	GLY
3	c	2190	ALA
3	c	2191	PRO
3	c	2192	GLY
3	c	2285	ILE
4	d	2218	VAL
4	d	2264	LYS
5	e	2049	PRO
6	f	2017	VAL
7	h	2021	ALA
10	k	2007	ALA
10	k	2008	ILE
11	l	2009	PRO
13	o	2076	THR
13	o	2077	SER
13	o	2130	GLN
13	o	2245	PRO
15	u	2040	VAL
15	u	2051	TYR
15	u	2052	GLY
15	u	2072	TYR
16	v	2038	ALA
17	x	2014	PRO
1	A	32	TRP
1	A	141	PRO
1	A	160	ILE

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	239	PHE
1	A	243	GLU
1	A	317	TRP
1	A	335	ASN
2	B	186	GLY
2	B	201	HIS
2	B	230	ARG
2	B	328	GLY
2	B	396	GLY
3	C	43	ILE
3	C	183	GLY
3	C	219	GLY
3	C	295	THR
3	C	453	ALA
4	D	109	GLY
4	D	156	VAL
4	D	219	GLU
4	D	292	ASN
5	E	10	SER
6	F	40	GLN
7	H	23	GLY
10	K	11	PRO
10	K	17	PRO
13	O	56	PRO
13	O	131	PRO
13	O	206	GLY
13	O	216	GLU
14	T	4	ILE
15	U	48	GLY
15	U	51	TYR
15	U	63	ALA
15	U	73	PRO
15	U	120	ALA
15	U	121	LEU
15	U	125	GLY
15	U	131	GLY
16	V	82	TYR
19	Z	32	ASP
1	a	2032	TRP
1	a	2160	ILE
1	a	2225	ARG

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Mol	Chain	Res	Type
1	a	2239	PHE
1	a	2242	GLU
1	a	2243	GLU
1	a	2308	ASP
2	b	2186	GLY
2	b	2201	HIS
2	b	2230	ARG
2	b	2328	GLY
2	b	2396	GLY
3	c	2137	PRO
3	c	2183	GLY
3	c	2219	GLY
3	c	2227	VAL
3	c	2295	THR
3	c	2453	ALA
4	d	2109	GLY
4	d	2219	GLU
4	d	2292	ASN
4	d	2299	ILE
5	e	2010	SER
6	f	2040	GLN
7	h	2023	GLY
10	k	2011	PRO
11	l	2008	GLN
13	o	2056	PRO
13	o	2078	LEU
13	o	2101	ILE
13	o	2161	GLY
13	o	2206	GLY
14	t	2004	ILE
15	u	2048	GLY
15	u	2063	ALA
15	u	2073	PRO
15	u	2120	ALA
15	u	2121	LEU
15	u	2131	GLY
16	v	2082	TYR
1	A	215	HIS
2	B	187	PRO
2	B	222	PRO
2	B	223	GLN
2	B	312	TYR

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Mol	Chain	Res	Type
2	B	319	PRO
2	B	361	ALA
3	C	80	PRO
3	C	110	PRO
3	C	191	PRO
3	C	223	TRP
3	C	334	PRO
3	C	355	THR
3	C	415	ASN
3	C	454	GLY
4	D	260	ALA
4	D	299	ILE
7	H	22	PRO
9	J	28	PHE
13	O	28	GLY
13	O	78	LEU
13	O	149	PRO
13	O	161	GLY
16	V	16	GLY
16	V	99	ASP
1	a	2191	ASN
1	a	2259	ILE
1	a	2317	TRP
2	b	2187	PRO
2	b	2222	PRO
2	b	2223	GLN
2	b	2319	PRO
2	b	2361	ALA
3	c	2110	PRO
3	c	2152	LYS
3	c	2223	TRP
3	c	2355	THR
3	c	2413	GLU
3	c	2415	ASN
4	d	2239	GLN
4	d	2260	ALA
4	d	2343	GLU
6	f	2019	TRP
7	h	2022	PRO
9	j	2028	PHE
10	k	2017	PRO
13	o	2131	PRO

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Mol	Chain	Res	Type
13	o	2149	PRO
13	o	2180	GLU
13	o	2216	GLU
15	u	2125	GLY
16	v	2016	GLY
19	z	2032	ASP
1	A	167	SER
1	A	191	ASN
1	A	208	GLY
1	A	259	ILE
1	A	300	PHE
1	A	301	ASN
1	A	334	ARG
3	C	46	SER
3	C	85	GLY
3	C	152	LYS
3	C	195	ASP
3	C	298	PRO
3	C	420	VAL
4	D	132	ILE
4	D	166	SER
4	D	239	GLN
4	D	343	GLU
13	O	114	GLU
14	T	27	PRO
16	V	133	GLY
19	Z	29	SER
1	a	2167	SER
1	a	2208	GLY
1	a	2215	HIS
1	a	2300	PHE
1	a	2301	ASN
2	b	2188	ASP
2	b	2312	TYR
3	c	2043	ILE
3	c	2334	PRO
3	c	2411	ALA
3	c	2420	VAL
4	d	2166	SER
13	o	2047	PRO
13	o	2114	GLU
14	t	2027	PRO

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Mol	Chain	Res	Type
16	v	2021	LEU
16	v	2102	PRO
16	v	2131	GLY
2	B	188	ASP
3	C	413	GLU
4	D	131	GLU
6	F	19	TRP
8	I	32	PRO
10	K	16	LEU
13	O	47	PRO
13	O	180	GLU
16	V	102	PRO
16	V	107	LEU
16	V	131	GLY
1	a	2116	ILE
1	a	2244	GLU
2	b	2047	PRO
3	c	2046	SER
3	c	2080	PRO
3	c	2454	GLY
4	d	2101	PHE
5	e	2057	GLN
10	k	2016	LEU
12	m	2005	GLN
13	o	2028	GLY
16	v	2133	GLY
19	z	2029	SER
1	A	116	ILE
2	B	47	PRO
3	C	380	ILE
11	L	2	GLU
14	T	3	THR
3	c	2085	GLY
3	c	2195	ASP
3	c	2298	PRO
3	c	2338	GLY
4	d	2113	PHE
4	d	2132	ILE
11	l	2002	GLU
12	m	2017	VAL
13	o	2175	PRO
1	A	63	ILE

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Mol	Chain	Res	Type
2	B	16	PRO
3	C	101	PRO
3	C	117	VAL
13	O	159	PRO
13	O	244	GLU
1	a	2046	ILE
1	a	2063	ILE
2	b	2264	PRO
13	o	2159	PRO
2	B	211	ILE
2	B	322	GLY
3	C	338	GLY
13	O	122	VAL
2	b	2016	PRO
2	b	2211	ILE
2	b	2322	GLY
13	o	2122	VAL
10	K	2	LEU
11	L	4	ASN
2	b	2008	VAL
9	j	2016	VAL
2	B	8	VAL
3	C	410	VAL
4	D	275	PRO
12	M	17	VAL
3	c	2380	ILE
4	d	2156	VAL
8	i	2008	VAL
8	i	2032	PRO
10	k	2002	LEU
13	o	2244	GLU
13	O	175	PRO
4	d	2095	PRO
4	d	2275	PRO
19	z	2013	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	244 (90%)	26 (10%)	7	28
1	a	270/280 (96%)	249 (92%)	21 (8%)	10	34
2	B	377/407 (93%)	355 (94%)	22 (6%)	17	44
2	b	377/407 (93%)	355 (94%)	22 (6%)	17	44
3	C	326/374 (87%)	306 (94%)	20 (6%)	15	43
3	c	326/374 (87%)	307 (94%)	19 (6%)	17	44
4	D	275/283 (97%)	257 (94%)	18 (6%)	14	41
4	d	275/283 (97%)	253 (92%)	22 (8%)	10	34
5	E	68/73 (93%)	65 (96%)	3 (4%)	24	53
5	e	68/73 (93%)	64 (94%)	4 (6%)	16	44
6	F	27/39 (69%)	25 (93%)	2 (7%)	11	36
6	f	27/39 (69%)	24 (89%)	3 (11%)	5	23
7	H	44/55 (80%)	41 (93%)	3 (7%)	13	39
7	h	44/55 (80%)	42 (96%)	2 (4%)	23	53
8	I	35/35 (100%)	31 (89%)	4 (11%)	4	22
8	i	35/35 (100%)	33 (94%)	2 (6%)	17	45
9	J	26/28 (93%)	25 (96%)	1 (4%)	28	57
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	13	40
10	k	30/30 (100%)	30 (100%)	0	100	100
11	L	35/35 (100%)	31 (89%)	4 (11%)	4	22
11	l	35/35 (100%)	31 (89%)	4 (11%)	4	22
12	M	27/33 (82%)	26 (96%)	1 (4%)	29	58
12	m	27/33 (82%)	26 (96%)	1 (4%)	29	58
13	O	208/208 (100%)	187 (90%)	21 (10%)	6	26
13	o	208/208 (100%)	190 (91%)	18 (9%)	8	31
14	T	28/29 (97%)	28 (100%)	0	100	100
14	t	28/29 (97%)	28 (100%)	0	100	100
15	U	89/112 (80%)	85 (96%)	4 (4%)	23	53
15	u	89/112 (80%)	84 (94%)	5 (6%)	17	45
16	V	117/117 (100%)	112 (96%)	5 (4%)	25	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/117 (100%)	112 (96%)	5 (4%)	25	54
17	X	33/42 (79%)	30 (91%)	3 (9%)	7	30
17	x	33/42 (79%)	29 (88%)	4 (12%)	4	20
19	Z	48/52 (92%)	42 (88%)	6 (12%)	3	19
19	z	48/52 (92%)	46 (96%)	2 (4%)	25	54
All	All	4126/4464 (92%)	3847 (93%)	279 (7%)	13	39

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	25	ASP
1	A	27	ARG
1	A	29	TYR
1	A	52	PHE
1	A	70	SER
1	A	84	PRO
1	A	162	PRO
1	A	170	ASP
1	A	172	MET
1	A	177	SER
1	A	180	PHE
1	A	183	MET
1	A	187	GLN
1	A	212	CYS
1	A	214	MET
1	A	237	TYR
1	A	269	ARG
1	A	284	TRP
1	A	295	PHE
1	A	298	ASN
1	A	301	ASN
1	A	317	TRP
1	A	325	ASN
1	A	335	ASN
1	A	342	ASP
2	B	8	VAL
2	B	48	SER
2	B	57	ARG
2	B	130	GLU

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Mol	Chain	Res	Type
2	B	139	PHE
2	B	167	TRP
2	B	216	HIS
2	B	240	SER
2	B	246	PHE
2	B	255	THR
2	B	285	ASN
2	B	286	ARG
2	B	311	PHE
2	B	318	ASN
2	B	334	ASP
2	B	340	TRP
2	B	362	PHE
2	B	372	ASP
2	B	385	ARG
2	B	402	TYR
2	B	409	GLN
2	B	479	PHE
3	C	110	PRO
3	C	127	PHE
3	C	139	THR
3	C	149	TYR
3	C	198	VAL
3	C	201	ASN
3	C	264	PHE
3	C	289	PHE
3	C	290	VAL
3	C	292	PHE
3	C	293	ASN
3	C	294	ASN
3	C	295	THR
3	C	313	GLN
3	C	321	ASP
3	C	340	TYR
3	C	343	ARG
3	C	368	PRO
3	C	400	PRO
3	C	443	TRP
4	D	29	PHE
4	D	32	TRP
4	D	58	TRP
4	D	61	HIS

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Mol	Chain	Res	Type
4	D	73	PHE
4	D	91	LEU
4	D	142	ASN
4	D	168	PHE
4	D	180	ARG
4	D	188	PHE
4	D	192	THR
4	D	211	CYS
4	D	220	ASN
4	D	254	SER
4	D	261	PHE
4	D	262	SER
4	D	336	HIS
4	D	340	VAL
5	E	16	VAL
5	E	30	PHE
5	E	49	PRO
6	F	12	TYR
6	F	31	PHE
7	H	26	THR
7	H	48	TYR
7	H	57	VAL
8	I	16	VAL
8	I	18	LEU
8	I	27	ASP
8	I	30	ARG
9	J	38	SER
10	K	6	TYR
10	K	36	PHE
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
11	L	36	PHE
12	M	28	GLN
13	O	3	GLN
13	O	21	THR
13	O	34	SER
13	O	39	ARG
13	O	46	GLN
13	O	47	PRO
13	O	65	PHE
13	O	68	THR

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Mol	Chain	Res	Type
13	O	104	GLN
13	O	110	MET
13	O	126	VAL
13	O	142	PHE
13	O	147	ASN
13	O	162	ARG
13	O	166	SER
13	O	174	LEU
13	O	190	PHE
13	O	193	THR
13	O	219	GLN
13	O	225	MET
13	O	245	PRO
15	U	51	TYR
15	U	59	ASN
15	U	61	ASN
15	U	132	LEU
16	V	4	THR
16	V	40	CYS
16	V	55	ARG
16	V	78	ASN
16	V	130	TRP
17	X	13	THR
17	X	14	PRO
17	X	47	GLN
19	Z	5	PHE
19	Z	32	ASP
19	Z	34	ASP
19	Z	41	PHE
19	Z	42	LEU
19	Z	51	VAL
1	a	2015	GLU
1	a	2024	THR
1	a	2025	ASP
1	a	2027	ARG
1	a	2029	TYR
1	a	2033	PHE
1	a	2040	THR
1	a	2045	THR
1	a	2070	SER
1	a	2111	PRO
1	a	2180	PHE

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Mol	Chain	Res	Type
1	a	2187	GLN
1	a	2237	TYR
1	a	2269	ARG
1	a	2278	TRP
1	a	2284	TRP
1	a	2286	THR
1	a	2295	PHE
1	a	2317	TRP
1	a	2335	ASN
1	a	2342	ASP
2	b	2008	VAL
2	b	2048	SER
2	b	2057	ARG
2	b	2130	GLU
2	b	2139	PHE
2	b	2167	TRP
2	b	2216	HIS
2	b	2240	SER
2	b	2246	PHE
2	b	2255	THR
2	b	2286	ARG
2	b	2311	PHE
2	b	2318	ASN
2	b	2334	ASP
2	b	2340	TRP
2	b	2362	PHE
2	b	2372	ASP
2	b	2385	ARG
2	b	2392	PHE
2	b	2402	TYR
2	b	2409	GLN
2	b	2479	PHE
3	c	2046	SER
3	c	2110	PRO
3	c	2127	PHE
3	c	2139	THR
3	c	2149	TYR
3	c	2198	VAL
3	c	2201	ASN
3	c	2264	PHE
3	c	2285	ILE
3	c	2289	PHE

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Mol	Chain	Res	Type
3	c	2292	PHE
3	c	2293	ASN
3	c	2294	ASN
3	c	2304	PRO
3	c	2310	SER
3	c	2321	ASP
3	c	2340	TYR
3	c	2403	SER
3	c	2443	TRP
4	d	2029	PHE
4	d	2032	TRP
4	d	2058	TRP
4	d	2061	HIS
4	d	2073	PHE
4	d	2081	PRO
4	d	2091	LEU
4	d	2130	PHE
4	d	2147	SER
4	d	2165	SER
4	d	2168	PHE
4	d	2180	ARG
4	d	2188	PHE
4	d	2192	THR
4	d	2211	CYS
4	d	2220	ASN
4	d	2235	PHE
4	d	2254	SER
4	d	2261	PHE
4	d	2262	SER
4	d	2336	HIS
4	d	2350	ASN
5	e	2030	PHE
5	e	2049	PRO
5	e	2050	ARG
5	e	2053	SER
6	f	2012	TYR
6	f	2031	PHE
6	f	2043	GLN
7	h	2024	TRP
7	h	2026	THR
8	i	2027	ASP
8	i	2030	ARG

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Mol	Chain	Res	Type
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
11	l	2036	PHE
12	m	2028	GLN
13	o	2005	LEU
13	o	2006	THR
13	o	2021	THR
13	o	2039	ARG
13	o	2047	PRO
13	o	2060	ARG
13	o	2068	THR
13	o	2103	PHE
13	o	2104	GLN
13	o	2110	MET
13	o	2147	ASN
13	o	2159	PRO
13	o	2166	SER
13	o	2174	LEU
13	o	2193	THR
13	o	2225	MET
13	o	2239	PHE
13	o	2245	PRO
15	u	2051	TYR
15	u	2059	ASN
15	u	2061	ASN
15	u	2128	TYR
15	u	2132	LEU
16	v	2004	THR
16	v	2040	CYS
16	v	2050	PRO
16	v	2055	ARG
16	v	2093	PRO
17	x	2011	THR
17	x	2013	THR
17	x	2014	PRO
17	x	2047	GLN
19	z	2005	PHE
19	z	2051	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	199	GLN
1	A	296	ASN
1	A	301	ASN
1	A	303	ASN
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
2	B	233	ASN
2	B	285	ASN
2	B	318	ASN
2	B	331	ASN
2	B	374	ASN
2	B	395	GLN
2	B	438	ASN
3	C	39	ASN
3	C	201	ASN
3	C	294	ASN
3	C	311	GLN
3	C	378	ASN
4	D	83	ASN
4	D	87	HIS
4	D	106	GLN
4	D	129	GLN
4	D	164	GLN
4	D	186	GLN
4	D	255	GLN
4	D	263	ASN
4	D	322	ASN
4	D	338	ASN
4	D	350	ASN
5	E	81	GLN
6	F	40	GLN
6	F	43	GLN
10	K	31	GLN
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
12	M	4	ASN

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Mol	Chain	Res	Type
12	M	28	GLN
13	O	36	GLN
13	O	46	GLN
13	O	61	GLN
13	O	124	ASN
13	O	132	ASN
13	O	147	ASN
13	O	155	ASN
13	O	200	ASN
13	O	219	GLN
15	U	59	ASN
15	U	61	ASN
15	U	82	ASN
15	U	130	ASN
16	V	25	GLN
19	Z	6	GLN
1	a	2019	ASN
1	a	2092	HIS
1	a	2165	GLN
1	a	2187	GLN
1	a	2199	GLN
1	a	2296	ASN
1	a	2301	ASN
1	a	2303	ASN
1	a	2322	ASN
1	a	2325	ASN
1	a	2335	ASN
2	b	2285	ASN
2	b	2318	ASN
2	b	2331	ASN
2	b	2343	HIS
2	b	2374	ASN
2	b	2395	GLN
2	b	2438	ASN
3	c	2039	ASN
3	c	2201	ASN
3	c	2294	ASN
3	c	2322	GLN
3	c	2405	ASN
4	d	2083	ASN
4	d	2087	HIS
4	d	2129	GLN

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Mol	Chain	Res	Type
4	d	2142	ASN
4	d	2164	GLN
4	d	2186	GLN
4	d	2190	ASN
4	d	2250	ASN
4	d	2255	GLN
4	d	2263	ASN
4	d	2322	ASN
4	d	2338	ASN
4	d	2350	ASN
6	f	2040	GLN
6	f	2043	GLN
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
12	m	2004	ASN
12	m	2028	GLN
13	o	2036	GLN
13	o	2046	GLN
13	o	2061	GLN
13	o	2124	ASN
13	o	2147	ASN
13	o	2155	ASN
13	o	2236	GLN
15	u	2059	ASN
15	u	2061	ASN
15	u	2108	ASN
15	u	2111	HIS
15	u	2130	ASN
16	v	2078	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 2 are monoatomic - leaving 106 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	522	2	63,73,73	1.84	10 (15%)	74,113,113	2.01	13 (17%)
23	CLA	B	517	2	63,73,73	1.65	9 (14%)	74,113,113	2.06	12 (16%)
23	CLA	c	2487	-	63,73,73	1.94	13 (20%)	74,113,113	1.94	14 (18%)
25	PL9	A	353	-	45,45,55	2.32	19 (42%)	56,57,69	2.18	17 (30%)
25	PL9	d	2358	-	45,45,55	2.37	19 (42%)	56,57,69	1.75	12 (21%)
23	CLA	b	2523	2	63,73,73	1.92	10 (15%)	74,113,113	2.15	12 (16%)
23	CLA	C	476	3	63,73,73	1.87	8 (12%)	74,113,113	2.02	13 (17%)
23	CLA	d	2355	-	63,73,73	1.64	8 (12%)	74,113,113	2.23	15 (20%)
23	CLA	C	474	3	63,73,73	1.72	9 (14%)	74,113,113	2.11	13 (17%)
23	CLA	c	2485	-	63,73,73	1.70	10 (15%)	74,113,113	2.01	12 (16%)
22	OEC	A	347	1,21,3	0,13,13	-	-	-	-	-
23	CLA	D	356	4	63,73,73	1.88	13 (20%)	74,113,113	2.03	10 (13%)
23	CLA	c	2478	3	63,73,73	1.83	8 (12%)	74,113,113	2.14	15 (20%)
27	BCR	C	489	-	41,41,41	1.78	7 (17%)	56,56,56	2.00	16 (28%)
23	CLA	b	2522	2	63,73,73	1.72	11 (17%)	74,113,113	2.01	13 (17%)
27	BCR	F	48	-	41,41,41	2.03	7 (17%)	56,56,56	2.55	22 (39%)
27	BCR	b	2527	-	41,41,41	1.92	7 (17%)	56,56,56	2.24	20 (35%)
23	CLA	b	2515	2	63,73,73	1.70	12 (19%)	74,113,113	2.06	15 (20%)
24	PHO	A	351	-	50,69,69	1.14	4 (8%)	48,99,99	1.65	12 (25%)
23	CLA	A	349	-	63,73,73	1.72	9 (14%)	74,113,113	2.31	14 (18%)
23	CLA	B	527	-	63,73,73	2.00	11 (17%)	74,113,113	2.07	14 (18%)
23	CLA	C	480	3	63,73,73	1.79	8 (12%)	74,113,113	1.95	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	482	3	63,73,73	2.01	9 (14%)	74,113,113	2.08	11 (14%)
23	CLA	c	2481	3	63,73,73	1.86	10 (15%)	74,113,113	2.22	13 (17%)
25	PL9	a	2352	-	45,45,55	2.32	18 (40%)	56,57,69	2.21	17 (30%)
24	PHO	a	2350	-	50,69,69	1.22	6 (12%)	48,99,99	1.69	12 (25%)
23	CLA	C	486	3	63,73,73	1.82	9 (14%)	74,113,113	1.99	13 (17%)
28	HEC	E	84	5,6	32,50,50	2.35	14 (43%)	30,82,82	2.86	15 (50%)
23	CLA	C	483	3	63,73,73	1.95	12 (19%)	74,113,113	2.21	13 (17%)
28	HEC	V	138	16	32,50,50	6.15	21 (65%)	30,82,82	3.12	11 (36%)
23	CLA	B	511	2	63,73,73	1.80	14 (22%)	74,113,113	2.26	15 (20%)
23	CLA	c	2476	3	63,73,73	1.97	10 (15%)	74,113,113	1.97	12 (16%)
27	BCR	B	528	-	41,41,41	2.03	7 (17%)	56,56,56	2.23	21 (37%)
23	CLA	d	2357	4	63,73,73	1.95	9 (14%)	74,113,113	2.03	10 (13%)
23	CLA	b	2519	2	63,73,73	1.86	14 (22%)	74,113,113	2.39	11 (14%)
23	CLA	b	2516	2	63,73,73	2.17	15 (23%)	74,113,113	2.04	14 (18%)
23	CLA	B	515	2	63,73,73	1.76	8 (12%)	74,113,113	2.04	16 (21%)
23	CLA	c	2474	3	63,73,73	1.71	10 (15%)	74,113,113	2.06	11 (14%)
21	BCT	d	2353	20	3,3,3	1.94	1 (33%)	2,3,3	0.13	0
28	HEC	v	2138	16	32,50,50	3.07	17 (53%)	30,82,82	3.85	14 (46%)
23	CLA	C	484	3	63,73,73	2.06	10 (15%)	74,113,113	1.96	12 (16%)
27	BCR	k	2050	-	41,41,41	2.02	15 (36%)	56,56,56	1.92	17 (30%)
23	CLA	b	2525	2	63,73,73	1.94	11 (17%)	74,113,113	2.04	9 (12%)
23	CLA	b	2524	-	63,73,73	1.67	11 (17%)	74,113,113	2.22	14 (18%)
23	CLA	b	2513	2	63,73,73	1.97	10 (15%)	74,113,113	2.36	17 (22%)
25	PL9	D	357	-	45,45,55	2.32	18 (40%)	56,57,69	1.75	12 (21%)
27	BCR	C	488	-	41,41,41	1.82	9 (21%)	56,56,56	2.02	18 (32%)
23	CLA	B	524	-	63,73,73	1.71	10 (15%)	74,113,113	2.23	12 (16%)
23	CLA	C	481	3	63,73,73	1.76	9 (14%)	74,113,113	2.22	10 (13%)
23	CLA	B	525	2	63,73,73	1.86	11 (17%)	74,113,113	2.00	9 (12%)
23	CLA	C	479	3	63,73,73	1.78	9 (14%)	74,113,113	2.24	18 (24%)
27	BCR	K	50	-	41,41,41	1.97	14 (34%)	56,56,56	1.95	17 (30%)
27	BCR	c	2489	-	41,41,41	1.97	8 (19%)	56,56,56	2.02	18 (32%)
23	CLA	C	478	3	63,73,73	1.76	9 (14%)	74,113,113	2.11	14 (18%)
23	CLA	c	2482	3	63,73,73	2.01	12 (19%)	74,113,113	2.00	12 (16%)
27	BCR	j	2053	-	41,41,41	2.19	8 (19%)	56,56,56	2.15	21 (37%)
23	CLA	B	520	2	63,73,73	1.88	11 (17%)	74,113,113	2.50	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	487	-	63,73,73	1.85	13 (20%)	74,113,113	1.97	14 (18%)
27	BCR	d	2360	-	41,41,41	2.00	7 (17%)	56,56,56	2.50	21 (37%)
23	CLA	a	2351	1	63,73,73	1.82	10 (15%)	74,113,113	2.03	12 (16%)
23	CLA	B	516	2	63,73,73	2.16	13 (20%)	74,113,113	2.03	13 (17%)
23	CLA	c	2480	3	63,73,73	1.78	7 (11%)	74,113,113	1.97	10 (13%)
23	CLA	A	352	1	63,73,73	1.76	11 (17%)	74,113,113	2.02	12 (16%)
23	CLA	C	475	-	63,73,73	2.00	14 (22%)	74,113,113	2.06	11 (14%)
23	CLA	a	2349	-	63,73,73	1.86	8 (12%)	74,113,113	1.82	12 (16%)
24	PHO	d	2356	-	50,69,69	1.16	5 (10%)	48,99,99	1.72	14 (29%)
27	BCR	c	2488	-	41,41,41	2.00	9 (21%)	56,56,56	2.01	19 (33%)
23	CLA	b	2512	2	63,73,73	1.90	10 (15%)	74,113,113	2.17	13 (17%)
27	BCR	b	2528	-	41,41,41	2.09	10 (24%)	56,56,56	2.25	22 (39%)
23	CLA	b	2517	2	63,73,73	1.72	11 (17%)	74,113,113	2.02	11 (14%)
23	CLA	b	2521	2	63,73,73	1.85	12 (19%)	74,113,113	1.77	10 (13%)
23	CLA	a	2348	1	63,73,73	1.74	10 (15%)	74,113,113	1.90	13 (17%)
23	CLA	D	354	4	63,73,73	1.93	10 (15%)	74,113,113	2.02	11 (14%)
23	CLA	c	2486	3	63,73,73	1.83	8 (12%)	74,113,113	2.03	14 (18%)
26	LMT	d	2359	-	36,36,36	1.36	4 (11%)	47,47,47	1.93	7 (14%)
23	CLA	B	512	2	63,73,73	1.95	9 (14%)	74,113,113	2.11	10 (13%)
21	BCT	D	353	20	3,3,3	2.10	1 (33%)	2,3,3	0.22	0
27	BCR	B	529	-	41,41,41	2.12	8 (19%)	56,56,56	2.32	21 (37%)
23	CLA	B	521	2	63,73,73	1.80	10 (15%)	74,113,113	1.77	10 (13%)
23	CLA	b	2518	2	63,73,73	1.89	11 (17%)	74,113,113	2.10	10 (13%)
26	LMT	B	526	-	36,36,36	1.35	4 (11%)	47,47,47	1.93	8 (17%)
23	CLA	d	2354	4	63,73,73	1.87	10 (15%)	74,113,113	2.05	11 (14%)
23	CLA	B	523	2	63,73,73	1.83	8 (12%)	74,113,113	2.15	11 (14%)
23	CLA	b	2511	2	63,73,73	1.79	11 (17%)	74,113,113	2.25	14 (18%)
27	BCR	J	53	-	41,41,41	1.94	6 (14%)	56,56,56	2.14	21 (37%)
23	CLA	c	2477	3	63,73,73	1.87	11 (17%)	74,113,113	2.26	15 (20%)
23	CLA	b	2520	2	63,73,73	1.96	12 (19%)	74,113,113	2.52	13 (17%)
23	CLA	B	514	-	63,73,73	1.75	12 (19%)	74,113,113	2.07	14 (18%)
23	CLA	A	348	1	63,73,73	1.67	10 (15%)	74,113,113	1.91	14 (18%)
21	BCT	A	346	22	3,3,3	1.14	0	2,3,3	0.80	0
23	CLA	b	2514	-	63,73,73	1.72	12 (19%)	74,113,113	2.08	14 (18%)
23	CLA	c	2475	-	63,73,73	2.00	14 (22%)	74,113,113	1.98	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	513	2	63,73,73	2.02	11 (17%)	74,113,113	2.35	16 (21%)
23	CLA	C	485	-	63,73,73	1.67	10 (15%)	74,113,113	1.97	14 (18%)
23	CLA	b	2526	-	63,73,73	1.91	10 (15%)	74,113,113	2.09	15 (20%)
23	CLA	B	518	2	63,73,73	1.76	7 (11%)	74,113,113	2.12	12 (16%)
28	HEC	e	2084	5,6	32,50,50	2.41	13 (40%)	30,82,82	2.69	12 (40%)
23	CLA	c	2484	3	63,73,73	1.93	11 (17%)	74,113,113	1.98	11 (14%)
22	OEC	a	2347	1,21,3	0,13,13	-	-	-	-	-
23	CLA	C	477	3	63,73,73	1.92	11 (17%)	74,113,113	2.27	15 (20%)
24	PHO	D	355	-	50,69,69	1.07	4 (8%)	48,99,99	1.77	14 (29%)
21	BCT	a	2346	22	3,3,3	1.80	1 (33%)	2,3,3	1.34	0
23	CLA	A	350	-	63,73,73	1.90	8 (12%)	74,113,113	1.87	12 (16%)
23	CLA	B	519	2	63,73,73	1.88	15 (23%)	74,113,113	2.47	13 (17%)
23	CLA	c	2483	3	63,73,73	1.97	10 (15%)	74,113,113	2.19	13 (17%)
23	CLA	c	2479	3	63,73,73	1.77	10 (15%)	74,113,113	2.28	18 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	522	2	1/1/15/20	14/37/115/115	-
23	CLA	B	517	2	1/1/15/20	13/37/115/115	-
23	CLA	c	2487	-	1/1/15/20	12/37/115/115	-
25	PL9	A	353	-	-	10/41/61/73	0/1/1/1
25	PL9	d	2358	-	-	12/41/61/73	0/1/1/1
23	CLA	b	2523	2	1/1/15/20	8/37/115/115	-
23	CLA	C	476	3	1/1/15/20	10/37/115/115	-
23	CLA	d	2355	-	1/1/15/20	12/37/115/115	-
23	CLA	C	474	3	1/1/15/20	11/37/115/115	-
23	CLA	c	2485	-	1/1/15/20	12/37/115/115	-
27	BCR	b	2527	-	-	5/29/63/63	0/2/2/2
23	CLA	D	356	4	1/1/15/20	4/37/115/115	-
23	CLA	c	2478	3	1/1/15/20	14/37/115/115	-
27	BCR	C	489	-	-	2/29/63/63	0/2/2/2
23	CLA	b	2522	2	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	F	48	-	-	3/29/63/63	0/2/2/2
22	OEC	A	347	1,21,3	-	-	0/6/5/5
23	CLA	b	2515	2	1/1/15/20	15/37/115/115	-
24	PHO	A	351	-	-	9/37/103/103	0/5/6/6
23	CLA	A	349	-	1/1/15/20	12/37/115/115	-
23	CLA	B	527	-	1/1/15/20	13/37/115/115	-
23	CLA	C	480	3	1/1/15/20	14/37/115/115	-
23	CLA	C	482	3	1/1/15/20	9/37/115/115	-
23	CLA	c	2481	3	1/1/15/20	6/37/115/115	-
25	PL9	a	2352	-	-	10/41/61/73	0/1/1/1
24	PHO	a	2350	-	-	9/37/103/103	0/5/6/6
23	CLA	C	486	3	1/1/15/20	5/37/115/115	-
28	HEC	E	84	5,6	-	2/10/54/54	-
23	CLA	C	483	3	1/1/15/20	10/37/115/115	-
28	HEC	V	138	16	-	2/10/54/54	-
23	CLA	B	511	2	1/1/15/20	14/37/115/115	-
23	CLA	c	2476	3	1/1/15/20	10/37/115/115	-
27	BCR	B	528	-	-	5/29/63/63	0/2/2/2
23	CLA	d	2357	4	1/1/15/20	4/37/115/115	-
23	CLA	b	2519	2	1/1/15/20	6/37/115/115	-
23	CLA	b	2516	2	1/1/15/20	6/37/115/115	-
23	CLA	B	515	2	1/1/15/20	15/37/115/115	-
23	CLA	c	2474	3	1/1/15/20	11/37/115/115	-
28	HEC	v	2138	16	-	4/10/54/54	-
23	CLA	C	484	3	1/1/15/20	14/37/115/115	-
27	BCR	k	2050	-	-	3/29/63/63	0/2/2/2
23	CLA	b	2525	2	1/1/15/20	11/37/115/115	-
23	CLA	b	2524	-	1/1/15/20	13/37/115/115	-
23	CLA	b	2513	2	1/1/15/20	11/37/115/115	-
25	PL9	D	357	-	-	12/41/61/73	0/1/1/1
27	BCR	C	488	-	-	6/29/63/63	0/2/2/2
23	CLA	B	524	-	1/1/15/20	13/37/115/115	-
23	CLA	C	481	3	1/1/15/20	7/37/115/115	-
23	CLA	B	525	2	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	479	3	1/1/15/20	10/37/115/115	-
27	BCR	K	50	-	-	3/29/63/63	0/2/2/2
27	BCR	c	2489	-	-	2/29/63/63	0/2/2/2
23	CLA	C	478	3	1/1/15/20	14/37/115/115	-
23	CLA	c	2482	3	1/1/15/20	10/37/115/115	-
27	BCR	j	2053	-	-	4/29/63/63	0/2/2/2
23	CLA	B	520	2	1/1/15/20	3/37/115/115	-
23	CLA	C	487	-	1/1/15/20	13/37/115/115	-
27	BCR	d	2360	-	-	4/29/63/63	0/2/2/2
23	CLA	a	2351	1	1/1/15/20	7/37/115/115	-
23	CLA	B	516	2	1/1/15/20	6/37/115/115	-
23	CLA	c	2480	3	1/1/15/20	14/37/115/115	-
23	CLA	A	352	1	1/1/15/20	7/37/115/115	-
23	CLA	C	475	-	1/1/15/20	9/37/115/115	-
23	CLA	a	2349	-	1/1/15/20	6/37/115/115	-
24	PHO	d	2356	-	-	11/37/103/103	0/5/6/6
27	BCR	c	2488	-	-	5/29/63/63	0/2/2/2
23	CLA	b	2512	2	1/1/15/20	10/37/115/115	-
27	BCR	b	2528	-	-	6/29/63/63	0/2/2/2
23	CLA	b	2517	2	1/1/15/20	13/37/115/115	-
23	CLA	b	2521	2	1/1/15/20	4/37/115/115	-
23	CLA	a	2348	1	1/1/15/20	12/37/115/115	-
23	CLA	D	354	4	1/1/15/20	8/37/115/115	-
23	CLA	c	2486	3	1/1/15/20	5/37/115/115	-
26	LMT	d	2359	-	-	8/21/61/61	0/2/2/2
23	CLA	B	512	2	1/1/15/20	10/37/115/115	-
27	BCR	B	529	-	-	6/29/63/63	0/2/2/2
23	CLA	B	521	2	1/1/15/20	4/37/115/115	-
23	CLA	b	2518	2	1/1/15/20	10/37/115/115	-
26	LMT	B	526	-	-	8/21/61/61	0/2/2/2
23	CLA	d	2354	4	1/1/15/20	8/37/115/115	-
23	CLA	B	523	2	1/1/15/20	8/37/115/115	-
23	CLA	b	2511	2	1/1/15/20	14/37/115/115	-
27	BCR	J	53	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	2477	3	1/1/15/20	15/37/115/115	-
23	CLA	b	2520	2	1/1/15/20	5/37/115/115	-
23	CLA	B	514	-	1/1/15/20	14/37/115/115	-
23	CLA	A	348	1	1/1/15/20	12/37/115/115	-
23	CLA	b	2514	-	1/1/15/20	14/37/115/115	-
23	CLA	c	2475	-	1/1/15/20	10/37/115/115	-
23	CLA	B	513	2	1/1/15/20	12/37/115/115	-
23	CLA	C	485	-	1/1/15/20	12/37/115/115	-
23	CLA	b	2526	-	1/1/15/20	13/37/115/115	-
23	CLA	B	518	2	1/1/15/20	10/37/115/115	-
28	HEC	e	2084	5,6	-	2/10/54/54	-
23	CLA	c	2484	3	1/1/15/20	15/37/115/115	-
22	OEC	a	2347	1,21,3	-	-	0/6/5/5
23	CLA	C	477	3	1/1/15/20	15/37/115/115	-
24	PHO	D	355	-	-	13/37/103/103	0/5/6/6
23	CLA	A	350	-	1/1/15/20	7/37/115/115	-
23	CLA	B	519	2	1/1/15/20	6/37/115/115	-
23	CLA	c	2483	3	1/1/15/20	10/37/115/115	-
23	CLA	c	2479	3	1/1/15/20	10/37/115/115	-

All (1043) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	V	138	HEC	C2B-C3B	12.37	1.54	1.40
23	C	484	CLA	CHB-C4A	11.59	1.43	1.33
23	B	512	CLA	CHB-C4A	11.44	1.43	1.33
23	B	516	CLA	CHB-C4A	11.42	1.43	1.33
23	B	513	CLA	CHB-C4A	11.41	1.43	1.33
23	C	482	CLA	CHB-C4A	11.09	1.43	1.33
28	V	138	HEC	C1D-ND	11.08	1.58	1.36
23	c	2476	CLA	CHB-C4A	11.02	1.43	1.33
23	b	2516	CLA	CHB-C4A	10.99	1.43	1.33
23	b	2513	CLA	CHB-C4A	10.96	1.43	1.33
23	b	2512	CLA	CHB-C4A	10.92	1.43	1.33
23	c	2482	CLA	CHB-C4A	10.91	1.43	1.33
23	d	2357	CLA	CHB-C4A	10.91	1.43	1.33
23	c	2483	CLA	CHB-C4A	10.88	1.43	1.33
23	C	483	CLA	CHB-C4A	10.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2523	CLA	CHB-C4A	10.61	1.43	1.33
23	b	2525	CLA	CHB-C4A	10.60	1.42	1.33
23	c	2481	CLA	CHB-C4A	10.57	1.42	1.33
23	C	476	CLA	CHB-C4A	10.54	1.42	1.33
23	c	2484	CLA	CHB-C4A	10.49	1.42	1.33
23	D	354	CLA	CHB-C4A	10.41	1.42	1.33
28	V	138	HEC	C3C-C2C	10.36	1.52	1.40
23	D	356	CLA	CHB-C4A	10.34	1.42	1.33
23	B	527	CLA	CHB-C4A	10.33	1.42	1.33
23	A	350	CLA	CHB-C4A	10.32	1.42	1.33
23	a	2349	CLA	CHB-C4A	10.27	1.42	1.33
28	V	138	HEC	CMC-C2C	10.15	1.75	1.51
28	V	138	HEC	C1B-NB	10.10	1.56	1.36
23	b	2518	CLA	CHB-C4A	10.09	1.42	1.33
23	b	2520	CLA	CHB-C4A	9.99	1.42	1.33
23	d	2354	CLA	CHB-C4A	9.93	1.42	1.33
28	V	138	HEC	C4B-C3B	9.90	1.61	1.43
23	B	525	CLA	CHB-C4A	9.87	1.42	1.33
23	C	480	CLA	CHB-C4A	9.86	1.42	1.33
23	B	522	CLA	CHB-C4A	9.83	1.42	1.33
23	c	2480	CLA	CHB-C4A	9.75	1.42	1.33
23	B	523	CLA	CHB-C4A	9.74	1.42	1.33
28	V	138	HEC	CMB-C2B	9.73	1.74	1.51
23	b	2526	CLA	CHB-C4A	9.65	1.42	1.33
23	C	481	CLA	CHB-C4A	9.54	1.42	1.33
23	c	2478	CLA	CHB-C4A	9.49	1.41	1.33
23	b	2521	CLA	CHB-C4A	9.47	1.41	1.33
23	B	521	CLA	CHB-C4A	9.43	1.41	1.33
23	C	477	CLA	CHB-C4A	9.39	1.41	1.33
23	C	479	CLA	CHB-C4A	9.37	1.41	1.33
23	a	2351	CLA	CHB-C4A	9.14	1.41	1.33
23	B	520	CLA	CHB-C4A	9.14	1.41	1.33
23	c	2486	CLA	CHB-C4A	9.08	1.41	1.33
23	B	518	CLA	CHB-C4A	9.03	1.41	1.33
23	c	2479	CLA	CHB-C4A	8.95	1.41	1.33
28	V	138	HEC	C1C-NC	8.93	1.54	1.36
23	c	2477	CLA	CHB-C4A	8.90	1.41	1.33
23	c	2475	CLA	CHB-C4A	8.83	1.41	1.33
23	C	474	CLA	CHB-C4A	8.82	1.41	1.33
23	C	475	CLA	CHB-C4A	8.80	1.41	1.33
23	C	486	CLA	CHB-C4A	8.79	1.41	1.33
23	A	352	CLA	CHB-C4A	8.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	524	CLA	CHB-C4A	8.65	1.41	1.33
23	b	2517	CLA	CHB-C4A	8.59	1.41	1.33
28	V	138	HEC	CMD-C2D	8.57	1.68	1.51
23	c	2474	CLA	CHB-C4A	8.55	1.41	1.33
23	C	478	CLA	CHB-C4A	8.47	1.40	1.33
23	b	2522	CLA	CHB-C4A	8.46	1.40	1.33
23	b	2524	CLA	CHB-C4A	8.32	1.40	1.33
23	A	349	CLA	CHB-C4A	8.30	1.40	1.33
23	B	515	CLA	CHB-C4A	8.30	1.40	1.33
27	j	2053	BCR	C30-C25	8.18	1.64	1.53
23	b	2519	CLA	CHB-C4A	8.14	1.40	1.33
23	B	511	CLA	CHB-C4A	8.12	1.40	1.33
23	b	2511	CLA	CHB-C4A	8.11	1.40	1.33
23	C	485	CLA	CHB-C4A	8.05	1.40	1.33
23	a	2348	CLA	CHB-C4A	8.04	1.40	1.33
23	c	2487	CLA	CHB-C4A	7.74	1.40	1.33
23	c	2485	CLA	CHB-C4A	7.74	1.40	1.33
23	B	519	CLA	CHB-C4A	7.69	1.40	1.33
23	B	517	CLA	CHB-C4A	7.63	1.40	1.33
27	F	48	BCR	C30-C25	7.53	1.63	1.53
23	d	2355	CLA	CHB-C4A	7.51	1.40	1.33
23	b	2515	CLA	CHB-C4A	7.49	1.40	1.33
23	B	514	CLA	CHB-C4A	7.38	1.39	1.33
28	V	138	HEC	C4D-ND	7.33	1.51	1.36
23	A	348	CLA	CHB-C4A	6.98	1.39	1.33
27	J	53	BCR	C30-C25	6.96	1.62	1.53
28	v	2138	HEC	C3C-C2C	6.61	1.48	1.40
27	B	529	BCR	C30-C25	6.59	1.62	1.53
23	c	2487	CLA	MG-NA	6.54	2.21	2.06
27	B	528	BCR	C30-C25	6.53	1.62	1.53
23	b	2514	CLA	CHB-C4A	6.50	1.39	1.33
23	C	487	CLA	CHB-C4A	6.49	1.39	1.33
27	b	2528	BCR	C30-C25	6.41	1.62	1.53
27	d	2360	BCR	C30-C25	6.36	1.61	1.53
28	v	2138	HEC	CMD-C2D	6.19	1.64	1.51
28	V	138	HEC	CMA-C3A	6.16	1.66	1.51
23	C	487	CLA	MG-NA	6.16	2.20	2.06
27	C	489	BCR	C30-C25	6.07	1.61	1.53
27	c	2489	BCR	C30-C25	6.04	1.61	1.53
28	v	2138	HEC	CMC-C2C	5.98	1.65	1.51
23	C	486	CLA	MG-NA	5.76	2.19	2.06
25	D	357	PL9	C31-C29	5.75	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	V	138	HEC	C2A-C3A	5.73	1.54	1.37
23	D	354	CLA	MG-NA	5.63	2.19	2.06
28	v	2138	HEC	CMB-C2B	5.59	1.64	1.51
23	b	2526	CLA	MG-NA	5.54	2.19	2.06
23	B	527	CLA	MG-NA	5.52	2.19	2.06
28	e	2084	HEC	C1B-NB	5.51	1.47	1.36
23	d	2354	CLA	MG-NA	5.47	2.19	2.06
27	c	2488	BCR	C1-C6	5.43	1.60	1.53
28	v	2138	HEC	C1C-NC	5.40	1.47	1.36
25	d	2358	PL9	C53-C6	-5.33	1.39	1.50
27	b	2527	BCR	C30-C25	5.28	1.60	1.53
28	V	138	HEC	C4D-CHA	-5.27	1.26	1.41
23	a	2348	CLA	MG-NA	5.25	2.18	2.06
27	B	529	BCR	C26-C25	5.23	1.43	1.34
23	c	2486	CLA	MG-NA	5.22	2.18	2.06
25	D	357	PL9	C53-C6	-5.20	1.40	1.50
25	d	2358	PL9	C52-C5	-5.20	1.40	1.50
27	c	2489	BCR	C1-C6	5.07	1.60	1.53
23	c	2476	CLA	MG-NA	5.03	2.18	2.06
27	j	2053	BCR	C26-C25	5.00	1.42	1.34
23	B	513	CLA	CAA-C2A	5.00	1.63	1.54
23	C	482	CLA	MG-NA	4.99	2.18	2.06
23	c	2482	CLA	MG-NA	4.99	2.18	2.06
25	a	2352	PL9	C53-C6	-4.98	1.40	1.50
27	b	2527	BCR	C5-C6	4.97	1.42	1.34
25	d	2358	PL9	C31-C29	4.93	1.61	1.51
23	B	516	CLA	MG-NA	4.93	2.18	2.06
23	c	2477	CLA	MG-NA	4.93	2.18	2.06
27	j	2053	BCR	C5-C6	4.91	1.42	1.34
23	C	477	CLA	MG-NA	4.86	2.17	2.06
25	A	353	PL9	C52-C5	-4.84	1.40	1.50
28	e	2084	HEC	CMB-C2B	4.81	1.63	1.51
28	V	138	HEC	O2D-CGD	-4.81	1.14	1.30
27	B	528	BCR	C26-C25	4.81	1.42	1.34
23	b	2521	CLA	MG-NA	4.77	2.17	2.06
25	a	2352	PL9	C7-C3	4.76	1.57	1.51
27	c	2488	BCR	C30-C25	4.76	1.59	1.53
28	V	138	HEC	O1A-CGA	4.75	1.37	1.22
28	v	2138	HEC	C1B-NB	4.73	1.46	1.36
25	A	353	PL9	C53-C6	-4.72	1.41	1.50
23	C	484	CLA	MG-NA	4.70	2.17	2.06
27	F	48	BCR	C1-C6	4.68	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	e	2084	HEC	CMD-C2D	4.67	1.60	1.51
27	b	2528	BCR	C2-C1	4.66	1.64	1.54
23	a	2349	CLA	MG-NA	4.66	2.17	2.06
23	C	481	CLA	MG-NA	4.65	2.17	2.06
25	a	2352	PL9	C22-C23	-4.61	1.36	1.50
23	A	348	CLA	MG-NA	4.60	2.17	2.06
28	E	84	HEC	CMB-C2B	4.59	1.62	1.51
27	b	2528	BCR	C26-C25	4.59	1.42	1.34
23	A	350	CLA	MG-NA	4.58	2.17	2.06
27	B	528	BCR	C5-C6	4.56	1.42	1.34
23	C	480	CLA	MG-NA	4.56	2.17	2.06
24	d	2356	PHO	C3A-C2A	-4.54	1.50	1.54
23	c	2487	CLA	MG-NC	4.53	2.17	2.06
23	c	2481	CLA	MG-NA	4.53	2.17	2.06
23	b	2522	CLA	MG-NA	4.51	2.17	2.06
25	a	2352	PL9	C52-C5	-4.51	1.41	1.50
23	c	2484	CLA	MG-NA	4.50	2.17	2.06
23	b	2513	CLA	CAA-C2A	4.50	1.62	1.54
25	A	353	PL9	C22-C23	-4.49	1.36	1.50
23	B	520	CLA	CAA-CBA	-4.48	1.39	1.52
23	b	2516	CLA	MG-NA	4.48	2.16	2.06
25	D	357	PL9	C52-C5	-4.47	1.41	1.50
23	B	515	CLA	MG-NA	4.47	2.16	2.06
23	B	522	CLA	MG-NA	4.46	2.16	2.06
23	c	2480	CLA	MG-NA	4.46	2.16	2.06
27	C	488	BCR	C30-C25	4.44	1.59	1.53
27	d	2360	BCR	C1-C6	4.44	1.59	1.53
25	A	353	PL9	C7-C3	4.41	1.57	1.51
27	B	529	BCR	C2-C1	4.41	1.64	1.54
27	b	2527	BCR	C26-C25	4.38	1.41	1.34
23	C	478	CLA	MG-NA	4.36	2.16	2.06
27	J	53	BCR	C5-C6	4.36	1.41	1.34
23	B	521	CLA	MG-NA	4.35	2.16	2.06
28	E	84	HEC	CMD-C2D	4.33	1.60	1.51
23	b	2520	CLA	CAA-CBA	-4.33	1.39	1.52
23	C	479	CLA	MG-NA	4.32	2.16	2.06
27	c	2488	BCR	C29-C30	4.31	1.64	1.54
23	B	527	CLA	MG-NC	4.31	2.16	2.06
23	b	2526	CLA	MG-NC	4.30	2.16	2.06
27	d	2360	BCR	C5-C6	4.29	1.41	1.34
27	d	2360	BCR	C29-C30	4.29	1.63	1.54
27	k	2050	BCR	C1-C6	4.29	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	523	CLA	CAA-CBA	-4.28	1.40	1.52
23	b	2515	CLA	MG-NA	4.28	2.16	2.06
23	b	2523	CLA	CAA-CBA	-4.27	1.40	1.52
27	c	2489	BCR	C29-C30	4.25	1.63	1.54
28	E	84	HEC	CMA-C3A	4.25	1.61	1.51
23	c	2478	CLA	MG-NA	4.25	2.16	2.06
28	V	138	HEC	C3D-C2D	4.23	1.50	1.37
23	B	525	CLA	MG-NA	4.23	2.16	2.06
25	d	2358	PL9	C23-C24	4.22	1.42	1.33
23	C	475	CLA	MG-NA	4.22	2.16	2.06
23	C	487	CLA	MG-NC	4.22	2.16	2.06
23	c	2475	CLA	MG-NA	4.22	2.16	2.06
23	b	2517	CLA	MG-NA	4.17	2.16	2.06
23	C	487	CLA	C4C-C3C	4.17	1.52	1.45
27	C	488	BCR	C29-C30	4.14	1.63	1.54
25	A	353	PL9	C33-C34	4.14	1.42	1.33
25	d	2358	PL9	C18-C19	4.14	1.42	1.33
23	c	2485	CLA	MG-NA	4.13	2.16	2.06
23	b	2525	CLA	MG-NA	4.13	2.16	2.06
23	C	483	CLA	MG-NA	4.12	2.16	2.06
27	d	2360	BCR	C26-C25	4.11	1.41	1.34
23	C	475	CLA	CAA-C2A	4.09	1.61	1.54
23	d	2357	CLA	MG-NC	4.09	2.16	2.06
23	b	2514	CLA	C1B-CHB	-4.08	1.29	1.41
28	E	84	HEC	C2A-C1A	4.07	1.51	1.42
27	b	2527	BCR	C2-C1	4.06	1.63	1.54
23	c	2483	CLA	MG-NA	4.06	2.15	2.06
23	c	2474	CLA	MG-NA	4.03	2.15	2.06
27	C	488	BCR	C1-C6	4.02	1.58	1.53
25	a	2352	PL9	C28-C29	4.02	1.42	1.33
23	c	2477	CLA	CAA-CBA	-4.01	1.40	1.52
23	A	352	CLA	MG-NA	4.01	2.15	2.06
27	b	2527	BCR	C29-C30	4.01	1.63	1.54
23	b	2516	CLA	CAA-C2A	4.01	1.61	1.54
23	B	514	CLA	CAA-CBA	-4.00	1.40	1.52
28	e	2084	HEC	C4B-C3B	3.99	1.50	1.43
27	d	2360	BCR	C2-C1	3.99	1.63	1.54
23	b	2514	CLA	CAA-CBA	-3.99	1.40	1.52
27	F	48	BCR	C26-C25	3.98	1.41	1.34
23	A	352	CLA	MG-NC	3.98	2.15	2.06
23	c	2479	CLA	CAA-CBA	-3.98	1.41	1.52
27	j	2053	BCR	C2-C1	3.98	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	2528	BCR	C1-C6	3.94	1.58	1.53
23	a	2348	CLA	CHC-C1C	3.94	1.44	1.34
23	C	484	CLA	MG-NC	3.94	2.15	2.06
27	C	489	BCR	C29-C30	3.94	1.63	1.54
27	B	528	BCR	C29-C30	3.93	1.63	1.54
23	c	2487	CLA	C4C-C3C	3.93	1.51	1.45
28	e	2084	HEC	C1C-NC	3.92	1.44	1.36
27	J	53	BCR	C29-C30	3.91	1.63	1.54
27	j	2053	BCR	C29-C30	3.90	1.63	1.54
23	B	514	CLA	C1B-CHB	-3.90	1.30	1.41
27	c	2488	BCR	C2-C1	3.89	1.63	1.54
25	D	357	PL9	C18-C19	3.86	1.42	1.33
23	D	356	CLA	MG-NC	3.86	2.15	2.06
25	d	2358	PL9	C7-C3	3.85	1.56	1.51
23	b	2524	CLA	MG-NA	3.85	2.15	2.06
23	C	476	CLA	MG-NC	3.85	2.15	2.06
27	b	2528	BCR	C29-C30	3.84	1.62	1.54
23	C	477	CLA	C1D-ND	-3.83	1.32	1.37
23	c	2486	CLA	MG-NC	3.83	2.15	2.06
23	A	349	CLA	MG-NA	3.83	2.15	2.06
23	C	487	CLA	CAA-C2A	3.82	1.61	1.54
27	J	53	BCR	C26-C25	3.82	1.40	1.34
23	B	519	CLA	O2A-CGA	3.81	1.44	1.33
25	D	357	PL9	C7-C3	3.81	1.56	1.51
27	B	528	BCR	C2-C1	3.80	1.62	1.54
23	b	2518	CLA	MG-NA	3.80	2.15	2.06
23	A	348	CLA	CHC-C1C	3.80	1.43	1.34
27	C	488	BCR	C2-C1	3.79	1.62	1.54
23	B	512	CLA	MG-NA	3.79	2.15	2.06
23	b	2516	CLA	C2-C3	3.78	1.41	1.33
23	b	2519	CLA	O2A-CGA	3.78	1.44	1.33
23	B	513	CLA	MG-NC	3.77	2.15	2.06
27	K	50	BCR	C23-C22	-3.77	1.37	1.46
27	B	529	BCR	C1-C6	3.76	1.58	1.53
23	C	476	CLA	MG-NA	3.76	2.15	2.06
23	a	2351	CLA	MG-NA	3.75	2.15	2.06
23	C	485	CLA	MG-NA	3.74	2.15	2.06
25	A	353	PL9	C28-C29	3.74	1.41	1.33
23	c	2475	CLA	CAA-C2A	3.73	1.60	1.54
23	B	519	CLA	C1D-ND	-3.73	1.33	1.37
27	K	50	BCR	C30-C25	3.72	1.58	1.53
23	d	2357	CLA	MG-NA	3.72	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	482	CLA	CAA-C2A	3.72	1.60	1.54
28	E	84	HEC	C1B-NB	3.72	1.43	1.36
27	k	2050	BCR	C19-C18	-3.71	1.38	1.46
28	v	2138	HEC	O1A-CGA	3.71	1.34	1.22
27	k	2050	BCR	C23-C22	-3.70	1.38	1.46
28	E	84	HEC	CMC-C2C	3.70	1.60	1.51
23	d	2355	CLA	C1D-ND	-3.69	1.33	1.37
27	F	48	BCR	C2-C1	3.69	1.62	1.54
23	b	2511	CLA	CHC-C1C	3.69	1.43	1.34
23	C	475	CLA	MG-NC	3.68	2.15	2.06
23	C	477	CLA	CAA-CBA	-3.68	1.41	1.52
23	a	2351	CLA	MG-NC	3.67	2.15	2.06
23	c	2475	CLA	C2-C3	3.67	1.41	1.33
23	B	517	CLA	MG-NA	3.67	2.15	2.06
23	B	524	CLA	MG-NA	3.67	2.15	2.06
27	k	2050	BCR	C29-C30	3.66	1.62	1.54
23	B	523	CLA	MG-NA	3.66	2.15	2.06
25	A	353	PL9	C38-C39	3.65	1.43	1.32
24	a	2350	PHO	CBD-CGD	3.65	1.57	1.52
23	c	2487	CLA	CAA-C2A	3.65	1.60	1.54
23	b	2513	CLA	MG-NA	3.65	2.14	2.06
27	c	2489	BCR	C2-C1	3.65	1.62	1.54
23	B	511	CLA	MG-NC	3.64	2.14	2.06
24	A	351	PHO	C3A-C2A	-3.64	1.51	1.54
27	F	48	BCR	C29-C30	3.63	1.62	1.54
23	B	514	CLA	MG-NA	3.63	2.14	2.06
21	D	353	BCT	O1-C	3.62	1.38	1.25
23	C	485	CLA	C1B-CHB	-3.62	1.30	1.41
23	c	2485	CLA	MG-NC	3.62	2.14	2.06
27	B	529	BCR	C29-C30	3.61	1.62	1.54
23	B	524	CLA	C1B-CHB	-3.60	1.31	1.41
23	B	511	CLA	CHC-C1C	3.60	1.43	1.34
23	C	475	CLA	C2-C3	3.60	1.41	1.33
27	K	50	BCR	C19-C18	-3.59	1.38	1.46
23	b	2511	CLA	MG-NA	3.58	2.14	2.06
23	A	348	CLA	C3B-C2B	-3.57	1.35	1.40
23	B	519	CLA	C1B-CHB	-3.57	1.31	1.41
27	C	489	BCR	C2-C1	3.57	1.62	1.54
26	B	526	LMT	C3B-C2B	-3.57	1.43	1.52
23	b	2523	CLA	CHC-C1C	3.57	1.43	1.34
28	e	2084	HEC	C3A-C4A	3.57	1.50	1.42
23	b	2514	CLA	MG-NA	3.56	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2479	CLA	MG-NA	3.56	2.14	2.06
23	b	2520	CLA	CHC-C1C	3.56	1.43	1.34
23	B	523	CLA	MG-NC	3.56	2.14	2.06
23	b	2512	CLA	MG-NA	3.55	2.14	2.06
23	c	2482	CLA	CAA-C2A	3.55	1.60	1.54
23	c	2476	CLA	CHC-C1C	3.55	1.43	1.34
24	a	2350	PHO	C3A-C2A	-3.54	1.51	1.54
25	D	357	PL9	C23-C24	3.54	1.41	1.33
27	J	53	BCR	C2-C1	3.54	1.62	1.54
23	C	475	CLA	C5-C3	3.54	1.58	1.51
23	B	513	CLA	MG-NA	3.54	2.14	2.06
27	K	50	BCR	C29-C30	3.51	1.62	1.54
28	v	2138	HEC	O2D-CGD	-3.50	1.19	1.30
25	a	2352	PL9	C31-C29	3.50	1.58	1.51
23	B	511	CLA	MG-NA	3.50	2.14	2.06
27	c	2489	BCR	C26-C25	3.50	1.40	1.34
23	b	2523	CLA	MG-NA	3.49	2.14	2.06
23	C	474	CLA	MG-NA	3.48	2.14	2.06
27	F	48	BCR	C5-C6	3.48	1.40	1.34
23	b	2519	CLA	MG-NA	3.48	2.14	2.06
23	D	356	CLA	MG-NA	3.47	2.14	2.06
23	B	515	CLA	C1B-CHB	-3.47	1.31	1.41
23	b	2520	CLA	MG-NC	3.47	2.14	2.06
23	b	2513	CLA	MG-NC	3.47	2.14	2.06
23	C	484	CLA	CHC-C1C	3.46	1.43	1.34
23	d	2355	CLA	CHC-C1C	3.46	1.43	1.34
23	B	518	CLA	MG-NC	3.46	2.14	2.06
25	a	2352	PL9	C13-C14	3.45	1.41	1.33
23	C	474	CLA	MG-NC	3.43	2.14	2.06
23	B	520	CLA	CHC-C1C	3.43	1.43	1.34
25	d	2358	PL9	C33-C34	3.43	1.41	1.33
23	c	2475	CLA	C5-C3	3.43	1.58	1.51
23	b	2516	CLA	C5-C3	3.42	1.58	1.51
23	b	2516	CLA	C1-C2	3.42	1.58	1.49
23	B	511	CLA	CAA-CBA	-3.41	1.42	1.52
23	b	2511	CLA	MG-NC	3.41	2.14	2.06
23	C	482	CLA	MG-NC	3.41	2.14	2.06
23	b	2515	CLA	C1B-CHB	-3.41	1.31	1.41
23	B	516	CLA	C5-C3	3.40	1.58	1.51
23	B	512	CLA	MG-NC	3.40	2.14	2.06
23	C	483	CLA	MG-NC	3.40	2.14	2.06
23	B	516	CLA	C1-C2	3.39	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	353	PL9	C13-C14	3.39	1.40	1.33
23	C	483	CLA	C5-C3	3.39	1.58	1.51
23	A	349	CLA	C1D-ND	-3.39	1.33	1.37
23	c	2477	CLA	O2A-CGA	3.39	1.43	1.33
23	C	481	CLA	MG-NC	3.38	2.14	2.06
27	c	2488	BCR	C26-C25	3.38	1.40	1.34
23	c	2484	CLA	MG-NC	3.38	2.14	2.06
23	b	2524	CLA	C1B-CHB	-3.38	1.31	1.41
23	b	2518	CLA	CAA-CBA	-3.38	1.42	1.52
23	B	520	CLA	MG-NA	3.38	2.14	2.06
27	k	2050	BCR	C2-C1	3.38	1.61	1.54
23	b	2519	CLA	C1B-CHB	-3.37	1.31	1.41
23	C	486	CLA	CAA-C2A	3.37	1.60	1.54
23	c	2475	CLA	O2A-CGA	3.37	1.43	1.33
23	B	520	CLA	MG-NC	3.37	2.14	2.06
25	A	353	PL9	C31-C29	3.37	1.58	1.51
23	c	2485	CLA	C1B-CHB	-3.37	1.31	1.41
23	B	523	CLA	CHC-C1C	3.36	1.42	1.34
23	B	518	CLA	MG-NA	3.36	2.14	2.06
26	d	2359	LMT	O1'-C1'	3.35	1.45	1.40
23	b	2520	CLA	MG-NA	3.35	2.14	2.06
25	a	2352	PL9	C38-C39	3.35	1.42	1.32
28	v	2138	HEC	CAD-C3D	-3.34	1.43	1.52
21	d	2353	BCT	O1-C	3.34	1.37	1.25
23	b	2511	CLA	C1B-CHB	-3.34	1.31	1.41
23	b	2518	CLA	CHC-C1C	3.33	1.42	1.34
23	c	2482	CLA	MG-NC	3.33	2.14	2.06
23	B	517	CLA	C1B-CHB	-3.32	1.31	1.41
28	e	2084	HEC	C2B-C3B	3.32	1.44	1.40
23	B	521	CLA	CHC-C1C	3.32	1.42	1.34
23	c	2477	CLA	MG-NC	3.31	2.14	2.06
23	C	479	CLA	CAA-CBA	-3.30	1.43	1.52
23	d	2355	CLA	MG-NA	3.29	2.14	2.06
23	B	518	CLA	CAA-CBA	-3.29	1.43	1.52
23	c	2478	CLA	MG-NC	3.29	2.14	2.06
23	c	2476	CLA	MG-NC	3.29	2.14	2.06
23	B	516	CLA	C2-C3	3.29	1.40	1.33
23	a	2348	CLA	C1B-CHB	-3.29	1.31	1.41
23	c	2475	CLA	MG-NC	3.29	2.14	2.06
23	b	2519	CLA	C1D-ND	-3.28	1.33	1.37
23	b	2515	CLA	CAA-CBA	-3.28	1.43	1.52
27	B	529	BCR	C24-C23	3.28	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2525	CLA	MG-NC	3.28	2.14	2.06
27	C	489	BCR	C1-C6	3.28	1.58	1.53
25	D	357	PL9	C28-C29	3.28	1.40	1.33
23	b	2519	CLA	CAA-CBA	-3.27	1.43	1.52
23	b	2521	CLA	C4-C3	3.26	1.58	1.50
28	E	84	HEC	C1C-NC	3.26	1.43	1.36
27	c	2489	BCR	C5-C6	3.26	1.40	1.34
25	D	357	PL9	C30-C29	3.24	1.58	1.50
23	C	486	CLA	MG-NC	3.23	2.13	2.06
27	k	2050	BCR	C30-C25	3.23	1.57	1.53
23	B	519	CLA	CAA-CBA	-3.23	1.43	1.52
23	c	2483	CLA	CHC-C1C	3.23	1.42	1.34
23	B	519	CLA	MG-ND	-3.22	1.99	2.05
23	B	512	CLA	CHC-C1C	3.22	1.42	1.34
23	c	2475	CLA	CHC-C1C	3.22	1.42	1.34
28	V	138	HEC	O2A-CGA	-3.22	1.20	1.30
24	D	355	PHO	C3A-C2A	-3.21	1.51	1.54
23	A	350	CLA	MG-NC	3.21	2.13	2.06
23	B	521	CLA	MG-NC	3.21	2.13	2.06
23	C	477	CLA	O2A-CGA	3.21	1.42	1.33
23	d	2354	CLA	CAA-C2A	3.21	1.59	1.54
23	A	349	CLA	C1D-C2D	-3.21	1.39	1.45
25	A	353	PL9	C23-C24	3.20	1.40	1.33
23	A	348	CLA	C1B-CHB	-3.20	1.32	1.41
23	b	2523	CLA	MG-NC	3.19	2.13	2.06
23	B	515	CLA	CAA-CBA	-3.18	1.43	1.52
25	d	2358	PL9	C13-C14	3.18	1.40	1.33
23	B	518	CLA	CHC-C1C	3.17	1.42	1.34
23	c	2486	CLA	CAA-C2A	3.17	1.59	1.54
23	B	516	CLA	CAA-C2A	3.16	1.59	1.54
23	B	514	CLA	CHC-C1C	3.16	1.42	1.34
23	a	2349	CLA	CAA-CBA	-3.15	1.43	1.52
23	b	2525	CLA	C1D-ND	-3.15	1.33	1.37
23	C	485	CLA	MG-NC	3.15	2.13	2.06
23	A	350	CLA	C1D-C2D	-3.14	1.39	1.45
27	C	489	BCR	C26-C25	3.14	1.39	1.34
27	k	2050	BCR	C26-C25	3.14	1.39	1.34
23	c	2483	CLA	C5-C3	3.14	1.57	1.51
23	C	476	CLA	CAA-C2A	3.14	1.59	1.54
23	C	475	CLA	CHC-C1C	3.13	1.42	1.34
23	C	478	CLA	MG-NC	3.13	2.13	2.06
28	V	138	HEC	CBD-CGD	-3.13	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	2359	LMT	C3B-C2B	-3.13	1.44	1.52
23	C	480	CLA	CAA-CBA	-3.13	1.43	1.52
23	b	2519	CLA	C1-C2	3.13	1.58	1.49
23	b	2516	CLA	MG-NC	3.13	2.13	2.06
23	B	515	CLA	CHC-C1C	3.13	1.42	1.34
23	D	354	CLA	CHC-C1C	3.13	1.42	1.34
23	b	2511	CLA	CAA-CBA	-3.12	1.43	1.52
23	c	2477	CLA	CHC-C1C	3.12	1.42	1.34
27	b	2527	BCR	C1-C6	3.12	1.57	1.53
23	C	475	CLA	O2A-CGA	3.11	1.42	1.33
23	C	477	CLA	MG-NC	3.11	2.13	2.06
27	K	50	BCR	C1-C6	3.11	1.57	1.53
25	d	2358	PL9	C28-C29	3.11	1.40	1.33
23	d	2357	CLA	CHC-C1C	3.10	1.42	1.34
21	a	2346	BCT	O1-C	3.10	1.36	1.25
23	d	2355	CLA	C1B-CHB	-3.10	1.32	1.41
23	B	518	CLA	C1B-CHB	-3.10	1.32	1.41
23	B	522	CLA	C1D-ND	-3.09	1.33	1.37
23	b	2525	CLA	CAA-C2A	3.09	1.59	1.54
23	B	511	CLA	C1B-CHB	-3.09	1.32	1.41
23	B	525	CLA	C1D-ND	-3.08	1.33	1.37
25	a	2352	PL9	C33-C34	3.08	1.40	1.33
25	D	357	PL9	C33-C34	3.07	1.40	1.33
23	D	356	CLA	CHC-C1C	3.07	1.42	1.34
23	C	482	CLA	C5-C3	3.07	1.57	1.51
23	c	2481	CLA	CAA-CBA	-3.07	1.43	1.52
23	b	2521	CLA	CHC-C1C	3.07	1.42	1.34
23	C	478	CLA	C1B-CHB	-3.06	1.32	1.41
23	B	520	CLA	C1-C2	3.06	1.57	1.49
23	C	483	CLA	CHC-C1C	3.06	1.42	1.34
23	B	520	CLA	O2A-CGA	3.06	1.42	1.33
23	B	527	CLA	CHC-C1C	3.06	1.42	1.34
25	a	2352	PL9	C23-C24	3.06	1.40	1.33
23	c	2475	CLA	C4-C3	3.06	1.58	1.50
23	A	350	CLA	C1D-ND	-3.06	1.33	1.37
23	D	354	CLA	CAA-C2A	3.06	1.59	1.54
23	c	2484	CLA	CAA-C2A	3.06	1.59	1.54
23	d	2354	CLA	MG-NC	3.05	2.13	2.06
23	b	2520	CLA	C1-C2	3.05	1.57	1.49
23	A	352	CLA	CAA-C2A	3.04	1.59	1.54
24	a	2350	PHO	C4A-C3A	-3.04	1.46	1.51
23	A	348	CLA	MG-NC	3.03	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	476	CLA	CHC-C1C	3.03	1.42	1.34
27	K	50	BCR	C2-C1	3.03	1.61	1.54
23	c	2486	CLA	C1B-CHB	-3.03	1.32	1.41
23	c	2479	CLA	MG-NC	3.03	2.13	2.06
23	b	2514	CLA	C5-C3	3.03	1.57	1.51
28	e	2084	HEC	O1A-CGA	3.02	1.32	1.22
23	B	519	CLA	C1-C2	3.02	1.57	1.49
28	E	84	HEC	C2B-C3B	3.02	1.44	1.40
27	c	2488	BCR	C5-C6	3.01	1.39	1.34
23	c	2478	CLA	C1B-CHB	-3.01	1.32	1.41
23	b	2517	CLA	C1B-CHB	-3.00	1.32	1.41
23	d	2354	CLA	CHC-C1C	3.00	1.41	1.34
23	a	2349	CLA	MG-NC	3.00	2.13	2.06
23	C	475	CLA	C1B-CHB	-2.99	1.32	1.41
27	K	50	BCR	C26-C25	2.99	1.39	1.34
23	c	2485	CLA	CAA-CBA	-2.99	1.43	1.52
23	B	522	CLA	MG-NC	2.99	2.13	2.06
23	C	484	CLA	CAA-C2A	2.98	1.59	1.54
23	c	2475	CLA	C1-C2	2.98	1.57	1.49
23	c	2480	CLA	MG-NC	2.98	2.13	2.06
23	c	2483	CLA	CAA-CBA	-2.98	1.44	1.52
23	b	2517	CLA	CHC-C1C	2.98	1.41	1.34
23	B	513	CLA	CHC-C1C	2.97	1.41	1.34
27	C	488	BCR	C5-C6	2.97	1.39	1.34
27	C	489	BCR	C5-C6	2.97	1.39	1.34
23	C	475	CLA	C1-C2	2.97	1.57	1.49
23	b	2516	CLA	CHC-C1C	2.97	1.41	1.34
26	d	2359	LMT	C2-C1	2.97	1.63	1.51
23	c	2484	CLA	CHC-C1C	2.96	1.41	1.34
23	c	2482	CLA	C5-C3	2.96	1.57	1.51
23	B	521	CLA	C4-C3	2.96	1.57	1.50
23	b	2512	CLA	MG-NC	2.96	2.13	2.06
23	C	474	CLA	CAA-CBA	-2.96	1.44	1.52
23	B	516	CLA	MG-NC	2.95	2.13	2.06
23	c	2481	CLA	MG-NC	2.95	2.13	2.06
23	c	2474	CLA	MG-NC	2.95	2.13	2.06
23	c	2474	CLA	CHC-C1C	2.95	1.41	1.34
23	B	522	CLA	C1D-C2D	-2.95	1.39	1.45
23	B	519	CLA	CHC-C1C	2.94	1.41	1.34
23	B	512	CLA	C4-C3	2.94	1.57	1.50
23	B	517	CLA	MG-NC	2.94	2.13	2.06
26	B	526	LMT	C2-C1	2.94	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	488	BCR	C26-C25	2.94	1.39	1.34
23	c	2480	CLA	CHC-C1C	2.94	1.41	1.34
23	b	2514	CLA	CHC-C1C	2.93	1.41	1.34
23	A	349	CLA	CHC-C1C	2.93	1.41	1.34
23	C	483	CLA	CAA-CBA	-2.93	1.44	1.52
23	C	487	CLA	C1B-CHB	-2.92	1.32	1.41
23	c	2484	CLA	C4-C3	2.92	1.57	1.50
23	B	522	CLA	CHC-C1C	2.92	1.41	1.34
23	C	481	CLA	CHC-C1C	2.91	1.41	1.34
24	A	351	PHO	C4A-C3A	-2.91	1.46	1.51
23	c	2480	CLA	CAA-CBA	-2.91	1.44	1.52
23	c	2478	CLA	CHC-C1C	2.90	1.41	1.34
23	b	2521	CLA	CAA-CBA	-2.90	1.44	1.52
23	c	2474	CLA	C4-C3	2.90	1.57	1.50
23	B	517	CLA	CHC-C1C	2.90	1.41	1.34
27	K	50	BCR	C12-C13	-2.90	1.39	1.46
23	b	2512	CLA	CHC-C1C	2.89	1.41	1.34
23	C	486	CLA	C1B-CHB	-2.89	1.32	1.41
23	c	2481	CLA	CHC-C1C	2.89	1.41	1.34
23	B	516	CLA	CAA-CBA	-2.88	1.44	1.52
23	b	2518	CLA	MG-NC	2.88	2.13	2.06
23	C	484	CLA	C4-C3	2.88	1.57	1.50
23	B	524	CLA	O2A-CGA	2.88	1.41	1.33
23	b	2515	CLA	MG-NC	2.88	2.13	2.06
28	E	84	HEC	O1A-CGA	2.87	1.31	1.22
23	d	2357	CLA	C4-C3	2.87	1.57	1.50
23	D	354	CLA	MG-NC	2.87	2.13	2.06
23	A	349	CLA	C1B-CHB	-2.87	1.33	1.41
23	C	474	CLA	CHC-C1C	2.86	1.41	1.34
23	b	2520	CLA	C2-C3	2.86	1.39	1.33
23	c	2483	CLA	MG-NC	2.86	2.13	2.06
23	c	2477	CLA	C1D-C2D	-2.86	1.39	1.45
23	C	475	CLA	C4-C3	2.85	1.57	1.50
23	b	2517	CLA	MG-NC	2.85	2.13	2.06
28	v	2138	HEC	CMA-C3A	2.85	1.58	1.51
23	b	2511	CLA	C1-C2	2.85	1.57	1.49
23	d	2355	CLA	O2A-CGA	2.85	1.41	1.33
25	d	2358	PL9	C30-C29	2.85	1.57	1.50
23	B	519	CLA	C5-C3	2.85	1.57	1.51
23	b	2521	CLA	MG-NC	2.84	2.13	2.06
23	b	2518	CLA	C1B-CHB	-2.84	1.33	1.41
23	c	2479	CLA	C1B-CHB	-2.84	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2485	CLA	CHC-C1C	2.84	1.41	1.34
23	b	2517	CLA	CAA-CBA	-2.83	1.44	1.52
23	B	525	CLA	MG-NC	2.83	2.13	2.06
23	b	2512	CLA	CAA-C2A	2.82	1.59	1.54
23	C	485	CLA	CHC-C1C	2.82	1.41	1.34
23	d	2357	CLA	C5-C3	2.82	1.57	1.51
25	a	2352	PL9	C17-C18	-2.80	1.42	1.50
23	A	350	CLA	CHC-C1C	2.80	1.41	1.34
23	c	2487	CLA	CHD-C1D	2.80	1.43	1.38
23	c	2474	CLA	CAA-CBA	-2.80	1.44	1.52
23	b	2516	CLA	CAA-CBA	-2.79	1.44	1.52
27	K	50	BCR	C33-C5	2.79	1.55	1.50
23	C	479	CLA	C1B-CHB	-2.79	1.33	1.41
23	c	2475	CLA	C1B-CHB	-2.79	1.33	1.41
23	b	2520	CLA	C4-C3	2.78	1.57	1.50
23	c	2486	CLA	CHC-C1C	2.78	1.41	1.34
23	C	477	CLA	CHC-C1C	2.78	1.41	1.34
23	C	474	CLA	C1B-CHB	-2.78	1.33	1.41
23	B	521	CLA	CAA-CBA	-2.78	1.44	1.52
27	B	528	BCR	C33-C5	2.78	1.55	1.50
23	C	480	CLA	CHC-C1C	2.77	1.41	1.34
23	b	2520	CLA	O2A-CGA	2.77	1.41	1.33
23	B	524	CLA	CAA-C2A	2.77	1.59	1.54
23	A	350	CLA	CAA-CBA	-2.77	1.44	1.52
23	c	2483	CLA	C4-C3	2.76	1.57	1.50
23	B	516	CLA	CHC-C1C	2.76	1.41	1.34
23	a	2351	CLA	C1B-CHB	-2.76	1.33	1.41
28	E	84	HEC	C3A-C4A	2.76	1.48	1.42
23	c	2477	CLA	C1D-ND	-2.75	1.34	1.37
28	E	84	HEC	C4B-C3B	2.75	1.48	1.43
23	B	525	CLA	CAA-C2A	2.74	1.59	1.54
23	B	516	CLA	C6-C5	2.74	1.62	1.52
23	a	2349	CLA	C1D-ND	-2.74	1.34	1.37
23	C	480	CLA	C1D-ND	-2.74	1.34	1.37
23	C	476	CLA	C1D-C2D	-2.74	1.39	1.45
26	d	2359	LMT	C4'-C5'	2.74	1.60	1.52
23	c	2487	CLA	C4-C3	2.73	1.57	1.50
23	A	352	CLA	C4-C3	2.73	1.57	1.50
23	C	486	CLA	CHC-C1C	2.73	1.41	1.34
23	b	2515	CLA	CHC-C1C	2.73	1.41	1.34
25	D	357	PL9	C13-C14	2.73	1.39	1.33
23	B	522	CLA	C1B-CHB	-2.73	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	352	CLA	C1B-CHB	-2.72	1.33	1.41
28	V	138	HEC	C1B-CHB	2.72	1.48	1.41
25	d	2358	PL9	C8-C9	2.72	1.39	1.33
23	b	2519	CLA	C1D-C2D	-2.72	1.40	1.45
23	b	2524	CLA	O2A-CGA	2.72	1.41	1.33
23	a	2351	CLA	C4C-C3C	2.71	1.49	1.45
23	A	348	CLA	CAA-CBA	-2.71	1.44	1.52
23	C	478	CLA	CHC-C1C	2.71	1.41	1.34
25	a	2352	PL9	C35-C34	2.71	1.57	1.50
27	b	2528	BCR	C38-C26	2.71	1.55	1.50
23	b	2511	CLA	O2A-CGA	2.70	1.41	1.33
23	A	352	CLA	CHC-C1C	2.70	1.41	1.34
23	B	524	CLA	C1D-ND	-2.70	1.34	1.37
23	C	479	CLA	C1D-ND	-2.70	1.34	1.37
23	B	514	CLA	C5-C3	2.70	1.56	1.51
23	B	517	CLA	CAA-CBA	-2.70	1.44	1.52
23	a	2351	CLA	CHC-C1C	2.70	1.41	1.34
27	k	2050	BCR	C12-C13	-2.69	1.40	1.46
23	B	527	CLA	C4-C3	2.69	1.57	1.50
23	C	477	CLA	C1D-C2D	-2.69	1.40	1.45
25	d	2358	PL9	C2-C3	2.69	1.41	1.34
23	b	2513	CLA	CHC-C1C	2.69	1.41	1.34
25	d	2358	PL9	C35-C34	2.68	1.57	1.50
23	B	511	CLA	C1-C2	2.68	1.56	1.49
23	a	2348	CLA	MG-NC	2.68	2.12	2.06
23	c	2474	CLA	C1B-CHB	-2.68	1.33	1.41
27	k	2050	BCR	C17-C18	-2.68	1.29	1.35
23	c	2478	CLA	CAA-C2A	2.68	1.59	1.54
23	b	2526	CLA	CHC-C1C	2.67	1.41	1.34
27	K	50	BCR	C17-C18	-2.67	1.29	1.35
23	B	515	CLA	MG-NC	2.67	2.12	2.06
23	b	2522	CLA	CHC-C1C	2.67	1.41	1.34
27	b	2528	BCR	C24-C23	2.67	1.41	1.33
25	A	353	PL9	C30-C29	2.67	1.57	1.50
23	c	2482	CLA	CHC-C1C	2.67	1.41	1.34
25	D	357	PL9	C8-C9	2.67	1.39	1.33
28	v	2138	HEC	C4D-CHA	-2.66	1.33	1.41
23	C	484	CLA	C1D-ND	-2.66	1.34	1.37
23	b	2520	CLA	C5-C3	2.66	1.56	1.51
23	b	2524	CLA	CHC-C1C	2.66	1.41	1.34
27	j	2053	BCR	C38-C26	2.66	1.55	1.50
23	B	520	CLA	C2-C3	2.65	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2351	CLA	CAA-C2A	2.65	1.58	1.54
23	b	2514	CLA	MG-NC	2.64	2.12	2.06
25	D	357	PL9	C38-C39	2.64	1.40	1.32
28	e	2084	HEC	CMA-C3A	2.64	1.57	1.51
23	c	2479	CLA	CHC-C1C	2.64	1.41	1.34
25	D	357	PL9	C2-C3	2.64	1.41	1.34
23	B	516	CLA	C4-C3	2.63	1.57	1.50
23	B	521	CLA	C1B-CHB	-2.63	1.33	1.41
23	a	2351	CLA	C4-C3	2.63	1.57	1.50
23	A	349	CLA	O2A-CGA	2.63	1.41	1.33
23	b	2522	CLA	MG-NC	2.63	2.12	2.06
23	c	2480	CLA	C1B-CHB	-2.63	1.33	1.41
23	d	2355	CLA	C1D-C2D	-2.63	1.40	1.45
23	b	2522	CLA	C4-C3	2.63	1.57	1.50
25	A	353	PL9	C27-C28	-2.62	1.42	1.50
23	C	485	CLA	CAA-CBA	-2.62	1.45	1.52
27	k	2050	BCR	C33-C5	2.61	1.55	1.50
25	a	2352	PL9	C30-C29	2.61	1.57	1.50
23	D	356	CLA	C4-C3	2.60	1.57	1.50
23	C	481	CLA	C4-C3	2.60	1.57	1.50
23	C	475	CLA	CAA-CBA	-2.60	1.45	1.52
23	b	2513	CLA	C1D-C2D	-2.60	1.40	1.45
23	a	2349	CLA	C1D-C2D	-2.60	1.40	1.45
25	d	2358	PL9	C38-C39	2.60	1.40	1.32
23	b	2522	CLA	C1B-CHB	-2.60	1.33	1.41
23	c	2475	CLA	CAA-CBA	-2.59	1.45	1.52
28	e	2084	HEC	C2A-C1A	2.59	1.48	1.42
23	b	2512	CLA	C4-C3	2.59	1.57	1.50
23	B	523	CLA	C1B-CHB	-2.59	1.33	1.41
23	B	524	CLA	CHC-C1C	2.59	1.40	1.34
23	b	2521	CLA	C5-C3	2.59	1.56	1.51
23	B	514	CLA	MG-NC	2.59	2.12	2.06
25	a	2352	PL9	C27-C28	-2.58	1.42	1.50
23	C	478	CLA	CAA-C2A	2.58	1.58	1.54
23	b	2525	CLA	C1B-CHB	-2.58	1.33	1.41
26	B	526	LMT	O1'-C1'	2.58	1.44	1.40
23	b	2515	CLA	C4-C3	2.58	1.57	1.50
23	B	512	CLA	CAA-C2A	2.57	1.58	1.54
25	A	353	PL9	C35-C34	2.57	1.57	1.50
23	B	517	CLA	C1D-ND	-2.57	1.34	1.37
23	b	2523	CLA	C5-C3	2.57	1.56	1.51
23	b	2518	CLA	C4-C3	2.57	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	520	CLA	C1B-CHB	-2.56	1.33	1.41
25	a	2352	PL9	C8-C9	2.56	1.39	1.33
26	B	526	LMT	C4'-C5'	2.56	1.59	1.52
24	d	2356	PHO	C4A-C3A	-2.56	1.47	1.51
23	b	2519	CLA	CHC-C1C	2.56	1.40	1.34
23	b	2524	CLA	C1D-ND	-2.55	1.34	1.37
23	c	2476	CLA	CAA-C2A	2.55	1.58	1.54
23	C	481	CLA	CAA-CBA	-2.55	1.45	1.52
23	b	2512	CLA	C1D-C2D	-2.55	1.40	1.45
23	B	511	CLA	O2A-CGA	2.54	1.40	1.33
27	c	2489	BCR	C33-C5	2.54	1.55	1.50
23	C	487	CLA	CHD-C1D	2.54	1.43	1.38
24	a	2350	PHO	CAA-CBA	-2.54	1.45	1.52
25	A	353	PL9	C17-C18	-2.54	1.42	1.50
23	b	2525	CLA	C1D-C2D	-2.53	1.40	1.45
28	v	2138	HEC	C3D-C2D	2.53	1.45	1.37
23	B	511	CLA	C1D-C2D	-2.53	1.40	1.45
23	c	2485	CLA	CBA-CGA	-2.53	1.43	1.50
25	D	357	PL9	C35-C34	2.53	1.56	1.50
23	C	478	CLA	O2A-CGA	2.53	1.40	1.33
23	B	519	CLA	C2-C3	2.52	1.38	1.33
23	c	2487	CLA	C1B-CHB	-2.52	1.34	1.41
27	c	2488	BCR	C19-C18	-2.52	1.40	1.46
23	c	2483	CLA	C1D-ND	-2.52	1.34	1.37
23	A	352	CLA	C1D-C2D	-2.52	1.40	1.45
23	B	527	CLA	C4C-C3C	2.52	1.49	1.45
23	b	2512	CLA	C1D-ND	-2.52	1.34	1.37
23	C	485	CLA	C4-C3	2.52	1.56	1.50
25	D	357	PL9	C32-C33	-2.52	1.42	1.50
23	c	2481	CLA	C4-C3	2.52	1.56	1.50
23	B	513	CLA	C1D-C2D	-2.51	1.40	1.45
23	A	349	CLA	CAA-CBA	-2.51	1.45	1.52
23	c	2485	CLA	C1D-ND	-2.51	1.34	1.37
23	B	519	CLA	MG-NC	2.51	2.12	2.06
23	c	2485	CLA	C4-C3	2.51	1.56	1.50
23	d	2354	CLA	C5-C3	2.50	1.56	1.51
23	c	2483	CLA	C2-C3	2.50	1.38	1.33
23	C	487	CLA	C4-C3	2.50	1.56	1.50
23	b	2513	CLA	C1D-ND	-2.50	1.34	1.37
23	c	2481	CLA	C1D-C2D	-2.50	1.40	1.45
23	b	2525	CLA	C4-C3	2.49	1.56	1.50
23	b	2516	CLA	C1D-ND	-2.49	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	j	2053	BCR	C33-C5	2.49	1.54	1.50
23	b	2519	CLA	C4-C3	2.49	1.56	1.50
23	b	2522	CLA	C1D-C2D	-2.49	1.40	1.45
24	d	2356	PHO	CHA-CBD	2.48	1.55	1.52
23	B	527	CLA	C1-C2	2.48	1.56	1.49
27	B	529	BCR	C38-C26	2.48	1.54	1.50
23	b	2517	CLA	C1D-C2D	-2.48	1.40	1.45
23	a	2348	CLA	CAA-CBA	-2.48	1.45	1.52
25	A	353	PL9	C8-C9	2.47	1.38	1.33
23	b	2519	CLA	C2-C3	2.47	1.38	1.33
23	b	2522	CLA	C5-C3	2.47	1.56	1.51
23	c	2479	CLA	C1D-ND	-2.47	1.34	1.37
23	b	2511	CLA	C1D-C2D	-2.47	1.40	1.45
23	a	2348	CLA	C1D-ND	-2.47	1.34	1.37
23	b	2514	CLA	C4-C3	2.47	1.56	1.50
27	K	50	BCR	C16-C15	-2.47	1.29	1.36
23	D	354	CLA	C1D-C2D	-2.46	1.40	1.45
24	a	2350	PHO	CHA-CBD	2.46	1.54	1.52
23	b	2513	CLA	C4-C3	2.46	1.56	1.50
23	A	349	CLA	CAA-C2A	2.46	1.58	1.54
23	A	348	CLA	C1D-C2D	-2.46	1.40	1.45
23	D	356	CLA	C1C-C2C	2.46	1.49	1.44
23	C	477	CLA	C1B-CHB	-2.46	1.34	1.41
23	b	2526	CLA	C4C-C3C	2.46	1.49	1.45
23	C	475	CLA	C1D-ND	-2.46	1.34	1.37
28	E	84	HEC	C2A-C3A	2.45	1.44	1.37
23	B	525	CLA	C3B-C2B	-2.45	1.37	1.40
23	B	519	CLA	MG-NA	2.45	2.12	2.06
23	b	2526	CLA	C4-C3	2.45	1.56	1.50
23	d	2354	CLA	C1D-ND	-2.45	1.34	1.37
23	b	2526	CLA	CMB-C2B	2.44	1.56	1.51
27	c	2488	BCR	C33-C5	2.44	1.54	1.50
24	a	2350	PHO	C4-C3	2.44	1.56	1.50
27	k	2050	BCR	C16-C15	-2.44	1.29	1.36
23	B	527	CLA	C1B-CHB	-2.43	1.34	1.41
23	b	2515	CLA	C1D-ND	-2.43	1.34	1.37
23	C	486	CLA	C5-C3	2.42	1.56	1.51
23	B	525	CLA	C1B-CHB	-2.42	1.34	1.41
23	b	2522	CLA	CAA-C2A	2.42	1.58	1.54
23	b	2516	CLA	C6-C5	2.42	1.61	1.52
23	B	524	CLA	MG-NC	2.42	2.12	2.06
23	a	2349	CLA	CHC-C1C	2.41	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2513	CLA	C1B-CHB	-2.41	1.34	1.41
23	b	2523	CLA	C1B-CHB	-2.41	1.34	1.41
23	B	527	CLA	C2-C3	2.41	1.38	1.33
23	b	2524	CLA	C1D-C2D	-2.41	1.40	1.45
23	c	2481	CLA	C1B-CHB	-2.40	1.34	1.41
23	a	2351	CLA	C1D-C2D	-2.40	1.40	1.45
23	c	2476	CLA	C1D-C2D	-2.40	1.40	1.45
23	D	356	CLA	CAA-CBA	-2.40	1.45	1.52
23	d	2354	CLA	C1D-C2D	-2.40	1.40	1.45
23	B	520	CLA	C4-C3	2.40	1.56	1.50
23	b	2511	CLA	C1C-C2C	2.40	1.49	1.44
23	B	514	CLA	C4-C3	2.40	1.56	1.50
23	b	2522	CLA	C1D-ND	-2.40	1.34	1.37
23	C	480	CLA	MG-NC	2.39	2.12	2.06
23	B	527	CLA	CMB-C2B	2.39	1.56	1.51
23	C	479	CLA	CHC-C1C	2.39	1.40	1.34
23	B	515	CLA	C4-C3	2.38	1.56	1.50
23	B	521	CLA	C1D-ND	-2.38	1.34	1.37
23	C	485	CLA	C1D-ND	-2.38	1.34	1.37
23	c	2487	CLA	C5-C3	2.37	1.56	1.51
23	c	2478	CLA	C2-C3	2.37	1.38	1.33
23	d	2354	CLA	C1B-CHB	-2.37	1.34	1.41
23	C	477	CLA	C1-C2	2.37	1.55	1.49
23	c	2486	CLA	C4-C3	2.37	1.56	1.50
23	b	2520	CLA	C1B-CHB	-2.37	1.34	1.41
23	C	482	CLA	C1-C2	2.37	1.55	1.49
23	B	511	CLA	C1D-ND	-2.36	1.34	1.37
23	b	2511	CLA	C1D-ND	-2.36	1.34	1.37
28	V	138	HEC	O1D-CGD	2.36	1.29	1.22
23	b	2521	CLA	CMB-C2B	2.35	1.56	1.51
25	d	2358	PL9	C32-C33	-2.35	1.43	1.50
23	C	480	CLA	C1B-CHB	-2.35	1.34	1.41
23	b	2526	CLA	C1B-CHB	-2.35	1.34	1.41
23	B	525	CLA	C4-C3	2.35	1.56	1.50
23	b	2516	CLA	O2A-CGA	2.34	1.40	1.33
23	C	483	CLA	C4-C3	2.34	1.56	1.50
23	b	2523	CLA	C1C-C2C	2.34	1.49	1.44
23	A	348	CLA	CBA-CGA	-2.34	1.43	1.50
23	b	2524	CLA	CAA-C2A	2.34	1.58	1.54
23	b	2523	CLA	C4-C3	2.34	1.56	1.50
23	B	519	CLA	C4-C3	2.33	1.56	1.50
23	D	354	CLA	C1-C2	2.33	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2516	CLA	C4-C3	2.33	1.56	1.50
27	J	53	BCR	C38-C26	2.33	1.54	1.50
24	A	351	PHO	CBD-CGD	2.33	1.55	1.52
24	D	355	PHO	C4A-C3A	-2.32	1.47	1.51
23	C	482	CLA	C4-C3	2.32	1.56	1.50
23	c	2482	CLA	C4C-C3C	2.32	1.49	1.45
23	b	2514	CLA	C1D-ND	-2.32	1.34	1.37
23	c	2475	CLA	C1D-ND	-2.32	1.34	1.37
23	C	483	CLA	C1B-CHB	-2.32	1.34	1.41
23	b	2524	CLA	MG-ND	-2.32	2.01	2.05
23	B	513	CLA	C1B-CHB	-2.32	1.34	1.41
23	b	2521	CLA	C1D-ND	-2.31	1.34	1.37
23	D	356	CLA	C1D-C2D	-2.31	1.40	1.45
23	c	2480	CLA	C4-C3	2.31	1.56	1.50
23	d	2357	CLA	CAA-CBA	-2.31	1.46	1.52
23	d	2357	CLA	CAA-C2A	2.31	1.58	1.54
28	E	84	HEC	C1D-ND	2.31	1.41	1.36
24	A	351	PHO	C4-C3	2.30	1.56	1.50
23	A	352	CLA	C1D-ND	-2.30	1.34	1.37
23	c	2476	CLA	C1D-ND	-2.30	1.34	1.37
23	D	356	CLA	CMD-C2D	2.30	1.55	1.50
23	C	483	CLA	CAA-C2A	2.29	1.58	1.54
23	B	513	CLA	C2-C3	2.29	1.38	1.33
23	C	481	CLA	C1D-ND	-2.29	1.34	1.37
23	B	523	CLA	C5-C3	2.29	1.56	1.51
25	A	353	PL9	C2-C3	2.28	1.40	1.34
27	j	2053	BCR	C1-C6	2.28	1.56	1.53
27	C	488	BCR	C23-C22	-2.28	1.41	1.46
23	c	2476	CLA	CMB-C2B	2.28	1.56	1.51
23	c	2487	CLA	CHC-C1C	2.28	1.40	1.34
23	B	519	CLA	C3B-C2B	-2.28	1.37	1.40
28	V	138	HEC	CBA-CGA	-2.28	1.45	1.50
23	C	487	CLA	OBD-CAD	2.28	1.26	1.22
23	B	519	CLA	C1D-C2D	-2.27	1.40	1.45
23	b	2517	CLA	C4-C3	2.27	1.56	1.50
23	c	2482	CLA	C4-C3	2.27	1.56	1.50
25	a	2352	PL9	C40-C39	2.27	1.56	1.50
28	v	2138	HEC	CBA-CGA	-2.27	1.45	1.50
27	b	2527	BCR	C38-C26	2.27	1.54	1.50
23	b	2525	CLA	C3B-C2B	-2.26	1.37	1.40
23	b	2525	CLA	OBD-CAD	2.26	1.26	1.22
27	K	50	BCR	C20-C21	-2.26	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	474	CLA	C4-C3	2.26	1.56	1.50
23	b	2515	CLA	C3A-C4A	-2.26	1.44	1.51
23	C	486	CLA	C4-C3	2.25	1.56	1.50
24	d	2356	PHO	C4-C3	2.25	1.56	1.50
23	B	523	CLA	C4-C3	2.25	1.56	1.50
25	d	2358	PL9	C37-C38	-2.25	1.43	1.50
23	c	2477	CLA	CMB-C2B	2.25	1.56	1.51
23	B	513	CLA	C4-C3	2.25	1.56	1.50
23	C	480	CLA	C4-C3	2.25	1.56	1.50
28	v	2138	HEC	O2A-CGA	-2.25	1.23	1.30
25	A	353	PL9	C21-C19	-2.25	1.46	1.51
27	B	529	BCR	C7-C6	2.25	1.52	1.45
23	c	2487	CLA	CMA-C3A	2.24	1.57	1.53
24	D	355	PHO	CBD-CGD	2.24	1.55	1.52
23	B	525	CLA	OBD-CAD	2.24	1.26	1.22
27	k	2050	BCR	C20-C21	-2.24	1.36	1.43
23	B	524	CLA	C1D-C2D	-2.24	1.40	1.45
23	c	2484	CLA	C1D-ND	-2.24	1.34	1.37
23	B	524	CLA	O2A-C1	2.24	1.52	1.46
23	c	2476	CLA	C4-C3	2.23	1.56	1.50
23	b	2525	CLA	CHC-C1C	2.23	1.40	1.34
23	D	354	CLA	C1B-CHB	-2.23	1.34	1.41
23	C	479	CLA	C1D-C2D	-2.23	1.40	1.45
23	c	2482	CLA	C1-C2	2.23	1.55	1.49
23	c	2478	CLA	O2A-CGA	2.22	1.39	1.33
23	C	474	CLA	C1-C2	2.22	1.55	1.49
23	B	512	CLA	C1D-ND	-2.22	1.34	1.37
27	C	489	BCR	C33-C5	2.22	1.54	1.50
23	B	521	CLA	C1-C2	2.21	1.55	1.49
23	b	2519	CLA	C1C-NC	-2.21	1.34	1.37
27	k	2050	BCR	C5-C6	2.21	1.38	1.34
23	d	2357	CLA	CMD-C2D	2.21	1.55	1.50
23	D	354	CLA	C5-C3	2.20	1.55	1.51
27	b	2528	BCR	C7-C6	2.20	1.52	1.45
23	c	2476	CLA	C1C-C2C	2.20	1.49	1.44
27	k	2050	BCR	C16-C17	-2.20	1.36	1.43
23	B	515	CLA	C3A-C4A	-2.20	1.44	1.51
23	c	2485	CLA	CHD-C1D	2.20	1.42	1.38
23	b	2518	CLA	C1D-ND	-2.19	1.35	1.37
27	c	2488	BCR	C23-C22	-2.19	1.41	1.46
23	C	486	CLA	C1D-C2D	-2.19	1.41	1.45
23	B	513	CLA	C1D-ND	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2523	CLA	CBA-CGA	-2.19	1.44	1.50
23	d	2355	CLA	CAA-CBA	-2.19	1.46	1.52
27	K	50	BCR	C16-C17	-2.19	1.36	1.43
27	b	2528	BCR	C5-C6	2.19	1.38	1.34
23	b	2526	CLA	C1D-C2D	-2.19	1.41	1.45
23	C	484	CLA	C1-C2	2.19	1.55	1.49
23	B	512	CLA	C1D-C2D	-2.19	1.41	1.45
23	C	478	CLA	C1D-C2D	-2.19	1.41	1.45
23	B	517	CLA	C3A-C4A	-2.18	1.44	1.51
23	a	2348	CLA	C3B-C2B	-2.18	1.37	1.40
23	B	522	CLA	C4-C3	2.18	1.56	1.50
23	C	487	CLA	C5-C3	2.18	1.55	1.51
23	b	2518	CLA	O2A-CGA	2.18	1.39	1.33
23	b	2521	CLA	C1B-CHB	-2.18	1.34	1.41
28	E	84	HEC	C4D-ND	2.18	1.40	1.36
23	b	2524	CLA	MG-NC	2.18	2.11	2.06
25	A	353	PL9	C18-C19	2.17	1.38	1.33
23	c	2482	CLA	C1D-ND	-2.17	1.35	1.37
25	a	2352	PL9	C2-C3	2.17	1.40	1.34
23	C	485	CLA	CHD-C1D	2.17	1.42	1.38
28	e	2084	HEC	C1D-ND	2.17	1.40	1.36
23	C	482	CLA	CHC-C1C	2.17	1.39	1.34
25	D	357	PL9	C37-C38	-2.17	1.43	1.50
23	c	2479	CLA	C4-C3	2.17	1.56	1.50
23	C	481	CLA	C1B-CHB	-2.16	1.35	1.41
23	B	514	CLA	C1-C2	2.16	1.55	1.49
23	c	2484	CLA	C1B-CHB	-2.16	1.35	1.41
23	D	356	CLA	C1B-CHB	-2.16	1.35	1.41
23	b	2514	CLA	C1-C2	2.16	1.55	1.49
27	d	2360	BCR	C24-C23	2.16	1.39	1.33
23	B	511	CLA	C3A-C4A	-2.15	1.44	1.51
23	B	514	CLA	C3A-C4A	-2.15	1.44	1.51
23	C	483	CLA	C2-C3	2.15	1.38	1.33
23	b	2519	CLA	C5-C3	2.15	1.55	1.51
23	C	479	CLA	MG-NC	2.15	2.11	2.06
25	D	357	PL9	C7-C8	-2.14	1.47	1.50
23	B	517	CLA	C4-C3	2.14	1.55	1.50
23	D	354	CLA	C1D-ND	-2.13	1.35	1.37
23	D	356	CLA	C5-C3	2.13	1.55	1.51
28	v	2138	HEC	O1D-CGD	2.13	1.29	1.22
28	v	2138	HEC	CBC-CAC	-2.13	1.41	1.49
23	B	514	CLA	O2A-CGA	2.13	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2515	CLA	C1D-C2D	-2.13	1.41	1.45
23	c	2487	CLA	CMD-C2D	2.13	1.55	1.50
25	a	2352	PL9	C21-C19	-2.13	1.46	1.51
27	C	488	BCR	C19-C18	-2.12	1.41	1.46
23	c	2484	CLA	C5-C3	2.12	1.55	1.51
23	A	352	CLA	C4C-C3C	2.12	1.48	1.45
23	b	2524	CLA	O2A-C1	2.12	1.51	1.46
23	B	514	CLA	C1D-ND	-2.12	1.35	1.37
25	A	353	PL9	C40-C39	2.12	1.56	1.50
23	B	525	CLA	CHC-C1C	2.12	1.39	1.34
23	d	2354	CLA	C1-C2	2.12	1.55	1.49
23	C	474	CLA	C1C-NC	-2.12	1.34	1.37
23	C	483	CLA	C1D-ND	-2.12	1.35	1.37
23	b	2521	CLA	C1-C2	2.12	1.55	1.49
23	c	2484	CLA	C1-C2	2.12	1.55	1.49
23	B	511	CLA	C5-C3	2.12	1.55	1.51
23	C	483	CLA	C1-C2	2.11	1.55	1.49
23	b	2518	CLA	C3B-C2B	-2.11	1.37	1.40
23	C	475	CLA	C1D-C2D	-2.11	1.41	1.45
23	B	511	CLA	C4-C3	2.11	1.55	1.50
23	B	522	CLA	CAA-C2A	2.11	1.57	1.54
23	b	2516	CLA	C1B-CHB	-2.11	1.35	1.41
23	B	516	CLA	O2A-CGA	2.10	1.39	1.33
25	d	2358	PL9	C36-C34	-2.10	1.47	1.51
27	K	50	BCR	C15-C14	-2.10	1.36	1.43
23	C	481	CLA	C1D-C2D	-2.10	1.41	1.45
23	b	2515	CLA	CBA-CGA	-2.10	1.44	1.50
23	B	521	CLA	C5-C3	2.10	1.55	1.51
23	b	2520	CLA	C1D-C2D	-2.10	1.41	1.45
23	C	479	CLA	C1-C2	2.10	1.55	1.49
23	B	516	CLA	C1B-CHB	-2.09	1.35	1.41
23	b	2526	CLA	CHD-C1D	2.09	1.42	1.38
27	B	528	BCR	C38-C26	2.09	1.54	1.50
23	c	2481	CLA	C1D-ND	-2.09	1.35	1.37
24	d	2356	PHO	CAA-CBA	-2.09	1.46	1.52
23	C	487	CLA	CMA-C3A	2.08	1.57	1.53
23	c	2477	CLA	C1B-CHB	-2.08	1.35	1.41
23	A	350	CLA	C1B-CHB	-2.08	1.35	1.41
23	D	356	CLA	CAA-C2A	2.08	1.57	1.54
28	v	2138	HEC	C1B-CHB	2.08	1.46	1.41
23	C	478	CLA	C2-C3	2.08	1.37	1.33
23	A	352	CLA	CMB-C2B	2.07	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2512	CLA	C5-C3	2.07	1.55	1.51
23	c	2479	CLA	C3A-C4A	-2.07	1.45	1.51
23	c	2486	CLA	C5-C3	2.07	1.55	1.51
23	c	2474	CLA	C4C-C3C	2.07	1.48	1.45
23	a	2351	CLA	C1D-ND	-2.07	1.35	1.37
23	B	520	CLA	C5-C3	2.07	1.55	1.51
23	a	2349	CLA	C1B-CHB	-2.07	1.35	1.41
23	b	2516	CLA	CHD-C1D	2.07	1.42	1.38
23	c	2481	CLA	C1C-C2C	2.07	1.48	1.44
23	c	2482	CLA	CMD-C2D	2.07	1.55	1.50
23	C	476	CLA	C4-C3	2.06	1.55	1.50
25	D	357	PL9	C36-C34	-2.06	1.47	1.51
27	F	48	BCR	C24-C23	2.06	1.39	1.33
23	b	2515	CLA	CHD-C1D	2.06	1.42	1.38
23	B	513	CLA	MG-ND	-2.06	2.01	2.05
23	C	487	CLA	CMD-C2D	2.05	1.55	1.50
23	b	2522	CLA	C1C-NC	-2.05	1.34	1.37
23	B	518	CLA	C1D-ND	-2.05	1.35	1.37
23	c	2479	CLA	C1-C2	2.05	1.55	1.49
23	c	2484	CLA	C1C-C2C	2.05	1.48	1.44
23	b	2514	CLA	C3A-C4A	-2.05	1.45	1.51
23	b	2514	CLA	O2A-CGA	2.04	1.39	1.33
23	B	522	CLA	C5-C3	2.04	1.55	1.51
23	C	485	CLA	CBA-CGA	-2.04	1.44	1.50
24	D	355	PHO	C4-C3	2.04	1.55	1.50
28	e	2084	HEC	CBA-CGA	-2.04	1.45	1.50
23	b	2517	CLA	C3A-C4A	-2.04	1.45	1.51
28	e	2084	HEC	C2A-C3A	2.03	1.43	1.37
23	C	487	CLA	C4D-CHA	2.03	1.45	1.38
27	C	488	BCR	C40-C30	-2.03	1.49	1.53
23	b	2517	CLA	O2A-CGA	2.03	1.39	1.33
23	A	348	CLA	C4-C3	2.03	1.55	1.50
23	a	2348	CLA	C4-C3	2.03	1.55	1.50
27	k	2050	BCR	C38-C26	2.03	1.54	1.50
23	c	2474	CLA	C1-C2	2.03	1.54	1.49
23	c	2477	CLA	C1-C2	2.03	1.54	1.49
23	c	2483	CLA	C1B-CHB	-2.02	1.35	1.41
23	B	512	CLA	C1B-CHB	-2.02	1.35	1.41
27	c	2489	BCR	C38-C26	2.02	1.54	1.50
23	C	476	CLA	C1B-CHB	-2.02	1.35	1.41
23	C	482	CLA	C4C-C3C	2.02	1.48	1.45
25	d	2358	PL9	C22-C23	-2.02	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2521	CLA	O2A-CGA	2.02	1.39	1.33
23	b	2513	CLA	C2-C3	2.02	1.37	1.33
23	B	525	CLA	C1D-C2D	-2.02	1.41	1.45
23	a	2348	CLA	CBA-CGA	-2.02	1.44	1.50
23	b	2512	CLA	C1B-CHB	-2.02	1.35	1.41
25	d	2358	PL9	C7-C8	-2.02	1.47	1.50
23	D	356	CLA	C1D-ND	-2.01	1.35	1.37
23	b	2518	CLA	MG-ND	-2.01	2.01	2.05
23	c	2475	CLA	C6-C5	2.01	1.59	1.52
23	c	2482	CLA	C1B-CHB	-2.01	1.35	1.41
23	B	511	CLA	C1C-C2C	2.01	1.48	1.44
23	b	2517	CLA	C1D-ND	-2.01	1.35	1.37
23	c	2487	CLA	C4D-CHA	2.01	1.45	1.38
23	b	2519	CLA	MG-NC	2.01	2.11	2.06
23	C	484	CLA	C5-C3	2.01	1.55	1.51
23	C	484	CLA	OBD-CAD	2.01	1.25	1.22
23	c	2474	CLA	C1D-C2D	-2.00	1.41	1.45
27	b	2528	BCR	C37-C22	2.00	1.54	1.50
23	B	527	CLA	CMD-C2D	2.00	1.54	1.50
23	C	477	CLA	C1C-NC	-2.00	1.34	1.37

All (1365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	C4A-NA-C1A	14.75	113.41	106.68
23	B	513	CLA	C4A-NA-C1A	14.60	113.34	106.68
23	c	2479	CLA	C4A-NA-C1A	14.27	113.19	106.68
23	B	511	CLA	C4A-NA-C1A	14.15	113.13	106.68
23	B	519	CLA	C4A-NA-C1A	13.99	113.06	106.68
23	b	2511	CLA	C4A-NA-C1A	13.96	113.05	106.68
23	d	2357	CLA	C4A-NA-C1A	13.85	113.00	106.68
23	D	356	CLA	C4A-NA-C1A	13.83	112.99	106.68
23	C	479	CLA	C4A-NA-C1A	13.81	112.98	106.68
23	b	2512	CLA	C4A-NA-C1A	13.75	112.95	106.68
23	b	2523	CLA	C4A-NA-C1A	13.68	112.92	106.68
23	B	523	CLA	C4A-NA-C1A	13.52	112.85	106.68
23	B	512	CLA	C4A-NA-C1A	13.41	112.80	106.68
23	B	517	CLA	C4A-NA-C1A	13.35	112.77	106.68
23	C	483	CLA	C4A-NA-C1A	13.32	112.76	106.68
23	A	352	CLA	C4A-NA-C1A	13.32	112.75	106.68
23	A	349	CLA	C4A-NA-C1A	13.25	112.72	106.68
23	b	2525	CLA	C4A-NA-C1A	13.24	112.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2522	CLA	C4A-NA-C1A	13.20	112.70	106.68
23	B	524	CLA	C4A-NA-C1A	13.19	112.70	106.68
23	C	476	CLA	C4A-NA-C1A	13.18	112.69	106.68
23	c	2483	CLA	C4A-NA-C1A	13.16	112.69	106.68
23	c	2478	CLA	C4A-NA-C1A	13.14	112.67	106.68
23	B	522	CLA	C4A-NA-C1A	13.14	112.67	106.68
23	a	2351	CLA	C4A-NA-C1A	13.07	112.64	106.68
23	b	2520	CLA	C4A-NA-C1A	13.07	112.64	106.68
23	C	474	CLA	C4A-NA-C1A	13.05	112.63	106.68
23	C	478	CLA	C4A-NA-C1A	13.01	112.61	106.68
23	C	482	CLA	C4A-NA-C1A	13.00	112.61	106.68
23	b	2518	CLA	C4A-NA-C1A	12.96	112.59	106.68
23	B	518	CLA	C4A-NA-C1A	12.96	112.59	106.68
23	b	2524	CLA	C4A-NA-C1A	12.92	112.57	106.68
23	B	525	CLA	C4A-NA-C1A	12.91	112.57	106.68
23	c	2484	CLA	C4A-NA-C1A	12.90	112.56	106.68
23	C	481	CLA	C4A-NA-C1A	12.84	112.54	106.68
23	b	2519	CLA	C4A-NA-C1A	12.83	112.53	106.68
23	c	2481	CLA	C4A-NA-C1A	12.80	112.52	106.68
23	c	2480	CLA	C4A-NA-C1A	12.78	112.51	106.68
23	b	2517	CLA	C4A-NA-C1A	12.72	112.48	106.68
23	B	520	CLA	C4A-NA-C1A	12.68	112.46	106.68
23	c	2486	CLA	C4A-NA-C1A	12.65	112.45	106.68
23	C	480	CLA	C4A-NA-C1A	12.61	112.43	106.68
23	d	2355	CLA	C4A-NA-C1A	12.61	112.43	106.68
23	C	484	CLA	C4A-NA-C1A	12.60	112.43	106.68
23	B	516	CLA	C4A-NA-C1A	12.60	112.43	106.68
23	b	2516	CLA	C4A-NA-C1A	12.58	112.42	106.68
23	c	2474	CLA	C4A-NA-C1A	12.54	112.40	106.68
23	c	2476	CLA	C4A-NA-C1A	12.50	112.38	106.68
23	C	475	CLA	C4A-NA-C1A	12.43	112.35	106.68
23	c	2482	CLA	C4A-NA-C1A	12.38	112.33	106.68
23	B	514	CLA	C4A-NA-C1A	12.37	112.32	106.68
23	b	2514	CLA	C4A-NA-C1A	12.34	112.31	106.68
23	C	486	CLA	C4A-NA-C1A	12.30	112.29	106.68
23	b	2515	CLA	C4A-NA-C1A	12.10	112.20	106.68
23	b	2526	CLA	C4A-NA-C1A	12.02	112.16	106.68
23	c	2485	CLA	C4A-NA-C1A	11.99	112.15	106.68
23	A	348	CLA	C4A-NA-C1A	11.83	112.08	106.68
23	B	527	CLA	C4A-NA-C1A	11.80	112.06	106.68
23	B	515	CLA	C4A-NA-C1A	11.72	112.03	106.68
23	c	2475	CLA	C4A-NA-C1A	11.69	112.01	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	485	CLA	C4A-NA-C1A	11.56	111.95	106.68
23	d	2354	CLA	C4A-NA-C1A	11.53	111.94	106.68
23	D	354	CLA	C4A-NA-C1A	11.50	111.92	106.68
23	a	2348	CLA	C4A-NA-C1A	11.49	111.92	106.68
23	b	2521	CLA	C4A-NA-C1A	11.33	111.85	106.68
23	A	350	CLA	C4A-NA-C1A	11.28	111.83	106.68
23	c	2477	CLA	C4A-NA-C1A	11.28	111.83	106.68
23	B	521	CLA	C4A-NA-C1A	11.24	111.81	106.68
23	C	477	CLA	C4A-NA-C1A	11.14	111.76	106.68
23	C	487	CLA	C4A-NA-C1A	11.06	111.72	106.68
23	a	2349	CLA	C4A-NA-C1A	10.96	111.68	106.68
23	c	2487	CLA	C4A-NA-C1A	10.36	111.41	106.68
23	B	520	CLA	CBA-CAA-C2A	9.79	142.93	113.79
23	b	2520	CLA	CBA-CAA-C2A	9.77	142.88	113.79
28	V	138	HEC	CBD-CAD-C3D	-9.64	96.33	112.54
26	d	2359	LMT	O1'-C1-C2	9.19	140.53	109.37
26	B	526	LMT	O1'-C1-C2	9.17	140.49	109.37
28	E	84	HEC	CBB-CAB-C3B	-8.97	106.50	127.49
28	e	2084	HEC	CBB-CAB-C3B	-8.92	106.62	127.49
28	v	2138	HEC	CBB-CAB-C3B	-8.91	106.63	127.49
23	A	349	CLA	C1-C2-C3	8.19	139.61	126.20
28	V	138	HEC	CBB-CAB-C3B	-8.10	108.53	127.49
28	v	2138	HEC	CMC-C2C-C3C	8.07	135.30	125.82
23	C	477	CLA	CBA-CAA-C2A	7.90	137.30	113.79
23	d	2355	CLA	C1-C2-C3	7.80	138.98	126.20
23	c	2477	CLA	CBA-CAA-C2A	7.80	137.00	113.79
23	B	519	CLA	C1-C2-C3	7.66	138.74	126.20
23	d	2354	CLA	C1-C2-C3	7.61	138.66	126.20
23	D	354	CLA	C1-C2-C3	7.57	138.59	126.20
23	b	2519	CLA	C1-C2-C3	7.52	138.52	126.20
23	B	520	CLA	CAA-C2A-C1A	-7.51	87.37	111.97
28	v	2138	HEC	CMD-C2D-C1D	-7.50	117.47	128.46
23	b	2520	CLA	CAA-C2A-C1A	-7.49	87.43	111.97
28	v	2138	HEC	CMD-C2D-C3D	7.41	138.92	124.94
23	C	481	CLA	CBA-CAA-C2A	6.96	134.49	113.79
23	b	2524	CLA	C1-C2-C3	6.92	137.53	126.20
27	b	2527	BCR	C33-C5-C6	6.90	132.01	124.48
27	B	528	BCR	C33-C5-C6	6.90	132.01	124.48
28	v	2138	HEC	CBD-CAD-C3D	-6.86	101.00	112.54
23	c	2481	CLA	CBA-CAA-C2A	6.74	133.84	113.79
23	B	524	CLA	C1-C2-C3	6.64	137.08	126.20
25	a	2352	PL9	C22-C23-C24	6.49	142.47	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2520	CLA	CAA-CBA-CGA	-6.48	94.80	113.21
23	B	520	CLA	CAA-CBA-CGA	-6.43	94.95	113.21
23	b	2519	CLA	CBA-CAA-C2A	6.43	132.92	113.79
27	B	529	BCR	C38-C26-C25	6.33	131.40	124.48
25	D	357	PL9	C37-C36-C34	6.27	133.97	113.19
25	d	2358	PL9	C37-C36-C34	6.25	133.88	113.19
23	B	519	CLA	CBA-CAA-C2A	6.23	132.33	113.79
27	d	2360	BCR	C33-C5-C6	6.21	131.26	124.48
23	c	2477	CLA	CAA-C2A-C1A	-6.20	91.66	111.97
23	C	483	CLA	CBA-CAA-C2A	6.19	132.20	113.79
23	C	477	CLA	CAA-C2A-C1A	-6.11	91.96	111.97
28	v	2138	HEC	C4C-C3C-C2C	6.05	112.89	106.35
27	F	48	BCR	C33-C5-C6	5.95	130.97	124.48
27	B	529	BCR	C20-C21-C22	-5.94	118.94	127.28
23	c	2483	CLA	CBA-CAA-C2A	5.94	131.48	113.79
27	j	2053	BCR	C33-C5-C6	5.90	130.92	124.48
27	b	2527	BCR	C38-C26-C25	5.90	130.92	124.48
27	F	48	BCR	C16-C17-C18	5.88	135.53	127.28
25	A	353	PL9	C22-C23-C24	5.88	141.08	127.62
25	A	353	PL9	C37-C36-C34	5.85	132.56	113.19
23	B	519	CLA	CAA-C2A-C1A	-5.76	93.09	111.97
23	b	2519	CLA	CAA-C2A-C1A	-5.74	93.15	111.97
25	a	2352	PL9	C37-C36-C34	5.74	132.20	113.19
27	B	528	BCR	C38-C26-C25	5.74	130.75	124.48
27	J	53	BCR	C33-C5-C6	5.72	130.72	124.48
27	J	53	BCR	C38-C26-C25	5.71	130.72	124.48
27	d	2360	BCR	C16-C17-C18	5.71	135.29	127.28
27	b	2528	BCR	C38-C26-C25	5.69	130.70	124.48
28	e	2084	HEC	CBC-CAC-C3C	-5.65	114.28	127.49
27	c	2489	BCR	C33-C5-C6	5.63	130.63	124.48
27	j	2053	BCR	C38-C26-C25	5.54	130.53	124.48
27	b	2528	BCR	C20-C21-C22	-5.52	119.53	127.28
28	E	84	HEC	CBC-CAC-C3C	-5.52	114.57	127.49
27	C	489	BCR	C33-C5-C6	5.50	130.49	124.48
27	F	48	BCR	C38-C26-C25	5.49	130.47	124.48
23	C	475	CLA	O2A-CGA-CBA	5.43	128.40	111.83
23	c	2475	CLA	O2A-CGA-CBA	5.39	128.27	111.83
27	K	50	BCR	C38-C26-C25	5.34	130.31	124.48
23	C	481	CLA	CAA-CBA-CGA	-5.29	98.19	113.21
23	B	516	CLA	O2A-CGA-CBA	5.27	127.90	111.83
23	b	2516	CLA	O2A-CGA-CBA	5.22	127.76	111.83
23	B	512	CLA	C1-C2-C3	5.22	134.75	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2481	CLA	CAA-CBA-CGA	-5.22	98.38	113.21
27	d	2360	BCR	C38-C26-C25	5.15	130.10	124.48
28	e	2084	HEC	CBA-CAA-C2A	-5.12	104.11	112.55
27	k	2050	BCR	C38-C26-C25	5.06	130.00	124.48
23	b	2512	CLA	C1-C2-C3	5.04	134.46	126.20
28	E	84	HEC	CBA-CAA-C2A	-5.00	104.30	112.55
27	C	488	BCR	C38-C26-C25	4.99	129.93	124.48
28	V	138	HEC	CMD-C2D-C1D	-4.99	121.14	128.46
23	c	2478	CLA	C1-C2-C3	4.96	134.32	126.20
25	A	353	PL9	C35-C34-C36	-4.95	106.63	115.23
27	C	488	BCR	C33-C5-C6	4.92	129.85	124.48
27	F	48	BCR	C11-C10-C9	4.89	134.14	127.28
28	v	2138	HEC	C1D-C2D-C3D	-4.86	103.61	107.00
27	K	50	BCR	C33-C5-C6	4.82	129.75	124.48
27	c	2488	BCR	C38-C26-C25	4.82	129.75	124.48
27	c	2488	BCR	C33-C5-C6	4.80	129.72	124.48
24	D	355	PHO	O2D-CGD-CBD	4.78	116.20	110.95
27	d	2360	BCR	C11-C10-C9	4.73	133.92	127.28
25	a	2352	PL9	C35-C34-C36	-4.71	107.05	115.23
27	B	529	BCR	C2-C1-C6	4.70	117.27	110.44
23	c	2477	CLA	C7-C6-C5	-4.69	100.77	113.26
23	C	478	CLA	C1-C2-C3	4.68	133.87	126.20
26	d	2359	LMT	C1B-O1B-C4'	-4.68	106.88	117.98
27	k	2050	BCR	C33-C5-C6	4.68	129.59	124.48
23	B	518	CLA	CBA-CAA-C2A	4.67	127.70	113.79
23	c	2483	CLA	CAA-C2A-C1A	-4.66	96.70	111.97
23	C	477	CLA	CAA-CBA-CGA	-4.65	100.00	113.21
23	C	477	CLA	C7-C6-C5	-4.63	100.93	113.26
27	F	48	BCR	C8-C9-C10	-4.61	111.76	119.01
23	c	2479	CLA	CAA-CBA-CGA	-4.60	100.16	113.21
23	b	2523	CLA	CBA-CAA-C2A	4.58	127.41	113.79
23	B	523	CLA	CBA-CAA-C2A	4.57	127.39	113.79
23	b	2518	CLA	CBA-CAA-C2A	4.56	127.38	113.79
23	c	2477	CLA	CAA-CBA-CGA	-4.54	100.31	113.21
27	c	2489	BCR	C38-C26-C25	4.54	129.44	124.48
23	C	483	CLA	CAA-C2A-C1A	-4.54	97.11	111.97
27	C	489	BCR	C38-C26-C25	4.52	129.42	124.48
25	A	353	PL9	C36-C34-C33	4.52	131.30	121.17
27	b	2528	BCR	C2-C1-C6	4.48	116.94	110.44
24	a	2350	PHO	O2D-CGD-CBD	4.48	115.86	110.95
25	a	2352	PL9	C26-C24-C23	-4.46	111.17	121.17
24	A	351	PHO	O2D-CGD-CBD	4.44	115.82	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	526	LMT	C1B-O1B-C4'	-4.44	107.46	117.98
27	B	529	BCR	C21-C20-C19	4.43	136.04	123.20
23	B	511	CLA	CBA-CAA-C2A	4.43	126.98	113.79
27	F	48	BCR	C7-C8-C9	4.43	132.79	126.23
23	B	527	CLA	C1-O2A-CGA	4.42	127.36	116.65
23	b	2511	CLA	CBA-CAA-C2A	4.42	126.95	113.79
25	a	2352	PL9	C36-C34-C33	4.42	131.08	121.17
27	d	2360	BCR	C8-C9-C10	-4.41	112.07	119.01
23	b	2524	CLA	C1-O2A-CGA	4.39	127.29	116.65
23	b	2513	CLA	CAA-CBA-CGA	4.39	125.68	113.21
25	D	357	PL9	C35-C34-C36	-4.39	107.61	115.23
23	b	2526	CLA	C1-O2A-CGA	4.38	127.26	116.65
27	b	2528	BCR	C21-C20-C19	4.37	135.88	123.20
27	K	50	BCR	C2-C1-C6	4.36	116.77	110.44
27	B	528	BCR	C2-C1-C6	4.33	116.73	110.44
27	k	2050	BCR	C2-C1-C6	4.31	116.70	110.44
23	B	513	CLA	CAA-CBA-CGA	4.31	125.44	113.21
23	B	524	CLA	C1-O2A-CGA	4.30	127.06	116.65
23	D	356	CLA	C1-C2-C3	4.30	133.24	126.20
28	v	2138	HEC	CBC-CAC-C3C	-4.30	117.43	127.49
28	V	138	HEC	CMD-C2D-C3D	4.29	133.03	124.94
23	C	479	CLA	CAA-CBA-CGA	-4.28	101.07	113.21
23	a	2351	CLA	C1-C2-C3	4.25	133.16	126.20
23	c	2476	CLA	C1-C2-C3	4.25	133.16	126.20
23	d	2357	CLA	C1-C2-C3	4.25	133.16	126.20
25	d	2358	PL9	C35-C34-C36	-4.24	107.87	115.23
28	V	138	HEC	C4C-C3C-C2C	4.23	110.92	106.35
23	c	2487	CLA	CMB-C2B-C1B	-4.22	122.28	128.46
23	C	487	CLA	CAC-C3C-C4C	4.19	130.24	124.79
27	d	2360	BCR	C7-C8-C9	4.16	132.39	126.23
23	B	513	CLA	CBA-CAA-C2A	4.14	126.10	113.79
27	C	488	BCR	C16-C17-C18	4.10	133.03	127.28
23	c	2481	CLA	CAA-C2A-C1A	-4.08	98.59	111.97
23	B	519	CLA	CAA-CBA-CGA	-4.06	101.67	113.21
27	b	2527	BCR	C33-C5-C4	-4.06	104.94	113.60
23	b	2518	CLA	O2A-CGA-CBA	4.06	124.22	111.83
23	c	2482	CLA	C1-C2-C3	4.06	132.85	126.20
27	b	2527	BCR	C2-C1-C6	4.05	116.33	110.44
27	b	2527	BCR	C29-C30-C25	4.02	116.28	110.44
27	d	2360	BCR	C23-C24-C25	4.02	137.74	127.00
25	A	353	PL9	C26-C24-C23	-4.02	112.15	121.17
27	C	489	BCR	C2-C1-C6	4.02	116.27	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	518	CLA	O2A-CGA-CBA	4.01	124.08	111.83
23	C	487	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
27	c	2488	BCR	C29-C30-C25	4.01	116.27	110.44
23	C	482	CLA	C1-C2-C3	4.01	132.77	126.20
27	J	53	BCR	C29-C30-C25	4.01	116.27	110.44
23	C	479	CLA	CBA-CAA-C2A	4.00	125.69	113.79
23	C	476	CLA	C1-C2-C3	4.00	132.75	126.20
28	v	2138	HEC	CMB-C2B-C1B	-3.99	122.60	128.46
23	C	482	CLA	C1-O2A-CGA	3.99	126.31	116.65
23	b	2526	CLA	C7-C6-C5	-3.98	102.64	113.26
25	a	2352	PL9	C7-C8-C9	3.98	133.68	126.83
23	B	511	CLA	CAA-C2A-C1A	-3.96	99.00	111.97
27	C	489	BCR	C29-C30-C25	3.96	116.19	110.44
27	B	528	BCR	C29-C30-C25	3.95	116.18	110.44
27	B	529	BCR	C30-C25-C26	-3.95	117.24	122.64
23	c	2479	CLA	CBA-CAA-C2A	3.94	125.53	113.79
23	b	2526	CLA	CAA-CBA-CGA	-3.94	102.03	113.21
23	B	527	CLA	C7-C6-C5	-3.93	102.78	113.26
23	a	2348	CLA	C1-O2A-CGA	3.93	126.17	116.65
23	b	2511	CLA	CAA-C2A-C1A	-3.92	99.12	111.97
25	D	357	PL9	C30-C29-C31	3.92	122.03	115.23
23	c	2487	CLA	CAC-C3C-C4C	3.91	129.88	124.79
28	E	84	HEC	C4C-C3C-C2C	3.91	110.58	106.35
27	c	2488	BCR	C16-C17-C18	3.90	132.75	127.28
24	a	2350	PHO	C1-C2-C3	3.90	132.59	126.20
25	A	353	PL9	C7-C8-C9	3.90	133.55	126.83
23	B	514	CLA	O2A-CGA-CBA	3.88	123.67	111.83
23	B	514	CLA	CBA-CAA-C2A	3.86	125.28	113.79
23	C	481	CLA	CAA-C2A-C1A	-3.86	99.33	111.97
27	F	48	BCR	C2-C1-C6	3.86	116.04	110.44
23	b	2516	CLA	O2A-C1-C2	3.85	122.93	108.11
23	b	2513	CLA	CBA-CAA-C2A	3.85	125.25	113.79
23	B	518	CLA	CAA-C2A-C1A	-3.85	99.37	111.97
23	A	348	CLA	C1-O2A-CGA	3.84	125.96	116.65
23	c	2482	CLA	C1-O2A-CGA	3.84	125.96	116.65
23	B	516	CLA	O2A-C1-C2	3.84	122.88	108.11
23	B	511	CLA	CAA-CBA-CGA	-3.84	102.31	113.21
27	b	2528	BCR	C30-C25-C26	-3.82	117.41	122.64
27	c	2489	BCR	C2-C1-C6	3.82	115.99	110.44
27	C	489	BCR	C23-C24-C25	3.81	137.19	127.00
23	b	2514	CLA	CAA-C2A-C3A	-3.81	102.69	113.00
23	b	2512	CLA	C1-O2A-CGA	3.81	125.87	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2519	CLA	CAA-CBA-CGA	-3.81	102.39	113.21
23	B	513	CLA	C7-C6-C5	-3.81	103.12	113.26
27	F	48	BCR	C23-C24-C25	3.81	137.17	127.00
27	b	2528	BCR	C29-C30-C25	3.81	115.97	110.44
23	B	527	CLA	CAA-CBA-CGA	-3.81	102.40	113.21
27	K	50	BCR	C29-C30-C25	3.80	115.97	110.44
23	c	2476	CLA	C7-C6-C5	-3.80	103.12	113.26
23	A	349	CLA	CBA-CAA-C2A	3.80	125.09	113.79
27	d	2360	BCR	C29-C30-C25	3.79	115.95	110.44
23	d	2355	CLA	CBA-CAA-C2A	3.78	125.04	113.79
27	B	528	BCR	C33-C5-C4	-3.78	105.53	113.60
27	d	2360	BCR	C2-C1-C6	3.77	115.92	110.44
23	b	2525	CLA	CED-O2D-CGD	3.76	124.45	115.92
25	d	2358	PL9	C30-C29-C31	3.76	121.75	115.23
23	A	349	CLA	O2A-CGA-CBA	3.76	123.29	111.83
23	C	474	CLA	CBA-CAA-C2A	3.75	124.94	113.79
28	V	138	HEC	O1D-CGD-CBD	-3.74	111.22	123.09
23	A	350	CLA	CBA-CAA-C2A	3.74	124.93	113.79
23	B	514	CLA	CAA-C2A-C1A	-3.74	99.71	111.97
24	a	2350	PHO	OBD-CAD-CBD	-3.74	120.34	125.82
23	b	2518	CLA	CAA-C2A-C1A	-3.73	99.76	111.97
23	B	523	CLA	CAA-CBA-CGA	-3.73	102.63	113.21
23	C	478	CLA	C2A-C1A-CHA	3.72	130.32	123.87
23	c	2474	CLA	CBA-CAA-C2A	3.71	124.84	113.79
25	A	353	PL9	C21-C22-C23	-3.71	93.65	112.02
25	A	353	PL9	C27-C26-C24	-3.71	100.89	113.19
23	b	2514	CLA	CBA-CAA-C2A	3.71	124.83	113.79
24	D	355	PHO	C7-C6-C5	-3.71	103.37	113.26
23	C	479	CLA	CAA-C2A-C1A	-3.71	99.82	111.97
23	B	514	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
23	b	2523	CLA	CAA-CBA-CGA	-3.71	102.68	113.21
23	b	2514	CLA	O2A-CGA-CBA	3.71	123.14	111.83
23	b	2526	CLA	C6-C5-C3	3.71	122.50	113.47
27	c	2489	BCR	C29-C30-C25	3.71	115.82	110.44
27	k	2050	BCR	C29-C30-C25	3.70	115.82	110.44
23	B	520	CLA	C1-C2-C3	3.70	132.27	126.20
23	B	523	CLA	CAA-C2A-C1A	-3.70	99.85	111.97
23	B	525	CLA	CED-O2D-CGD	3.69	124.30	115.92
27	b	2527	BCR	C24-C23-C22	3.69	131.70	126.23
23	c	2480	CLA	CBA-CAA-C2A	3.69	124.79	113.79
24	d	2356	PHO	O2D-CGD-CBD	3.68	114.99	110.95
23	B	512	CLA	C1-O2A-CGA	3.68	125.56	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	527	CLA	C6-C5-C3	3.68	122.42	113.47
27	B	529	BCR	C1-C6-C5	-3.67	117.62	122.64
27	c	2489	BCR	C23-C24-C25	3.67	136.80	127.00
23	c	2479	CLA	CAA-C2A-C1A	-3.66	99.97	111.97
23	b	2511	CLA	CAA-CBA-CGA	-3.66	102.81	113.21
23	b	2514	CLA	CAA-C2A-C1A	-3.66	99.98	111.97
27	F	48	BCR	C29-C30-C25	3.65	115.75	110.44
23	c	2478	CLA	C2A-C1A-CHA	3.65	130.21	123.87
27	J	53	BCR	C24-C23-C22	3.65	131.64	126.23
27	b	2528	BCR	C1-C6-C5	-3.65	117.65	122.64
27	B	528	BCR	C24-C23-C22	3.64	131.62	126.23
23	A	352	CLA	C1-C2-C3	3.63	132.15	126.20
23	b	2523	CLA	CAA-C2A-C1A	-3.63	100.09	111.97
23	B	515	CLA	CBA-CAA-C2A	3.62	124.58	113.79
23	b	2520	CLA	C1-C2-C3	3.62	132.13	126.20
23	C	480	CLA	CBA-CAA-C2A	3.62	124.56	113.79
25	a	2352	PL9	C27-C26-C24	-3.62	101.19	113.19
23	b	2513	CLA	C7-C6-C5	-3.62	103.62	113.26
23	a	2349	CLA	CBA-CAA-C2A	3.62	124.55	113.79
28	e	2084	HEC	CMD-C2D-C1D	-3.61	123.17	128.46
27	j	2053	BCR	C24-C23-C22	3.61	131.57	126.23
23	b	2523	CLA	CED-O2D-CGD	3.60	124.08	115.92
27	B	529	BCR	C29-C30-C25	3.60	115.67	110.44
23	d	2355	CLA	O2A-CGA-CBA	3.60	122.81	111.83
23	c	2483	CLA	O2A-CGA-CBA	3.60	122.80	111.83
27	C	488	BCR	C29-C30-C25	3.59	115.66	110.44
23	C	484	CLA	C1-C2-C3	3.59	132.07	126.20
27	F	48	BCR	C16-C15-C14	3.59	130.86	123.52
27	C	488	BCR	C23-C24-C25	3.58	136.57	127.00
25	a	2352	PL9	C21-C22-C23	-3.57	94.33	112.02
23	B	515	CLA	CED-O2D-CGD	3.57	124.02	115.92
23	B	513	CLA	C1-C2-C3	3.57	132.05	126.20
25	D	357	PL9	C36-C34-C33	3.57	129.17	121.17
23	C	479	CLA	C7-C6-C5	-3.56	103.77	113.26
23	c	2475	CLA	CED-O2D-CGD	3.56	123.99	115.92
25	a	2352	PL9	C32-C31-C29	3.55	124.94	113.19
23	a	2349	CLA	C7-C6-C5	-3.55	103.81	113.26
23	c	2478	CLA	O2A-CGA-CBA	3.54	122.62	111.83
23	b	2525	CLA	C7-C6-C5	-3.53	103.86	113.26
23	C	478	CLA	O2A-CGA-CBA	3.53	122.59	111.83
23	c	2486	CLA	C1-C2-C3	3.53	131.98	126.20
23	C	474	CLA	C1-O2A-CGA	3.53	125.19	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	353	PL9	C32-C31-C29	3.53	124.87	113.19
28	E	84	HEC	CMA-C3A-C2A	3.52	131.59	124.94
23	b	2515	CLA	CBA-CAA-C2A	3.52	124.27	113.79
25	d	2358	PL9	C36-C34-C33	3.52	129.07	121.17
27	d	2360	BCR	C33-C5-C4	-3.52	106.09	113.60
23	b	2515	CLA	C1-C2-C3	3.52	131.96	126.20
23	B	523	CLA	CED-O2D-CGD	3.51	123.88	115.92
23	B	527	CLA	O2A-C1-C2	-3.51	94.60	108.11
23	c	2477	CLA	O2A-CGA-CBA	3.51	122.54	111.83
27	J	53	BCR	C2-C1-C6	3.50	115.53	110.44
23	B	521	CLA	CED-O2D-CGD	3.50	123.86	115.92
23	b	2513	CLA	C1-C2-C3	3.50	131.93	126.20
23	A	350	CLA	C7-C6-C5	-3.50	103.94	113.26
23	C	477	CLA	O2A-CGA-CBA	3.49	122.49	111.83
27	d	2360	BCR	C16-C15-C14	3.49	130.66	123.52
24	A	351	PHO	C1-C2-C3	3.48	131.90	126.20
23	C	483	CLA	O2A-CGA-CBA	3.48	122.45	111.83
27	b	2527	BCR	C38-C26-C27	-3.48	106.17	113.60
23	b	2526	CLA	O2A-C1-C2	-3.48	94.73	108.11
24	a	2350	PHO	C7-C6-C5	-3.47	104.00	113.26
27	c	2488	BCR	C23-C24-C25	3.47	136.27	127.00
23	c	2479	CLA	C7-C6-C5	-3.47	104.01	113.26
23	b	2512	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
24	d	2356	PHO	C7-C6-C5	-3.47	104.02	113.26
27	J	53	BCR	C33-C5-C4	-3.47	106.20	113.60
23	b	2526	CLA	CBA-CAA-C2A	3.46	124.08	113.79
23	C	477	CLA	CED-O2D-CGD	3.45	123.75	115.92
27	j	2053	BCR	C7-C8-C9	3.45	131.34	126.23
23	c	2477	CLA	CED-O2D-CGD	3.45	123.73	115.92
23	c	2484	CLA	C1-C2-C3	3.44	131.84	126.20
23	d	2354	CLA	O2A-CGA-CBA	3.44	122.34	111.83
23	B	524	CLA	C7-C6-C5	-3.44	104.09	113.26
23	B	515	CLA	CAA-C2A-C3A	-3.44	103.70	113.00
28	V	138	HEC	CMB-C2B-C1B	-3.44	123.42	128.46
23	B	527	CLA	CBA-CAA-C2A	3.43	124.00	113.79
23	C	486	CLA	C7-C6-C5	-3.43	104.13	113.26
23	b	2520	CLA	O2D-CGD-CBD	3.42	117.22	111.23
23	D	354	CLA	O2A-CGA-CBA	3.42	122.27	111.83
27	c	2488	BCR	C8-C9-C10	-3.42	113.63	119.01
23	C	478	CLA	CMB-C2B-C1B	-3.42	123.45	128.46
23	C	485	CLA	CED-O2D-CGD	3.42	123.67	115.92
23	C	476	CLA	C7-C6-C5	-3.41	104.18	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2481	CLA	C7-C6-C5	-3.41	104.19	113.26
23	b	2515	CLA	CED-O2D-CGD	3.41	123.64	115.92
27	F	48	BCR	C33-C5-C4	-3.40	106.35	113.60
23	C	483	CLA	C1-C2-C3	3.40	131.76	126.20
27	C	488	BCR	C2-C1-C6	3.39	115.37	110.44
23	C	486	CLA	C1-C2-C3	3.37	131.72	126.20
27	j	2053	BCR	C2-C1-C6	3.37	115.33	110.44
27	j	2053	BCR	C33-C5-C4	-3.37	106.41	113.60
23	b	2524	CLA	C5-C3-C2	-3.37	113.61	121.17
23	c	2485	CLA	CED-O2D-CGD	3.37	123.56	115.92
23	b	2515	CLA	C1-O2A-CGA	3.36	124.79	116.65
23	c	2478	CLA	CMB-C2B-C1B	-3.36	123.53	128.46
27	B	528	BCR	C38-C26-C27	-3.36	106.44	113.60
27	j	2053	BCR	C8-C9-C10	-3.35	113.74	119.01
23	B	515	CLA	CAA-CBA-CGA	-3.35	103.70	113.21
24	A	351	PHO	C7-C6-C5	-3.35	104.34	113.26
27	F	48	BCR	C38-C26-C27	-3.35	106.46	113.60
23	B	515	CLA	C1-C2-C3	3.34	131.68	126.20
23	b	2521	CLA	CED-O2D-CGD	3.34	123.49	115.92
23	B	517	CLA	O2A-CGA-CBA	3.34	122.02	111.83
27	b	2527	BCR	C23-C24-C25	3.34	135.92	127.00
27	c	2488	BCR	C2-C1-C6	3.34	115.29	110.44
23	c	2479	CLA	CED-O2D-CGD	3.34	123.48	115.92
27	B	529	BCR	C33-C5-C6	3.34	128.12	124.48
23	c	2487	CLA	CED-O2D-CGD	3.33	123.48	115.92
27	b	2528	BCR	C33-C5-C6	3.33	128.12	124.48
23	b	2515	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
23	B	525	CLA	C1-C2-C3	3.33	131.65	126.20
23	c	2486	CLA	C7-C6-C5	-3.33	104.40	113.26
27	j	2053	BCR	C29-C30-C25	3.32	115.27	110.44
25	D	357	PL9	C32-C31-C29	3.32	124.19	113.19
24	A	351	PHO	OBD-CAD-CBD	-3.32	120.95	125.82
26	B	526	LMT	C1-O1'-C1'	-3.31	108.02	113.68
23	c	2486	CLA	O2A-CGA-CBA	3.31	121.92	111.83
23	B	512	CLA	C7-C6-C5	-3.31	104.45	113.26
23	C	481	CLA	C7-C6-C5	-3.30	104.46	113.26
23	b	2513	CLA	O2A-CGA-CBA	3.30	121.90	111.83
27	c	2489	BCR	C7-C8-C9	3.30	131.12	126.23
27	j	2053	BCR	C23-C22-C21	-3.30	113.83	119.01
23	C	475	CLA	CED-O2D-CGD	3.29	123.38	115.92
27	C	488	BCR	C8-C9-C10	-3.29	113.84	119.01
27	B	529	BCR	C38-C26-C27	-3.29	106.59	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	2358	PL9	C32-C31-C29	3.28	124.06	113.19
23	B	522	CLA	CMB-C2B-C1B	-3.28	123.65	128.46
23	b	2519	CLA	CED-O2D-CGD	3.28	123.35	115.92
27	K	50	BCR	C7-C8-C9	3.28	131.08	126.23
23	c	2474	CLA	C7-C6-C5	-3.27	104.54	113.26
23	c	2484	CLA	CED-O2D-CGD	3.27	123.33	115.92
23	B	511	CLA	CED-O2D-CGD	3.27	123.33	115.92
27	B	528	BCR	C23-C24-C25	3.27	135.72	127.00
27	k	2050	BCR	C7-C8-C9	3.26	131.06	126.23
23	c	2478	CLA	CED-O2D-CGD	3.26	123.31	115.92
23	C	474	CLA	C1-C2-C3	3.26	131.54	126.20
23	b	2511	CLA	CED-O2D-CGD	3.26	123.30	115.92
27	C	488	BCR	C38-C26-C27	-3.25	106.66	113.60
23	c	2474	CLA	C1-O2A-CGA	3.25	124.53	116.65
23	B	519	CLA	O2A-CGA-CBA	3.25	121.75	111.83
23	C	485	CLA	C7-C6-C5	-3.25	104.60	113.26
23	b	2522	CLA	CMB-C2B-C1B	-3.25	123.70	128.46
23	B	515	CLA	C1-O2A-CGA	3.25	124.51	116.65
23	c	2474	CLA	O2D-CGD-CBD	3.24	116.89	111.23
23	C	480	CLA	O2A-CGA-CBA	3.23	121.69	111.83
23	b	2512	CLA	C7-C6-C5	-3.22	104.67	113.26
27	C	489	BCR	C33-C5-C4	-3.22	106.72	113.60
23	c	2483	CLA	C1-C2-C3	3.22	131.47	126.20
23	b	2517	CLA	O2A-CGA-CBA	3.22	121.66	111.83
23	C	486	CLA	O2A-CGA-CBA	3.22	121.64	111.83
23	B	525	CLA	C7-C6-C5	-3.21	104.70	113.26
23	b	2513	CLA	CED-O2D-CGD	3.21	123.20	115.92
23	B	524	CLA	C5-C3-C2	-3.21	113.97	121.17
27	F	48	BCR	C34-C9-C8	3.20	122.98	118.09
27	d	2360	BCR	C30-C25-C26	-3.20	118.26	122.64
23	b	2524	CLA	C7-C6-C5	-3.19	104.75	113.26
23	b	2515	CLA	CAA-CBA-CGA	-3.19	104.14	113.21
24	D	355	PHO	O2A-CGA-CBA	3.19	121.57	111.83
28	e	2084	HEC	C4C-C3C-C2C	3.19	109.80	106.35
23	b	2525	CLA	C1-C2-C3	3.19	131.42	126.20
23	B	513	CLA	CED-O2D-CGD	3.19	123.15	115.92
27	B	528	BCR	C8-C7-C6	3.18	135.50	127.00
23	B	513	CLA	C2A-C1A-CHA	3.18	129.39	123.87
23	b	2522	CLA	CED-O2D-CGD	3.18	123.13	115.92
23	c	2474	CLA	O2A-CGA-CBA	3.18	121.52	111.83
27	F	48	BCR	C30-C25-C26	-3.18	118.29	122.64
26	B	526	LMT	O1B-C1B-C2B	3.18	115.91	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2351	CLA	CAA-C2A-C3A	-3.18	104.42	113.00
24	D	355	PHO	CED-O2D-CGD	3.17	123.11	115.92
23	c	2480	CLA	O2A-CGA-CBA	3.17	121.51	111.83
26	d	2359	LMT	O1B-C1B-C2B	3.17	115.89	108.09
23	C	479	CLA	CED-O2D-CGD	3.17	123.11	115.92
24	d	2356	PHO	O2A-CGA-CBA	3.17	121.50	111.83
27	d	2360	BCR	C38-C26-C27	-3.17	106.84	113.60
23	b	2519	CLA	O2A-CGA-CBA	3.16	121.48	111.83
23	C	474	CLA	O2A-CGA-CBA	3.16	121.47	111.83
27	J	53	BCR	C8-C7-C6	3.16	135.44	127.00
23	b	2517	CLA	CED-O2D-CGD	3.16	123.08	115.92
24	d	2356	PHO	C12-C11-C10	-3.16	99.13	113.28
23	C	487	CLA	CED-O2D-CGD	3.16	123.08	115.92
23	B	512	CLA	CMB-C2B-C1B	-3.16	123.83	128.46
23	B	513	CLA	O2A-CGA-CBA	3.15	121.45	111.83
26	d	2359	LMT	C1-O1'-C1'	-3.14	108.31	113.68
23	B	518	CLA	CAA-C2A-C3A	-3.14	104.52	113.00
23	B	516	CLA	CBA-CAA-C2A	3.13	123.11	113.79
23	c	2477	CLA	C6-C5-C3	3.13	121.09	113.47
27	J	53	BCR	C23-C22-C21	-3.12	114.11	119.01
23	B	515	CLA	C7-C6-C5	-3.12	104.95	113.26
23	b	2517	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
23	a	2348	CLA	O2D-CGD-CBD	3.11	116.67	111.23
23	C	484	CLA	CED-O2D-CGD	3.11	122.96	115.92
23	b	2525	CLA	O2A-CGA-CBA	3.11	121.31	111.83
24	a	2350	PHO	CED-O2D-CGD	3.11	122.96	115.92
23	B	525	CLA	O2A-CGA-CBA	3.11	121.31	111.83
24	D	355	PHO	C12-C11-C10	-3.10	99.37	113.28
25	a	2352	PL9	C25-C24-C23	3.10	131.59	123.63
27	d	2360	BCR	C34-C9-C8	3.09	122.81	118.09
23	c	2485	CLA	O2D-CGD-CBD	3.09	116.63	111.23
23	C	481	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	B	522	CLA	CED-O2D-CGD	3.09	122.92	115.92
23	c	2485	CLA	C7-C6-C5	-3.09	105.04	113.26
23	b	2524	CLA	O2A-CGA-CBA	3.09	121.24	111.83
27	c	2488	BCR	C38-C26-C27	-3.08	107.02	113.60
23	A	348	CLA	C7-C6-C5	-3.08	105.05	113.26
23	C	485	CLA	CBA-CAA-C2A	3.08	122.95	113.79
24	d	2356	PHO	CAA-C2A-C3A	-3.08	104.69	113.00
23	b	2518	CLA	CED-O2D-CGD	3.07	122.89	115.92
24	D	355	PHO	CAA-C2A-C3A	-3.07	104.71	113.00
23	d	2357	CLA	O2D-CGD-CBD	3.07	116.59	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2526	CLA	C2A-C1A-CHA	3.07	129.19	123.87
23	c	2481	CLA	CED-O2D-CGD	3.07	122.87	115.92
27	C	489	BCR	C7-C8-C9	3.06	130.77	126.23
23	c	2480	CLA	CED-O2D-CGD	3.06	122.86	115.92
27	c	2489	BCR	C33-C5-C4	-3.06	107.08	113.60
23	c	2486	CLA	O2D-CGD-CBD	3.06	116.58	111.23
24	A	351	PHO	CED-O2D-CGD	3.06	122.85	115.92
23	b	2514	CLA	CED-O2D-CGD	3.06	122.85	115.92
27	b	2528	BCR	C38-C26-C27	-3.06	107.08	113.60
23	c	2475	CLA	O2A-C1-C2	3.06	119.87	108.11
24	d	2356	PHO	C4A-C3A-C2A	3.05	105.75	102.84
23	B	511	CLA	C1-C2-C3	3.05	131.20	126.20
23	C	478	CLA	CED-O2D-CGD	3.05	122.84	115.92
23	C	475	CLA	O2A-C1-C2	3.05	119.85	108.11
27	b	2527	BCR	C8-C7-C6	3.05	135.14	127.00
23	A	352	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
23	a	2348	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
27	J	53	BCR	C7-C8-C9	3.04	130.74	126.23
27	J	53	BCR	C8-C9-C10	-3.04	114.22	119.01
27	B	528	BCR	C30-C25-C26	-3.04	118.48	122.64
27	j	2053	BCR	C8-C7-C6	3.04	135.12	127.00
23	c	2474	CLA	C1-C2-C3	3.04	131.17	126.20
23	b	2516	CLA	CBA-CAA-C2A	3.04	122.83	113.79
23	B	517	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
23	B	524	CLA	CED-O2D-CGD	3.03	122.79	115.92
23	a	2349	CLA	O2A-CGA-CBA	3.03	121.08	111.83
23	b	2511	CLA	C1-C2-C3	3.03	131.16	126.20
23	b	2513	CLA	C2A-C1A-CHA	3.02	129.11	123.87
27	b	2527	BCR	C30-C25-C26	-3.02	118.50	122.64
23	c	2481	CLA	O2A-CGA-CBA	3.02	121.05	111.83
23	A	349	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
27	B	528	BCR	C1-C6-C5	-3.02	118.51	122.64
23	A	352	CLA	C7-C6-C5	-3.02	105.22	113.26
27	C	488	BCR	C33-C5-C4	-3.02	107.17	113.60
23	B	523	CLA	O2A-CGA-CBA	3.02	121.03	111.83
27	b	2527	BCR	C1-C6-C5	-3.01	118.52	122.64
23	b	2526	CLA	CED-O2D-CGD	3.01	122.75	115.92
23	b	2511	CLA	C1-O2A-CGA	3.01	123.94	116.65
28	V	138	HEC	C3B-C4B-NB	-3.01	105.26	110.94
23	C	482	CLA	CBA-CAA-C2A	3.01	122.75	113.79
27	F	48	BCR	C30-C25-C24	3.01	123.81	115.65
23	C	485	CLA	O2D-CGD-CBD	3.01	116.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	2355	CLA	CMB-C2B-C1B	-3.01	124.05	128.46
23	B	519	CLA	CED-O2D-CGD	3.01	122.73	115.92
23	C	474	CLA	O2D-CGD-CBD	3.00	116.48	111.23
23	C	482	CLA	O2D-CGD-CBD	3.00	116.48	111.23
24	d	2356	PHO	CED-O2D-CGD	3.00	122.72	115.92
27	J	53	BCR	C38-C26-C27	-3.00	107.20	113.60
23	B	524	CLA	O2A-CGA-CBA	3.00	120.97	111.83
23	B	520	CLA	CED-O2D-CGD	2.99	122.70	115.92
23	A	350	CLA	O2A-CGA-CBA	2.98	120.93	111.83
27	F	48	BCR	C1-C6-C5	-2.98	118.56	122.64
23	C	475	CLA	O1A-CGA-CBA	-2.97	112.16	123.78
23	b	2523	CLA	CMB-C2B-C1B	-2.97	124.11	128.46
27	j	2053	BCR	C38-C26-C27	-2.97	107.27	113.60
23	B	520	CLA	O2D-CGD-CBD	2.97	116.42	111.23
23	B	527	CLA	C2A-C1A-CHA	2.97	129.01	123.87
27	c	2489	BCR	C8-C9-C10	-2.96	114.35	119.01
23	c	2475	CLA	O1A-CGA-CBA	-2.96	112.19	123.78
23	b	2517	CLA	CMB-C2B-C1B	-2.96	124.12	128.46
23	b	2524	CLA	CED-O2D-CGD	2.96	122.63	115.92
25	A	353	PL9	C7-C3-C4	2.96	119.35	116.91
23	B	513	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
25	d	2358	PL9	C8-C7-C3	2.96	119.67	112.03
23	B	527	CLA	CED-O2D-CGD	2.96	122.62	115.92
23	A	348	CLA	CED-O2D-CGD	2.96	122.62	115.92
23	B	518	CLA	CED-O2D-CGD	2.95	122.62	115.92
27	C	489	BCR	C30-C25-C24	2.95	123.66	115.65
23	c	2482	CLA	CBA-CAA-C2A	2.95	122.58	113.79
24	D	355	PHO	C4A-C3A-C2A	2.95	105.65	102.84
24	d	2356	PHO	C1-C2-C3	2.95	131.03	126.20
23	B	517	CLA	O2D-CGD-CBD	2.95	116.38	111.23
23	B	524	CLA	CMB-C2B-C1B	-2.94	124.14	128.46
23	c	2482	CLA	CED-O2D-CGD	2.94	122.59	115.92
23	b	2523	CLA	O2A-CGA-CBA	2.94	120.81	111.83
23	b	2517	CLA	O2D-CGD-CBD	2.94	116.37	111.23
23	C	483	CLA	CED-O2D-CGD	2.94	122.58	115.92
23	C	487	CLA	C1-O2A-CGA	2.93	123.74	116.65
23	c	2474	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
23	a	2351	CLA	C1-O2A-CGA	2.93	123.74	116.65
23	d	2355	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
23	a	2351	CLA	CED-O2D-CGD	2.93	122.55	115.92
28	e	2084	HEC	O1D-CGD-CBD	-2.92	113.82	123.09
23	c	2483	CLA	CED-O2D-CGD	2.92	122.54	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	477	CLA	C6-C5-C3	2.92	120.58	113.47
23	d	2354	CLA	CBA-CAA-C2A	2.91	122.46	113.79
23	c	2486	CLA	C6-C5-C3	2.91	120.55	113.47
23	b	2519	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
23	B	514	CLA	CMB-C2B-C1B	-2.90	124.20	128.46
23	a	2351	CLA	C7-C6-C5	-2.90	105.53	113.26
23	B	522	CLA	C1-C2-C3	2.90	130.95	126.20
27	c	2489	BCR	C30-C25-C24	2.90	123.52	115.65
27	K	50	BCR	C23-C22-C21	-2.90	114.45	119.01
23	A	348	CLA	O2D-CGD-CBD	2.89	116.29	111.23
23	B	520	CLA	O2A-CGA-CBA	2.89	120.65	111.83
23	c	2485	CLA	CBA-CAA-C2A	2.89	122.39	113.79
28	E	84	HEC	CMB-C2B-C1B	-2.88	124.23	128.46
23	B	523	CLA	CMB-C2B-C1B	-2.88	124.23	128.46
23	C	480	CLA	CED-O2D-CGD	2.88	122.46	115.92
23	b	2518	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
23	B	513	CLA	O2D-CGD-CBD	2.88	116.27	111.23
23	c	2487	CLA	C1-O2A-CGA	2.88	123.62	116.65
23	C	482	CLA	CED-O2D-CGD	2.88	122.44	115.92
23	b	2514	CLA	CMB-C2B-C1B	-2.88	124.24	128.46
28	E	84	HEC	O1D-CGD-CBD	-2.88	113.97	123.09
23	b	2513	CLA	O2D-CGD-CBD	2.87	116.25	111.23
23	D	354	CLA	O2A-C1-C2	2.87	119.14	108.11
23	b	2512	CLA	CED-O2D-CGD	2.86	122.41	115.92
23	C	474	CLA	CED-O2D-CGD	2.86	122.41	115.92
23	B	527	CLA	C1-C2-C3	2.86	130.89	126.20
23	C	486	CLA	C2A-C1A-CHA	2.86	128.83	123.87
23	A	348	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
23	c	2484	CLA	O2A-CGA-CBA	2.86	120.55	111.83
27	c	2489	BCR	C38-C26-C27	-2.86	107.50	113.60
27	k	2050	BCR	C34-C9-C8	2.86	122.45	118.09
23	b	2513	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
23	C	486	CLA	C6-C5-C3	2.86	120.42	113.47
23	A	349	CLA	CMB-C2B-C1B	-2.85	124.27	128.46
27	C	489	BCR	C38-C26-C27	-2.85	107.51	113.60
23	b	2515	CLA	C7-C6-C5	-2.85	105.67	113.26
28	E	84	HEC	CMD-C2D-C1D	-2.84	124.29	128.46
23	c	2486	CLA	CED-O2D-CGD	2.84	122.36	115.92
23	B	519	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
23	C	474	CLA	C7-C6-C5	-2.83	105.71	113.26
27	k	2050	BCR	C23-C22-C21	-2.83	114.55	119.01
28	v	2138	HEC	CMA-C3A-C2A	2.83	130.28	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	2360	BCR	C30-C25-C24	2.83	123.31	115.65
23	C	484	CLA	O2A-CGA-CBA	2.82	120.45	111.83
27	K	50	BCR	C36-C18-C19	2.82	122.40	118.09
28	E	84	HEC	CMC-C2C-C3C	2.82	129.13	125.82
23	B	521	CLA	CMB-C2B-C1B	-2.82	124.33	128.46
23	a	2349	CLA	CAA-C2A-C1A	-2.81	102.75	111.97
23	C	477	CLA	CMB-C2B-C1B	-2.81	124.33	128.46
27	K	50	BCR	C23-C24-C25	2.81	134.51	127.00
23	b	2522	CLA	C1-C2-C3	2.81	130.80	126.20
27	B	529	BCR	C1-C6-C7	2.81	123.27	115.65
23	b	2511	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
23	C	474	CLA	CAA-C2A-C1A	-2.81	102.78	111.97
23	b	2513	CLA	C6-C5-C3	2.80	120.30	113.47
27	k	2050	BCR	C8-C9-C10	-2.80	114.60	119.01
23	A	350	CLA	O2D-CGD-CBD	2.80	116.13	111.23
23	b	2524	CLA	CMB-C2B-C1B	-2.80	124.35	128.46
23	B	514	CLA	CED-O2D-CGD	2.80	122.26	115.92
23	c	2485	CLA	O2A-CGA-CBA	2.80	120.36	111.83
23	B	517	CLA	CMB-C2B-C1B	-2.80	124.36	128.46
23	C	476	CLA	O2A-CGA-CBA	2.80	120.36	111.83
25	a	2352	PL9	C7-C3-C4	2.79	119.21	116.91
23	b	2520	CLA	O2A-CGA-CBA	2.79	120.36	111.83
23	b	2520	CLA	CED-O2D-CGD	2.79	122.25	115.92
23	C	486	CLA	CED-O2D-CGD	2.79	122.24	115.92
23	c	2485	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
27	c	2488	BCR	C33-C5-C4	-2.78	107.66	113.60
28	E	84	HEC	CMD-C2D-C3D	2.78	130.19	124.94
27	B	528	BCR	C8-C9-C10	-2.78	114.63	119.01
23	B	517	CLA	CED-O2D-CGD	2.78	122.23	115.92
23	b	2515	CLA	C2A-C1A-CHA	2.78	128.70	123.87
27	k	2050	BCR	C36-C18-C19	2.78	122.34	118.09
23	A	352	CLA	C1-O2A-CGA	2.78	123.39	116.65
23	d	2354	CLA	O2D-CGD-CBD	2.78	116.08	111.23
23	B	513	CLA	C6-C5-C3	2.78	120.23	113.47
23	B	519	CLA	O2D-CGD-CBD	2.77	116.08	111.23
25	D	357	PL9	C8-C7-C3	2.77	119.20	112.03
23	A	349	CLA	CED-O2D-CGD	2.77	122.20	115.92
27	k	2050	BCR	C38-C26-C27	-2.77	107.69	113.60
23	c	2485	CLA	C12-C11-C10	-2.77	100.86	113.28
24	A	351	PHO	C4A-C3A-C2A	2.77	105.47	102.84
23	B	511	CLA	C1-O2A-CGA	2.77	123.35	116.65
23	a	2348	CLA	C7-C6-C5	-2.77	105.89	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	476	CLA	O2D-CGD-CBD	2.76	116.06	111.23
23	c	2485	CLA	C1-C2-C3	2.76	130.72	126.20
23	C	480	CLA	C7-C6-C5	-2.76	105.90	113.26
23	D	356	CLA	O2D-CGD-CBD	2.76	116.06	111.23
23	d	2355	CLA	C5-C3-C2	-2.76	114.97	121.17
23	c	2484	CLA	C1-O2A-CGA	2.76	123.33	116.65
27	F	48	BCR	C24-C23-C22	2.76	130.32	126.23
23	B	515	CLA	C2A-C1A-CHA	2.76	128.65	123.87
23	c	2483	CLA	C6-C5-C3	2.75	120.18	113.47
23	C	485	CLA	C1-C2-C3	2.75	130.71	126.20
27	K	50	BCR	C8-C9-C10	-2.75	114.68	119.01
25	A	353	PL9	C27-C28-C29	-2.75	121.32	127.62
23	c	2480	CLA	C7-C6-C5	-2.75	105.93	113.26
23	c	2476	CLA	O2D-CGD-CBD	2.75	116.04	111.23
25	d	2358	PL9	C22-C21-C19	-2.75	104.07	113.19
23	C	475	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
27	B	529	BCR	C35-C13-C12	2.75	122.28	118.09
23	b	2514	CLA	CAA-CBA-CGA	-2.75	105.41	113.21
27	k	2050	BCR	C23-C24-C25	2.75	134.33	127.00
23	B	513	CLA	C2A-C3A-C4A	2.74	106.30	101.87
25	a	2352	PL9	C32-C33-C34	-2.74	121.35	127.62
23	B	511	CLA	CMB-C2B-C1B	-2.74	124.44	128.46
23	b	2526	CLA	CMB-C2B-C1B	-2.74	124.45	128.46
27	K	50	BCR	C38-C26-C27	-2.73	107.77	113.60
23	C	486	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
27	b	2528	BCR	C33-C5-C4	-2.73	107.77	113.60
23	b	2513	CLA	C2A-C3A-C4A	2.73	106.28	101.87
23	C	487	CLA	C1-C2-C3	2.73	130.67	126.20
26	d	2359	LMT	C3'-C4'-C5'	-2.73	104.89	110.93
23	C	485	CLA	C12-C11-C10	-2.72	101.07	113.28
27	C	488	BCR	C19-C18-C17	-2.72	114.73	119.01
23	C	485	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
26	B	526	LMT	C3'-C4'-C5'	-2.72	104.90	110.93
23	c	2479	CLA	O2A-CGA-CBA	2.72	120.12	111.83
23	C	483	CLA	CAA-CBA-CGA	-2.71	105.50	113.21
23	C	481	CLA	CED-O2D-CGD	2.71	122.07	115.92
27	b	2528	BCR	C1-C6-C7	2.71	123.00	115.65
23	c	2476	CLA	O2A-CGA-CBA	2.71	120.10	111.83
27	d	2360	BCR	C1-C6-C5	-2.71	118.94	122.64
24	d	2356	PHO	C6-C5-C3	2.70	120.05	113.47
27	k	2050	BCR	C37-C22-C23	2.70	122.22	118.09
23	b	2522	CLA	O2A-CGA-CBA	2.70	120.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E	84	HEC	CMB-C2B-C3B	2.70	129.00	125.82
23	d	2354	CLA	CED-O2D-CGD	2.70	122.03	115.92
23	c	2483	CLA	C7-C6-C5	-2.70	106.08	113.26
23	b	2517	CLA	C2A-C1A-CHA	2.70	128.54	123.87
23	B	522	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	d	2354	CLA	O2A-C1-C2	2.69	118.48	108.11
23	b	2521	CLA	CMB-C2B-C1B	-2.69	124.52	128.46
23	B	518	CLA	CMD-C2D-C1D	2.69	129.46	124.73
27	C	489	BCR	C8-C9-C10	-2.69	114.78	119.01
23	C	487	CLA	O2A-CGA-CBA	2.69	120.02	111.83
23	C	482	CLA	C2A-C3A-C4A	2.69	106.21	101.87
23	d	2355	CLA	CED-O2D-CGD	2.68	122.00	115.92
27	B	529	BCR	C37-C22-C21	-2.68	118.47	122.82
23	D	356	CLA	CED-O2D-CGD	2.68	122.00	115.92
23	A	349	CLA	C5-C3-C2	-2.68	115.15	121.17
23	B	527	CLA	CMB-C2B-C1B	-2.68	124.53	128.46
23	c	2478	CLA	O2D-CGD-CBD	2.68	115.91	111.23
24	D	355	PHO	C1-C2-C3	2.68	130.58	126.20
23	B	515	CLA	O2D-CGD-CBD	2.67	115.90	111.23
23	C	478	CLA	C1-O2A-CGA	2.67	123.12	116.65
23	b	2515	CLA	CMB-C2B-C1B	-2.67	124.54	128.46
23	c	2486	CLA	C2A-C1A-CHA	2.67	128.50	123.87
23	c	2482	CLA	C2A-C3A-C4A	2.67	106.18	101.87
28	e	2084	HEC	CMB-C2B-C1B	-2.67	124.55	128.46
27	K	50	BCR	C37-C22-C23	2.66	122.16	118.09
27	d	2360	BCR	C24-C23-C22	2.66	130.18	126.23
27	b	2527	BCR	C23-C22-C21	-2.66	114.82	119.01
23	A	350	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
23	c	2474	CLA	CED-O2D-CGD	2.66	121.95	115.92
27	j	2053	BCR	C37-C22-C23	2.66	122.16	118.09
23	B	517	CLA	C2A-C1A-CHA	2.66	128.49	123.87
23	c	2476	CLA	CED-O2D-CGD	2.66	121.95	115.92
23	C	483	CLA	C2A-C3A-C4A	2.66	106.16	101.87
27	K	50	BCR	C33-C5-C4	-2.66	107.93	113.60
27	F	48	BCR	C8-C7-C6	2.65	134.08	127.00
27	c	2489	BCR	C1-C6-C5	-2.65	119.02	122.64
27	J	53	BCR	C30-C25-C26	-2.65	119.02	122.64
27	b	2528	BCR	C35-C13-C12	2.65	122.13	118.09
23	A	352	CLA	CED-O2D-CGD	2.64	121.91	115.92
23	b	2511	CLA	C2A-C1A-CHA	2.64	128.45	123.87
27	c	2488	BCR	C15-C16-C17	-2.64	118.11	123.52
23	B	525	CLA	CBA-CAA-C2A	2.64	121.65	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	489	BCR	C30-C25-C26	-2.64	119.03	122.64
27	C	488	BCR	C36-C18-C19	2.64	122.12	118.09
23	c	2475	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
27	C	489	BCR	C1-C6-C5	-2.64	119.03	122.64
27	c	2489	BCR	C21-C20-C19	2.64	130.84	123.20
23	b	2525	CLA	O2D-CGD-CBD	2.63	115.84	111.23
27	d	2360	BCR	C20-C21-C22	2.63	130.97	127.28
23	b	2512	CLA	CMB-C2B-C3B	2.63	129.94	124.68
23	c	2483	CLA	CAA-CBA-CGA	-2.63	105.73	113.21
28	e	2084	HEC	CMD-C2D-C3D	2.63	129.90	124.94
23	c	2487	CLA	C1-C2-C3	2.63	130.50	126.20
23	b	2524	CLA	O2D-CGD-CBD	2.62	115.82	111.23
25	A	353	PL9	C25-C24-C23	2.62	130.37	123.63
23	C	483	CLA	C6-C5-C3	2.62	119.86	113.47
23	C	479	CLA	O2A-CGA-CBA	2.62	119.82	111.83
23	B	524	CLA	O2D-CGD-CBD	2.62	115.81	111.23
23	b	2525	CLA	CBA-CAA-C2A	2.62	121.58	113.79
23	b	2518	CLA	CMD-C2D-C1D	2.61	129.33	124.73
23	B	511	CLA	O2A-CGA-CBA	2.61	119.81	111.83
27	C	488	BCR	C34-C9-C8	2.61	122.08	118.09
23	B	522	CLA	C2A-C1A-CHA	2.61	128.40	123.87
24	a	2350	PHO	C4A-C3A-C2A	2.61	105.33	102.84
24	d	2356	PHO	CBA-CAA-C2A	2.61	121.47	113.78
23	b	2513	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
23	B	520	CLA	CMD-C2D-C1D	2.61	129.32	124.73
27	B	529	BCR	C33-C5-C4	-2.61	108.04	113.60
25	a	2352	PL9	C27-C28-C29	-2.60	121.66	127.62
23	d	2355	CLA	CMD-C2D-C1D	2.60	129.31	124.73
23	C	477	CLA	O2D-CGD-CBD	2.60	115.78	111.23
23	c	2487	CLA	O2A-CGA-CBA	2.60	119.76	111.83
23	B	514	CLA	CAA-CBA-CGA	-2.60	105.83	113.21
23	A	349	CLA	CAA-C2A-C3A	-2.60	105.99	113.00
23	C	480	CLA	CAA-C2A-C1A	-2.59	103.47	111.97
27	b	2528	BCR	C30-C25-C24	2.59	122.68	115.65
23	b	2519	CLA	O2D-CGD-CBD	2.59	115.76	111.23
27	b	2528	BCR	C23-C24-C25	2.59	133.91	127.00
23	C	482	CLA	CMB-C2B-C1B	-2.58	124.68	128.46
23	b	2519	CLA	O2A-C1-C2	2.58	118.03	108.11
23	b	2512	CLA	C6-C5-C3	2.58	119.75	113.47
23	c	2487	CLA	CMB-C2B-C3B	2.58	129.83	124.68
23	B	511	CLA	C2A-C1A-CHA	2.57	128.34	123.87
27	B	528	BCR	C23-C22-C21	-2.57	114.96	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	478	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
23	C	484	CLA	C1-O2A-CGA	2.57	122.88	116.65
23	b	2525	CLA	C2A-C3A-C4A	2.57	106.02	101.87
25	D	357	PL9	C22-C21-C19	-2.57	104.66	113.19
23	C	483	CLA	O2D-CGD-CBD	2.57	115.72	111.23
23	C	475	CLA	CMB-C2B-C1B	-2.57	124.69	128.46
23	b	2521	CLA	O2A-CGA-CBA	2.57	119.66	111.83
27	d	2360	BCR	C8-C7-C6	2.57	133.86	127.00
24	A	351	PHO	O2A-CGA-CBA	2.57	119.66	111.83
27	C	488	BCR	C15-C16-C17	-2.57	118.27	123.52
27	k	2050	BCR	C33-C5-C4	-2.56	108.13	113.60
24	D	355	PHO	CBA-CAA-C2A	2.56	121.33	113.78
27	b	2528	BCR	C37-C22-C21	-2.56	118.66	122.82
23	c	2477	CLA	O2A-C1-C2	2.56	117.97	108.11
27	c	2488	BCR	C19-C18-C17	-2.56	114.98	119.01
23	B	523	CLA	C7-C6-C5	-2.56	106.43	113.26
27	b	2527	BCR	C7-C8-C9	2.56	130.02	126.23
27	b	2528	BCR	C34-C9-C8	2.56	122.00	118.09
24	a	2350	PHO	O2A-CGA-CBA	2.56	119.63	111.83
27	d	2360	BCR	C15-C16-C17	-2.55	118.29	123.52
23	C	479	CLA	C6-C5-C3	2.55	119.68	113.47
23	C	485	CLA	O2A-CGA-CBA	2.55	119.61	111.83
23	c	2482	CLA	CMB-C2B-C1B	-2.55	124.72	128.46
23	a	2348	CLA	C2A-C3A-C4A	2.55	105.98	101.87
27	C	489	BCR	C8-C7-C6	2.55	133.80	127.00
23	A	350	CLA	CMB-C2B-C1B	-2.55	124.72	128.46
23	C	487	CLA	CMB-C2B-C3B	2.55	129.77	124.68
23	B	511	CLA	CAA-C2A-C3A	-2.55	106.12	113.00
23	C	484	CLA	CBA-CAA-C2A	2.55	121.37	113.79
23	c	2487	CLA	C7-C6-C5	-2.54	106.49	113.26
23	b	2523	CLA	C7-C6-C5	-2.54	106.49	113.26
23	c	2477	CLA	CMB-C2B-C1B	-2.54	124.74	128.46
23	b	2522	CLA	C2A-C1A-CHA	2.54	128.27	123.87
28	V	138	HEC	C4C-CHD-C1D	2.54	131.10	123.67
23	C	476	CLA	CED-O2D-CGD	2.54	121.67	115.92
23	C	477	CLA	O2A-C1-C2	2.54	117.86	108.11
23	B	513	CLA	CAA-C2A-C1A	-2.54	103.67	111.97
27	C	489	BCR	C21-C20-C19	2.53	130.54	123.20
23	B	515	CLA	CMB-C2B-C1B	-2.53	124.74	128.46
23	C	485	CLA	C2A-C3A-C4A	2.53	105.96	101.87
23	c	2484	CLA	CBA-CAA-C2A	2.53	121.33	113.79
23	c	2477	CLA	O2D-CGD-CBD	2.53	115.66	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2474	CLA	CMB-C2B-C1B	-2.53	124.75	128.46
25	d	2358	PL9	C31-C29-C28	-2.53	115.48	121.17
23	B	512	CLA	C6-C5-C3	2.53	119.63	113.47
25	D	357	PL9	C31-C29-C28	-2.53	115.49	121.17
23	c	2478	CLA	C1-O2A-CGA	2.53	122.77	116.65
23	c	2480	CLA	O2D-CGD-CBD	2.53	115.65	111.23
27	b	2527	BCR	C37-C22-C23	2.53	121.95	118.09
23	C	481	CLA	C2A-C3A-C4A	2.52	105.95	101.87
23	B	514	CLA	O2A-C1-C2	2.52	117.82	108.11
27	B	529	BCR	C23-C24-C25	2.52	133.73	127.00
23	b	2511	CLA	CMB-C2B-C1B	-2.52	124.77	128.46
23	C	480	CLA	CMB-C2B-C1B	-2.52	124.77	128.46
24	a	2350	PHO	CMA-C3A-C4A	-2.52	109.19	114.61
23	b	2517	CLA	CBA-CAA-C2A	2.52	121.28	113.79
23	c	2485	CLA	C2A-C3A-C4A	2.52	105.93	101.87
23	D	354	CLA	CBA-CAA-C2A	2.51	121.28	113.79
24	D	355	PHO	OBD-CAD-CBD	-2.51	122.13	125.82
25	A	353	PL9	C30-C29-C31	2.51	119.58	115.23
23	b	2526	CLA	C1-C2-C3	2.50	130.30	126.20
27	c	2488	BCR	C11-C10-C9	2.50	130.79	127.28
27	c	2488	BCR	C34-C9-C8	2.50	121.91	118.09
27	j	2053	BCR	C35-C13-C12	2.50	121.91	118.09
23	c	2483	CLA	O2D-CGD-CBD	2.50	115.60	111.23
27	b	2527	BCR	C8-C9-C10	-2.50	115.08	119.01
23	c	2481	CLA	CMB-C2B-C1B	-2.49	124.80	128.46
23	c	2485	CLA	CMB-C2B-C1B	-2.49	124.81	128.46
23	C	483	CLA	C7-C6-C5	-2.49	106.62	113.26
23	B	519	CLA	O2A-C1-C2	2.49	117.69	108.11
23	b	2522	CLA	CMB-C2B-C3B	2.49	129.66	124.68
25	d	2358	PL9	C7-C3-C4	2.49	118.96	116.91
23	C	486	CLA	C2A-C3A-C4A	2.49	105.89	101.87
23	b	2518	CLA	CMB-C2B-C1B	-2.49	124.81	128.46
23	c	2480	CLA	CAA-C2A-C1A	-2.48	103.83	111.97
23	c	2484	CLA	CMB-C2B-C1B	-2.48	124.82	128.46
23	c	2478	CLA	C2A-C3A-C4A	2.48	105.88	101.87
23	c	2479	CLA	C6-C7-C8	2.48	124.21	115.97
23	B	516	CLA	O2D-CGD-CBD	2.48	115.56	111.23
23	a	2348	CLA	CED-O2D-CGD	2.48	121.54	115.92
23	b	2514	CLA	O2A-C1-C2	2.48	117.64	108.11
23	B	521	CLA	O2A-CGA-CBA	2.48	119.39	111.83
23	A	350	CLA	C1-O2A-CGA	2.48	122.64	116.65
28	E	84	HEC	O1A-CGA-CBA	-2.47	115.24	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	351	PHO	CAA-C2A-C3A	-2.47	106.31	113.00
27	F	48	BCR	C15-C16-C17	-2.47	118.46	123.52
23	c	2486	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
23	c	2478	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
23	A	352	CLA	O2D-CGD-CBD	2.46	115.54	111.23
23	D	354	CLA	CED-O2D-CGD	2.46	121.50	115.92
27	B	529	BCR	C34-C9-C8	2.46	121.85	118.09
23	C	481	CLA	CMB-C2B-C1B	-2.46	124.85	128.46
27	j	2053	BCR	C30-C25-C26	-2.46	119.27	122.64
23	B	516	CLA	C2A-C3A-C4A	2.46	105.85	101.87
23	c	2486	CLA	C2A-C3A-C4A	2.46	105.84	101.87
23	b	2516	CLA	C5-C3-C2	2.46	126.69	121.17
23	B	522	CLA	C1-O2A-CGA	2.46	122.61	116.65
23	b	2513	CLA	C1-O2A-CGA	2.46	122.61	116.65
23	C	479	CLA	C2A-C1A-CHA	2.46	128.13	123.87
24	d	2356	PHO	OBD-CAD-CBD	-2.46	122.22	125.82
23	c	2475	CLA	CMD-C2D-C1D	2.46	129.06	124.73
24	D	355	PHO	C6-C5-C3	2.46	119.45	113.47
23	C	482	CLA	C6-C5-C3	2.46	119.45	113.47
27	j	2053	BCR	C16-C17-C18	2.45	130.72	127.28
23	a	2351	CLA	O2D-CGD-CBD	2.45	115.52	111.23
27	F	48	BCR	C20-C21-C22	2.45	130.72	127.28
25	A	353	PL9	C32-C33-C34	-2.45	122.02	127.62
23	B	522	CLA	CMB-C2B-C3B	2.44	129.57	124.68
23	A	348	CLA	O2A-C1-C2	2.44	117.50	108.11
27	B	529	BCR	C24-C23-C22	2.44	129.84	126.23
23	A	349	CLA	O2D-CGD-CBD	2.44	115.50	111.23
24	d	2356	PHO	CMB-C2B-C3B	2.44	129.55	124.68
23	c	2476	CLA	C1-O2A-CGA	2.44	122.55	116.65
27	c	2489	BCR	C30-C25-C26	-2.44	119.31	122.64
23	C	480	CLA	O2D-CGD-CBD	2.43	115.49	111.23
27	c	2488	BCR	C32-C1-C6	2.43	114.06	110.24
23	B	512	CLA	CMB-C2B-C3B	2.43	129.54	124.68
23	d	2357	CLA	C1-O2A-CGA	2.43	122.53	116.65
23	C	486	CLA	CBA-CAA-C2A	2.43	121.02	113.79
23	B	525	CLA	O2D-CGD-CBD	2.43	115.47	111.23
23	c	2486	CLA	CBA-CAA-C2A	2.42	121.00	113.79
23	c	2479	CLA	C2A-C1A-CHA	2.42	128.06	123.87
23	b	2511	CLA	O2D-CGD-CBD	2.41	115.45	111.23
28	E	84	HEC	CBD-CAD-C3D	-2.41	108.48	112.54
27	j	2053	BCR	C1-C6-C5	-2.41	119.34	122.64
28	v	2138	HEC	O1D-CGD-CBD	-2.41	115.44	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2479	CLA	C1-C2-C3	2.41	130.15	126.20
23	A	350	CLA	CMA-C3A-C2A	-2.41	104.66	113.98
23	d	2357	CLA	C7-C6-C5	-2.41	106.84	113.26
23	b	2512	CLA	O2A-CGA-CBA	2.41	119.18	111.83
23	b	2516	CLA	O1A-CGA-CBA	-2.41	114.36	123.78
23	a	2349	CLA	O2D-CGD-CBD	2.41	115.44	111.23
23	a	2349	CLA	C1-O2A-CGA	2.41	122.47	116.65
23	B	520	CLA	C2A-C3A-C4A	2.40	105.75	101.87
23	D	356	CLA	C1-O2A-CGA	2.40	122.47	116.65
25	d	2358	PL9	C20-C19-C21	-2.40	111.06	115.23
28	e	2084	HEC	CMB-C2B-C3B	2.40	128.64	125.82
23	C	484	CLA	C7-C6-C5	-2.40	106.87	113.26
23	B	516	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
23	b	2514	CLA	O2D-CGD-CBD	2.40	115.42	111.23
23	D	354	CLA	C2A-C3A-C4A	2.40	105.74	101.87
23	B	517	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
23	b	2511	CLA	O2A-CGA-CBA	2.40	119.15	111.83
23	c	2482	CLA	O2D-CGD-CBD	2.40	115.42	111.23
23	b	2521	CLA	C1-O2A-CGA	2.40	122.45	116.65
23	b	2514	CLA	CMB-C2B-C3B	2.39	129.47	124.68
23	B	517	CLA	C7-C6-C5	-2.39	106.88	113.26
27	F	48	BCR	C36-C18-C19	2.39	121.74	118.09
27	B	529	BCR	C30-C25-C24	2.39	122.14	115.65
23	b	2515	CLA	O2D-CGD-CBD	2.39	115.41	111.23
23	B	524	CLA	CMB-C2B-C3B	2.39	129.46	124.68
23	B	512	CLA	CED-O2D-CGD	2.39	121.33	115.92
23	C	478	CLA	O2D-CGD-CBD	2.39	115.40	111.23
23	D	356	CLA	C7-C6-C5	-2.39	106.90	113.26
23	A	350	CLA	C2A-C3A-C4A	2.38	105.72	101.87
23	C	486	CLA	O2D-CGD-CBD	2.38	115.39	111.23
23	C	479	CLA	C6-C7-C8	2.38	123.88	115.97
23	B	521	CLA	CMD-C2D-C1D	2.38	128.92	124.73
23	b	2513	CLA	CMB-C2B-C1B	-2.38	124.97	128.46
23	B	516	CLA	O1A-CGA-CBA	-2.38	114.47	123.78
25	a	2352	PL9	C15-C14-C16	-2.38	111.10	115.23
23	d	2355	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
23	B	511	CLA	O2D-CGD-CBD	2.38	115.39	111.23
27	c	2488	BCR	C36-C18-C19	2.38	121.72	118.09
23	B	523	CLA	CMD-C2D-C1D	2.38	128.91	124.73
27	K	50	BCR	C34-C9-C8	2.38	121.72	118.09
23	c	2479	CLA	C6-C5-C3	2.38	119.26	113.47
27	J	53	BCR	C1-C6-C5	-2.38	119.39	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	2528	BCR	C20-C19-C18	-2.38	119.85	126.36
23	c	2477	CLA	C6-C7-C8	2.37	123.85	115.97
23	D	354	CLA	CMB-C2B-C1B	-2.37	124.98	128.46
27	C	489	BCR	C34-C9-C8	2.37	121.71	118.09
23	d	2354	CLA	C2A-C3A-C4A	2.37	105.70	101.87
23	b	2519	CLA	CMB-C2B-C1B	-2.37	124.99	128.46
23	B	518	CLA	O2D-CGD-CBD	2.37	115.36	111.23
23	B	513	CLA	CMB-C2B-C1B	-2.36	124.99	128.46
23	b	2516	CLA	CAA-C2A-C1A	-2.36	104.23	111.97
23	c	2487	CLA	CHD-C4C-C3C	2.36	128.22	124.77
23	A	352	CLA	CAA-CBA-CGA	2.36	119.91	113.21
27	B	528	BCR	C16-C17-C18	2.36	130.59	127.28
23	B	516	CLA	C5-C3-C2	2.36	126.46	121.17
24	D	355	PHO	CHA-C4D-C3D	2.36	115.90	111.19
23	C	475	CLA	CMD-C2D-C1D	2.35	128.88	124.73
27	J	53	BCR	C37-C22-C23	2.35	121.69	118.09
23	c	2484	CLA	C7-C6-C5	-2.35	106.99	113.26
23	b	2516	CLA	CMB-C2B-C1B	-2.35	125.01	128.46
23	C	487	CLA	C2A-C1A-CHA	2.35	127.94	123.87
23	C	477	CLA	C6-C7-C8	2.35	123.77	115.97
23	b	2515	CLA	CAA-C2A-C1A	-2.35	104.29	111.97
23	C	479	CLA	CAA-C2A-C3A	-2.34	106.66	113.00
28	V	138	HEC	O2D-CGD-O1D	2.34	129.36	123.33
27	j	2053	BCR	C30-C25-C24	2.34	122.00	115.65
23	b	2524	CLA	C2A-C3A-C4A	2.34	105.65	101.87
26	d	2359	LMT	C3-C2-C1	-2.34	103.29	113.47
23	B	514	CLA	CMB-C2B-C3B	2.34	129.36	124.68
23	d	2357	CLA	CED-O2D-CGD	2.34	121.22	115.92
23	c	2478	CLA	C7-C6-C5	-2.34	107.03	113.26
23	B	525	CLA	C2A-C3A-C4A	2.34	105.65	101.87
23	B	512	CLA	O2A-CGA-CBA	2.34	118.97	111.83
23	C	487	CLA	CHD-C4C-C3C	2.34	128.18	124.77
27	d	2360	BCR	C36-C18-C19	2.34	121.66	118.09
25	D	357	PL9	C7-C8-C9	2.34	130.86	126.83
23	a	2349	CLA	CMA-C3A-C2A	-2.34	104.95	113.98
23	C	485	CLA	CMB-C2B-C1B	-2.34	125.03	128.46
23	B	523	CLA	C16-C15-C13	2.34	123.73	115.97
23	D	356	CLA	C2A-C3A-C4A	2.34	105.64	101.87
23	A	349	CLA	CMD-C2D-C1D	2.33	128.84	124.73
23	b	2522	CLA	C7-C6-C5	-2.33	107.05	113.26
27	B	528	BCR	C12-C13-C14	-2.33	115.34	119.01
23	c	2487	CLA	C2A-C1A-CHA	2.33	127.91	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	474	CLA	CMB-C2B-C1B	-2.33	125.04	128.46
24	d	2356	PHO	CHA-C4D-C3D	2.33	115.84	111.19
24	a	2350	PHO	CHA-C4D-C3D	2.33	115.84	111.19
23	a	2351	CLA	C2A-C3A-C4A	2.32	105.62	101.87
23	B	522	CLA	C7-C6-C5	-2.32	107.07	113.26
28	v	2138	HEC	CMB-C2B-C3B	2.32	128.55	125.82
27	J	53	BCR	C30-C25-C24	2.32	121.95	115.65
27	c	2488	BCR	C30-C25-C26	-2.32	119.46	122.64
23	C	482	CLA	CAA-CBA-CGA	2.32	119.80	113.21
23	d	2354	CLA	CMB-C2B-C1B	-2.32	125.06	128.46
23	b	2516	CLA	CED-O2D-CGD	2.32	121.17	115.92
23	A	352	CLA	C2A-C3A-C4A	2.32	105.61	101.87
23	B	517	CLA	CBA-CAA-C2A	2.32	120.69	113.79
25	d	2358	PL9	C7-C8-C9	2.32	130.82	126.83
25	a	2352	PL9	C30-C29-C31	2.31	119.24	115.23
27	b	2527	BCR	C34-C9-C8	2.31	121.62	118.09
23	b	2523	CLA	C16-C15-C13	2.31	123.65	115.97
23	D	356	CLA	O2A-CGA-CBA	2.31	118.88	111.83
23	c	2483	CLA	C2A-C3A-C4A	2.31	105.60	101.87
23	B	511	CLA	CMB-C2B-C3B	2.31	129.30	124.68
27	b	2527	BCR	C35-C13-C12	2.31	121.61	118.09
23	a	2348	CLA	C12-C11-C10	-2.31	102.95	113.28
27	c	2489	BCR	C34-C9-C8	2.30	121.61	118.09
23	A	348	CLA	C12-C11-C10	-2.30	102.96	113.28
23	d	2357	CLA	O2A-CGA-CBA	2.30	118.85	111.83
23	D	354	CLA	C1-O2A-CGA	2.30	122.22	116.65
23	b	2516	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
27	b	2528	BCR	C7-C8-C9	2.30	129.63	126.23
23	C	476	CLA	CMB-C2B-C1B	-2.30	125.09	128.46
23	c	2482	CLA	CAA-CBA-CGA	2.30	119.73	113.21
23	B	524	CLA	C4-C3-C5	2.30	119.21	115.23
23	b	2521	CLA	CMD-C2D-C1D	2.29	128.77	124.73
25	D	357	PL9	C20-C19-C21	-2.29	111.25	115.23
23	b	2526	CLA	O2D-CGD-CBD	2.29	115.24	111.23
23	b	2511	CLA	C7-C6-C5	-2.29	107.15	113.26
23	C	476	CLA	CBA-CAA-C2A	2.29	120.62	113.79
27	b	2527	BCR	C16-C17-C18	2.29	130.49	127.28
23	B	518	CLA	CMB-C2B-C1B	-2.29	125.10	128.46
23	b	2523	CLA	CMD-C2D-C1D	2.29	128.76	124.73
23	d	2357	CLA	C2A-C3A-C4A	2.28	105.56	101.87
23	B	521	CLA	C1-O2A-CGA	2.28	122.18	116.65
23	A	348	CLA	O2A-CGA-CBA	2.28	118.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	525	CLA	C6-C5-C3	2.28	119.02	113.47
23	C	484	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
23	b	2521	CLA	CAA-CBA-CGA	-2.28	106.75	113.21
24	A	351	PHO	CHA-C4D-C3D	2.27	115.74	111.19
23	c	2479	CLA	O2D-CGD-CBD	2.27	115.20	111.23
23	c	2484	CLA	CMD-C2D-C1D	2.27	128.73	124.73
23	b	2516	CLA	C6-C7-C8	2.27	123.52	115.97
23	C	479	CLA	O2D-CGD-CBD	2.27	115.20	111.23
27	B	528	BCR	C7-C8-C9	2.27	129.60	126.23
23	b	2522	CLA	CBA-CAA-C2A	2.27	120.55	113.79
23	C	480	CLA	CMD-C2D-C1D	2.27	128.73	124.73
27	B	528	BCR	C37-C22-C23	2.27	121.56	118.09
23	C	476	CLA	C2A-C3A-C4A	2.27	105.53	101.87
27	B	529	BCR	C20-C19-C18	-2.27	120.14	126.36
23	B	523	CLA	C2A-C3A-C4A	2.27	105.53	101.87
23	d	2354	CLA	C7-C6-C5	-2.26	107.23	113.26
26	B	526	LMT	C3-C2-C1	-2.26	103.63	113.47
23	B	516	CLA	C6-C7-C8	2.26	123.48	115.97
27	c	2489	BCR	C11-C10-C9	2.26	130.45	127.28
23	A	352	CLA	C12-C11-C10	-2.26	103.15	113.28
23	c	2481	CLA	O2D-CGD-CBD	2.26	115.18	111.23
23	C	484	CLA	C2A-C3A-C4A	2.26	105.52	101.87
23	a	2348	CLA	O2A-CGA-CBA	2.26	118.72	111.83
24	A	351	PHO	C12-C11-C10	-2.26	103.16	113.28
24	A	351	PHO	CMA-C3A-C4A	-2.26	109.75	114.61
23	c	2480	CLA	CMD-C2D-C1D	2.26	128.70	124.73
23	c	2476	CLA	CMB-C2B-C1B	-2.26	125.15	128.46
23	A	352	CLA	C2A-C1A-CHA	2.26	127.78	123.87
23	B	516	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
23	C	487	CLA	C7-C6-C5	-2.26	107.25	113.26
23	a	2348	CLA	O2A-C1-C2	2.25	116.78	108.11
23	b	2514	CLA	C3A-C2A-C1A	2.25	104.71	101.34
23	b	2515	CLA	C2A-C3A-C4A	2.25	105.50	101.87
23	b	2526	CLA	C2A-C3A-C4A	2.25	105.50	101.87
27	J	53	BCR	C16-C17-C18	2.25	130.43	127.28
23	a	2348	CLA	CMB-C2B-C1B	-2.25	125.16	128.46
27	j	2053	BCR	C15-C14-C13	2.25	130.43	127.28
23	B	521	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
28	e	2084	HEC	O1A-CGA-CBA	-2.24	115.99	123.09
23	C	475	CLA	C2A-C1A-CHA	2.24	127.75	123.87
23	b	2520	CLA	CMD-C2D-C1D	2.24	128.67	124.73
23	a	2349	CLA	C2A-C3A-C4A	2.24	105.48	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	349	CLA	C1-O2A-CGA	2.24	122.06	116.65
23	b	2517	CLA	CAA-C2A-C1A	-2.24	104.65	111.97
27	c	2489	BCR	C8-C7-C6	2.23	132.97	127.00
23	D	354	CLA	C7-C6-C5	-2.23	107.31	113.26
23	c	2487	CLA	O2D-CGD-CBD	2.23	115.13	111.23
23	A	349	CLA	C2A-C3A-C4A	2.23	105.47	101.87
23	B	515	CLA	C2A-C3A-C4A	2.23	105.47	101.87
27	C	488	BCR	C30-C25-C26	-2.23	119.59	122.64
23	D	354	CLA	O2D-CGD-CBD	2.23	115.13	111.23
23	B	511	CLA	C7-C6-C5	-2.23	107.32	113.26
23	B	520	CLA	C1-O2A-CGA	2.23	122.04	116.65
23	C	479	CLA	C1-C2-C3	2.23	129.84	126.20
28	v	2138	HEC	CMC-C2C-C1C	-2.23	125.19	128.46
23	B	522	CLA	CBA-CAA-C2A	2.22	120.41	113.79
23	a	2351	CLA	C12-C11-C10	-2.22	103.31	113.28
23	d	2355	CLA	O2D-CGD-CBD	2.22	115.11	111.23
23	c	2479	CLA	C2A-C3A-C4A	2.22	105.45	101.87
27	J	53	BCR	C35-C13-C12	2.21	121.47	118.09
23	b	2516	CLA	O2D-CGD-CBD	2.21	115.10	111.23
23	b	2516	CLA	C2A-C3A-C4A	2.21	105.44	101.87
23	C	482	CLA	CMD-C2D-C1D	2.21	128.62	124.73
23	C	483	CLA	CMB-C2B-C1B	-2.21	125.22	128.46
28	E	84	HEC	O2A-CGA-CBA	2.21	120.98	114.00
24	D	355	PHO	CMB-C2B-C3B	2.21	129.10	124.68
23	c	2476	CLA	C12-C11-C10	-2.21	103.38	113.28
25	a	2352	PL9	C8-C7-C3	2.21	117.73	112.03
27	F	48	BCR	C40-C30-C25	2.21	113.70	110.24
23	C	478	CLA	C7-C6-C5	-2.20	107.39	113.26
23	b	2517	CLA	C7-C6-C5	-2.20	107.39	113.26
27	B	529	BCR	C7-C8-C9	2.20	129.49	126.23
23	c	2480	CLA	CMB-C2B-C1B	-2.20	125.23	128.46
23	B	524	CLA	C2A-C3A-C4A	2.20	105.42	101.87
25	a	2352	PL9	O1-C4-C3	-2.20	118.41	120.73
23	B	513	CLA	C1-O2A-CGA	2.20	121.97	116.65
23	B	514	CLA	O2D-CGD-CBD	2.20	115.07	111.23
23	C	477	CLA	C16-C15-C13	2.20	123.27	115.97
23	C	484	CLA	CMB-C2B-C1B	-2.20	125.24	128.46
27	C	488	BCR	C37-C22-C23	2.20	121.44	118.09
23	b	2520	CLA	C2A-C3A-C4A	2.19	105.41	101.87
23	B	515	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
23	c	2481	CLA	C2A-C3A-C4A	2.19	105.41	101.87
23	c	2475	CLA	CMB-C2B-C1B	-2.19	125.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	515	CLA	O2A-CGA-CBA	2.19	118.52	111.83
27	j	2053	BCR	C36-C18-C19	2.19	121.43	118.09
23	D	356	CLA	CMB-C2B-C1B	-2.19	125.25	128.46
23	b	2516	CLA	CMD-C2D-C1D	2.19	128.58	124.73
23	b	2520	CLA	CMB-C2B-C1B	-2.19	125.25	128.46
24	a	2350	PHO	CAA-C2A-C3A	-2.19	107.09	113.00
27	K	50	BCR	C1-C6-C5	-2.19	119.65	122.64
23	B	514	CLA	C2A-C1A-CHA	2.19	127.66	123.87
23	a	2351	CLA	O2A-CGA-CBA	2.18	118.49	111.83
23	b	2525	CLA	C6-C5-C3	2.18	118.78	113.47
23	C	479	CLA	CMB-C2B-C1B	-2.18	125.26	128.46
23	b	2524	CLA	C4-C3-C5	2.18	119.01	115.23
27	J	53	BCR	C36-C18-C19	2.17	121.41	118.09
23	c	2487	CLA	C2A-C3A-C4A	2.17	105.38	101.87
23	b	2524	CLA	CMB-C2B-C3B	2.17	129.02	124.68
23	c	2475	CLA	C2A-C1A-CHA	2.17	127.64	123.87
23	d	2355	CLA	C2A-C3A-C4A	2.17	105.38	101.87
27	c	2488	BCR	C23-C22-C21	-2.17	115.60	119.01
23	a	2351	CLA	CAA-CBA-CGA	2.17	119.37	113.21
23	C	483	CLA	CMD-C2D-C1D	2.17	128.55	124.73
23	C	478	CLA	C2A-C3A-C4A	2.17	105.37	101.87
27	J	53	BCR	C20-C21-C22	2.17	130.32	127.28
23	a	2351	CLA	C2A-C1A-CHA	2.17	127.62	123.87
23	C	484	CLA	O2D-CGD-CBD	2.16	115.01	111.23
23	b	2515	CLA	CMB-C2B-C3B	2.16	129.01	124.68
23	C	484	CLA	CMD-C2D-C1D	2.16	128.53	124.73
23	b	2512	CLA	O2D-CGD-CBD	2.16	115.01	111.23
27	C	488	BCR	C11-C10-C9	2.16	130.31	127.28
23	B	522	CLA	C6-C5-C3	2.16	118.73	113.47
27	c	2489	BCR	C32-C1-C6	2.16	113.63	110.24
23	c	2479	CLA	C1-O2A-CGA	2.16	121.87	116.65
27	j	2053	BCR	C34-C9-C8	2.16	121.38	118.09
24	d	2356	PHO	CMA-C3A-C4A	-2.16	109.96	114.61
23	B	518	CLA	C12-C11-C10	-2.16	103.62	113.28
23	b	2514	CLA	C2A-C1A-CHA	2.16	127.61	123.87
23	C	479	CLA	CMD-C2D-C1D	2.15	128.52	124.73
23	c	2486	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
23	c	2481	CLA	C2D-C1D-ND	2.15	112.26	110.13
27	c	2488	BCR	C37-C22-C23	2.15	121.38	118.09
23	C	487	CLA	C2A-C3A-C4A	2.15	105.35	101.87
23	B	514	CLA	CMD-C2D-C1D	2.15	128.52	124.73
23	b	2526	CLA	C6-C7-C8	2.15	123.12	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	521	CLA	C7-C6-C5	-2.15	107.53	113.26
24	A	351	PHO	O1D-CGD-CBD	-2.15	121.46	124.72
25	D	357	PL9	C7-C3-C4	2.15	118.68	116.91
23	b	2522	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	B	519	CLA	CMB-C2B-C1B	-2.15	125.31	128.46
23	c	2476	CLA	CBA-CAA-C2A	2.15	120.18	113.79
23	b	2511	CLA	CMB-C2B-C3B	2.15	128.97	124.68
23	B	516	CLA	CMB-C2B-C1B	-2.15	125.31	128.46
23	C	485	CLA	CMB-C2B-C3B	2.14	128.97	124.68
23	C	485	CLA	C1-O2A-CGA	2.14	121.84	116.65
23	A	349	CLA	C2D-C1D-ND	2.14	112.25	110.13
23	B	517	CLA	CMD-C2D-C1D	2.14	128.50	124.73
23	C	477	CLA	C2A-C3A-C4A	2.14	105.33	101.87
23	a	2349	CLA	CED-O2D-CGD	2.14	120.77	115.92
23	C	475	CLA	CAA-CBA-CGA	2.14	119.28	113.21
27	B	529	BCR	C16-C17-C18	2.14	130.28	127.28
23	b	2513	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
23	b	2518	CLA	O2A-C1-C2	2.14	116.33	108.11
23	C	476	CLA	C12-C11-C10	-2.13	103.72	113.28
23	c	2478	CLA	CAA-CBA-CGA	2.13	119.26	113.21
23	d	2354	CLA	C1-O2A-CGA	2.13	121.81	116.65
27	B	528	BCR	C34-C9-C8	2.13	121.34	118.09
23	c	2476	CLA	C2A-C3A-C4A	2.13	105.31	101.87
27	C	488	BCR	C1-C6-C7	2.13	121.42	115.65
28	E	84	HEC	C1D-C2D-C3D	-2.13	105.52	107.00
23	C	479	CLA	C2A-C3A-C4A	2.13	105.30	101.87
23	b	2523	CLA	CMB-C2B-C3B	2.12	128.93	124.68
23	B	527	CLA	C2A-C3A-C4A	2.12	105.30	101.87
25	A	353	PL9	C8-C7-C3	2.12	117.52	112.03
27	c	2488	BCR	C1-C6-C7	2.12	121.41	115.65
23	c	2482	CLA	CMD-C2D-C1D	2.12	128.47	124.73
24	a	2350	PHO	C12-C11-C10	-2.12	103.78	113.28
23	B	519	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	b	2512	CLA	C2A-C3A-C4A	2.12	105.29	101.87
23	c	2476	CLA	CMA-C3A-C2A	-2.12	105.79	113.98
23	C	476	CLA	C1-O2A-CGA	2.12	121.78	116.65
23	b	2514	CLA	CMD-C2D-C1D	2.12	128.45	124.73
23	a	2349	CLA	CAA-C2A-C3A	-2.11	107.28	113.00
24	D	355	PHO	CMA-C3A-C4A	-2.11	110.06	114.61
27	c	2489	BCR	C1-C6-C7	2.11	121.38	115.65
27	b	2528	BCR	C37-C22-C23	2.11	121.32	118.09
23	b	2515	CLA	CMD-C2D-C1D	2.11	128.45	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	526	LMT	O1'-C1'-C2'	2.11	111.48	108.27
23	c	2479	CLA	CHB-C4A-NA	2.11	127.45	124.40
23	c	2478	CLA	CMB-C2B-C3B	2.11	128.90	124.68
23	b	2522	CLA	C16-C15-C13	2.11	122.97	115.97
23	A	348	CLA	CMB-C2B-C1B	-2.11	125.37	128.46
23	C	476	CLA	CMA-C3A-C2A	-2.11	105.83	113.98
23	b	2517	CLA	C3A-C2A-C1A	2.11	104.50	101.34
23	c	2480	CLA	C2A-C3A-C4A	2.11	105.27	101.87
23	A	350	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
23	B	520	CLA	CMB-C2B-C1B	-2.11	125.37	128.46
23	b	2521	CLA	CMB-C2B-C3B	2.11	128.89	124.68
23	C	478	CLA	C12-C11-C10	-2.11	103.84	113.28
27	C	488	BCR	C1-C6-C5	-2.10	119.76	122.64
23	b	2518	CLA	C12-C11-C10	-2.10	103.85	113.28
23	C	474	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
23	d	2355	CLA	CMB-C2B-C3B	2.10	128.89	124.68
23	B	521	CLA	CBA-CAA-C2A	2.10	120.05	113.79
27	B	528	BCR	C36-C18-C19	2.10	121.30	118.09
23	c	2474	CLA	C2A-C3A-C4A	2.10	105.26	101.87
27	J	53	BCR	C11-C10-C9	2.10	130.22	127.28
23	B	522	CLA	C2A-C3A-C4A	2.10	105.26	101.87
23	b	2521	CLA	C7-C6-C5	-2.10	107.67	113.26
23	c	2482	CLA	O2A-CGA-CBA	2.10	118.23	111.83
23	C	479	CLA	C1-O2A-CGA	2.10	121.72	116.65
23	B	511	CLA	CHB-C4A-NA	2.09	127.42	124.40
23	B	515	CLA	CMD-C2D-C1D	2.09	128.41	124.73
23	B	514	CLA	C3A-C2A-C1A	2.09	104.47	101.34
23	b	2524	CLA	C12-C11-C10	-2.09	103.90	113.28
27	k	2050	BCR	C1-C6-C7	2.09	121.33	115.65
23	d	2357	CLA	CMB-C2B-C1B	-2.09	125.39	128.46
23	b	2526	CLA	CMB-C2B-C3B	2.09	128.86	124.68
24	a	2350	PHO	CMB-C2B-C3B	2.09	128.86	124.68
23	B	518	CLA	O2A-C1-C2	2.09	116.15	108.11
27	B	529	BCR	C10-C11-C12	2.09	129.25	123.20
23	d	2357	CLA	C6-C5-C3	2.09	118.56	113.47
27	C	489	BCR	C11-C10-C9	2.09	130.21	127.28
23	c	2478	CLA	C12-C11-C10	-2.09	103.93	113.28
27	K	50	BCR	C1-C6-C7	2.09	121.31	115.65
23	a	2348	CLA	CMA-C3A-C2A	-2.08	105.92	113.98
27	k	2050	BCR	C16-C17-C18	2.08	130.20	127.28
23	c	2479	CLA	CMD-C2D-C1D	2.08	128.40	124.73
23	c	2483	CLA	CMB-C2B-C1B	-2.08	125.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	521	CLA	C2A-C3A-C4A	2.08	105.23	101.87
23	C	474	CLA	C2A-C3A-C4A	2.08	105.23	101.87
23	c	2477	CLA	C16-C15-C13	2.08	122.88	115.97
25	A	353	PL9	O1-C4-C3	-2.08	118.54	120.73
27	J	53	BCR	C23-C24-C25	2.08	132.55	127.00
23	A	348	CLA	CMA-C3A-C2A	-2.08	105.95	113.98
23	B	527	CLA	C6-C7-C8	2.08	122.87	115.97
23	A	348	CLA	C2A-C1A-CHA	2.08	127.47	123.87
23	c	2481	CLA	C4D-CHA-C1A	2.08	123.72	121.24
23	c	2482	CLA	C6-C5-C3	2.07	118.52	113.47
23	A	352	CLA	O2A-CGA-CBA	2.07	118.16	111.83
27	b	2528	BCR	C16-C17-C18	2.07	130.19	127.28
23	C	487	CLA	CMD-C2D-C1D	2.07	128.38	124.73
27	b	2527	BCR	C12-C13-C14	-2.07	115.75	119.01
26	d	2359	LMT	O6B-C6B-C5B	2.07	118.37	111.33
23	C	486	CLA	CMD-C2D-C1D	2.06	128.36	124.73
23	a	2348	CLA	C16-C15-C13	2.06	122.83	115.97
23	d	2355	CLA	C1-O2A-CGA	2.06	121.64	116.65
23	C	478	CLA	CMB-C2B-C3B	2.06	128.81	124.68
23	A	348	CLA	C2A-C3A-C4A	2.06	105.20	101.87
23	b	2521	CLA	CBA-CAA-C2A	2.06	119.92	113.79
23	b	2512	CLA	C12-C11-C10	-2.06	104.05	113.28
23	b	2520	CLA	C1-O2A-CGA	2.06	121.64	116.65
23	B	522	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
23	B	518	CLA	C2A-C1A-CHA	2.06	127.44	123.87
23	b	2522	CLA	C6-C5-C3	2.06	118.48	113.47
23	B	513	CLA	CMA-C3A-C2A	-2.06	106.03	113.98
27	B	528	BCR	C15-C14-C13	2.06	130.16	127.28
23	c	2478	CLA	CMD-C2D-C1D	2.06	128.35	124.73
23	c	2479	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
27	K	50	BCR	C19-C18-C17	-2.05	115.78	119.01
23	c	2484	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
23	C	487	CLA	O2D-CGD-CBD	2.05	114.82	111.23
23	c	2477	CLA	CMB-C2B-C3B	2.05	128.78	124.68
27	j	2053	BCR	C23-C24-C25	2.05	132.47	127.00
23	C	480	CLA	C12-C11-C10	-2.05	104.11	113.28
23	C	478	CLA	CAA-CBA-CGA	2.05	119.02	113.21
23	B	512	CLA	C2A-C3A-C4A	2.05	105.17	101.87
23	c	2477	CLA	C2A-C3A-C4A	2.05	105.17	101.87
23	c	2484	CLA	C2A-C3A-C4A	2.04	105.17	101.87
23	C	476	CLA	C6-C5-C3	2.04	118.44	113.47
27	K	50	BCR	C16-C17-C18	2.04	130.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	477	CLA	CMB-C2B-C3B	2.04	128.76	124.68
23	b	2513	CLA	C12-C11-C10	-2.04	104.13	113.28
23	a	2349	CLA	CMB-C2B-C1B	-2.04	125.47	128.46
23	D	356	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
23	B	519	CLA	C2A-C1A-CHA	2.04	127.40	123.87
23	C	474	CLA	C6-C7-C8	2.04	122.73	115.97
23	C	480	CLA	C2A-C3A-C4A	2.04	105.16	101.87
28	v	2138	HEC	O2D-CGD-O1D	2.04	128.57	123.33
23	B	517	CLA	CMB-C2B-C3B	2.03	128.75	124.68
23	c	2483	CLA	CMD-C2D-C1D	2.03	128.31	124.73
23	c	2479	CLA	CMB-C2B-C1B	-2.03	125.48	128.46
23	c	2487	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
28	V	138	HEC	CAA-CBA-CGA	-2.03	108.36	113.83
23	A	348	CLA	C16-C15-C13	2.03	122.70	115.97
23	d	2355	CLA	C4-C3-C5	2.03	118.75	115.23
23	b	2524	CLA	C2A-C1A-CHA	2.03	127.38	123.87
23	c	2486	CLA	C1-O2A-CGA	2.02	121.55	116.65
27	k	2050	BCR	C19-C18-C17	-2.02	115.83	119.01
27	b	2528	BCR	C10-C11-C12	2.02	129.05	123.20
23	C	481	CLA	O2D-CGD-CBD	2.02	114.76	111.23
23	b	2522	CLA	C2A-C3A-C4A	2.02	105.13	101.87
23	C	475	CLA	C12-C11-C10	-2.02	104.23	113.28
25	D	357	PL9	C25-C24-C26	-2.02	111.73	115.23
23	B	527	CLA	CMB-C2B-C3B	2.02	128.71	124.68
23	C	485	CLA	CMD-C2D-C1D	2.02	128.28	124.73
23	A	350	CLA	CED-O2D-CGD	2.02	120.49	115.92
27	B	528	BCR	C30-C25-C24	2.02	121.12	115.65
27	b	2528	BCR	C35-C13-C14	-2.01	119.55	122.82
23	c	2485	CLA	C1-O2A-CGA	2.01	121.52	116.65
28	e	2084	HEC	O2A-CGA-CBA	2.01	120.36	114.00
25	d	2358	PL9	C25-C24-C26	-2.01	111.74	115.23
25	A	353	PL9	C15-C14-C16	-2.01	111.74	115.23
26	B	526	LMT	C1'-O5'-C5'	2.01	117.64	113.72
23	B	515	CLA	CMB-C2B-C3B	2.01	128.70	124.68
23	C	486	CLA	CMB-C2B-C1B	-2.01	125.51	128.46
23	C	479	CLA	C3A-C2A-C1A	2.01	104.35	101.34
27	k	2050	BCR	C35-C13-C12	2.01	121.15	118.09
23	b	2512	CLA	CMD-C2D-C1D	2.01	128.26	124.73
27	b	2527	BCR	C15-C14-C13	2.01	130.09	127.28
23	b	2523	CLA	C2D-C1D-ND	2.00	112.11	110.13
23	c	2481	CLA	C1-C2-C3	2.00	129.48	126.20
28	e	2084	HEC	CMC-C2C-C3C	2.00	128.18	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	516	CLA	CMD-C2D-C1D	2.00	128.25	124.73
23	b	2520	CLA	C7-C6-C5	-2.00	107.93	113.26
23	c	2486	CLA	CMD-C2D-C1D	2.00	128.25	124.73

All (72) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	348	CLA	ND
23	A	349	CLA	ND
23	A	350	CLA	ND
23	A	352	CLA	ND
23	B	511	CLA	ND
23	B	512	CLA	ND
23	B	513	CLA	ND
23	B	514	CLA	ND
23	B	515	CLA	ND
23	B	516	CLA	ND
23	B	517	CLA	ND
23	B	518	CLA	ND
23	B	519	CLA	ND
23	B	520	CLA	ND
23	B	521	CLA	ND
23	B	522	CLA	ND
23	B	523	CLA	ND
23	B	524	CLA	ND
23	B	525	CLA	ND
23	B	527	CLA	ND
23	C	474	CLA	ND
23	C	475	CLA	ND
23	C	476	CLA	ND
23	C	477	CLA	ND
23	C	478	CLA	ND
23	C	479	CLA	ND
23	C	480	CLA	ND
23	C	481	CLA	ND
23	C	482	CLA	ND
23	C	483	CLA	ND
23	C	484	CLA	ND
23	C	485	CLA	ND
23	C	486	CLA	ND
23	C	487	CLA	ND
23	D	354	CLA	ND

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Mol	Chain	Res	Type	Atom
23	D	356	CLA	ND
23	a	2348	CLA	ND
23	a	2349	CLA	ND
23	a	2351	CLA	ND
23	b	2511	CLA	ND
23	b	2512	CLA	ND
23	b	2513	CLA	ND
23	b	2514	CLA	ND
23	b	2515	CLA	ND
23	b	2516	CLA	ND
23	b	2517	CLA	ND
23	b	2518	CLA	ND
23	b	2519	CLA	ND
23	b	2520	CLA	ND
23	b	2521	CLA	ND
23	b	2522	CLA	ND
23	b	2523	CLA	ND
23	b	2524	CLA	ND
23	b	2525	CLA	ND
23	b	2526	CLA	ND
23	c	2474	CLA	ND
23	c	2475	CLA	ND
23	c	2476	CLA	ND
23	c	2477	CLA	ND
23	c	2478	CLA	ND
23	c	2479	CLA	ND
23	c	2480	CLA	ND
23	c	2481	CLA	ND
23	c	2482	CLA	ND
23	c	2483	CLA	ND
23	c	2484	CLA	ND
23	c	2485	CLA	ND
23	c	2486	CLA	ND
23	c	2487	CLA	ND
23	d	2354	CLA	ND
23	d	2355	CLA	ND
23	d	2357	CLA	ND

All (911) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	348	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	B	512	CLA	CBD-CGD-O2D-CED
23	B	513	CLA	CAD-CBD-CGD-O1D
23	B	513	CLA	CAD-CBD-CGD-O2D
23	B	513	CLA	O2A-C1-C2-C3
23	B	514	CLA	CBD-CGD-O2D-CED
23	B	514	CLA	C6-C7-C8-C9
23	B	515	CLA	CAD-CBD-CGD-O1D
23	B	515	CLA	CAD-CBD-CGD-O2D
23	B	515	CLA	O2A-C1-C2-C3
23	B	517	CLA	CAD-CBD-CGD-O1D
23	B	517	CLA	CAD-CBD-CGD-O2D
23	B	518	CLA	C6-C7-C8-C9
23	B	519	CLA	O2A-C1-C2-C3
23	B	520	CLA	CHA-CBD-CGD-O1D
23	B	520	CLA	CHA-CBD-CGD-O2D
23	B	522	CLA	CBD-CGD-O2D-CED
23	B	524	CLA	C2-C1-O2A-CGA
23	B	524	CLA	C14-C13-C15-C16
23	B	525	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	C6-C7-C8-C9
23	C	476	CLA	CBD-CGD-O2D-CED
23	C	477	CLA	CBD-CGD-O2D-CED
23	C	478	CLA	CAD-CBD-CGD-O1D
23	C	478	CLA	CAD-CBD-CGD-O2D
23	C	479	CLA	CHA-CBD-CGD-O1D
23	C	479	CLA	CHA-CBD-CGD-O2D
23	C	481	CLA	CBD-CGD-O2D-CED
23	C	482	CLA	CBD-CGD-O2D-CED
23	C	483	CLA	CHA-CBD-CGD-O1D
23	C	483	CLA	CHA-CBD-CGD-O2D
23	C	483	CLA	C6-C7-C8-C9
23	C	484	CLA	C6-C7-C8-C9
23	C	485	CLA	CHA-CBD-CGD-O1D
23	C	485	CLA	CHA-CBD-CGD-O2D
23	C	486	CLA	CHA-CBD-CGD-O2D
23	C	487	CLA	CBD-CGD-O2D-CED
23	a	2348	CLA	C2-C1-O2A-CGA
23	b	2512	CLA	CBD-CGD-O2D-CED
23	b	2513	CLA	CAD-CBD-CGD-O1D
23	b	2513	CLA	CAD-CBD-CGD-O2D
23	b	2513	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	b	2514	CLA	CBD-CGD-O2D-CED
23	b	2514	CLA	C6-C7-C8-C9
23	b	2515	CLA	CAD-CBD-CGD-O1D
23	b	2515	CLA	CAD-CBD-CGD-O2D
23	b	2515	CLA	O2A-C1-C2-C3
23	b	2517	CLA	CAD-CBD-CGD-O1D
23	b	2517	CLA	CAD-CBD-CGD-O2D
23	b	2518	CLA	C6-C7-C8-C9
23	b	2519	CLA	O2A-C1-C2-C3
23	b	2520	CLA	CHA-CBD-CGD-O1D
23	b	2520	CLA	CHA-CBD-CGD-O2D
23	b	2522	CLA	CBD-CGD-O2D-CED
23	b	2524	CLA	C2-C1-O2A-CGA
23	b	2524	CLA	C14-C13-C15-C16
23	b	2526	CLA	CBD-CGD-O2D-CED
23	b	2526	CLA	C6-C7-C8-C9
23	c	2476	CLA	CBD-CGD-O2D-CED
23	c	2477	CLA	CBD-CGD-O2D-CED
23	c	2478	CLA	CAD-CBD-CGD-O1D
23	c	2478	CLA	CAD-CBD-CGD-O2D
23	c	2479	CLA	CHA-CBD-CGD-O1D
23	c	2479	CLA	CHA-CBD-CGD-O2D
23	c	2481	CLA	CBD-CGD-O2D-CED
23	c	2482	CLA	CBD-CGD-O2D-CED
23	c	2483	CLA	CHA-CBD-CGD-O1D
23	c	2483	CLA	CHA-CBD-CGD-O2D
23	c	2483	CLA	C6-C7-C8-C9
23	c	2485	CLA	CHA-CBD-CGD-O1D
23	c	2485	CLA	CHA-CBD-CGD-O2D
23	c	2486	CLA	CHA-CBD-CGD-O2D
23	c	2487	CLA	CBD-CGD-O2D-CED
24	D	355	PHO	CBD-CGD-O2D-CED
24	d	2356	PHO	CBD-CGD-O2D-CED
25	A	353	PL9	C18-C19-C21-C22
25	A	353	PL9	C20-C19-C21-C22
25	d	2358	PL9	C29-C31-C32-C33
26	B	526	LMT	C2'-C1'-O1'-C1
26	B	526	LMT	O5'-C1'-O1'-C1
26	d	2359	LMT	C2'-C1'-O1'-C1
26	d	2359	LMT	O5'-C1'-O1'-C1
27	B	529	BCR	C6-C7-C8-C9
27	B	529	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	B	529	BCR	C7-C8-C9-C34
27	B	529	BCR	C22-C23-C24-C25
27	C	488	BCR	C6-C7-C8-C9
27	C	488	BCR	C7-C8-C9-C10
27	C	488	BCR	C7-C8-C9-C34
27	C	489	BCR	C6-C7-C8-C9
27	C	489	BCR	C22-C23-C24-C25
27	F	48	BCR	C6-C7-C8-C9
27	F	48	BCR	C22-C23-C24-C25
27	J	53	BCR	C6-C7-C8-C9
27	J	53	BCR	C22-C23-C24-C25
27	K	50	BCR	C22-C23-C24-C25
27	b	2527	BCR	C7-C8-C9-C10
27	b	2528	BCR	C6-C7-C8-C9
27	b	2528	BCR	C7-C8-C9-C10
27	b	2528	BCR	C7-C8-C9-C34
27	b	2528	BCR	C22-C23-C24-C25
27	c	2488	BCR	C6-C7-C8-C9
27	c	2488	BCR	C7-C8-C9-C10
27	c	2488	BCR	C7-C8-C9-C34
27	c	2489	BCR	C6-C7-C8-C9
27	c	2489	BCR	C22-C23-C24-C25
27	d	2360	BCR	C6-C7-C8-C9
27	j	2053	BCR	C6-C7-C8-C9
27	j	2053	BCR	C22-C23-C24-C25
27	k	2050	BCR	C22-C23-C24-C25
23	C	480	CLA	O1D-CGD-O2D-CED
23	C	484	CLA	O1D-CGD-O2D-CED
23	c	2480	CLA	O1D-CGD-O2D-CED
23	c	2484	CLA	O1D-CGD-O2D-CED
23	A	349	CLA	O1D-CGD-O2D-CED
23	B	512	CLA	O1D-CGD-O2D-CED
23	B	513	CLA	O1D-CGD-O2D-CED
23	B	527	CLA	O1D-CGD-O2D-CED
23	b	2512	CLA	O1D-CGD-O2D-CED
23	b	2526	CLA	O1D-CGD-O2D-CED
23	c	2478	CLA	O1D-CGD-O2D-CED
23	A	349	CLA	CBD-CGD-O2D-CED
23	B	511	CLA	CBD-CGD-O2D-CED
23	B	513	CLA	CBD-CGD-O2D-CED
23	B	515	CLA	CBD-CGD-O2D-CED
23	B	516	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	524	CLA	CBD-CGD-O2D-CED
23	C	478	CLA	CBD-CGD-O2D-CED
23	C	479	CLA	CBD-CGD-O2D-CED
23	C	480	CLA	CBD-CGD-O2D-CED
23	C	484	CLA	CBD-CGD-O2D-CED
23	b	2511	CLA	CBD-CGD-O2D-CED
23	b	2513	CLA	CBD-CGD-O2D-CED
23	b	2515	CLA	CBD-CGD-O2D-CED
23	b	2516	CLA	CBD-CGD-O2D-CED
23	b	2524	CLA	CBD-CGD-O2D-CED
23	b	2525	CLA	CBD-CGD-O2D-CED
23	c	2478	CLA	CBD-CGD-O2D-CED
23	c	2479	CLA	CBD-CGD-O2D-CED
23	c	2480	CLA	CBD-CGD-O2D-CED
23	c	2484	CLA	CBD-CGD-O2D-CED
23	d	2355	CLA	CBD-CGD-O2D-CED
23	c	2487	CLA	C2C-C3C-CAC-CBC
23	C	487	CLA	C2C-C3C-CAC-CBC
23	C	478	CLA	O1D-CGD-O2D-CED
23	b	2513	CLA	O1D-CGD-O2D-CED
23	d	2355	CLA	O1D-CGD-O2D-CED
23	C	482	CLA	O1D-CGD-O2D-CED
23	C	487	CLA	O1D-CGD-O2D-CED
23	b	2522	CLA	O1D-CGD-O2D-CED
23	c	2482	CLA	O1D-CGD-O2D-CED
23	c	2487	CLA	O1D-CGD-O2D-CED
24	D	355	PHO	O1D-CGD-O2D-CED
23	B	522	CLA	O1D-CGD-O2D-CED
23	C	476	CLA	O1D-CGD-O2D-CED
23	C	477	CLA	O1D-CGD-O2D-CED
23	C	481	CLA	O1D-CGD-O2D-CED
23	c	2476	CLA	O1D-CGD-O2D-CED
23	c	2477	CLA	O1D-CGD-O2D-CED
23	c	2481	CLA	O1D-CGD-O2D-CED
24	d	2356	PHO	O1D-CGD-O2D-CED
23	A	349	CLA	C13-C15-C16-C17
23	d	2355	CLA	C13-C15-C16-C17
23	B	514	CLA	O1D-CGD-O2D-CED
23	C	487	CLA	C4C-C3C-CAC-CBC
23	c	2487	CLA	C4C-C3C-CAC-CBC
23	C	474	CLA	CBD-CGD-O2D-CED
23	C	475	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	483	CLA	CBD-CGD-O2D-CED
23	c	2474	CLA	CBD-CGD-O2D-CED
23	c	2475	CLA	CBD-CGD-O2D-CED
23	c	2483	CLA	CBD-CGD-O2D-CED
23	B	515	CLA	O1D-CGD-O2D-CED
23	B	516	CLA	O1D-CGD-O2D-CED
23	B	525	CLA	O1D-CGD-O2D-CED
23	b	2514	CLA	O1D-CGD-O2D-CED
23	b	2525	CLA	O1D-CGD-O2D-CED
23	b	2516	CLA	O1D-CGD-O2D-CED
23	B	517	CLA	C4-C3-C5-C6
23	B	518	CLA	C4-C3-C5-C6
23	B	522	CLA	C4-C3-C5-C6
23	C	479	CLA	C4-C3-C5-C6
23	C	480	CLA	C4-C3-C5-C6
23	b	2517	CLA	C4-C3-C5-C6
23	b	2518	CLA	C4-C3-C5-C6
23	b	2522	CLA	C4-C3-C5-C6
23	c	2479	CLA	C4-C3-C5-C6
23	c	2480	CLA	C4-C3-C5-C6
25	D	357	PL9	C25-C24-C26-C27
25	a	2352	PL9	C20-C19-C21-C22
25	d	2358	PL9	C25-C24-C26-C27
23	B	517	CLA	C2-C3-C5-C6
23	B	518	CLA	C2-C3-C5-C6
23	C	479	CLA	C2-C3-C5-C6
23	C	480	CLA	C2-C3-C5-C6
23	b	2517	CLA	C2-C3-C5-C6
23	b	2518	CLA	C2-C3-C5-C6
23	c	2479	CLA	C2-C3-C5-C6
23	c	2480	CLA	C2-C3-C5-C6
25	a	2352	PL9	C18-C19-C21-C22
23	b	2511	CLA	O1D-CGD-O2D-CED
23	B	511	CLA	O1D-CGD-O2D-CED
23	B	524	CLA	O1D-CGD-O2D-CED
23	b	2515	CLA	O1D-CGD-O2D-CED
23	b	2524	CLA	O1D-CGD-O2D-CED
26	B	526	LMT	O5B-C5B-C6B-O6B
26	d	2359	LMT	O5B-C5B-C6B-O6B
23	c	2479	CLA	O1D-CGD-O2D-CED
23	B	514	CLA	C4-C3-C5-C6
23	B	521	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	484	CLA	C4-C3-C5-C6
23	b	2514	CLA	C4-C3-C5-C6
23	b	2521	CLA	C4-C3-C5-C6
23	c	2484	CLA	C4-C3-C5-C6
25	A	353	PL9	C35-C34-C36-C37
25	D	357	PL9	C35-C34-C36-C37
25	a	2352	PL9	C35-C34-C36-C37
25	d	2358	PL9	C35-C34-C36-C37
23	B	516	CLA	C2-C3-C5-C6
23	B	521	CLA	C2-C3-C5-C6
23	B	522	CLA	C2-C3-C5-C6
23	C	484	CLA	C2-C3-C5-C6
23	b	2516	CLA	C2-C3-C5-C6
23	b	2521	CLA	C2-C3-C5-C6
23	b	2522	CLA	C2-C3-C5-C6
23	c	2484	CLA	C2-C3-C5-C6
25	D	357	PL9	C33-C34-C36-C37
25	d	2358	PL9	C33-C34-C36-C37
25	D	357	PL9	C14-C16-C17-C18
25	D	357	PL9	C29-C31-C32-C33
25	d	2358	PL9	C14-C16-C17-C18
23	A	348	CLA	C2A-CAA-CBA-CGA
23	a	2348	CLA	C2A-CAA-CBA-CGA
23	C	479	CLA	O1D-CGD-O2D-CED
23	B	518	CLA	CBD-CGD-O2D-CED
23	a	2349	CLA	CBD-CGD-O2D-CED
23	b	2518	CLA	CBD-CGD-O2D-CED
23	A	350	CLA	CBD-CGD-O2D-CED
23	B	516	CLA	C4-C3-C5-C6
23	b	2516	CLA	C4-C3-C5-C6
23	B	514	CLA	C2-C3-C5-C6
23	b	2514	CLA	C2-C3-C5-C6
25	A	353	PL9	C33-C34-C36-C37
25	D	357	PL9	C23-C24-C26-C27
25	a	2352	PL9	C33-C34-C36-C37
25	d	2358	PL9	C23-C24-C26-C27
23	A	349	CLA	C6-C7-C8-C9
23	B	511	CLA	C11-C10-C8-C9
23	B	514	CLA	C11-C12-C13-C14
23	B	522	CLA	C14-C13-C15-C16
23	B	523	CLA	C6-C7-C8-C9
23	B	524	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	474	CLA	C11-C12-C13-C14
23	C	475	CLA	C6-C7-C8-C9
23	C	477	CLA	C6-C7-C8-C9
23	C	477	CLA	C14-C13-C15-C16
23	C	481	CLA	C6-C7-C8-C9
23	b	2511	CLA	C11-C10-C8-C9
23	b	2514	CLA	C11-C12-C13-C14
23	b	2522	CLA	C14-C13-C15-C16
23	b	2523	CLA	C6-C7-C8-C9
23	b	2524	CLA	C6-C7-C8-C9
23	c	2474	CLA	C11-C12-C13-C14
23	c	2475	CLA	C6-C7-C8-C9
23	c	2477	CLA	C6-C7-C8-C9
23	c	2477	CLA	C14-C13-C15-C16
23	c	2481	CLA	C6-C7-C8-C9
23	c	2484	CLA	C6-C7-C8-C9
23	d	2355	CLA	C6-C7-C8-C9
23	C	475	CLA	O1D-CGD-O2D-CED
23	C	483	CLA	O1D-CGD-O2D-CED
23	c	2483	CLA	O1D-CGD-O2D-CED
27	B	528	BCR	C7-C8-C9-C34
27	J	53	BCR	C7-C8-C9-C34
27	b	2527	BCR	C7-C8-C9-C34
27	j	2053	BCR	C7-C8-C9-C34
27	J	53	BCR	C7-C8-C9-C10
27	j	2053	BCR	C7-C8-C9-C10
23	A	349	CLA	C2A-CAA-CBA-CGA
23	B	524	CLA	C2A-CAA-CBA-CGA
23	b	2524	CLA	C2A-CAA-CBA-CGA
23	d	2355	CLA	C2A-CAA-CBA-CGA
26	B	526	LMT	C4B-C5B-C6B-O6B
26	d	2359	LMT	C4B-C5B-C6B-O6B
23	C	478	CLA	C2-C1-O2A-CGA
23	c	2478	CLA	C2-C1-O2A-CGA
23	B	516	CLA	C15-C16-C17-C18
23	a	2351	CLA	C13-C15-C16-C17
23	b	2516	CLA	C15-C16-C17-C18
23	A	348	CLA	C12-C13-C15-C16
23	B	512	CLA	C11-C10-C8-C7
23	B	517	CLA	C11-C12-C13-C15
23	B	523	CLA	C12-C13-C15-C16
23	C	478	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	a	2348	CLA	C12-C13-C15-C16
23	b	2511	CLA	C11-C12-C13-C15
23	b	2512	CLA	C11-C10-C8-C7
23	b	2517	CLA	C11-C12-C13-C15
23	b	2523	CLA	C12-C13-C15-C16
23	c	2478	CLA	C6-C7-C8-C10
23	A	352	CLA	C13-C15-C16-C17
23	a	2348	CLA	C10-C11-C12-C13
23	c	2474	CLA	O1D-CGD-O2D-CED
25	A	353	PL9	C29-C31-C32-C33
25	a	2352	PL9	C29-C31-C32-C33
26	B	526	LMT	O1'-C1-C2-C3
23	A	348	CLA	C10-C11-C12-C13
23	b	2513	CLA	C15-C16-C17-C18
23	B	513	CLA	C15-C16-C17-C18
23	C	484	CLA	C10-C11-C12-C13
23	a	2348	CLA	C5-C6-C7-C8
23	c	2481	CLA	C5-C6-C7-C8
23	c	2484	CLA	C10-C11-C12-C13
23	B	511	CLA	C2A-CAA-CBA-CGA
23	B	519	CLA	C2A-CAA-CBA-CGA
23	C	479	CLA	C2A-CAA-CBA-CGA
23	b	2511	CLA	C2A-CAA-CBA-CGA
23	b	2519	CLA	C2A-CAA-CBA-CGA
23	c	2479	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	C13-C15-C16-C17
26	d	2359	LMT	O1'-C1-C2-C3
23	c	2475	CLA	O1D-CGD-O2D-CED
27	d	2360	BCR	C22-C23-C24-C25
23	A	348	CLA	C5-C6-C7-C8
23	B	514	CLA	C10-C11-C12-C13
23	C	480	CLA	C5-C6-C7-C8
23	C	481	CLA	C5-C6-C7-C8
23	C	482	CLA	C13-C15-C16-C17
23	D	354	CLA	C5-C6-C7-C8
23	b	2514	CLA	C10-C11-C12-C13
23	c	2480	CLA	C5-C6-C7-C8
23	c	2482	CLA	C13-C15-C16-C17
23	d	2354	CLA	C5-C6-C7-C8
23	B	527	CLA	C15-C16-C17-C18
23	b	2525	CLA	C10-C11-C12-C13
23	C	474	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	525	CLA	C10-C11-C12-C13
23	C	474	CLA	C13-C15-C16-C17
23	b	2526	CLA	C15-C16-C17-C18
23	b	2525	CLA	C15-C16-C17-C18
23	d	2357	CLA	C5-C6-C7-C8
23	B	521	CLA	C2A-CAA-CBA-CGA
23	C	478	CLA	C2A-CAA-CBA-CGA
23	b	2517	CLA	C2A-CAA-CBA-CGA
23	b	2521	CLA	C2A-CAA-CBA-CGA
23	c	2478	CLA	C2A-CAA-CBA-CGA
23	B	515	CLA	C5-C6-C7-C8
23	C	485	CLA	C5-C6-C7-C8
23	b	2522	CLA	C5-C6-C7-C8
23	c	2482	CLA	C5-C6-C7-C8
23	B	512	CLA	C10-C11-C12-C13
23	B	513	CLA	C5-C6-C7-C8
23	B	525	CLA	C15-C16-C17-C18
23	b	2512	CLA	C10-C11-C12-C13
23	b	2515	CLA	C15-C16-C17-C18
23	d	2357	CLA	C13-C15-C16-C17
23	B	515	CLA	C15-C16-C17-C18
23	B	522	CLA	C5-C6-C7-C8
23	D	356	CLA	C5-C6-C7-C8
23	D	356	CLA	C13-C15-C16-C17
23	c	2485	CLA	C5-C6-C7-C8
23	b	2514	CLA	C5-C6-C7-C8
23	C	482	CLA	C5-C6-C7-C8
23	C	484	CLA	C5-C6-C7-C8
25	D	357	PL9	C9-C11-C12-C13
25	d	2358	PL9	C9-C11-C12-C13
23	B	518	CLA	C10-C11-C12-C13
23	b	2513	CLA	C5-C6-C7-C8
27	B	528	BCR	C7-C8-C9-C10
23	B	517	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	C2A-CAA-CBA-CGA
23	D	354	CLA	O2A-C1-C2-C3
23	d	2354	CLA	O2A-C1-C2-C3
23	B	522	CLA	C13-C15-C16-C17
23	b	2518	CLA	C10-C11-C12-C13
23	B	518	CLA	O1D-CGD-O2D-CED
23	B	514	CLA	C5-C6-C7-C8
23	C	474	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	c	2474	CLA	C2-C1-O2A-CGA
23	d	2355	CLA	C2-C1-O2A-CGA
26	B	526	LMT	C2-C1-O1'-C1'
26	d	2359	LMT	C2-C1-O1'-C1'
23	b	2518	CLA	O1D-CGD-O2D-CED
23	B	515	CLA	C10-C11-C12-C13
23	b	2515	CLA	C5-C6-C7-C8
23	B	525	CLA	C2A-CAA-CBA-CGA
23	b	2525	CLA	C2A-CAA-CBA-CGA
23	B	513	CLA	C13-C15-C16-C17
23	b	2522	CLA	C13-C15-C16-C17
23	B	511	CLA	C11-C12-C13-C15
23	c	2483	CLA	C15-C16-C17-C18
23	c	2484	CLA	C5-C6-C7-C8
23	b	2515	CLA	C10-C11-C12-C13
23	A	350	CLA	C10-C11-C12-C13
23	C	479	CLA	C10-C11-C12-C13
23	a	2349	CLA	C10-C11-C12-C13
27	B	528	BCR	C1-C6-C7-C8
27	B	528	BCR	C5-C6-C7-C8
27	B	529	BCR	C1-C6-C7-C8
27	B	529	BCR	C5-C6-C7-C8
27	b	2527	BCR	C1-C6-C7-C8
27	b	2527	BCR	C5-C6-C7-C8
27	b	2528	BCR	C1-C6-C7-C8
27	b	2528	BCR	C5-C6-C7-C8
23	C	483	CLA	C15-C16-C17-C18
23	b	2513	CLA	C13-C15-C16-C17
23	C	474	CLA	C2A-CAA-CBA-CGA
23	B	515	CLA	C4-C3-C5-C6
23	a	2349	CLA	O1D-CGD-O2D-CED
23	B	520	CLA	C10-C11-C12-C13
27	B	528	BCR	C6-C7-C8-C9
23	B	523	CLA	C5-C6-C7-C8
23	c	2478	CLA	C5-C6-C7-C8
28	v	2138	HEC	C3A-C2A-CAA-CBA
23	A	350	CLA	C4-C3-C5-C6
23	a	2349	CLA	C2-C3-C5-C6
23	c	2476	CLA	C10-C11-C12-C13
23	c	2477	CLA	C5-C6-C7-C8
23	c	2479	CLA	C10-C11-C12-C13
23	d	2355	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	523	CLA	C15-C16-C17-C18
23	C	478	CLA	C5-C6-C7-C8
23	C	483	CLA	C10-C11-C12-C13
23	b	2523	CLA	C15-C16-C17-C18
23	B	522	CLA	C15-C16-C17-C18
23	C	477	CLA	C5-C6-C7-C8
23	b	2520	CLA	C10-C11-C12-C13
24	d	2356	PHO	C10-C11-C12-C13
23	C	476	CLA	C10-C11-C12-C13
23	b	2522	CLA	C15-C16-C17-C18
23	c	2477	CLA	C15-C16-C17-C18
24	D	355	PHO	C10-C11-C12-C13
23	b	2522	CLA	C2C-C3C-CAC-CBC
23	a	2349	CLA	C4-C3-C5-C6
23	A	350	CLA	C2-C3-C5-C6
23	A	349	CLA	C10-C11-C12-C13
23	B	527	CLA	C13-C15-C16-C17
23	b	2523	CLA	C5-C6-C7-C8
24	a	2350	PHO	C10-C11-C12-C13
23	c	2480	CLA	C15-C16-C17-C18
23	c	2483	CLA	C10-C11-C12-C13
23	B	511	CLA	C6-C7-C8-C10
23	B	512	CLA	C11-C12-C13-C15
23	B	514	CLA	C6-C7-C8-C10
23	B	514	CLA	C11-C12-C13-C15
23	B	519	CLA	C11-C12-C13-C15
23	C	477	CLA	C11-C10-C8-C7
23	C	477	CLA	C12-C13-C15-C16
23	C	480	CLA	C11-C10-C8-C7
23	C	482	CLA	C11-C12-C13-C15
23	b	2511	CLA	C6-C7-C8-C10
23	b	2512	CLA	C11-C12-C13-C15
23	b	2513	CLA	C11-C12-C13-C15
23	b	2514	CLA	C11-C12-C13-C15
23	b	2519	CLA	C11-C12-C13-C15
23	c	2477	CLA	C11-C10-C8-C7
23	c	2477	CLA	C12-C13-C15-C16
23	c	2482	CLA	C11-C12-C13-C15
24	D	355	PHO	C11-C10-C8-C7
24	d	2356	PHO	C6-C7-C8-C10
23	B	517	CLA	C5-C6-C7-C8
23	c	2487	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	522	CLA	C2C-C3C-CAC-CBC
23	C	477	CLA	C15-C16-C17-C18
23	A	349	CLA	C11-C10-C8-C9
23	B	512	CLA	C11-C10-C8-C9
23	B	513	CLA	C11-C12-C13-C14
23	B	522	CLA	C11-C10-C8-C9
23	B	525	CLA	C11-C12-C13-C14
23	C	477	CLA	C11-C10-C8-C9
23	C	480	CLA	C11-C10-C8-C9
23	C	485	CLA	C6-C7-C8-C9
23	b	2512	CLA	C11-C10-C8-C9
23	c	2477	CLA	C11-C10-C8-C9
23	c	2480	CLA	C11-C10-C8-C9
23	d	2355	CLA	C11-C10-C8-C9
24	A	351	PHO	C6-C7-C8-C9
24	D	355	PHO	C11-C10-C8-C9
24	D	355	PHO	C14-C13-C15-C16
24	a	2350	PHO	C6-C7-C8-C9
24	a	2350	PHO	C11-C12-C13-C14
24	d	2356	PHO	C11-C10-C8-C9
23	b	2526	CLA	C13-C15-C16-C17
23	A	350	CLA	O1D-CGD-O2D-CED
23	A	348	CLA	C13-C15-C16-C17
23	a	2348	CLA	C13-C15-C16-C17
23	b	2517	CLA	C5-C6-C7-C8
23	B	525	CLA	C5-C6-C7-C8
24	A	351	PHO	C10-C11-C12-C13
23	C	477	CLA	C13-C15-C16-C17
23	C	487	CLA	C5-C6-C7-C8
23	c	2477	CLA	C13-C15-C16-C17
23	A	350	CLA	C5-C6-C7-C8
23	a	2349	CLA	C5-C6-C7-C8
24	A	351	PHO	O2A-C1-C2-C3
24	D	355	PHO	O2A-C1-C2-C3
24	a	2350	PHO	O2A-C1-C2-C3
24	d	2356	PHO	O2A-C1-C2-C3
27	b	2527	BCR	C6-C7-C8-C9
26	B	526	LMT	C11-C10-C9-C8
23	C	475	CLA	CAA-CBA-CGA-O2A
23	b	2525	CLA	C5-C6-C7-C8
23	A	349	CLA	C2-C1-O2A-CGA
23	b	2511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	353	PL9	C25-C24-C26-C27
23	c	2486	CLA	C10-C11-C12-C13
23	B	511	CLA	C6-C7-C8-C9
23	B	515	CLA	C6-C7-C8-C9
23	B	517	CLA	C11-C10-C8-C9
23	B	523	CLA	C14-C13-C15-C16
23	C	482	CLA	C11-C12-C13-C14
23	b	2511	CLA	C6-C7-C8-C9
23	b	2513	CLA	C11-C12-C13-C14
23	b	2514	CLA	C14-C13-C15-C16
23	b	2517	CLA	C11-C10-C8-C9
23	b	2522	CLA	C11-C10-C8-C9
23	b	2523	CLA	C14-C13-C15-C16
23	b	2525	CLA	C11-C12-C13-C14
23	c	2482	CLA	C11-C12-C13-C14
23	c	2485	CLA	C6-C7-C8-C9
24	A	351	PHO	C11-C12-C13-C14
24	D	355	PHO	C6-C7-C8-C9
24	d	2356	PHO	C6-C7-C8-C9
24	d	2356	PHO	C14-C13-C15-C16
26	d	2359	LMT	C11-C10-C9-C8
23	b	2514	CLA	C15-C16-C17-C18
23	C	486	CLA	C10-C11-C12-C13
23	c	2475	CLA	CAA-CBA-CGA-O2A
23	A	352	CLA	C6-C7-C8-C10
23	B	513	CLA	C11-C12-C13-C15
23	B	514	CLA	C12-C13-C15-C16
23	B	517	CLA	C11-C10-C8-C7
23	B	518	CLA	C6-C7-C8-C10
23	B	522	CLA	C11-C10-C8-C7
23	B	524	CLA	C6-C7-C8-C10
23	B	524	CLA	C12-C13-C15-C16
23	B	525	CLA	C11-C12-C13-C15
23	B	527	CLA	C6-C7-C8-C10
23	C	474	CLA	C11-C12-C13-C15
23	C	474	CLA	C12-C13-C15-C16
23	C	475	CLA	C11-C10-C8-C7
23	C	483	CLA	C6-C7-C8-C10
23	C	485	CLA	C6-C7-C8-C10
23	a	2351	CLA	C6-C7-C8-C10
23	b	2514	CLA	C6-C7-C8-C10
23	b	2514	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	2517	CLA	C11-C10-C8-C7
23	b	2518	CLA	C6-C7-C8-C10
23	b	2522	CLA	C11-C10-C8-C7
23	b	2523	CLA	C6-C7-C8-C10
23	b	2524	CLA	C12-C13-C15-C16
23	b	2526	CLA	C6-C7-C8-C10
23	c	2474	CLA	C11-C12-C13-C15
23	c	2475	CLA	C11-C10-C8-C7
23	c	2480	CLA	C11-C10-C8-C7
23	c	2483	CLA	C6-C7-C8-C10
23	c	2485	CLA	C6-C7-C8-C10
24	A	351	PHO	C6-C7-C8-C10
24	A	351	PHO	C11-C12-C13-C15
24	D	355	PHO	C6-C7-C8-C10
24	D	355	PHO	C12-C13-C15-C16
24	a	2350	PHO	C6-C7-C8-C10
24	a	2350	PHO	C11-C12-C13-C15
24	d	2356	PHO	C11-C10-C8-C7
24	d	2356	PHO	C12-C13-C15-C16
23	C	480	CLA	C15-C16-C17-C18
25	a	2352	PL9	C25-C24-C26-C27
25	A	353	PL9	C23-C24-C26-C27
23	B	511	CLA	C4-C3-C5-C6
25	a	2352	PL9	C23-C24-C26-C27
27	K	50	BCR	C1-C6-C7-C8
27	d	2360	BCR	C5-C6-C7-C8
27	k	2050	BCR	C1-C6-C7-C8
23	B	511	CLA	C5-C6-C7-C8
23	B	514	CLA	C15-C16-C17-C18
25	D	357	PL9	C4-C3-C7-C8
25	d	2358	PL9	C4-C3-C7-C8
23	A	348	CLA	C14-C13-C15-C16
23	B	514	CLA	C14-C13-C15-C16
23	B	522	CLA	C6-C7-C8-C9
23	C	479	CLA	C14-C13-C15-C16
23	a	2348	CLA	C14-C13-C15-C16
23	b	2515	CLA	C6-C7-C8-C9
23	b	2522	CLA	C6-C7-C8-C9
23	b	2511	CLA	C5-C6-C7-C8
23	B	523	CLA	C6-C7-C8-C10
23	B	525	CLA	C11-C10-C8-C7
23	b	2524	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	2525	CLA	C11-C10-C8-C7
23	b	2525	CLA	C11-C12-C13-C15
23	b	2526	CLA	C12-C13-C15-C16
23	c	2474	CLA	C12-C13-C15-C16
23	c	2483	CLA	C11-C12-C13-C15
23	b	2515	CLA	C4-C3-C5-C6
23	b	2517	CLA	O1D-CGD-O2D-CED
28	v	2138	HEC	C1A-C2A-CAA-CBA
23	A	352	CLA	C4-C3-C5-C6
24	d	2356	PHO	C5-C6-C7-C8
23	b	2518	CLA	C11-C12-C13-C14
23	c	2479	CLA	C14-C13-C15-C16
23	b	2522	CLA	C4C-C3C-CAC-CBC
23	C	486	CLA	CAA-CBA-CGA-O2A
23	c	2486	CLA	CAA-CBA-CGA-O2A
24	D	355	PHO	C5-C6-C7-C8
23	B	519	CLA	C4-C3-C5-C6
23	c	2487	CLA	C4-C3-C5-C6
23	b	2524	CLA	C10-C11-C12-C13
23	c	2475	CLA	C10-C11-C12-C13
23	a	2351	CLA	C4-C3-C5-C6
23	b	2519	CLA	C4-C3-C5-C6
23	B	522	CLA	C4C-C3C-CAC-CBC
23	C	477	CLA	C2A-CAA-CBA-CGA
23	c	2477	CLA	C2A-CAA-CBA-CGA
23	b	2517	CLA	CBD-CGD-O2D-CED
23	B	511	CLA	C12-C13-C15-C16
23	B	512	CLA	C12-C13-C15-C16
23	B	523	CLA	C11-C10-C8-C7
23	B	527	CLA	C12-C13-C15-C16
23	C	477	CLA	C11-C12-C13-C15
23	C	478	CLA	C12-C13-C15-C16
23	C	481	CLA	C6-C7-C8-C10
23	C	483	CLA	C11-C12-C13-C15
23	b	2511	CLA	C12-C13-C15-C16
23	b	2512	CLA	C12-C13-C15-C16
23	b	2523	CLA	C11-C10-C8-C7
23	c	2477	CLA	C11-C12-C13-C15
23	c	2478	CLA	C12-C13-C15-C16
23	c	2481	CLA	C6-C7-C8-C10
23	B	524	CLA	C10-C11-C12-C13
23	A	352	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	512	CLA	C14-C13-C15-C16
23	B	518	CLA	C11-C12-C13-C14
23	C	478	CLA	C14-C13-C15-C16
23	b	2511	CLA	C14-C13-C15-C16
23	b	2525	CLA	C11-C10-C8-C9
23	c	2474	CLA	C14-C13-C15-C16
23	c	2478	CLA	C14-C13-C15-C16
24	A	351	PHO	C5-C6-C7-C8
24	a	2350	PHO	C5-C6-C7-C8
23	C	476	CLA	C4-C3-C5-C6
23	c	2476	CLA	C4-C3-C5-C6
23	A	352	CLA	C2-C3-C5-C6
23	C	476	CLA	CAD-CBD-CGD-O2D
23	C	480	CLA	CAD-CBD-CGD-O2D
23	c	2476	CLA	CAD-CBD-CGD-O2D
23	c	2480	CLA	CAD-CBD-CGD-O2D
23	C	476	CLA	CAD-CBD-CGD-O1D
23	C	480	CLA	CAD-CBD-CGD-O1D
23	C	486	CLA	CHA-CBD-CGD-O1D
23	c	2476	CLA	CAD-CBD-CGD-O1D
23	c	2480	CLA	CAD-CBD-CGD-O1D
23	c	2486	CLA	CHA-CBD-CGD-O1D
27	C	488	BCR	C23-C24-C25-C30
27	F	48	BCR	C5-C6-C7-C8
23	B	515	CLA	C2-C3-C5-C6
23	B	519	CLA	C2-C3-C5-C6
23	C	475	CLA	C10-C11-C12-C13
23	a	2348	CLA	CBD-CGD-O2D-CED
25	A	353	PL9	C4-C3-C7-C8
25	a	2352	PL9	C4-C3-C7-C8
25	D	357	PL9	C2-C3-C7-C8
23	B	511	CLA	C14-C13-C15-C16
23	B	525	CLA	C11-C10-C8-C9
23	C	474	CLA	C14-C13-C15-C16
23	C	475	CLA	C11-C10-C8-C9
23	a	2351	CLA	C6-C7-C8-C9
23	b	2512	CLA	C14-C13-C15-C16
23	d	2354	CLA	C11-C12-C13-C15
23	B	517	CLA	O1D-CGD-O2D-CED
23	C	478	CLA	C4-C3-C5-C6
23	d	2354	CLA	C4-C3-C5-C6
25	D	357	PL9	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	d	2358	PL9	C16-C17-C18-C19
23	a	2348	CLA	O1D-CGD-O2D-CED
23	d	2355	CLA	CAA-CBA-CGA-O2A
25	A	353	PL9	C12-C11-C9-C10
23	B	511	CLA	CAA-CBA-CGA-O2A
23	A	349	CLA	CAA-CBA-CGA-O2A
23	C	484	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	O1D-CGD-O2D-CED
23	b	2511	CLA	CAA-CBA-CGA-O2A
23	C	487	CLA	C4-C3-C5-C6
23	d	2355	CLA	C4-C3-C5-C6
23	C	480	CLA	CAA-CBA-CGA-O2A
23	c	2484	CLA	CAA-CBA-CGA-O2A
23	a	2351	CLA	C2-C3-C5-C6
23	B	527	CLA	C5-C6-C7-C8
25	d	2358	PL9	C2-C3-C7-C8
23	B	515	CLA	C14-C13-C15-C16
23	B	517	CLA	C11-C12-C13-C14
23	C	478	CLA	C6-C7-C8-C9
23	C	485	CLA	C11-C10-C8-C9
23	c	2475	CLA	C11-C10-C8-C9
23	c	2478	CLA	C6-C7-C8-C9
23	c	2482	CLA	C6-C7-C8-C9
23	c	2485	CLA	C11-C10-C8-C9
23	C	476	CLA	C13-C15-C16-C17
23	C	479	CLA	C15-C16-C17-C18
23	A	349	CLA	C4-C3-C5-C6
23	c	2478	CLA	C4-C3-C5-C6
23	A	349	CLA	C2-C3-C5-C6
23	C	476	CLA	C2-C3-C5-C6
23	b	2519	CLA	C2-C3-C5-C6
23	c	2476	CLA	C2-C3-C5-C6
23	b	2516	CLA	CAA-CBA-CGA-O2A
23	c	2482	CLA	C6-C7-C8-C10
23	B	514	CLA	C13-C15-C16-C17
23	B	516	CLA	CAA-CBA-CGA-O2A
23	b	2526	CLA	C5-C6-C7-C8
23	c	2480	CLA	CAA-CBA-CGA-O2A
23	d	2355	CLA	C2-C3-C5-C6
23	B	518	CLA	C5-C6-C7-C8
23	b	2514	CLA	C13-C15-C16-C17
23	c	2479	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	A	348	CLA	CBD-CGD-O2D-CED
23	C	485	CLA	C2-C1-O2A-CGA
23	c	2476	CLA	C13-C15-C16-C17
25	a	2352	PL9	C12-C11-C9-C10
23	C	475	CLA	CAA-CBA-CGA-O1A
28	v	2138	HEC	CAD-CBD-CGD-O1D
23	A	352	CLA	C11-C12-C13-C14
23	B	512	CLA	C6-C7-C8-C9
23	B	527	CLA	C14-C13-C15-C16
23	C	474	CLA	C6-C7-C8-C9
23	C	482	CLA	C6-C7-C8-C9
23	C	482	CLA	C14-C13-C15-C16
23	D	354	CLA	C6-C7-C8-C9
23	D	354	CLA	C11-C12-C13-C14
23	a	2351	CLA	C11-C12-C13-C14
23	b	2512	CLA	C6-C7-C8-C9
23	b	2526	CLA	C14-C13-C15-C16
23	c	2474	CLA	C6-C7-C8-C9
23	c	2482	CLA	C14-C13-C15-C16
23	c	2483	CLA	C11-C12-C13-C14
23	d	2354	CLA	C11-C12-C13-C14
28	E	84	HEC	CAD-CBD-CGD-O1D
27	c	2488	BCR	C23-C24-C25-C30
27	k	2050	BCR	C5-C6-C7-C8
28	V	138	HEC	CAD-CBD-CGD-O1D
28	e	2084	HEC	CAD-CBD-CGD-O1D
23	c	2478	CLA	C2-C3-C5-C6
23	B	512	CLA	C5-C6-C7-C8
23	B	511	CLA	C11-C10-C8-C7
23	B	515	CLA	C12-C13-C15-C16
23	B	522	CLA	C12-C13-C15-C16
23	B	527	CLA	C11-C10-C8-C7
23	C	482	CLA	C6-C7-C8-C10
23	C	485	CLA	C11-C10-C8-C7
23	C	487	CLA	C12-C13-C15-C16
23	D	354	CLA	C11-C12-C13-C15
23	a	2348	CLA	C11-C10-C8-C7
23	b	2511	CLA	C11-C10-C8-C7
23	b	2515	CLA	C12-C13-C15-C16
23	b	2522	CLA	C12-C13-C15-C16
23	b	2526	CLA	C11-C10-C8-C7
23	c	2485	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	2487	CLA	C12-C13-C15-C16
23	c	2475	CLA	CAA-CBA-CGA-O1A
23	B	517	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	C2A-CAA-CBA-CGA
23	b	2526	CLA	C2A-CAA-CBA-CGA
23	b	2518	CLA	C5-C6-C7-C8
23	c	2484	CLA	C15-C16-C17-C18
23	B	517	CLA	CAA-CBA-CGA-O2A
23	C	478	CLA	C2-C3-C5-C6
23	c	2476	CLA	C2-C1-O2A-CGA
28	v	2138	HEC	CAD-CBD-CGD-O2D
23	B	524	CLA	C11-C12-C13-C14
23	C	487	CLA	C14-C13-C15-C16
23	b	2517	CLA	C11-C12-C13-C14
23	b	2524	CLA	C11-C12-C13-C14
27	C	488	BCR	C22-C23-C24-C25
27	c	2488	BCR	C22-C23-C24-C25
24	a	2350	PHO	C4-C3-C5-C6
25	d	2358	PL9	C20-C19-C21-C22
28	E	84	HEC	CAD-CBD-CGD-O2D
23	b	2517	CLA	CAA-CBA-CGA-O2A
23	B	511	CLA	C2-C3-C5-C6
23	b	2511	CLA	C2-C3-C5-C6
23	b	2515	CLA	C2-C3-C5-C6
23	C	485	CLA	C10-C11-C12-C13
23	a	2351	CLA	C5-C6-C7-C8
28	e	2084	HEC	CAD-CBD-CGD-O2D
23	C	484	CLA	C15-C16-C17-C18
23	B	518	CLA	CAA-CBA-CGA-O2A
23	c	2485	CLA	C2A-CAA-CBA-CGA
23	C	476	CLA	CAA-CBA-CGA-O2A
23	b	2524	CLA	C4-C3-C5-C6
24	A	351	PHO	C4-C3-C5-C6
25	D	357	PL9	C20-C19-C21-C22
23	B	519	CLA	CAA-CBA-CGA-O2A
23	b	2519	CLA	CAA-CBA-CGA-O2A
23	d	2354	CLA	C2-C3-C5-C6
23	b	2518	CLA	CAA-CBA-CGA-O2A
23	c	2476	CLA	CAA-CBA-CGA-O2A
28	V	138	HEC	CAD-CBD-CGD-O2D
24	D	355	PHO	CHA-CBD-CGD-O1D
25	A	353	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
23	b	2512	CLA	C5-C6-C7-C8
23	B	524	CLA	C11-C12-C13-C15
23	B	521	CLA	C11-C10-C8-C9
23	C	483	CLA	C11-C12-C13-C14
23	C	484	CLA	C11-C12-C13-C14
23	b	2515	CLA	C14-C13-C15-C16
23	b	2521	CLA	C11-C10-C8-C9
23	c	2477	CLA	C11-C12-C13-C14
23	c	2484	CLA	C11-C12-C13-C14
23	c	2487	CLA	C14-C13-C15-C16
23	d	2354	CLA	C6-C7-C8-C9
23	C	484	CLA	C2A-CAA-CBA-CGA
23	B	513	CLA	C2-C1-O2A-CGA
23	C	476	CLA	C2-C1-O2A-CGA
23	c	2484	CLA	C2-C1-O2A-CGA
23	c	2485	CLA	C2-C1-O2A-CGA
23	c	2487	CLA	C2-C3-C5-C6
23	c	2487	CLA	O2A-C1-C2-C3
26	d	2359	LMT	C4-C5-C6-C7
23	c	2485	CLA	C10-C11-C12-C13
26	B	526	LMT	C4-C5-C6-C7
23	c	2484	CLA	C2A-CAA-CBA-CGA
23	b	2520	CLA	CBD-CGD-O2D-CED
23	C	477	CLA	C11-C12-C13-C14
23	D	356	CLA	C14-C13-C15-C16
23	b	2523	CLA	C11-C10-C8-C9
23	d	2357	CLA	C14-C13-C15-C16
23	c	2485	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	CAA-CBA-CGA-O2A
23	C	485	CLA	CAA-CBA-CGA-O2A
23	a	2348	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	C11-C10-C8-C7
23	C	475	CLA	C6-C7-C8-C10
23	C	477	CLA	C6-C7-C8-C10
23	C	484	CLA	C11-C12-C13-C15
23	D	354	CLA	C6-C7-C8-C10
23	b	2524	CLA	C11-C12-C13-C15
23	b	2526	CLA	C11-C12-C13-C15
23	c	2477	CLA	C6-C7-C8-C10
23	c	2480	CLA	C11-C12-C13-C15
23	c	2484	CLA	C11-C12-C13-C15
23	d	2354	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	d	2355	CLA	C6-C7-C8-C10
27	C	488	BCR	C23-C24-C25-C26
27	K	50	BCR	C5-C6-C7-C8
27	d	2360	BCR	C1-C6-C7-C8
23	C	480	CLA	C2-C1-O2A-CGA
23	C	484	CLA	C2-C1-O2A-CGA
24	A	351	PHO	C2-C1-O2A-CGA
24	a	2350	PHO	C2-C1-O2A-CGA
23	A	352	CLA	C5-C6-C7-C8
23	c	2487	CLA	CAA-CBA-CGA-O2A
23	B	524	CLA	C4-C3-C5-C6
23	D	354	CLA	C4-C3-C5-C6
23	b	2515	CLA	CAA-CBA-CGA-O2A
25	a	2352	PL9	C12-C11-C9-C8
23	B	525	CLA	C14-C13-C15-C16
23	b	2525	CLA	C14-C13-C15-C16
23	b	2526	CLA	C11-C12-C13-C14
23	c	2480	CLA	C11-C12-C13-C14
23	c	2475	CLA	C4-C3-C5-C6
23	D	354	CLA	C2-C3-C5-C6
23	B	515	CLA	CAA-CBA-CGA-O2A
23	C	485	CLA	C2A-CAA-CBA-CGA
23	C	487	CLA	CAA-CBA-CGA-O2A
23	C	477	CLA	C2-C1-O2A-CGA
23	b	2513	CLA	C2-C1-O2A-CGA
23	c	2477	CLA	C2-C1-O2A-CGA
23	c	2480	CLA	C2-C1-O2A-CGA
24	D	355	PHO	C2-C1-O2A-CGA
23	A	349	CLA	C6-C7-C8-C10
23	B	527	CLA	C11-C12-C13-C15
23	C	478	CLA	C11-C12-C13-C15
23	C	480	CLA	C11-C12-C13-C15
23	C	484	CLA	C6-C7-C8-C10
23	c	2475	CLA	C6-C7-C8-C10
23	c	2478	CLA	C11-C12-C13-C15
23	c	2484	CLA	C6-C7-C8-C10
23	C	487	CLA	O2A-C1-C2-C3
23	b	2524	CLA	C5-C6-C7-C8
23	D	356	CLA	C2A-CAA-CBA-CGA
23	b	2520	CLA	O1D-CGD-O2D-CED
23	c	2482	CLA	C4-C3-C5-C6
25	D	357	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
25	d	2358	PL9	C15-C14-C16-C17
23	C	481	CLA	C15-C16-C17-C18
23	B	523	CLA	C11-C10-C8-C9
23	B	527	CLA	C11-C12-C13-C14
23	C	480	CLA	C11-C12-C13-C14
23	C	486	CLA	CAA-CBA-CGA-O1A
23	C	487	CLA	C10-C11-C12-C13
23	a	2348	CLA	CAA-CBA-CGA-O1A
23	C	485	CLA	CAA-CBA-CGA-O1A
23	B	524	CLA	C5-C6-C7-C8
23	B	515	CLA	CAA-CBA-CGA-O1A
23	c	2485	CLA	CAA-CBA-CGA-O1A
23	c	2481	CLA	C15-C16-C17-C18
23	A	348	CLA	CAA-CBA-CGA-O1A
23	b	2515	CLA	CAA-CBA-CGA-O1A
23	d	2357	CLA	C2A-CAA-CBA-CGA
23	c	2486	CLA	CAA-CBA-CGA-O1A
23	C	487	CLA	C2-C3-C5-C6
23	A	350	CLA	CAD-CBD-CGD-O2D
23	C	481	CLA	CAD-CBD-CGD-O2D
23	c	2484	CLA	CAD-CBD-CGD-O2D
23	B	525	CLA	C2-C1-O2A-CGA
23	C	487	CLA	CAA-CBA-CGA-O1A
23	c	2487	CLA	CAA-CBA-CGA-O1A
23	b	2522	CLA	CAA-CBA-CGA-O2A
23	B	513	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	CAA-CBA-CGA-O2A
23	C	474	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

50 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	522	CLA	12	0
23	B	517	CLA	3	0
25	A	353	PL9	8	0
23	C	476	CLA	4	0
23	C	474	CLA	11	0
22	A	347	OEC	1	0
23	D	356	CLA	8	0
27	C	489	BCR	11	0
27	F	48	BCR	3	0

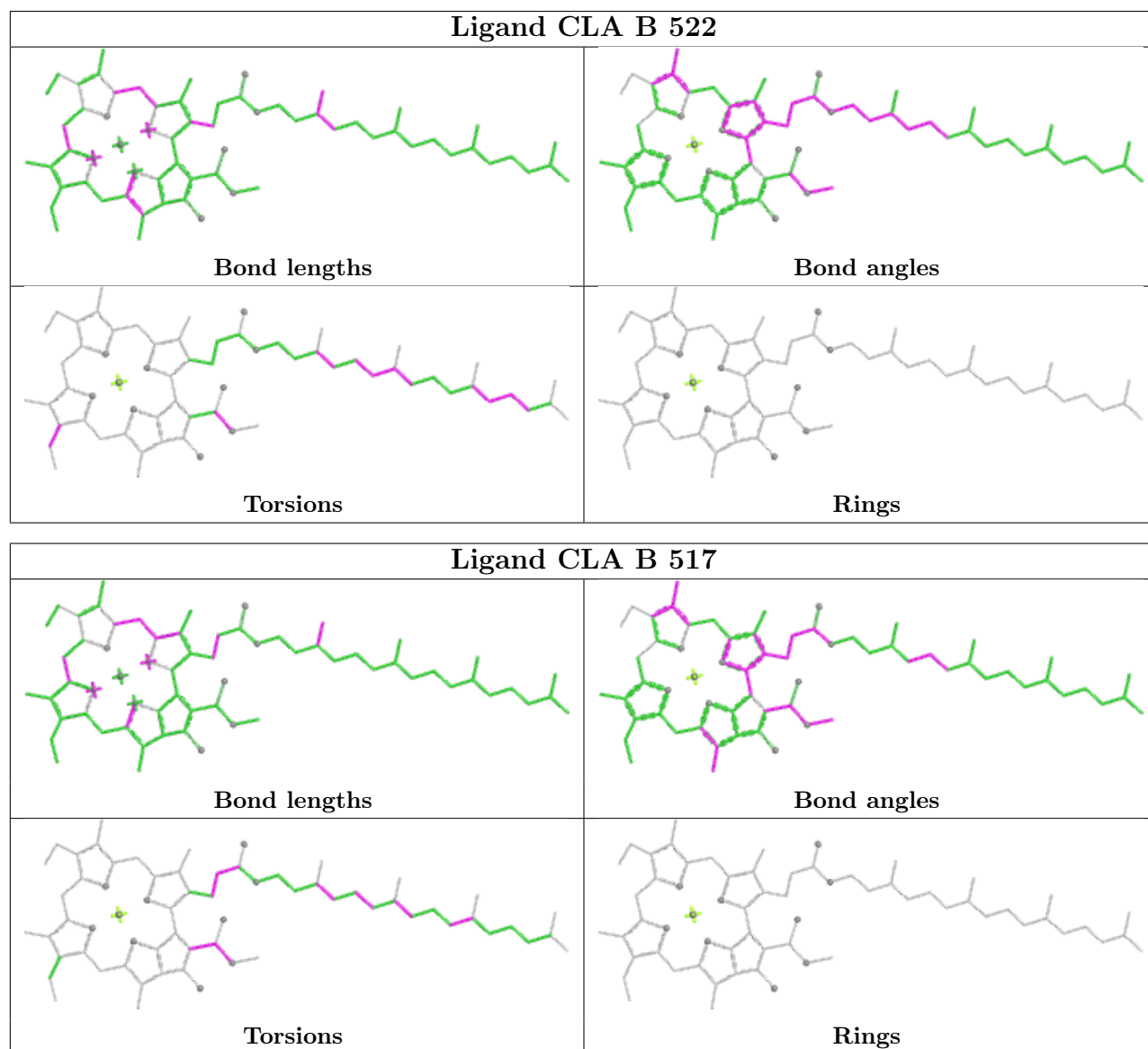
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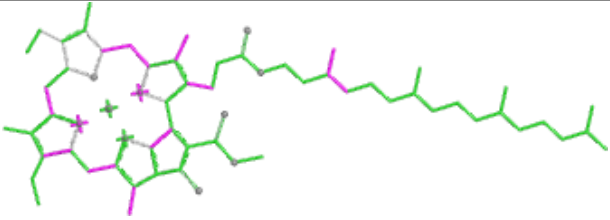
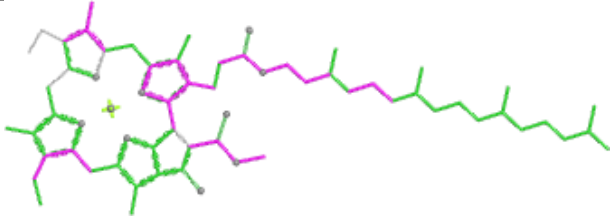
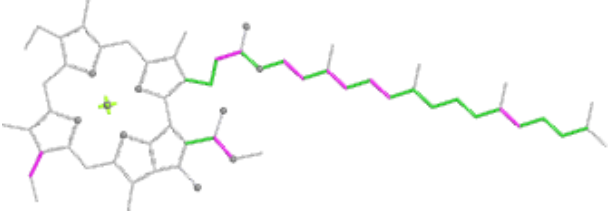
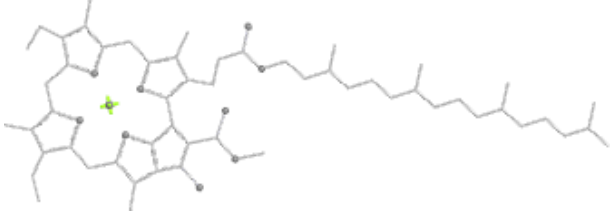
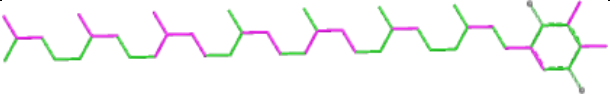
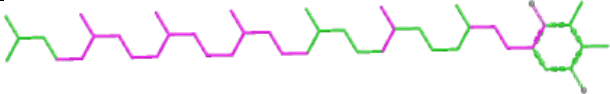
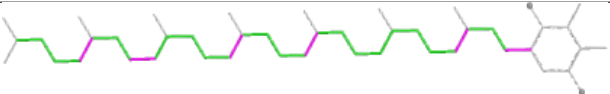
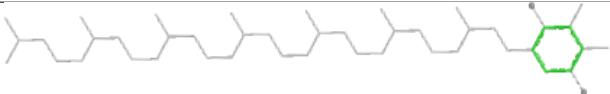


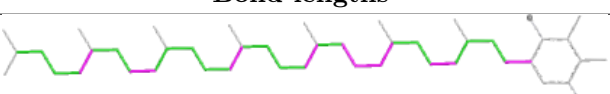
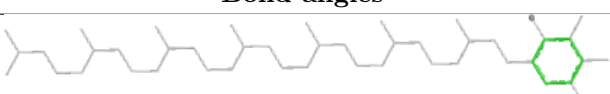
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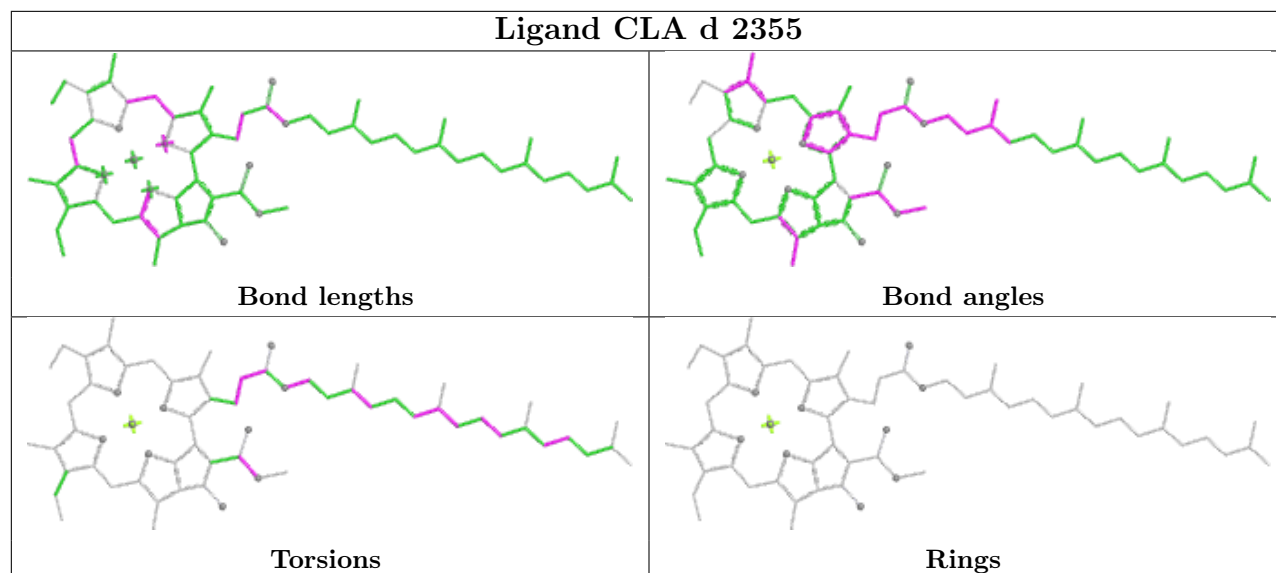
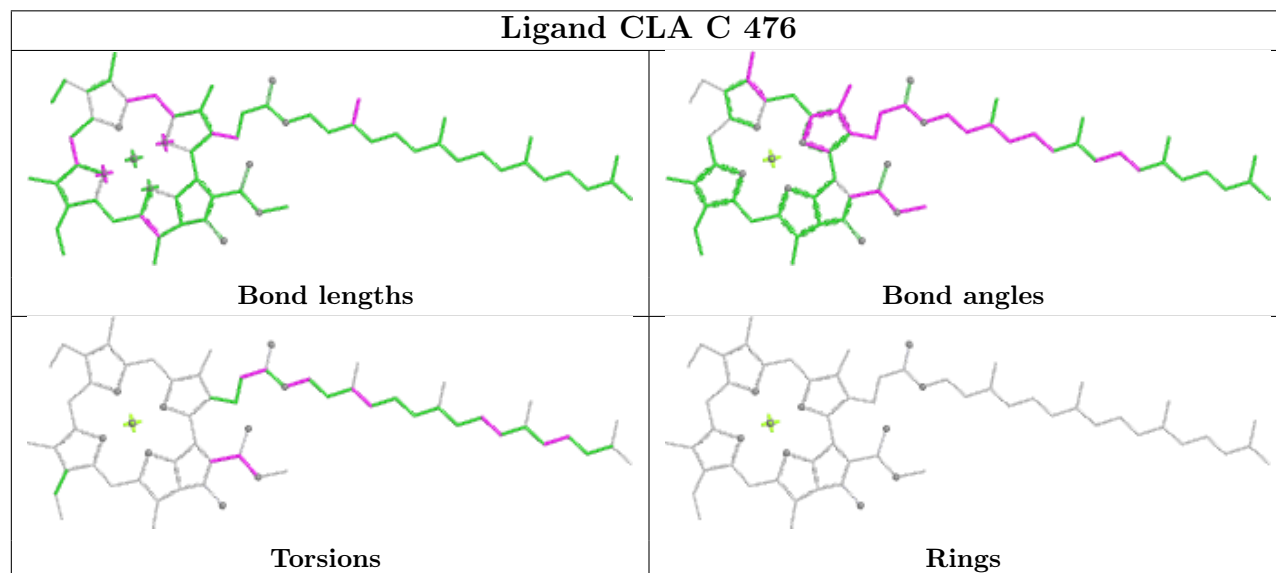
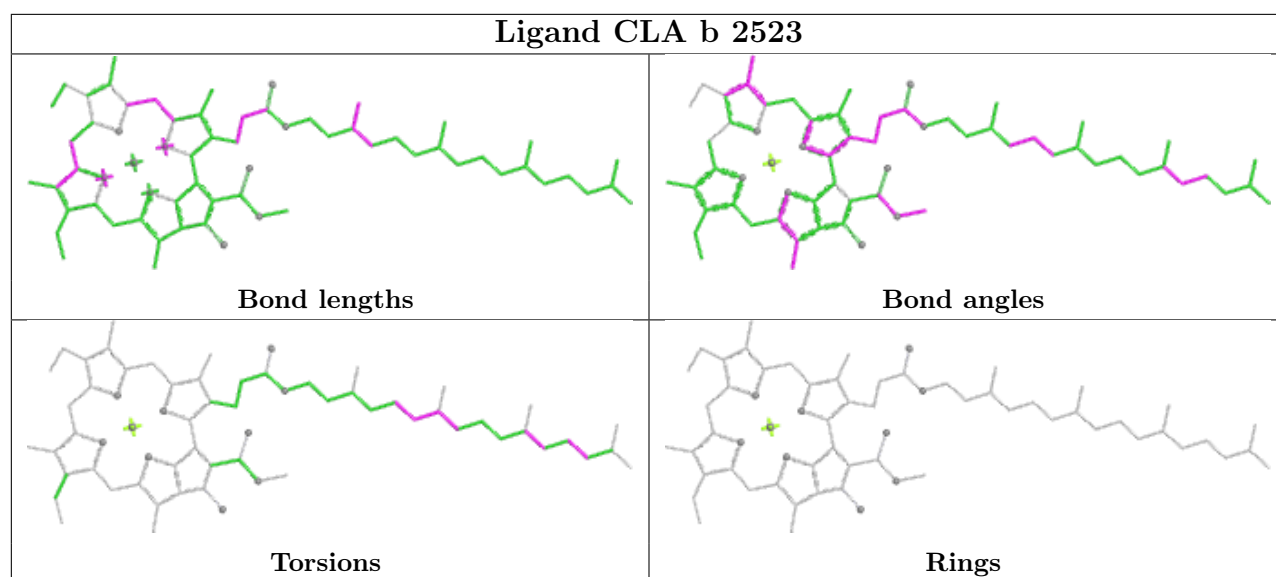
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	351	PHO	6	0
23	A	349	CLA	5	0
23	B	527	CLA	5	0
23	C	480	CLA	6	0
23	C	482	CLA	6	0
23	C	486	CLA	18	0
28	E	84	HEC	19	0
23	C	483	CLA	11	0
28	V	138	HEC	8	0
23	B	511	CLA	5	0
27	B	528	BCR	3	0
23	B	515	CLA	8	0
23	C	484	CLA	1	0
25	D	357	PL9	5	0
27	C	488	BCR	12	0
23	B	524	CLA	22	0
23	C	481	CLA	4	0
23	B	525	CLA	7	0
23	C	479	CLA	13	0
27	K	50	BCR	13	0
23	C	478	CLA	6	0
23	B	520	CLA	10	0
23	C	487	CLA	17	0
23	B	516	CLA	8	0
23	A	352	CLA	1	0
23	C	475	CLA	5	0
23	D	354	CLA	10	0
23	B	512	CLA	7	0
27	B	529	BCR	13	0
23	B	521	CLA	9	0
23	B	523	CLA	7	0
27	J	53	BCR	2	0
23	B	514	CLA	4	0
23	A	348	CLA	14	0
23	B	513	CLA	7	0
23	C	485	CLA	10	0
23	B	518	CLA	16	0
23	C	477	CLA	8	0
24	D	355	PHO	8	0
23	A	350	CLA	10	0
23	B	519	CLA	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

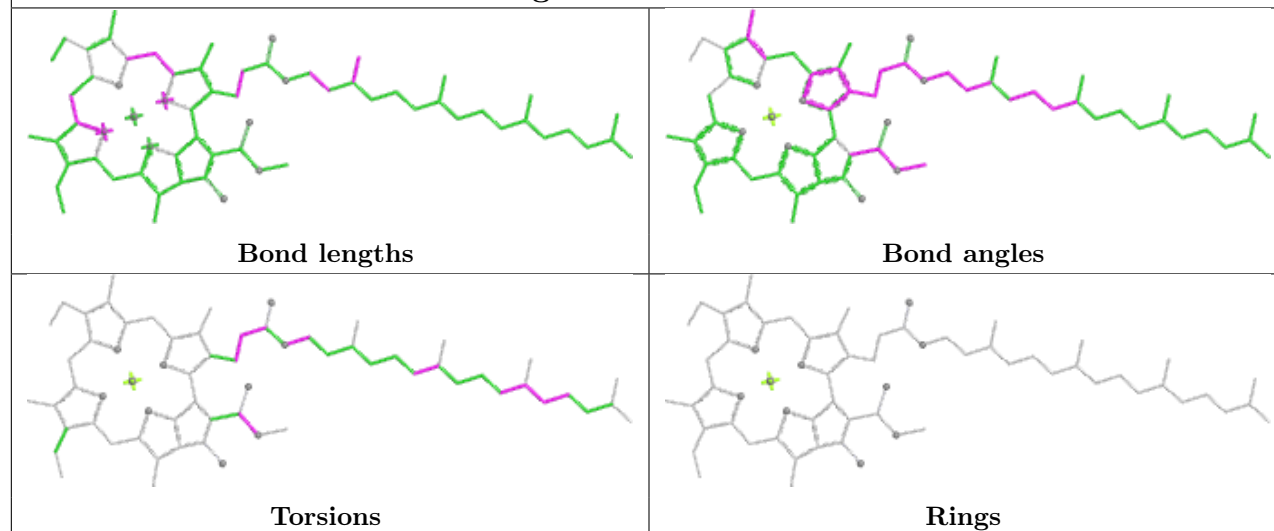
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



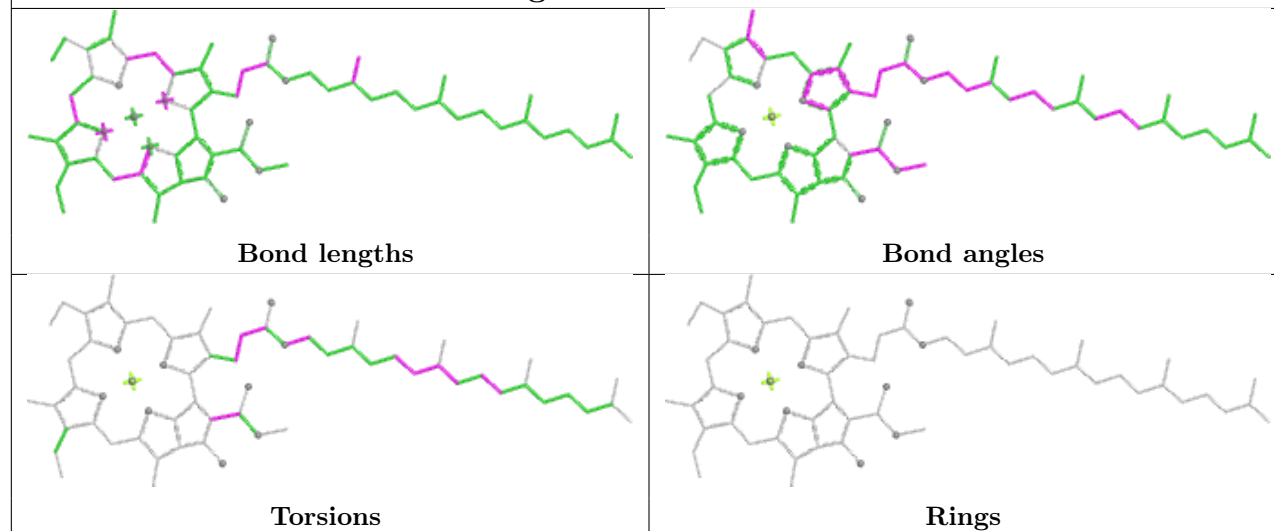
Ligand CLA c 2487	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 A 353	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 d 2358	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



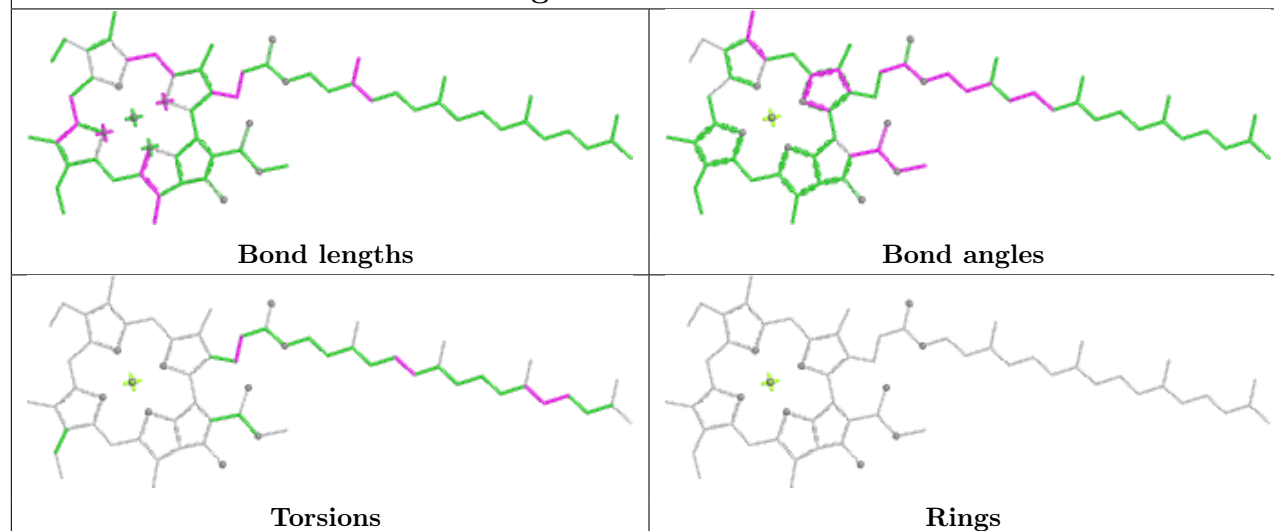
Ligand CLA C 474

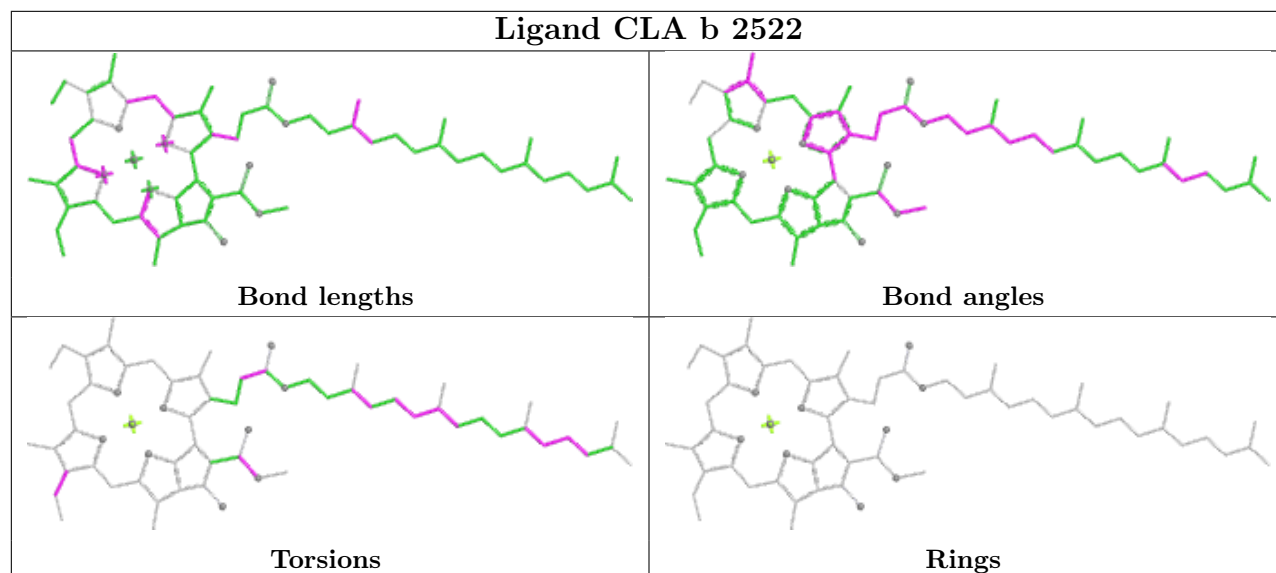
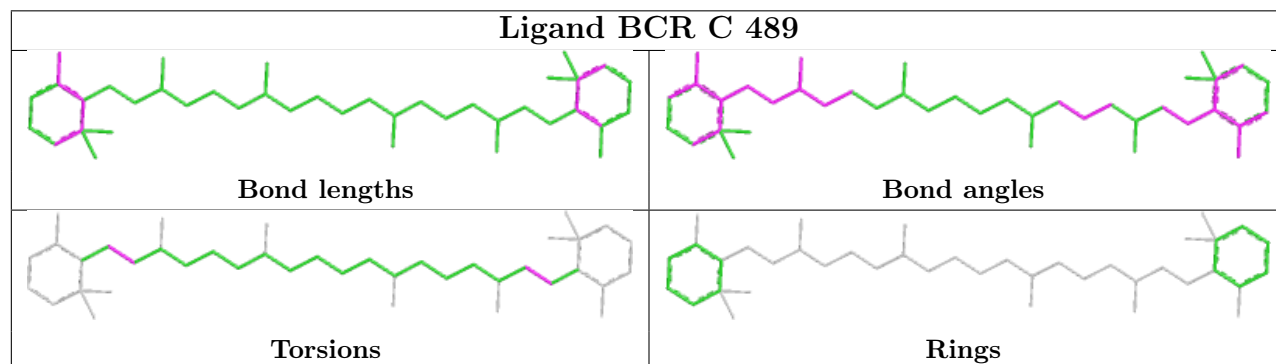
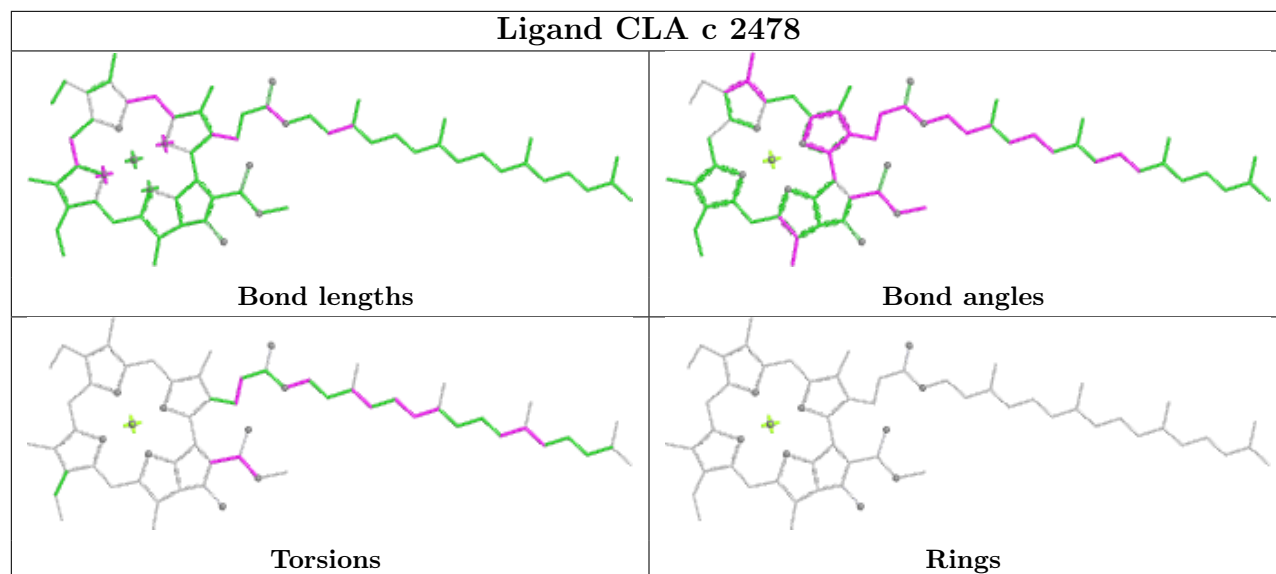


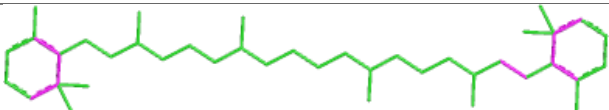
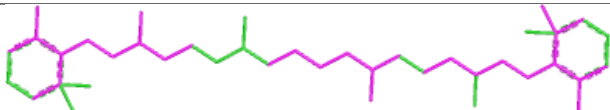
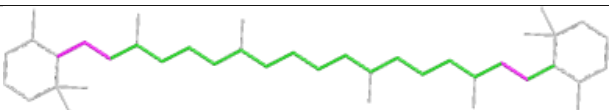
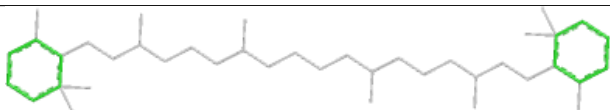
Ligand CLA c 2485



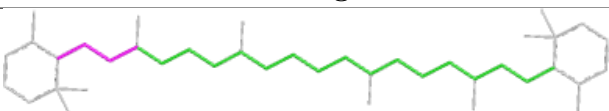
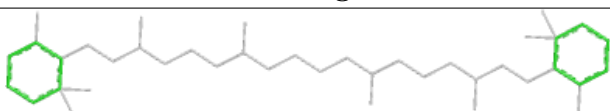


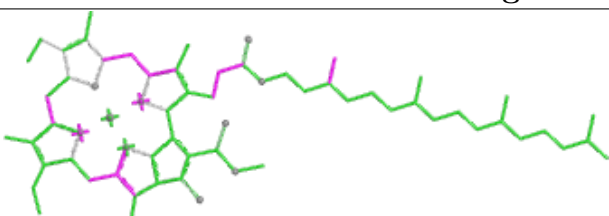
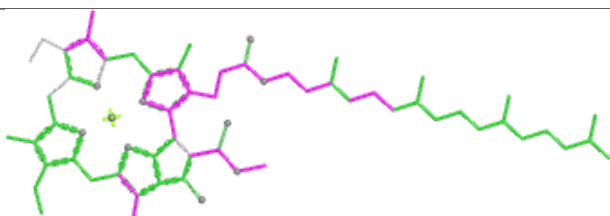
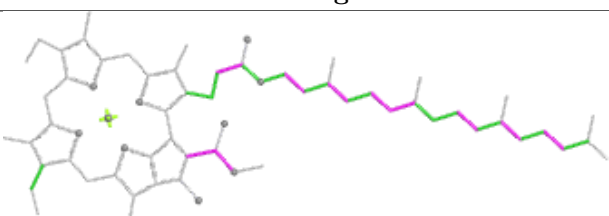
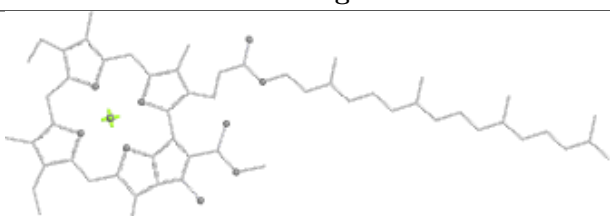
Ligand CLA D 356

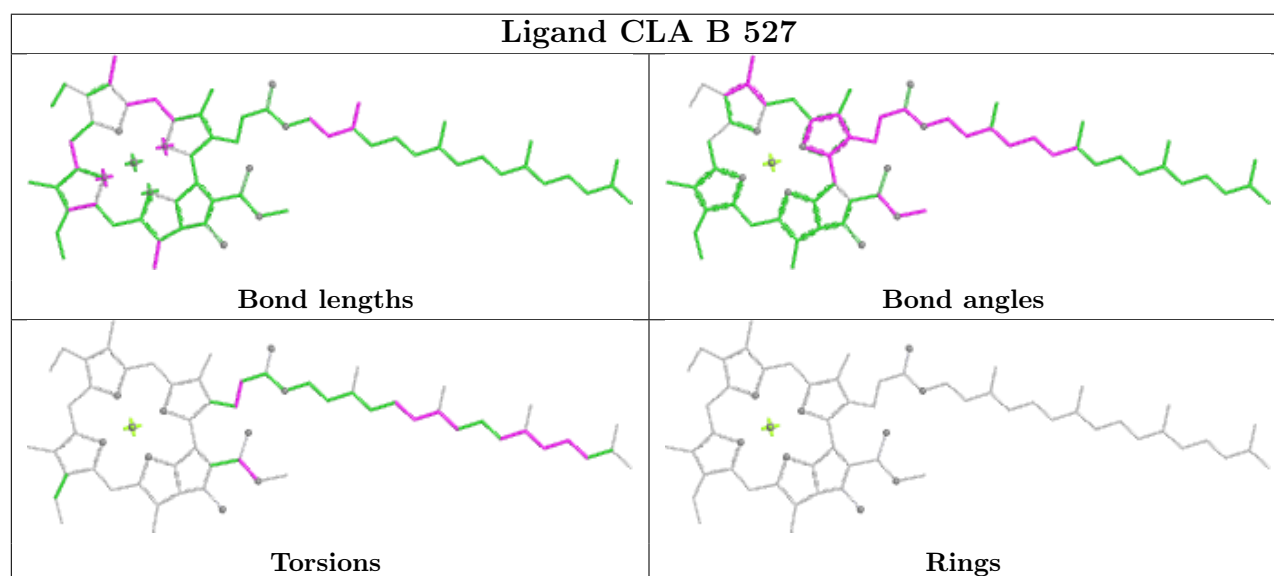
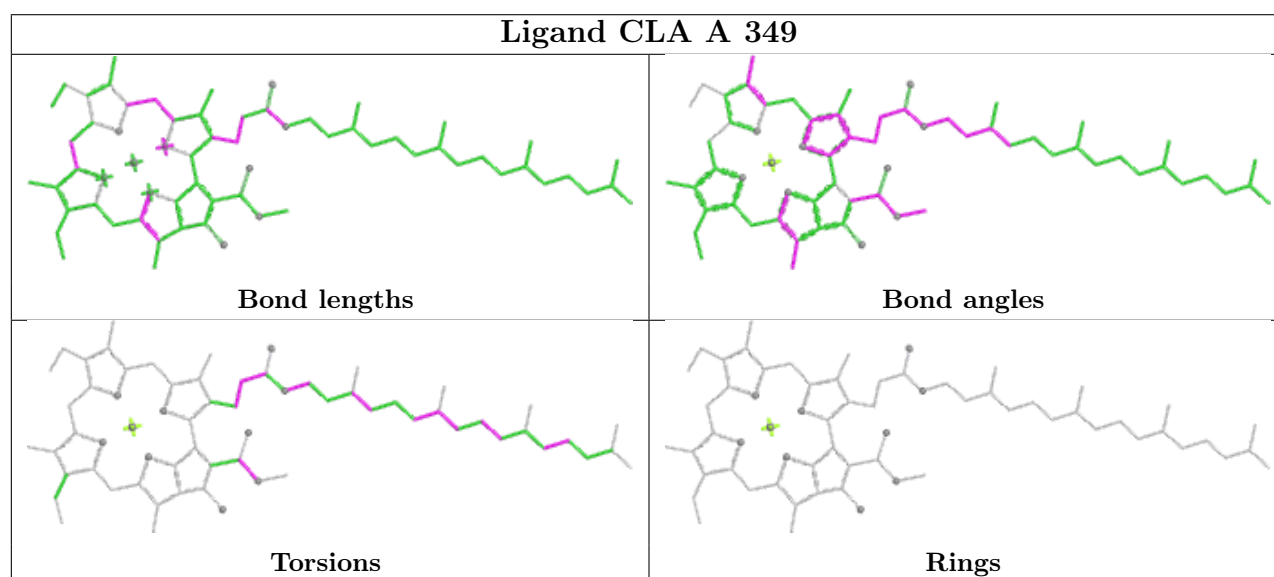
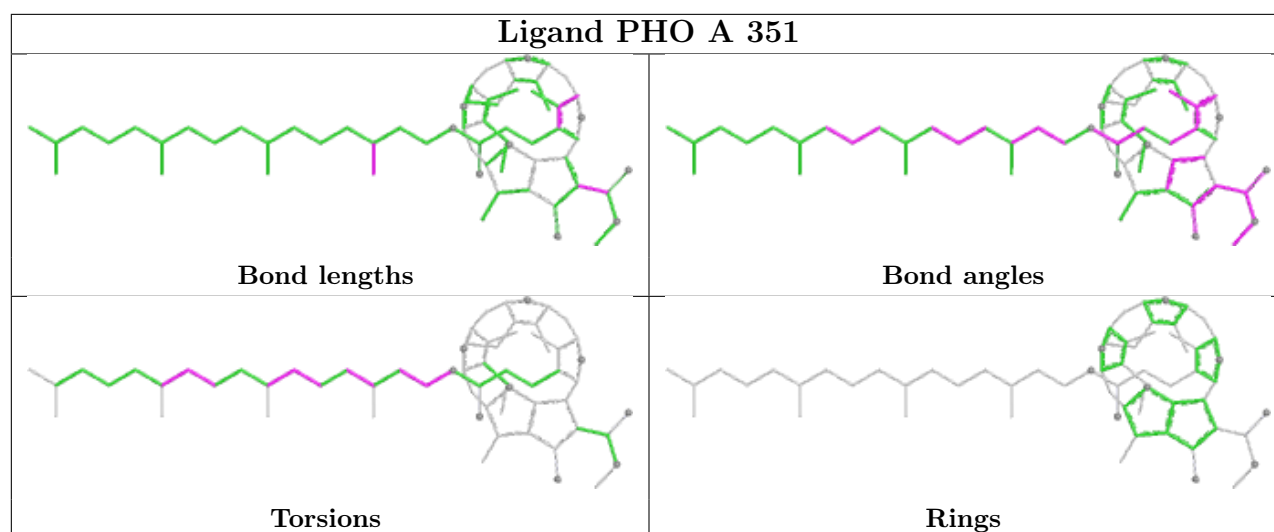




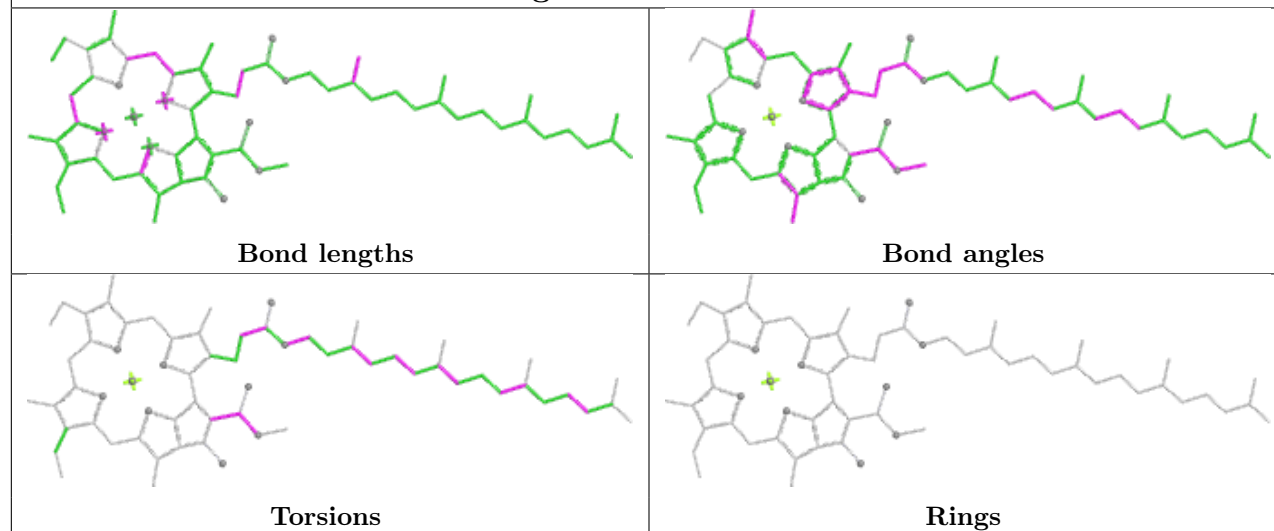
Ligand BCR F 48	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 2527	
	
Bond lengths	Bond angles
	
Torsions	Rings

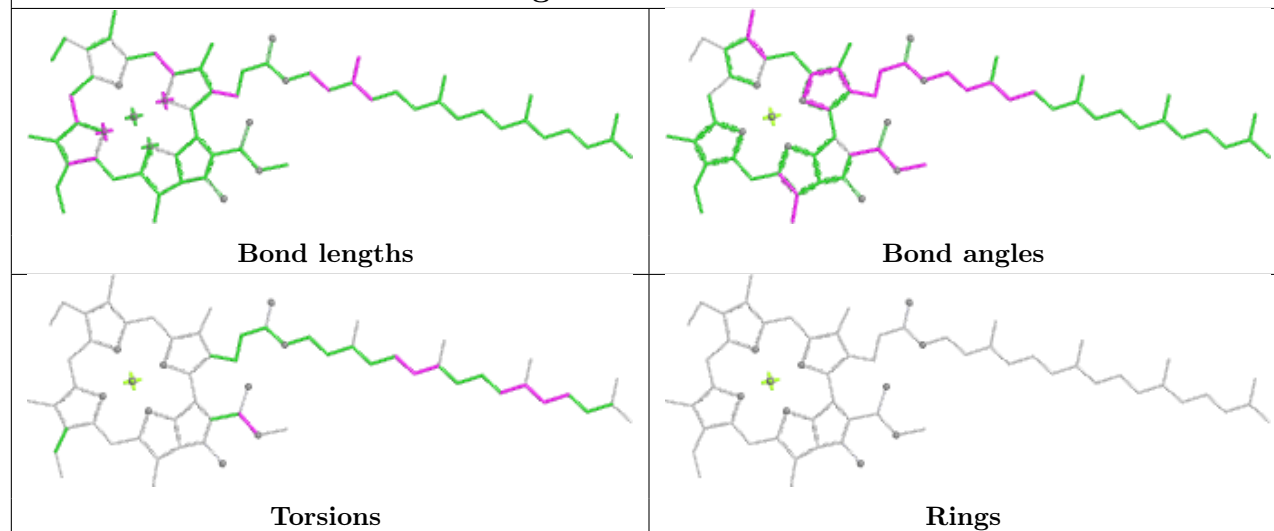
Ligand CLA b 2515	
	
Bond lengths	Bond angles
	
Torsions	Rings



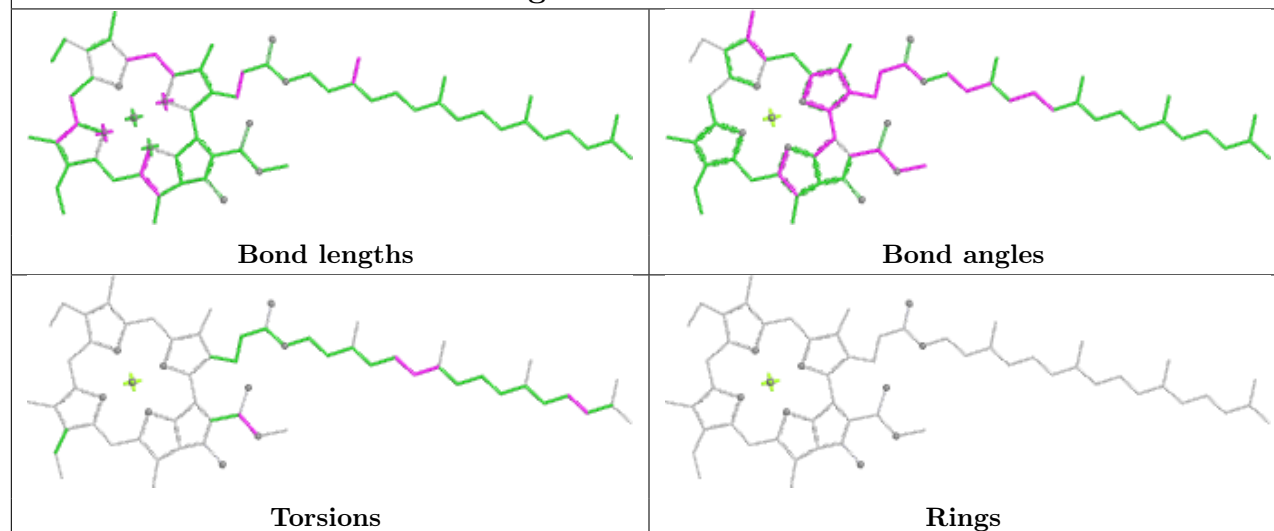
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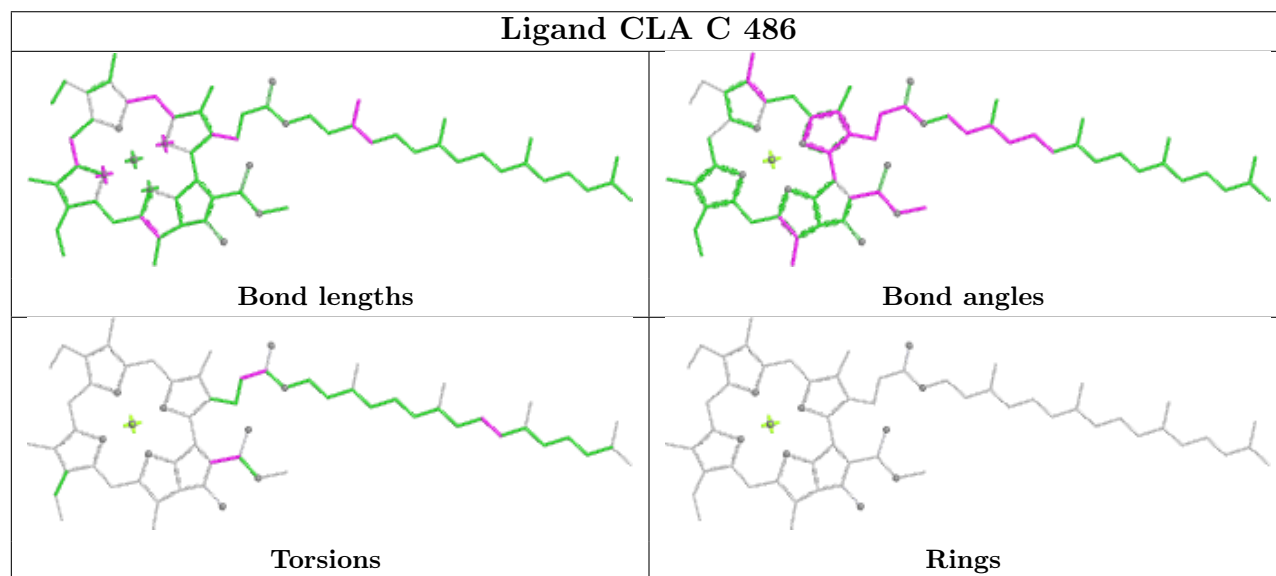
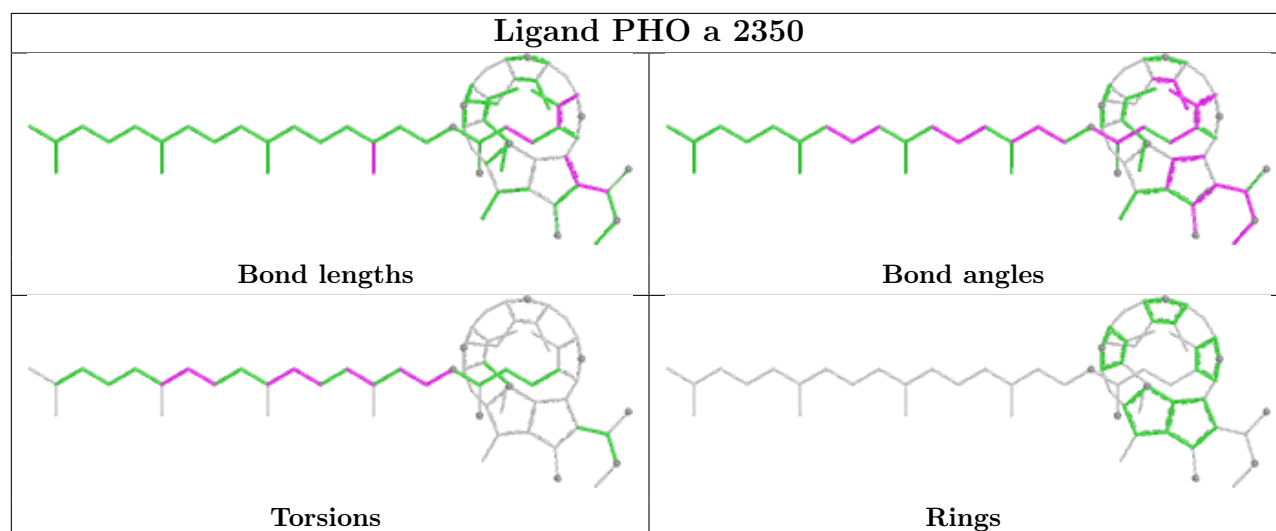
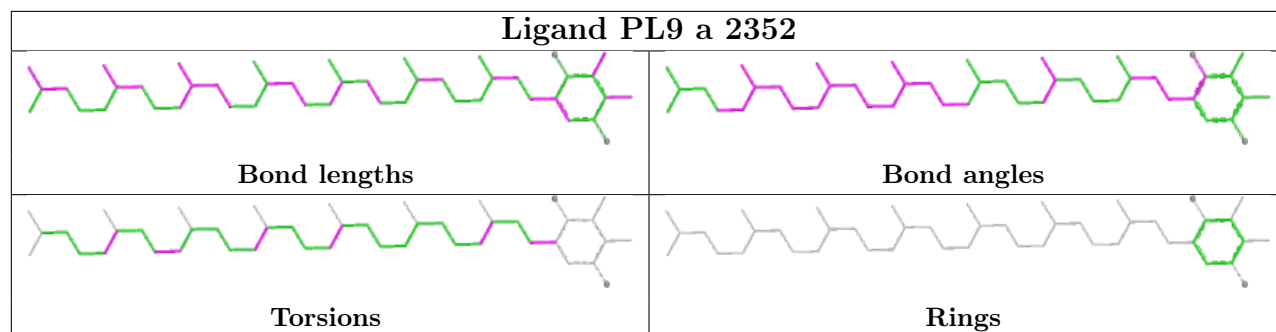


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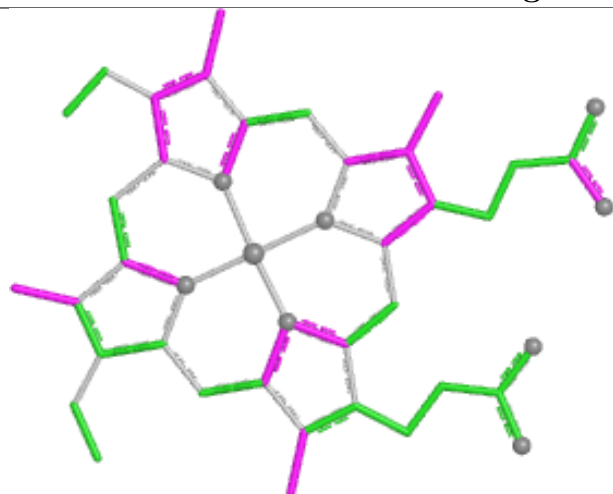


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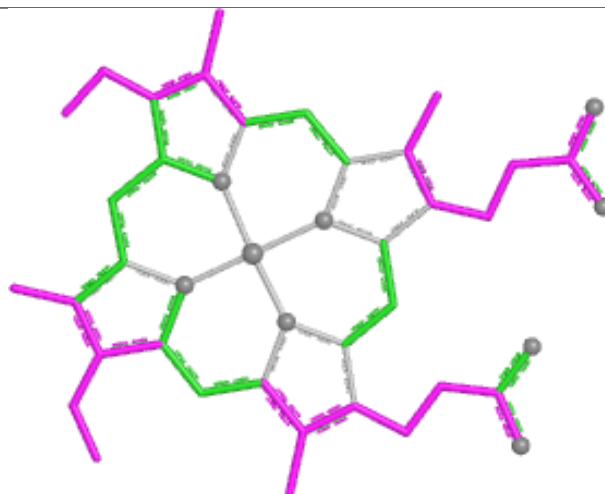




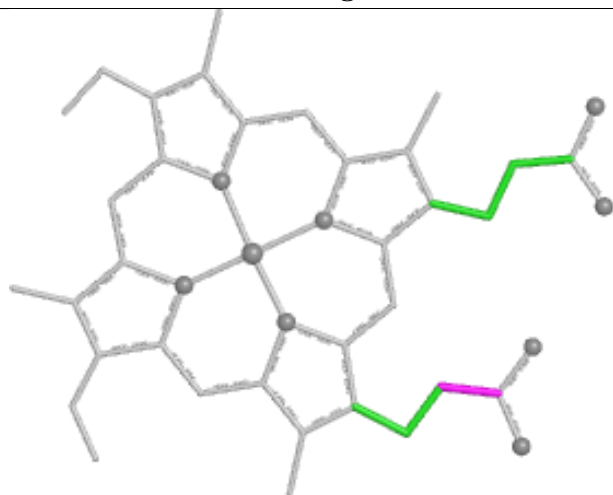
Ligand HEC E 84



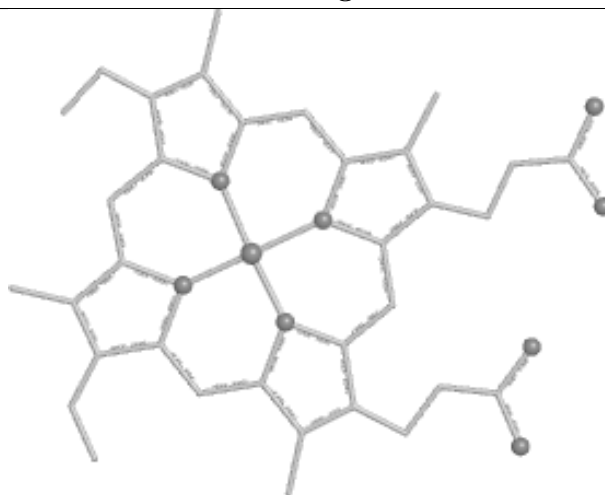
Bond lengths



Bond angles

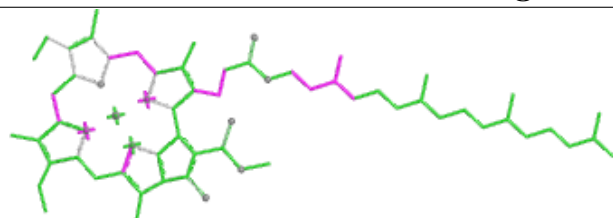


Torsions

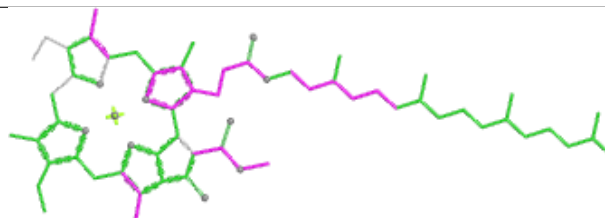


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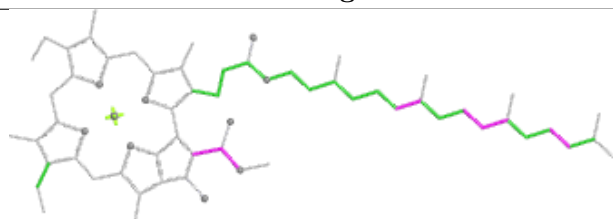
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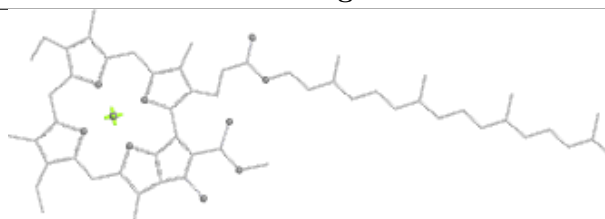
Bond lengths



Bond angles

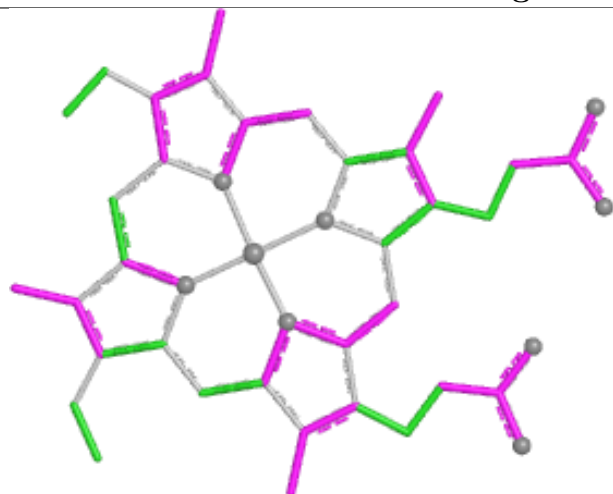


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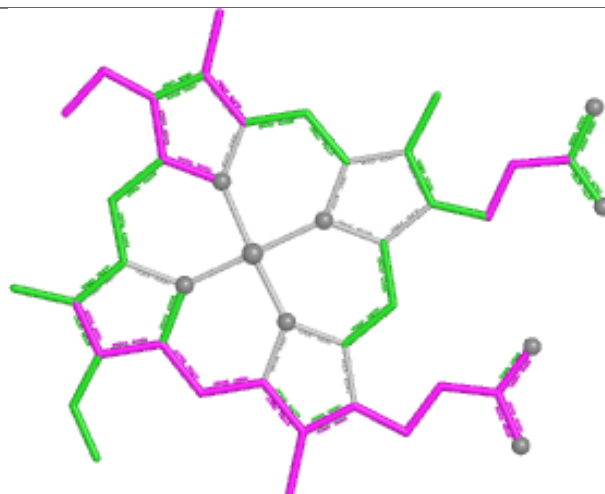


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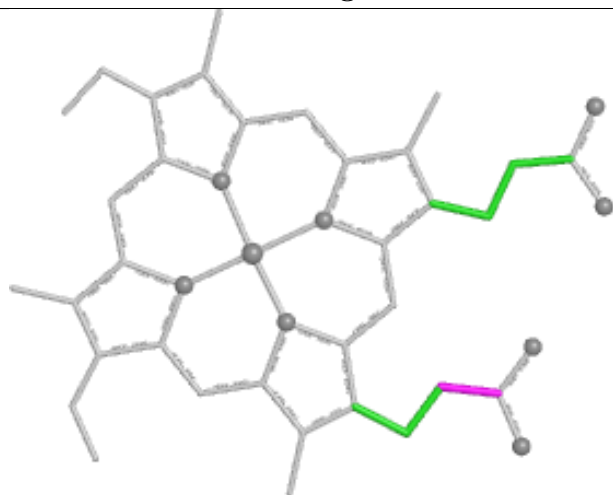
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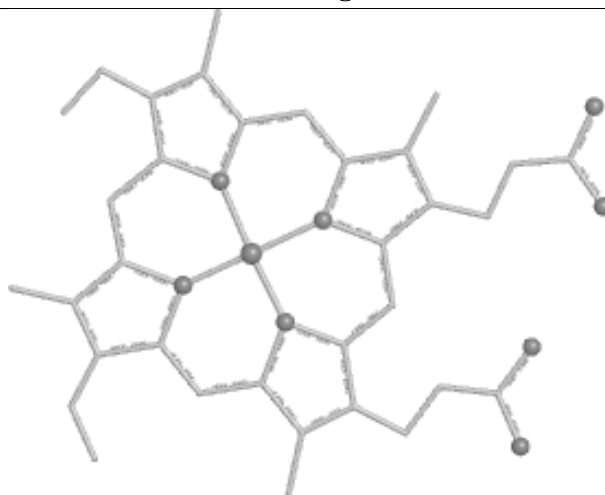
Bond lengths



Bond angles

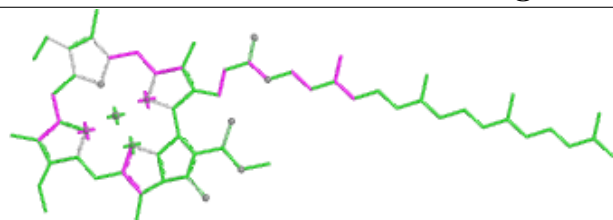


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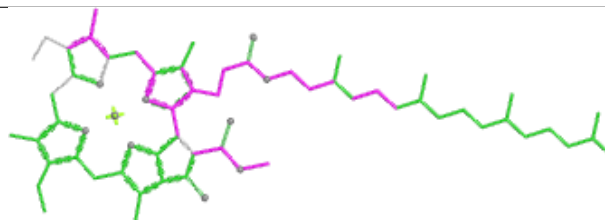


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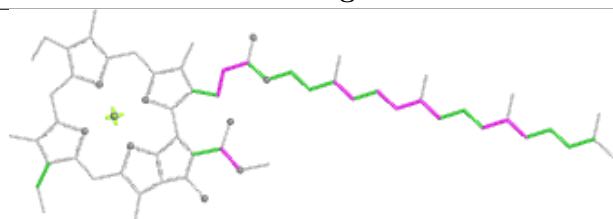
Ligand CLA B 511



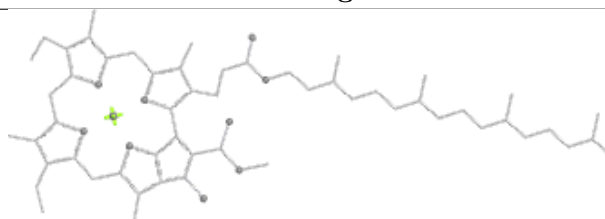
Bond lengths



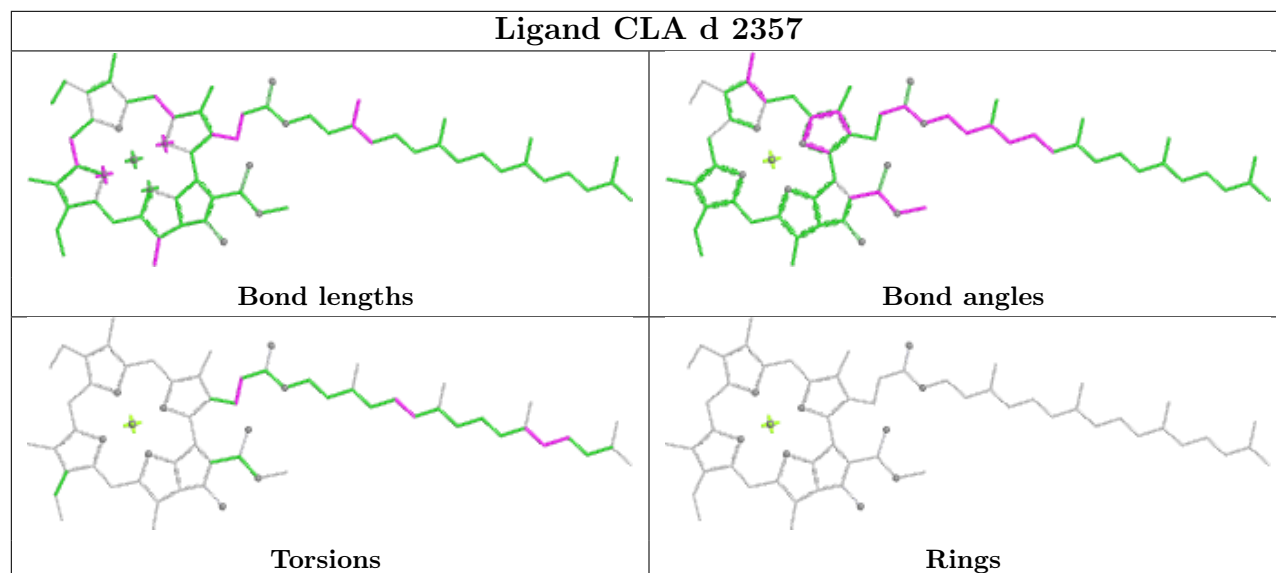
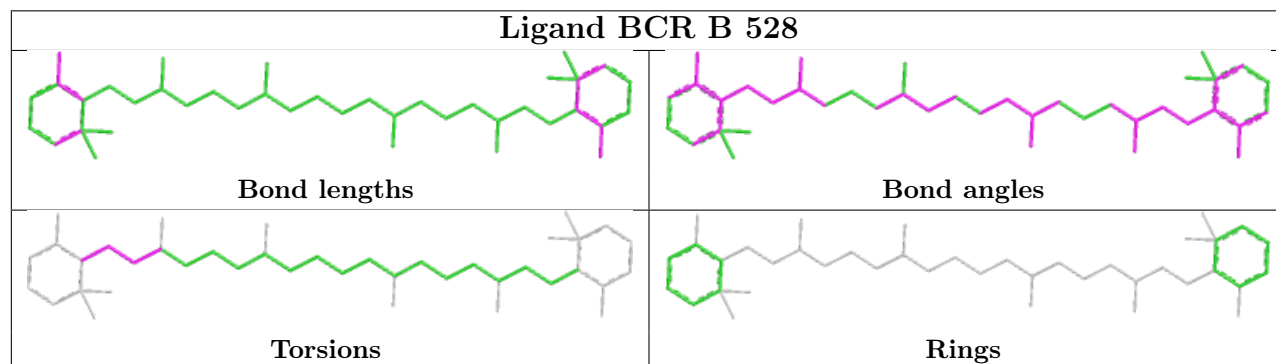
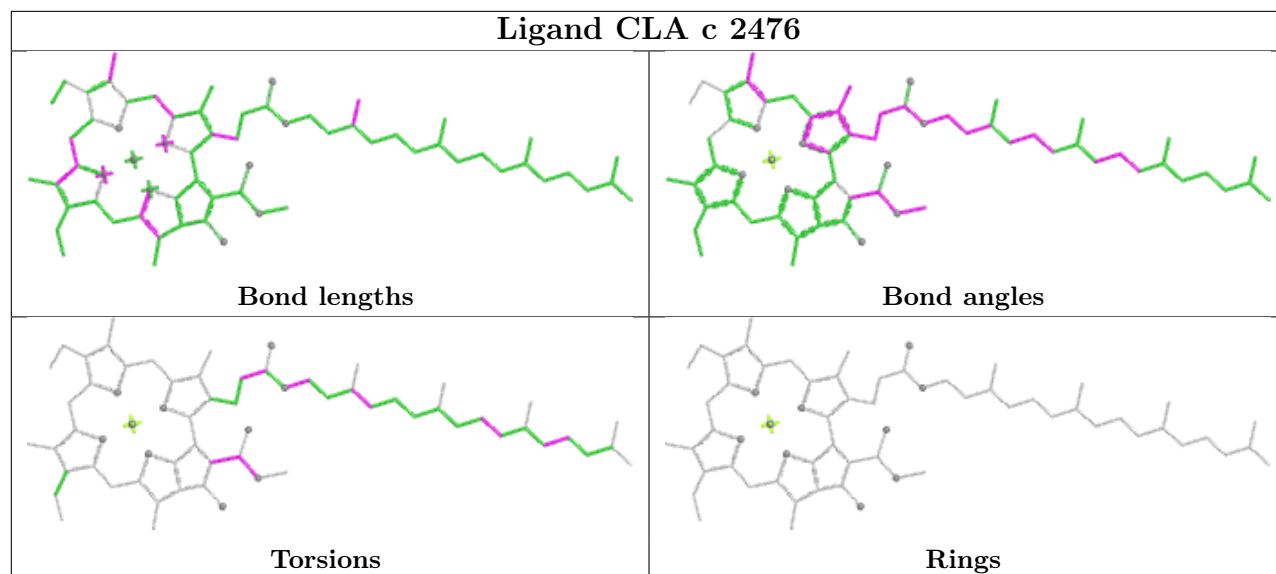
Bond angles

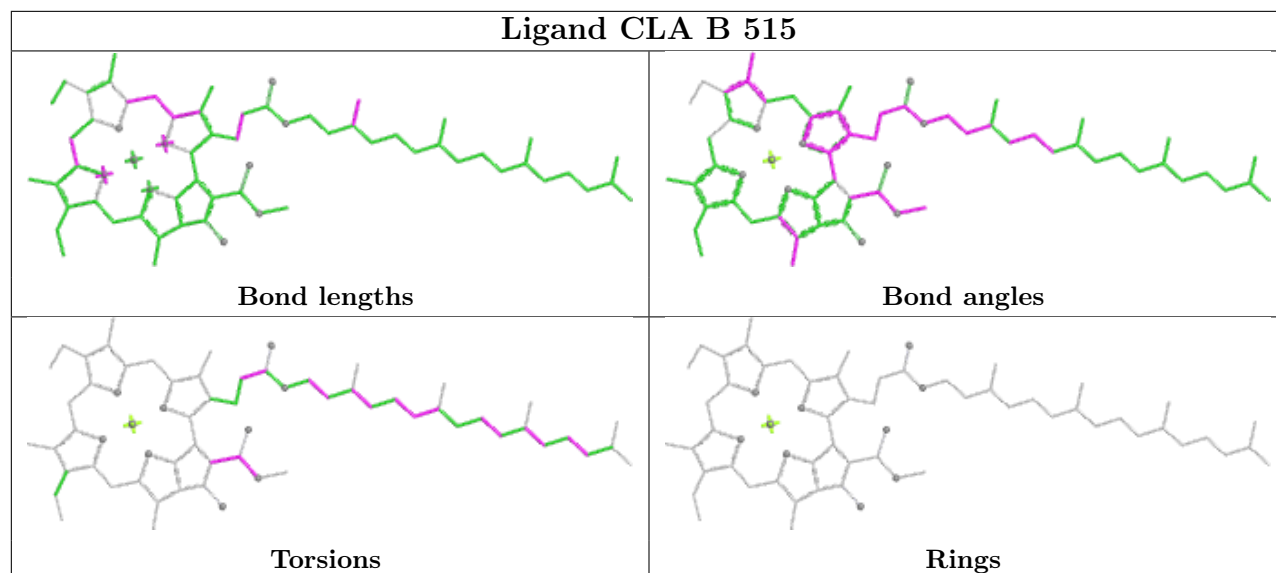
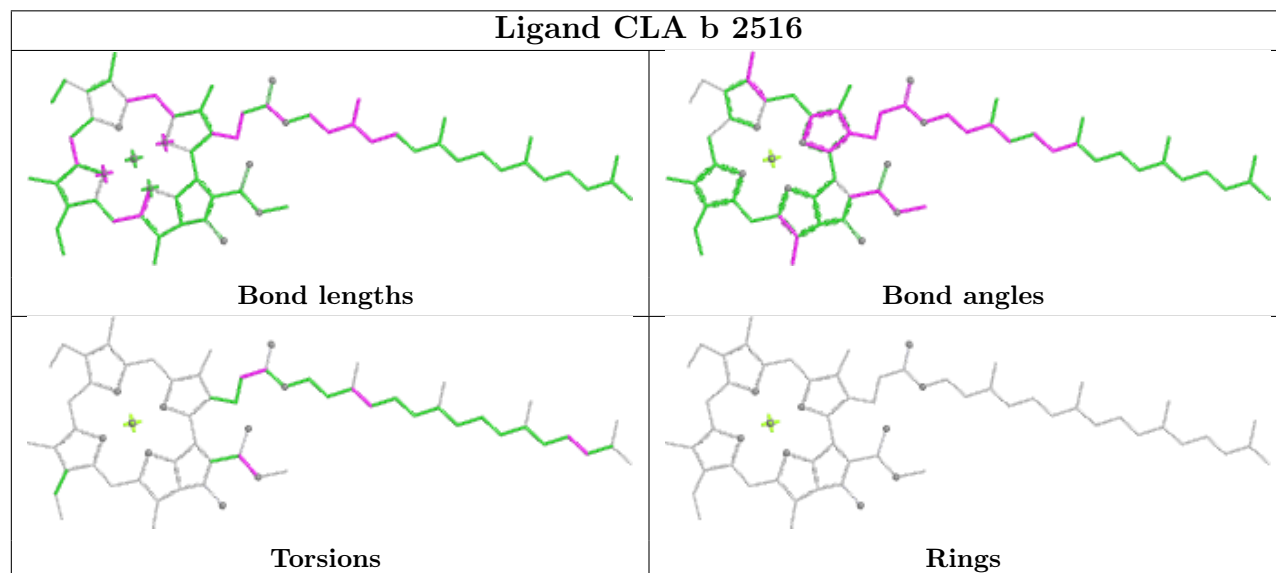
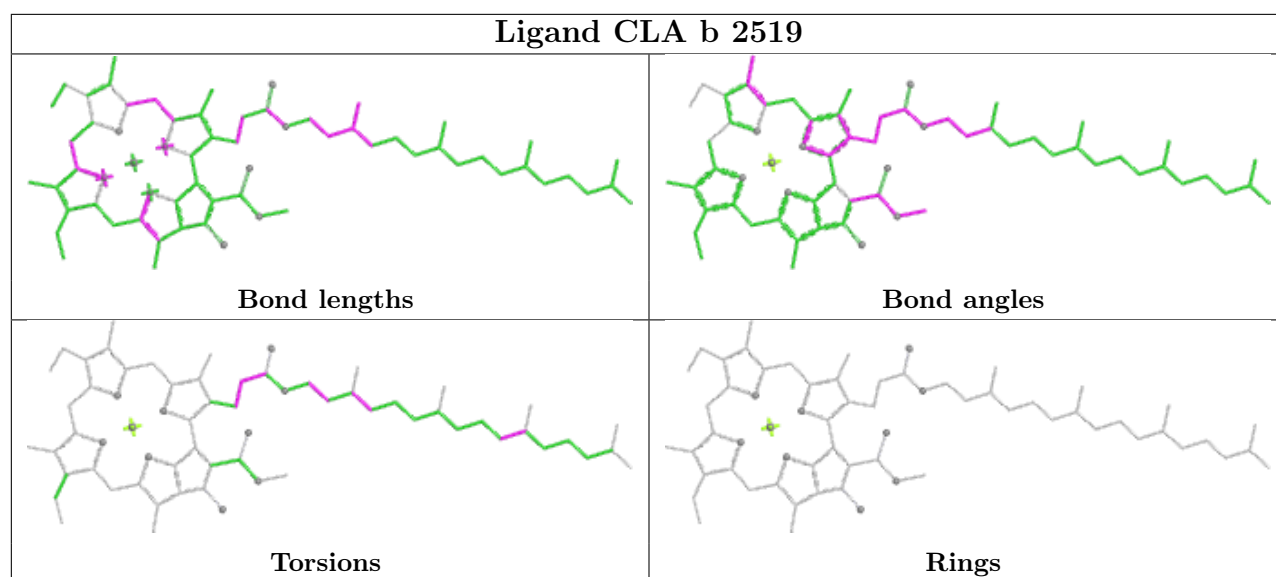


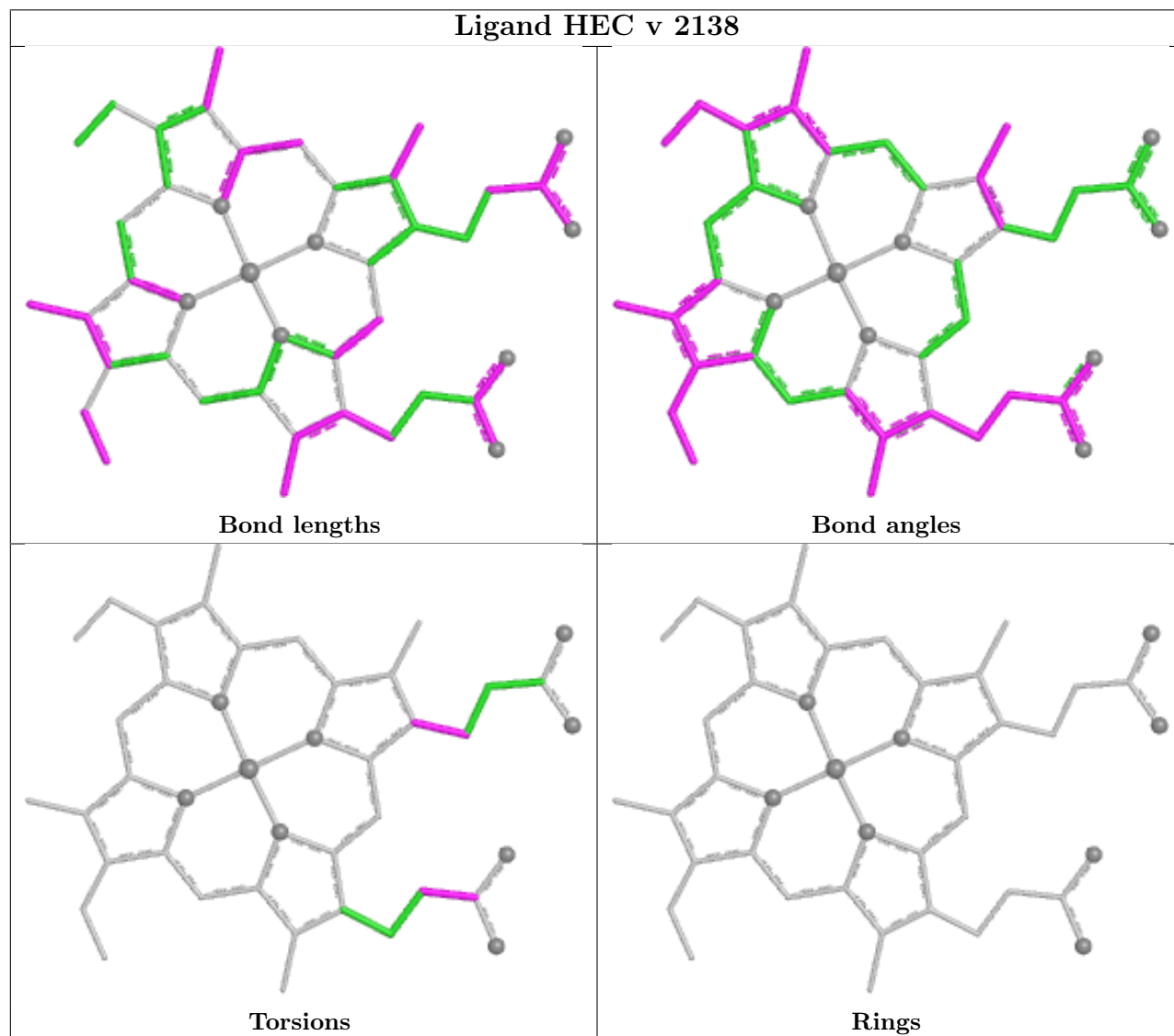
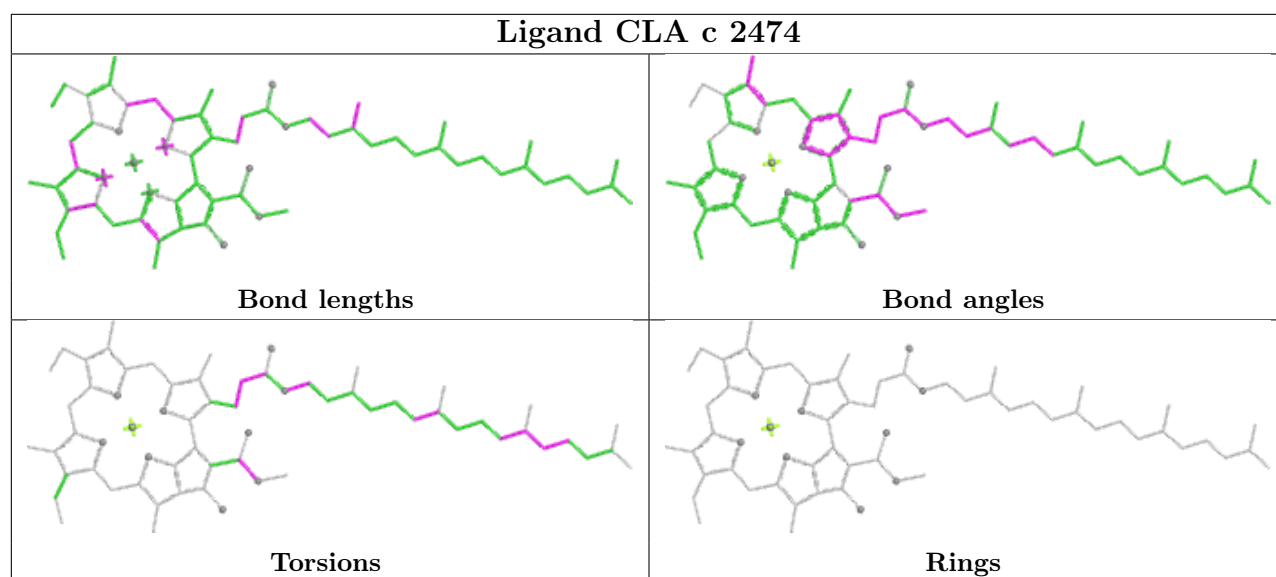
Torsions

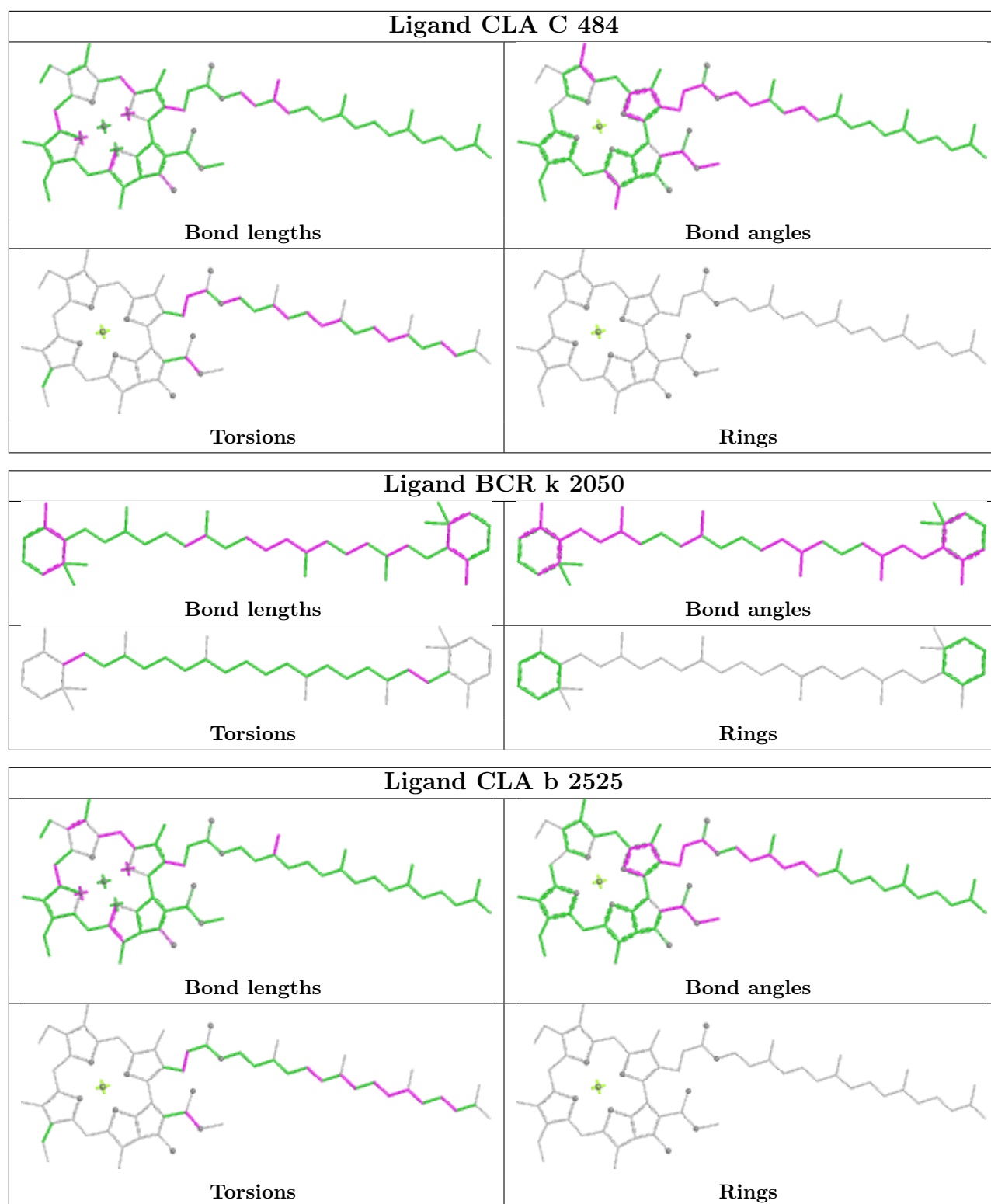


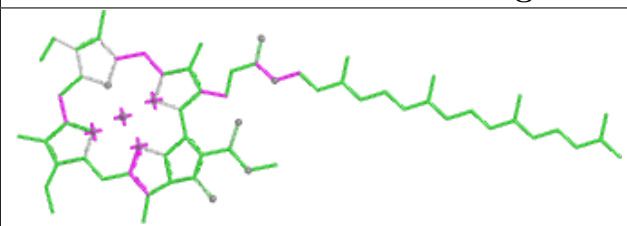
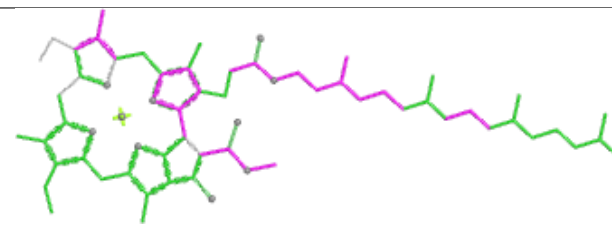
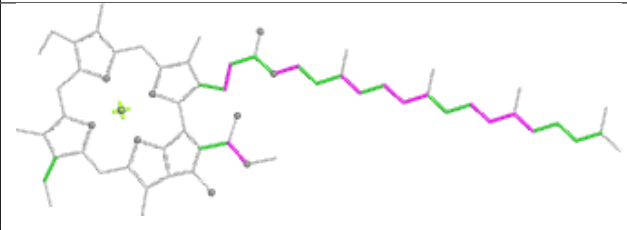
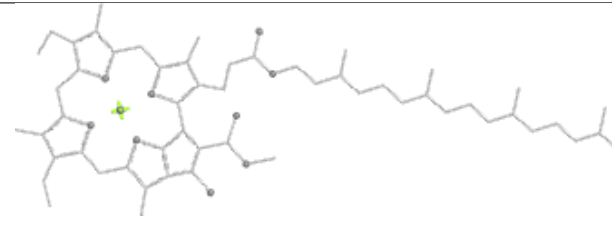
Rings

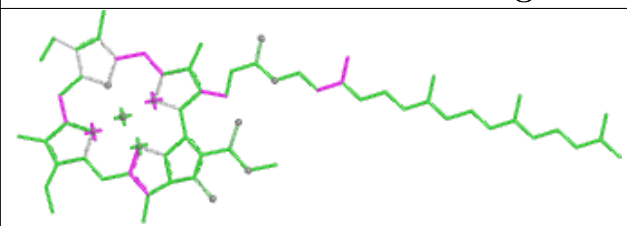
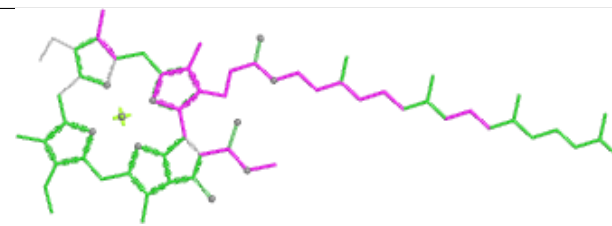
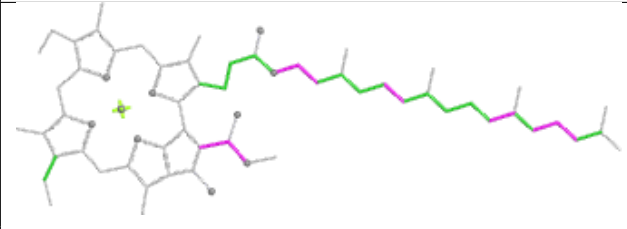
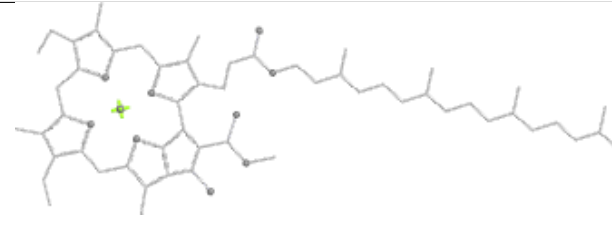


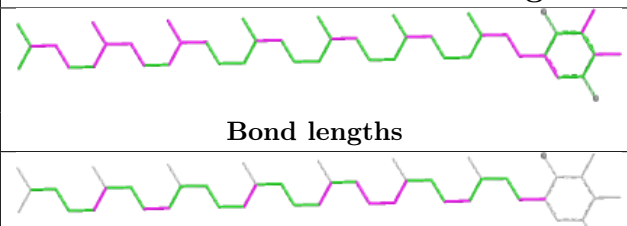
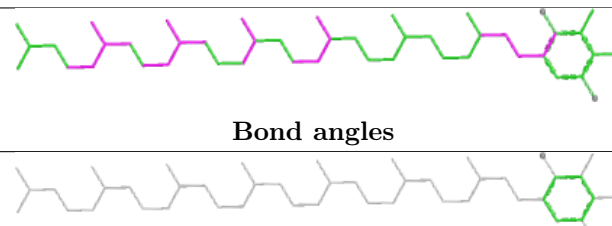




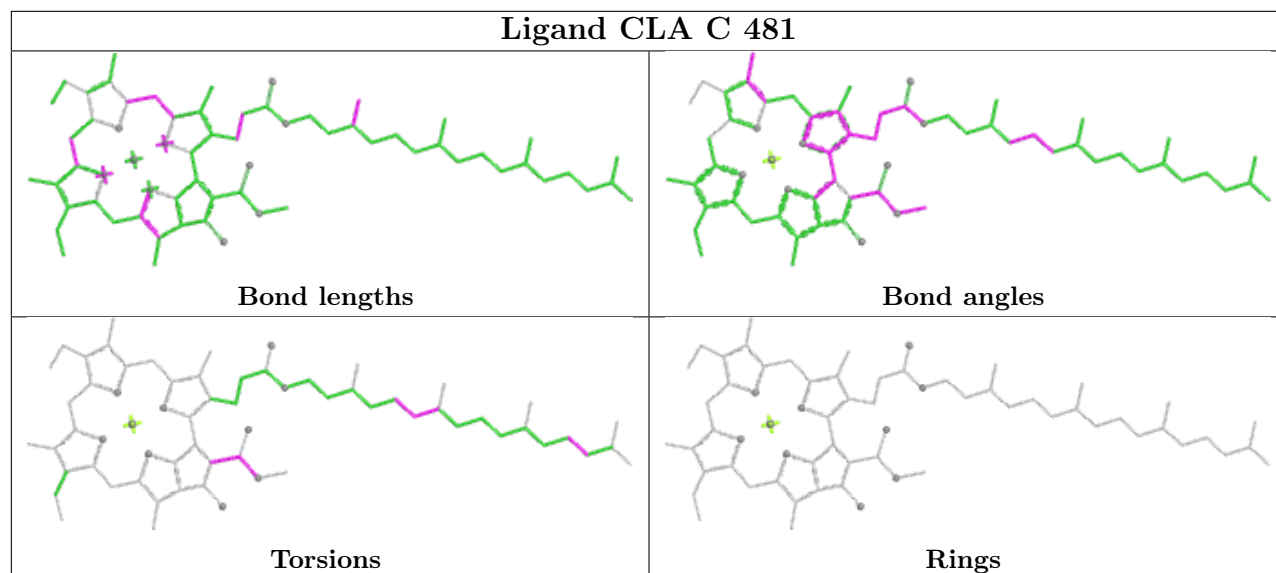
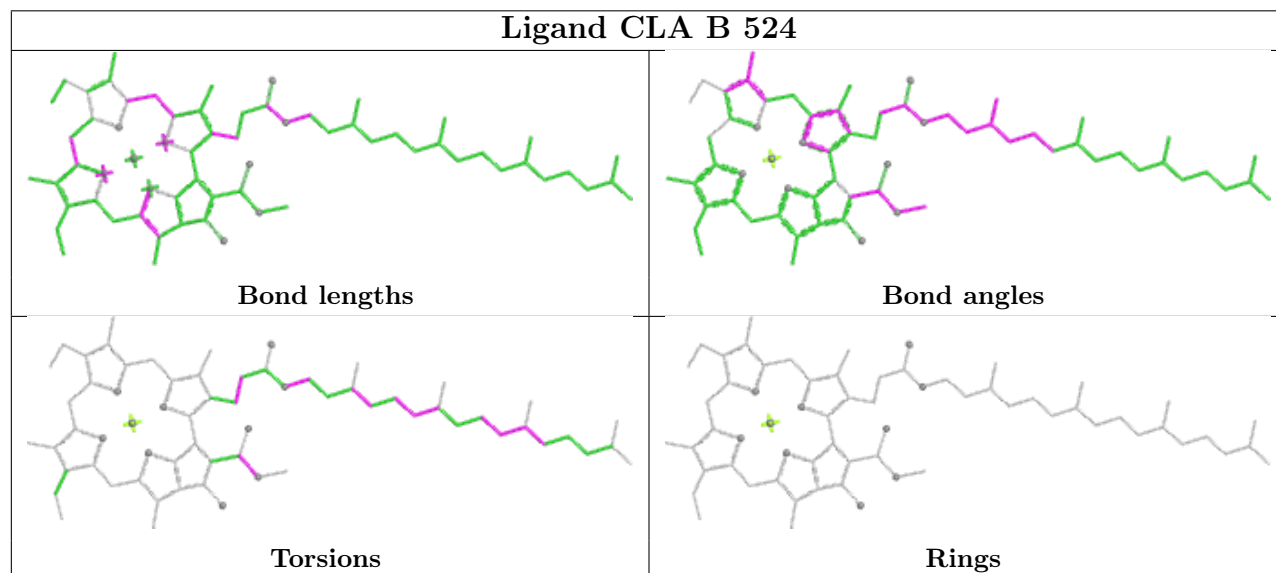
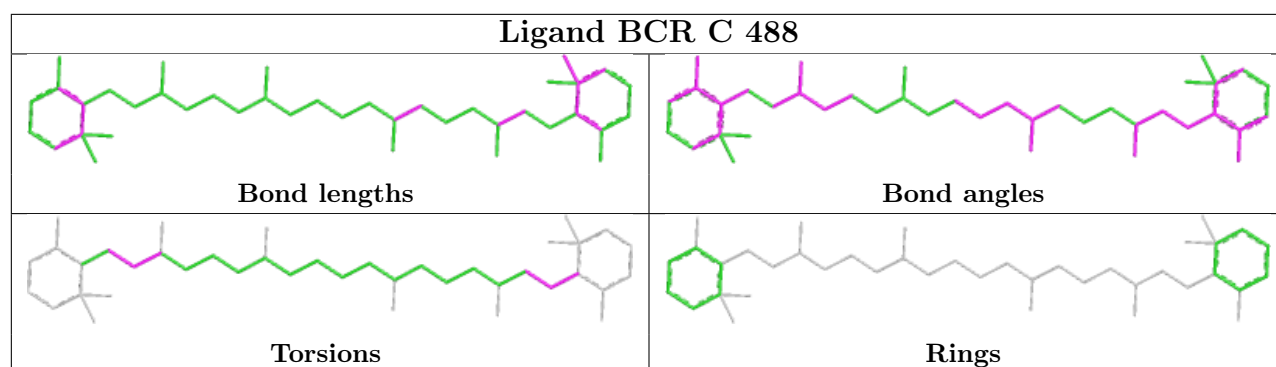




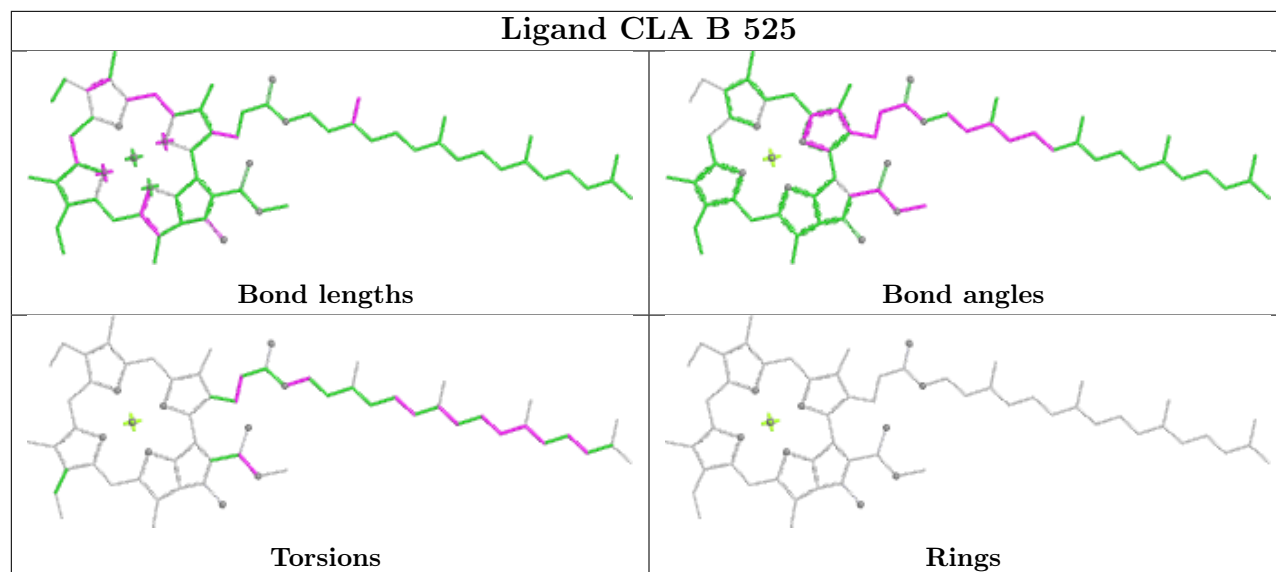
Ligand CLA b 2524	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 2513	
	
Bond lengths	Bond angles
	
Torsions	Rings

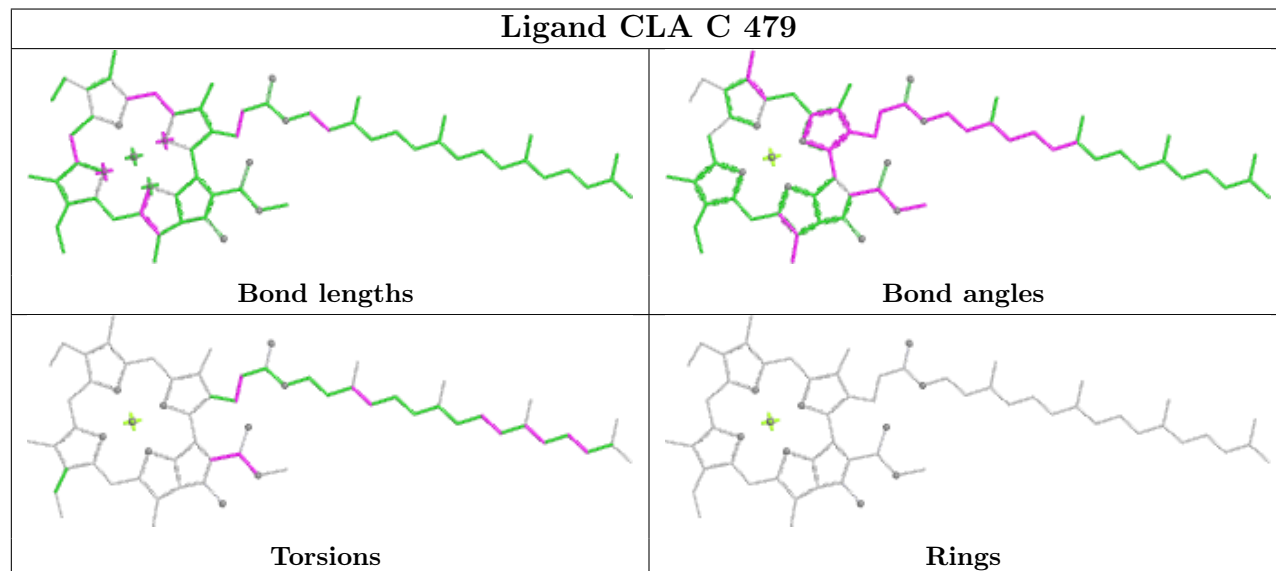
Ligand PL9 D 357	
	
Bond lengths	Bond angles
	
Torsions	Rings



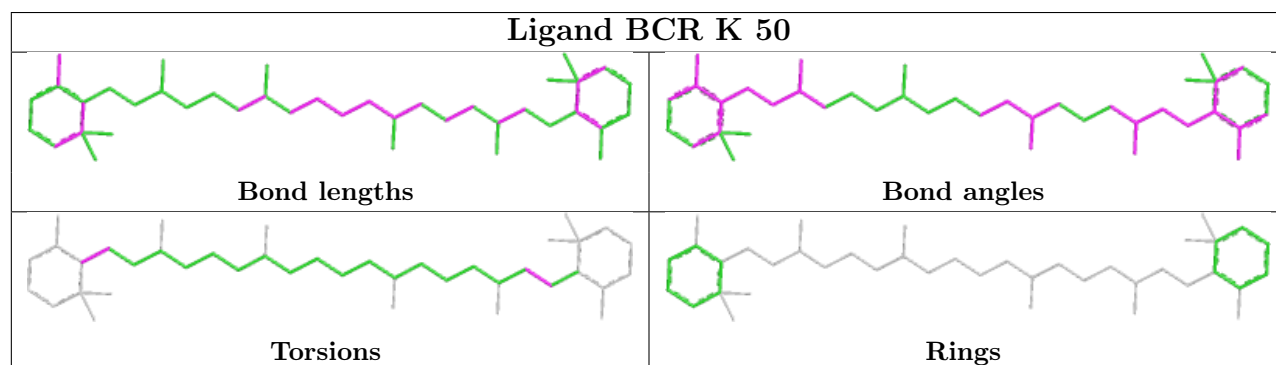
Ligand CLA B 525

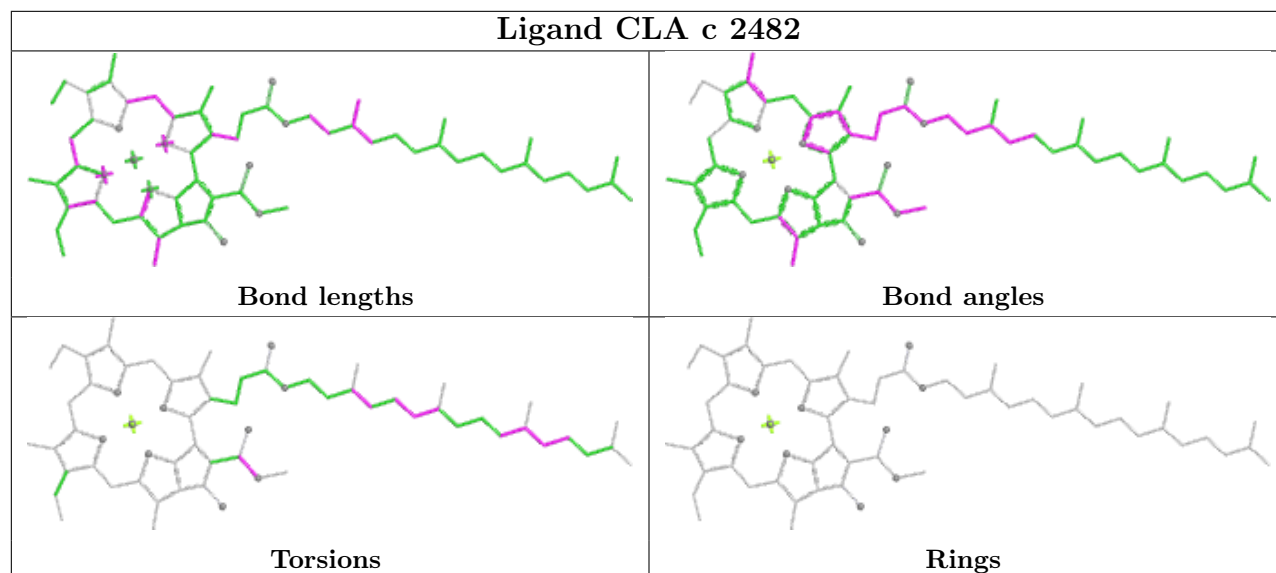
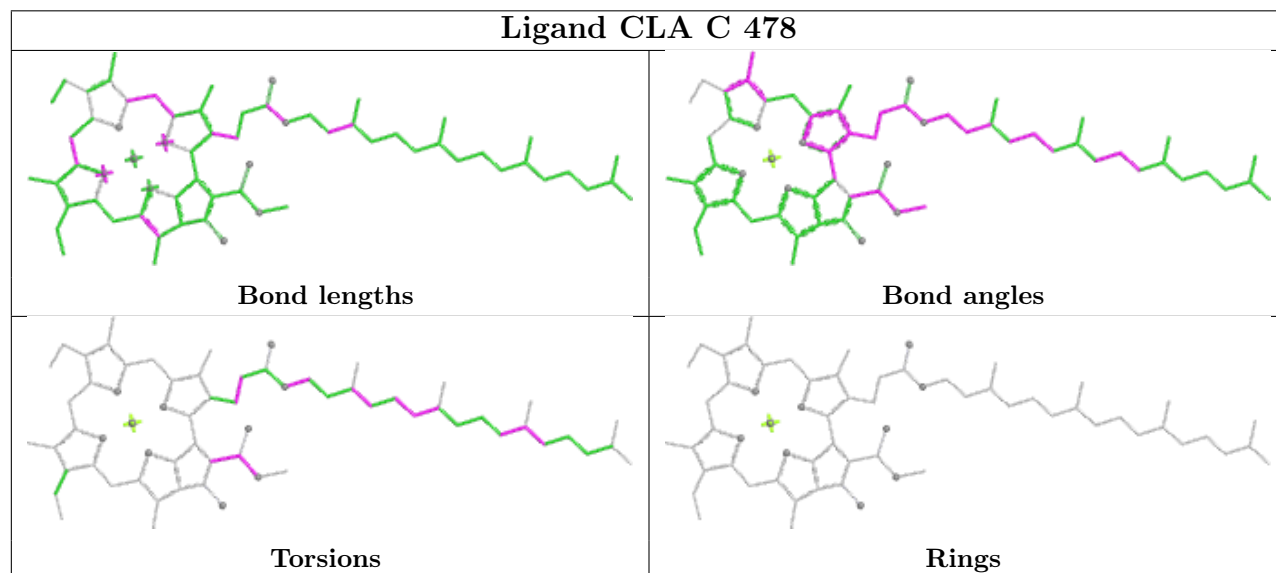
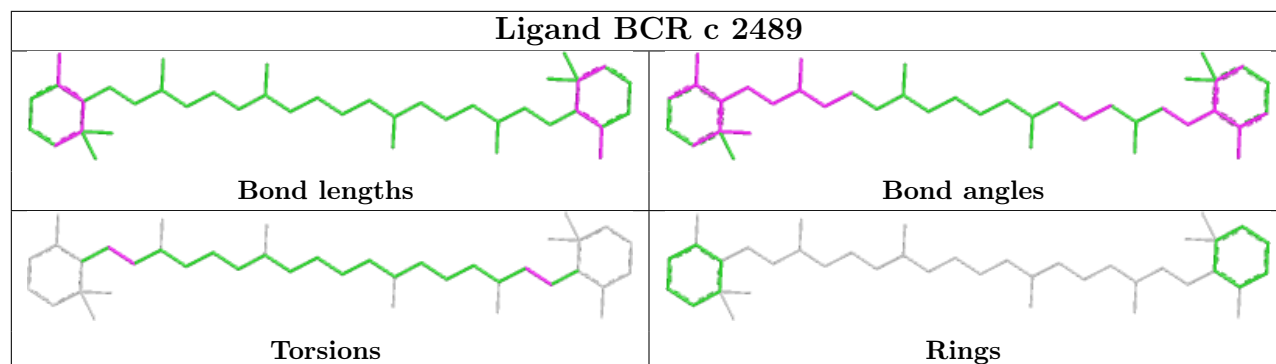


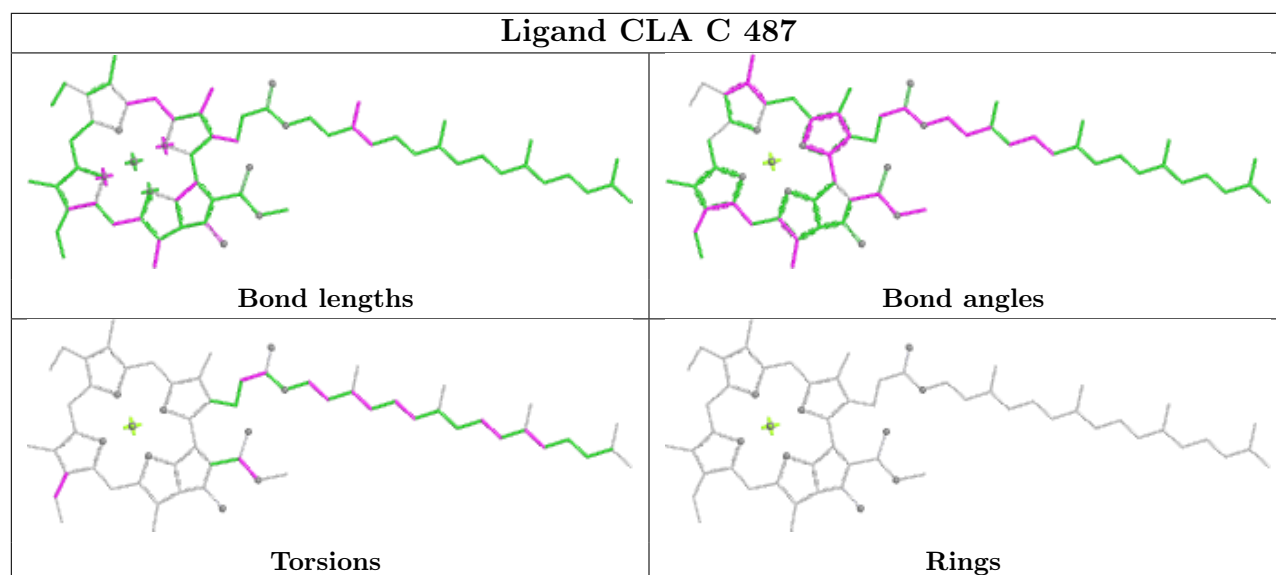
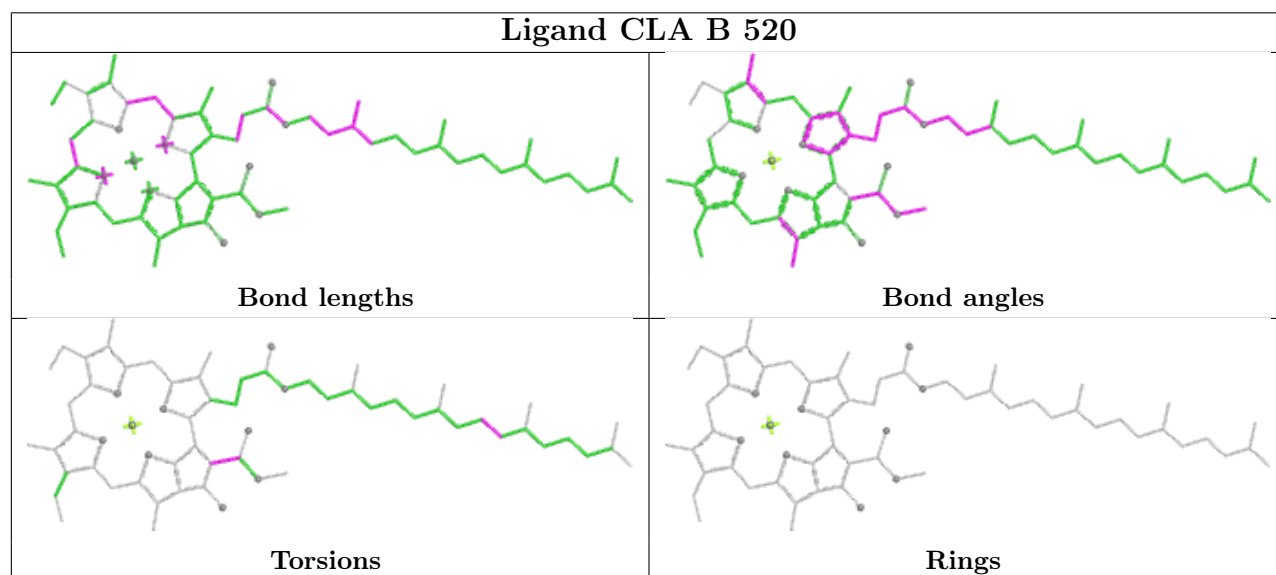
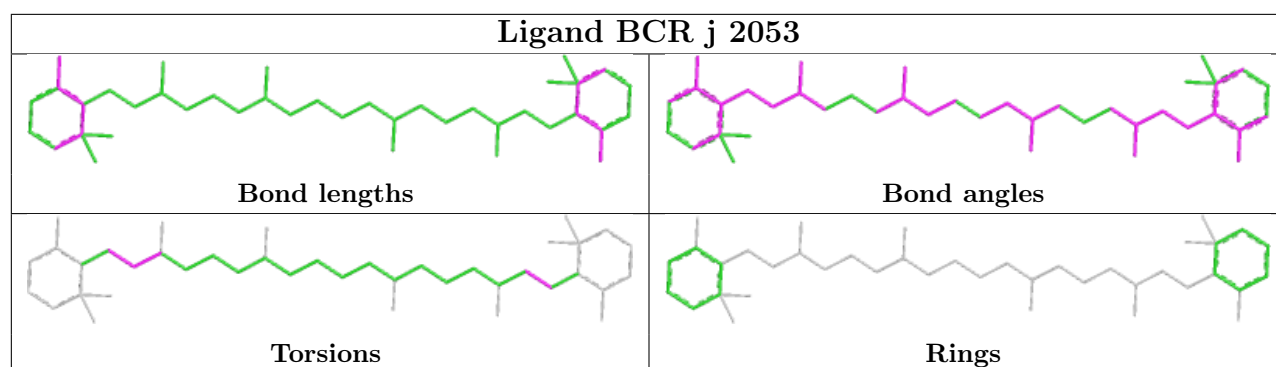
Ligand CLA C 479

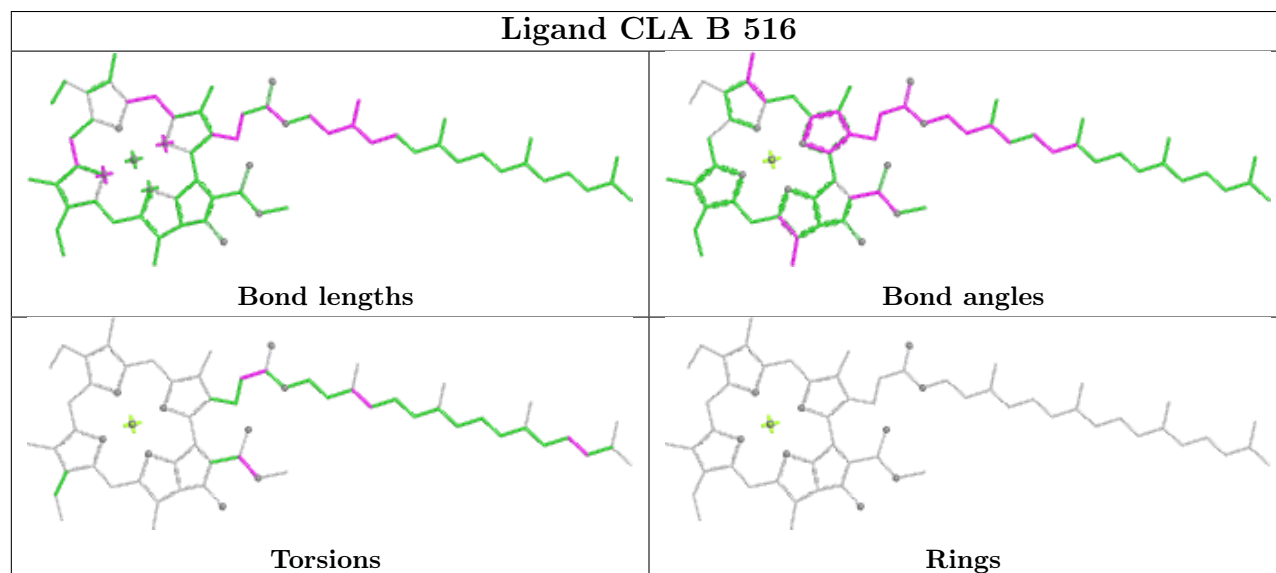
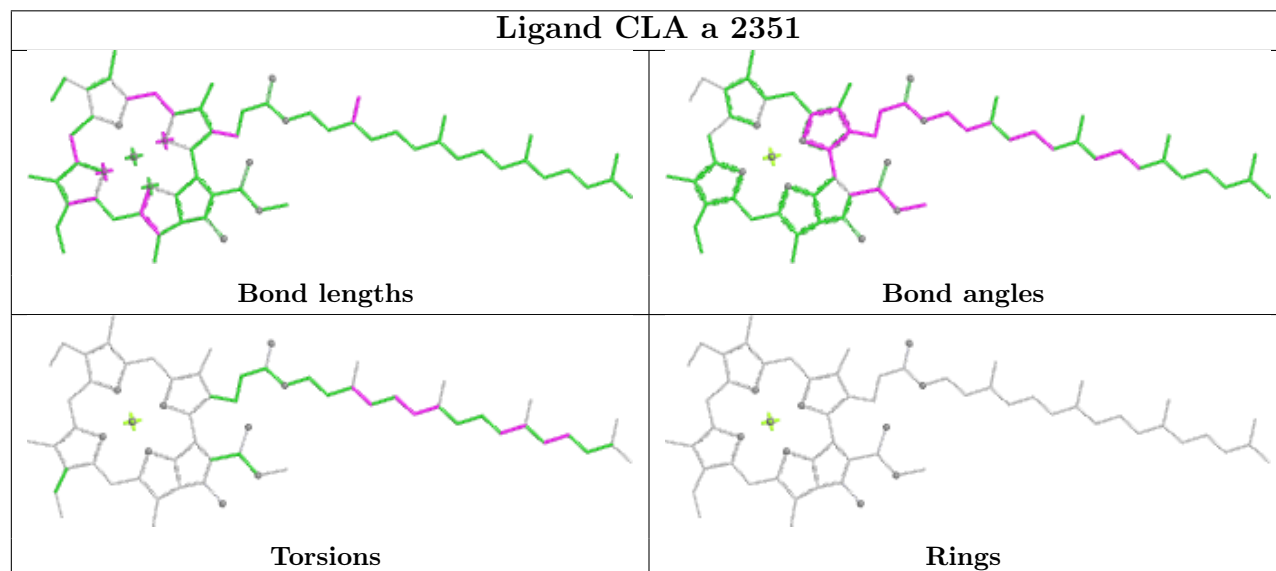
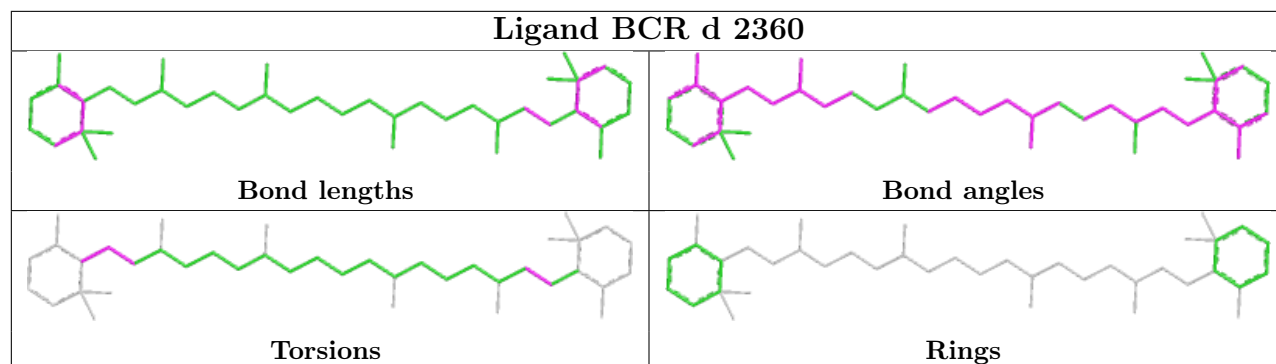


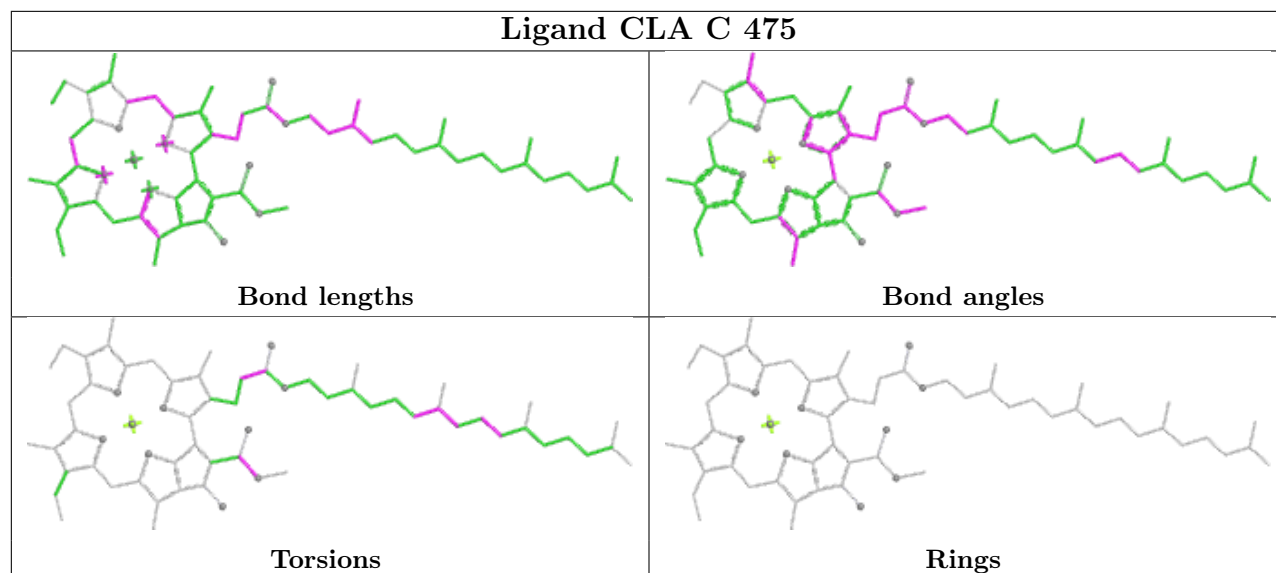
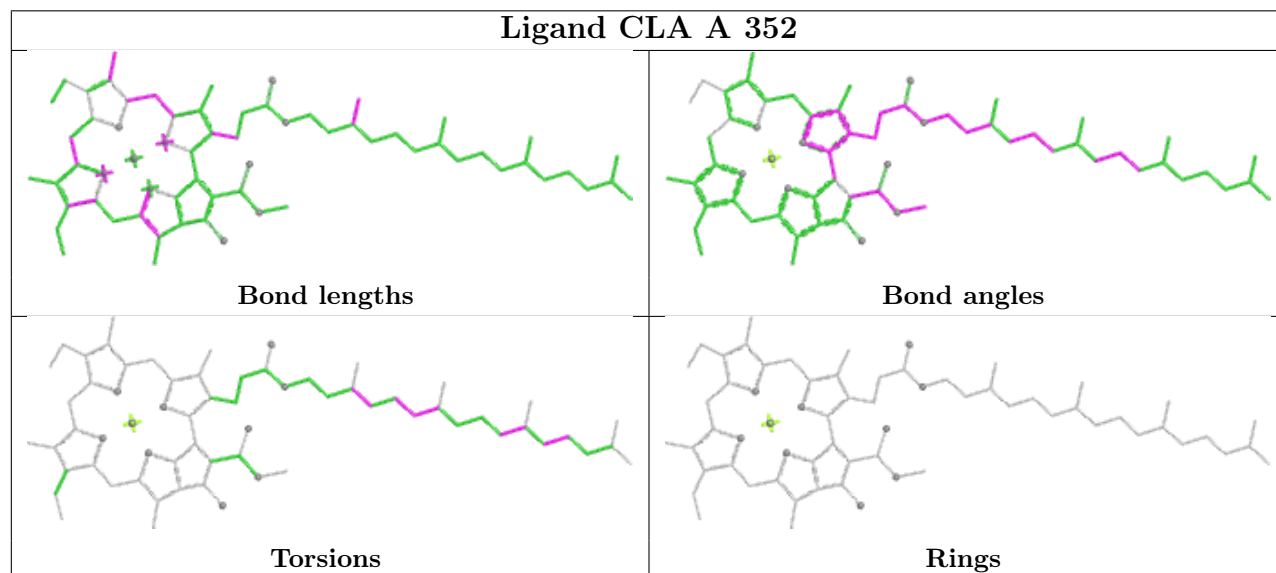
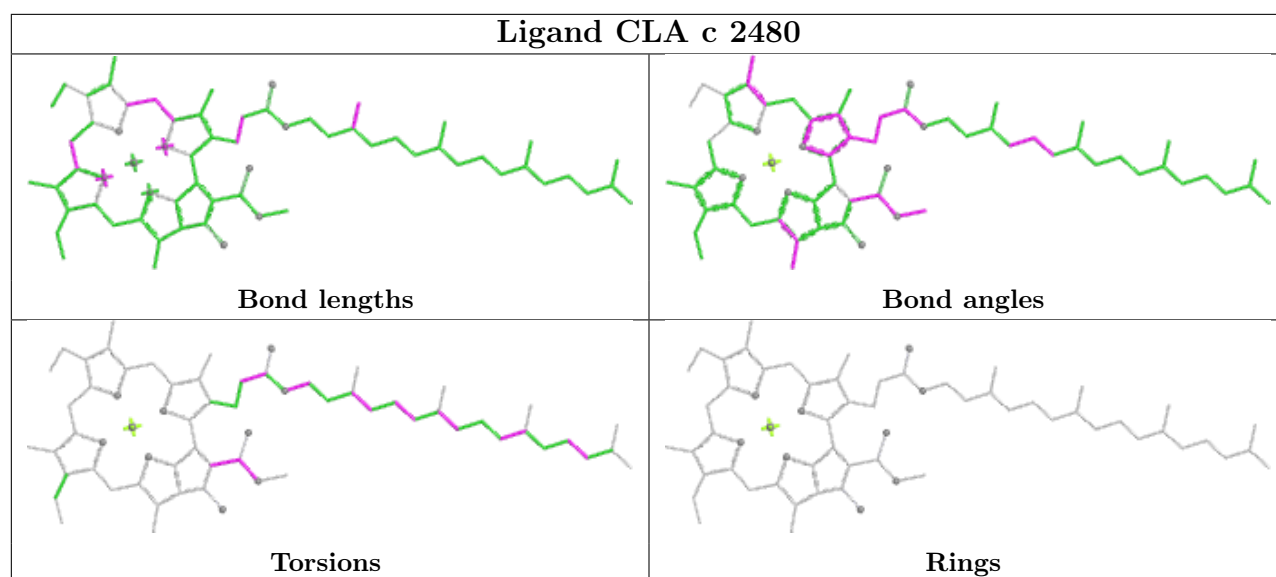
Ligand BCR K 50

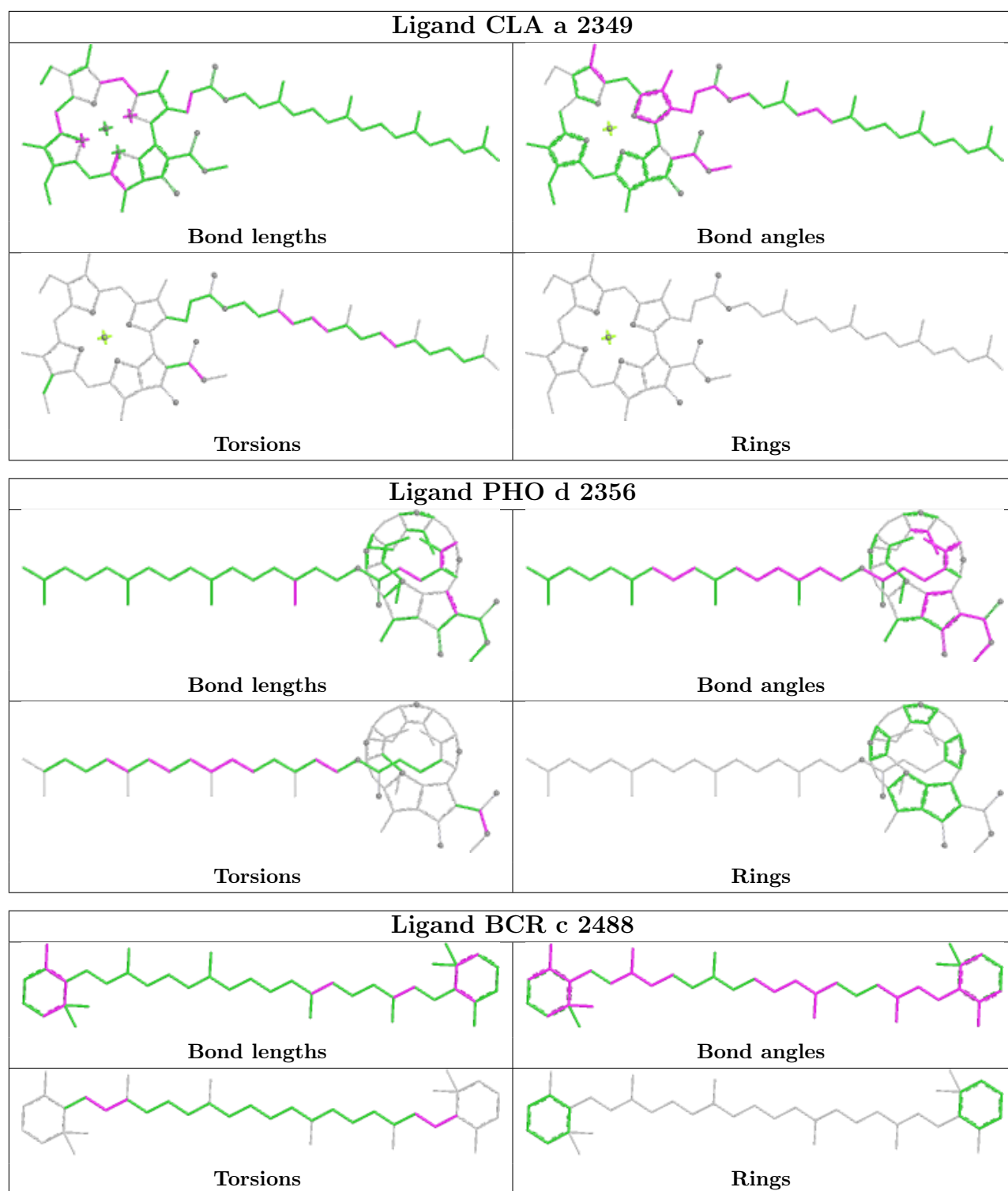


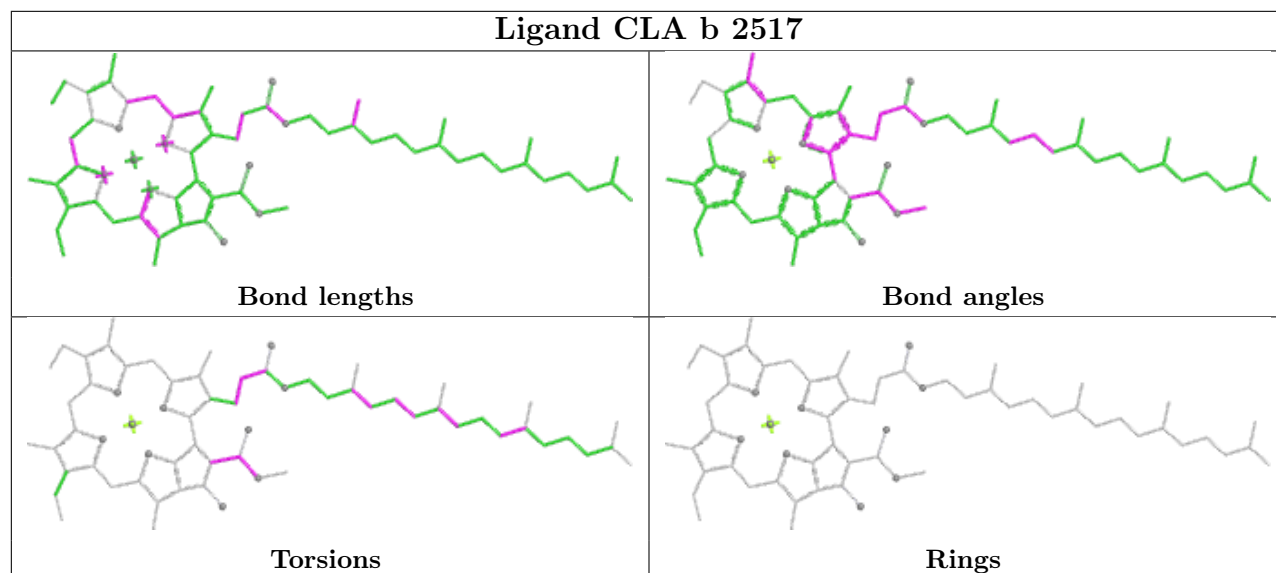
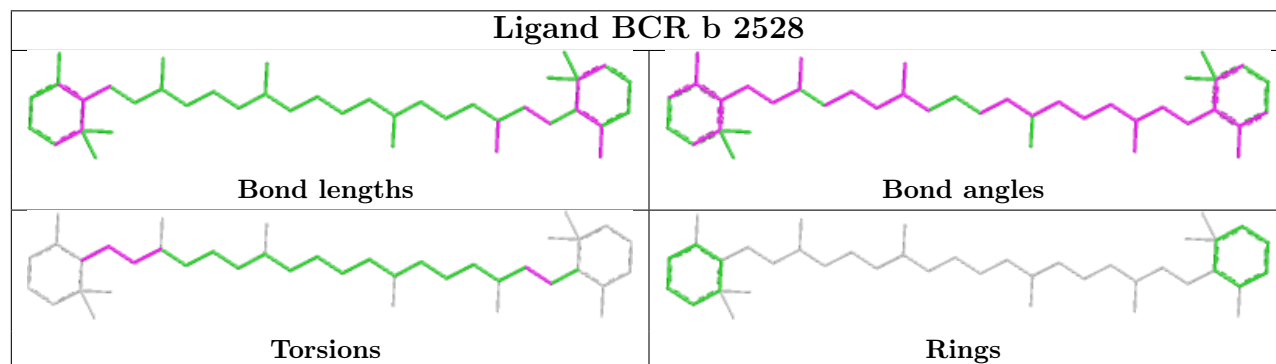
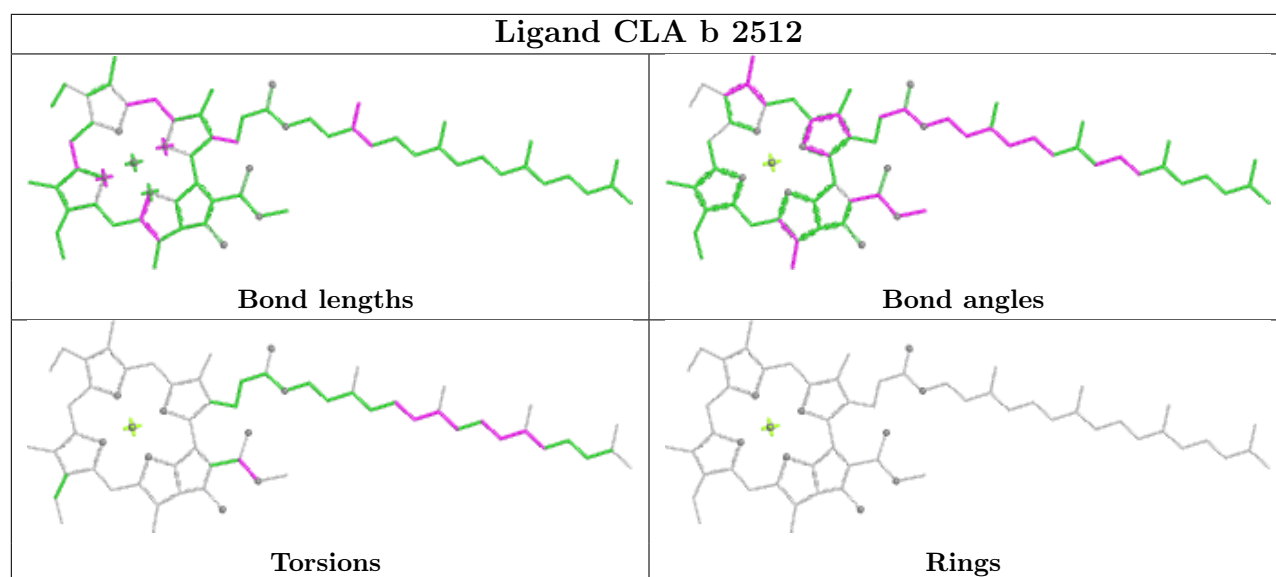


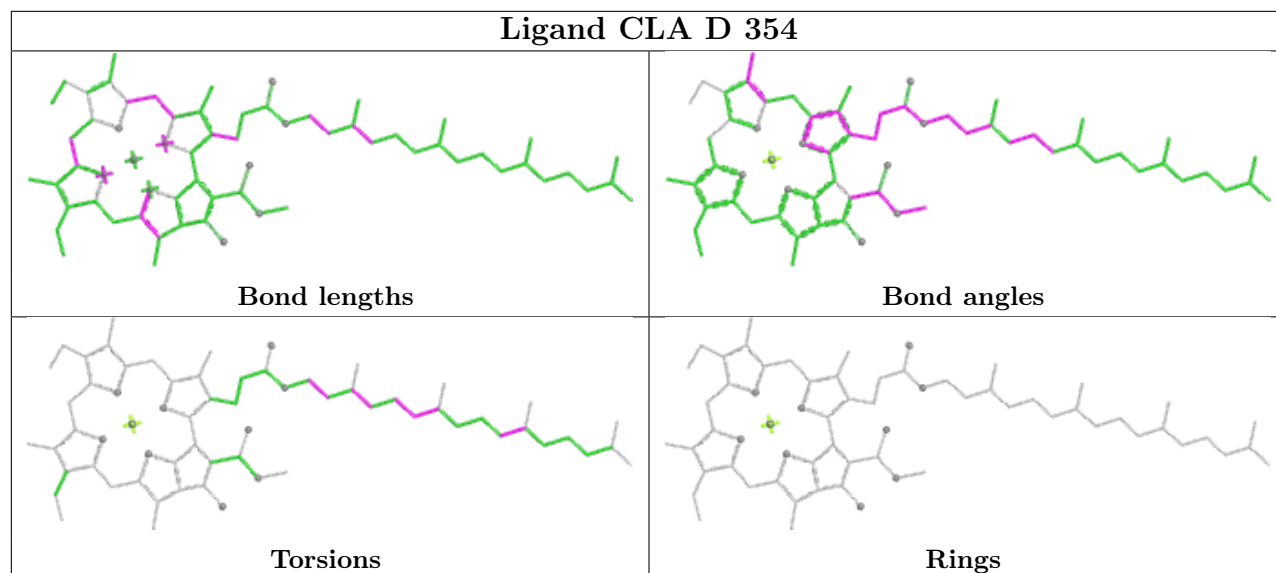
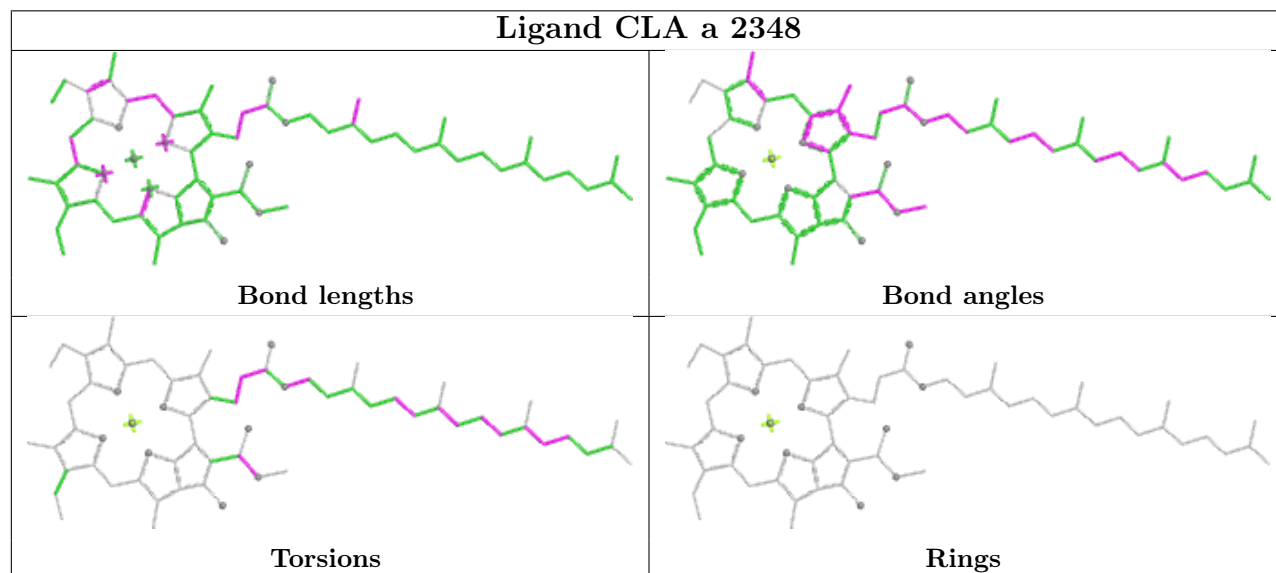
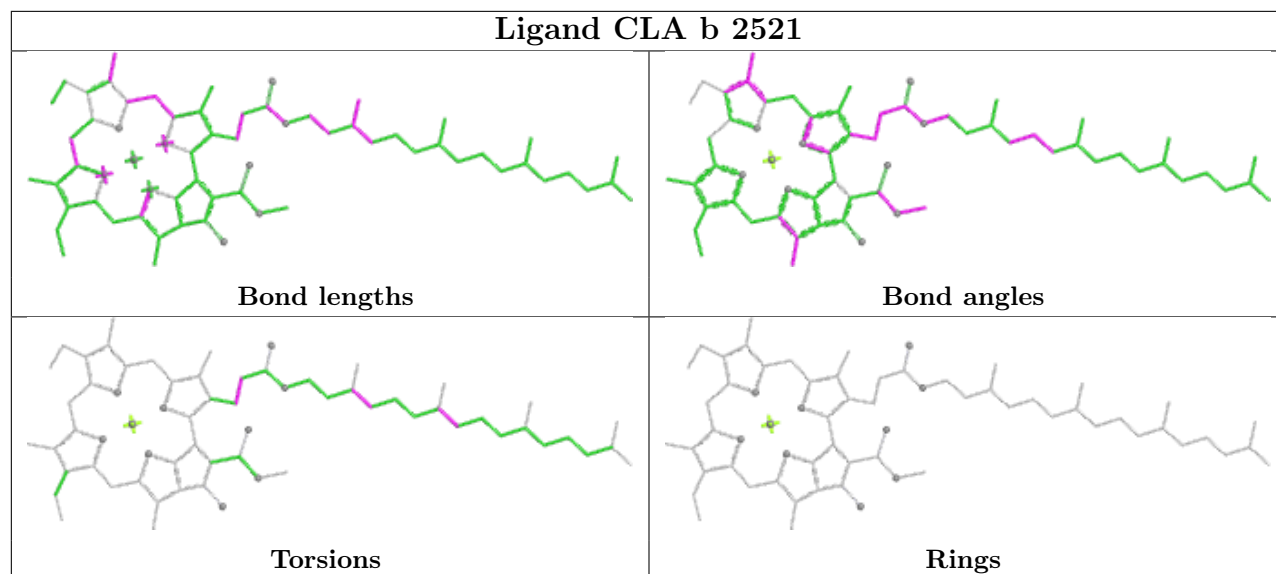


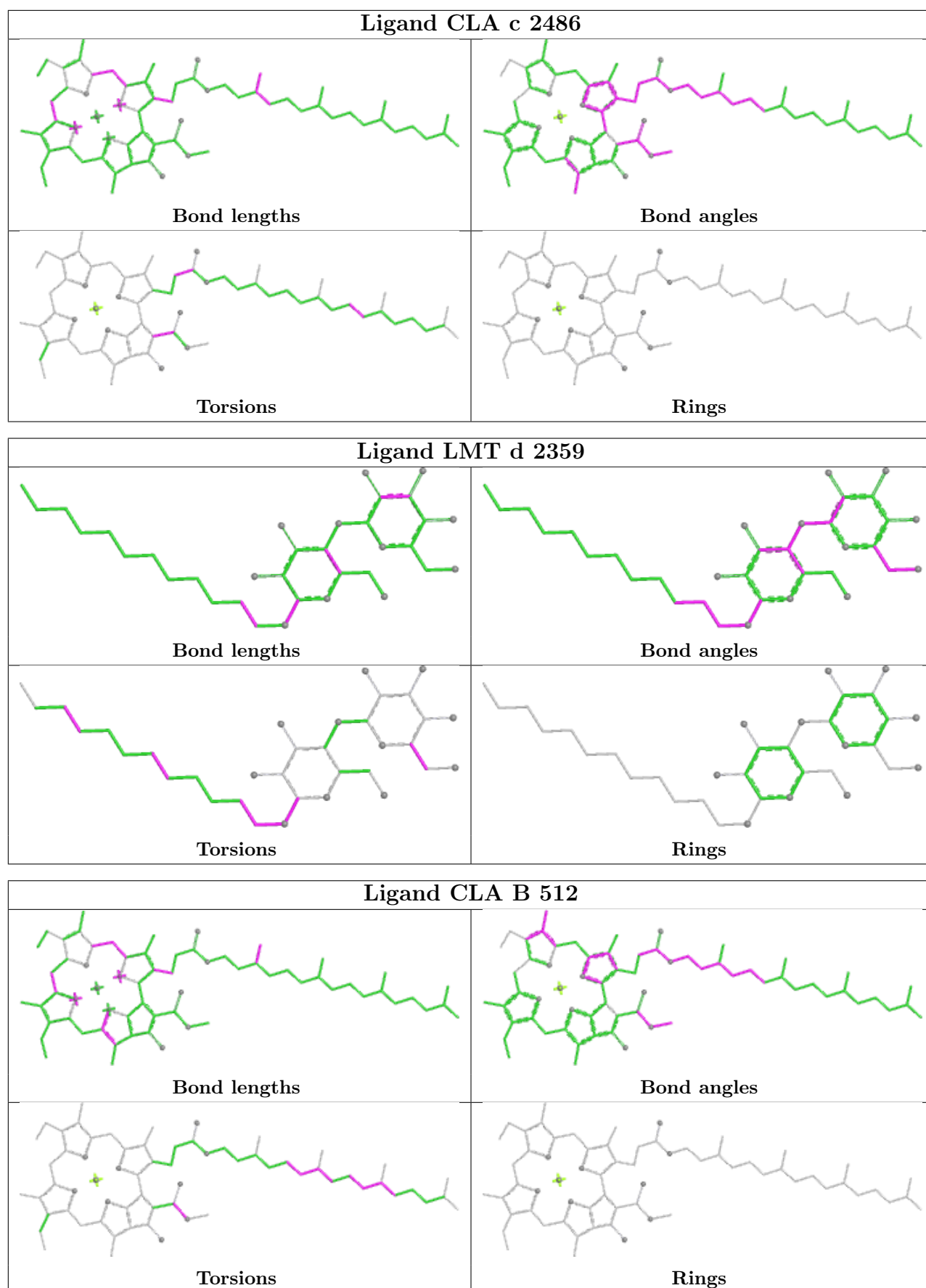


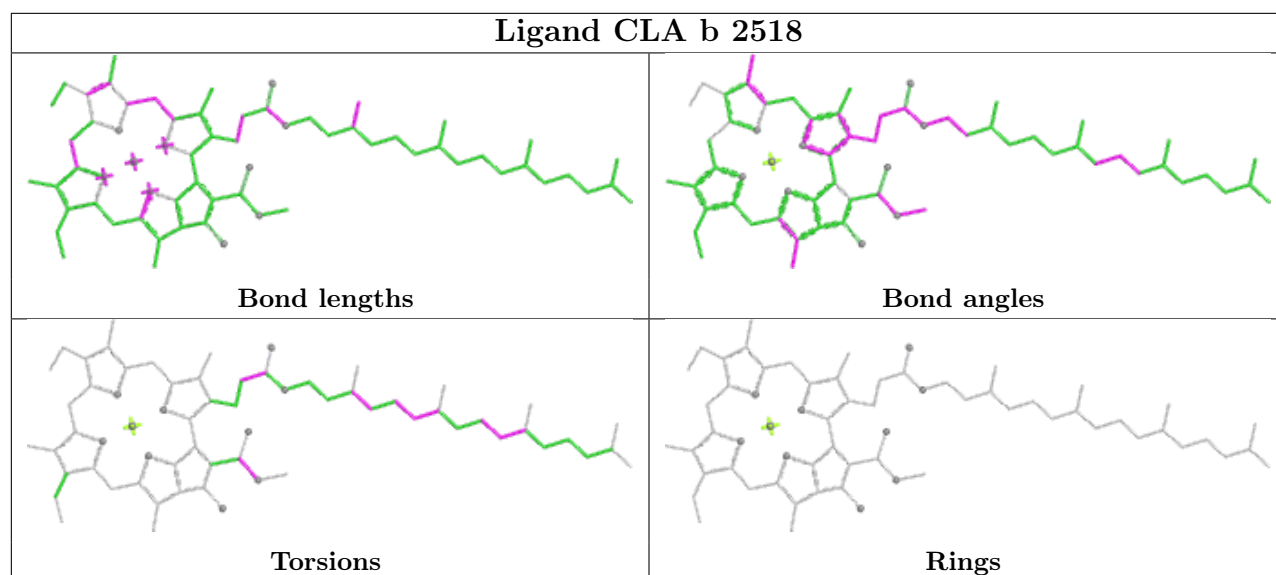
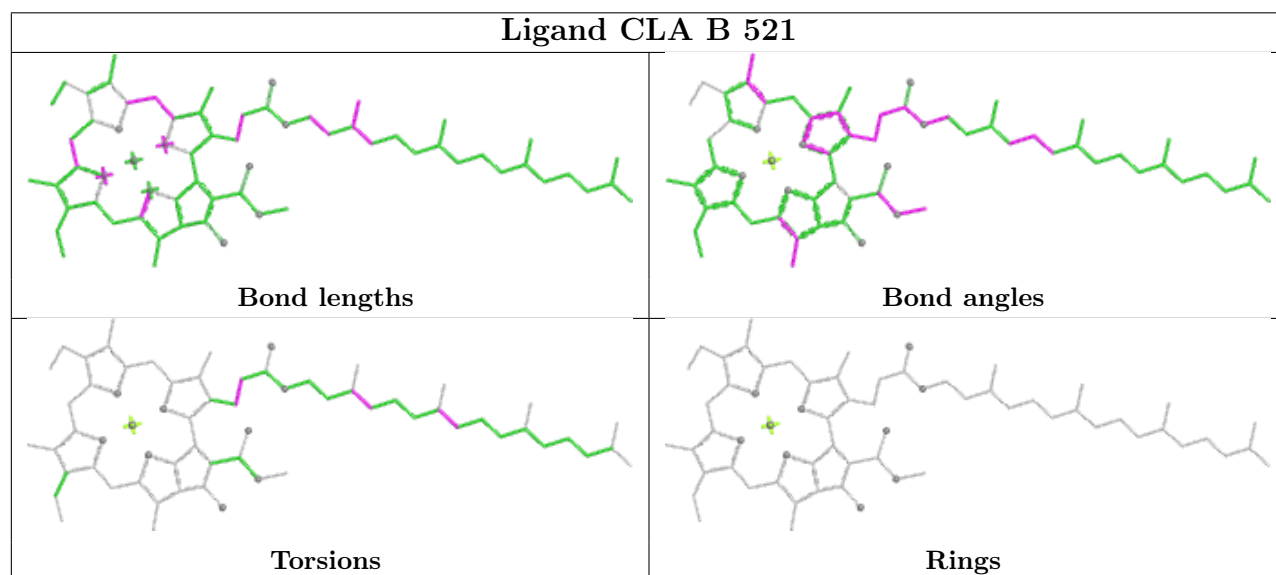
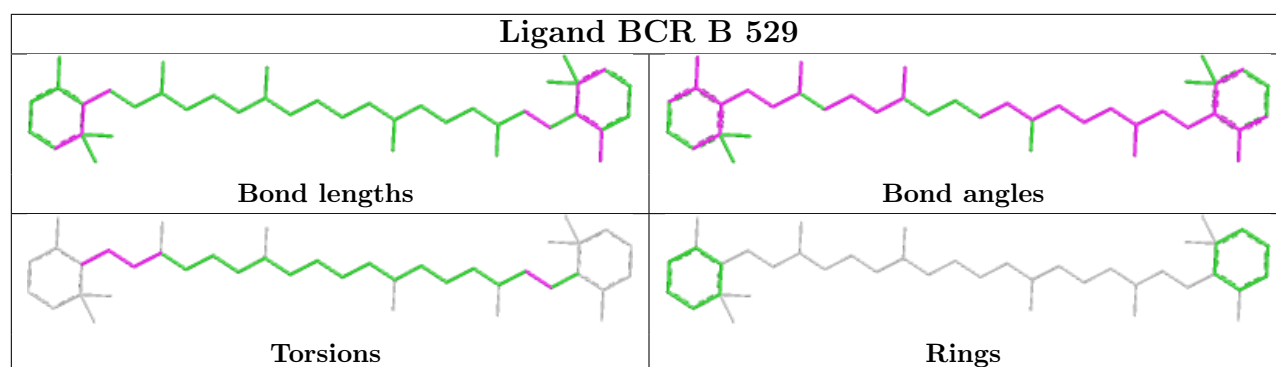


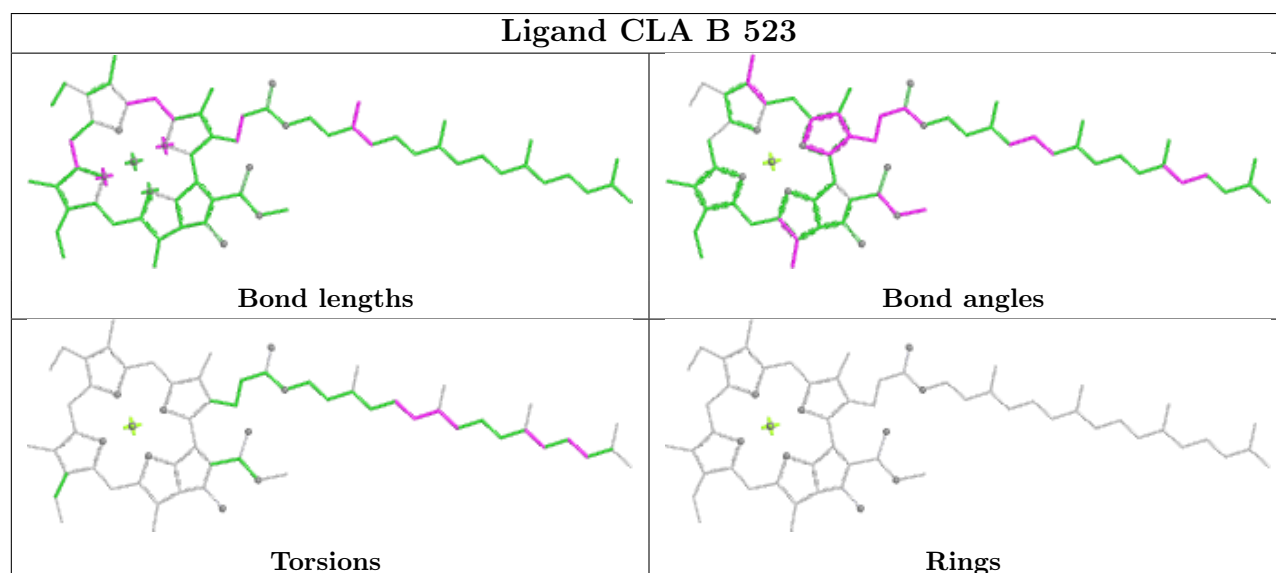
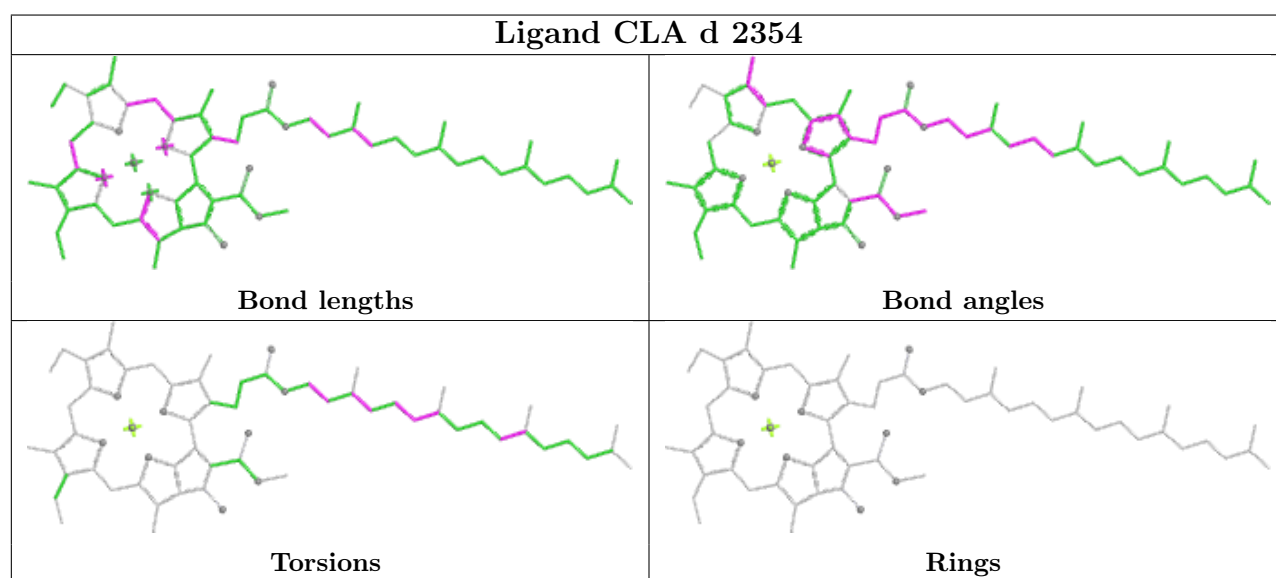
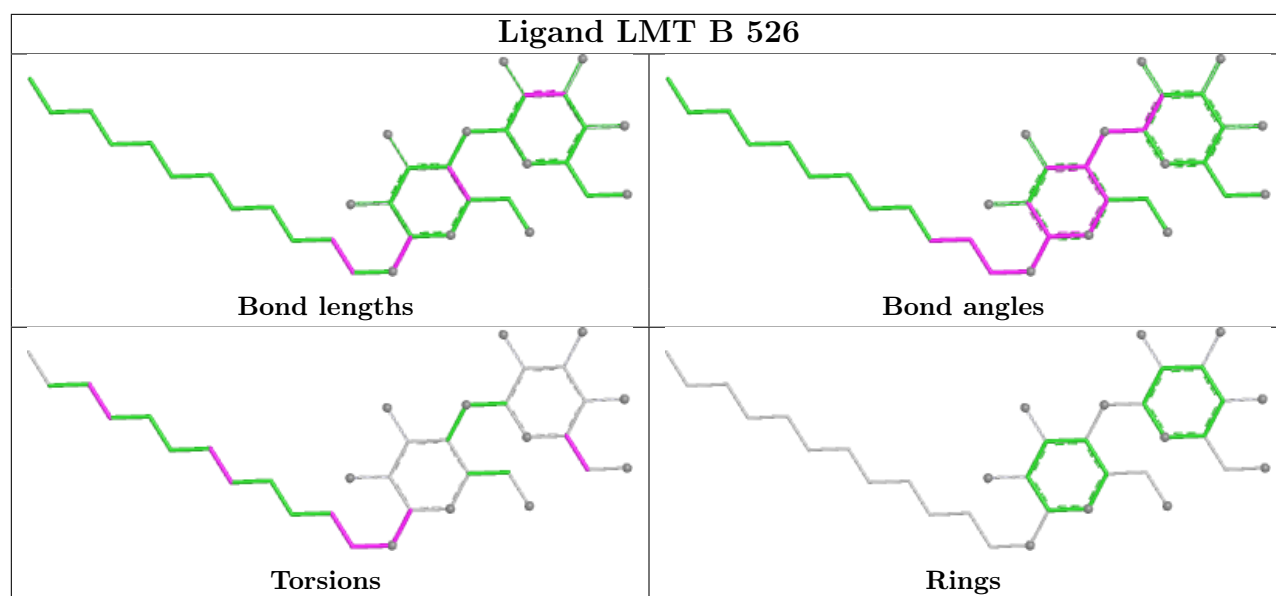


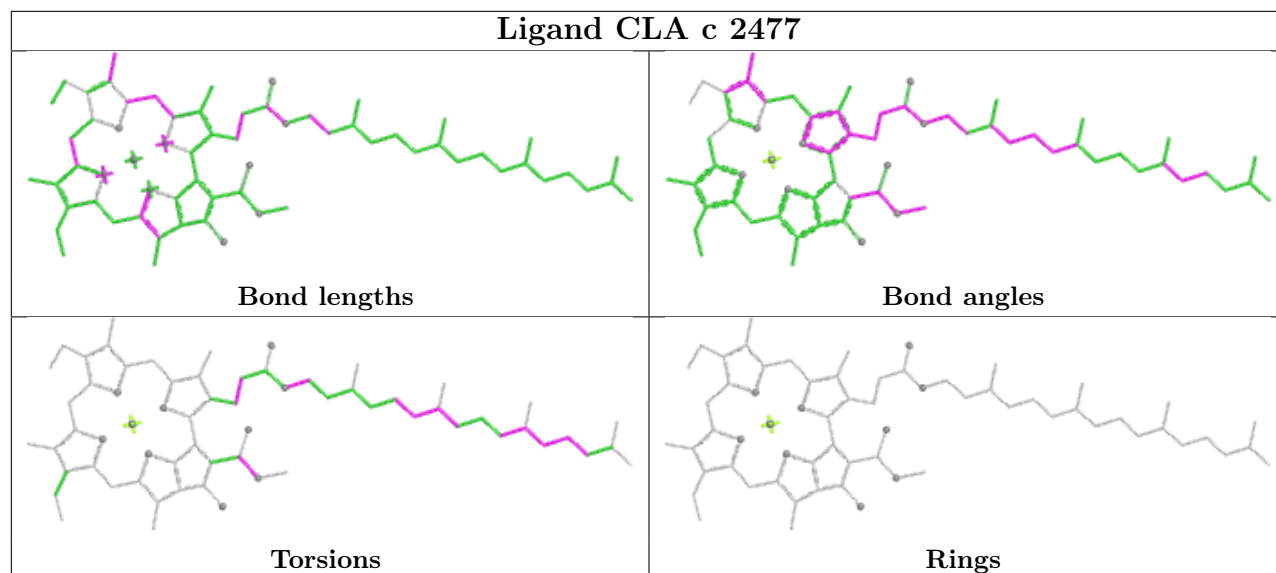
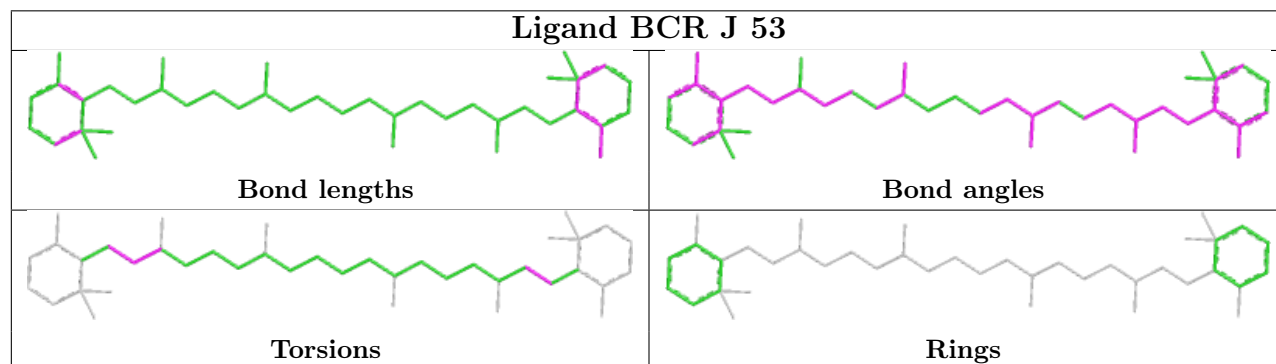
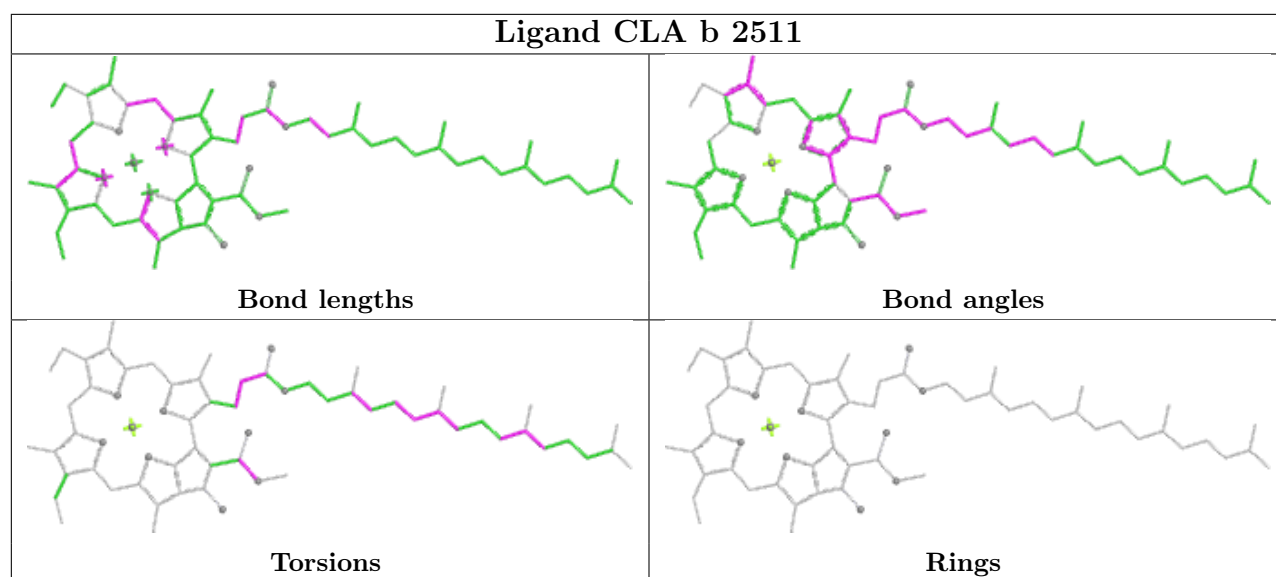


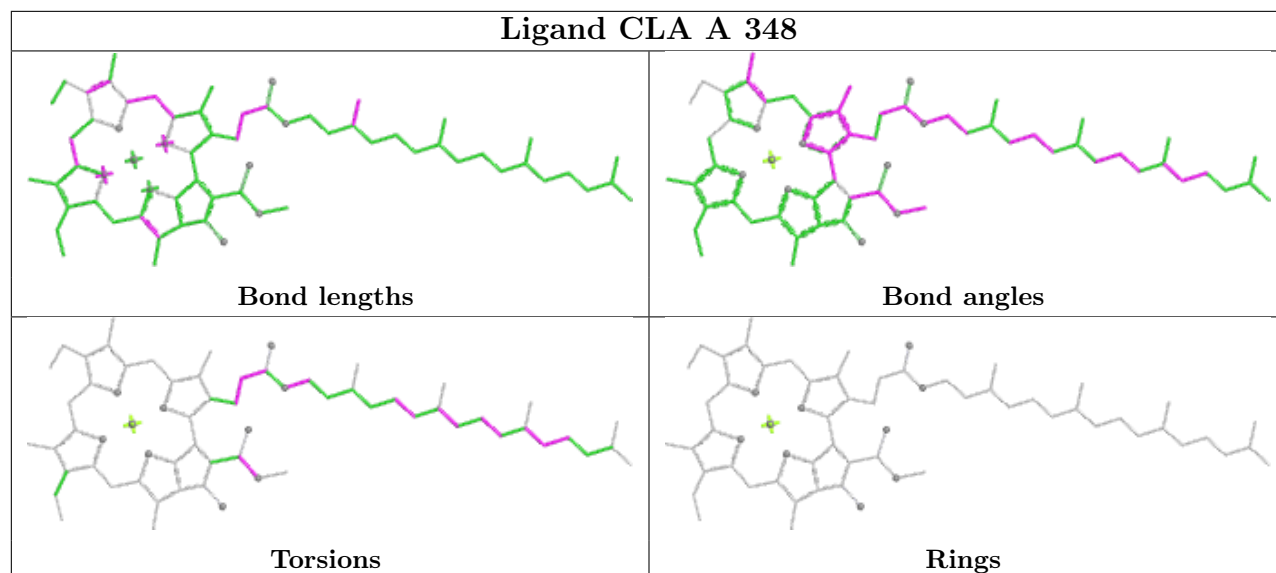
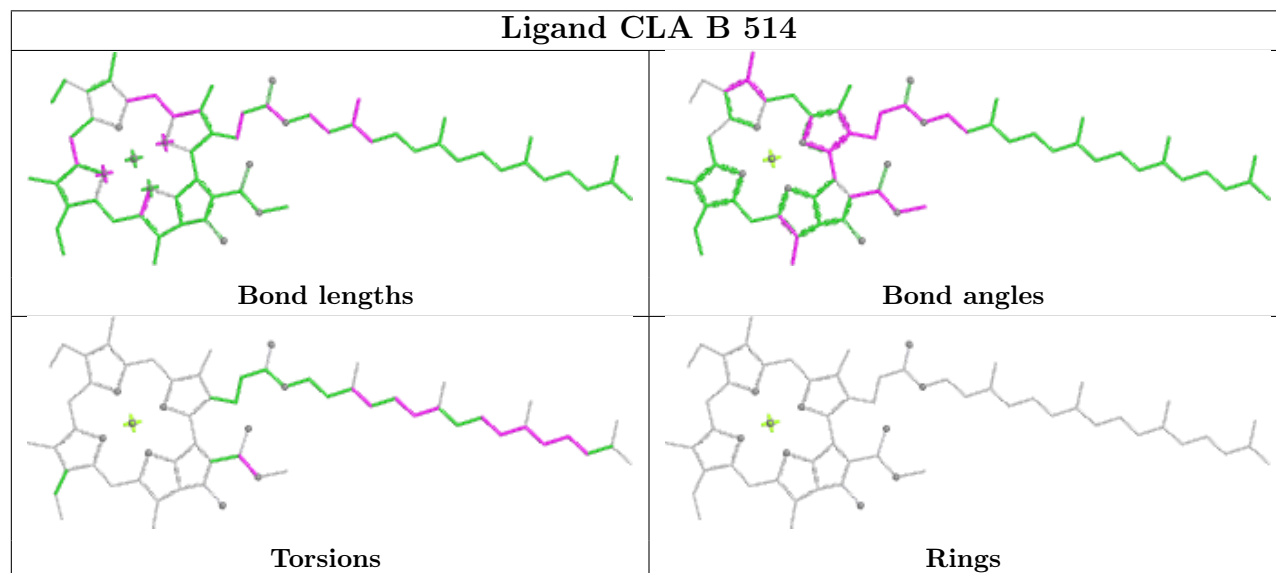
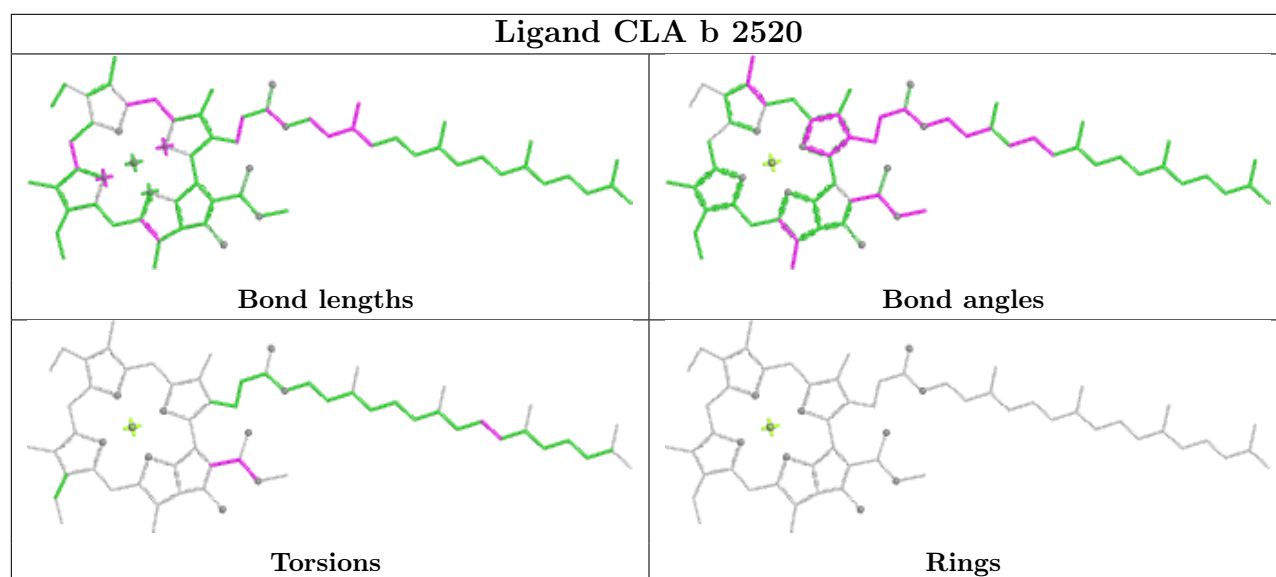


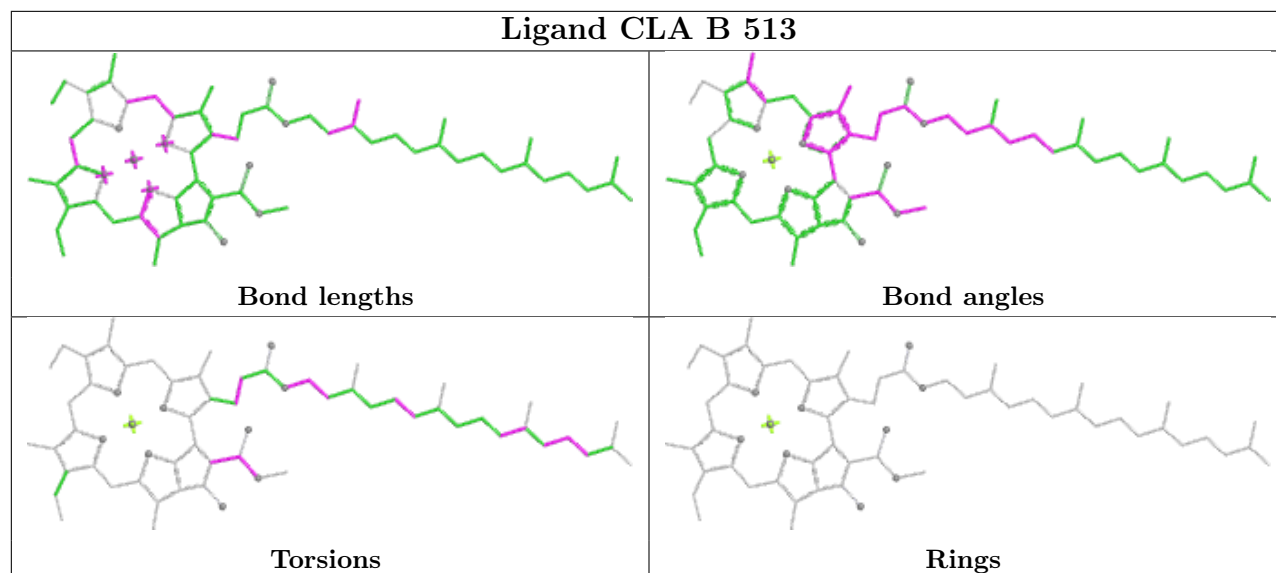
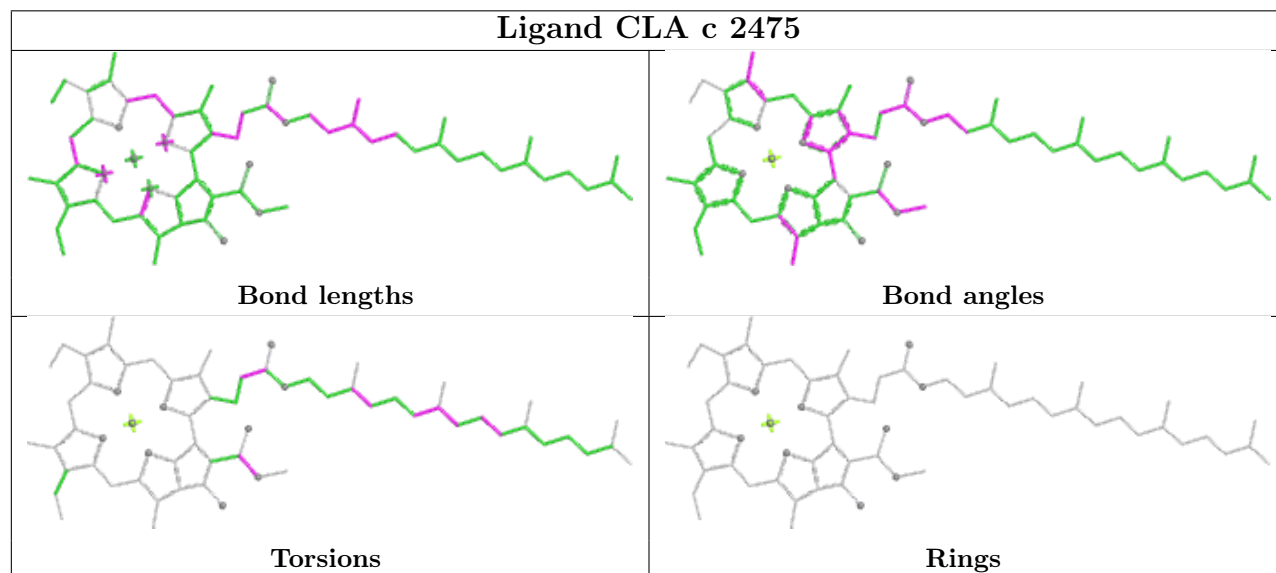
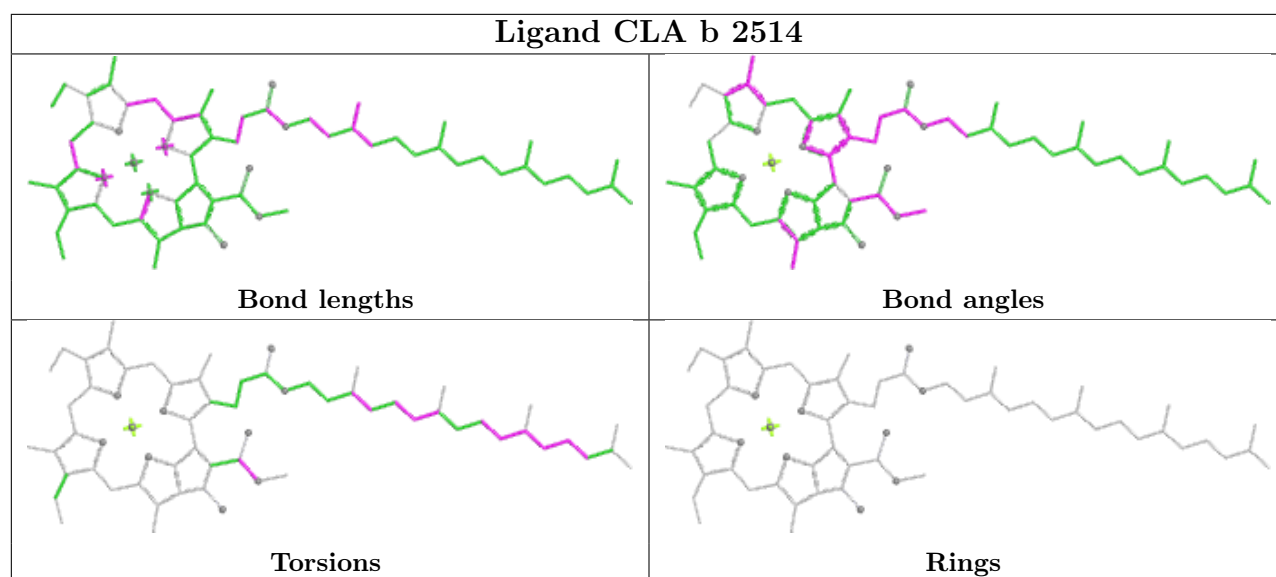


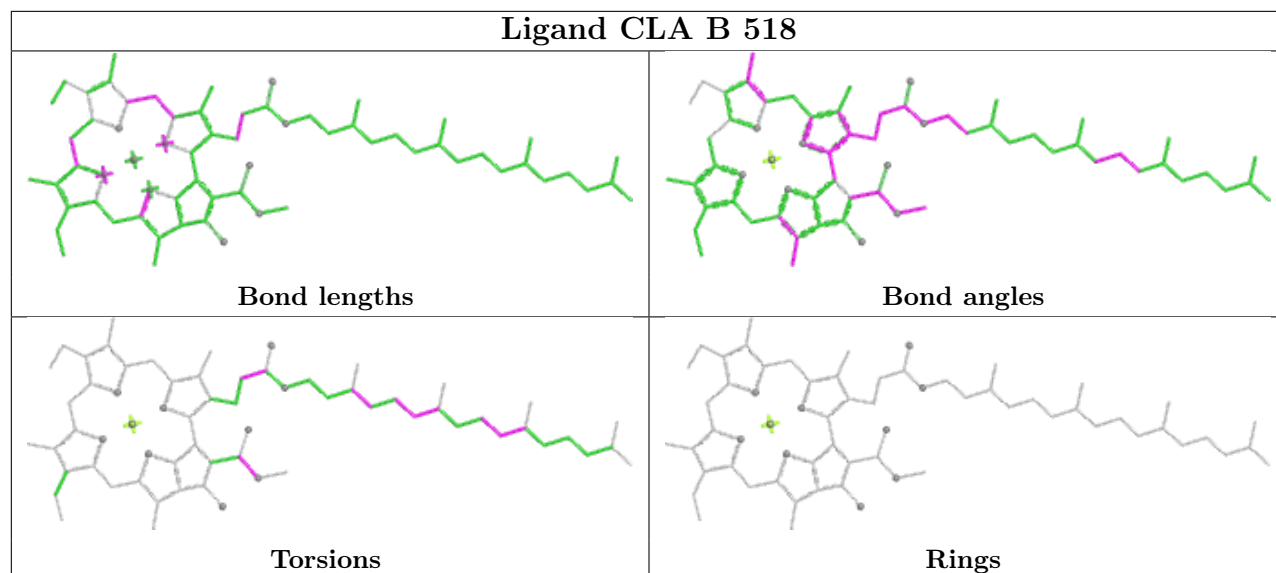
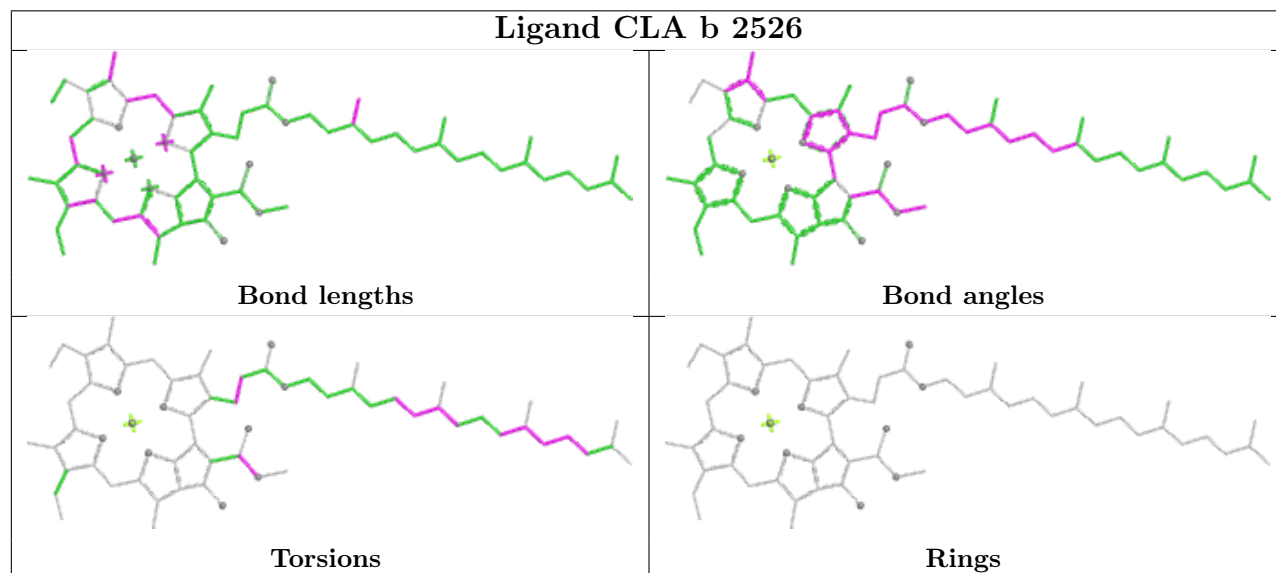
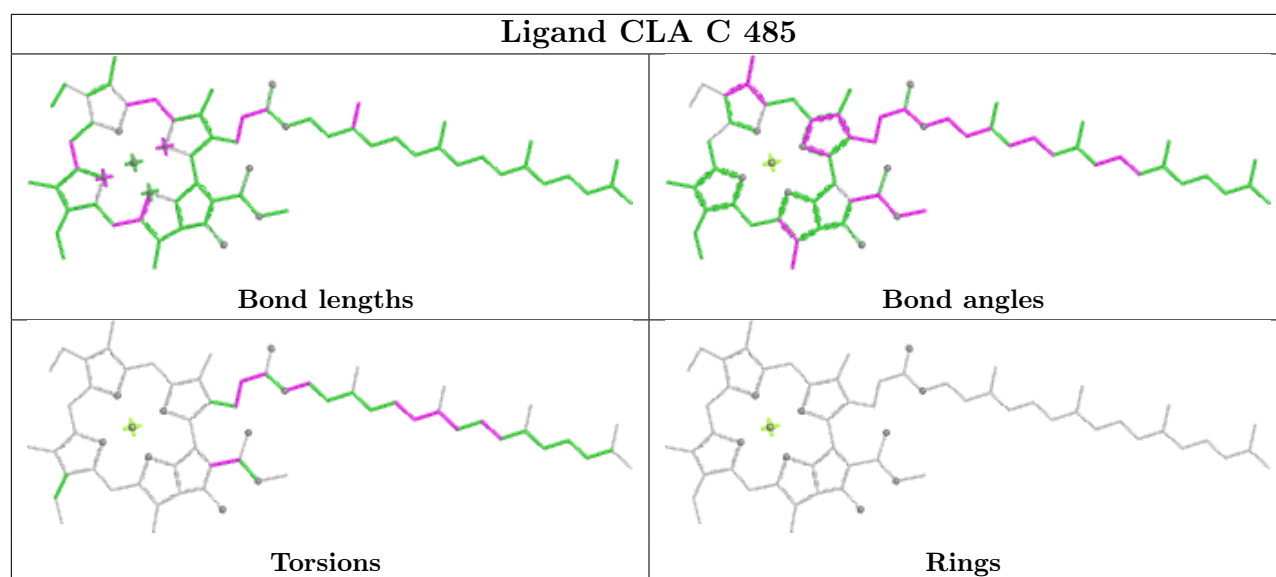




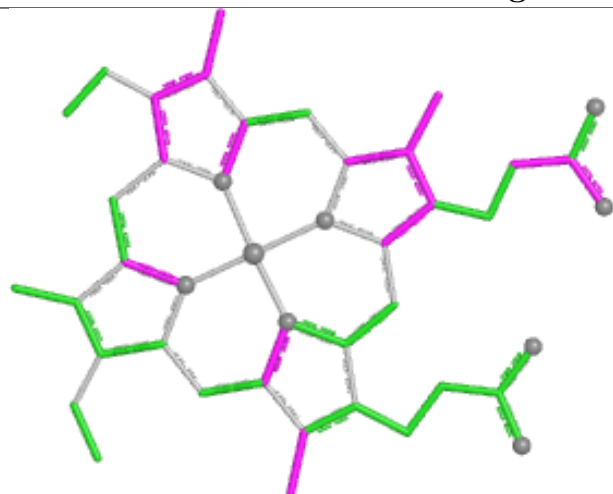




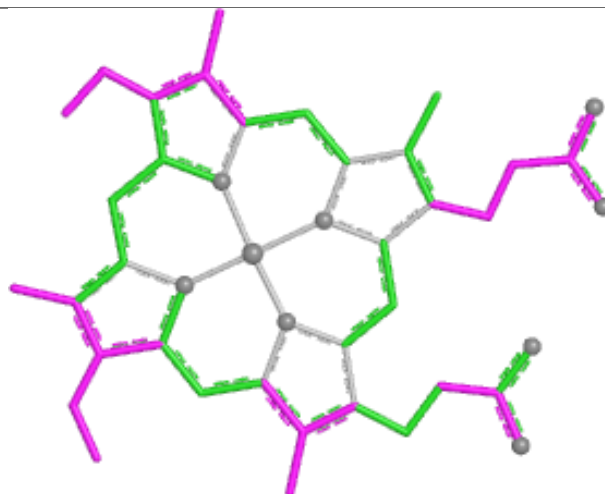




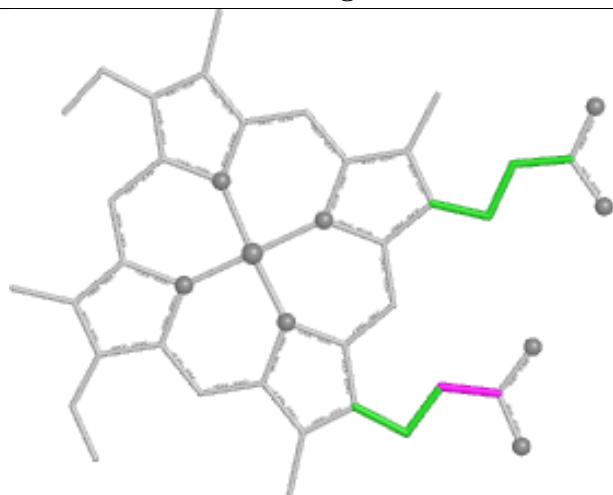
Ligand HEC e 2084



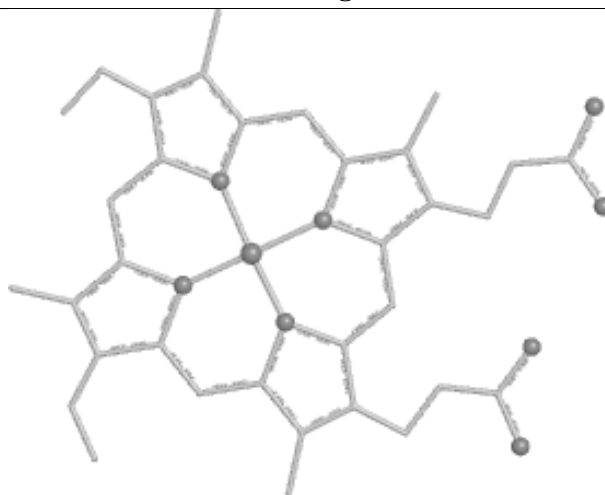
Bond lengths



Bond angles

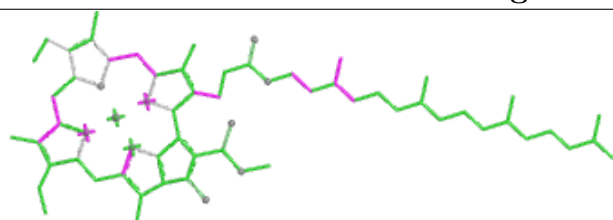


Torsions

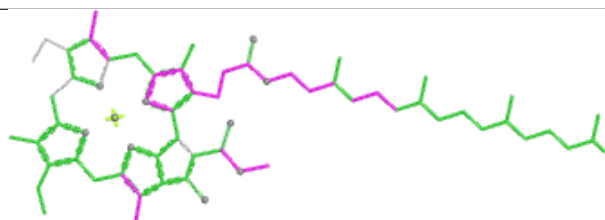


Rings

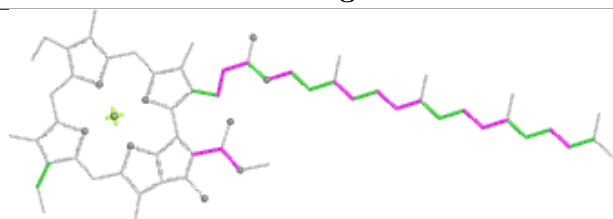
Ligand CLA c 2484



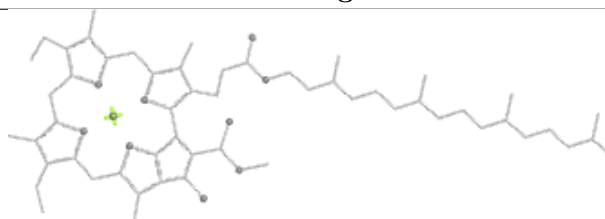
Bond lengths



Bond angles

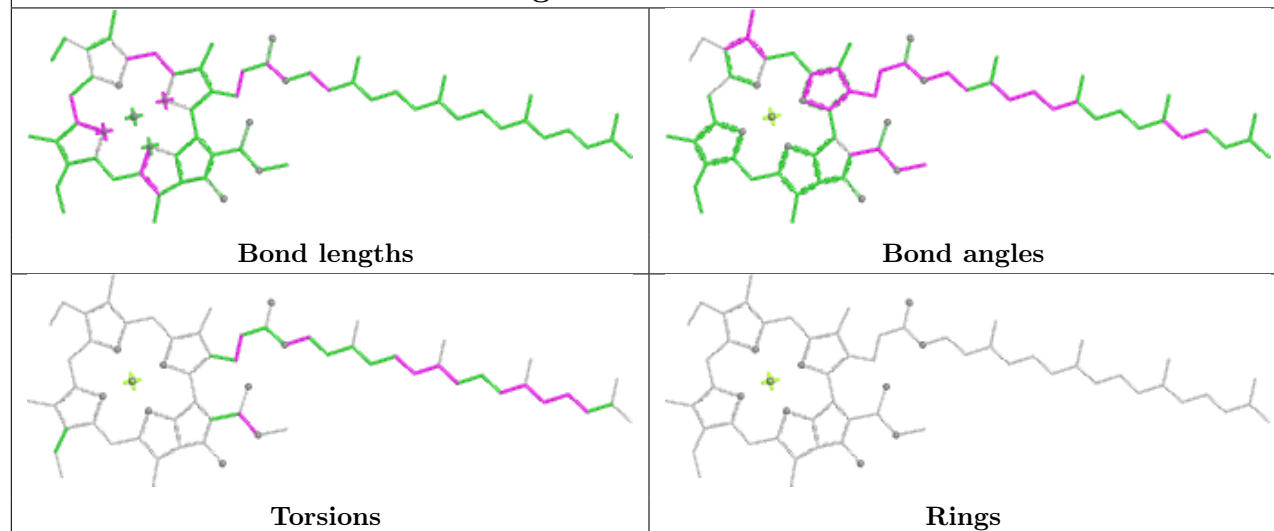


Torsions

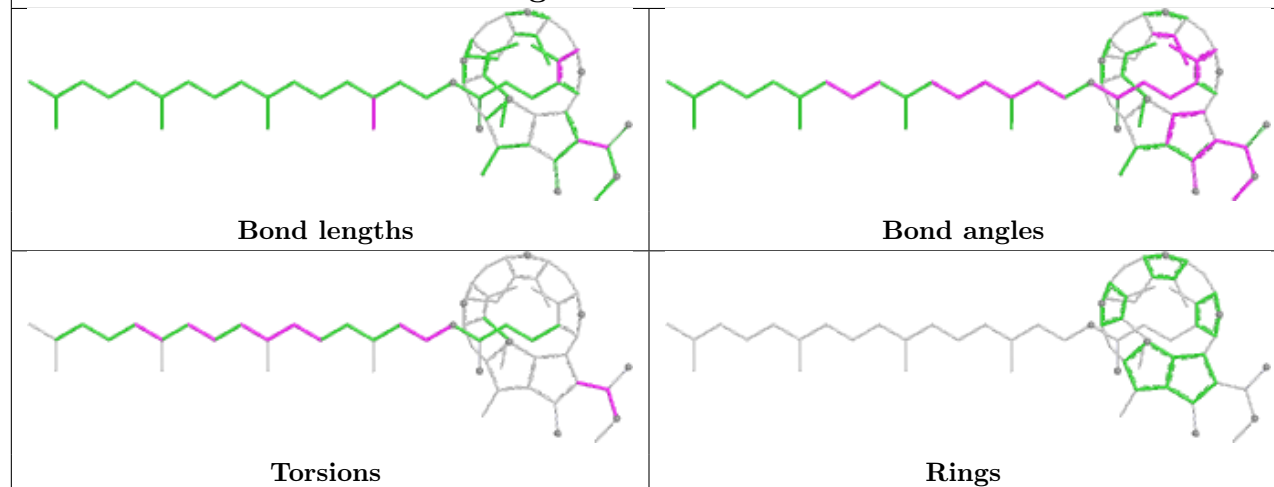


Rings

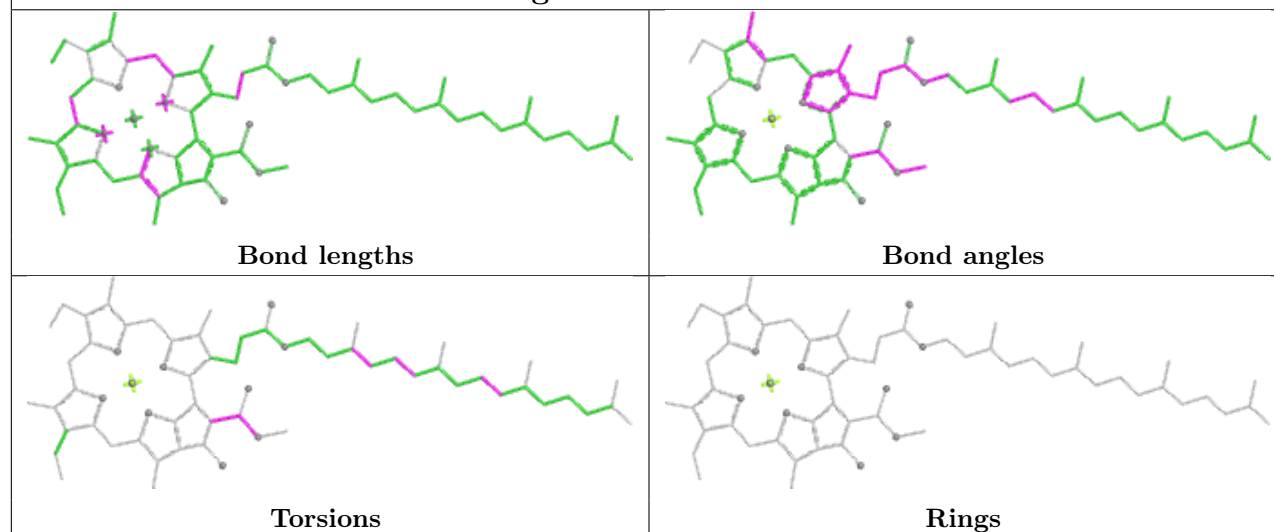
Ligand CLA C 477



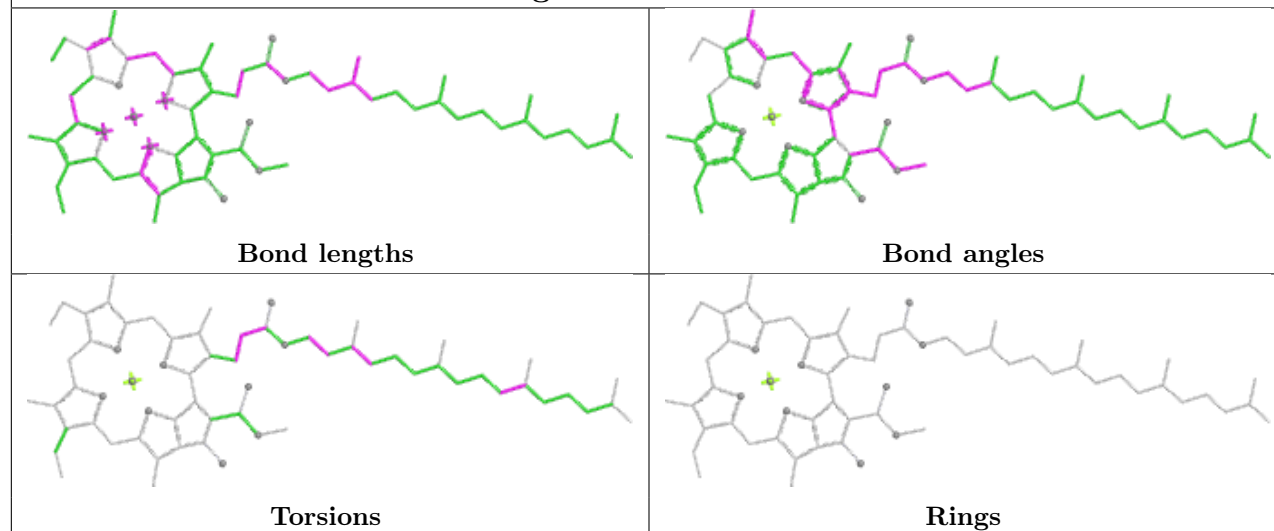
Ligand PHO D 355



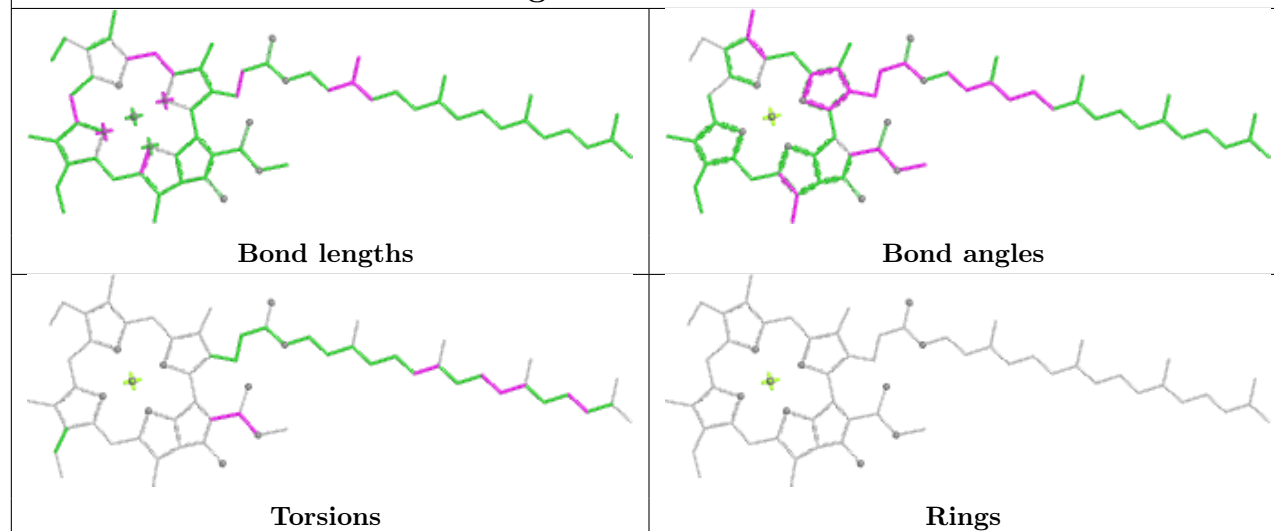
Ligand CLA A 350



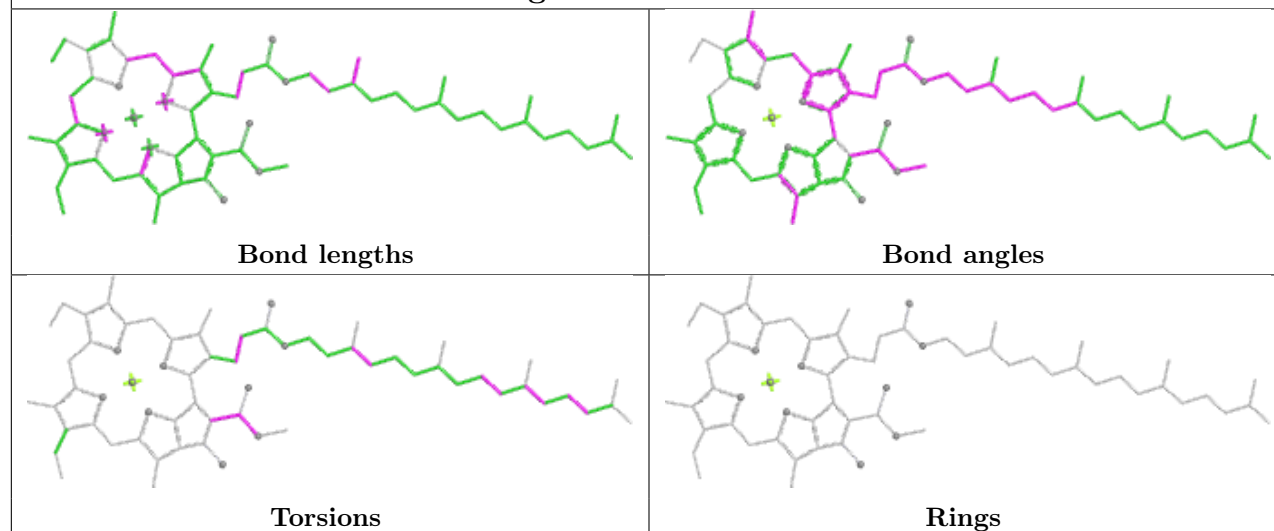
Ligand CLA B 519



Ligand CLA c 2483



Ligand CLA c 2479



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/344 (96%)	0.43	15 (4%) 39 27	33, 60, 91, 104	0
1	a	333/344 (96%)	0.41	15 (4%) 39 27	39, 63, 92, 105	0
2	B	476/510 (93%)	0.49	29 (6%) 28 21	39, 65, 89, 105	0
2	b	476/510 (93%)	0.43	18 (3%) 44 30	39, 65, 89, 106	0
3	C	421/473 (89%)	0.47	17 (4%) 43 29	34, 69, 89, 103	0
3	c	421/473 (89%)	0.55	22 (5%) 34 24	36, 71, 90, 107	0
4	D	339/352 (96%)	0.37	18 (5%) 33 24	22, 60, 92, 106	0
4	d	339/352 (96%)	0.37	16 (4%) 37 26	31, 62, 92, 106	0
5	E	76/84 (90%)	0.45	2 (2%) 57 39	55, 76, 94, 107	0
5	e	76/84 (90%)	0.73	6 (7%) 20 16	60, 79, 96, 107	0
6	F	33/45 (73%)	0.33	2 (6%) 28 21	49, 68, 92, 107	0
6	f	33/45 (73%)	0.43	1 (3%) 52 35	49, 70, 92, 101	0
7	H	53/66 (80%)	0.25	3 (5%) 30 23	46, 73, 104, 106	0
7	h	53/66 (80%)	0.29	1 (1%) 66 46	56, 74, 106, 109	0
8	I	38/38 (100%)	0.89	6 (15%) 6 6	60, 76, 100, 102	0
8	i	38/38 (100%)	0.50	3 (7%) 20 16	59, 76, 100, 104	0
9	J	38/40 (95%)	0.34	3 (7%) 20 16	60, 79, 99, 103	0
9	j	38/40 (95%)	0.71	2 (5%) 33 24	61, 82, 98, 107	0
10	K	37/37 (100%)	0.13	0 100 100	61, 71, 95, 95	0
10	k	37/37 (100%)	0.29	0 100 100	65, 73, 96, 97	0
11	L	37/37 (100%)	0.31	1 (2%) 56 38	39, 58, 101, 104	0
11	l	37/37 (100%)	0.37	2 (5%) 32 23	34, 61, 99, 101	0
12	M	30/36 (83%)	-0.05	0 100 100	45, 56, 78, 88	0
12	m	30/36 (83%)	0.10	0 100 100	44, 56, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	246/246 (100%)	0.61	15 (6%) 28 21	41, 75, 100, 110	0
13	o	246/246 (100%)	0.65	12 (4%) 36 25	46, 75, 99, 107	0
14	T	31/32 (96%)	0.06	0 100 100	27, 54, 86, 89	0
14	t	31/32 (96%)	0.01	1 (3%) 50 34	32, 53, 90, 93	0
15	U	105/134 (78%)	0.52	9 (8%) 18 14	41, 67, 91, 104	0
15	u	105/134 (78%)	0.52	9 (8%) 18 14	46, 68, 92, 103	0
16	V	137/137 (100%)	0.20	0 100 100	42, 66, 80, 88	0
16	v	137/137 (100%)	0.32	4 (2%) 54 36	46, 70, 85, 90	0
17	X	40/50 (80%)	0.13	1 (2%) 58 40	67, 74, 102, 109	0
17	x	40/50 (80%)	0.11	1 (2%) 58 40	67, 77, 104, 108	0
18	N	0/37	-	-	-	-
18	n	0/37	-	-	-	-
19	Z	58/62 (93%)	0.28	2 (3%) 48 32	62, 80, 93, 102	0
19	z	58/62 (93%)	0.41	2 (3%) 48 32	70, 81, 94, 106	0
All	All	5056/5520 (91%)	0.44	238 (4%) 37 26	22, 68, 95, 110	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	2006	TYR	6.4
8	I	28	PRO	6.1
4	D	242	GLU	6.0
2	B	328	GLY	5.8
1	a	2026	ASN	5.6
3	C	47	GLY	5.6
8	I	25	SER	5.6
13	O	246	ALA	5.4
9	j	2040	LEU	5.3
3	C	293	ASN	5.3
1	A	264	SER	5.0
15	U	35	THR	4.9
1	A	245	THR	4.8
8	I	2	GLU	4.8
9	J	39	SER	4.6
2	B	224	ARG	4.6
15	u	2052	GLY	4.6
5	e	2010	SER	4.4
5	e	2009	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
14	t	2002	GLU	4.2
15	U	38	GLU	4.2
2	B	72	THR	4.2
1	a	2226	GLU	4.1
3	c	2172	ALA	4.1
13	o	2134	THR	4.1
13	O	34	SER	4.1
2	B	6	TYR	4.0
16	v	2100	ILE	4.0
2	b	2091	TRP	3.9
9	J	40	LEU	3.8
2	b	2471	ALA	3.8
4	d	2041	ALA	3.8
2	B	87	ASP	3.7
11	L	11	GLU	3.7
13	o	2034	SER	3.7
13	o	2100	GLY	3.6
1	A	342	ASP	3.6
3	C	366	LEU	3.6
2	b	2271	THR	3.6
2	B	235	GLU	3.6
4	d	2262	SER	3.5
7	H	21	ALA	3.5
2	b	2122	LEU	3.4
4	D	55	VAL	3.4
4	d	2053	THR	3.4
2	b	2078	TRP	3.4
13	O	218	GLU	3.3
2	b	2441	GLY	3.3
5	E	13	ILE	3.2
2	b	2188	ASP	3.2
8	I	29	ALA	3.2
15	u	2134	LYS	3.2
4	d	2054	PHE	3.2
19	Z	30	PRO	3.2
3	C	294	ASN	3.1
5	E	9	PHE	3.1
2	B	327	THR	3.1
2	b	2388	SER	3.1
8	I	26	GLY	3.1
1	A	263	ALA	3.1
13	O	99	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLY	3.1
4	D	230	SER	3.1
2	b	2326	ARG	3.1
1	A	344	ALA	3.0
1	a	2305	SER	3.0
2	B	198	VAL	3.0
11	l	2017	LEU	3.0
3	c	2148	GLY	3.0
2	b	2163	GLY	2.9
17	X	19	PHE	2.9
13	o	2166	SER	2.9
2	B	361	ALA	2.9
16	v	2126	LEU	2.9
1	a	2133	LEU	2.9
1	A	166	GLY	2.9
1	A	167	SER	2.9
1	A	112	TYR	2.9
13	O	196	GLN	2.9
3	C	72	LEU	2.8
13	o	2099	ASP	2.8
3	c	2064	ALA	2.8
4	D	255	GLN	2.8
9	J	38	SER	2.8
2	B	405	GLU	2.7
3	C	104	GLU	2.7
15	U	128	TYR	2.7
4	d	2090	LEU	2.7
8	i	2024	LEU	2.7
3	c	2288	CYS	2.7
3	c	2086	LEU	2.7
7	h	2021	ALA	2.7
4	d	2213	ILE	2.7
1	A	26	ASN	2.7
2	B	226	TYR	2.7
2	B	115	TRP	2.7
3	C	277	GLY	2.7
3	C	195	ASP	2.7
3	c	2270	ALA	2.6
15	u	2044	ASP	2.6
2	B	89	GLY	2.6
1	a	2338	ASN	2.6
13	o	2101	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
15	U	56	ASP	2.6
3	C	257	PHE	2.6
13	O	31	PRO	2.6
2	B	440	ASP	2.6
15	u	2126	ASP	2.6
4	D	95	PRO	2.5
4	D	105	CYS	2.5
1	A	222	SER	2.5
3	c	2090	PRO	2.5
13	o	2019	CYS	2.5
2	B	122	LEU	2.5
3	c	2366	LEU	2.5
2	B	326	ARG	2.5
6	f	2013	PRO	2.5
8	i	2028	PRO	2.5
6	F	27	VAL	2.5
15	u	2042	VAL	2.5
19	Z	15	LEU	2.5
3	c	2437	PHE	2.5
15	U	126	ASP	2.5
3	C	270	ALA	2.5
3	C	142	GLU	2.5
1	a	2165	GLN	2.5
4	d	2224	GLN	2.5
3	c	2158	THR	2.5
16	v	2136	TYR	2.5
3	C	446	GLY	2.4
2	B	330	MET	2.4
4	d	2223	PHE	2.4
6	F	26	ALA	2.4
3	c	2161	LEU	2.4
2	B	78	TRP	2.4
2	B	193	TYR	2.4
15	U	131	GLY	2.4
1	A	142	TRP	2.4
13	o	2052	VAL	2.3
4	d	2017	ILE	2.3
4	d	2132	ILE	2.3
13	O	138	THR	2.3
15	U	96	GLY	2.3
4	d	2222	LEU	2.3
1	A	139	MET	2.3

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Mol	Chain	Res	Type	RSRZ
13	O	204	VAL	2.3
17	x	2038	ILE	2.3
1	a	2188	ALA	2.3
1	a	2143	ILE	2.3
2	b	2181	VAL	2.3
4	D	256	ILE	2.3
2	b	2344	ALA	2.3
3	c	2384	ILE	2.3
1	a	2301	ASN	2.3
5	e	2018	TYR	2.3
13	O	33	ASP	2.3
4	D	90	LEU	2.3
13	o	2200	ASN	2.3
16	v	2046	THR	2.3
13	O	111	ALA	2.3
15	U	40	VAL	2.3
2	B	7	ARG	2.3
5	e	2082	LEU	2.3
1	a	2245	THR	2.3
4	D	225	ASP	2.3
4	D	234	ALA	2.3
13	O	202	ALA	2.3
15	u	2031	ALA	2.3
11	l	2005	PRO	2.2
3	C	138	GLU	2.2
2	B	124	ARG	2.2
4	D	241	GLU	2.2
13	O	100	GLY	2.2
2	B	303	SER	2.2
4	D	295	SER	2.2
15	u	2058	ASN	2.2
3	c	2269	GLU	2.2
1	A	261	GLN	2.2
2	B	465	GLY	2.2
7	H	61	TRP	2.2
13	o	2121	THR	2.2
8	I	30	ARG	2.2
4	d	2242	GLU	2.2
19	z	2003	ILE	2.2
13	O	19	CYS	2.2
3	C	320	ARG	2.2
15	u	2048	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	o	2176	GLN	2.2
4	d	2115	ALA	2.2
8	i	2030	ARG	2.2
3	c	2346	THR	2.2
15	u	2109	LEU	2.2
3	c	2373	ASN	2.2
5	e	2013	ILE	2.1
1	a	2343	LEU	2.1
19	z	2015	LEU	2.1
1	a	2023	SER	2.1
3	c	2104	GLU	2.1
4	D	344	GLU	2.1
3	c	2183	GLY	2.1
1	a	2082	VAL	2.1
4	d	2080	THR	2.1
4	d	2313	THR	2.1
4	D	228	GLY	2.1
13	O	136	ILE	2.1
4	D	106	GLN	2.1
4	d	2264	LYS	2.1
2	b	2084	THR	2.1
1	A	19	ASN	2.1
2	B	299	GLU	2.1
2	B	341	LYS	2.1
1	a	2037	MET	2.1
3	c	2315	MET	2.1
2	B	14	ASN	2.1
2	B	318	ASN	2.1
7	H	20	VAL	2.1
13	O	43	LEU	2.1
2	b	2072	THR	2.1
2	b	2225	LEU	2.1
3	c	2292	PHE	2.1
3	c	2039	ASN	2.1
1	a	2220	THR	2.0
3	C	401	LEU	2.0
3	c	2096	GLY	2.0
4	D	267	LEU	2.0
15	U	63	ALA	2.0
2	B	191	ASN	2.0
5	e	2011	ASP	2.0
4	D	232	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	2097	ALA	2.0
2	b	2129	GLY	2.0
3	C	98	GLY	2.0
3	C	288	CYS	2.0
3	c	2229	ASN	2.0
9	j	2038	SER	2.0
13	o	2198	SER	2.0
4	D	233	ARG	2.0
2	B	90	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CLA	C	487	65/65	0.49	0.24	87,101,114,118	0
23	CLA	c	2487	65/65	0.53	0.22	88,101,114,118	0
27	BCR	c	2489	40/40	0.53	0.20	85,90,100,100	0
26	LMT	d	2359	35/35	0.55	0.26	73,82,91,92	0
27	BCR	j	2053	40/40	0.56	0.14	71,87,100,101	0
27	BCR	k	2050	40/40	0.57	0.25	80,85,97,101	0
27	BCR	B	529	40/40	0.59	0.23	76,93,105,106	0
27	BCR	J	53	40/40	0.63	0.15	70,88,100,100	0
27	BCR	K	50	40/40	0.65	0.22	79,85,96,101	0
27	BCR	C	489	40/40	0.66	0.24	85,90,100,100	0
25	PL9	D	357	45/55	0.66	0.24	71,80,86,88	0
25	PL9	d	2358	45/55	0.67	0.22	70,80,87,89	0
23	CLA	c	2475	65/65	0.67	0.19	66,80,97,102	0
27	BCR	b	2528	40/40	0.67	0.23	77,92,105,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	527	65/65	0.68	0.16	84,89,106,109	0
23	CLA	b	2526	65/65	0.70	0.16	82,89,106,110	0
23	CLA	C	482	65/65	0.71	0.17	71,80,97,98	0
23	CLA	c	2486	65/65	0.71	0.22	79,84,92,94	0
27	BCR	d	2360	40/40	0.72	0.21	67,79,91,93	0
23	CLA	d	2357	65/65	0.72	0.21	68,77,91,95	0
23	CLA	c	2484	65/65	0.72	0.17	77,87,101,102	0
27	BCR	c	2488	40/40	0.73	0.23	76,84,93,96	0
23	CLA	b	2511	65/65	0.75	0.20	58,81,92,97	0
23	CLA	B	511	65/65	0.75	0.21	58,81,92,97	0
25	PL9	a	2352	45/55	0.75	0.15	77,85,90,91	0
25	PL9	A	353	45/55	0.76	0.16	77,86,91,92	0
23	CLA	B	523	65/65	0.76	0.18	60,64,94,109	0
23	CLA	C	484	65/65	0.76	0.16	76,87,101,102	0
26	LMT	B	526	35/35	0.77	0.21	72,82,90,91	0
23	CLA	c	2482	65/65	0.77	0.15	72,81,97,98	0
23	CLA	C	477	65/65	0.77	0.17	71,79,97,100	0
23	CLA	b	2525	65/65	0.77	0.17	73,80,89,91	0
21	BCT	d	2353	4/4	0.78	0.13	66,68,69,69	0
21	BCT	A	346	4/4	0.78	0.14	70,70,71,74	0
23	CLA	c	2480	65/65	0.78	0.17	65,80,82,87	0
23	CLA	c	2474	65/65	0.79	0.17	70,76,88,89	0
23	CLA	b	2517	65/65	0.79	0.17	64,71,80,89	0
23	CLA	B	520	65/65	0.79	0.15	63,68,79,79	0
23	CLA	A	352	65/65	0.79	0.18	48,65,101,102	0
23	CLA	b	2523	65/65	0.80	0.16	59,64,94,108	0
23	CLA	c	2477	65/65	0.80	0.16	73,79,98,101	0
23	CLA	B	514	65/65	0.80	0.17	60,67,79,82	0
27	BCR	B	528	40/40	0.80	0.19	63,79,85,87	0
23	CLA	C	483	65/65	0.80	0.14	67,73,101,106	0
23	CLA	c	2483	65/65	0.80	0.16	68,74,100,106	0
23	CLA	B	525	65/65	0.80	0.16	72,80,89,92	0
23	CLA	C	474	65/65	0.81	0.17	69,76,87,89	0
23	CLA	b	2513	65/65	0.81	0.18	45,57,102,106	0
23	CLA	C	485	65/65	0.81	0.18	64,75,91,95	0
27	BCR	b	2527	40/40	0.81	0.15	64,78,84,86	0
23	CLA	B	519	65/65	0.81	0.15	58,67,90,91	0
23	CLA	a	2349	65/65	0.82	0.14	36,54,93,95	0
23	CLA	c	2479	65/65	0.82	0.16	57,76,80,84	0
23	CLA	a	2351	65/65	0.82	0.16	50,66,101,102	0
23	CLA	c	2481	65/65	0.82	0.15	55,60,85,89	0
23	CLA	b	2520	65/65	0.82	0.14	61,68,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	516	65/65	0.82	0.16	44,55,92,93	0
23	CLA	c	2476	65/65	0.82	0.16	50,64,75,78	0
23	CLA	B	515	65/65	0.83	0.16	45,66,84,87	0
23	CLA	c	2485	65/65	0.83	0.17	61,75,90,94	0
23	CLA	b	2514	65/65	0.83	0.17	59,67,79,82	0
23	CLA	b	2516	65/65	0.83	0.14	42,54,93,94	0
21	BCT	a	2346	4/4	0.83	0.14	71,72,73,76	0
24	PHO	a	2350	64/64	0.83	0.18	56,66,81,82	0
23	CLA	D	356	65/65	0.83	0.15	69,77,90,95	0
23	CLA	b	2521	65/65	0.83	0.18	67,71,80,82	0
27	BCR	C	488	40/40	0.84	0.23	75,83,92,95	0
23	CLA	C	486	65/65	0.84	0.18	78,84,91,95	0
27	BCR	F	48	40/40	0.84	0.15	66,80,91,92	0
23	CLA	C	475	65/65	0.84	0.17	66,80,97,103	0
24	PHO	D	355	64/64	0.84	0.16	62,69,103,111	0
23	CLA	B	524	65/65	0.84	0.17	56,68,75,88	0
23	CLA	B	521	65/65	0.85	0.16	67,72,80,81	0
23	CLA	b	2522	65/65	0.85	0.15	69,75,87,88	0
23	CLA	C	476	65/65	0.85	0.15	49,62,75,78	0
24	PHO	d	2356	64/64	0.85	0.16	62,70,103,111	0
28	HEC	e	2084	43/43	0.85	0.23	75,79,100,108	0
23	CLA	b	2519	65/65	0.86	0.13	60,66,90,91	0
23	CLA	B	512	65/65	0.86	0.13	37,50,63,67	0
23	CLA	C	481	65/65	0.86	0.16	54,60,84,88	0
23	CLA	B	522	65/65	0.86	0.16	71,75,87,88	0
23	CLA	B	518	65/65	0.86	0.15	51,61,86,89	0
23	CLA	c	2478	65/65	0.87	0.19	55,66,87,92	0
23	CLA	C	480	65/65	0.87	0.16	64,79,82,87	0
23	CLA	B	517	65/65	0.87	0.16	65,71,79,89	0
23	CLA	b	2515	65/65	0.87	0.15	43,66,84,87	0
23	CLA	A	350	65/65	0.87	0.15	36,52,92,95	0
23	CLA	C	478	65/65	0.87	0.18	55,65,87,91	0
23	CLA	b	2524	65/65	0.87	0.17	56,68,76,89	0
23	CLA	b	2518	65/65	0.88	0.18	53,60,86,88	0
23	CLA	b	2512	65/65	0.88	0.13	34,50,63,66	0
23	CLA	A	348	65/65	0.88	0.14	44,50,65,70	0
23	CLA	d	2354	65/65	0.88	0.12	40,47,75,80	0
23	CLA	B	513	65/65	0.88	0.16	46,57,102,106	0
24	PHO	A	351	64/64	0.88	0.15	55,65,80,82	0
23	CLA	d	2355	65/65	0.89	0.14	19,32,75,86	0
23	CLA	a	2348	65/65	0.89	0.14	44,50,65,69	0
23	CLA	D	354	65/65	0.89	0.14	42,46,76,81	0

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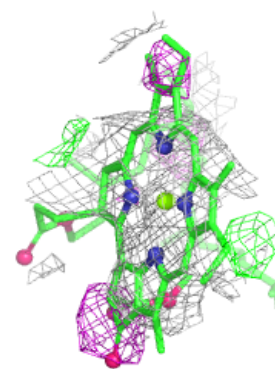
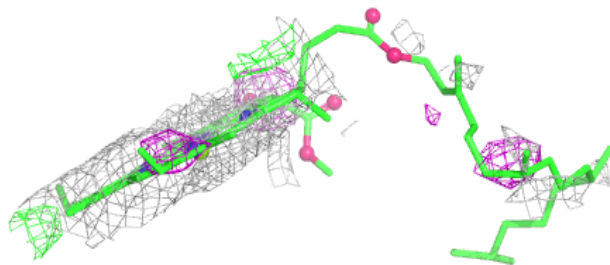
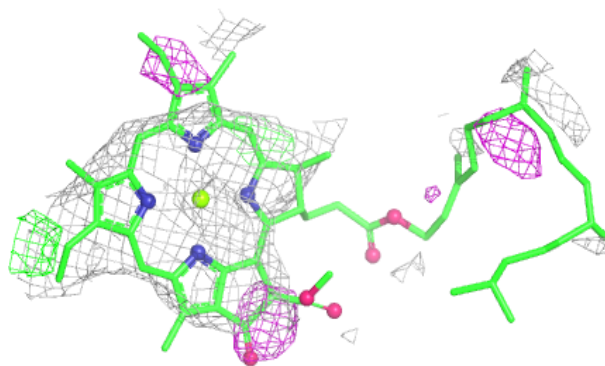
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	C	479	65/65	0.90	0.14	57,76,80,83	0
21	BCT	D	353	4/4	0.90	0.12	66,66,69,69	0
23	CLA	A	349	65/65	0.91	0.12	19,31,76,86	0
28	HEC	E	84	43/43	0.93	0.18	64,79,100,108	0
28	HEC	V	138	43/43	0.94	0.17	44,49,56,57	0
22	OEC	A	347	9/9	0.94	0.06	66,69,73,74	0
28	HEC	v	2138	43/43	0.94	0.12	40,50,55,57	0
22	OEC	a	2347	9/9	0.95	0.06	68,70,74,75	0
20	FE	a	2345	1/1	0.98	0.03	67,67,67,67	0
20	FE	A	345	1/1	0.99	0.04	58,58,58,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

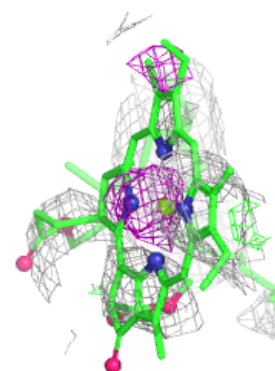
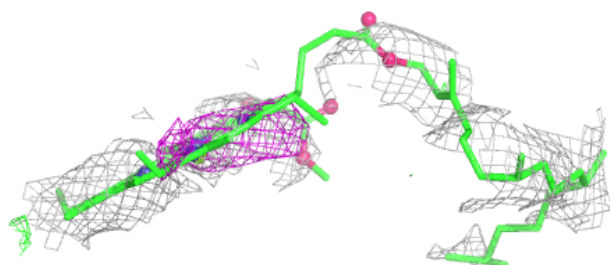
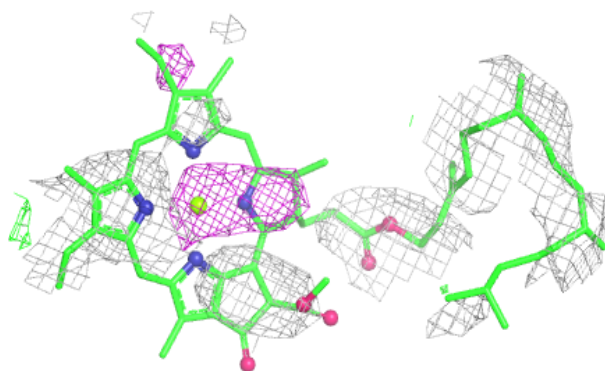
Electron density around CLA C 487:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

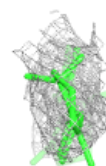
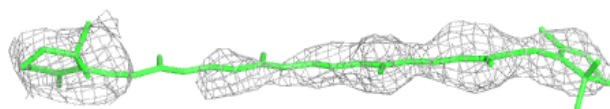
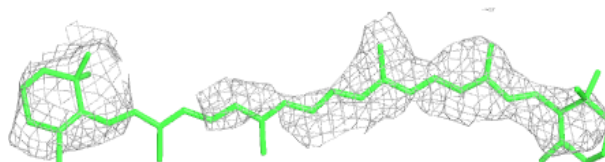


Electron density around CLA c 2487:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

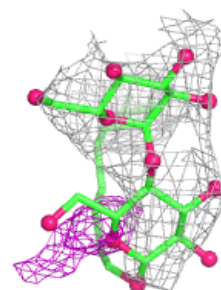
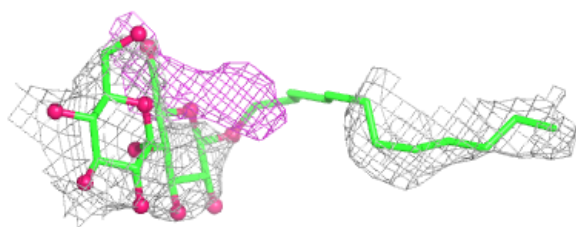
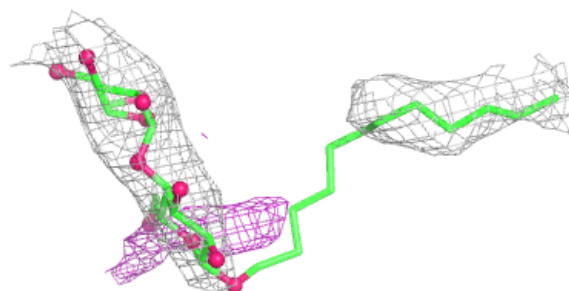
**Electron density around BCR c 2489:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

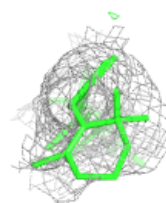
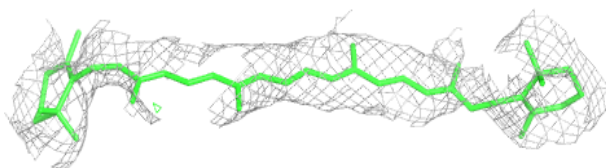
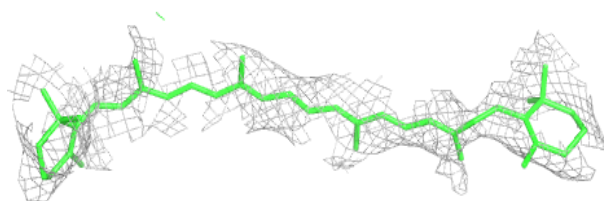


Electron density around LMT d 2359:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

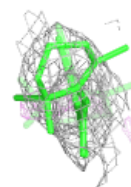
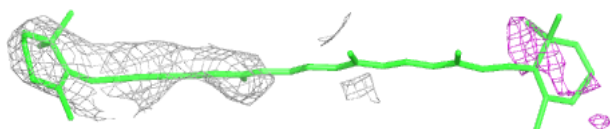
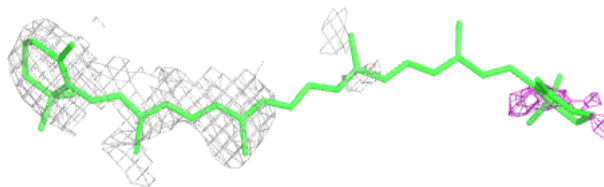
**Electron density around BCR j 2053:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

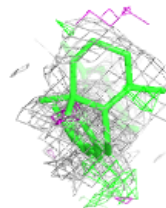
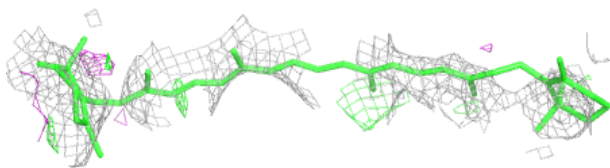
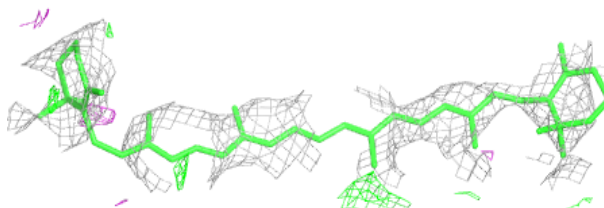


Electron density around BCR k 2050:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

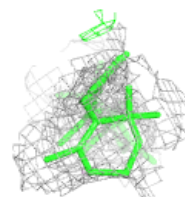
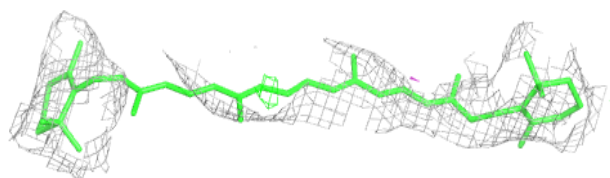
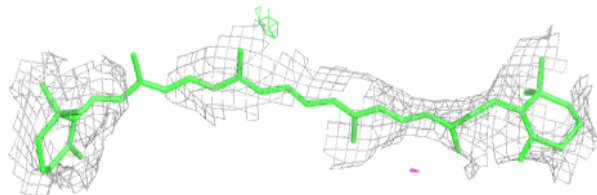
**Electron density around BCR B 529:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

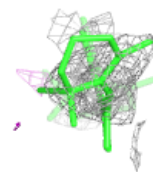
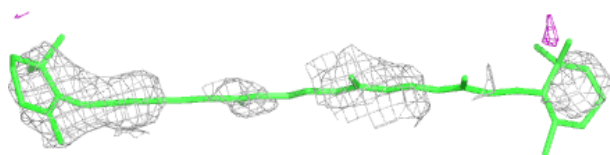
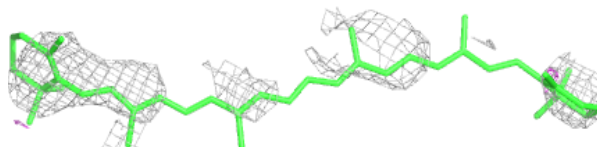


Electron density around BCR J 53:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

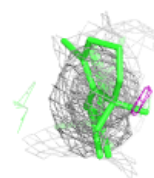
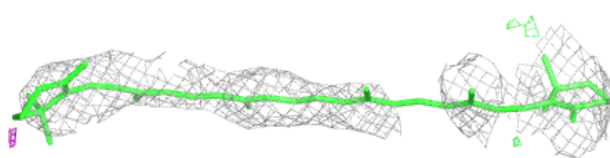
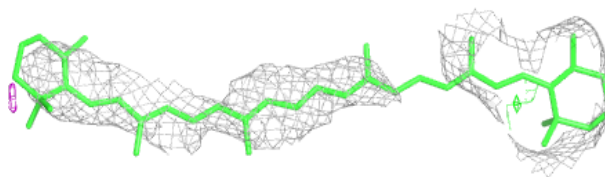
**Electron density around BCR K 50:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

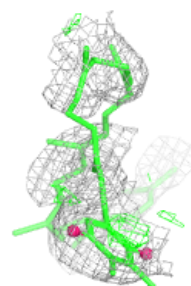
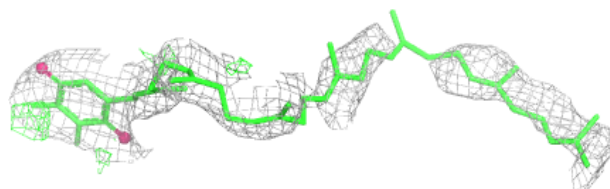
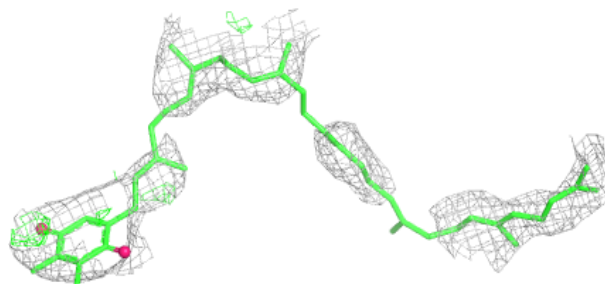


Electron density around BCR C 489:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

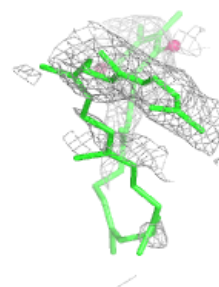
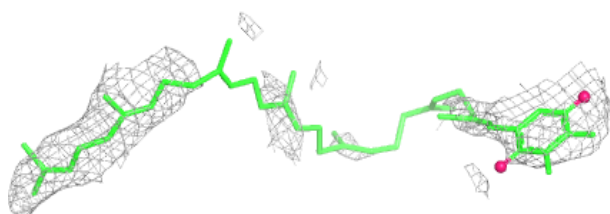
**Electron density around PL9 D 357:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

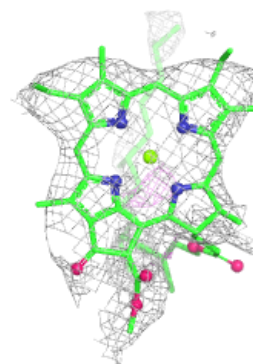
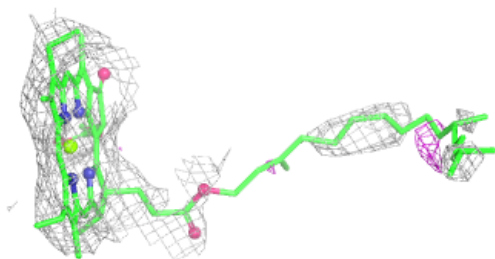
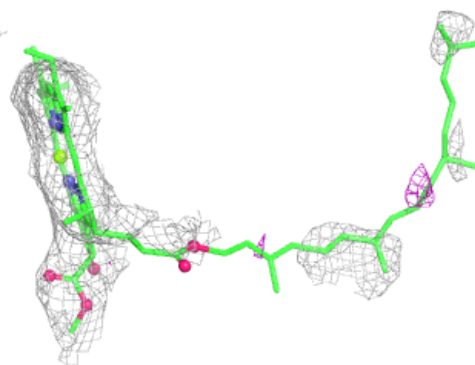


Electron density around PL9 d 2358:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

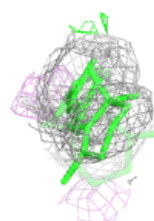
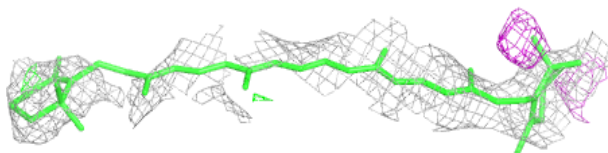
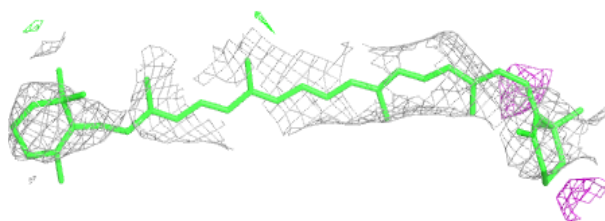
**Electron density around CLA c 2475:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

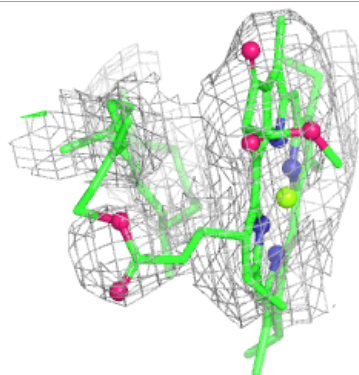
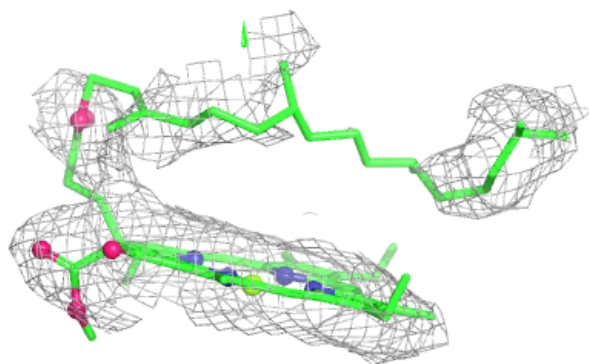
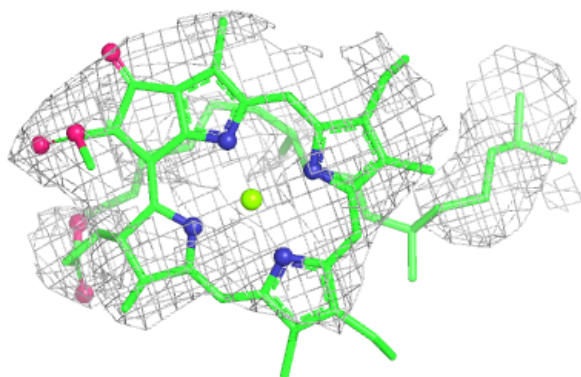


Electron density around BCR b 2528:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

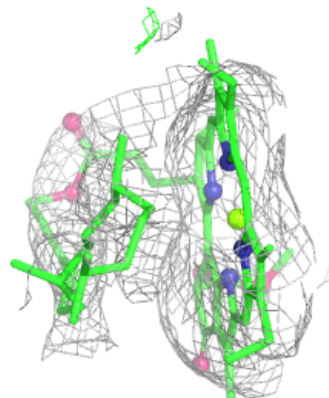
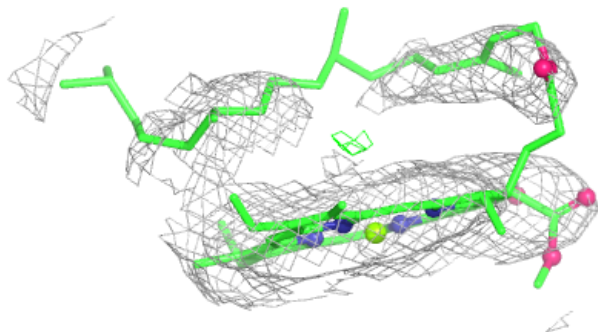
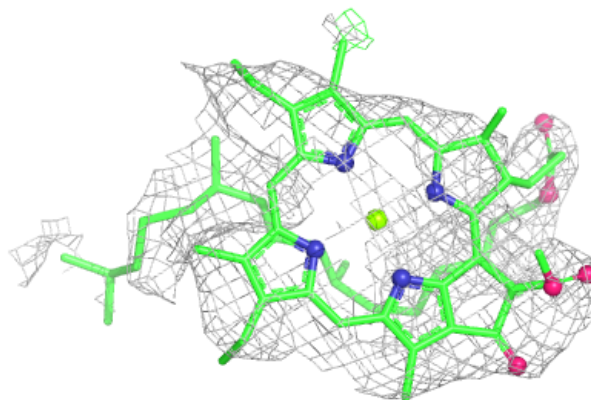
**Electron density around CLA B 527:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

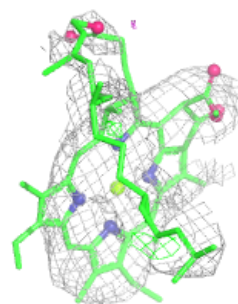
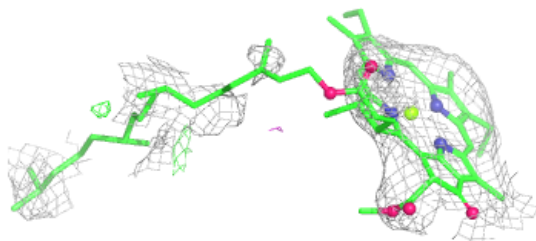
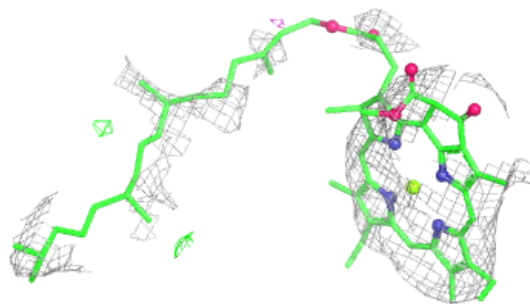


Electron density around CLA b 2526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

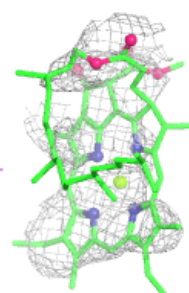
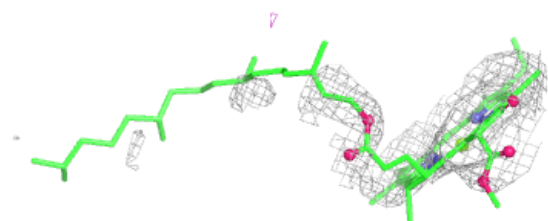
**Electron density around CLA C 482:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

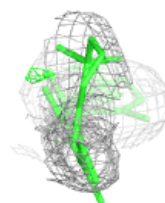
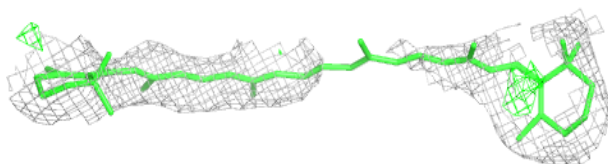
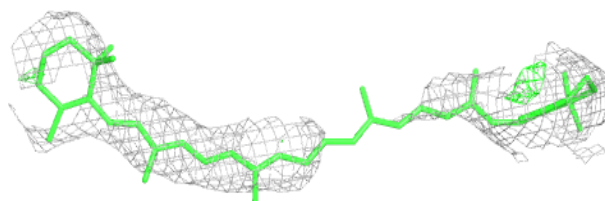


Electron density around CLA c 2486:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

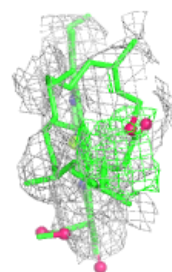
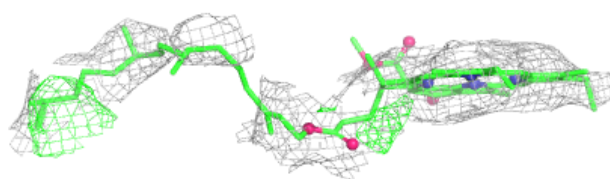
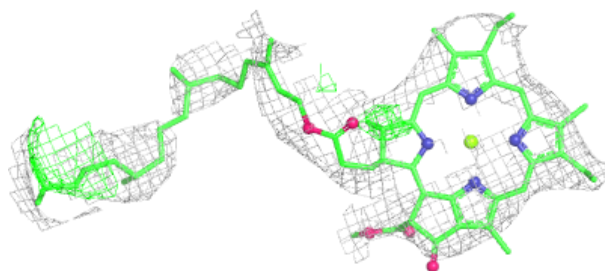
**Electron density around BCR d 2360:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

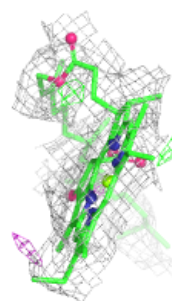
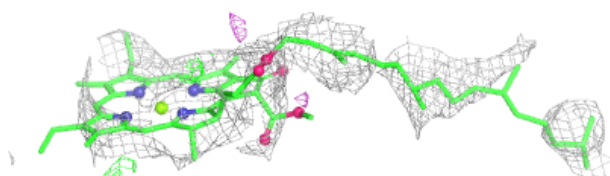
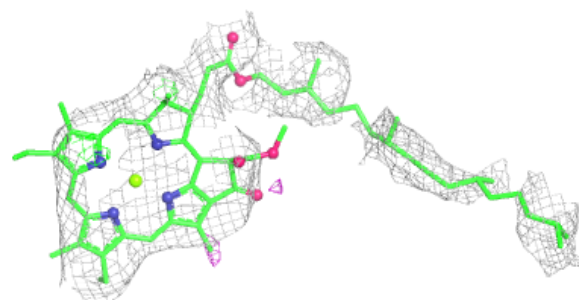


Electron density around CLA d 2357:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

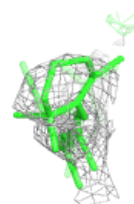
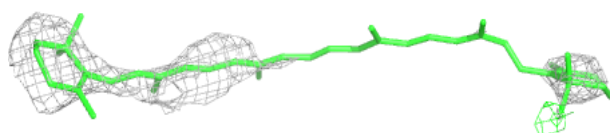
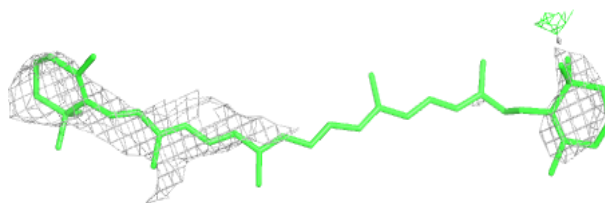
**Electron density around CLA c 2484:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

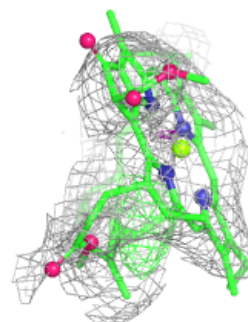
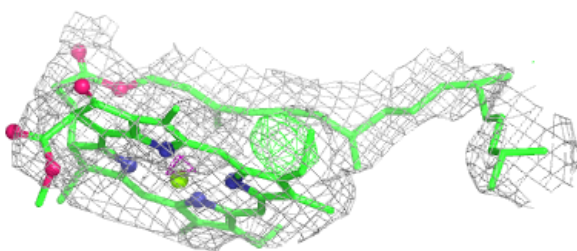
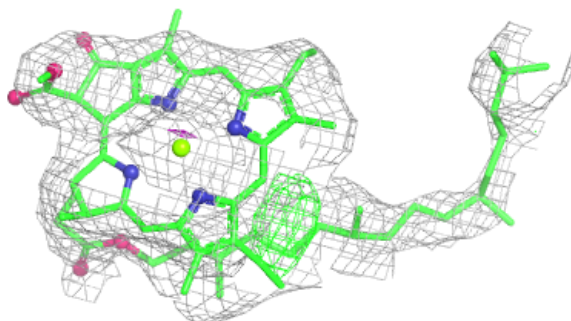


Electron density around BCR c 2488:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

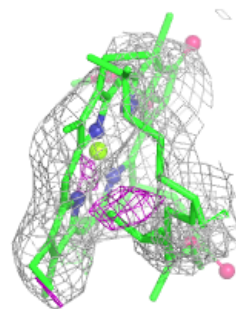
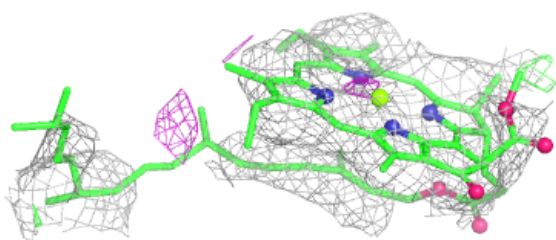
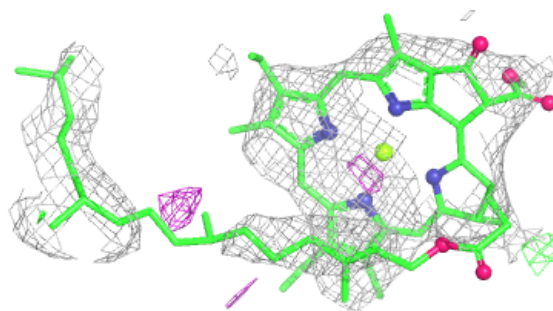
**Electron density around CLA b 2511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

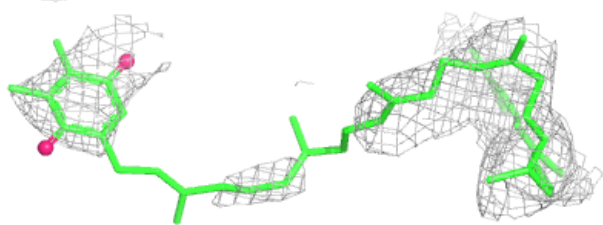
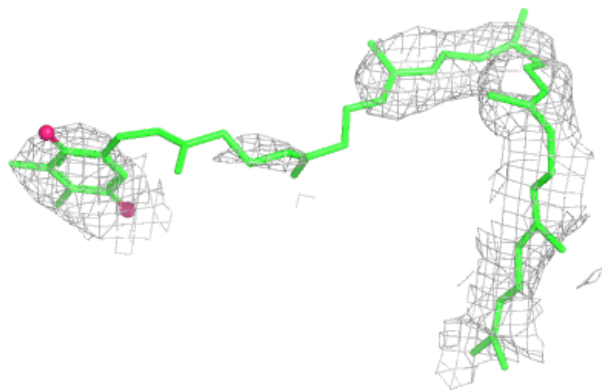


Electron density around CLA B 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

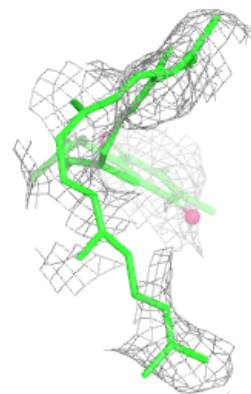
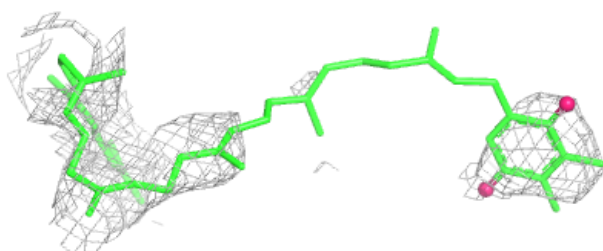
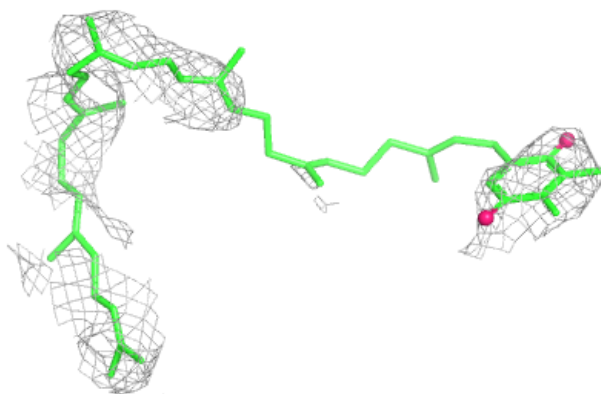
**Electron density around PL9 a 2352:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

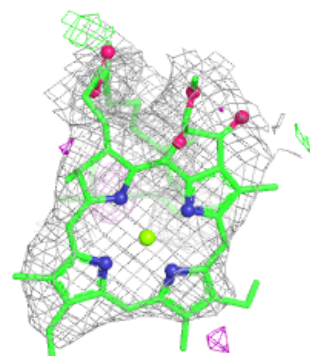
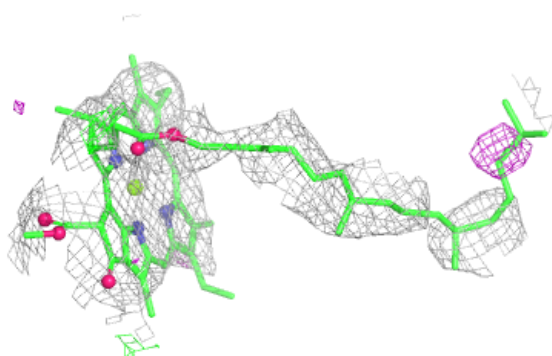
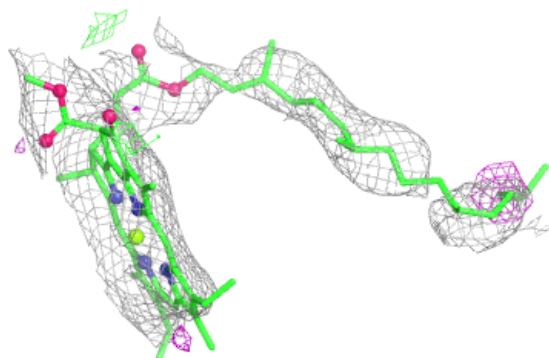


Electron density around PL9 A 353:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

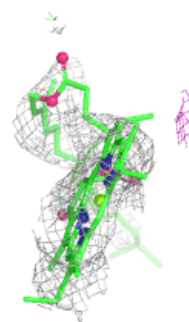
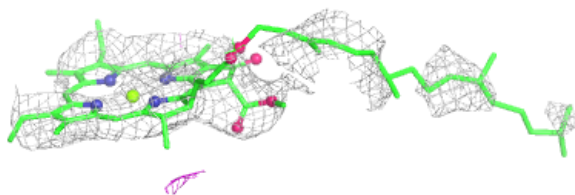
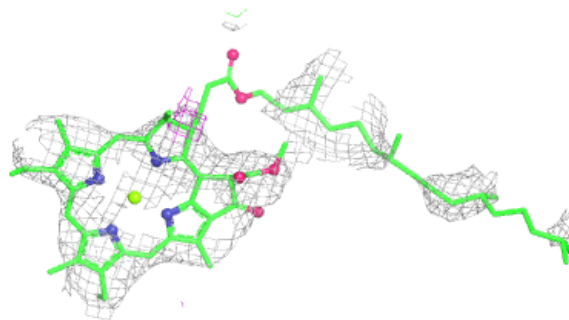
**Electron density around CLA B 523:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

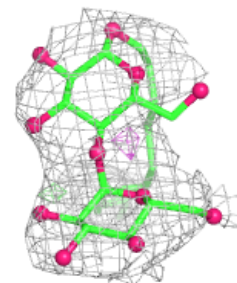
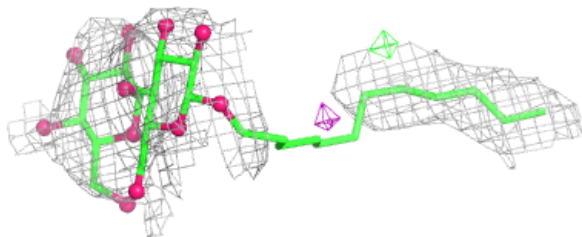
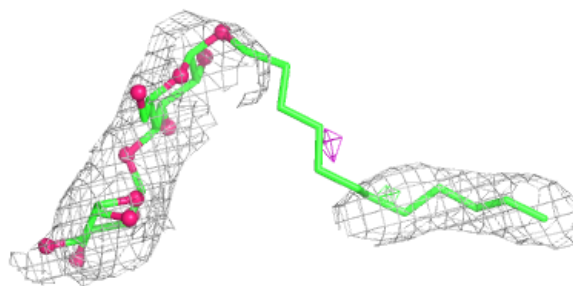


Electron density around CLA C 484:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

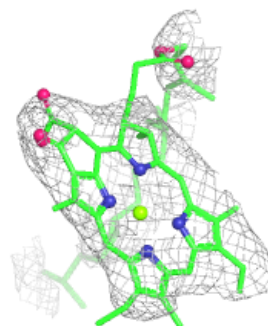
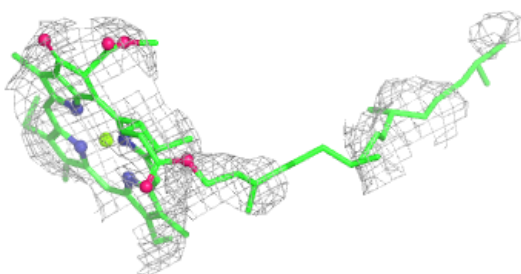
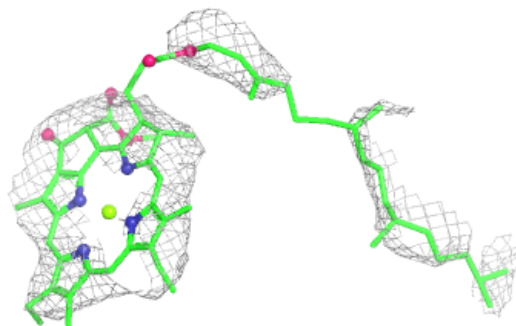
**Electron density around LMT B 526:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

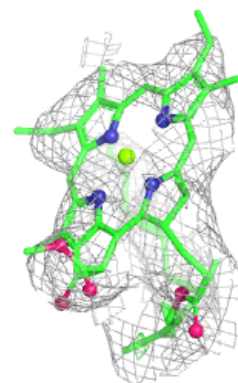
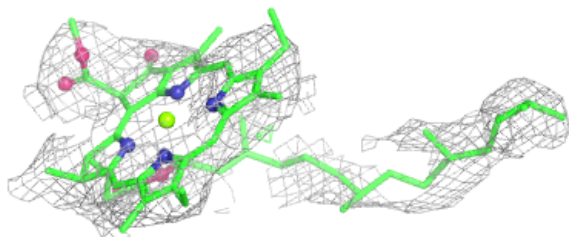
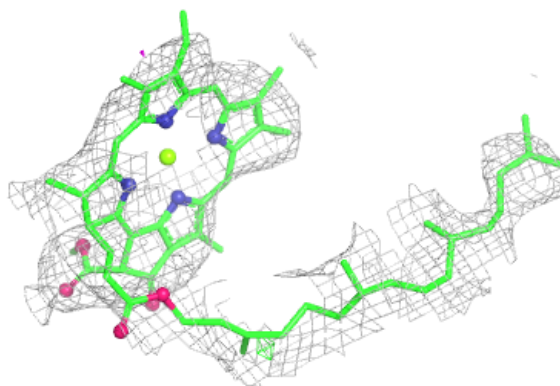


Electron density around CLA c 2482:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

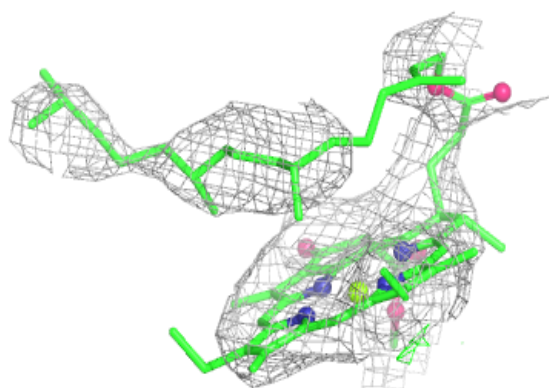
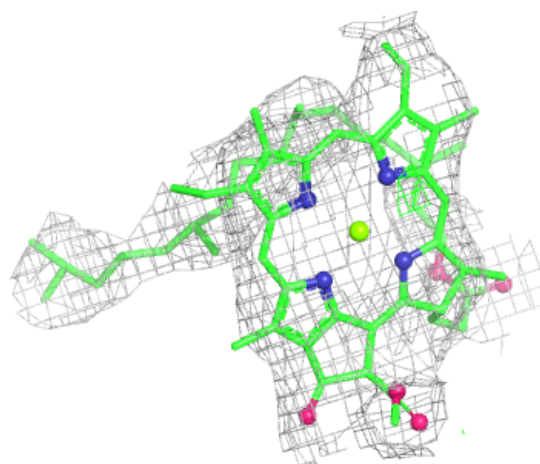
**Electron density around CLA C 477:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



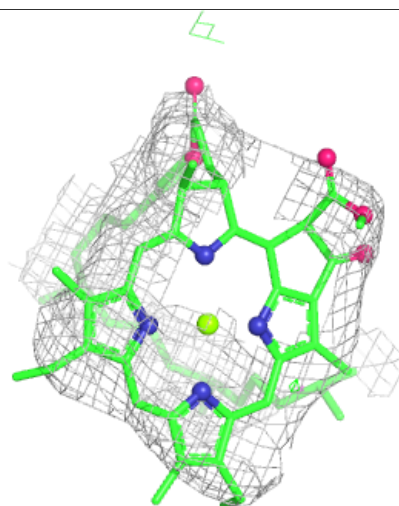
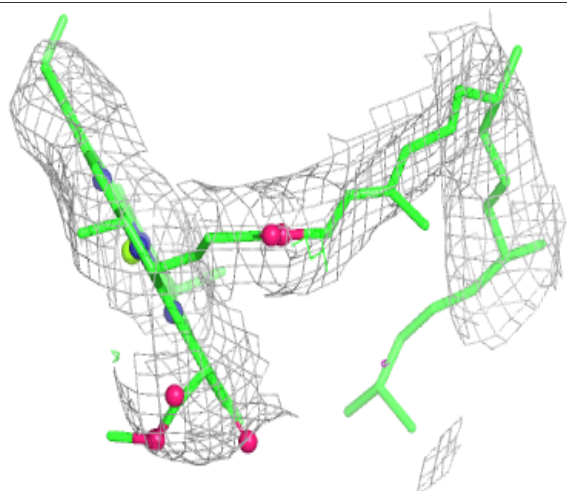
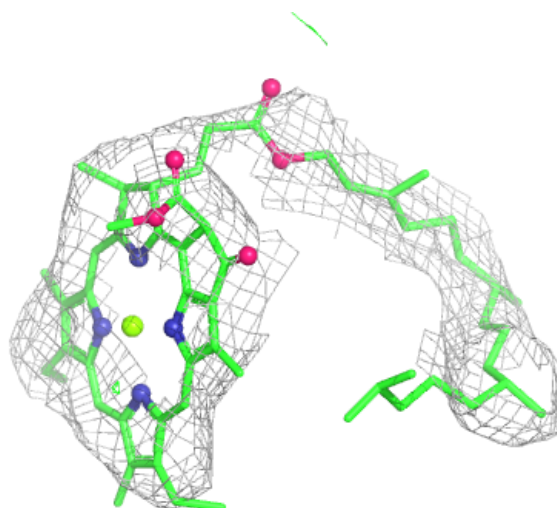
Electron density around CLA b 2525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



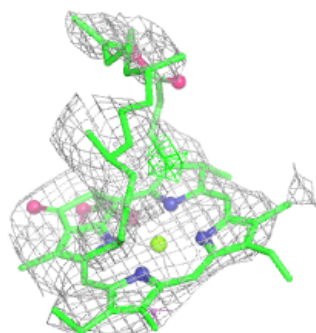
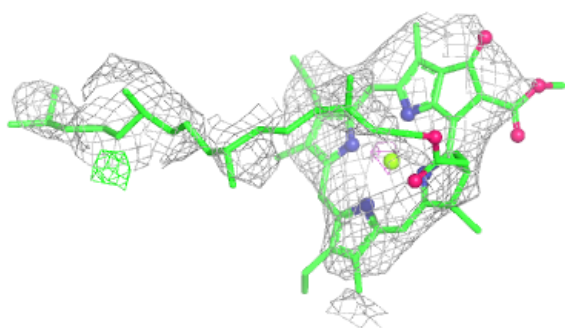
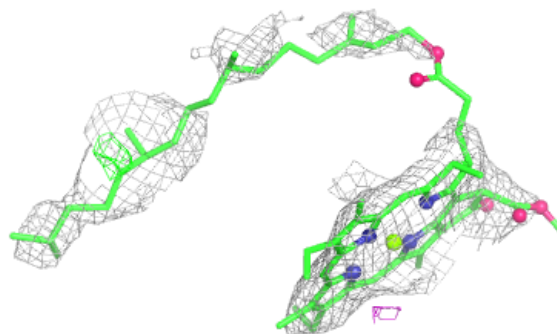
Electron density around CLA c 2480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

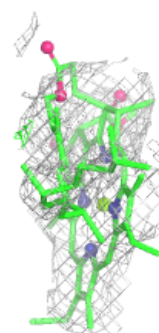
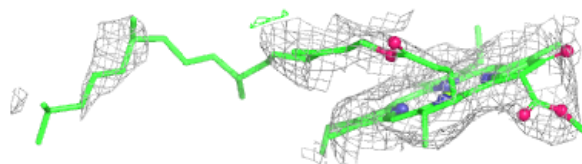
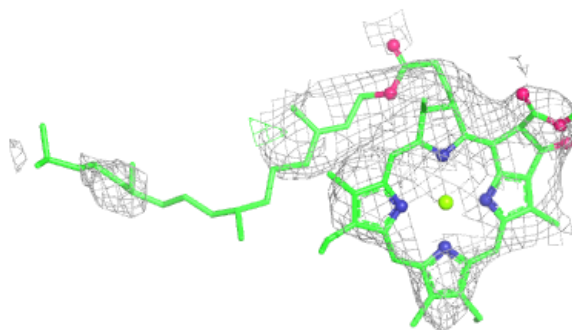


Electron density around CLA c 2474:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

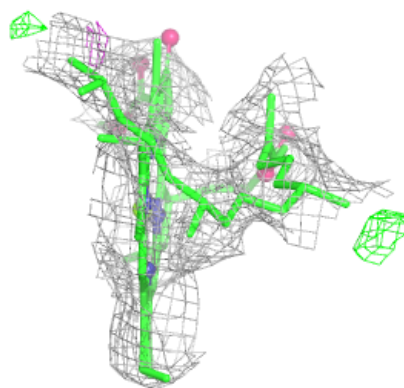
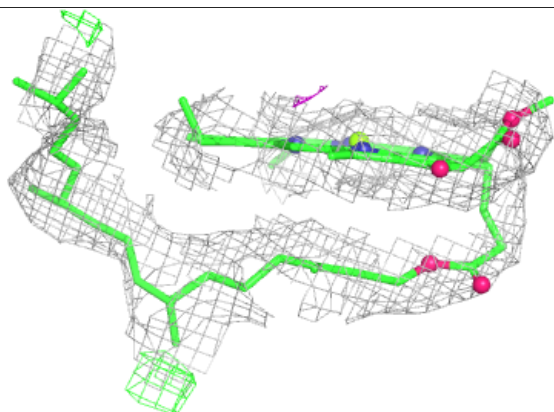
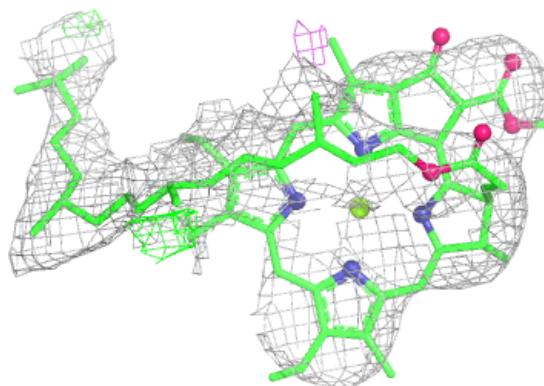
**Electron density around CLA b 2517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

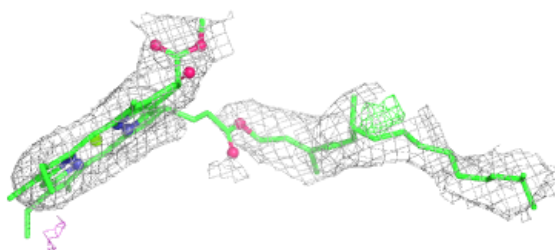
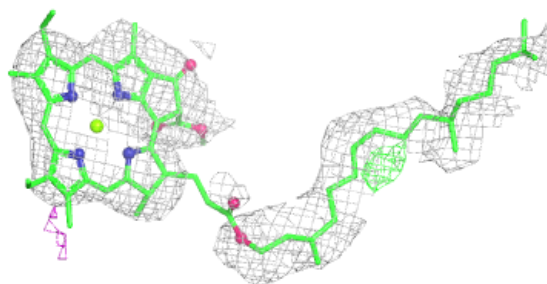


Electron density around CLA B 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

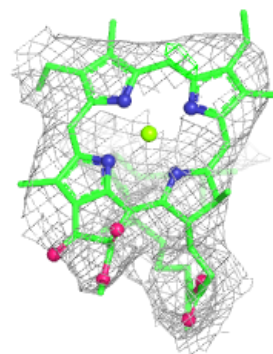
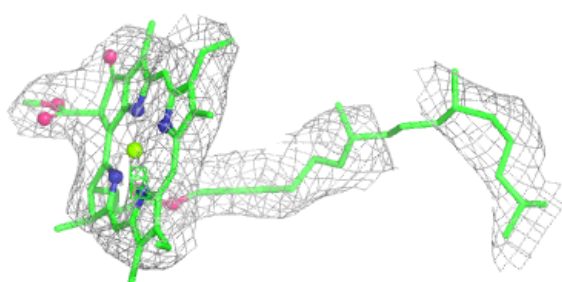
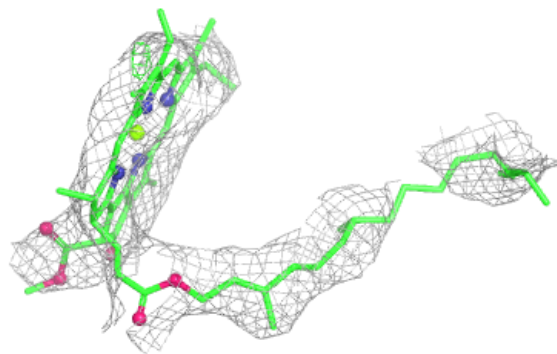
**Electron density around CLA A 352:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

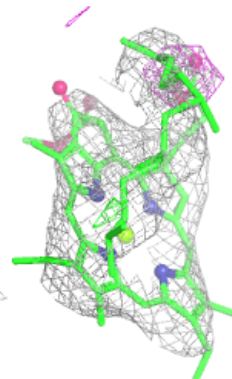
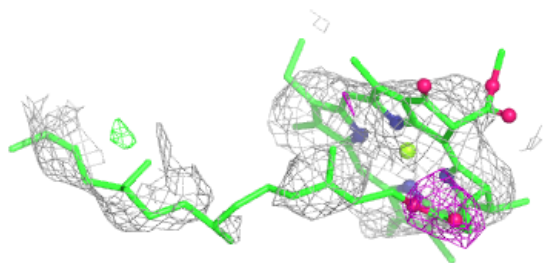
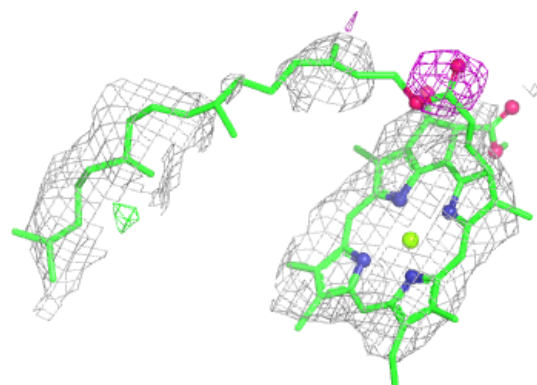


Electron density around CLA b 2523:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

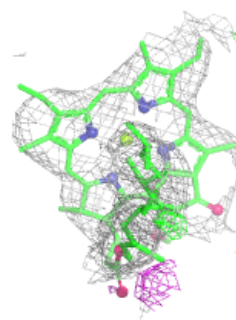
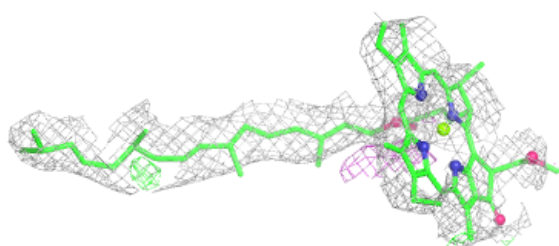
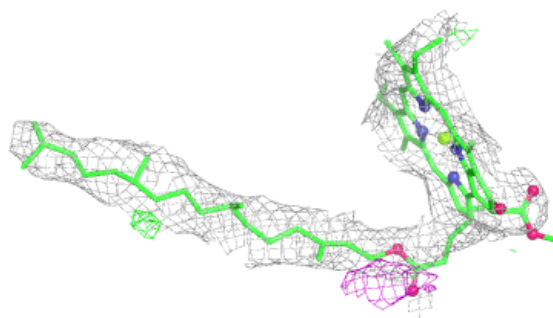
**Electron density around CLA c 2477:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

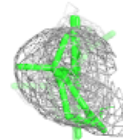
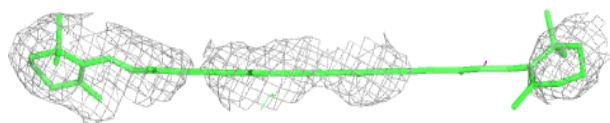
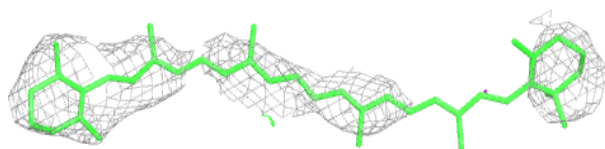


Electron density around CLA B 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

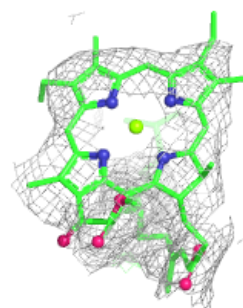
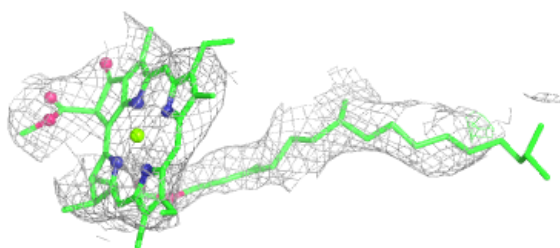
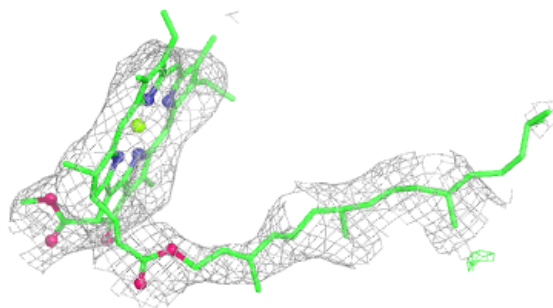
**Electron density around BCR B 528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

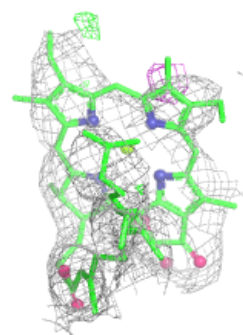
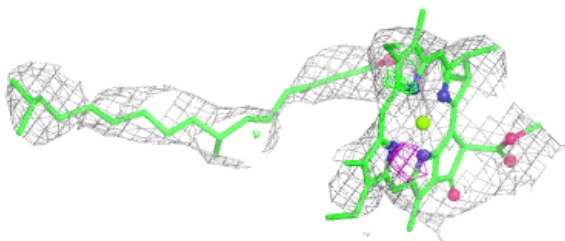
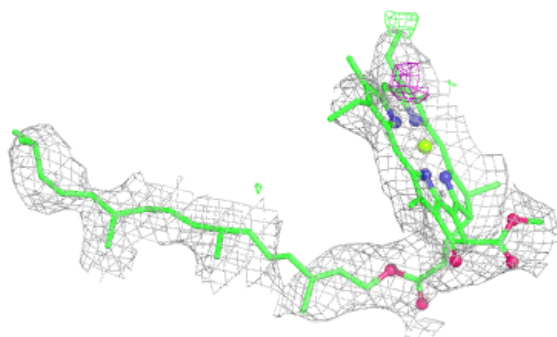


Electron density around CLA C 483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

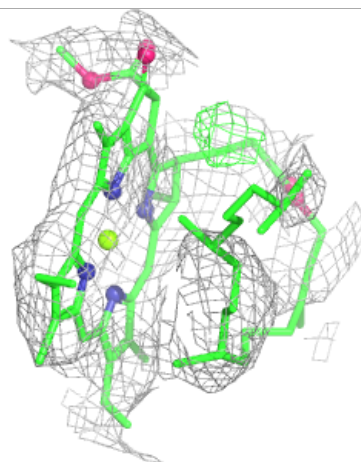
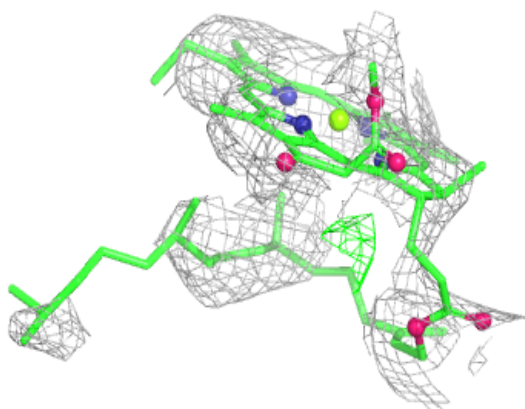
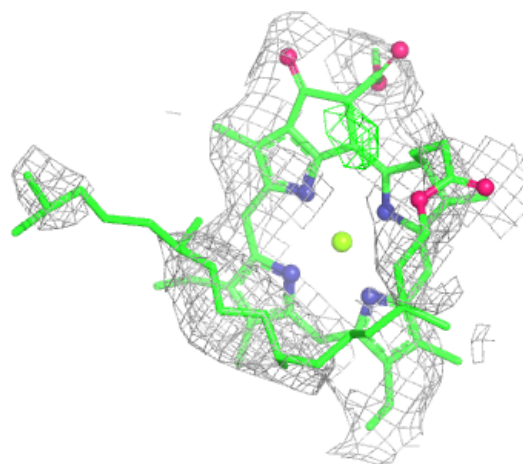
**Electron density around CLA c 2483:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



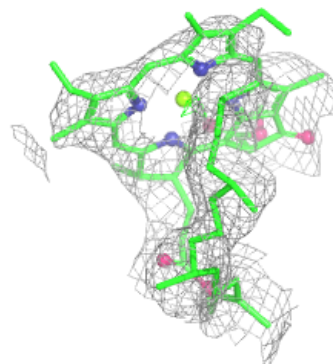
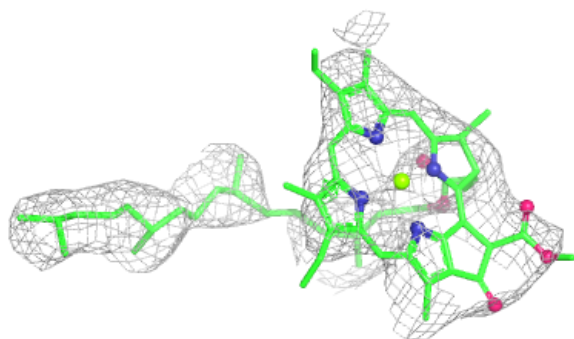
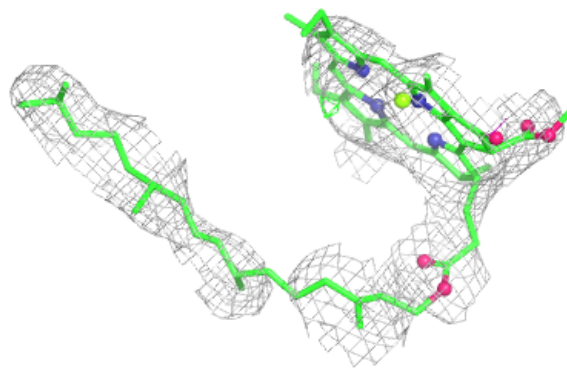
Electron density around CLA B 525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



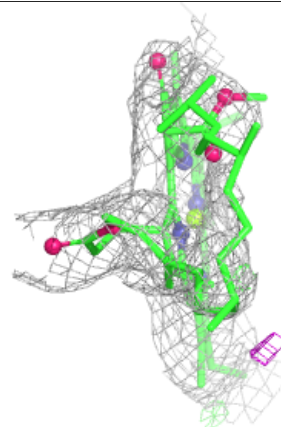
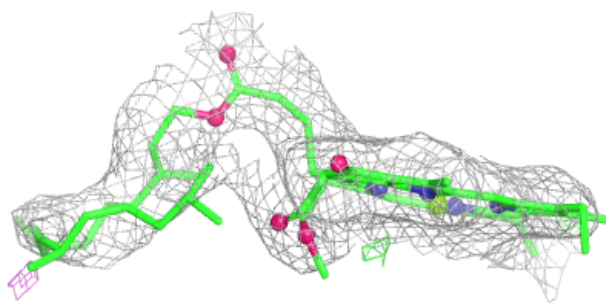
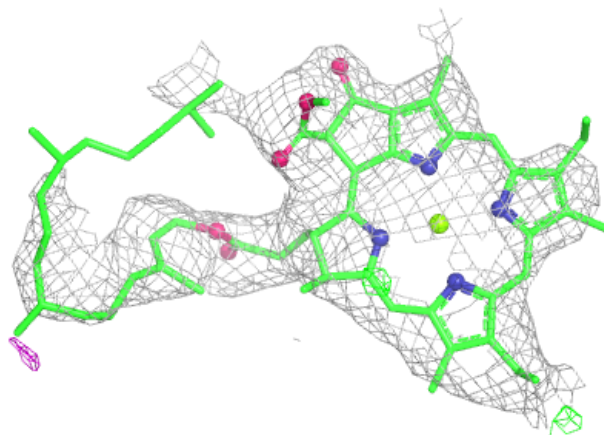
Electron density around CLA C 474:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



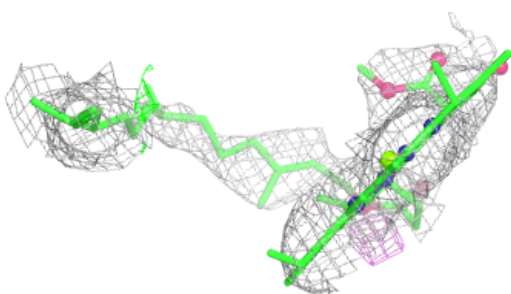
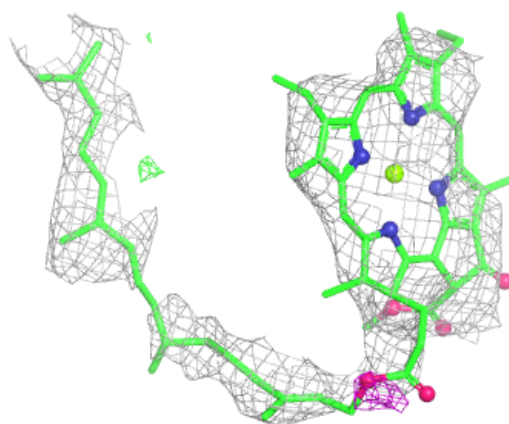
Electron density around CLA b 2513:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

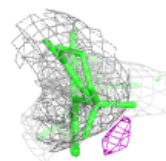
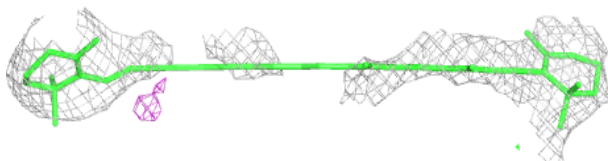
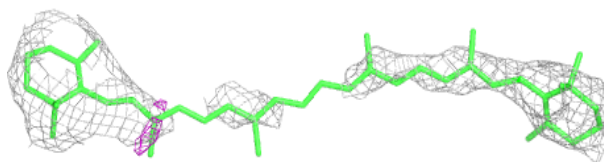


Electron density around CLA C 485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

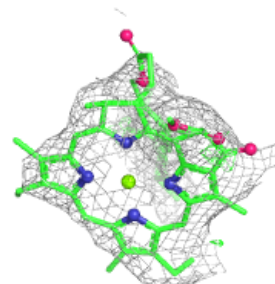
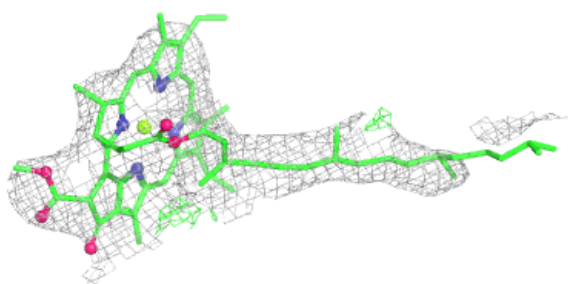
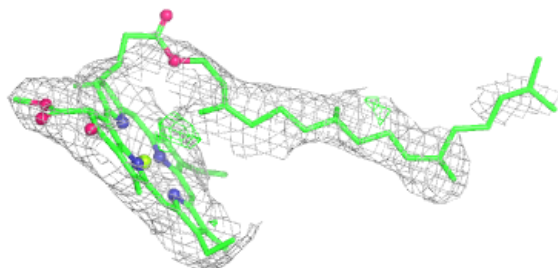
**Electron density around BCR b 2527:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

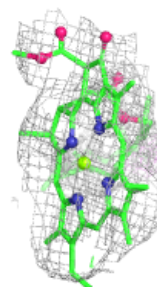
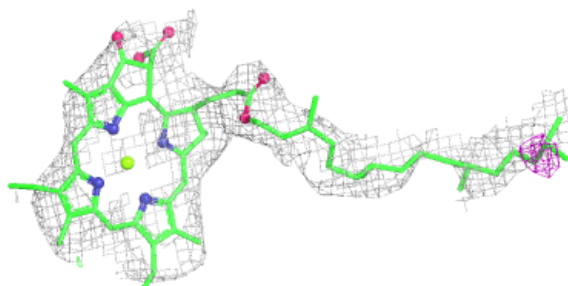


Electron density around CLA B 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

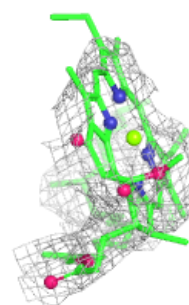
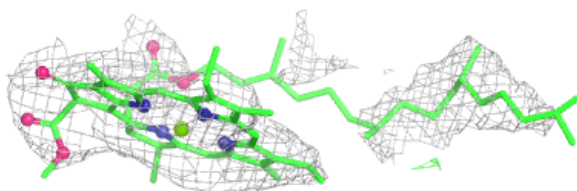
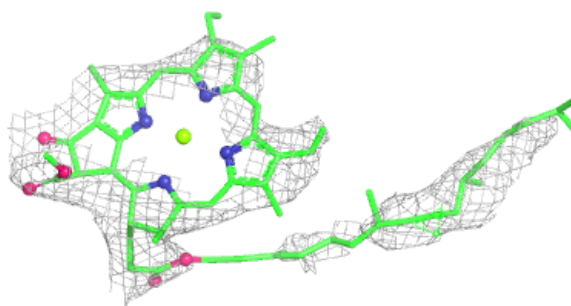
**Electron density around CLA a 2349:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

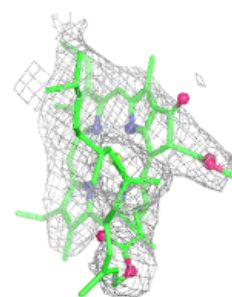
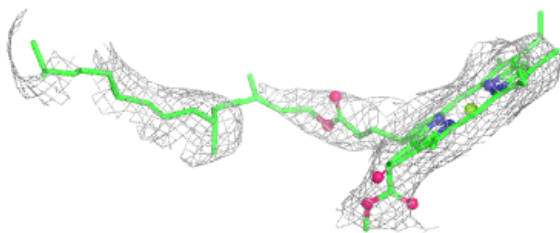
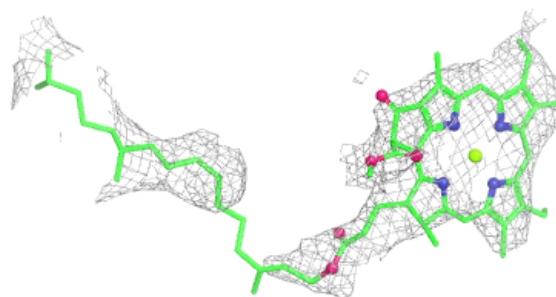


Electron density around CLA c 2479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

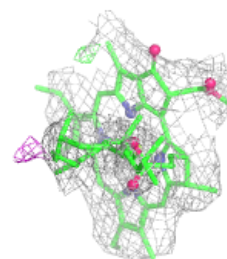
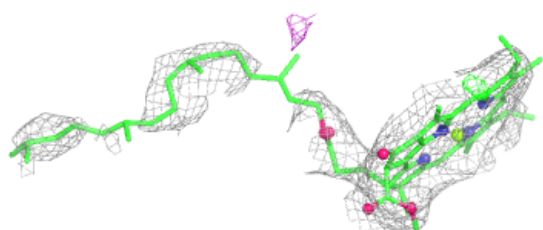
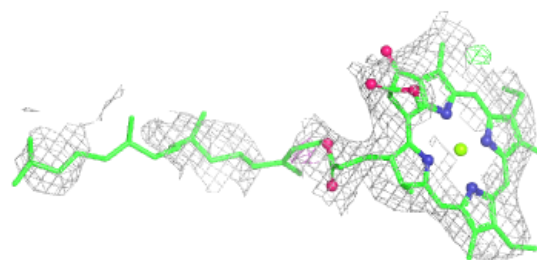
**Electron density around CLA a 2351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

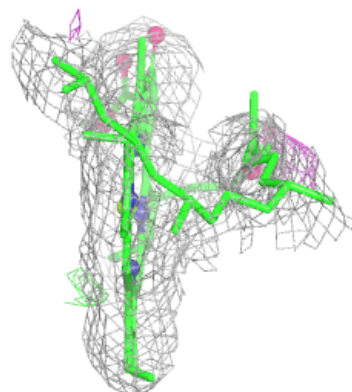
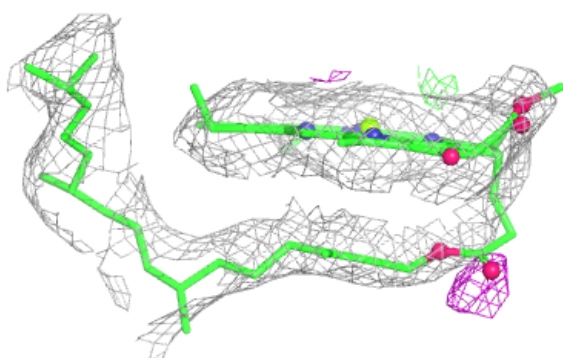
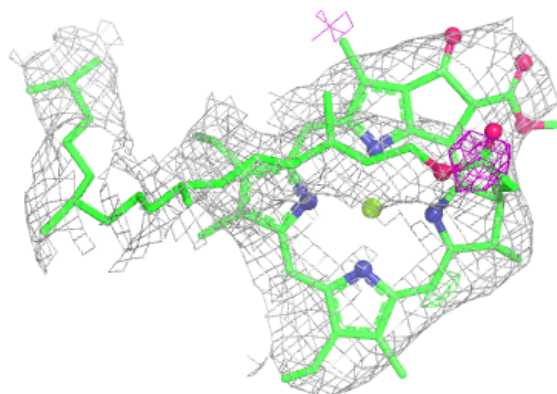


Electron density around CLA c 2481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

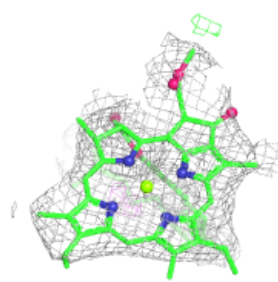
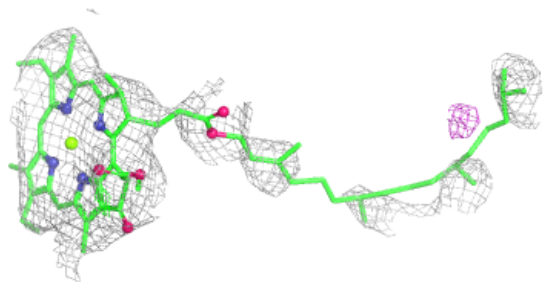
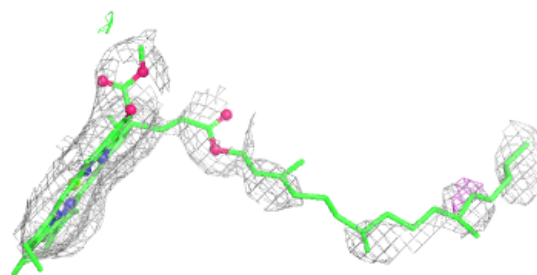
**Electron density around CLA b 2520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



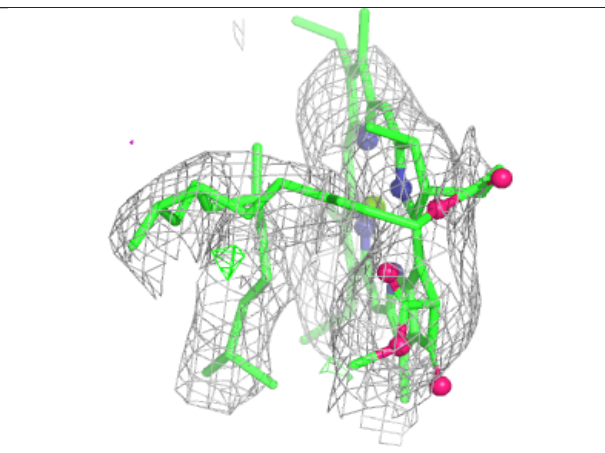
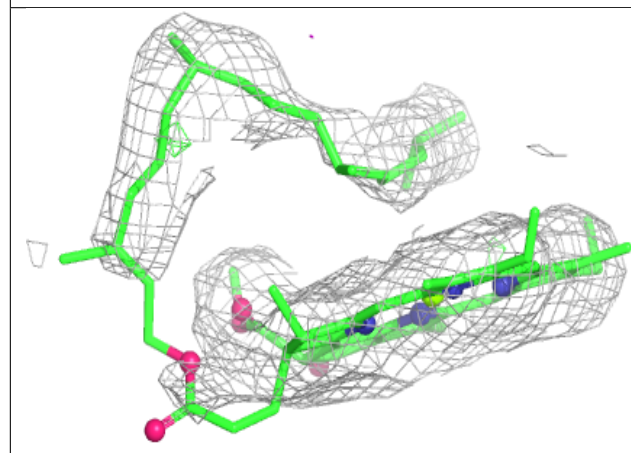
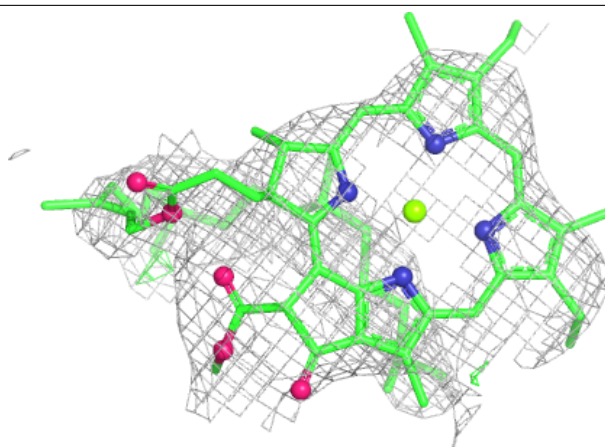
Electron density around CLA B 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



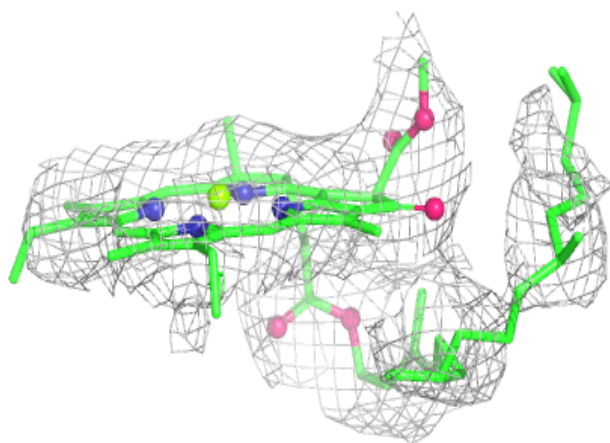
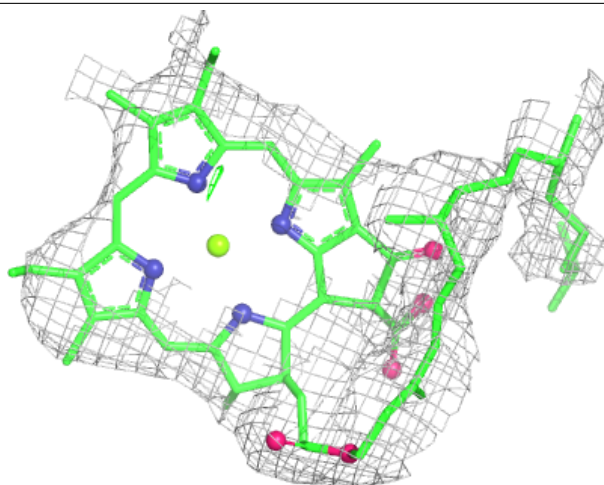
Electron density around CLA c 2476:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



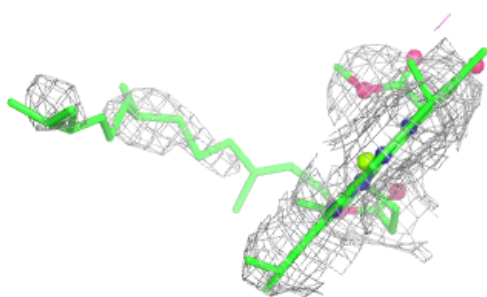
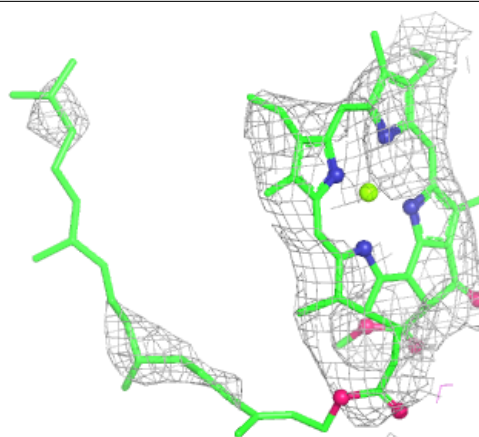
Electron density around CLA B 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



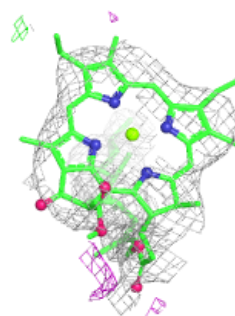
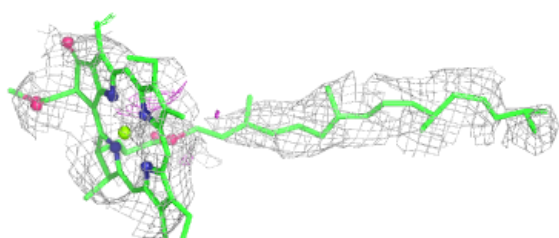
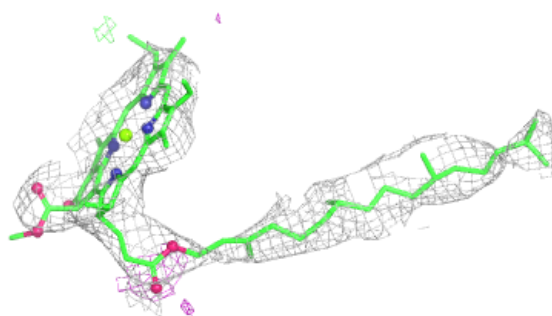
Electron density around CLA c 2485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

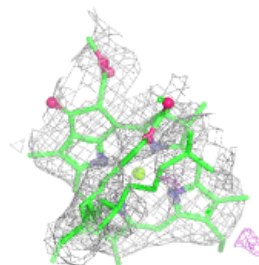
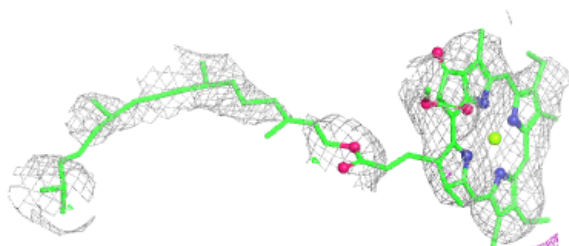
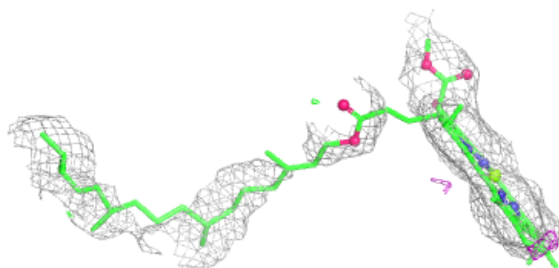


Electron density around CLA b 2514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

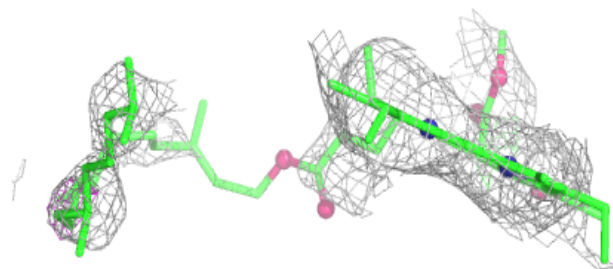
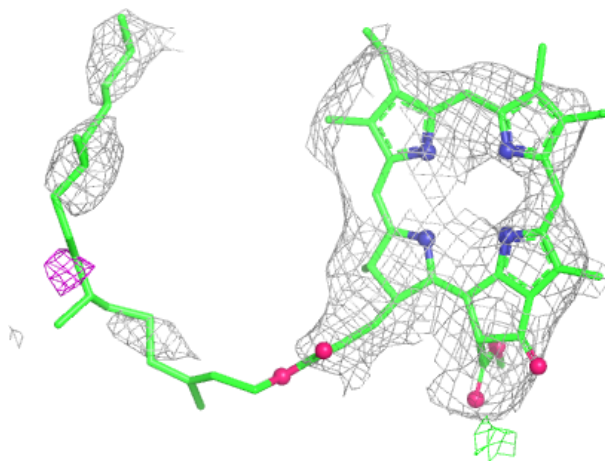
**Electron density around CLA b 2516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



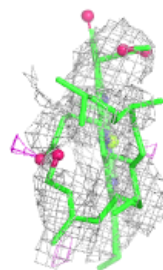
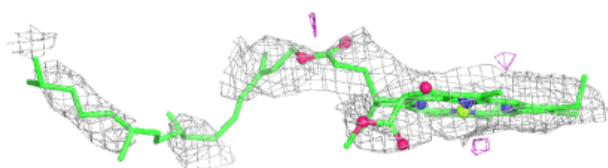
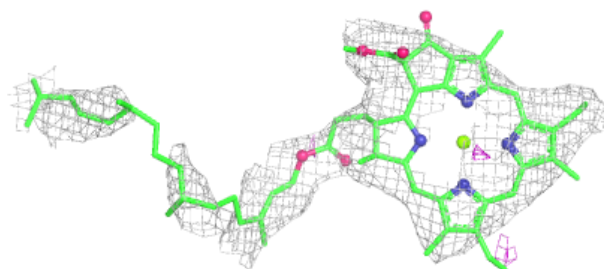
Electron density around PHO a 2350:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

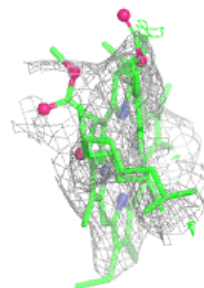
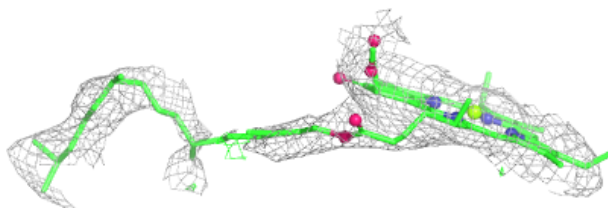
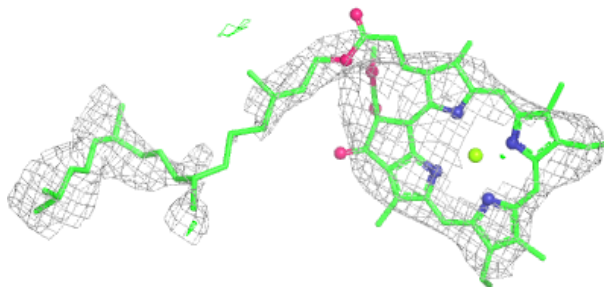


Electron density around CLA D 356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

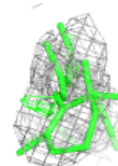
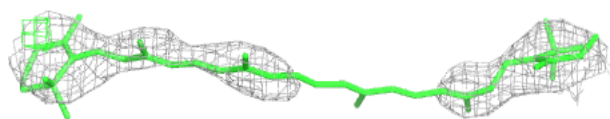
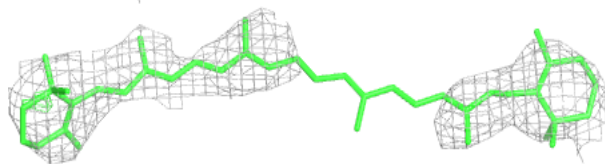
**Electron density around CLA b 2521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

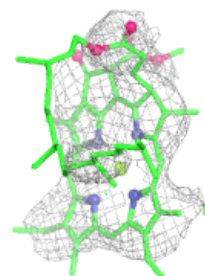
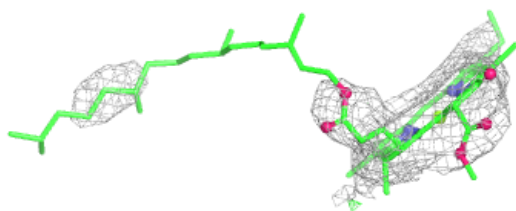
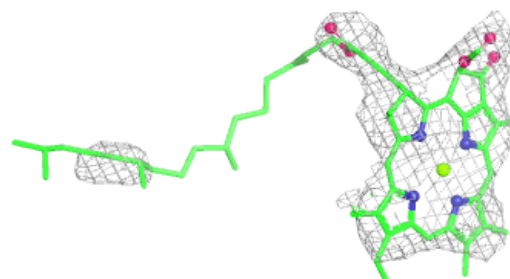


Electron density around BCR C 488:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

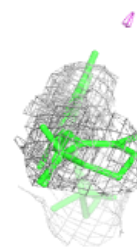
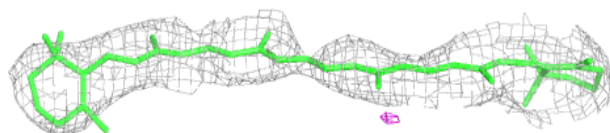
**Electron density around CLA C 486:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

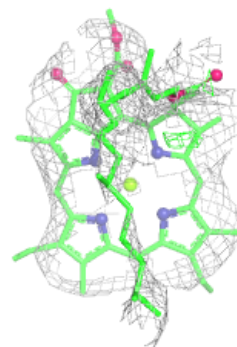
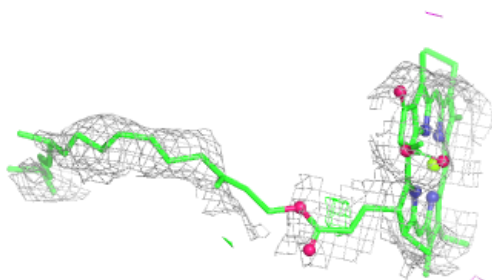


Electron density around BCR F 48:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

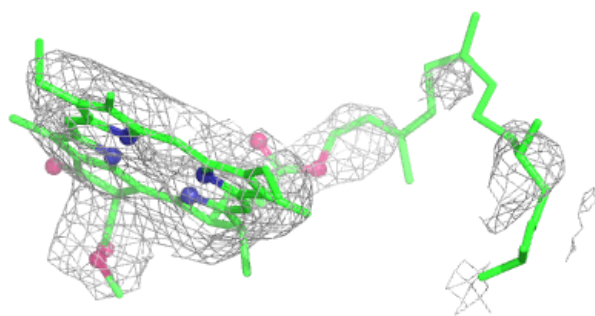
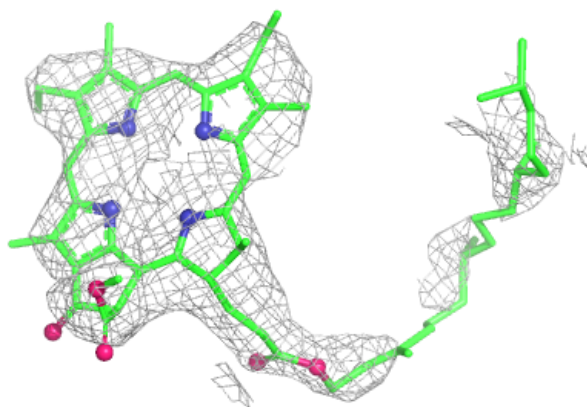
**Electron density around CLA C 475:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



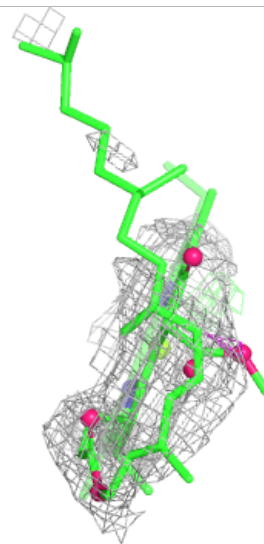
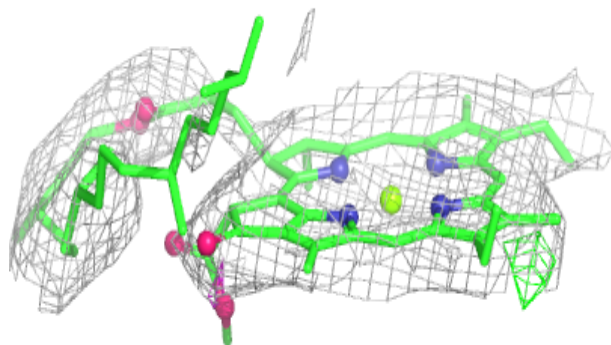
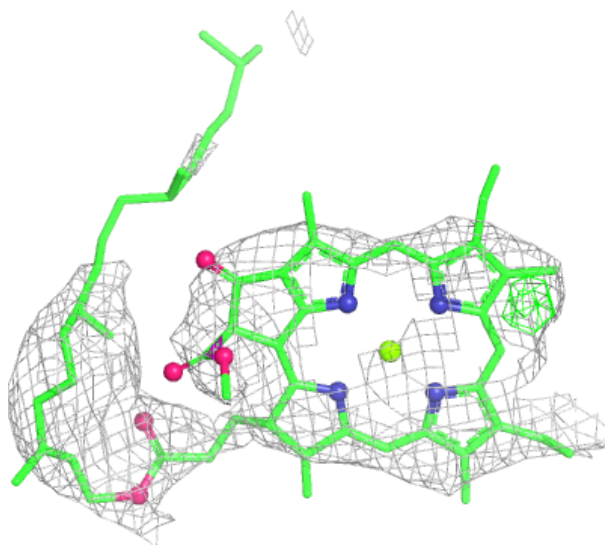
Electron density around PHO D 355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



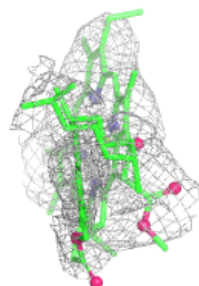
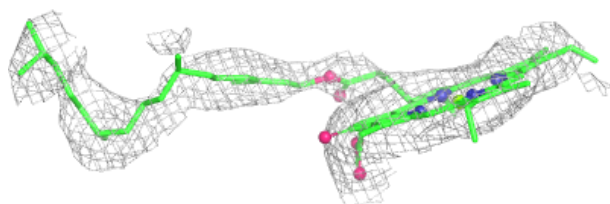
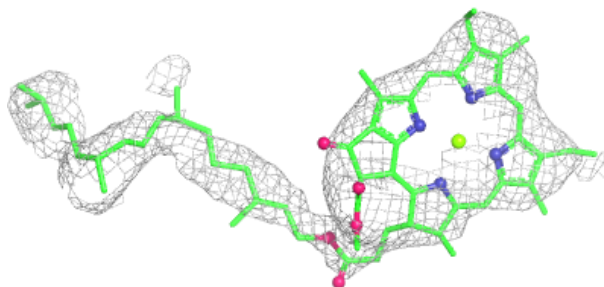
Electron density around CLA B 524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

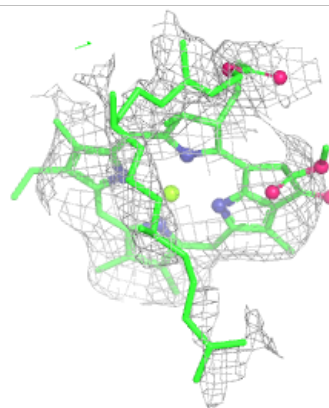
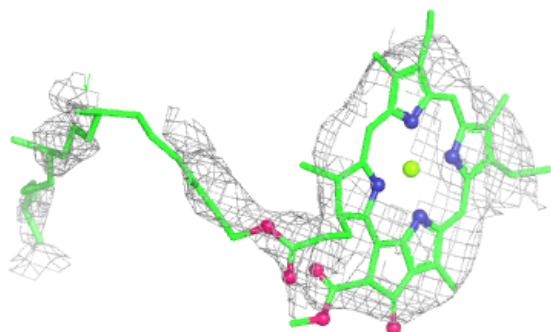
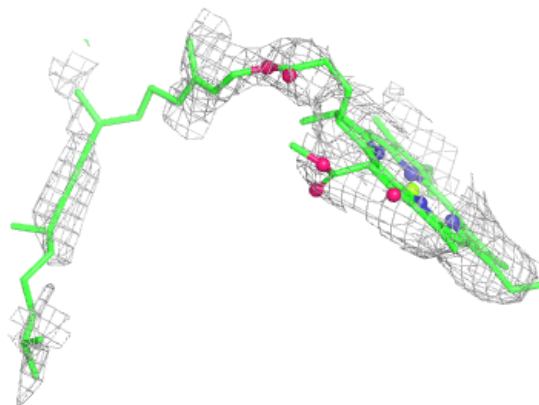


Electron density around CLA B 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

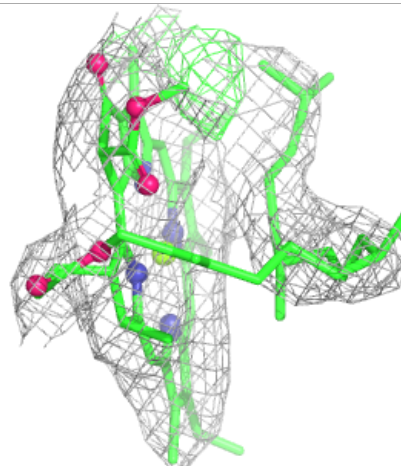
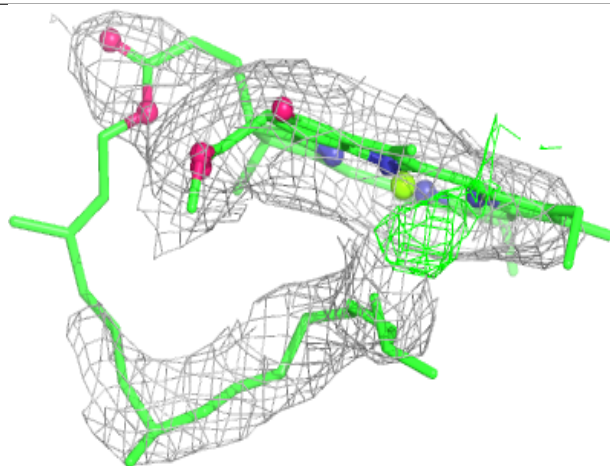
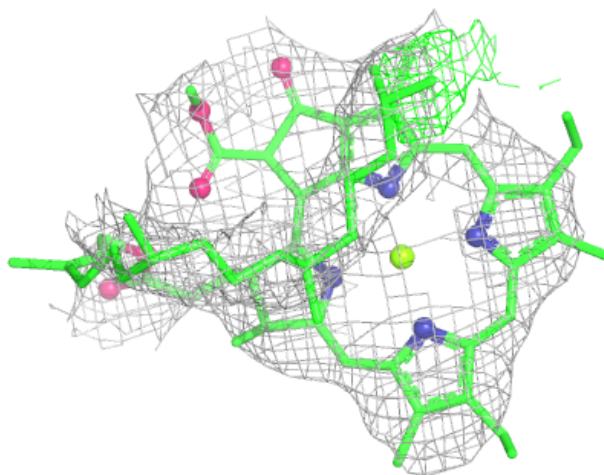
**Electron density around CLA b 2522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



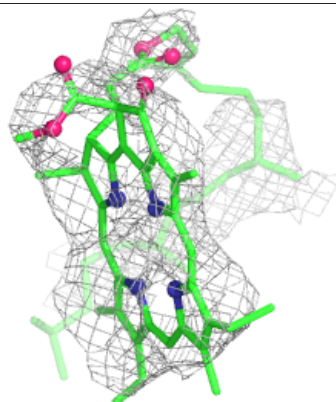
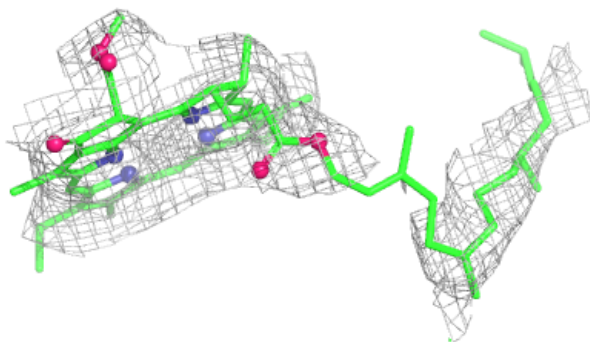
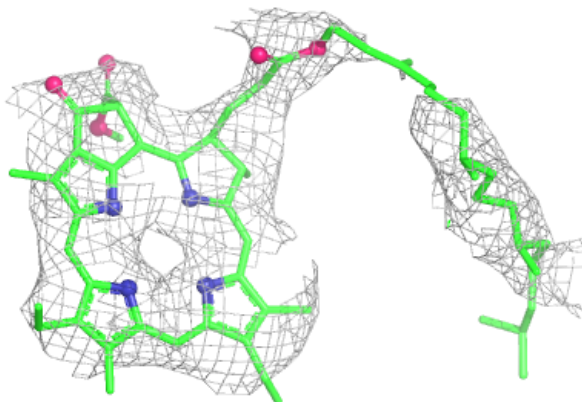
Electron density around CLA C 476:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



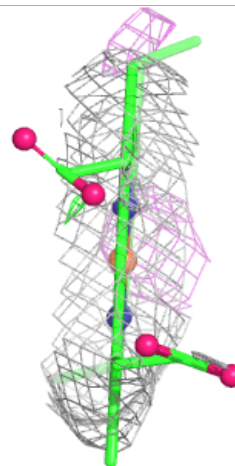
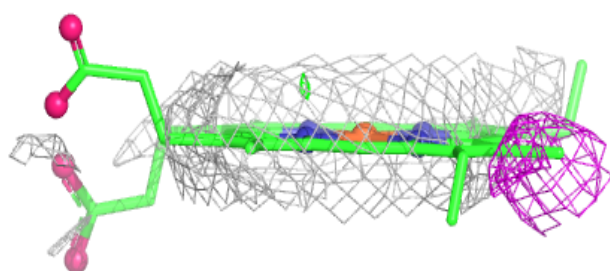
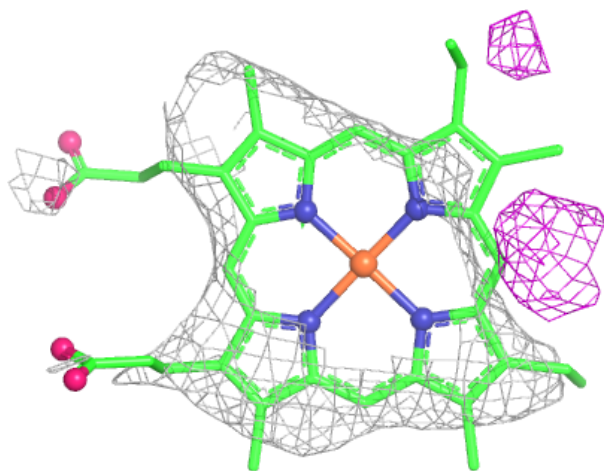
Electron density around PHO d 2356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



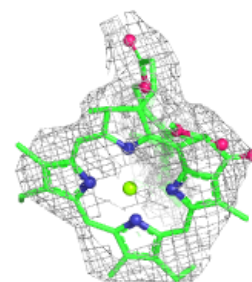
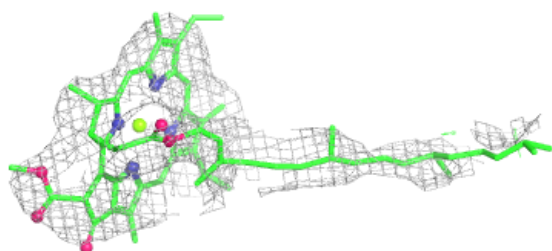
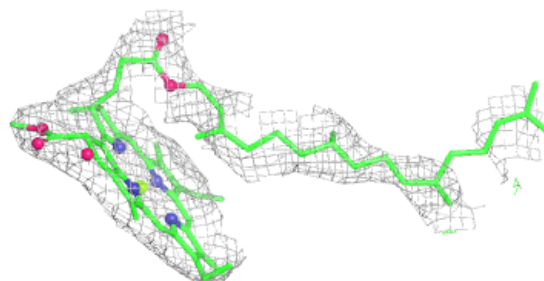
Electron density around HEC e 2084:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



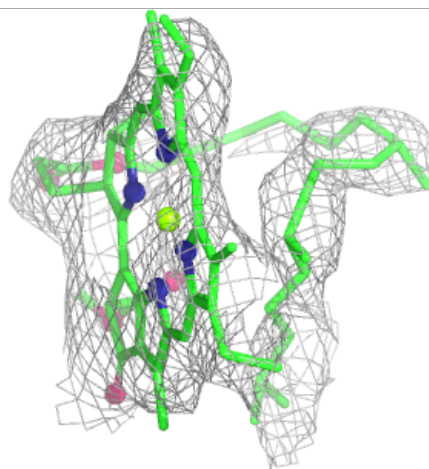
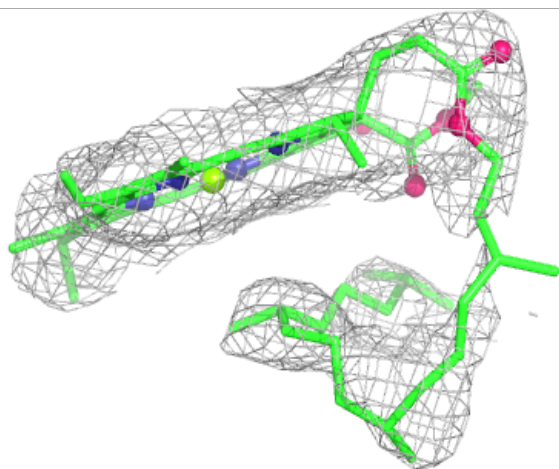
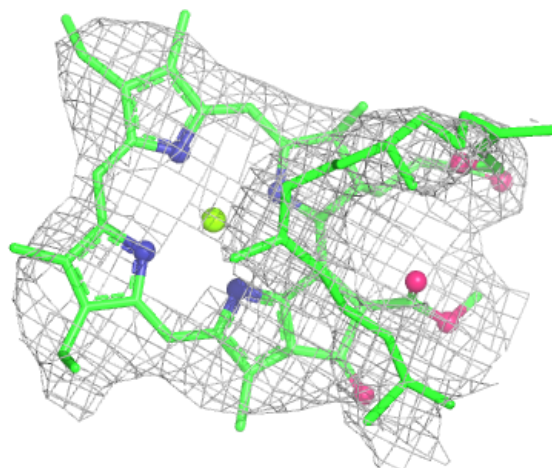
Electron density around CLA b 2519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



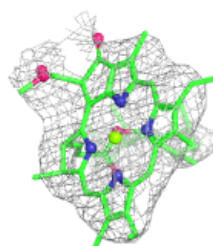
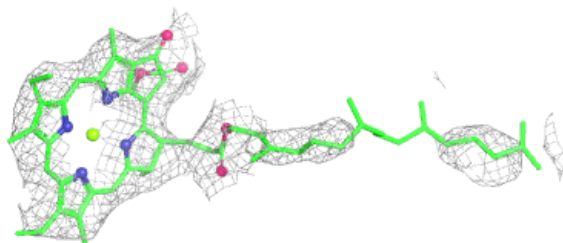
Electron density around CLA B 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

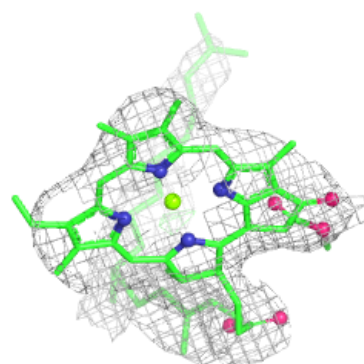
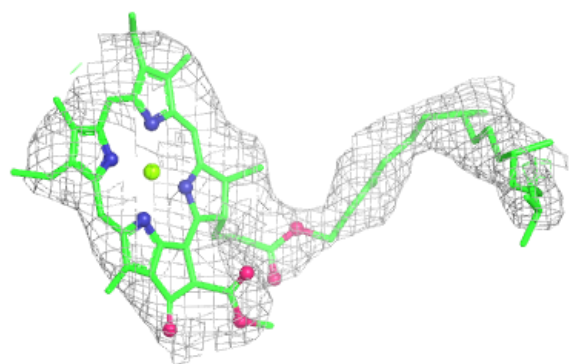
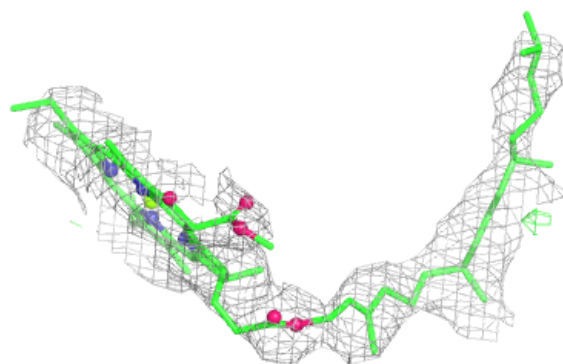


Electron density around CLA C 481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

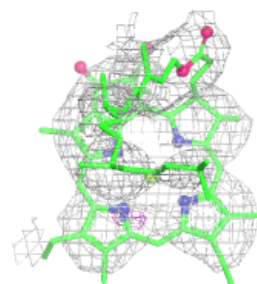
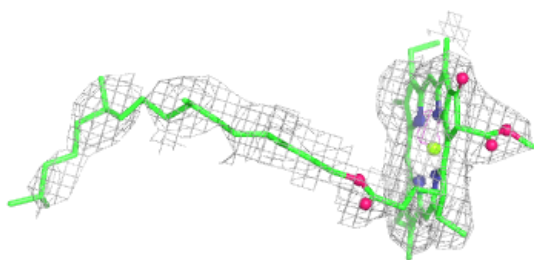
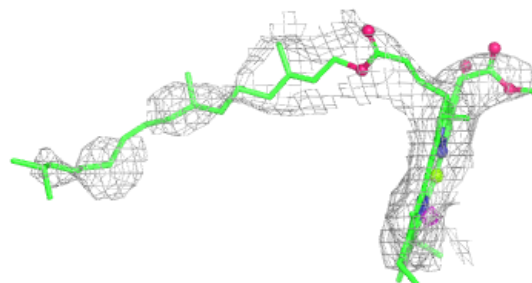
**Electron density around CLA B 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

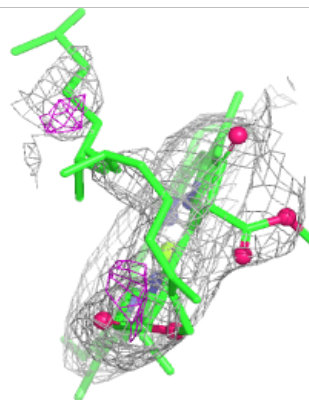
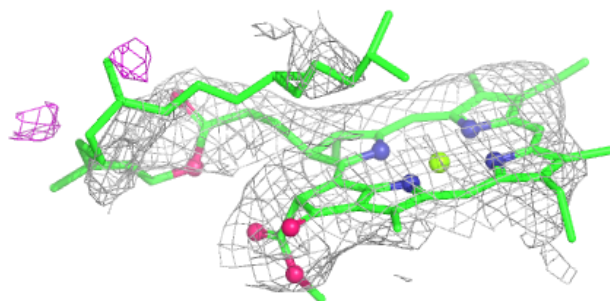
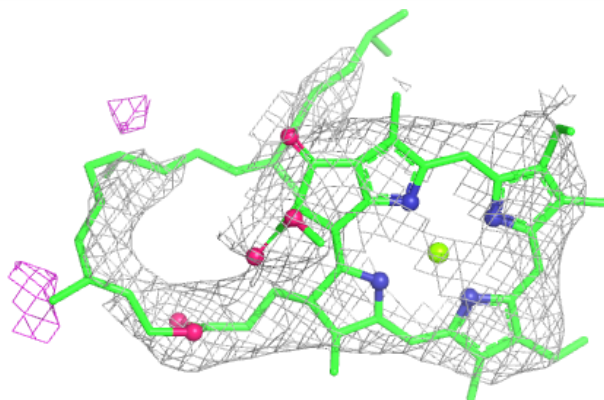


Electron density around CLA B 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

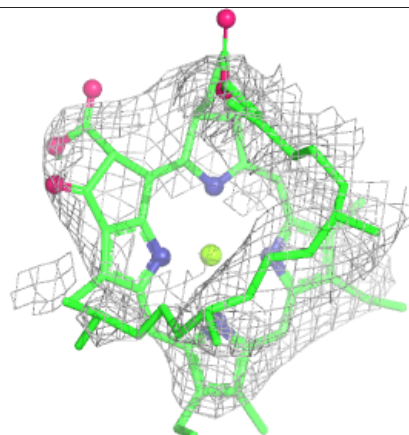
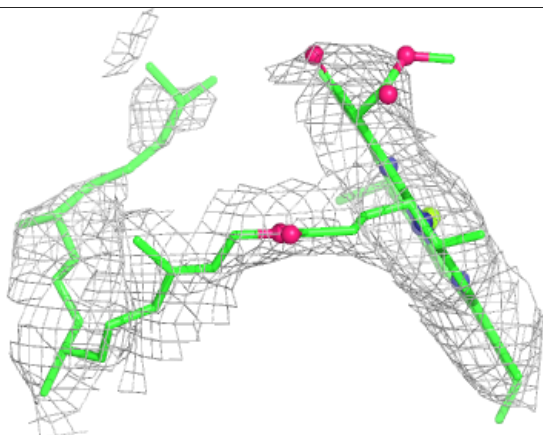
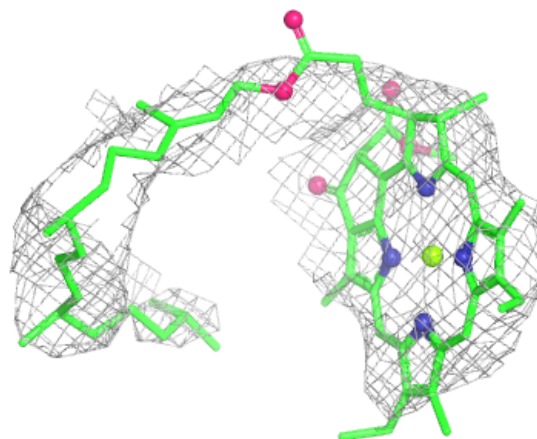
**Electron density around CLA c 2478:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



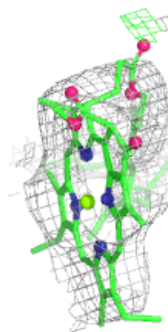
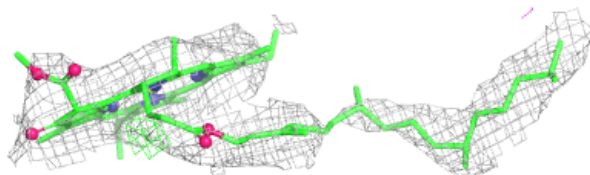
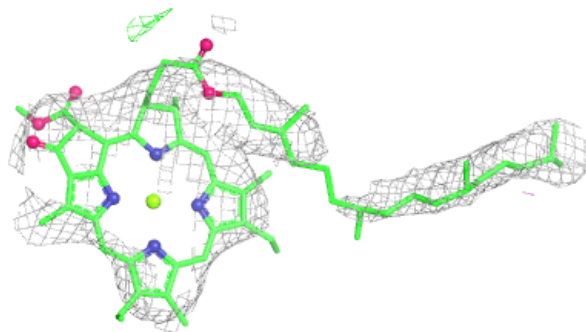
Electron density around CLA C 480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

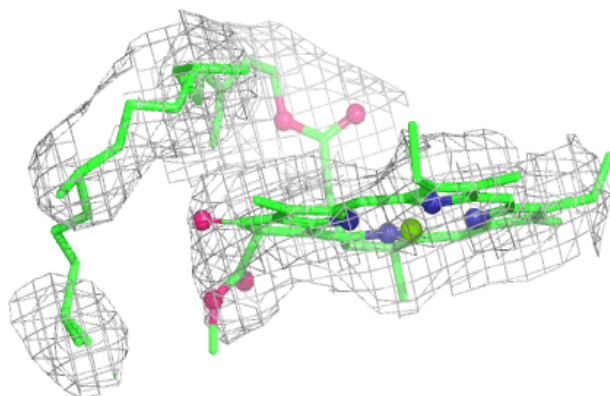
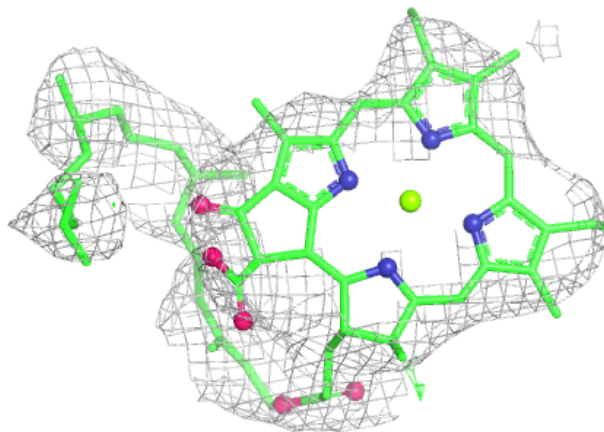


Electron density around CLA B 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

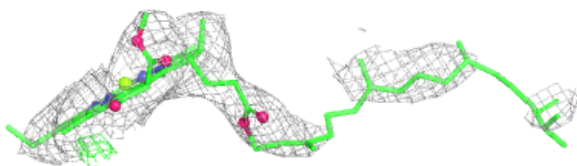
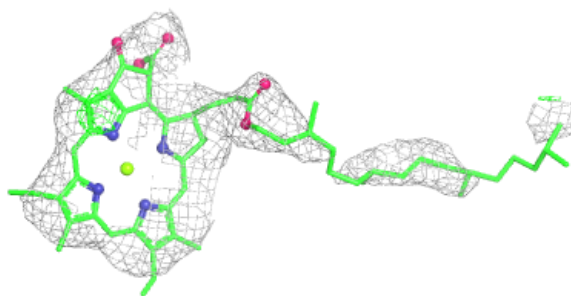
**Electron density around CLA b 2515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



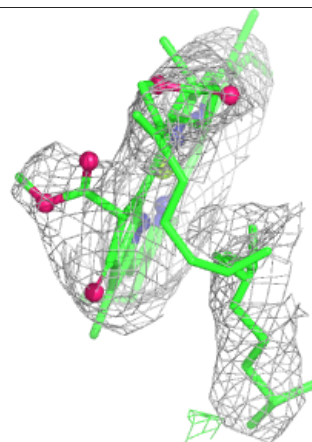
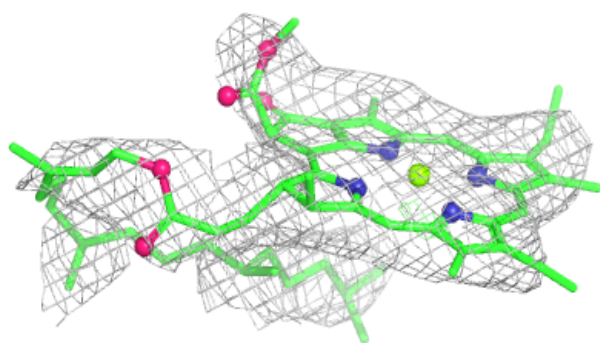
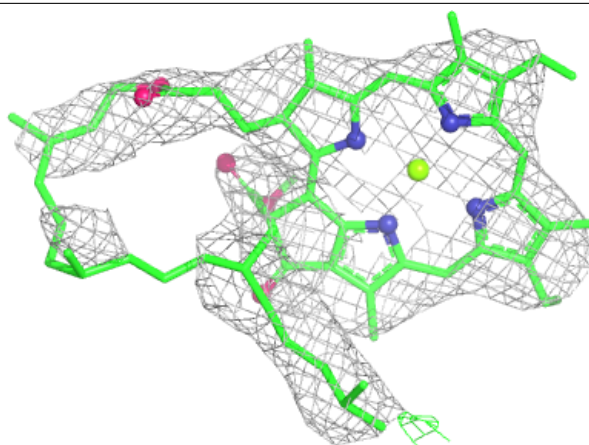
Electron density around CLA A 350:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



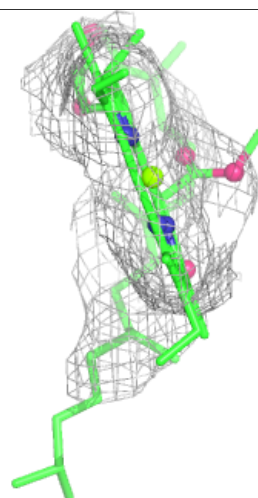
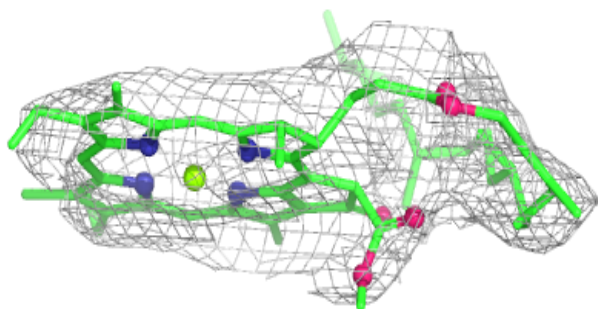
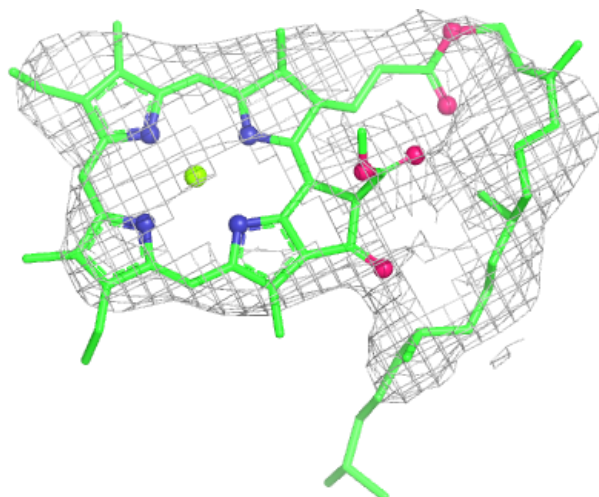
Electron density around CLA C 478:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



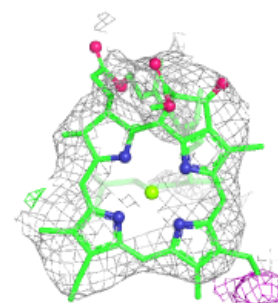
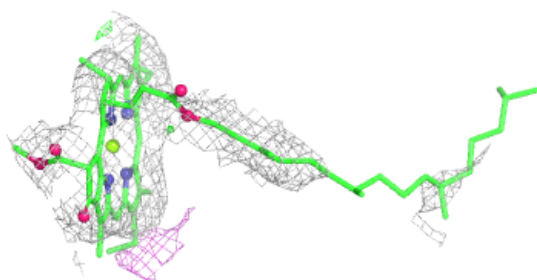
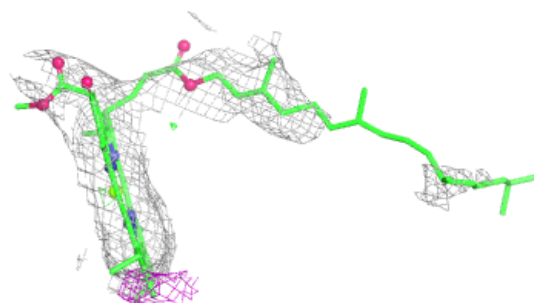
Electron density around CLA b 2524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



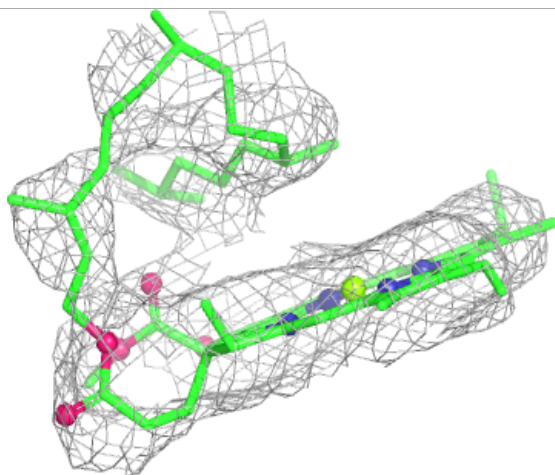
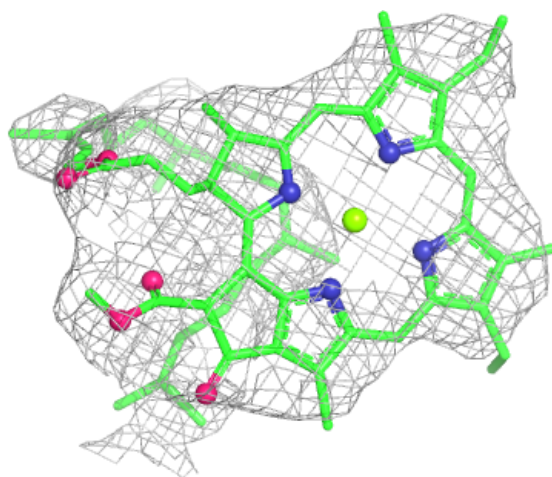
Electron density around CLA b 2518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



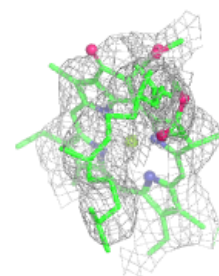
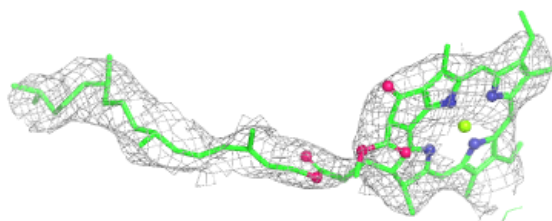
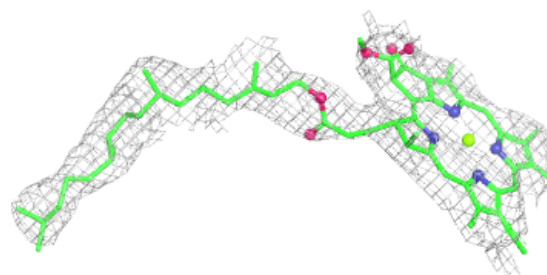
Electron density around CLA b 2512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

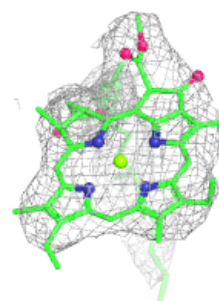
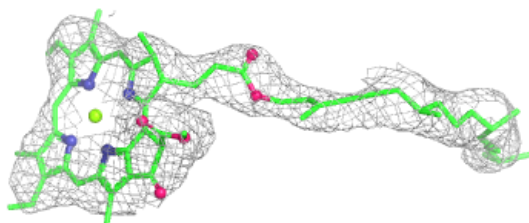
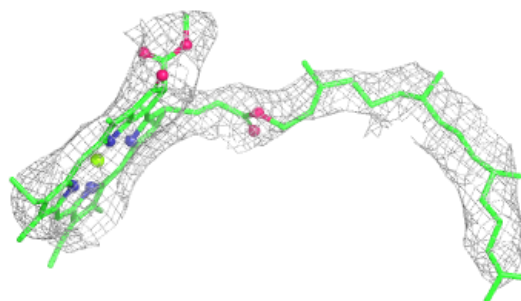


Electron density around CLA A 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

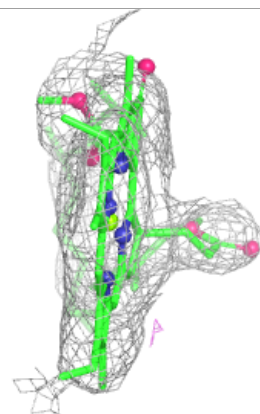
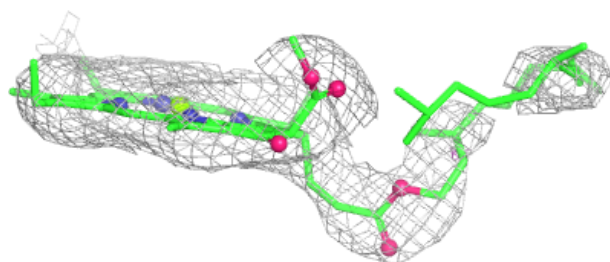
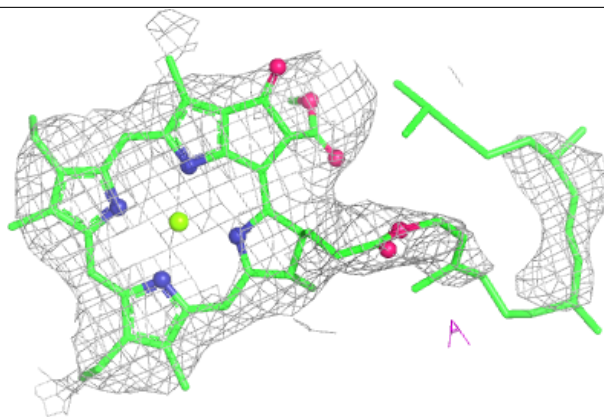
**Electron density around CLA d 2354:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

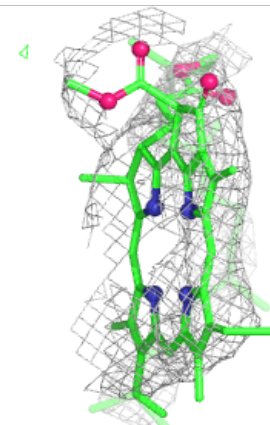
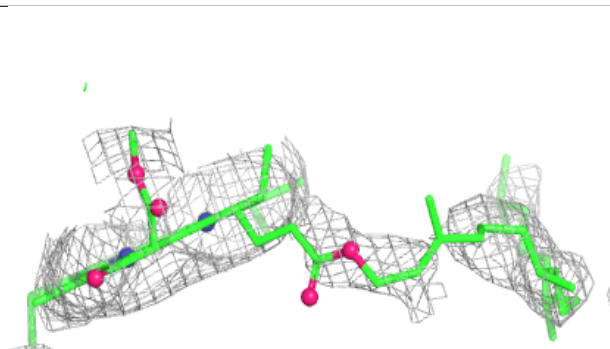
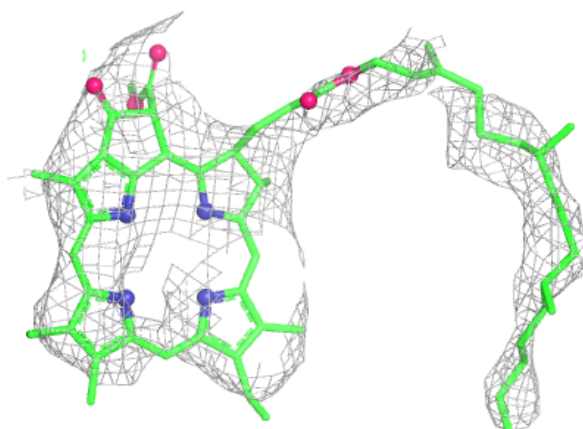


Electron density around CLA B 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

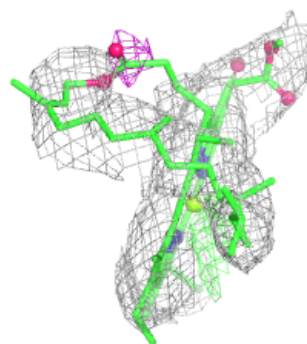
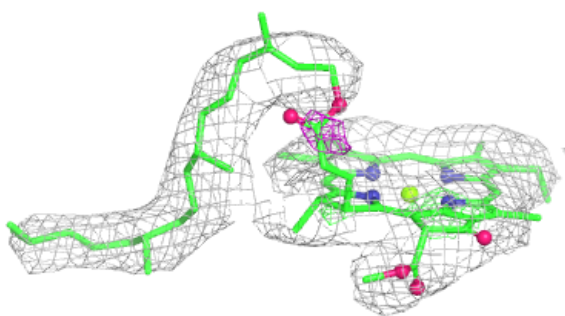
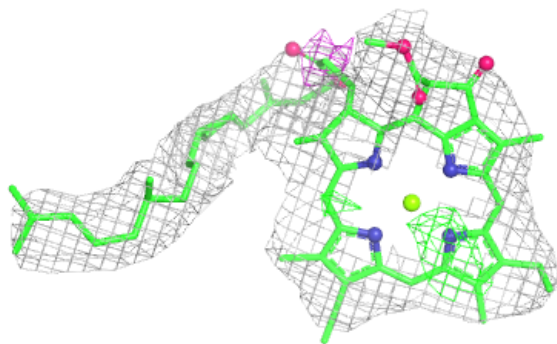
**Electron density around PHO A 351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

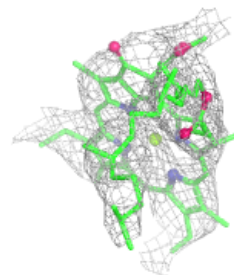
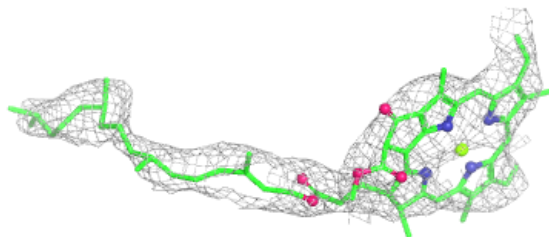
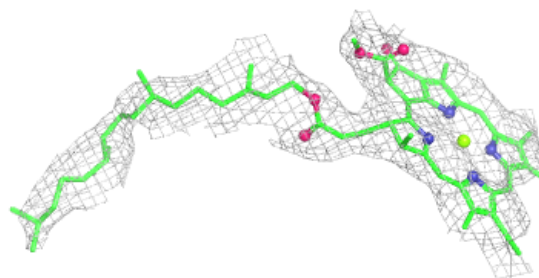


Electron density around CLA d 2355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

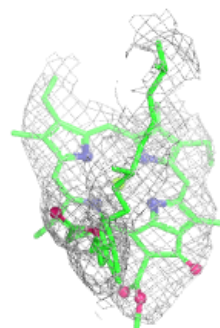
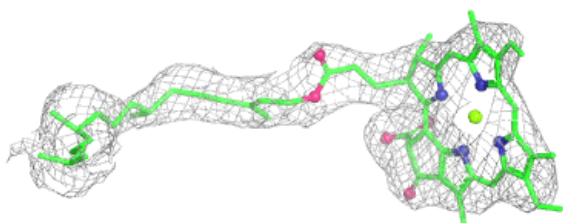
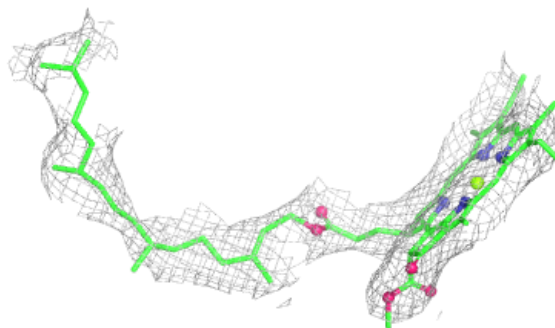
**Electron density around CLA a 2348:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

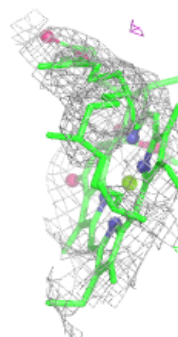
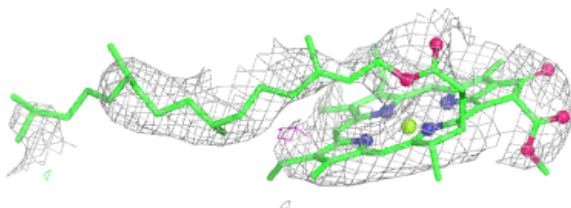
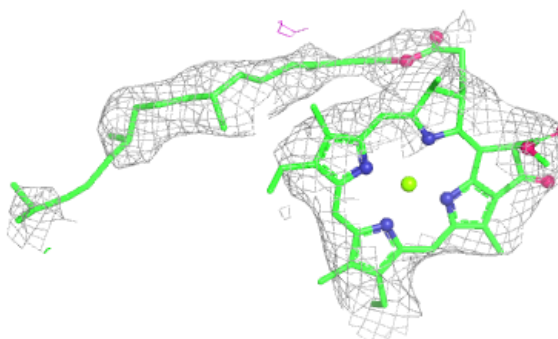


Electron density around CLA D 354:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

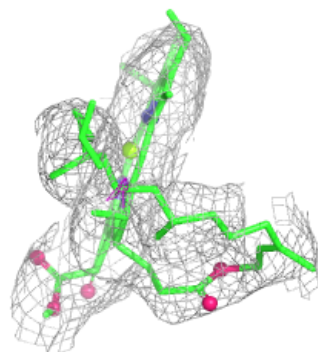
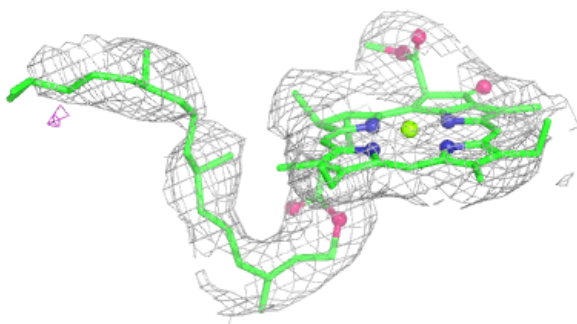
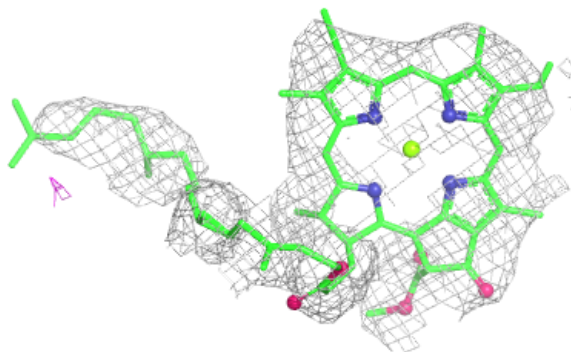
**Electron density around CLA C 479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



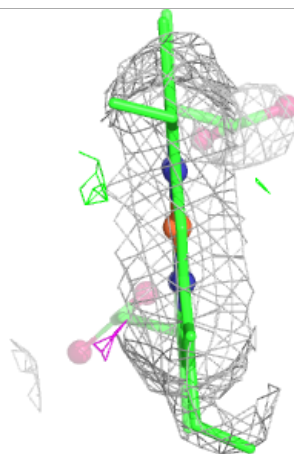
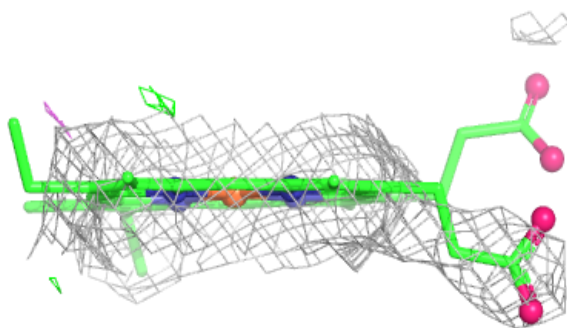
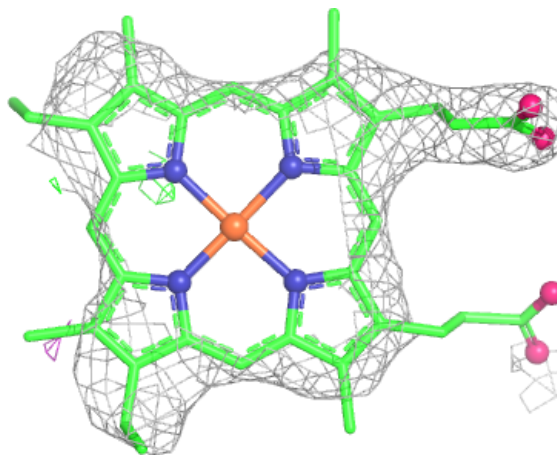
Electron density around CLA A 349:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



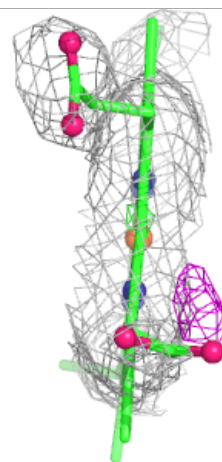
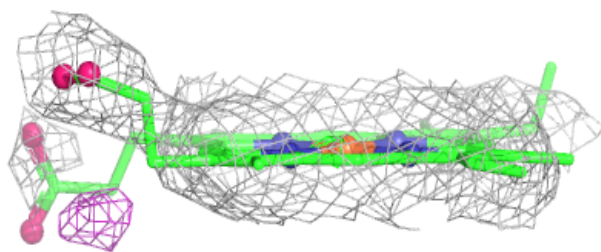
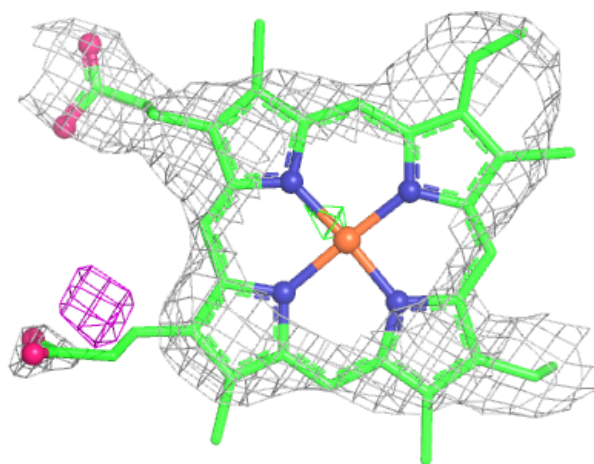
Electron density around HEC E 84:

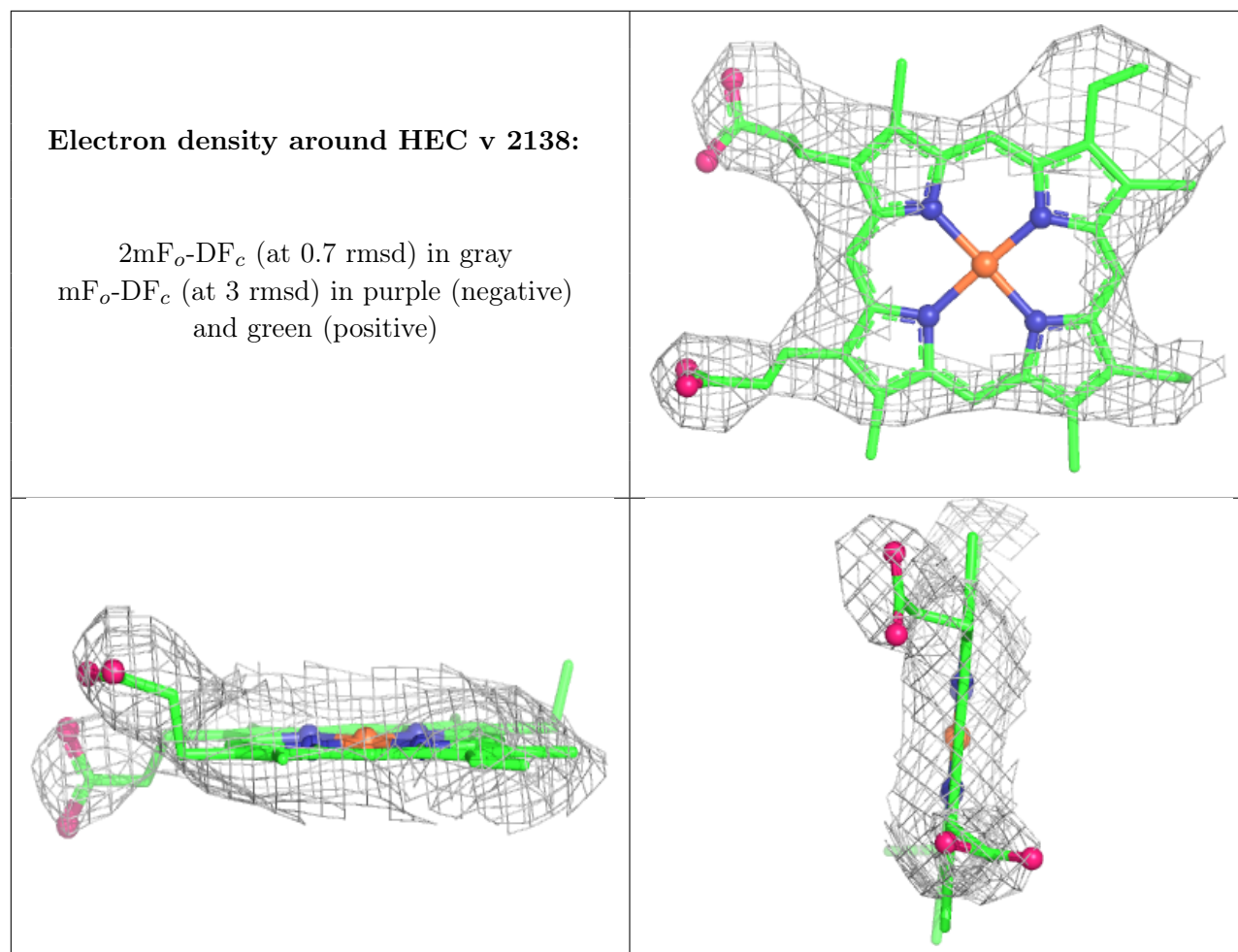
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC V 138:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.