



## Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 04:03 pm GMT

PDB ID : 9HEI / pdb\_00009hei  
EMDB ID : EMD-52077  
Title : Universal Photosystem II Intermediate with Light-Dependent Water-Ferrocyanide Oxydo-reductase activity from Chlamydomonas reinhardtii  
Authors : Nelson, N.; Klaiman, D.; Fadeeva, M.; Kandiah, E.  
Deposited on : 2024-11-14  
Resolution : 2.92 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

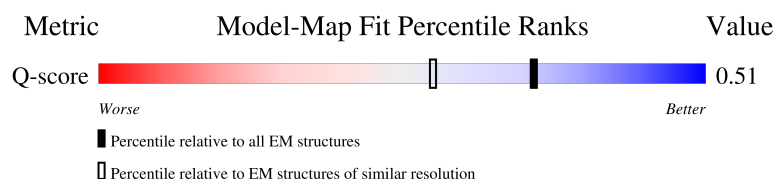
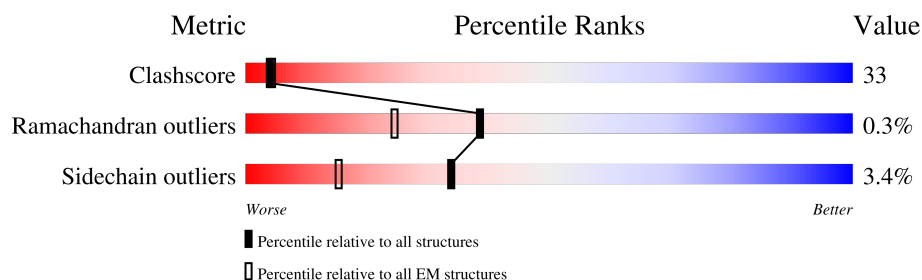
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 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.







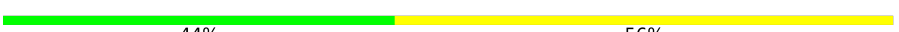

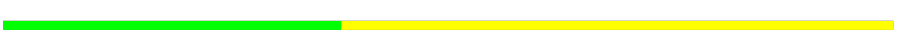





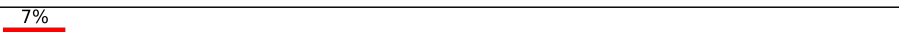



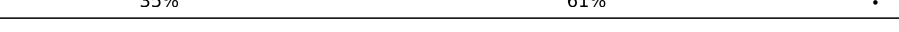
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13007 ( 2.42 - 3.42 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	
2	B	480	
3	V	32	
4	C	449	

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Mol	Chain	Length	Quality of chain
5	D	348	
6	E	75	
7	F	31	
8	H	66	
9	I	34	
10	J	36	
11	K	37	
12	L	35	
13	M	29	
14	O	240	
15	P	188	
16	Q	148	
17	T	30	
18	X	32	
19	Z	61	
20	U	23	
21	W	44	

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
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	408	X	-	-	-
25	CLA	B	501	X	-	-	-
25	CLA	B	502	X	-	-	-
25	CLA	B	503	X	-	X	-
25	CLA	B	504	X	-	-	-
25	CLA	B	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	506	X	-	-	-
25	CLA	B	507	X	-	-	-
25	CLA	B	508	X	-	-	-
25	CLA	B	509	X	-	X	-
25	CLA	B	510	X	-	-	-
25	CLA	B	511	X	-	-	-
25	CLA	B	512	X	-	-	-
25	CLA	B	513	X	-	-	-
25	CLA	B	514	X	-	-	-
25	CLA	B	515	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	X	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	H	101	X	-	-	-
29	LMG	W	201	-	-	X	-

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 24697 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	318	Total	C	N	O	S	0	0
			2491	1635	409	432	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		

- Molecule 3 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	75	Total	C	N	O	0	0
			610	399	101	110		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	66	Total	C	N	O	S	0	0
			501	336	74	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			262	178	40	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			223	154	31	38		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1192	746	214	232			

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

- Molecule 18 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	32	Total	C	N	O	S	0	0
			220	146	35	39			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

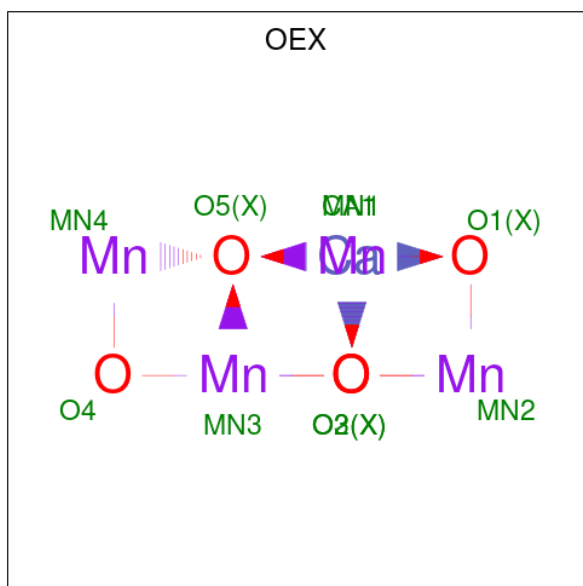
- Molecule 20 is a protein called Photosystem II reaction center protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	23	Total	C	N	O	S	0	0
			176	109	30	37			

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	44	Total	C	N	O	S	0	0
			344	226	57	59	2		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

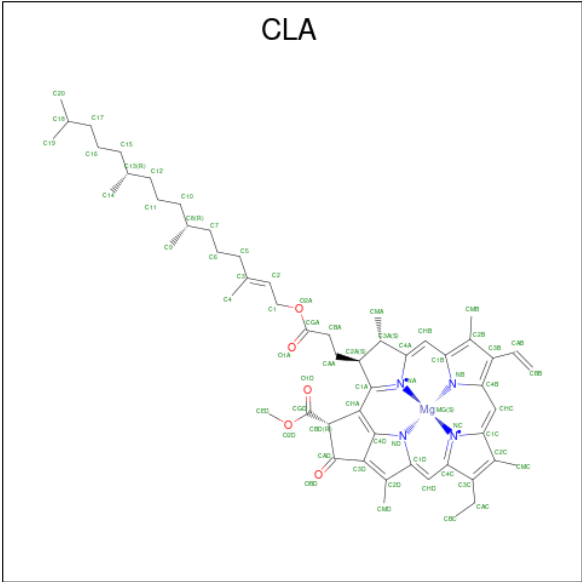
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Fe	0
			1	1	

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).





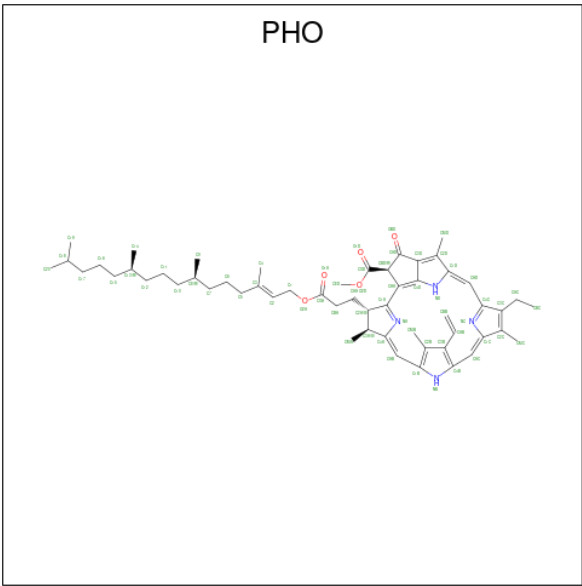
Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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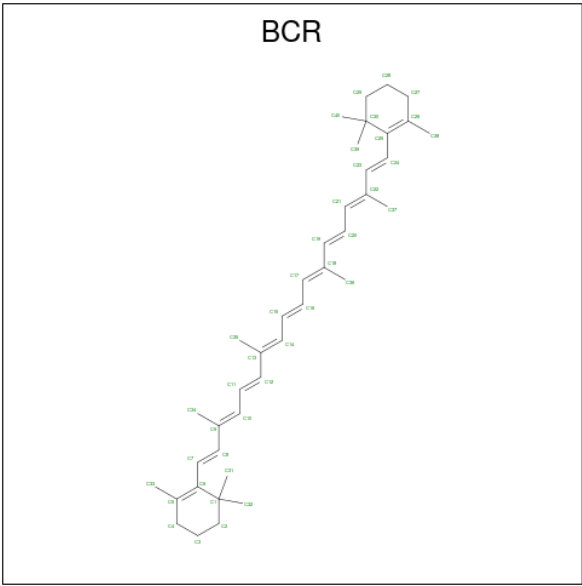
Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	H	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



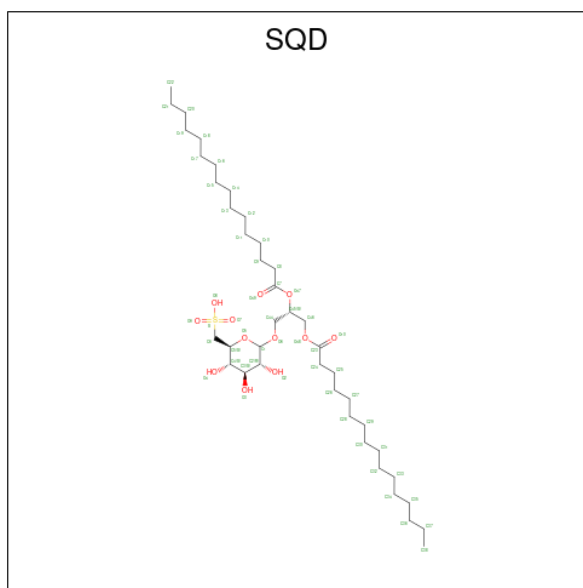
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	

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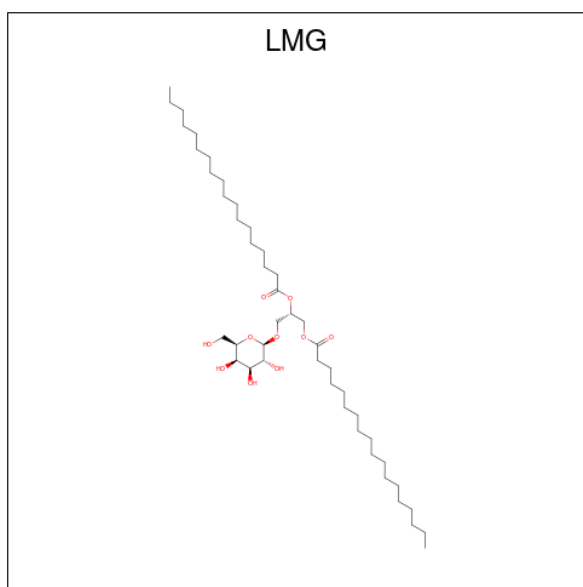
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	K	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



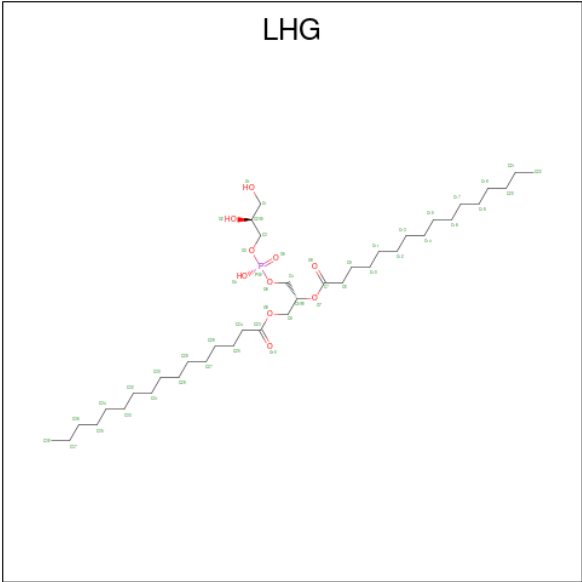
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C O S 51 38 12 1	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



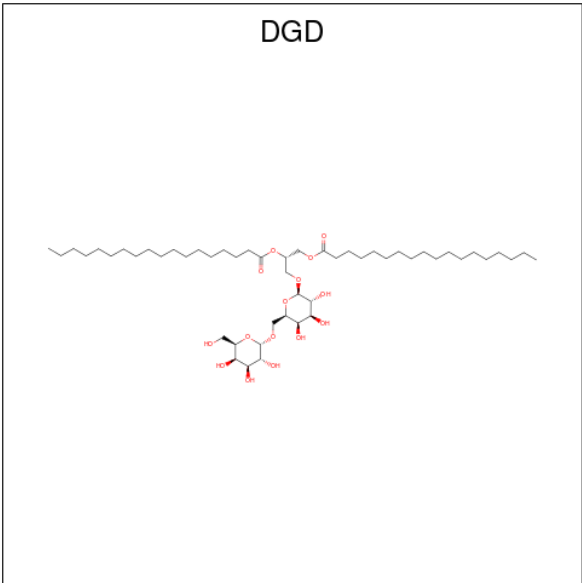
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			43	33	10	
29	B	1	Total	C	O	0
			48	38	10	
29	C	1	Total	C	O	0
			51	41	10	
29	D	1	Total	C	O	0
			36	26	10	
29	W	1	Total	C	O	0
			48	38	10	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



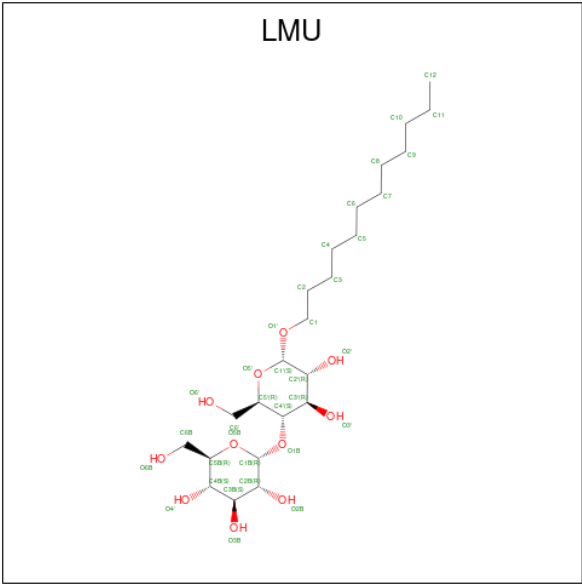
Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			44	33	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



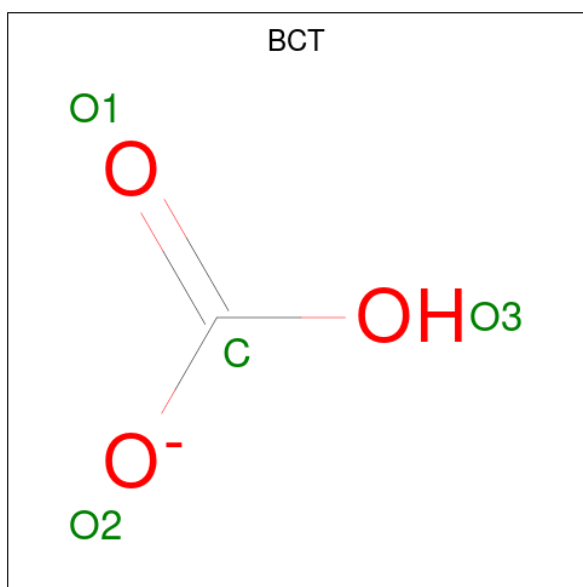
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			52	37	15	
31	C	1	Total	C	O	0
			54	39	15	
31	C	1	Total	C	O	0
			54	39	15	

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



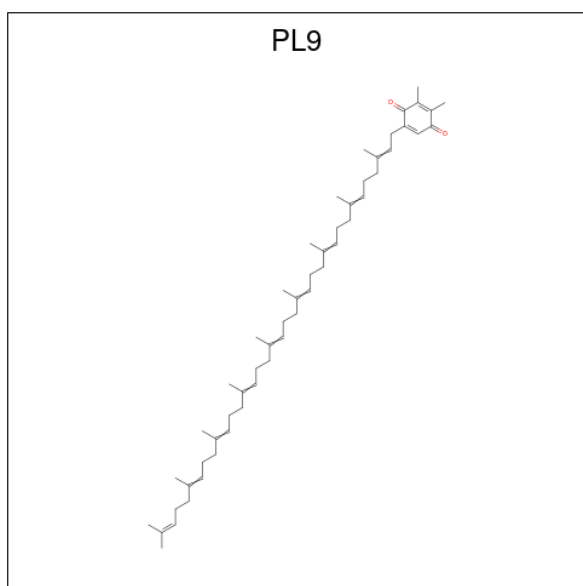
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	

- Molecule 34 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 (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).

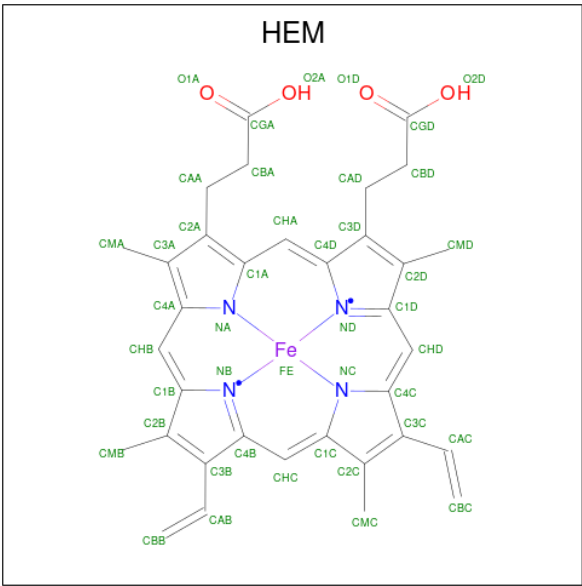


Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			55	53	2	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:



C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					AltConf
35	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

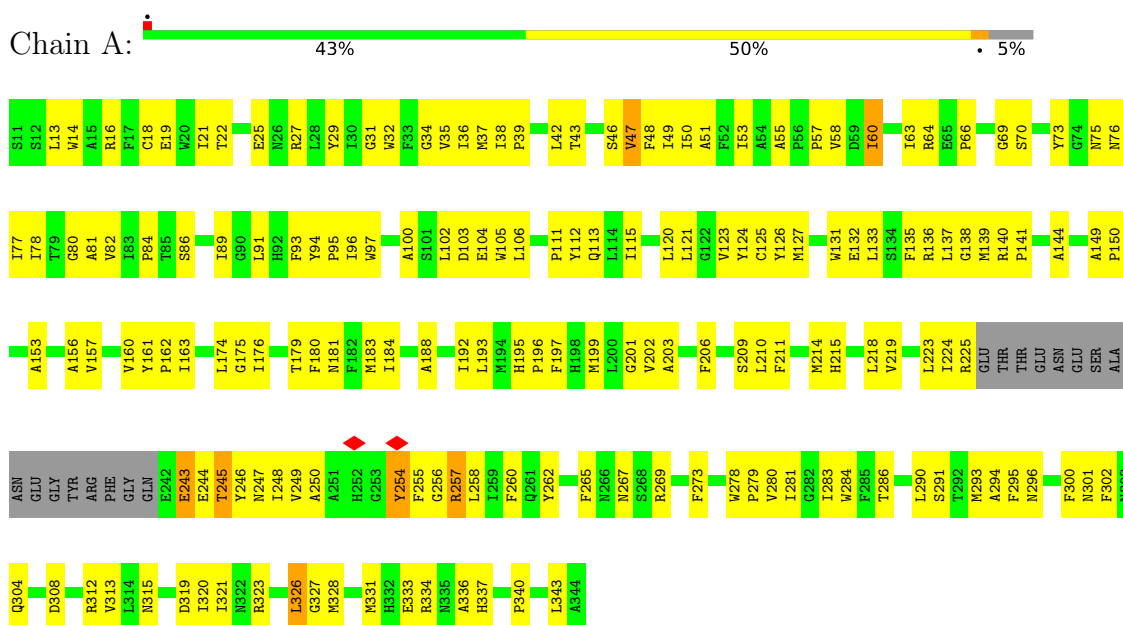
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	2	Total	O	0
			2	2	
36	B	2	Total	O	0
			2	2	
36	C	2	Total	O	0
			2	2	
36	D	1	Total	O	0
			1	1	

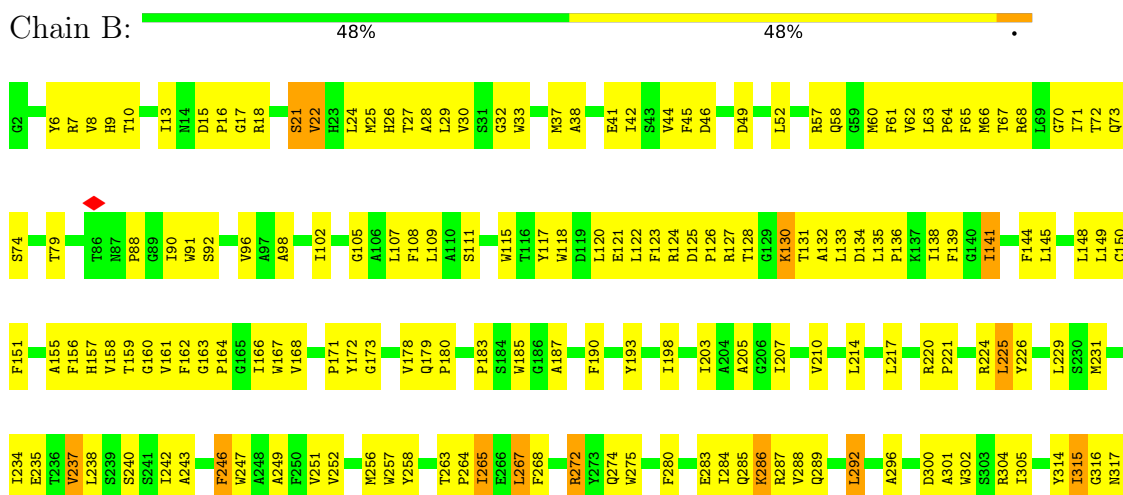
### 3 Residue-property plots

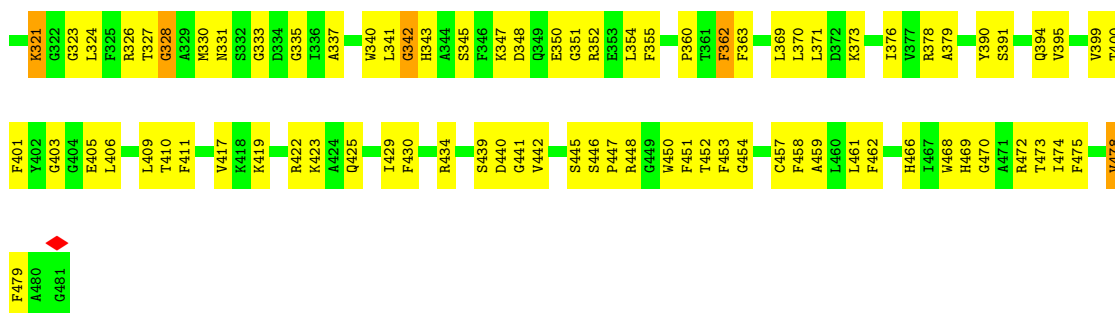
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 II protein D1

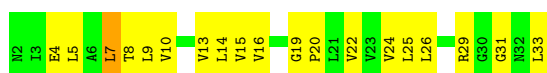


#### • Molecule 2: Photosystem II CP47 reaction center protein

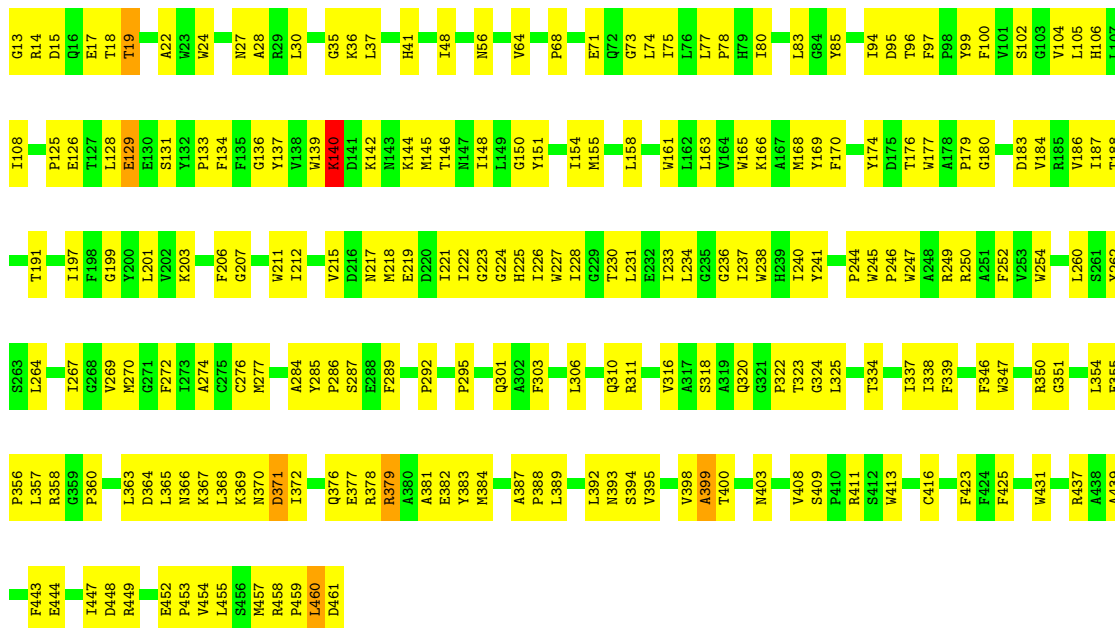




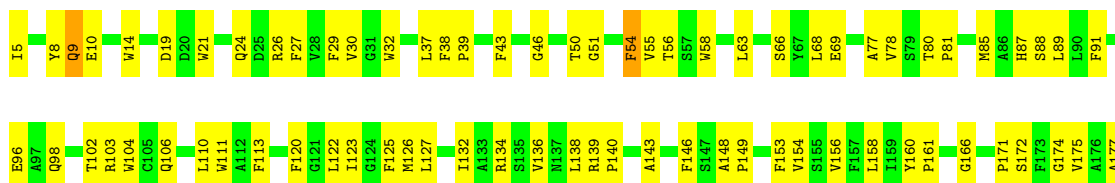
• Molecule 3: Photosystem II reaction center protein Psb30

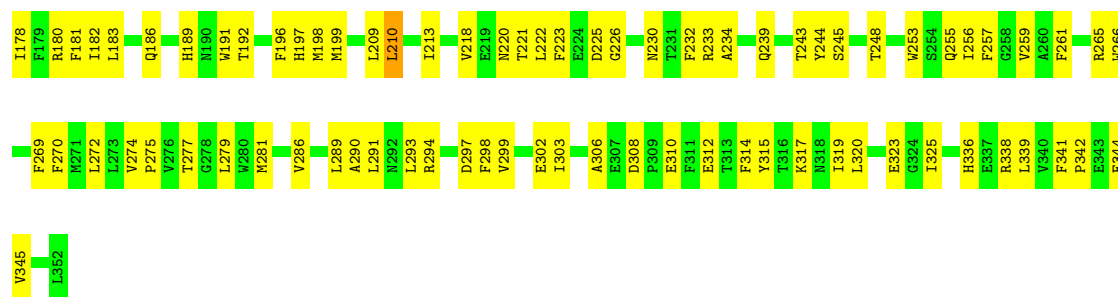


• Molecule 4: Photosystem II CP43 reaction center protein



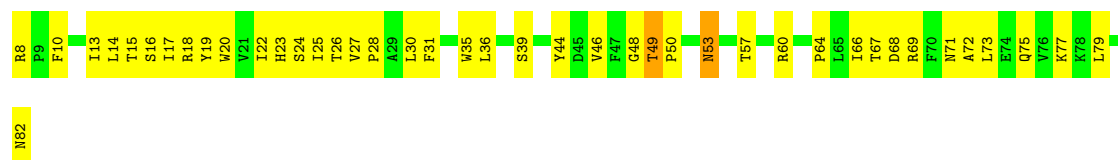
• Molecule 5: Photosystem II D2 protein





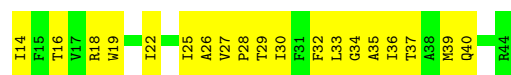
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 44% 53%



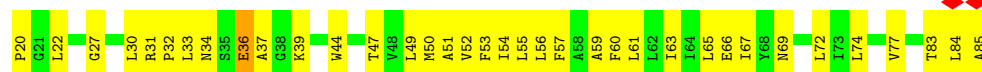
- Molecule 7: Cytochrome b559 subunit beta

Chain F: 39% 61%



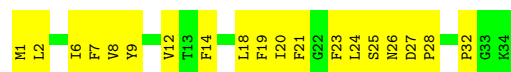
- Molecule 8: Photosystem II reaction center protein H

Chain H: 45% 53%



- Molecule 9: Photosystem II reaction center protein I

Chain I: 44% 56%

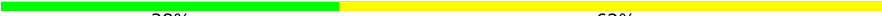


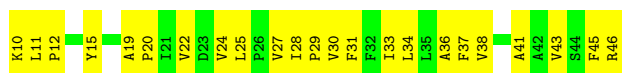
- Molecule 10: Photosystem II reaction center protein J

Chain J: 53% 44%



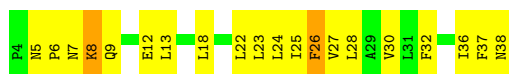
- Molecule 11: Photosystem II reaction center protein K

Chain K:  38% 62%



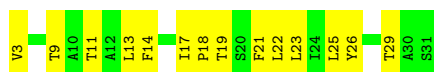
- Molecule 12: Photosystem II reaction center protein L

Chain L:  43% 51% 6%



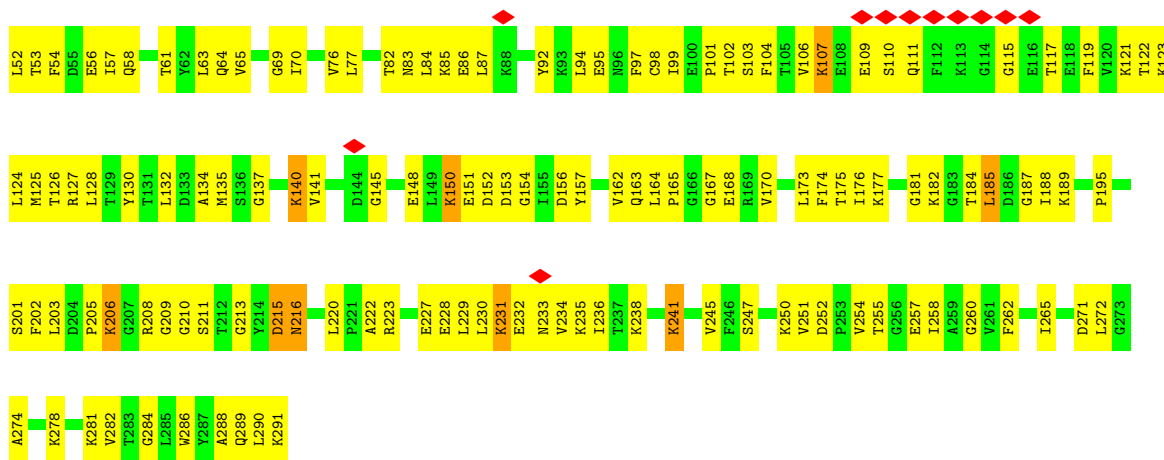
- Molecule 13: Photosystem II reaction center protein M

Chain M:  52% 48%



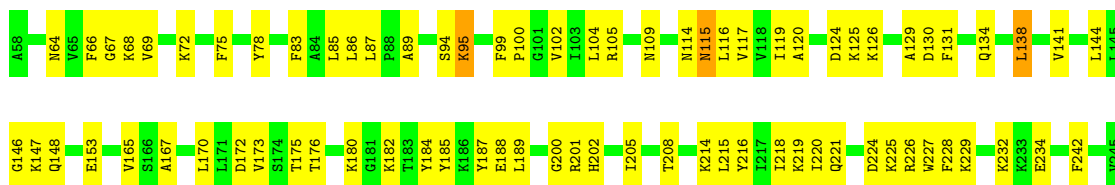
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:  5% 45% 52%



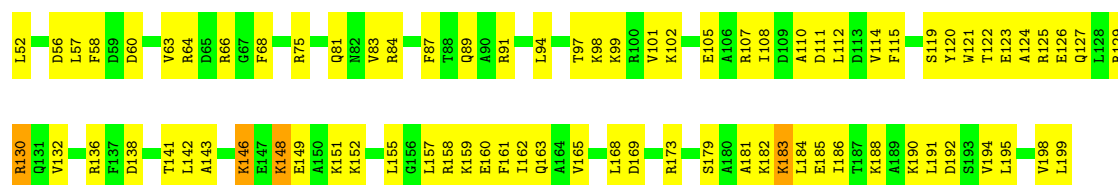
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:  60% 39%



- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain Q:  47% 51%



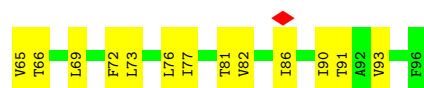
- Molecule 17: Photosystem II reaction center protein T

Chain T:  7% 67% 33%



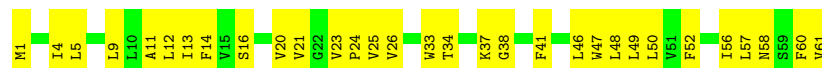
- Molecule 18: 4.1 kDa photosystem II subunit

Chain X:  59% 41%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  49% 51%



- Molecule 20: Photosystem II reaction center protein U

Chain U:  35% 61%



- Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W:  50% 39% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	361852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.9	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ( $\text{\AA}$ )	210.0, 210.0, 210.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.84, 0.84, 0.84	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, CLA, PHO, LHG, SQD, BCR, LMG, OEX, LMU, CL, HEM, FE2, DGD, BCT

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	0.94	0/2570	1.14	0/3505
2	B	0.93	0/3883	1.13	3/5286 (0.1%)
3	V	0.98	0/224	1.29	0/307
4	C	0.92	0/3619	1.14	0/4931
5	D	0.92	0/2866	1.12	0/3909
6	E	0.92	0/628	1.16	0/857
7	F	0.91	0/258	1.16	0/349
8	H	0.93	0/512	1.18	0/701
9	I	0.89	0/283	1.13	0/383
10	J	0.93	0/268	1.19	0/366
11	K	0.92	0/309	1.08	0/425
12	L	0.90	0/298	1.09	0/405
13	M	0.93	0/227	1.18	0/311
14	O	0.98	0/1839	1.09	0/2482
15	P	0.97	0/1473	1.09	2/1987 (0.1%)
16	Q	0.90	0/1204	1.19	0/1616
17	T	0.90	0/254	1.15	0/343
18	X	0.95	0/222	1.31	0/301
19	Z	0.93	0/469	1.20	0/644
20	U	0.96	0/176	1.20	0/235
21	W	0.88	0/354	1.13	0/481
All	All	0.93	0/21936	1.14	5/29824 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	200	GLY	CA-C-O	-6.30	118.12	122.22
15	P	146	GLY	CA-C-O	-6.02	118.12	122.45
2	B	342	GLY	CA-C-O	-5.86	118.23	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	GLY	CA-C-O	-5.57	118.30	122.37
2	B	335	GLY	CA-C-O	-5.40	118.25	122.52

There are no chirality outliers.

There are no planarity outliers.

## 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	2491	0	2415	210	0
2	B	3755	0	3642	271	0
3	V	224	0	256	20	0
4	C	3498	0	3372	239	0
5	D	2771	0	2655	172	0
6	E	610	0	599	42	0
7	F	251	0	263	17	0
8	H	501	0	531	40	0
9	I	275	0	287	21	0
10	J	262	0	276	20	0
11	K	297	0	308	42	0
12	L	290	0	298	24	0
13	M	223	0	245	18	0
14	O	1808	0	1813	119	0
15	P	1444	0	1414	70	0
16	Q	1192	0	1216	88	0
17	T	247	0	260	12	0
18	X	220	0	244	13	0
19	Z	458	0	490	25	0
20	U	176	0	184	17	0
21	W	344	0	334	29	0
22	A	10	0	0	0	0
23	A	1	0	0	0	0
24	A	2	0	0	0	0
25	A	174	0	167	42	0
25	B	927	0	962	187	0
25	C	789	0	804	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	186	0	193	29	0
25	H	61	0	60	12	0
26	A	64	0	74	6	0
26	D	64	0	74	12	0
27	A	40	0	56	19	0
27	B	80	0	112	20	0
27	C	120	0	168	34	0
27	D	40	0	56	9	0
27	K	40	0	56	12	0
28	A	51	0	68	15	0
29	B	91	0	122	19	0
29	C	51	0	72	12	0
29	D	36	0	42	6	0
29	W	48	0	66	23	0
30	B	93	0	135	15	0
30	D	88	0	122	15	0
31	C	160	0	194	35	0
32	C	35	0	46	5	0
33	D	4	0	0	1	0
34	D	55	0	80	6	0
35	F	43	0	30	6	0
36	A	2	0	0	0	0
36	B	2	0	0	1	0
36	C	2	0	0	0	0
36	D	1	0	0	0	0
All	All	24697	0	24861	1619	0

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 33.

All (1619) 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)
25:B:503:CLA:HAB	25:B:505:CLA:H172	1.36	1.07
1:A:333:GLU:HB3	1:A:336:ALA:HB3	1.39	1.00
2:B:157:HIS:CA	2:B:163:GLY:HA3	1.93	0.99
12:L:13:LEU:H	13:M:29:THR:HG21	1.25	0.98
2:B:157:HIS:HA	2:B:163:GLY:HA3	0.98	0.97
5:D:275:PRO:HB2	26:D:402:PHO:HBC1	1.47	0.97
2:B:157:HIS:HA	2:B:163:GLY:CA	1.94	0.96
29:C:520:LMG:H172	11:K:27:VAL:HG21	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:406:BCR:H403	10:J:27:LEU:HB2	1.44	0.96
6:E:8:ARG:HH22	6:E:16:SER:HB3	1.28	0.95
14:O:109:GLU:HA	14:O:117:THR:HA	1.49	0.95
15:P:116:LEU:HD13	15:P:220:ILE:HG12	1.50	0.93
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.51	0.91
25:B:510:CLA:H171	25:B:512:CLA:H101	1.54	0.90
25:A:408:CLA:H12	29:W:201:LMG:H111	1.52	0.90
28:A:410:SQD:H262	4:C:24:TRP:HB3	1.53	0.90
1:A:27:ARG:HA	4:C:460:LEU:HD11	1.54	0.89
4:C:392:LEU:HD21	31:C:519:DGD:HB71	1.55	0.89
1:A:50:ILE:HD12	27:A:409:BCR:H21C	1.54	0.88
2:B:117:TYR:HB3	8:H:22:LEU:HD21	1.56	0.88
31:C:517:DGD:HB41	29:W:201:LMG:H392	1.56	0.88
5:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.54	0.88
27:C:516:BCR:HC22	19:Z:9:LEU:HD21	1.56	0.87
2:B:30:VAL:HG12	25:B:505:CLA:HHD	1.56	0.87
4:C:134:PHE:HZ	25:C:512:CLA:HAB	1.39	0.87
2:B:122:LEU:HD11	8:H:30:LEU:HB2	1.57	0.86
2:B:247:TRP:HB2	25:B:508:CLA:HBC1	1.56	0.86
6:E:68:ASP:H	6:E:75:GLN:HE22	1.25	0.84
4:C:108:ILE:HB	27:C:514:BCR:H12C	1.59	0.83
2:B:25:MET:HA	2:B:25:MET:HE2	1.60	0.83
11:K:37:PHE:HB3	27:K:101:BCR:H291	1.59	0.83
20:U:110:ARG:HG2	20:U:111:LYS:HG3	1.58	0.83
4:C:272:PHE:HB3	31:C:517:DGD:HB71	1.59	0.83
25:C:507:CLA:H142	27:C:515:BCR:H16C	1.61	0.83
30:B:519:LHG:HC82	30:B:519:LHG:H361	1.60	0.82
25:C:510:CLA:HED1	25:C:510:CLA:H102	1.62	0.81
1:A:340:PRO:HB2	15:P:225:LYS:HE2	1.61	0.81
6:E:44:TYR:HA	6:E:49:THR:HG23	1.61	0.80
16:Q:101:VAL:HG21	16:Q:142:LEU:HD11	1.61	0.80
11:K:31:PHE:HB3	27:K:101:BCR:H16C	1.64	0.80
1:A:13:LEU:HA	1:A:16:ARG:HD3	1.64	0.80
25:B:507:CLA:H201	13:M:11:THR:HA	1.62	0.80
4:C:105:LEU:HD23	32:C:521:LMU:H71	1.61	0.80
14:O:157:TYR:HB3	14:O:177:LYS:HE2	1.60	0.80
4:C:368:LEU:HA	4:C:372:ILE:HD11	1.64	0.80
25:C:504:CLA:HAA2	31:C:518:DGD:HE1	1.64	0.79
5:D:66:SER:HB3	5:D:69:GLU:HG3	1.64	0.79
1:A:64:ARG:HG2	4:C:325:LEU:HD21	1.65	0.79
14:O:234:VAL:HG13	14:O:236:ILE:HG13	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:511:CLA:H72	27:C:516:BCR:H402	1.65	0.78
2:B:66:MET:HB3	2:B:71:ILE:HD12	1.65	0.78
5:D:192:THR:HG23	25:D:404:CLA:HBC2	1.65	0.78
14:O:82:THR:HA	14:O:250:LYS:HG2	1.63	0.78
2:B:124:ARG:HG3	8:H:20:PRO:HB3	1.64	0.78
2:B:105:GLY:HA3	27:B:517:BCR:H402	1.67	0.77
1:A:244:GLU:HB3	1:A:247:ASN:HB2	1.65	0.76
25:C:502:CLA:HBB1	25:C:502:CLA:HMB3	1.67	0.76
27:D:406:BCR:H363	7:F:32:PHE:HB3	1.67	0.76
2:B:29:LEU:HD11	27:B:516:BCR:H19C	1.68	0.76
25:C:510:CLA:HMB3	25:C:510:CLA:HBB1	1.68	0.76
5:D:56:THR:HG21	6:E:50:PRO:HD2	1.67	0.76
2:B:128:THR:HG21	2:B:130:LYS:HE2	1.67	0.76
25:B:510:CLA:HBB1	25:B:510:CLA:HMB3	1.66	0.76
14:O:97:PHE:HD1	14:O:288:ALA:HB2	1.49	0.76
1:A:100:ALA:HB2	21:W:64:ARG:HG2	1.67	0.76
4:C:364:ASP:HB2	4:C:367:LYS:HD3	1.68	0.76
3:V:26:LEU:HD23	3:V:33:LEU:HB3	1.68	0.76
1:A:131:TRP:HZ2	4:C:437:ARG:HG2	1.51	0.75
25:B:511:CLA:HBB1	25:B:511:CLA:HMB1	1.68	0.75
5:D:5:ILE:HG12	5:D:10:GLU:H	1.50	0.75
1:A:296:ASN:HB3	4:C:389:LEU:HA	1.68	0.75
2:B:237:VAL:HG22	25:B:511:CLA:HMD1	1.69	0.75
1:A:333:GLU:HB2	1:A:337:HIS:CE1	2.23	0.74
16:Q:184:LEU:HG	16:Q:188:LYS:HE2	1.70	0.74
25:B:505:CLA:HHC	25:B:505:CLA:HBB1	1.70	0.74
2:B:419:LYS:HG2	2:B:423:LYS:HE2	1.70	0.74
30:B:519:LHG:HC91	30:B:519:LHG:H332	1.68	0.73
25:B:501:CLA:HHC	25:B:501:CLA:HBB1	1.70	0.73
16:Q:157:LEU:O	16:Q:160:GLU:HG2	1.89	0.73
4:C:174:TYR:HA	4:C:184:VAL:HA	1.70	0.73
25:B:504:CLA:HBA2	25:B:511:CLA:H152	1.71	0.73
31:C:517:DGD:HB91	29:W:201:LMG:H411	1.71	0.72
19:Z:34:THR:HA	19:Z:37:LYS:HZ2	1.53	0.72
4:C:187:ILE:HD11	4:C:218:MET:HB3	1.70	0.72
2:B:348:ASP:HB3	2:B:354:LEU:HD11	1.71	0.72
4:C:129:GLU:HA	4:C:136:GLY:HA3	1.72	0.72
1:A:93:PHE:HZ	25:A:408:CLA:HAA2	1.53	0.72
2:B:468:TRP:CE2	2:B:472:ARG:HD2	2.25	0.72
1:A:78:ILE:HA	1:A:176:ILE:HD12	1.73	0.71
1:A:283:ILE:HG13	26:A:407:PHO:HBC3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD12	1:A:258:LEU:H	1.54	0.71
25:B:504:CLA:HBB1	25:B:504:CLA:HMB1	1.72	0.71
8:H:30:LEU:HA	8:H:33:LEU:HD13	1.73	0.70
4:C:64:VAL:HA	11:K:10:LYS:HZ2	1.56	0.70
4:C:354:LEU:HD23	4:C:358:ARG:HH21	1.56	0.70
15:P:94:SER:HB3	15:P:105:ARG:HD2	1.72	0.70
1:A:343:LEU:HA	4:C:389:LEU:HD11	1.73	0.70
2:B:73:GLN:HG2	2:B:79:THR:HG22	1.73	0.70
25:B:508:CLA:H72	25:H:101:CLA:H143	1.74	0.70
14:O:77:LEU:HD11	14:O:252:ASP:HB2	1.73	0.70
25:C:506:CLA:H11	25:C:507:CLA:H171	1.74	0.69
5:D:172:SER:HB2	5:D:177:ALA:HB1	1.73	0.69
1:A:77:ILE:HD11	17:T:6:TYR:HB3	1.74	0.69
29:C:520:LMG:H322	11:K:27:VAL:HG12	1.73	0.69
16:Q:160:GLU:HG3	16:Q:190:LYS:HD2	1.74	0.69
25:B:506:CLA:H93	25:B:506:CLA:HMD2	1.75	0.69
4:C:27:ASN:HB2	25:C:508:CLA:HBA1	1.72	0.69
29:D:410:LMG:H112	10:J:30:PHE:HB3	1.74	0.69
5:D:314:PHE:HA	5:D:317:LYS:HD3	1.73	0.69
11:K:31:PHE:HB3	27:K:101:BCR:C16	2.22	0.69
11:K:43:VAL:HG13	11:K:46:ARG:HG3	1.75	0.69
25:C:513:CLA:H2A	25:C:513:CLA:HED2	1.73	0.69
26:D:402:PHO:HBB1	26:D:402:PHO:HMB1	1.74	0.69
25:A:405:CLA:H152	26:A:407:PHO:HBA2	1.74	0.68
2:B:58:GLN:HG2	2:B:60:MET:HE2	1.75	0.68
15:P:120:ALA:HB1	15:P:214:LYS:HD3	1.75	0.68
1:A:184:ILE:HA	25:A:405:CLA:HBC1	1.75	0.68
5:D:191:TRP:CE3	5:D:289:LEU:HD11	2.28	0.68
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.75	0.68
2:B:18:ARG:HG3	2:B:118:TRP:HB3	1.76	0.68
2:B:65:PHE:HB3	25:B:505:CLA:HAA2	1.76	0.68
2:B:125:ASP:HB2	2:B:127:ARG:HH21	1.57	0.68
2:B:288:VAL:HG23	2:B:305:ILE:HD11	1.75	0.68
25:D:404:CLA:HHC	25:D:404:CLA:HBB1	1.75	0.68
11:K:38:VAL:CG2	27:K:101:BCR:H21C	2.23	0.68
4:C:388:PRO:HA	4:C:409:SER:HB2	1.76	0.67
15:P:134:GLN:HB3	15:P:187:TYR:HE1	1.59	0.67
29:B:520:LMG:H302	8:H:65:LEU:HD11	1.75	0.67
8:H:49:LEU:HG	8:H:53:PHE:CE2	2.30	0.67
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.76	0.67
2:B:275:TRP:CZ2	2:B:315:ILE:HG12	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:504:CLA:H122	25:B:509:CLA:H62	1.76	0.67
25:A:408:CLA:H142	29:W:201:LMG:H291	1.76	0.67
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.76	0.67
2:B:264:PRO:HB2	2:B:267:LEU:HB2	1.76	0.67
8:H:72:LEU:HD11	18:X:69:LEU:HA	1.77	0.67
25:C:509:CLA:H121	25:C:509:CLA:HBD	1.75	0.67
25:C:508:CLA:H102	11:K:33:ILE:HD11	1.76	0.67
6:E:35:TRP:HZ3	7:F:37:THR:HG22	1.60	0.67
2:B:117:TYR:HB3	8:H:22:LEU:CD2	2.24	0.66
4:C:449:ARG:HG3	5:D:223:PHE:HB3	1.77	0.66
4:C:139:TRP:O	4:C:140:LYS:HB3	1.92	0.66
25:C:506:CLA:HMB3	25:C:506:CLA:HBB1	1.77	0.66
2:B:327:THR:HG22	25:B:507:CLA:H11	1.75	0.66
4:C:384:MET:HE1	16:Q:75:ARG:HH11	1.60	0.66
19:Z:16:SER:HB2	19:Z:47:TRP:HE1	1.59	0.66
1:A:36:ILE:HG23	25:A:408:CLA:HBB1	1.78	0.66
25:B:513:CLA:H93	27:B:516:BCR:H362	1.78	0.66
27:C:515:BCR:HC32	9:I:23:PHE:HB3	1.77	0.66
6:E:35:TRP:HZ2	15:P:66:PHE:HE2	1.43	0.66
5:D:275:PRO:HB2	26:D:402:PHO:CBC	2.24	0.66
1:A:14:TRP:CH2	21:W:96:TRP:HE3	2.13	0.66
8:H:74:LEU:HB2	8:H:77:VAL:HG22	1.78	0.66
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.78	0.66
4:C:221:ILE:HA	27:C:515:BCR:H282	1.78	0.66
5:D:30:VAL:HA	5:D:38:PHE:HE2	1.60	0.66
15:P:64:ASN:ND2	15:P:67:GLY:HA3	2.11	0.66
25:B:504:CLA:H2	25:B:511:CLA:H122	1.78	0.66
4:C:350:ARG:HG2	4:C:358:ARG:HH12	1.60	0.66
25:A:408:CLA:H143	29:W:201:LMG:H112	1.78	0.65
25:B:512:CLA:H192	30:B:521:LHG:H352	1.78	0.65
14:O:109:GLU:HA	14:O:117:THR:CA	2.23	0.65
14:O:109:GLU:CA	14:O:117:THR:HA	2.23	0.65
15:P:205:ILE:HG12	15:P:219:LYS:HG2	1.76	0.65
2:B:265:ILE:HG21	2:B:274:GLN:HE22	1.62	0.65
4:C:146:THR:HG21	4:C:244:PRO:HD3	1.77	0.65
12:L:13:LEU:N	13:M:29:THR:HG21	2.03	0.65
1:A:63:ILE:HB	4:C:323:THR:HG21	1.79	0.65
1:A:199:MET:HB2	31:C:519:DGD:HAE1	1.77	0.65
10:J:11:PRO:HG2	10:J:14:LEU:HB2	1.78	0.65
1:A:304:GLN:HG2	1:A:313:VAL:HG11	1.78	0.65
4:C:104:VAL:HG12	27:C:514:BCR:HC8	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:501:CLA:H201	25:C:507:CLA:HBB1	1.79	0.64
25:C:507:CLA:H2A	25:C:507:CLA:HED2	1.79	0.64
2:B:108:PHE:HD2	2:B:109:LEU:HD12	1.62	0.64
25:C:508:CLA:H171	25:C:510:CLA:H152	1.79	0.64
2:B:327:THR:HG22	25:B:507:CLA:H42	1.79	0.64
6:E:15:THR:O	10:J:10:ILE:HG21	1.97	0.64
16:Q:122:THR:O	16:Q:126:GLU:HG2	1.98	0.64
1:A:29:TYR:H	5:D:255:GLN:HB3	1.63	0.64
27:C:515:BCR:H333	9:I:20:ILE:HG23	1.79	0.64
11:K:19:ALA:O	11:K:22:VAL:HG12	1.98	0.64
4:C:320:GLN:HG3	4:C:324:GLY:HA2	1.79	0.64
4:C:454:VAL:HG21	5:D:248:THR:HA	1.80	0.64
16:Q:102:LYS:HZ1	16:Q:199:LEU:HB2	1.62	0.64
16:Q:162:ILE:O	16:Q:165:VAL:HG22	1.98	0.64
25:D:401:CLA:H2A	25:D:401:CLA:HED2	1.79	0.64
4:C:225:HIS:HA	4:C:228:ILE:HG22	1.79	0.64
14:O:257:GLU:HG2	14:O:289:GLN:HG2	1.80	0.64
1:A:42:LEU:HD13	27:A:409:BCR:H11C	1.80	0.63
25:B:510:CLA:H151	25:B:512:CLA:O2D	1.99	0.63
25:C:502:CLA:H172	32:C:521:LMU:H52	1.80	0.63
11:K:28:ILE:HG21	27:K:101:BCR:H342	1.79	0.63
14:O:148:GLU:HG2	14:O:182:LYS:HG2	1.80	0.63
11:K:27:VAL:O	11:K:30:VAL:HG12	1.99	0.63
16:Q:161:PHE:CE1	16:Q:191:LEU:HB2	2.32	0.63
2:B:454:GLY:CA	29:B:518:LMG:H192	2.28	0.63
19:Z:12:LEU:HD13	19:Z:50:LEU:HB2	1.81	0.63
2:B:120:LEU:HB2	2:B:123:PHE:CE2	2.32	0.63
2:B:434:ARG:HB2	2:B:439:SER:HB2	1.81	0.63
5:D:80:THR:HG22	5:D:111:TRP:CE2	2.34	0.63
5:D:113:PHE:HZ	27:D:406:BCR:H323	1.64	0.63
16:Q:87:PHE:HB3	16:Q:91:ARG:NH1	2.13	0.63
2:B:30:VAL:HG11	25:B:511:CLA:H112	1.80	0.63
1:A:133:LEU:HD23	5:D:256:ILE:HG12	1.80	0.63
4:C:365:LEU:HD21	14:O:134:ALA:HB1	1.81	0.63
1:A:27:ARG:NH2	17:T:24:ARG:HE	1.96	0.62
2:B:162:PHE:CD2	25:B:506:CLA:HHD	2.34	0.62
27:B:516:BCR:H313	29:B:518:LMG:H112	1.80	0.62
14:O:235:LYS:HA	14:O:272:LEU:HB3	1.81	0.62
19:Z:48:LEU:HG	19:Z:52:PHE:CE2	2.34	0.62
1:A:262:TYR:HE2	1:A:265:PHE:HB2	1.63	0.62
25:A:405:CLA:H41	25:D:401:CLA:HAB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PHE:HD2	25:B:506:CLA:HHD	1.64	0.62
25:C:503:CLA:HMB3	32:C:521:LMU:H61	1.81	0.62
17:T:24:ARG:HH22	17:T:27:PRO:HG3	1.64	0.62
25:A:408:CLA:H111	29:W:201:LMG:H152	1.81	0.62
5:D:297:ASP:HB2	5:D:315:TYR:OH	1.99	0.62
2:B:71:ILE:HD13	2:B:96:VAL:HG21	1.81	0.62
5:D:85:MET:HE1	6:E:69:ARG:HA	1.81	0.62
7:F:16:THR:HG23	7:F:19:TRP:H	1.65	0.62
1:A:93:PHE:CZ	25:A:408:CLA:HAA2	2.33	0.62
30:B:521:LHG:H192	30:D:408:LHG:H172	1.80	0.62
14:O:65:VAL:HG13	14:O:70:ILE:HG13	1.81	0.62
14:O:109:GLU:CD	14:O:117:THR:HB	2.25	0.62
14:O:289:GLN:HB3	14:O:291:LYS:NZ	2.13	0.62
2:B:125:ASP:HB3	2:B:132:ALA:HB3	1.82	0.62
4:C:104:VAL:CG1	27:C:514:BCR:HC8	2.30	0.62
1:A:14:TRP:CH2	9:I:25:SER:HB2	2.35	0.62
4:C:448:ASP:O	4:C:449:ARG:HB2	2.00	0.62
16:Q:64:ARG:HA	16:Q:68:PHE:HB3	1.82	0.62
25:A:408:CLA:C1	29:W:201:LMG:H111	2.29	0.61
25:C:508:CLA:CAB	25:C:510:CLA:HMA3	2.29	0.61
25:C:513:CLA:HAB	27:C:514:BCR:H24C	1.82	0.61
13:M:17:ILE:HB	13:M:18:PRO:HD3	1.81	0.61
14:O:110:SER:HB3	14:O:115:GLY:HA3	1.81	0.61
28:A:410:SQD:H5	5:D:232:PHE:HB3	1.82	0.61
2:B:67:THR:HA	2:B:71:ILE:O	2.00	0.61
11:K:12:PRO:HB2	11:K:15:TYR:HD2	1.65	0.61
21:W:81:LEU:O	21:W:84:VAL:HG22	2.00	0.61
1:A:55:ALA:HA	27:A:409:BCR:H272	1.82	0.61
25:B:509:CLA:HBB2	25:H:101:CLA:H2	1.82	0.61
12:L:5:ASN:HD22	12:L:6:PRO:HD2	1.66	0.61
5:D:30:VAL:HA	5:D:38:PHE:CE2	2.35	0.61
13:M:21:PHE:CZ	13:M:25:LEU:HD11	2.36	0.61
25:B:503:CLA:HBA1	25:B:505:CLA:H43	1.82	0.61
14:O:216:ASN:H	14:O:216:ASN:HD22	1.49	0.61
16:Q:112:LEU:HD23	16:Q:184:LEU:HD13	1.82	0.61
1:A:121:LEU:HD23	25:C:505:CLA:H151	1.83	0.61
1:A:140:ARG:HH12	5:D:222:LEU:HB2	1.66	0.61
5:D:182:ILE:HG23	25:D:404:CLA:CHD	2.30	0.61
5:D:213:ILE:HD13	34:D:407:PL9:HC8	1.83	0.61
27:K:101:BCR:HC21	19:Z:13:ILE:HG23	1.83	0.61
15:P:116:LEU:HD11	15:P:218:ILE:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:125:LYS:HB3	15:P:130:ASP:HB2	1.83	0.61
25:B:501:CLA:C4D	25:B:501:CLA:H122	2.30	0.61
15:P:225:LYS:HD2	15:P:226:ARG:NH1	2.16	0.60
1:A:47:VAL:HG13	1:A:115:ILE:HG12	1.82	0.60
1:A:139:MET:HE3	5:D:221:THR:HG22	1.82	0.60
25:B:507:CLA:HBD	29:B:518:LMG:HC71	1.84	0.60
3:V:33:LEU:HD23	3:V:33:LEU:H	1.66	0.60
4:C:187:ILE:HG13	4:C:222:ILE:HG13	1.83	0.60
4:C:276:CYS:SG	31:C:517:DGD:HB72	2.41	0.60
4:C:358:ARG:HG2	4:C:363:LEU:HD23	1.83	0.60
25:C:504:CLA:H61	31:C:518:DGD:HB72	1.82	0.60
1:A:224:ILE:HA	5:D:265:ARG:HH12	1.65	0.60
16:Q:146:LYS:HE3	16:Q:198:VAL:HA	1.83	0.60
4:C:254:TRP:CZ3	25:C:507:CLA:HMC1	2.36	0.60
10:J:8:GLY:O	10:J:10:ILE:HG22	2.01	0.60
15:P:69:VAL:HG21	15:P:72:LYS:HG3	1.82	0.60
16:Q:105:GLU:HA	16:Q:191:LEU:HD21	1.82	0.60
16:Q:191:LEU:HG	16:Q:195:LEU:HD11	1.84	0.60
1:A:140:ARG:NH1	5:D:222:LEU:HB2	2.16	0.60
25:B:509:CLA:HBB2	25:H:101:CLA:C2	2.31	0.60
4:C:150:GLY:HA2	4:C:236:GLY:HA2	1.82	0.60
21:W:74:PHE:HA	29:W:201:LMG:C28	2.31	0.60
2:B:25:MET:HE1	2:B:108:PHE:HD1	1.67	0.60
4:C:161:TRP:CH2	4:C:226:ILE:HG23	2.36	0.60
6:E:17:ILE:HA	6:E:20:TRP:HD1	1.66	0.60
8:H:50:MET:HB2	25:H:101:CLA:C3D	2.32	0.60
1:A:124:TYR:HE2	25:C:505:CLA:H172	1.66	0.60
6:E:67:THR:HG23	20:U:109:LEU:HD12	1.83	0.60
14:O:135:MET:HA	14:O:154:GLY:HA3	1.84	0.60
4:C:100:PHE:HE2	27:C:514:BCR:HC32	1.67	0.60
4:C:272:PHE:HB3	31:C:517:DGD:HB92	1.82	0.60
10:J:33:GLY:HA2	10:J:36:VAL:HG12	1.84	0.60
2:B:234:ILE:O	2:B:237:VAL:HG13	2.01	0.59
2:B:265:ILE:HD13	2:B:265:ILE:H	1.67	0.59
5:D:160:TYR:HB3	5:D:161:PRO:HD3	1.82	0.59
25:D:405:CLA:NA	25:D:405:CLA:H12	2.17	0.59
6:E:68:ASP:HB3	6:E:71:ASN:HB2	1.83	0.59
11:K:28:ILE:HA	11:K:31:PHE:HD2	1.66	0.59
15:P:95:LYS:HB2	15:P:95:LYS:HZ2	1.67	0.59
16:Q:60:ASP:O	16:Q:63:VAL:HG22	2.02	0.59
28:A:410:SQD:H5	5:D:232:PHE:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:513:CLA:HMB3	27:C:514:BCR:H402	1.84	0.59
11:K:38:VAL:HG21	27:K:101:BCR:H19C	1.82	0.59
4:C:211:TRP:NE1	29:W:201:LMG:H342	2.17	0.59
1:A:132:GLU:O	1:A:136:ARG:HG2	2.02	0.59
10:J:32:TYR:CZ	10:J:36:VAL:HG11	2.37	0.59
25:B:503:CLA:CAB	25:B:505:CLA:H172	2.22	0.59
2:B:145:LEU:HB3	25:B:504:CLA:H171	1.84	0.59
4:C:303:PHE:HE2	4:C:377:GLU:HA	1.67	0.59
25:C:506:CLA:NC	25:C:507:CLA:H152	2.17	0.59
7:F:27:VAL:HB	7:F:28:PRO:HD3	1.85	0.59
14:O:157:TYR:HB2	14:O:173:LEU:HD21	1.84	0.59
14:O:209:GLY:H	14:O:213:GLY:HA3	1.67	0.59
9:I:8:VAL:O	9:I:12:VAL:HG23	2.03	0.59
11:K:27:VAL:HG23	11:K:31:PHE:HE2	1.67	0.59
15:P:75:PHE:CZ	15:P:234:GLU:HA	2.38	0.59
21:W:77:ASN:C	21:W:77:ASN:HD22	2.10	0.59
2:B:156:PHE:HA	2:B:161:VAL:HG22	1.83	0.59
5:D:68:LEU:HD23	6:E:49:THR:HG21	1.84	0.59
19:Z:34:THR:HA	19:Z:37:LYS:NZ	2.18	0.59
2:B:149:LEU:HD13	25:B:503:CLA:HBC1	1.85	0.59
25:C:501:CLA:HMD3	25:C:502:CLA:H112	1.85	0.59
5:D:156:VAL:HG12	5:D:171:PRO:HG2	1.85	0.59
2:B:149:LEU:HD22	25:B:503:CLA:HAC2	1.85	0.58
2:B:379:ALA:HB2	2:B:395:VAL:HG11	1.84	0.58
25:B:503:CLA:HBB1	25:B:503:CLA:HMB1	1.84	0.58
4:C:228:ILE:HD11	25:C:507:CLA:H93	1.85	0.58
5:D:259:VAL:HG21	30:D:408:LHG:H301	1.84	0.58
14:O:65:VAL:HG13	14:O:70:ILE:CG1	2.33	0.58
14:O:164:LEU:HB2	14:O:165:PRO:HD2	1.85	0.58
16:Q:168:LEU:HD22	16:Q:184:LEU:HA	1.85	0.58
27:B:517:BCR:H321	27:B:517:BCR:HC8	1.85	0.58
2:B:133:LEU:HB3	2:B:138:ILE:HD11	1.85	0.58
2:B:251:VAL:HG13	25:B:502:CLA:H43	1.85	0.58
25:C:509:CLA:HBB1	25:C:509:CLA:HMB1	1.86	0.58
14:O:229:LEU:HD12	14:O:230:LEU:N	2.19	0.58
1:A:211:PHE:HE2	1:A:278:TRP:CG	2.22	0.58
2:B:9:HIS:HB2	25:B:510:CLA:HBA1	1.84	0.58
25:B:503:CLA:HMC2	25:B:505:CLA:H161	1.86	0.58
4:C:131:SER:O	4:C:133:PRO:HD3	2.03	0.58
5:D:257:PHE:HA	30:D:408:LHG:H371	1.86	0.58
16:Q:107:ARG:O	16:Q:111:ASP:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ALA:HB1	2:B:300:ASP:HB2	1.86	0.58
25:B:514:CLA:HBB1	25:B:514:CLA:HMB1	1.85	0.58
5:D:113:PHE:CZ	27:D:406:BCR:H323	2.39	0.58
15:P:131:PHE:CE2	15:P:215:LEU:HD22	2.38	0.58
2:B:183:PRO:HB2	2:B:185:TRP:CD1	2.39	0.57
1:A:104:GLU:OE2	14:O:127:ARG:HG2	2.04	0.57
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.86	0.57
1:A:223:LEU:HA	1:A:248:ILE:HD12	1.86	0.57
2:B:190:PHE:HE2	8:H:60:PHE:HE1	1.52	0.57
2:B:347:LYS:HD2	2:B:351:GLY:HA2	1.85	0.57
2:B:400:THR:HG22	2:B:410:THR:HG23	1.86	0.57
2:B:394:GLN:HA	16:Q:52:LEU:HD22	1.86	0.57
25:B:509:CLA:H203	25:B:514:CLA:C3D	2.34	0.57
5:D:55:VAL:O	5:D:66:SER:HB2	2.03	0.57
2:B:149:LEU:HD12	25:B:504:CLA:H161	1.87	0.57
2:B:256:MET:HG3	2:B:448:ARG:HG3	1.85	0.57
25:B:513:CLA:HBC3	25:B:513:CLA:H102	1.85	0.57
4:C:201:LEU:HD11	27:C:515:BCR:H373	1.87	0.57
4:C:284:ALA:HB1	25:C:501:CLA:HAA2	1.84	0.57
25:C:501:CLA:H121	25:C:507:CLA:H62	1.87	0.57
31:C:518:DGD:HD3	29:C:520:LMG:HC3	1.86	0.57
5:D:189:HIS:HB3	5:D:289:LEU:HD22	1.87	0.57
8:H:74:LEU:HA	18:X:66:THR:HG21	1.86	0.57
2:B:360:PRO:HB2	2:B:363:PHE:HD1	1.68	0.57
25:B:503:CLA:CMC	25:B:505:CLA:H161	2.33	0.57
25:B:511:CLA:H102	25:B:511:CLA:H172	1.87	0.57
30:D:408:LHG:H322	17:T:21:ILE:HD11	1.86	0.57
8:H:52:VAL:O	8:H:56:LEU:HG	2.04	0.57
14:O:201:SER:O	14:O:203:LEU:HD12	2.05	0.57
4:C:17:GLU:HG3	4:C:18:THR:HG23	1.87	0.57
4:C:394:SER:HA	4:C:408:VAL:CG2	2.34	0.57
10:J:8:GLY:O	10:J:9:ARG:HG2	2.04	0.57
2:B:317:ASN:HA	2:B:330:MET:HE1	1.87	0.57
4:C:318:SER:HA	14:O:157:TYR:HE1	1.69	0.57
25:C:504:CLA:HAA2	31:C:518:DGD:HD61	1.87	0.57
14:O:125:MET:HE2	14:O:125:MET:HA	1.87	0.57
1:A:149:ALA:HB2	1:A:280:VAL:HG13	1.87	0.57
1:A:326:LEU:HD22	4:C:400:THR:HB	1.87	0.57
4:C:166:LYS:O	4:C:166:LYS:HD3	2.05	0.57
4:C:365:LEU:HD12	4:C:366:ASN:N	2.18	0.57
14:O:107:LYS:HG2	14:O:117:THR:OG1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:502:CLA:CGA	25:B:502:CLA:HBD	2.35	0.57
4:C:97:PHE:HZ	19:Z:58:ASN:HD21	1.53	0.57
4:C:431:TRP:CH2	30:D:409:LHG:HC61	2.40	0.57
25:C:507:CLA:H112	27:C:515:BCR:H16C	1.85	0.57
5:D:148:ALA:HB3	5:D:149:PRO:HD3	1.85	0.57
9:I:18:LEU:HD12	21:W:92:MET:HE2	1.86	0.57
12:L:22:LEU:O	12:L:25:ILE:HG13	2.04	0.57
14:O:184:THR:O	14:O:188:ILE:HG12	2.04	0.57
2:B:300:ASP:O	2:B:304:ARG:HG3	2.05	0.57
4:C:150:GLY:HA3	4:C:240:ILE:HG13	1.86	0.57
14:O:107:LYS:HA	14:O:119:PHE:HA	1.86	0.57
4:C:140:LYS:HB3	4:C:140:LYS:NZ	2.19	0.56
4:C:270:MET:HE3	25:C:501:CLA:H61	1.86	0.56
8:H:31:ARG:N	8:H:32:PRO:HD2	2.19	0.56
1:A:224:ILE:HG12	5:D:139:ARG:HD2	1.85	0.56
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.41	0.56
25:B:510:CLA:H152	25:B:512:CLA:H112	1.86	0.56
4:C:425:PHE:HA	25:C:508:CLA:HMC1	1.87	0.56
5:D:56:THR:HG22	5:D:69:GLU:CD	2.31	0.56
2:B:71:ILE:HD11	25:B:506:CLA:HMA2	1.86	0.56
2:B:376:ILE:HB	2:B:378:ARG:HE	1.69	0.56
2:B:468:TRP:O	2:B:472:ARG:HG3	2.04	0.56
25:B:510:CLA:C2D	30:B:519:LHG:H362	2.35	0.56
5:D:46:GLY:HA3	27:D:406:BCR:C34	2.35	0.56
14:O:163:GLN:NE2	14:O:167:GLY:HA2	2.20	0.56
15:P:115:ASN:HD21	15:P:221:GLN:HB3	1.70	0.56
16:Q:161:PHE:HA	16:Q:190:LYS:HB3	1.87	0.56
21:W:72:ARG:CZ	21:W:77:ASN:HA	2.35	0.56
2:B:27:THR:HG21	25:B:514:CLA:H2	1.87	0.56
4:C:351:GLY:O	4:C:355:GLU:HG2	2.06	0.56
5:D:14:TRP:HE1	18:X:91:THR:HA	1.70	0.56
13:M:19:THR:O	13:M:23:LEU:HG	2.06	0.56
28:A:410:SQD:H372	11:K:33:ILE:HG23	1.87	0.56
25:H:101:CLA:HMB1	25:H:101:CLA:HBB1	1.86	0.56
11:K:27:VAL:HG23	11:K:31:PHE:CE2	2.40	0.56
15:P:87:LEU:HD21	15:P:104:LEU:HD21	1.87	0.56
2:B:125:ASP:HB2	2:B:127:ARG:NH2	2.20	0.56
2:B:376:ILE:HD12	2:B:378:ARG:HH21	1.70	0.56
4:C:357:LEU:HD22	4:C:372:ILE:HD13	1.87	0.56
5:D:125:PHE:CE2	26:D:402:PHO:HBD	2.40	0.56
14:O:87:LEU:HD23	14:O:185:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:72:PHE:O	18:X:76:LEU:HG	2.05	0.56
1:A:93:PHE:HA	1:A:113:GLN:HE22	1.71	0.56
1:A:250:ALA:HA	1:A:255:PHE:HE1	1.70	0.56
1:A:319:ASP:O	1:A:323:ARG:HG2	2.06	0.56
25:C:501:CLA:H112	27:C:515:BCR:H17C	1.87	0.56
15:P:134:GLN:HB3	15:P:187:TYR:CE1	2.40	0.56
16:Q:112:LEU:HD21	16:Q:168:LEU:HD21	1.87	0.56
16:Q:146:LYS:HZ1	16:Q:198:VAL:HA	1.71	0.56
16:Q:158:ARG:O	16:Q:162:ILE:HG12	2.06	0.56
1:A:126:TYR:HE2	30:D:408:LHG:H383	1.71	0.56
1:A:150:PRO:HB2	25:A:405:CLA:H92	1.88	0.56
1:A:179:THR:O	1:A:183:MET:HG3	2.06	0.56
2:B:68:ARG:HH21	25:B:505:CLA:HBA1	1.70	0.56
31:C:518:DGD:HBF2	31:C:518:DGD:HBT2	1.87	0.56
20:U:107:LYS:HA	20:U:110:ARG:HH21	1.68	0.56
2:B:258:TYR:CZ	29:B:520:LMG:HC91	2.39	0.56
2:B:454:GLY:HA2	29:B:518:LMG:H192	1.88	0.56
25:B:509:CLA:H152	25:B:511:CLA:HBD	1.87	0.56
2:B:52:LEU:HB3	2:B:337:ALA:HB3	1.87	0.56
25:B:509:CLA:HHC	25:B:509:CLA:HBB1	1.87	0.56
4:C:27:ASN:HB2	25:C:508:CLA:CBA	2.35	0.56
4:C:148:ILE:HA	4:C:151:TYR:CD2	2.42	0.56
4:C:431:TRP:HH2	30:D:409:LHG:HC61	1.71	0.56
14:O:54:PHE:O	14:O:58:GLN:HG2	2.06	0.55
1:A:262:TYR:CE2	1:A:265:PHE:HB2	2.42	0.55
2:B:324:LEU:HD21	5:D:196:PHE:HE2	1.71	0.55
4:C:68:PRO:HD2	4:C:71:GLU:CD	2.32	0.55
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.36	0.55
1:A:202:VAL:HG11	25:A:406:CLA:C3D	2.36	0.55
2:B:24:LEU:HD21	25:B:515:CLA:CAB	2.35	0.55
2:B:391:SER:HB3	2:B:394:GLN:HG2	1.88	0.55
5:D:160:TYR:HA	5:D:290:ALA:HB2	1.87	0.55
15:P:172:ASP:HB3	15:P:188:GLU:HB3	1.87	0.55
21:W:64:ARG:HB2	21:W:66:ASN:ND2	2.22	0.55
1:A:284:TRP:HZ3	30:D:409:LHG:H321	1.72	0.55
28:A:410:SQD:H262	4:C:24:TRP:CB	2.32	0.55
25:C:501:CLA:H192	25:C:507:CLA:H162	1.89	0.55
2:B:124:ARG:HD3	2:B:131:THR:HG22	1.87	0.55
5:D:189:HIS:HA	5:D:294:ARG:HD3	1.88	0.55
16:Q:146:LYS:CE	16:Q:198:VAL:HA	2.36	0.55
1:A:106:LEU:HD11	27:A:409:BCR:H402	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:311:ARG:HD2	16:Q:68:PHE:HD1	1.70	0.55
25:C:510:CLA:H61	25:C:510:CLA:HMA1	1.89	0.55
5:D:50:THR:HG23	5:D:54:PHE:HE1	1.71	0.55
14:O:132:LEU:HG	14:O:174:PHE:CE2	2.42	0.55
2:B:440:ASP:HB2	5:D:299:VAL:HG11	1.87	0.55
4:C:413:TRP:HB3	25:C:504:CLA:HMB1	1.87	0.55
25:C:504:CLA:HAB	29:C:520:LMG:H421	1.88	0.55
14:O:227:GLU:C	14:O:229:LEU:H	2.14	0.55
15:P:69:VAL:HG11	15:P:72:LYS:HE2	1.87	0.55
15:P:120:ALA:HB1	15:P:214:LYS:CD	2.37	0.55
2:B:150:CYS:HB2	25:B:503:CLA:CMC	2.36	0.55
25:B:505:CLA:HHC	25:B:505:CLA:CBB	2.37	0.55
5:D:5:ILE:N	5:D:9:GLN:HA	2.22	0.55
13:M:21:PHE:CE2	13:M:25:LEU:HD11	2.42	0.55
2:B:7:ARG:HG2	2:B:10:THR:HG21	1.89	0.55
16:Q:149:GLU:HA	16:Q:152:LYS:HE2	1.89	0.55
25:C:510:CLA:H171	25:C:510:CLA:H121	1.89	0.55
2:B:247:TRP:CD1	25:B:503:CLA:H8	2.42	0.54
4:C:350:ARG:HG2	4:C:358:ARG:NH1	2.22	0.54
5:D:259:VAL:HG13	17:T:21:ILE:HG12	1.89	0.54
18:X:69:LEU:O	18:X:73:LEU:HG	2.07	0.54
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.89	0.54
31:C:518:DGD:HD1	29:C:520:LMG:O2	2.08	0.54
5:D:148:ALA:HB1	5:D:279:LEU:HB2	1.88	0.54
5:D:153:PHE:HB2	25:D:404:CLA:H61	1.89	0.54
14:O:289:GLN:HB3	14:O:291:LYS:HZ2	1.72	0.54
19:Z:58:ASN:HA	19:Z:61:VAL:HG12	1.89	0.54
25:A:408:CLA:H142	29:W:201:LMG:H312	1.89	0.54
2:B:422:ARG:O	2:B:425:GLN:HG2	2.07	0.54
6:E:15:THR:HA	10:J:10:ILE:HD13	1.88	0.54
14:O:209:GLY:N	14:O:213:GLY:HA3	2.22	0.54
14:O:216:ASN:HD22	14:O:216:ASN:N	2.04	0.54
1:A:43:THR:HA	27:A:409:BCR:C16	2.37	0.54
25:B:508:CLA:HMD1	25:B:509:CLA:HAB	1.89	0.54
27:B:516:BCR:HC21	29:B:518:LMG:H311	1.89	0.54
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.89	0.54
25:C:507:CLA:H151	25:C:507:CLA:H193	1.90	0.54
2:B:355:PHE:HZ	20:U:92:THR:HG21	1.72	0.54
4:C:306:LEU:HG	4:C:316:VAL:HG11	1.89	0.54
4:C:388:PRO:HA	4:C:409:SER:CB	2.38	0.54
7:F:36:ILE:O	7:F:40:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CZ2	4:C:437:ARG:HG2	2.39	0.54
25:C:501:CLA:H203	27:C:515:BCR:H14C	1.89	0.54
25:C:508:CLA:NC	25:C:510:CLA:H51	2.22	0.54
5:D:106:GLN:HE21	6:E:48:GLY:HA3	1.72	0.54
16:Q:192:ASP:HA	16:Q:195:LEU:HD12	1.88	0.54
18:X:90:ILE:HA	18:X:93:VAL:HG22	1.88	0.54
25:B:504:CLA:H111	25:B:514:CLA:H43	1.90	0.54
28:A:410:SQD:H342	11:K:37:PHE:CZ	2.43	0.54
2:B:469:HIS:O	2:B:473:THR:HG23	2.07	0.54
25:B:510:CLA:H62	25:B:512:CLA:HED3	1.89	0.54
6:E:26:THR:HB	35:F:101:HEM:HAB	1.89	0.54
11:K:41:ALA:HB2	27:K:101:BCR:H272	1.89	0.54
28:A:410:SQD:H242	4:C:24:TRP:CD1	2.43	0.53
2:B:468:TRP:CZ2	2:B:472:ARG:HD2	2.42	0.53
3:V:22:VAL:HG22	19:Z:21:VAL:HG13	1.89	0.53
11:K:31:PHE:HA	11:K:34:LEU:HD12	1.90	0.53
15:P:115:ASN:ND2	15:P:221:GLN:HB3	2.23	0.53
19:Z:1:MET:HB2	19:Z:4:ILE:HG12	1.90	0.53
5:D:126:MET:HE3	5:D:143:ALA:O	2.07	0.53
5:D:146:PHE:C	5:D:149:PRO:HD2	2.33	0.53
14:O:106:VAL:HG21	14:O:278:LYS:HE3	1.90	0.53
2:B:240:SER:HB2	25:B:509:CLA:C3B	2.38	0.53
25:B:505:CLA:H142	25:B:509:CLA:H2	1.91	0.53
35:F:101:HEM:HBA2	35:F:101:HEM:HHA	1.91	0.53
1:A:224:ILE:O	1:A:225:ARG:C	2.51	0.53
5:D:77:ALA:CB	5:D:174:GLY:HA3	2.38	0.53
26:D:402:PHO:H143	25:D:404:CLA:H171	1.89	0.53
1:A:25:GLU:HG3	4:C:458:ARG:HB2	1.90	0.53
5:D:298:PHE:HA	12:L:38:ASN:ND2	2.23	0.53
1:A:206:PHE:CD2	26:D:402:PHO:HBB2	2.44	0.53
1:A:211:PHE:HE2	1:A:278:TRP:CD2	2.27	0.53
2:B:6:TYR:HB2	30:B:519:LHG:H371	1.90	0.53
30:B:521:LHG:H151	12:L:24:LEU:HD13	1.90	0.53
4:C:104:VAL:HG13	27:C:516:BCR:H333	1.91	0.53
1:A:137:LEU:HA	4:C:457:MET:HE1	1.89	0.53
1:A:203:ALA:HA	25:A:406:CLA:O2A	2.07	0.53
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.44	0.53
25:B:509:CLA:H203	25:B:514:CLA:C2D	2.39	0.53
25:C:506:CLA:C1C	25:C:507:CLA:H122	2.39	0.53
16:Q:179:SER:O	16:Q:183:LYS:HB2	2.08	0.53
19:Z:5:LEU:HD13	19:Z:61:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:129:GLU:H	4:C:129:GLU:CD	2.15	0.53
4:C:163:LEU:HD21	25:C:501:CLA:HED2	1.91	0.53
31:C:517:DGD:HB41	29:W:201:LMG:H371	1.91	0.53
19:Z:9:LEU:O	19:Z:13:ILE:HG13	2.09	0.53
2:B:360:PRO:HB2	2:B:363:PHE:CD1	2.43	0.53
25:C:501:CLA:HMB1	27:C:515:BCR:H23C	1.91	0.53
5:D:58:TRP:O	6:E:64:PRO:HD2	2.09	0.53
5:D:303:ILE:HG12	14:O:220:LEU:HD11	1.91	0.53
1:A:35:VAL:HA	27:A:409:BCR:C32	2.38	0.52
1:A:69:GLY:O	1:A:73:TYR:HB2	2.09	0.52
2:B:122:LEU:HD12	8:H:27:GLY:HA2	1.90	0.52
2:B:475:PHE:CG	5:D:140:PRO:HD3	2.44	0.52
4:C:15:ASP:HB3	11:K:46:ARG:HB3	1.91	0.52
4:C:295:PRO:HB3	4:C:346:PHE:HB3	1.91	0.52
15:P:114:ASN:HA	15:P:221:GLN:O	2.10	0.52
1:A:224:ILE:HA	5:D:265:ARG:NH1	2.25	0.52
1:A:250:ALA:HA	1:A:255:PHE:CE1	2.43	0.52
5:D:199:MET:HE3	5:D:281:MET:HB3	1.92	0.52
30:D:408:LHG:H272	12:L:23:LEU:HD22	1.89	0.52
6:E:25:ILE:C	6:E:28:PRO:HD2	2.34	0.52
26:A:407:PHO:HBB1	26:A:407:PHO:HMB3	1.91	0.52
2:B:470:GLY:O	2:B:474:ILE:HG12	2.09	0.52
4:C:262:TYR:HB3	25:C:507:CLA:C3B	2.39	0.52
5:D:91:PHE:CE1	25:D:405:CLA:HAA2	2.45	0.52
12:L:32:PHE:O	12:L:36:ILE:HG12	2.09	0.52
1:A:300:PHE:HB3	1:A:302:PHE:CE2	2.45	0.52
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.43	0.52
25:B:501:CLA:HHC	25:B:501:CLA:CBB	2.37	0.52
25:B:503:CLA:H162	25:B:508:CLA:HAC1	1.91	0.52
3:V:7:LEU:HD21	11:K:20:PRO:HG2	1.90	0.52
5:D:38:PHE:HB2	5:D:39:PRO:HD3	1.92	0.52
16:Q:148:LYS:HB3	16:Q:148:LYS:NZ	2.25	0.52
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.92	0.52
1:A:38:ILE:HG22	27:A:409:BCR:H343	1.91	0.52
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.44	0.52
1:A:140:ARG:NH2	5:D:222:LEU:HB2	2.24	0.52
25:A:405:CLA:H192	25:D:401:CLA:H111	1.91	0.52
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.90	0.52
4:C:80:ILE:HG22	4:C:85:TYR:HB2	1.90	0.52
29:C:520:LMG:H211	11:K:30:VAL:HG11	1.91	0.52
1:A:214:MET:O	1:A:218:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:PHE:O	2:B:148:LEU:HG	2.09	0.52
2:B:333:GLY:HA2	2:B:440:ASP:OD1	2.08	0.52
25:B:503:CLA:C1D	25:B:505:CLA:H51	2.38	0.52
25:B:508:CLA:HBB1	25:B:508:CLA:HMB3	1.91	0.52
4:C:36:LYS:HG2	4:C:126:GLU:HA	1.90	0.52
1:A:278:TRP:HA	28:A:410:SQD:H161	1.90	0.52
2:B:71:ILE:CD1	2:B:96:VAL:HG21	2.39	0.52
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.44	0.52
4:C:245:TRP:HB2	4:C:247:TRP:NE1	2.25	0.52
31:C:519:DGD:HG32	10:J:35:TYR:CZ	2.45	0.52
1:A:27:ARG:HD3	1:A:27:ARG:C	2.34	0.52
1:A:111:PRO:O	1:A:115:ILE:HG13	2.10	0.52
25:A:408:CLA:HBA1	29:W:201:LMG:H122	1.91	0.52
27:A:409:BCR:H321	27:A:409:BCR:HC8	1.92	0.52
27:C:516:BCR:H391	11:K:36:ALA:HB2	1.92	0.52
5:D:134:ARG:HA	5:D:134:ARG:NE	2.24	0.52
25:D:404:CLA:HHC	25:D:404:CLA:CBB	2.40	0.52
11:K:43:VAL:HG12	11:K:46:ARG:H	1.74	0.52
25:B:504:CLA:H11	25:B:505:CLA:ND	2.24	0.52
25:B:510:CLA:H8	25:B:512:CLA:HED3	1.91	0.52
4:C:168:MET:HB2	4:C:169:TYR:CE1	2.45	0.52
4:C:267:ILE:HG12	25:C:502:CLA:HAC1	1.92	0.52
25:C:505:CLA:H43	27:C:515:BCR:HC7	1.92	0.52
5:D:26:ARG:O	5:D:27:PHE:C	2.53	0.52
26:D:402:PHO:HBB1	26:D:402:PHO:CMB	2.38	0.52
14:O:137:GLY:HA2	14:O:152:ASP:CG	2.35	0.52
16:Q:57:LEU:HD23	16:Q:58:PHE:N	2.24	0.52
16:Q:87:PHE:HB3	16:Q:91:ARG:HH12	1.75	0.52
1:A:181:ASN:HD22	5:D:314:PHE:HD1	1.57	0.51
1:A:245:THR:HB	33:D:403:BCT:O1	2.10	0.51
25:B:510:CLA:C3B	25:B:512:CLA:HMA2	2.41	0.51
3:V:8:THR:OG1	11:K:20:PRO:HB3	2.11	0.51
4:C:408:VAL:HB	4:C:413:TRP:HE1	1.75	0.51
25:C:501:CLA:H203	27:C:515:BCR:C14	2.40	0.51
20:U:95:LEU:HD12	20:U:107:LYS:HG3	1.91	0.51
4:C:68:PRO:HG3	16:Q:81:GLN:CD	2.34	0.51
25:C:511:CLA:H203	19:Z:20:VAL:HA	1.92	0.51
25:D:405:CLA:H12	25:D:405:CLA:C4A	2.40	0.51
14:O:86:GLU:OE2	14:O:251:VAL:HB	2.09	0.51
15:P:75:PHE:HZ	15:P:234:GLU:HA	1.76	0.51
1:A:86:SER:HB3	1:A:89:ILE:HD13	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:410:SQD:H242	4:C:24:TRP:CG	2.45	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.92	0.51
2:B:145:LEU:HD13	2:B:148:LEU:HD12	1.92	0.51
5:D:198:MET:HB3	25:D:401:CLA:O1D	2.09	0.51
2:B:264:PRO:HD2	2:B:268:PHE:HE2	1.75	0.51
5:D:189:HIS:HA	5:D:294:ARG:NE	2.25	0.51
10:J:40:SER:O	10:J:42:LEU:HG	2.11	0.51
15:P:173:VAL:HG12	15:P:187:TYR:HD1	1.75	0.51
15:P:184:TYR:CE2	15:P:208:THR:HG21	2.44	0.51
21:W:60:LEU:HD12	21:W:62:ASP:O	2.10	0.51
1:A:43:THR:O	1:A:47:VAL:HG12	2.10	0.51
1:A:53:ILE:C	1:A:70:SER:HB2	2.36	0.51
25:B:509:CLA:H192	25:B:514:CLA:HMD2	1.93	0.51
25:B:512:CLA:H52	25:B:512:CLA:HMA3	1.93	0.51
21:W:91:THR:O	21:W:95:ILE:HG13	2.10	0.51
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.70	0.51
2:B:187:ALA:HB2	25:B:501:CLA:HMD3	1.92	0.51
2:B:315:ILE:HD12	2:B:321:LYS:HG3	1.91	0.51
25:B:508:CLA:H43	25:H:101:CLA:H91	1.93	0.51
27:D:406:BCR:H23C	27:D:406:BCR:H291	1.92	0.51
14:O:101:PRO:HG3	14:O:174:PHE:CE2	2.45	0.51
15:P:134:GLN:NE2	15:P:175:THR:HB	2.25	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.93	0.51
4:C:176:THR:HG23	4:C:177:TRP:CD1	2.46	0.51
25:C:506:CLA:C1C	25:C:507:CLA:H152	2.40	0.51
5:D:37:LEU:HD22	5:D:125:PHE:HA	1.92	0.51
5:D:87:HIS:C	8:H:69:ASN:HD21	2.19	0.51
2:B:18:ARG:HG3	2:B:118:TRP:CB	2.40	0.51
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.46	0.51
3:V:26:LEU:HA	3:V:29:ARG:HH21	1.75	0.51
4:C:105:LEU:HA	27:C:514:BCR:H10C	1.93	0.51
5:D:104:TRP:HH2	5:D:113:PHE:HB2	1.76	0.51
6:E:16:SER:HA	10:J:7:THR:N	2.24	0.51
8:H:50:MET:O	8:H:54:ILE:HG13	2.11	0.51
11:K:24:VAL:O	11:K:27:VAL:HG22	2.10	0.51
1:A:76:ASN:O	1:A:80:GLY:N	2.40	0.51
1:A:93:PHE:CE2	1:A:95:PRO:HG3	2.46	0.51
2:B:247:TRP:CD2	25:B:503:CLA:H151	2.46	0.51
5:D:154:VAL:O	5:D:158:LEU:HB2	2.10	0.51
16:Q:124:ALA:O	16:Q:127:GLN:HB3	2.10	0.51
2:B:25:MET:HG3	27:B:516:BCR:H23C	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LEU:O	25:B:507:CLA:H43	2.11	0.51
4:C:249:ARG:HA	4:C:254:TRP:HE1	1.75	0.51
14:O:140:LYS:HG3	14:O:148:GLU:HB3	1.92	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
2:B:198:ILE:HG21	25:B:503:CLA:HED3	1.92	0.50
4:C:30:LEU:HD23	25:C:511:CLA:HED2	1.92	0.50
4:C:180:GLY:O	16:Q:136:ARG:HG3	2.11	0.50
15:P:226:ARG:H	15:P:226:ARG:HD2	1.76	0.50
20:U:93:LEU:HB3	20:U:96:ASP:CG	2.36	0.50
4:C:365:LEU:HA	4:C:368:LEU:HB2	1.93	0.50
25:C:511:CLA:C3B	27:C:516:BCR:H393	2.41	0.50
31:C:518:DGD:HA61	10:J:31:PHE:CE1	2.46	0.50
5:D:253:TRP:CG	34:D:407:PL9:HC71	2.46	0.50
1:A:27:ARG:HH21	17:T:24:ARG:HE	1.58	0.50
2:B:210:VAL:O	2:B:214:LEU:HG	2.11	0.50
25:B:509:CLA:HHC	25:B:509:CLA:CBB	2.41	0.50
25:B:513:CLA:H71	27:B:516:BCR:H20C	1.93	0.50
4:C:36:LYS:HE3	4:C:126:GLU:HG2	1.93	0.50
4:C:96:THR:HA	4:C:99:TYR:CD1	2.47	0.50
4:C:394:SER:HA	4:C:408:VAL:HG23	1.92	0.50
5:D:103:ARG:HH21	6:E:77:LYS:HA	1.75	0.50
5:D:269:PHE:O	5:D:272:LEU:HG	2.11	0.50
21:W:80:VAL:O	21:W:84:VAL:HG13	2.11	0.50
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.92	0.50
2:B:8:VAL:HB	25:B:513:CLA:O1D	2.12	0.50
2:B:38:ALA:O	2:B:42:ILE:HG12	2.11	0.50
2:B:46:ASP:H	2:B:58:GLN:CD	2.19	0.50
25:C:511:CLA:CHA	25:C:511:CLA:HBA2	2.40	0.50
8:H:36:GLU:HB2	8:H:39:LYS:HD3	1.93	0.50
20:U:93:LEU:HG	20:U:95:LEU:H	1.77	0.50
1:A:296:ASN:HD22	4:C:388:PRO:HG2	1.77	0.50
25:B:509:CLA:H193	25:B:511:CLA:HMD2	1.93	0.50
4:C:83:LEU:HD11	25:C:503:CLA:HBA1	1.92	0.50
5:D:55:VAL:HG21	5:D:110:LEU:HD12	1.94	0.50
14:O:122:THR:HG22	14:O:164:LEU:HA	1.94	0.50
1:A:51:ALA:HA	1:A:55:ALA:HB2	1.92	0.50
1:A:124:TYR:CD2	25:C:505:CLA:H152	2.47	0.50
25:B:507:CLA:H2	29:B:518:LMG:H161	1.94	0.50
4:C:13:GLY:HA2	25:C:511:CLA:O1A	2.12	0.50
15:P:99:PHE:HB3	15:P:100:PRO:HD2	1.93	0.50
16:Q:115:PHE:HB3	16:Q:120:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:14:ARG:HH11	4:C:14:ARG:HA	1.76	0.50
14:O:95:GLU:OE2	14:O:291:LYS:HD2	2.11	0.50
15:P:170:LEU:HD11	15:P:173:VAL:HG13	1.93	0.50
15:P:124:ASP:O	15:P:126:LYS:HD3	2.12	0.50
16:Q:83:VAL:HG13	16:Q:89:GLN:HE22	1.77	0.50
2:B:26:HIS:O	2:B:30:VAL:HG23	2.11	0.50
2:B:91:TRP:CD1	25:B:506:CLA:HBD	2.47	0.50
2:B:205:ALA:HA	25:B:502:CLA:HBC2	1.94	0.50
4:C:37:LEU:HD11	25:C:509:CLA:C1C	2.42	0.50
2:B:6:TYR:O	25:B:510:CLA:HBD	2.12	0.49
4:C:24:TRP:CE3	30:D:409:LHG:H102	2.47	0.49
4:C:94:ILE:HG13	4:C:95:ASP:H	1.77	0.49
12:L:37:PHE:HA	13:M:3:VAL:N	2.27	0.49
16:Q:123:GLU:O	16:Q:127:GLN:N	2.42	0.49
2:B:246:PHE:CZ	25:B:508:CLA:HBC2	2.47	0.49
2:B:327:THR:HB	29:B:518:LMG:HC8	1.93	0.49
2:B:343:HIS:O	2:B:401:PHE:HA	2.11	0.49
4:C:318:SER:HA	14:O:157:TYR:CE1	2.47	0.49
4:C:381:ALA:HB1	16:Q:75:ARG:HG3	1.94	0.49
6:E:68:ASP:H	6:E:75:GLN:NE2	2.03	0.49
11:K:25:LEU:O	11:K:28:ILE:HG12	2.12	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.93	0.49
2:B:257:TRP:CZ2	2:B:272:ARG:HG2	2.48	0.49
2:B:369:LEU:HD11	5:D:341:PHE:HD1	1.77	0.49
25:B:508:CLA:CHD	25:H:101:CLA:H101	2.42	0.49
4:C:104:VAL:O	4:C:108:ILE:HG12	2.12	0.49
12:L:37:PHE:O	13:M:3:VAL:HB	2.11	0.49
14:O:164:LEU:HD11	14:O:168:GLU:HB3	1.93	0.49
14:O:234:VAL:HG12	14:O:235:LYS:N	2.26	0.49
1:A:278:TRP:HA	28:A:410:SQD:C16	2.42	0.49
1:A:284:TRP:CD1	4:C:423:PHE:HZ	2.30	0.49
31:C:517:DGD:HB62	29:W:201:LMG:H411	1.95	0.49
5:D:77:ALA:HB2	5:D:174:GLY:HA3	1.95	0.49
5:D:89:LEU:HG	8:H:69:ASN:OD1	2.12	0.49
5:D:111:TRP:HE1	5:D:172:SER:HA	1.77	0.49
5:D:189:HIS:HA	5:D:294:ARG:CD	2.42	0.49
5:D:223:PHE:CZ	5:D:245:SER:HB2	2.48	0.49
6:E:53:ASN:H	6:E:53:ASN:HD22	1.61	0.49
8:H:51:ALA:O	8:H:55:LEU:HG	2.13	0.49
15:P:78:TYR:CE2	15:P:104:LEU:HD22	2.47	0.49
2:B:124:ARG:HA	2:B:131:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:PHE:CE1	2:B:203:ILE:HG23	2.47	0.49
2:B:164:PRO:HG3	25:B:506:CLA:O2D	2.12	0.49
2:B:167:TRP:HE3	2:B:178:VAL:HG23	1.76	0.49
2:B:256:MET:HA	2:B:263:THR:HG21	1.94	0.49
1:A:156:ALA:HA	1:A:160:VAL:HB	1.94	0.49
25:B:509:CLA:H111	25:B:514:CLA:CAA	2.42	0.49
4:C:247:TRP:CD1	21:W:103:LEU:HD22	2.47	0.49
4:C:254:TRP:HZ3	25:C:507:CLA:HMC1	1.75	0.49
18:X:82:VAL:O	18:X:86:ILE:HG13	2.13	0.49
21:W:81:LEU:O	21:W:85:LEU:HG	2.12	0.49
2:B:126:PRO:HD3	8:H:31:ARG:HH12	1.77	0.49
25:B:509:CLA:H111	25:B:514:CLA:HAA2	1.94	0.49
25:C:504:CLA:H42	31:C:518:DGD:HB31	1.95	0.49
14:O:95:GLU:HG2	14:O:289:GLN:O	2.12	0.49
14:O:247:SER:O	14:O:260:GLY:HA3	2.11	0.49
4:C:35:GLY:HA3	4:C:125:PRO:O	2.12	0.49
4:C:96:THR:HA	4:C:99:TYR:HD1	1.77	0.49
5:D:218:VAL:HG13	5:D:244:TYR:CD1	2.48	0.49
2:B:171:PRO:HA	8:H:84:LEU:HD12	1.95	0.49
2:B:172:TYR:CZ	2:B:283:GLU:HB2	2.48	0.49
25:C:501:CLA:HHC	25:C:501:CLA:HBB1	1.95	0.49
1:A:135:PHE:O	9:I:32:PRO:HD3	2.13	0.49
2:B:41:GLU:CD	2:B:62:VAL:HG22	2.38	0.49
2:B:74:SER:HA	2:B:92:SER:HB2	1.95	0.49
25:B:508:CLA:CMD	25:B:509:CLA:HAB	2.43	0.49
4:C:334:THR:O	14:O:69:GLY:HA2	2.12	0.49
27:D:406:BCR:C40	10:J:27:LEU:HB2	2.30	0.49
26:A:407:PHO:H161	25:D:401:CLA:H142	1.95	0.48
2:B:16:PRO:HB2	2:B:123:PHE:CD1	2.47	0.48
2:B:144:PHE:HD2	2:B:145:LEU:HD22	1.77	0.48
2:B:251:VAL:HG22	25:B:502:CLA:H102	1.93	0.48
3:V:19:GLY:HA3	27:K:101:BCR:H15C	1.93	0.48
25:C:506:CLA:HBB1	25:C:506:CLA:CMB	2.42	0.48
5:D:274:VAL:HG22	34:D:407:PL9:H222	1.95	0.48
9:I:9:TYR:HB3	21:W:85:LEU:HD21	1.94	0.48
14:O:53:THR:OG1	14:O:56:GLU:HG3	2.14	0.48
4:C:73:GLY:HA3	31:C:518:DGD:HE2	1.94	0.48
4:C:191:THR:O	4:C:223:GLY:HA3	2.14	0.48
4:C:207:GLY:HA2	31:C:517:DGD:O2D	2.13	0.48
5:D:80:THR:HB	5:D:81:PRO:HD2	1.95	0.48
21:W:74:PHE:CD2	29:W:201:LMG:H292	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TRP:HA	9:I:1:MET:SD	2.54	0.48
1:A:196:PRO:CB	31:C:519:DGD:HAT1	2.43	0.48
25:A:405:CLA:H61	25:D:401:CLA:CAB	2.43	0.48
2:B:127:ARG:HH22	8:H:37:ALA:HB3	1.78	0.48
2:B:450:TRP:CD1	25:B:507:CLA:HMA2	2.48	0.48
6:E:27:VAL:HB	6:E:28:PRO:HD3	1.94	0.48
1:A:140:ARG:HH22	5:D:222:LEU:HB2	1.77	0.48
2:B:238:LEU:O	2:B:242:ILE:HG13	2.13	0.48
25:B:512:CLA:HED1	25:B:512:CLA:H51	1.96	0.48
4:C:106:HIS:CE1	32:C:521:LMU:H81	2.47	0.48
4:C:108:ILE:HB	27:C:514:BCR:C12	2.38	0.48
4:C:277:MET:HB3	4:C:285:TYR:HE1	1.77	0.48
4:C:367:LYS:O	4:C:372:ILE:HG12	2.12	0.48
5:D:315:TYR:O	5:D:319:ILE:HG12	2.13	0.48
25:A:408:CLA:HBC3	9:I:7:PHE:HE2	1.78	0.48
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.94	0.48
2:B:283:GLU:O	2:B:287:ARG:HG2	2.12	0.48
25:B:507:CLA:NB	29:B:518:LMG:H152	2.28	0.48
25:C:507:CLA:H112	27:C:515:BCR:C16	2.43	0.48
25:C:509:CLA:H151	25:C:509:CLA:CAD	2.42	0.48
10:J:10:ILE:HD11	10:J:15:VAL:HG21	1.96	0.48
14:O:121:LYS:O	14:O:165:PRO:HD3	2.14	0.48
14:O:175:THR:OG1	14:O:177:LYS:HG3	2.13	0.48
14:O:227:GLU:C	14:O:229:LEU:N	2.72	0.48
16:Q:148:LYS:HZ3	16:Q:149:GLU:H	1.61	0.48
2:B:9:HIS:CE1	25:B:510:CLA:H11	2.49	0.48
25:C:504:CLA:HAB	29:C:520:LMG:C42	2.44	0.48
15:P:99:PHE:O	15:P:102:VAL:HG23	2.14	0.48
19:Z:37:LYS:HB2	19:Z:41:PHE:CZ	2.48	0.48
1:A:281:ILE:HG12	30:D:409:LHG:H352	1.94	0.48
25:B:514:CLA:HBD	25:B:514:CLA:HBA2	1.95	0.48
14:O:130:TYR:HH	21:W:60:LEU:HA	1.79	0.48
14:O:229:LEU:O	14:O:234:VAL:HG23	2.14	0.48
19:Z:33:TRP:CD1	19:Z:37:LYS:HZ1	2.32	0.48
20:U:97:LYS:C	20:U:97:LYS:HD3	2.38	0.48
1:A:21:ILE:HG21	1:A:32:TRP:CE3	2.48	0.48
25:A:405:CLA:HAB	5:D:182:ILE:HD13	1.94	0.48
2:B:13:ILE:HA	25:B:511:CLA:HAC2	1.96	0.48
2:B:328:GLY:HA2	29:B:518:LMG:O6	2.13	0.48
4:C:187:ILE:HG23	4:C:219:GLU:OE1	2.14	0.48
4:C:260:LEU:O	4:C:264:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:320:GLN:CG	4:C:324:GLY:HA2	2.43	0.48
25:C:501:CLA:H101	25:C:507:CLA:H92	1.96	0.48
9:I:20:ILE:O	9:I:24:LEU:HG	2.14	0.48
16:Q:184:LEU:O	16:Q:188:LYS:HG3	2.14	0.48
25:B:508:CLA:H142	25:D:405:CLA:HMB1	1.95	0.48
25:B:508:CLA:H202	5:D:120:PHE:HE2	1.78	0.48
25:B:512:CLA:H92	25:B:512:CLA:H61	1.72	0.48
4:C:389:LEU:HD13	4:C:398:VAL:HA	1.95	0.48
25:C:501:CLA:HMB2	25:C:501:CLA:H71	1.96	0.48
25:C:505:CLA:HBC2	27:C:515:BCR:H341	1.94	0.48
5:D:91:PHE:HE1	25:D:405:CLA:HAA2	1.79	0.48
14:O:150:LYS:HB2	14:O:150:LYS:NZ	2.28	0.48
1:A:140:ARG:HB2	5:D:220:ASN:HA	1.96	0.48
1:A:283:ILE:HA	1:A:286:THR:HG22	1.96	0.48
2:B:9:HIS:ND1	25:B:510:CLA:H11	2.28	0.48
2:B:10:THR:HG23	25:B:510:CLA:HAA2	1.95	0.48
2:B:183:PRO:HB2	2:B:185:TRP:NE1	2.28	0.48
4:C:174:TYR:CE2	4:C:183:ASP:HA	2.49	0.48
14:O:124:LEU:HA	14:O:162:VAL:HG23	1.96	0.48
1:A:58:VAL:HG22	1:A:106:LEU:O	2.14	0.47
1:A:201:GLY:HA3	1:A:286:THR:HB	1.95	0.47
2:B:121:GLU:HG3	8:H:31:ARG:HE	1.78	0.47
2:B:252:VAL:HG22	25:B:503:CLA:O2A	2.13	0.47
2:B:450:TRP:CH2	25:B:507:CLA:H12	2.49	0.47
25:B:507:CLA:HBC2	27:B:516:BCR:H311	1.95	0.47
6:E:71:ASN:HD22	20:U:113:ILE:HG22	1.79	0.47
21:W:60:LEU:HD13	21:W:61:VAL:H	1.77	0.47
4:C:142:LYS:HD3	4:C:254:TRP:CE2	2.49	0.47
7:F:26:ALA:O	7:F:30:ILE:HG12	2.14	0.47
9:I:2:LEU:O	9:I:6:ILE:HG13	2.14	0.47
11:K:45:PHE:O	11:K:46:ARG:C	2.57	0.47
1:A:37:MET:HB2	1:A:125:CYS:CB	2.43	0.47
2:B:283:GLU:HA	2:B:286:LYS:HZ3	1.78	0.47
2:B:478:VAL:HG12	5:D:139:ARG:HG3	1.96	0.47
25:B:507:CLA:H93	25:B:507:CLA:H111	1.68	0.47
27:B:517:BCR:HC21	29:B:518:LMG:H202	1.96	0.47
3:V:10:VAL:O	3:V:14:LEU:HG	2.14	0.47
25:C:506:CLA:C1D	25:C:507:CLA:H18	2.44	0.47
5:D:239:GLN:HE22	5:D:243:THR:HB	1.79	0.47
7:F:18:ARG:O	7:F:22:ILE:HG12	2.14	0.47
16:Q:195:LEU:HA	16:Q:198:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:46:LEU:O	19:Z:50:LEU:HG	2.14	0.47
1:A:38:ILE:CG2	27:A:409:BCR:H343	2.44	0.47
25:A:406:CLA:HBA1	25:A:406:CLA:H12	1.69	0.47
25:A:408:CLA:C4	25:A:408:CLA:H102	2.44	0.47
2:B:30:VAL:HG21	25:B:511:CLA:H91	1.96	0.47
2:B:57:ARG:NH2	2:B:331:ASN:HA	2.29	0.47
2:B:118:TRP:CZ2	12:L:5:ASN:HA	2.49	0.47
4:C:399:ALA:O	4:C:400:THR:C	2.57	0.47
25:C:511:CLA:H203	19:Z:20:VAL:HG22	1.97	0.47
12:L:8:LYS:HD2	12:L:8:LYS:C	2.40	0.47
14:O:103:SER:HA	21:W:61:VAL:HG23	1.97	0.47
14:O:228:GLU:O	14:O:232:GLU:HG2	2.14	0.47
1:A:18:CYS:HA	1:A:32:TRP:HH2	1.80	0.47
1:A:57:PRO:HB2	1:A:66:PRO:HB2	1.96	0.47
2:B:453:PHE:HB2	5:D:291:LEU:HD12	1.97	0.47
25:B:510:CLA:H2A	25:B:510:CLA:HED2	1.95	0.47
4:C:458:ARG:HG3	4:C:459:PRO:HD2	1.96	0.47
25:C:501:CLA:H193	25:C:506:CLA:C1B	2.44	0.47
25:C:508:CLA:HBC3	25:C:510:CLA:H92	1.97	0.47
5:D:302:GLU:HG2	5:D:315:TYR:OH	2.15	0.47
25:A:405:CLA:H203	25:D:401:CLA:H72	1.96	0.47
2:B:229:LEU:CD2	25:H:101:CLA:HBA1	2.44	0.47
2:B:288:VAL:HG21	2:B:302:TRP:CZ3	2.50	0.47
4:C:354:LEU:O	4:C:358:ARG:HG3	2.15	0.47
1:A:140:ARG:CZ	5:D:222:LEU:HB2	2.45	0.47
1:A:224:ILE:HD12	5:D:265:ARG:NH1	2.29	0.47
1:A:300:PHE:HZ	31:C:519:DGD:HB52	1.79	0.47
4:C:286:PRO:HB2	4:C:289:PHE:CD2	2.49	0.47
4:C:379:ARG:HG3	4:C:383:TYR:CE2	2.49	0.47
4:C:413:TRP:CD1	25:C:504:CLA:HMA2	2.49	0.47
27:C:516:BCR:C10	27:K:101:BCR:HC42	2.44	0.47
29:C:520:LMG:H142	11:K:24:VAL:HG22	1.97	0.47
5:D:122:LEU:HD23	26:D:402:PHO:H42	1.96	0.47
5:D:177:ALA:O	5:D:180:ARG:HG3	2.15	0.47
5:D:191:TRP:CE2	5:D:197:HIS:HB2	2.50	0.47
5:D:196:PHE:HA	5:D:199:MET:HE2	1.97	0.47
5:D:298:PHE:HA	12:L:38:ASN:HD21	1.80	0.47
34:D:407:PL9:H401	30:D:408:LHG:H212	1.95	0.47
16:Q:81:GLN:HA	16:Q:84:ARG:HE	1.78	0.47
20:U:111:LYS:HB2	20:U:111:LYS:NZ	2.30	0.47
27:A:409:BCR:H11C	27:A:409:BCR:H341	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:TRP:HB2	2:B:430:PHE:CE2	2.49	0.47
2:B:342:GLY:HA3	2:B:403:GLY:O	2.15	0.47
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.47
25:B:513:CLA:H62	25:B:513:CLA:H2	1.63	0.47
5:D:160:TYR:HA	5:D:290:ALA:CB	2.45	0.47
8:H:50:MET:SD	25:H:101:CLA:HAA1	2.54	0.47
15:P:138:LEU:HA	15:P:141:VAL:HG12	1.95	0.47
1:A:254:TYR:CG	5:D:136:VAL:HG13	2.49	0.47
28:A:410:SQD:H382	11:K:33:ILE:HD13	1.97	0.47
2:B:224:ARG:HD3	8:H:44:TRP:CE2	2.50	0.47
3:V:15:VAL:HG13	27:K:101:BCR:C10	2.45	0.47
4:C:287:SER:HA	4:C:411:ARG:HH21	1.79	0.47
4:C:310:GLN:OE1	4:C:369:LYS:HA	2.15	0.47
5:D:286:VAL:HG21	25:D:404:CLA:HED2	1.97	0.47
8:H:63:ILE:O	8:H:67:ILE:HG13	2.15	0.47
12:L:12:GLU:HA	13:M:29:THR:HG21	1.96	0.47
1:A:35:VAL:HG13	27:A:409:BCR:HC31	1.97	0.47
1:A:131:TRP:CD2	25:C:505:CLA:HMA1	2.50	0.47
1:A:256:GLY:C	1:A:258:LEU:N	2.72	0.47
2:B:25:MET:HE3	2:B:111:SER:HB3	1.96	0.47
2:B:44:VAL:HG23	2:B:60:MET:HE1	1.97	0.47
2:B:122:LEU:HD11	8:H:30:LEU:CB	2.39	0.47
2:B:247:TRP:CH2	25:B:502:CLA:H93	2.50	0.47
2:B:441:GLY:HA3	14:O:223:ARG:HD3	1.97	0.47
25:C:510:CLA:H121	25:C:510:CLA:C17	2.45	0.47
5:D:320:LEU:HD11	14:O:205:PRO:O	2.15	0.47
5:D:336:HIS:O	5:D:338:ARG:HG3	2.15	0.47
6:E:19:TYR:HA	6:E:22:ILE:HD12	1.97	0.47
11:K:25:LEU:HA	11:K:28:ILE:HG12	1.97	0.47
1:A:127:MET:HG2	1:A:144:ALA:HB1	1.97	0.46
25:A:406:CLA:H2	26:D:402:PHO:CAB	2.44	0.46
4:C:218:MET:SD	4:C:221:ILE:HD12	2.55	0.46
4:C:250:ARG:NH2	21:W:102:ASP:HA	2.29	0.46
4:C:354:LEU:HG	4:C:358:ARG:HE	1.79	0.46
8:H:72:LEU:CD1	18:X:69:LEU:HA	2.45	0.46
14:O:52:LEU:HA	14:O:56:GLU:OE1	2.15	0.46
1:A:137:LEU:HD12	1:A:139:MET:SD	2.55	0.46
1:A:176:ILE:HG22	1:A:180:PHE:CE2	2.51	0.46
1:A:301:ASN:C	4:C:393:ASN:HD21	2.23	0.46
25:A:406:CLA:H2A	25:A:406:CLA:HED2	1.98	0.46
2:B:249:ALA:HB3	2:B:459:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:501:CLA:HAB	25:B:502:CLA:HMC2	1.97	0.46
27:B:517:BCR:H323	29:B:518:LMG:H141	1.96	0.46
4:C:211:TRP:CE2	29:W:201:LMG:H342	2.49	0.46
25:C:504:CLA:CAA	31:C:518:DGD:HD61	2.45	0.46
7:F:25:ILE:C	7:F:28:PRO:HD2	2.41	0.46
8:H:59:ALA:O	8:H:63:ILE:HG13	2.16	0.46
16:Q:146:LYS:HB2	16:Q:151:LYS:HA	1.96	0.46
16:Q:181:ALA:O	16:Q:185:GLU:HG2	2.15	0.46
1:A:49:ILE:HA	34:D:407:PL9:H503	1.98	0.46
1:A:135:PHE:HD2	1:A:136:ARG:HH11	1.63	0.46
1:A:308:ASP:OD1	1:A:312:ARG:N	2.48	0.46
2:B:96:VAL:HG22	25:B:506:CLA:HBA1	1.98	0.46
25:C:506:CLA:CHC	25:C:507:CLA:H122	2.46	0.46
12:L:30:VAL:HG22	17:T:9:LEU:HB3	1.97	0.46
15:P:147:LYS:HE3	16:Q:52:LEU:HG	1.98	0.46
21:W:98:ILE:HA	21:W:101:LYS:NZ	2.30	0.46
25:B:504:CLA:H93	25:B:504:CLA:H62	1.76	0.46
4:C:74:LEU:HD13	4:C:77:LEU:HD22	1.98	0.46
4:C:246:PRO:HD2	21:W:103:LEU:HB2	1.98	0.46
5:D:158:LEU:C	5:D:161:PRO:HD2	2.40	0.46
5:D:319:ILE:O	5:D:323:GLU:HG3	2.16	0.46
11:K:30:VAL:O	11:K:33:ILE:HG22	2.16	0.46
12:L:13:LEU:HD23	13:M:26:TYR:HB2	1.98	0.46
12:L:24:LEU:O	12:L:28:LEU:HG	2.15	0.46
15:P:170:LEU:HD13	15:P:170:LEU:C	2.41	0.46
16:Q:115:PHE:HB2	16:Q:124:ALA:HB2	1.98	0.46
1:A:120:LEU:O	1:A:123:VAL:HG22	2.15	0.46
28:A:410:SQD:H461	5:D:232:PHE:CE2	2.51	0.46
25:B:508:CLA:H202	5:D:120:PHE:CE2	2.50	0.46
25:B:509:CLA:H93	25:B:514:CLA:HAA1	1.98	0.46
31:C:517:DGD:HB41	29:W:201:LMG:C39	2.37	0.46
14:O:132:LEU:HB3	14:O:135:MET:SD	2.56	0.46
1:A:161:TYR:HA	1:A:294:ALA:HB1	1.96	0.46
1:A:258:LEU:HD22	5:D:132:ILE:HG23	1.98	0.46
1:A:300:PHE:CZ	31:C:519:DGD:HB52	2.51	0.46
2:B:454:GLY:HA3	29:B:518:LMG:H192	1.96	0.46
25:B:506:CLA:H11	25:B:506:CLA:H52	1.68	0.46
4:C:272:PHE:CB	31:C:517:DGD:HB92	2.45	0.46
4:C:360:PRO:HG3	16:Q:122:THR:HG21	1.97	0.46
9:I:25:SER:O	9:I:26:ASN:C	2.57	0.46
1:A:36:ILE:HA	25:A:408:CLA:HBB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB3	25:A:405:CLA:H11	1.97	0.46
2:B:30:VAL:HG13	25:B:512:CLA:HMC2	1.96	0.46
2:B:247:TRP:HB2	25:B:508:CLA:CBC	2.38	0.46
27:B:516:BCR:C14	27:B:517:BCR:H11C	2.45	0.46
27:D:406:BCR:C20	29:D:410:LMG:H332	2.45	0.46
10:J:27:LEU:HA	10:J:30:PHE:CD2	2.50	0.46
14:O:189:LYS:HG3	14:O:245:VAL:HG22	1.98	0.46
14:O:238:LYS:HD3	15:P:153:GLU:CD	2.40	0.46
1:A:273:PHE:CE2	28:A:410:SQD:H112	2.51	0.46
25:A:405:CLA:H72	25:A:405:CLA:H111	1.29	0.46
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.97	0.46
2:B:441:GLY:HA2	14:O:222:ALA:HB3	1.98	0.46
25:B:510:CLA:H121	25:B:512:CLA:H151	1.98	0.46
27:B:517:BCR:HC31	29:B:518:LMG:H142	1.97	0.46
4:C:75:ILE:C	4:C:78:PRO:HD2	2.40	0.46
5:D:189:HIS:CE1	5:D:294:ARG:HH21	2.34	0.46
5:D:191:TRP:CZ2	5:D:197:HIS:HB2	2.51	0.46
7:F:26:ALA:HB1	35:F:101:HEM:CAC	2.46	0.46
15:P:129:ALA:HA	15:P:185:TYR:OH	2.15	0.46
15:P:228:PHE:HE1	15:P:229:LYS:HZ3	1.64	0.46
1:A:295:PHE:HB2	4:C:416:CYS:SG	2.56	0.46
2:B:120:LEU:HB2	2:B:123:PHE:CD2	2.51	0.46
25:C:506:CLA:CBB	25:C:507:CLA:H61	2.46	0.46
14:O:101:PRO:HB3	14:O:282:VAL:CG1	2.46	0.46
14:O:110:SER:HB3	14:O:115:GLY:CA	2.45	0.46
16:Q:108:ILE:HD11	16:Q:132:VAL:HG11	1.98	0.46
2:B:171:PRO:HG2	8:H:85:ALA:HB2	1.98	0.46
2:B:362:PHE:HE1	5:D:189:HIS:HE2	1.63	0.46
25:B:501:CLA:HBD	25:B:501:CLA:C2	2.46	0.46
25:B:508:CLA:H102	5:D:120:PHE:CE1	2.51	0.46
4:C:199:GLY:O	4:C:203:LYS:HG3	2.16	0.46
25:C:511:CLA:H12	25:C:511:CLA:HBA1	1.67	0.46
16:Q:146:LYS:NZ	16:Q:198:VAL:HA	2.31	0.46
1:A:246:TYR:O	1:A:247:ASN:C	2.59	0.45
2:B:57:ARG:HB3	2:B:331:ASN:OD1	2.16	0.45
4:C:94:ILE:HG13	4:C:95:ASP:N	2.30	0.45
14:O:271:ASP:HB3	14:O:274:ALA:HB3	1.98	0.45
16:Q:182:LYS:O	16:Q:186:ILE:HG13	2.16	0.45
1:A:48:PHE:CD1	26:A:407:PHO:H112	2.51	0.45
25:B:513:CLA:H3A	25:B:513:CLA:HBA2	1.47	0.45
4:C:387:ALA:HB1	4:C:388:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:510:CLA:HBB1	25:C:510:CLA:CMB	2.43	0.45
25:D:405:CLA:H91	25:D:405:CLA:HMD2	1.98	0.45
7:F:32:PHE:O	7:F:36:ILE:HG13	2.16	0.45
16:Q:83:VAL:HG13	16:Q:89:GLN:NE2	2.31	0.45
16:Q:101:VAL:HG21	16:Q:142:LEU:CD1	2.40	0.45
1:A:290:LEU:HA	1:A:293:MET:HE3	1.97	0.45
2:B:350:GLU:HG3	2:B:352:ARG:NH1	2.31	0.45
25:B:509:CLA:H13	25:B:514:CLA:CBA	2.46	0.45
4:C:269:VAL:HG13	29:W:201:LMG:H391	1.99	0.45
5:D:104:TRP:CH2	5:D:113:PHE:HB2	2.50	0.45
15:P:69:VAL:HG11	15:P:72:LYS:HG3	1.98	0.45
16:Q:98:LYS:HD2	16:Q:199:LEU:HD13	1.98	0.45
2:B:145:LEU:HA	2:B:148:LEU:HD12	1.98	0.45
4:C:197:ILE:HG13	4:C:227:TRP:CD1	2.52	0.45
4:C:357:LEU:HD21	4:C:376:GLN:OE1	2.16	0.45
25:C:501:CLA:ND	25:C:503:CLA:H62	2.31	0.45
25:C:504:CLA:H51	31:C:519:DGD:HB72	1.98	0.45
7:F:35:ALA:O	7:F:39:MET:HG3	2.17	0.45
9:I:12:VAL:HG11	29:W:201:LMG:H151	1.99	0.45
15:P:94:SER:CB	15:P:105:ARG:HD2	2.42	0.45
18:X:72:PHE:CE2	18:X:76:LEU:HD11	2.51	0.45
21:W:102:ASP:N	21:W:102:ASP:OD1	2.49	0.45
1:A:32:TRP:HB2	9:I:23:PHE:CE2	2.51	0.45
4:C:125:PRO:HG2	4:C:128:LEU:HD23	1.98	0.45
4:C:140:LYS:HB3	4:C:140:LYS:HZ2	1.79	0.45
5:D:50:THR:HG23	5:D:54:PHE:CE1	2.51	0.45
27:D:406:BCR:H14C	7:F:32:PHE:CE2	2.52	0.45
29:D:410:LMG:H312	29:D:410:LMG:C19	2.46	0.45
12:L:8:LYS:HD2	12:L:9:GLN:N	2.32	0.45
17:T:29:MET:HE3	17:T:30:ILE:HG12	1.98	0.45
2:B:25:MET:HG2	2:B:111:SER:OG	2.17	0.45
2:B:29:LEU:HD13	25:B:512:CLA:HMD3	1.99	0.45
2:B:369:LEU:HD11	5:D:341:PHE:CD1	2.51	0.45
25:C:501:CLA:HHC	25:C:501:CLA:CBB	2.46	0.45
5:D:220:ASN:HD21	30:D:409:LHG:H252	1.81	0.45
6:E:10:PHE:O	6:E:14:LEU:HD23	2.16	0.45
14:O:102:THR:H	14:O:284:GLY:CA	2.30	0.45
15:P:134:GLN:HG2	15:P:185:TYR:CD2	2.52	0.45
1:A:157:VAL:HG11	25:D:401:CLA:CMC	2.46	0.45
1:A:256:GLY:C	1:A:258:LEU:H	2.25	0.45
2:B:475:PHE:HB2	2:B:479:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:277:MET:HG3	25:C:501:CLA:H12	1.97	0.45
5:D:312:GLU:HB2	14:O:205:PRO:HG3	1.99	0.45
16:Q:129:ARG:O	16:Q:130:ARG:C	2.58	0.45
16:Q:136:ARG:HG2	16:Q:162:ILE:HD12	1.99	0.45
1:A:31:GLY:O	1:A:35:VAL:HG23	2.16	0.45
1:A:93:PHE:HB2	4:C:206:PHE:CG	2.51	0.45
2:B:98:ALA:O	2:B:102:ILE:HG12	2.16	0.45
2:B:167:TRP:HA	2:B:178:VAL:HA	1.98	0.45
2:B:340:TRP:O	2:B:405:GLU:HG3	2.17	0.45
25:B:507:CLA:O1A	29:B:518:LMG:H151	2.16	0.45
4:C:224:GLY:HA3	27:C:515:BCR:H402	1.98	0.45
4:C:322:PRO:HB3	14:O:201:SER:OG	2.17	0.45
5:D:149:PRO:O	25:D:404:CLA:H52	2.17	0.45
16:Q:111:ASP:O	16:Q:112:LEU:HB3	2.16	0.45
1:A:69:GLY:HA2	1:A:75:ASN:OD1	2.17	0.45
25:B:509:CLA:H121	25:B:509:CLA:O1A	2.17	0.45
25:B:513:CLA:H93	27:B:516:BCR:C36	2.44	0.45
4:C:262:TYR:CD1	25:C:505:CLA:HMD1	2.52	0.45
25:C:509:CLA:HBB1	25:C:509:CLA:CMB	2.46	0.45
25:C:509:CLA:H203	25:C:512:CLA:HAC1	1.98	0.45
25:C:510:CLA:H61	25:C:510:CLA:H2	1.61	0.45
29:D:410:LMG:H292	29:D:410:LMG:H172	1.99	0.45
14:O:228:GLU:HA	14:O:231:LYS:HZ3	1.81	0.45
14:O:241:LYS:HB2	14:O:241:LYS:NZ	2.32	0.45
15:P:75:PHE:HB3	15:P:86:LEU:HB3	1.98	0.45
15:P:167:ALA:HA	16:Q:56:ASP:OD1	2.17	0.45
16:Q:97:THR:O	16:Q:101:VAL:HG23	2.17	0.45
21:W:64:ARG:HB2	21:W:66:ASN:HD21	1.82	0.45
25:A:408:CLA:H143	29:W:201:LMG:H131	1.98	0.45
2:B:15:ASP:HB2	12:L:7:ASN:ND2	2.32	0.45
2:B:28:ALA:HB2	2:B:107:LEU:HB2	1.99	0.45
2:B:134:ASP:O	2:B:138:ILE:HG13	2.17	0.45
4:C:211:TRP:CE3	4:C:212:ILE:HG12	2.52	0.45
4:C:350:ARG:HD2	14:O:63:LEU:HD21	1.99	0.45
4:C:439:ALA:HA	4:C:444:GLU:OE1	2.17	0.45
25:C:504:CLA:C1B	31:C:518:DGD:HB82	2.46	0.45
5:D:342:PRO:O	5:D:345:VAL:HG12	2.17	0.45
14:O:128:LEU:HA	14:O:130:TYR:CE2	2.51	0.45
14:O:130:TYR:OH	21:W:60:LEU:HD13	2.17	0.45
16:Q:112:LEU:HA	16:Q:115:PHE:CD2	2.52	0.45
16:Q:149:GLU:HA	16:Q:152:LYS:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:CA	27:A:409:BCR:H272	2.45	0.44
1:A:249:VAL:HA	1:A:254:TYR:CE1	2.52	0.44
2:B:102:ILE:HA	27:B:517:BCR:C40	2.47	0.44
4:C:197:ILE:HG21	4:C:227:TRP:CD1	2.52	0.44
4:C:453:PRO:HB2	4:C:457:MET:HE3	1.98	0.44
9:I:27:ASP:N	9:I:28:PRO:CD	2.80	0.44
25:B:505:CLA:H41	25:B:505:CLA:H92	1.99	0.44
4:C:370:ASN:O	4:C:371:ASP:CB	2.64	0.44
5:D:19:ASP:HA	5:D:32:TRP:HE1	1.82	0.44
5:D:277:THR:O	5:D:281:MET:HG2	2.17	0.44
14:O:258:ILE:HG13	14:O:286:TRP:HZ3	1.83	0.44
15:P:99:PHE:CE1	15:P:144:LEU:HA	2.53	0.44
2:B:18:ARG:HA	2:B:21:SER:HG	1.83	0.44
2:B:139:PHE:CD1	25:B:509:CLA:HED2	2.51	0.44
2:B:159:THR:O	2:B:180:PRO:HB3	2.17	0.44
2:B:373:LYS:HD3	20:U:92:THR:HG22	1.98	0.44
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.98	0.44
25:B:506:CLA:HBA2	25:B:506:CLA:H3A	1.66	0.44
3:V:5:LEU:O	3:V:9:LEU:HG	2.17	0.44
4:C:137:TYR:HB2	4:C:145:MET:HE1	1.98	0.44
4:C:215:VAL:HG21	4:C:221:ILE:HG12	2.00	0.44
25:C:504:CLA:H102	31:C:518:DGD:HBF1	1.99	0.44
5:D:230:ASN:ND2	5:D:233:ARG:HG2	2.32	0.44
5:D:274:VAL:N	5:D:275:PRO:HD2	2.32	0.44
14:O:163:GLN:HE21	14:O:167:GLY:HA2	1.81	0.44
2:B:288:VAL:CG2	2:B:305:ILE:HD11	2.44	0.44
2:B:475:PHE:CD2	5:D:140:PRO:HD3	2.52	0.44
25:B:514:CLA:HMA2	25:B:515:CLA:CBB	2.47	0.44
30:B:519:LHG:HC62	5:D:269:PHE:CE1	2.53	0.44
26:D:402:PHO:HBA2	26:D:402:PHO:H3A	1.76	0.44
20:U:99:ASP:N	20:U:100:PRO:HD2	2.33	0.44
29:W:201:LMG:H391	29:W:201:LMG:C43	2.48	0.44
1:A:35:VAL:HA	27:A:409:BCR:H323	2.00	0.44
1:A:97:TRP:HB2	21:W:65:MET:CE	2.47	0.44
2:B:120:LEU:HG	8:H:22:LEU:HD23	1.99	0.44
2:B:354:LEU:HB3	2:B:370:LEU:HB3	1.99	0.44
25:B:510:CLA:H12	25:B:510:CLA:H51	1.72	0.44
29:C:520:LMG:H202	11:K:27:VAL:HB	2.00	0.44
15:P:214:LYS:HD2	15:P:216:TYR:CZ	2.51	0.44
1:A:18:CYS:HA	1:A:32:TRP:CH2	2.52	0.44
1:A:193:LEU:HD11	25:A:405:CLA:HMC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:409:BCR:H321	27:A:409:BCR:C8	2.48	0.44
2:B:61:PHE:C	2:B:64:PRO:HD2	2.43	0.44
25:B:503:CLA:NC	25:B:505:CLA:H93	2.32	0.44
25:B:504:CLA:H111	25:B:514:CLA:H11	1.98	0.44
4:C:104:VAL:HG22	27:C:516:BCR:HC41	1.99	0.44
4:C:277:MET:HB3	4:C:285:TYR:CE1	2.51	0.44
4:C:447:ILE:HB	5:D:223:PHE:CD1	2.53	0.44
32:C:521:LMU:H11	32:C:521:LMU:H42	1.26	0.44
5:D:87:HIS:CD2	5:D:166:GLY:HA2	2.53	0.44
5:D:226:GLY:HA3	5:D:234:ALA:HB2	2.00	0.44
15:P:148:GLN:CD	15:P:165:VAL:HG22	2.42	0.44
2:B:46:ASP:N	2:B:58:GLN:OE1	2.50	0.44
4:C:247:TRP:HH2	25:C:506:CLA:H12	1.82	0.44
6:E:18:ARG:O	6:E:22:ILE:HG13	2.18	0.44
9:I:19:PHE:CE2	9:I:23:PHE:HE2	2.36	0.44
12:L:12:GLU:HA	13:M:29:THR:CG2	2.48	0.44
12:L:18:LEU:HD22	13:M:26:TYR:CG	2.53	0.44
1:A:50:ILE:HG22	27:A:409:BCR:H271	1.99	0.44
1:A:267:ASN:ND2	1:A:269:ARG:H	2.15	0.44
2:B:30:VAL:HG22	25:B:512:CLA:C3C	2.48	0.44
2:B:144:PHE:CE1	2:B:210:VAL:HG13	2.53	0.44
2:B:224:ARG:HD3	8:H:44:TRP:CD2	2.53	0.44
2:B:264:PRO:HD2	2:B:268:PHE:CE2	2.52	0.44
2:B:275:TRP:CE2	2:B:315:ILE:HG12	2.53	0.44
3:V:16:VAL:HG22	27:K:101:BCR:H363	2.00	0.44
4:C:14:ARG:HG2	4:C:19:THR:HG21	2.00	0.44
25:C:505:CLA:H3A	25:C:505:CLA:HBA2	1.44	0.44
16:Q:142:LEU:HB3	16:Q:198:VAL:HB	2.00	0.44
17:T:29:MET:O	17:T:30:ILE:C	2.61	0.44
18:X:72:PHE:CE1	18:X:76:LEU:HD21	2.53	0.44
1:A:35:VAL:HA	27:A:409:BCR:H322	1.99	0.44
2:B:70:GLY:O	2:B:72:THR:HG23	2.18	0.44
2:B:458:PHE:HB3	25:B:504:CLA:HBC2	1.99	0.44
25:B:501:CLA:H2	25:B:501:CLA:HAA1	1.98	0.44
25:B:505:CLA:H3A	25:B:505:CLA:HBA2	1.36	0.44
25:B:506:CLA:H93	25:B:506:CLA:H62	1.80	0.44
25:B:508:CLA:C1A	25:B:508:CLA:CGA	2.96	0.44
30:B:519:LHG:H382	30:B:519:LHG:H351	1.64	0.44
30:B:521:LHG:H182	12:L:27:VAL:HG21	2.00	0.44
4:C:311:ARG:HD2	16:Q:68:PHE:CD1	2.53	0.44
6:E:57:THR:HG23	6:E:60:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:GLU:HB3	8:H:72:LEU:HB2	2.00	0.44
14:O:123:LYS:HG3	14:O:163:GLN:HB3	2.00	0.44
16:Q:143:ALA:HA	16:Q:146:LYS:HD3	1.99	0.44
1:A:63:ILE:HA	4:C:325:LEU:HD22	2.00	0.43
1:A:258:LEU:HD12	1:A:258:LEU:N	2.27	0.43
1:A:296:ASN:ND2	4:C:388:PRO:HG2	2.33	0.43
26:A:407:PHO:HBA2	26:A:407:PHO:H3A	1.65	0.43
2:B:141:ILE:O	2:B:145:LEU:HD23	2.18	0.43
25:B:507:CLA:H201	13:M:11:THR:CA	2.42	0.43
4:C:22:ALA:HB3	4:C:24:TRP:CE2	2.52	0.43
4:C:154:ILE:O	4:C:158:LEU:HD13	2.18	0.43
25:C:508:CLA:H8	25:C:510:CLA:HED3	1.99	0.43
25:C:509:CLA:H151	25:C:509:CLA:C3D	2.47	0.43
6:E:31:PHE:CZ	7:F:34:GLY:HA2	2.53	0.43
14:O:61:THR:OG1	14:O:64:GLN:HG3	2.18	0.43
14:O:140:LYS:HD3	14:O:140:LYS:C	2.43	0.43
16:Q:63:VAL:HA	16:Q:66:ARG:NE	2.33	0.43
1:A:97:TRP:HB2	21:W:65:MET:HE3	1.99	0.43
1:A:291:SER:O	1:A:294:ALA:HB3	2.18	0.43
25:B:503:CLA:H41	25:B:503:CLA:H61	1.73	0.43
4:C:41:HIS:CB	25:C:512:CLA:HMD1	2.48	0.43
10:J:32:TYR:CE1	10:J:36:VAL:HG11	2.52	0.43
14:O:234:VAL:O	14:O:235:LYS:C	2.61	0.43
15:P:119:ILE:HD12	15:P:144:LEU:HD21	2.00	0.43
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.99	0.43
1:A:209:SER:HB2	26:D:402:PHO:HMC2	2.01	0.43
1:A:210:LEU:HG	26:D:402:PHO:ND	2.33	0.43
2:B:26:HIS:CE1	25:B:511:CLA:HMA2	2.53	0.43
25:B:510:CLA:ND	25:B:512:CLA:H42	2.33	0.43
4:C:408:VAL:HB	4:C:413:TRP:NE1	2.33	0.43
27:C:516:BCR:H11C	27:C:516:BCR:H341	1.84	0.43
6:E:13:ILE:HG21	35:F:101:HEM:HAD1	2.00	0.43
15:P:116:LEU:HD12	15:P:117:VAL:N	2.33	0.43
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.53	0.43
1:A:51:ALA:C	1:A:53:ILE:H	2.26	0.43
1:A:103:ASP:HB2	14:O:125:MET:HE1	2.01	0.43
25:A:405:CLA:H141	25:D:401:CLA:H122	2.00	0.43
2:B:46:ASP:H	2:B:58:GLN:NE2	2.16	0.43
2:B:193:TYR:HB2	8:H:83:THR:HB	2.00	0.43
3:V:25:LEU:HB3	3:V:29:ARG:NH2	2.32	0.43
4:C:104:VAL:HG11	27:C:514:BCR:C5	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:453:PRO:O	4:C:457:MET:HG3	2.19	0.43
25:C:502:CLA:H42	25:C:503:CLA:C4C	2.48	0.43
25:H:101:CLA:H93	25:H:101:CLA:H62	1.77	0.43
15:P:78:TYR:HE2	15:P:83:PHE:CE2	2.35	0.43
25:B:507:CLA:H18	13:M:14:PHE:CD2	2.54	0.43
3:V:15:VAL:HG11	11:K:28:ILE:HD12	2.01	0.43
4:C:224:GLY:HA3	27:C:515:BCR:C40	2.49	0.43
4:C:458:ARG:HD3	4:C:459:PRO:HD2	1.99	0.43
25:C:506:CLA:HBB2	25:C:507:CLA:H61	2.01	0.43
5:D:134:ARG:HA	5:D:134:ARG:HE	1.83	0.43
5:D:199:MET:HG2	34:D:407:PL9:H321	2.01	0.43
5:D:339:LEU:HD13	5:D:341:PHE:HZ	1.84	0.43
16:Q:138:ASP:O	16:Q:141:THR:HG22	2.18	0.43
1:A:120:LEU:HB2	25:C:505:CLA:H193	2.01	0.43
1:A:283:ILE:O	1:A:286:THR:HG22	2.19	0.43
25:A:408:CLA:CMC	27:A:409:BCR:H12C	2.48	0.43
2:B:406:LEU:O	2:B:409:LEU:HB2	2.18	0.43
25:B:503:CLA:C16	25:B:508:CLA:HAC1	2.49	0.43
25:B:504:CLA:HHC	25:B:510:CLA:H201	2.01	0.43
4:C:144:LYS:HE3	4:C:148:ILE:HD11	2.01	0.43
4:C:301:GLN:HB2	4:C:384:MET:HG3	2.00	0.43
4:C:398:VAL:O	4:C:399:ALA:HB2	2.18	0.43
25:C:502:CLA:H112	25:C:502:CLA:H93	1.61	0.43
5:D:123:ILE:O	5:D:127:LEU:HG	2.18	0.43
6:E:64:PRO:HB3	6:E:79:LEU:HB3	2.00	0.43
6:E:67:THR:HB	20:U:112:ASP:CG	2.44	0.43
14:O:77:LEU:HD11	14:O:252:ASP:CB	2.47	0.43
14:O:181:GLY:HA2	14:O:189:LYS:O	2.18	0.43
16:Q:136:ARG:CZ	16:Q:162:ILE:HG23	2.49	0.43
2:B:49:ASP:OD2	2:B:52:LEU:HB2	2.18	0.43
2:B:292:LEU:HD13	2:B:301:ALA:HB2	2.00	0.43
2:B:466:HIS:CE1	25:B:508:CLA:C4D	3.02	0.43
25:B:501:CLA:H91	25:B:501:CLA:H111	1.82	0.43
3:V:29:ARG:HH22	19:Z:25:VAL:HG22	1.83	0.43
6:E:72:ALA:O	6:E:73:LEU:C	2.61	0.43
8:H:33:LEU:H	8:H:33:LEU:HD12	1.84	0.43
14:O:53:THR:O	14:O:57:ILE:HG13	2.19	0.43
14:O:262:PHE:HZ	14:O:282:VAL:HG12	1.83	0.43
15:P:85:LEU:HB3	15:P:242:PHE:HA	2.00	0.43
15:P:170:LEU:HD23	15:P:189:LEU:HG	2.01	0.43
19:Z:56:ILE:O	19:Z:60:PHE:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:HD2	15:P:89:ALA:O	2.19	0.43
2:B:17:GLY:HA2	2:B:123:PHE:CZ	2.54	0.43
2:B:45:PHE:HA	2:B:60:MET:HE3	2.00	0.43
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.99	0.43
25:B:511:CLA:H122	25:B:511:CLA:H162	1.92	0.43
3:V:4:GLU:HA	3:V:7:LEU:HD23	2.00	0.43
4:C:186:VAL:O	4:C:188:THR:HG23	2.19	0.43
25:C:501:CLA:H52	25:C:503:CLA:C9	2.48	0.43
25:C:504:CLA:NB	31:C:518:DGD:HB62	2.33	0.43
25:C:508:CLA:H152	25:C:510:CLA:H202	2.01	0.43
31:C:518:DGD:HB51	29:C:520:LMG:H381	2.01	0.43
5:D:19:ASP:HA	5:D:32:TRP:NE1	2.34	0.43
14:O:127:ARG:HA	21:W:64:ARG:NH2	2.33	0.43
1:A:149:ALA:N	1:A:150:PRO:HD2	2.34	0.43
1:A:254:TYR:OH	5:D:138:LEU:HD21	2.19	0.43
1:A:326:LEU:HD13	1:A:326:LEU:HA	1.79	0.43
25:B:507:CLA:H93	29:B:518:LMG:H331	2.01	0.43
25:B:508:CLA:HBB1	25:B:508:CLA:CMB	2.48	0.43
25:B:508:CLA:C4C	25:H:101:CLA:H101	2.48	0.43
25:B:511:CLA:H11	25:B:511:CLA:H52	1.70	0.43
30:B:521:LHG:H172	30:B:521:LHG:H201	1.82	0.43
3:V:15:VAL:HG11	11:K:28:ILE:CD1	2.48	0.43
4:C:311:ARG:HD3	16:Q:66:ARG:HG3	2.00	0.43
25:C:513:CLA:CHA	25:C:513:CLA:HBA2	2.44	0.43
29:D:410:LMG:H141	29:D:410:LMG:C10	2.48	0.43
7:F:29:THR:O	7:F:33:LEU:HG	2.18	0.43
13:M:21:PHE:O	13:M:25:LEU:HG	2.18	0.43
14:O:84:LEU:HD22	14:O:251:VAL:HG23	2.00	0.43
15:P:176:THR:O	15:P:184:TYR:N	2.51	0.43
16:Q:102:LYS:HE2	16:Q:199:LEU:HD22	2.00	0.43
19:Z:11:ALA:HA	19:Z:14:PHE:CD2	2.53	0.43
1:A:215:HIS:O	1:A:219:VAL:HG23	2.18	0.43
28:A:410:SQD:H5	5:D:232:PHE:HB2	2.00	0.43
27:B:517:BCR:HC31	29:B:518:LMG:C14	2.49	0.43
4:C:134:PHE:CZ	25:C:512:CLA:HAB	2.32	0.43
4:C:238:TRP:CH2	4:C:245:TRP:HZ2	2.37	0.43
31:C:518:DGD:HA21	29:C:520:LMG:H301	2.00	0.43
14:O:265:ILE:N	14:O:265:ILE:HD12	2.33	0.43
15:P:67:GLY:C	15:P:68:LYS:HD3	2.44	0.43
17:T:4:LEU:HD23	17:T:4:LEU:C	2.44	0.43
1:A:257:ARG:HA	1:A:260:PHE:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:405:CLA:H192	25:D:401:CLA:H8	2.01	0.42
2:B:220:ARG:HB3	2:B:221:PRO:HD2	2.01	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.54	0.42
25:B:510:CLA:C3D	30:B:519:LHG:H362	2.49	0.42
4:C:108:ILE:HG22	27:C:514:BCR:H353	2.01	0.42
4:C:151:TYR:O	4:C:155:MET:HG2	2.18	0.42
5:D:308:ASP:OD1	5:D:310:GLU:HG2	2.19	0.42
6:E:24:SER:O	6:E:28:PRO:HG2	2.19	0.42
7:F:40:GLN:OE1	10:J:33:GLY:HA3	2.19	0.42
16:Q:151:LYS:O	16:Q:155:LEU:HG	2.19	0.42
25:A:408:CLA:HBB1	25:A:408:CLA:HMB3	2.00	0.42
2:B:30:VAL:HG22	25:B:512:CLA:C4C	2.49	0.42
2:B:394:GLN:HB3	16:Q:52:LEU:CD1	2.49	0.42
4:C:183:ASP:OD1	16:Q:136:ARG:NH2	2.51	0.42
5:D:306:ALA:HA	14:O:208:ARG:HH21	1.83	0.42
11:K:28:ILE:N	11:K:29:PRO:CD	2.82	0.42
14:O:153:ASP:CG	14:O:154:GLY:H	2.27	0.42
16:Q:159:LYS:NZ	16:Q:163:GLN:HB2	2.34	0.42
2:B:22:VAL:HG22	25:B:513:CLA:HMB2	2.02	0.42
2:B:25:MET:CE	2:B:108:PHE:HA	2.48	0.42
4:C:378:ARG:O	4:C:382:GLU:HG3	2.18	0.42
29:D:410:LMG:HC71	7:F:40:GLN:HE22	1.84	0.42
6:E:66:ILE:HD11	6:E:72:ALA:CB	2.49	0.42
9:I:14:PHE:O	9:I:18:LEU:HD13	2.20	0.42
9:I:21:PHE:HA	9:I:24:LEU:HD12	2.01	0.42
15:P:85:LEU:N	15:P:85:LEU:HD23	2.34	0.42
15:P:201:ARG:HD3	15:P:221:GLN:OE1	2.19	0.42
16:Q:129:ARG:O	16:Q:132:VAL:N	2.52	0.42
19:Z:5:LEU:HD23	19:Z:5:LEU:C	2.44	0.42
30:B:521:LHG:H301	30:B:521:LHG:H272	1.58	0.42
4:C:165:TRP:HZ2	4:C:170:PHE:CE1	2.38	0.42
4:C:379:ARG:HD2	4:C:379:ARG:HA	1.88	0.42
4:C:392:LEU:HG	31:C:519:DGD:HB31	2.02	0.42
25:C:501:CLA:HMD2	25:C:503:CLA:H12	1.99	0.42
25:D:401:CLA:H92	30:D:408:LHG:H181	2.01	0.42
18:X:77:ILE:O	18:X:81:THR:HG23	2.19	0.42
1:A:127:MET:CG	1:A:144:ALA:HB1	2.49	0.42
4:C:37:LEU:HD23	4:C:137:TYR:OH	2.20	0.42
4:C:217:ASN:HD22	16:Q:173:ARG:HH21	1.66	0.42
29:C:520:LMG:C14	11:K:24:VAL:HG22	2.50	0.42
5:D:21:TRP:O	5:D:24:GLN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:102:THR:HG22	6:E:46:VAL:O	2.19	0.42
6:E:25:ILE:N	6:E:25:ILE:HD12	2.34	0.42
25:H:101:CLA:H91	25:H:101:CLA:H121	2.01	0.42
2:B:343:HIS:CE1	2:B:345:SER:HB2	2.55	0.42
25:B:507:CLA:H202	25:B:507:CLA:H162	1.78	0.42
4:C:48:ILE:HG23	25:C:510:CLA:HMC1	2.01	0.42
4:C:452:GLU:HB3	4:C:455:LEU:HD22	2.01	0.42
25:C:507:CLA:H2A	25:C:507:CLA:CED	2.48	0.42
25:C:507:CLA:HBD	25:C:509:CLA:H122	2.01	0.42
5:D:96:GLU:O	5:D:98:GLN:HG3	2.19	0.42
6:E:66:ILE:HD11	6:E:72:ALA:HB1	2.02	0.42
8:H:33:LEU:HD12	8:H:33:LEU:N	2.33	0.42
8:H:44:TRP:HB3	8:H:47:THR:HB	2.01	0.42
14:O:145:GLY:O	14:O:185:LEU:N	2.53	0.42
20:U:112:ASP:O	20:U:113:ILE:C	2.62	0.42
21:W:101:LYS:HD2	21:W:101:LYS:N	2.34	0.42
1:A:93:PHE:C	1:A:95:PRO:HD3	2.44	0.42
1:A:258:LEU:H	1:A:258:LEU:CD1	2.27	0.42
2:B:371:LEU:HD12	2:B:371:LEU:N	2.34	0.42
25:B:501:CLA:CBD	25:B:501:CLA:H102	2.50	0.42
25:B:503:CLA:HMB1	25:B:503:CLA:CBB	2.49	0.42
25:B:512:CLA:H52	25:B:512:CLA:H11	1.74	0.42
3:V:13:VAL:O	3:V:16:VAL:HG12	2.20	0.42
3:V:26:LEU:CD1	3:V:31:GLY:HA3	2.49	0.42
4:C:144:LYS:O	4:C:148:ILE:HG13	2.20	0.42
4:C:230:THR:O	4:C:234:LEU:HG	2.20	0.42
4:C:249:ARG:HA	4:C:254:TRP:CZ2	2.55	0.42
14:O:206:LYS:NZ	14:O:206:LYS:HB3	2.34	0.42
14:O:211:SER:OG	15:P:165:VAL:HG11	2.20	0.42
1:A:37:MET:HB2	1:A:125:CYS:HB2	2.01	0.42
1:A:64:ARG:CG	4:C:325:LEU:HD11	2.49	0.42
1:A:180:PHE:O	1:A:184:ILE:HG13	2.20	0.42
1:A:315:ASN:HD21	15:P:109:ASN:HD21	1.68	0.42
25:A:406:CLA:HED1	5:D:175:VAL:HG22	2.02	0.42
25:B:509:CLA:H161	25:B:509:CLA:CAD	2.50	0.42
4:C:140:LYS:O	4:C:142:LYS:N	2.52	0.42
4:C:179:PRO:HG3	16:Q:169:ASP:OD2	2.20	0.42
4:C:227:TRP:O	4:C:231:LEU:HD13	2.20	0.42
19:Z:38:GLY:HA2	19:Z:41:PHE:CD2	2.55	0.42
1:A:38:ILE:N	1:A:39:PRO:HD2	2.34	0.42
25:A:405:CLA:H191	30:D:408:LHG:H202	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HG2	2:B:115:TRP:HA	2.02	0.42
2:B:235:GLU:HB3	2:B:473:THR:HG22	2.01	0.42
2:B:343:HIS:HE1	2:B:345:SER:HB2	1.85	0.42
2:B:479:PHE:CZ	5:D:140:PRO:HD2	2.55	0.42
4:C:14:ARG:HA	4:C:14:ARG:NH1	2.35	0.42
5:D:55:VAL:HG21	5:D:110:LEU:CD1	2.50	0.42
15:P:227:TRP:CE2	15:P:232:LYS:HD3	2.55	0.42
16:Q:190:LYS:O	16:Q:194:VAL:HG23	2.19	0.42
1:A:138:GLY:CA	9:I:32:PRO:HG3	2.50	0.42
2:B:22:VAL:HG21	25:B:511:CLA:CAB	2.50	0.42
2:B:32:GLY:HA3	27:B:517:BCR:C17	2.49	0.42
2:B:445:SER:HB2	5:D:293:LEU:HD21	2.02	0.42
25:B:504:CLA:H102	25:B:504:CLA:H13	1.56	0.42
25:B:508:CLA:H92	25:B:508:CLA:H62	1.67	0.42
25:B:509:CLA:H111	25:B:509:CLA:H93	1.83	0.42
4:C:274:ALA:HB2	25:C:502:CLA:HMD2	2.02	0.42
15:P:134:GLN:HG2	15:P:185:TYR:CG	2.54	0.42
18:X:73:LEU:HA	18:X:76:LEU:HD12	2.01	0.42
1:A:255:PHE:HB2	1:A:257:ARG:HG3	2.00	0.41
2:B:362:PHE:HE1	5:D:189:HIS:NE2	2.18	0.41
2:B:409:LEU:HB3	2:B:411:PHE:CZ	2.55	0.41
14:O:84:LEU:CB	14:O:185:LEU:HD13	2.50	0.41
15:P:64:ASN:HD21	15:P:67:GLY:HA3	1.84	0.41
1:A:64:ARG:CZ	14:O:126:THR:HG21	2.51	0.41
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.02	0.41
1:A:196:PRO:HB2	31:C:519:DGD:CBB	2.51	0.41
2:B:251:VAL:HG11	25:B:503:CLA:H42	2.01	0.41
25:B:513:CLA:H72	25:B:513:CLA:C1C	2.50	0.41
4:C:292:PRO:HB3	4:C:383:TYR:CD1	2.54	0.41
25:C:510:CLA:NA	25:C:510:CLA:H122	2.35	0.41
12:L:7:ASN:O	12:L:9:GLN:HG2	2.19	0.41
12:L:26:PHE:HE1	17:T:9:LEU:HA	1.85	0.41
1:A:35:VAL:HG11	9:I:18:LEU:HB3	2.02	0.41
2:B:33:TRP:CG	25:B:512:CLA:HBC1	2.55	0.41
2:B:156:PHE:HA	2:B:161:VAL:CG2	2.50	0.41
2:B:390:TYR:HB2	5:D:344:GLU:OE2	2.20	0.41
25:B:514:CLA:HBB1	25:B:514:CLA:CMB	2.48	0.41
4:C:56:ASN:HD21	4:C:102:SER:HB3	1.84	0.41
25:C:509:CLA:H141	25:C:509:CLA:H161	1.90	0.41
5:D:261:PHE:HD1	5:D:266:TRP:CD1	2.38	0.41
10:J:13:TRP:CZ2	10:J:14:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:11:LEU:HD11	11:K:22:VAL:HG11	2.02	0.41
14:O:83:ASN:ND2	14:O:85:LYS:H	2.19	0.41
14:O:92:TYR:HB2	14:O:290:LEU:HD22	2.02	0.41
14:O:156:ASP:CG	14:O:177:LYS:HG2	2.45	0.41
15:P:115:ASN:C	15:P:115:ASN:HD22	2.28	0.41
1:A:37:MET:HB2	1:A:125:CYS:HB3	2.02	0.41
1:A:188:ALA:CB	1:A:328:MET:HB2	2.50	0.41
1:A:243:GLU:CD	1:A:243:GLU:H	2.28	0.41
2:B:168:VAL:HB	2:B:179:GLN:OE1	2.20	0.41
25:B:501:CLA:HBD	25:B:501:CLA:H102	2.02	0.41
25:B:513:CLA:H62	27:B:516:BCR:H372	2.01	0.41
29:B:520:LMG:H171	29:B:520:LMG:H141	1.90	0.41
4:C:339:PHE:HE2	4:C:354:LEU:HD21	1.84	0.41
16:Q:121:TRP:O	16:Q:125:ARG:HG3	2.19	0.41
29:W:201:LMG:H401	29:W:201:LMG:H372	1.83	0.41
1:A:46:SER:HB3	27:A:409:BCR:H17C	2.02	0.41
2:B:88:PRO:HB2	2:B:92:SER:HB3	2.02	0.41
2:B:333:GLY:H	2:B:439:SER:CB	2.33	0.41
25:B:512:CLA:H43	30:B:519:LHG:H372	2.03	0.41
4:C:237:ILE:O	4:C:241:TYR:HD1	2.04	0.41
4:C:249:ARG:HA	4:C:254:TRP:NE1	2.36	0.41
4:C:449:ARG:HE	5:D:225:ASP:CG	2.28	0.41
25:C:506:CLA:ND	25:C:507:CLA:H18	2.34	0.41
5:D:43:PHE:HB3	5:D:113:PHE:CZ	2.55	0.41
5:D:88:SER:HB2	6:E:69:ARG:CZ	2.50	0.41
15:P:188:GLU:CD	16:Q:64:ARG:HH22	2.28	0.41
16:Q:136:ARG:C	16:Q:158:ARG:HH21	2.28	0.41
1:A:22:THR:HG22	1:A:136:ARG:HH21	1.86	0.41
1:A:315:ASN:HD21	15:P:109:ASN:ND2	2.19	0.41
4:C:139:TRP:O	4:C:140:LYS:CB	2.64	0.41
4:C:245:TRP:O	4:C:249:ARG:HG3	2.20	0.41
4:C:252:PHE:CE2	25:C:506:CLA:HBA1	2.56	0.41
25:C:510:CLA:HED1	25:C:510:CLA:H72	2.02	0.41
25:C:510:CLA:HBA1	25:C:510:CLA:H3A	1.69	0.41
5:D:51:GLY:HA2	5:D:55:VAL:CG2	2.49	0.41
6:E:26:THR:HB	35:F:101:HEM:CAB	2.49	0.41
14:O:254:VAL:HG13	14:O:255:THR:HG23	2.02	0.41
16:Q:107:ARG:HB3	16:Q:127:GLN:NE2	2.36	0.41
21:W:97:PHE:HD1	21:W:102:ASP:CG	2.28	0.41
1:A:76:ASN:OD1	1:A:77:ILE:N	2.52	0.41
1:A:139:MET:O	4:C:443:PHE:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MET:HB3	25:A:406:CLA:O1D	2.21	0.41
2:B:158:VAL:HG13	2:B:166:ILE:HD13	2.01	0.41
2:B:160:GLY:HA2	2:B:163:GLY:O	2.20	0.41
2:B:275:TRP:O	20:U:102:LYS:HE3	2.21	0.41
25:B:503:CLA:H93	25:B:503:CLA:H62	1.81	0.41
25:B:507:CLA:HBC3	27:B:517:BCR:H10C	2.01	0.41
4:C:14:ARG:HD2	4:C:19:THR:HG23	2.02	0.41
4:C:142:LYS:HB3	4:C:244:PRO:HG2	2.01	0.41
31:C:517:DGD:C4B	29:W:201:LMG:H392	2.40	0.41
14:O:84:LEU:HB3	14:O:185:LEU:HD13	2.02	0.41
2:B:91:TRP:CZ2	25:B:506:CLA:H12	2.56	0.41
2:B:285:GLN:O	2:B:289:GLN:HG2	2.20	0.41
25:B:503:CLA:HMC3	25:B:505:CLA:H161	2.02	0.41
25:B:509:CLA:H172	25:B:511:CLA:CAD	2.51	0.41
4:C:165:TRP:O	4:C:169:TYR:N	2.52	0.41
4:C:269:VAL:HG13	29:W:201:LMG:C43	2.51	0.41
5:D:210:LEU:HD12	5:D:210:LEU:HA	1.84	0.41
7:F:14:ILE:HD12	7:F:14:ILE:N	2.35	0.41
11:K:43:VAL:CG1	11:K:46:ARG:HG3	2.48	0.41
15:P:226:ARG:HD2	15:P:226:ARG:N	2.34	0.41
16:Q:99:LYS:HE2	16:Q:99:LYS:HB3	1.94	0.41
1:A:258:LEU:HB3	5:D:29:PHE:HB2	2.03	0.41
1:A:320:ILE:HD11	5:D:63:LEU:HD21	2.02	0.41
1:A:327:GLY:O	1:A:331:MET:HG2	2.20	0.41
25:A:408:CLA:HBB1	25:A:408:CLA:CMB	2.51	0.41
25:A:408:CLA:HMC1	27:A:409:BCR:H12C	2.03	0.41
2:B:25:MET:HA	2:B:25:MET:CE	2.39	0.41
2:B:141:ILE:N	2:B:217:LEU:HD21	2.36	0.41
2:B:235:GLU:OE2	2:B:472:ARG:HD3	2.21	0.41
2:B:252:VAL:HG12	2:B:451:PHE:HE1	1.86	0.41
3:V:5:LEU:HD13	3:V:5:LEU:C	2.46	0.41
4:C:247:TRP:HA	4:C:250:ARG:NH2	2.35	0.41
4:C:350:ARG:CD	14:O:63:LEU:HD21	2.51	0.41
4:C:395:VAL:HG13	4:C:403:ASN:HA	2.02	0.41
4:C:460:LEU:HB3	4:C:461:ASP:H	1.66	0.41
25:C:507:CLA:H91	27:C:515:BCR:C17	2.51	0.41
5:D:146:PHE:O	5:D:149:PRO:HD2	2.20	0.41
13:M:18:PRO:O	13:M:22:LEU:HG	2.20	0.41
14:O:94:LEU:HG	14:O:97:PHE:HB2	2.03	0.41
14:O:119:PHE:CE2	14:O:281:LYS:HB2	2.56	0.41
14:O:177:LYS:HD2	14:O:195:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:180:LYS:HD3	15:P:182:LYS:NZ	2.36	0.41
16:Q:63:VAL:O	16:Q:68:PHE:HB2	2.21	0.41
16:Q:94:LEU:HD13	16:Q:94:LEU:C	2.46	0.41
16:Q:138:ASP:O	16:Q:142:LEU:HG	2.20	0.41
17:T:10:LEU:O	17:T:14:LEU:HG	2.20	0.41
19:Z:49:LEU:C	19:Z:49:LEU:HD13	2.46	0.41
20:U:110:ARG:NE	20:U:111:LYS:HE3	2.35	0.41
1:A:224:ILE:HA	1:A:224:ILE:HD12	1.95	0.41
2:B:462:PHE:CE1	25:B:504:CLA:HMC1	2.56	0.41
2:B:472:ARG:HA	2:B:479:PHE:CD2	2.56	0.41
4:C:41:HIS:HB3	25:C:512:CLA:OBD	2.20	0.41
4:C:323:THR:HG22	14:O:202:PHE:HE1	1.86	0.41
4:C:337:ILE:HD12	4:C:337:ILE:N	2.36	0.41
25:C:506:CLA:HBB2	25:C:507:CLA:HED1	2.03	0.41
25:C:507:CLA:HED2	25:C:507:CLA:H2	2.02	0.41
5:D:218:VAL:O	5:D:222:LEU:HG	2.21	0.41
6:E:23:HIS:HB3	6:E:27:VAL:HG23	2.02	0.41
15:P:226:ARG:H	15:P:226:ARG:CD	2.34	0.41
1:A:47:VAL:CG1	1:A:115:ILE:HG12	2.49	0.40
1:A:157:VAL:HG11	25:D:401:CLA:HMC2	2.03	0.40
1:A:249:VAL:HA	1:A:254:TYR:HE1	1.85	0.40
1:A:321:ILE:HG23	5:D:183:LEU:CD1	2.51	0.40
2:B:24:LEU:HD21	25:B:515:CLA:HAB	2.02	0.40
2:B:134:ASP:O	2:B:135:LEU:C	2.64	0.40
2:B:225:LEU:HD13	2:B:229:LEU:HD13	2.03	0.40
25:B:501:CLA:H12	25:B:501:CLA:H52	1.89	0.40
3:V:20:PRO:O	3:V:24:VAL:HG23	2.21	0.40
4:C:246:PRO:O	4:C:250:ARG:HG3	2.20	0.40
5:D:180:ARG:HG3	5:D:181:PHE:N	2.36	0.40
5:D:209:LEU:HD23	5:D:209:LEU:C	2.46	0.40
6:E:36:LEU:HA	6:E:39:SER:OG	2.21	0.40
6:E:77:LYS:HG2	6:E:82:ASN:OD1	2.21	0.40
8:H:57:PHE:CZ	8:H:61:LEU:HD21	2.56	0.40
14:O:99:ILE:HD11	14:O:176:ILE:HD13	2.03	0.40
14:O:187:GLY:O	14:O:189:LYS:HD3	2.21	0.40
14:O:215:ASP:O	14:O:233:ASN:HB2	2.21	0.40
16:Q:97:THR:HG21	16:Q:141:THR:CG2	2.51	0.40
16:Q:126:GLU:OE1	16:Q:126:GLU:HA	2.21	0.40
1:A:94:TYR:OH	1:A:104:GLU:HG2	2.21	0.40
2:B:115:TRP:CD2	27:B:516:BCR:H401	2.56	0.40
2:B:226:TYR:HA	2:B:231:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:HD2	1.83	0.40
2:B:280:PHE:O	2:B:284:ILE:HG13	2.21	0.40
25:B:501:CLA:HBD	25:B:501:CLA:H2	2.03	0.40
25:B:503:CLA:H8	25:B:503:CLA:H122	1.72	0.40
30:B:521:LHG:H351	30:B:521:LHG:H382	1.75	0.40
25:C:512:CLA:H12	25:C:512:CLA:HBA2	1.88	0.40
5:D:210:LEU:HD21	5:D:270:PHE:CE2	2.56	0.40
5:D:222:LEU:HD23	5:D:244:TYR:HB3	2.02	0.40
13:M:9:THR:O	13:M:13:LEU:HD13	2.22	0.40
1:A:25:GLU:HG3	4:C:458:ARG:CB	2.51	0.40
1:A:206:PHE:HB3	25:A:406:CLA:H2	2.03	0.40
1:A:340:PRO:CB	15:P:225:LYS:HE2	2.44	0.40
25:A:406:CLA:HAC2	25:D:404:CLA:CHA	2.51	0.40
25:A:408:CLA:C1B	9:I:12:VAL:HG22	2.51	0.40
2:B:133:LEU:HB3	2:B:138:ILE:CD1	2.50	0.40
2:B:323:GLY:N	2:B:326:ARG:HD2	2.36	0.40
2:B:341:LEU:HD22	2:B:429:ILE:HG22	2.04	0.40
2:B:457:CYS:O	2:B:461:LEU:HG	2.22	0.40
25:B:510:CLA:C1B	25:B:512:CLA:H12	2.51	0.40
25:B:515:CLA:CBB	25:B:515:CLA:HHC	2.52	0.40
4:C:355:GLU:HB2	4:C:356:PRO:HD3	2.02	0.40
25:C:505:CLA:H92	25:C:505:CLA:H61	1.73	0.40
25:D:401:CLA:H162	25:D:401:CLA:H141	1.76	0.40
14:O:289:GLN:HB3	14:O:291:LYS:HZ3	1.83	0.40
15:P:202:HIS:CD2	15:P:224:ASP:HA	2.56	0.40
16:Q:115:PHE:O	16:Q:119:SER:N	2.55	0.40
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.56	0.40
1:A:328:MET:HG2	5:D:325:ILE:HG12	2.04	0.40
1:A:334:ARG:HD2	14:O:203:LEU:CB	2.51	0.40
28:A:410:SQD:H362	11:K:37:PHE:CE1	2.55	0.40
2:B:37:MET:HE2	36:B:602:HOH:O	2.21	0.40
2:B:52:LEU:HB3	2:B:337:ALA:CB	2.49	0.40
4:C:28:ALA:HA	25:C:508:CLA:HMA2	2.03	0.40
4:C:233:ILE:O	4:C:237:ILE:HG13	2.21	0.40
5:D:14:TRP:HZ2	18:X:90:ILE:HG13	1.86	0.40
5:D:43:PHE:HB3	5:D:113:PHE:CE1	2.56	0.40
5:D:78:VAL:O	5:D:111:TRP:HD1	2.05	0.40
5:D:174:GLY:O	5:D:178:ILE:HG12	2.21	0.40
14:O:101:PRO:HB2	14:O:104:PHE:CZ	2.56	0.40
14:O:110:SER:O	14:O:111:GLN:C	2.63	0.40
16:Q:110:ALA:O	16:Q:111:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HD23	8:H:34:ASN:HD21	1.86	0.40
2:B:155:ALA:HB2	2:B:203:ILE:HG12	2.03	0.40
2:B:370:LEU:N	2:B:370:LEU:HD12	2.36	0.40
25:B:506:CLA:H2A	25:B:506:CLA:CED	2.52	0.40
25:B:507:CLA:H41	25:B:507:CLA:H62	1.70	0.40
4:C:447:ILE:HB	5:D:223:PHE:HD1	1.86	0.40
25:C:505:CLA:H62	25:C:505:CLA:H2	1.80	0.40
25:C:511:CLA:C2	25:C:511:CLA:H71	2.47	0.40
25:C:512:CLA:O2D	25:C:513:CLA:HBB2	2.21	0.40
10:J:27:LEU:HA	10:J:30:PHE:HD2	1.85	0.40
14:O:251:VAL:HG22	14:O:258:ILE:HG22	2.04	0.40
20:U:95:LEU:C	20:U:97:LYS:H	2.29	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	314/334 (94%)	295 (94%)	18 (6%)	1 (0%)	37	65
2	B	478/480 (100%)	458 (96%)	20 (4%)	0	100	100
3	V	30/32 (94%)	30 (100%)	0	0	100	100
4	C	447/449 (100%)	427 (96%)	17 (4%)	3 (1%)	19	47
5	D	346/348 (99%)	330 (95%)	14 (4%)	2 (1%)	22	51
6	E	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
8	H	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	33/35 (94%)	33 (100%)	0	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	O	238/240 (99%)	219 (92%)	18 (8%)	1 (0%)	30	59
15	P	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
16	Q	146/148 (99%)	139 (95%)	7 (5%)	0	100	100
17	T	28/30 (93%)	28 (100%)	0	0	100	100
18	X	30/32 (94%)	30 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
20	U	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
21	W	42/44 (96%)	42 (100%)	0	0	100	100
All	All	2692/2752 (98%)	2577 (96%)	108 (4%)	7 (0%)	38	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	8	TYR
4	C	140	LYS
1	A	141	PRO
4	C	371	ASP
4	C	399	ALA
5	D	9	GLN
14	O	210	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	259/272 (95%)	250 (96%)	9 (4%)	31	64
2	B	382/382 (100%)	363 (95%)	19 (5%)	20	50
3	V	26/26 (100%)	25 (96%)	1 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	352/352 (100%)	347 (99%)	5 (1%)	62	85
5	D	278/278 (100%)	276 (99%)	2 (1%)	81	93
6	E	66/66 (100%)	63 (96%)	3 (4%)	23	54
7	F	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	55 (98%)	1 (2%)	54	81
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	26 (96%)	1 (4%)	29	62
11	K	31/31 (100%)	31 (100%)	0	100	100
12	L	33/33 (100%)	31 (94%)	2 (6%)	15	42
13	M	25/25 (100%)	25 (100%)	0	100	100
14	O	195/195 (100%)	181 (93%)	14 (7%)	12	33
15	P	150/150 (100%)	147 (98%)	3 (2%)	50	78
16	Q	126/126 (100%)	121 (96%)	5 (4%)	27	59
17	T	27/27 (100%)	27 (100%)	0	100	100
18	X	23/23 (100%)	22 (96%)	1 (4%)	25	56
19	Z	51/51 (100%)	49 (96%)	2 (4%)	27	60
20	U	20/20 (100%)	18 (90%)	2 (10%)	6	19
21	W	35/35 (100%)	30 (86%)	5 (14%)	2	8
All	All	2218/2231 (99%)	2143 (97%)	75 (3%)	34	65

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	47	VAL
1	A	60	ILE
1	A	102	LEU
1	A	243	GLU
1	A	245	THR
1	A	254	TYR
1	A	257	ARG
1	A	326	LEU
2	B	21	SER
2	B	22	VAL
2	B	90	ILE
2	B	130	LYS

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Mol	Chain	Res	Type
2	B	141	ILE
2	B	207	ILE
2	B	225	LEU
2	B	237	VAL
2	B	246	PHE
2	B	265	ILE
2	B	267	LEU
2	B	272	ARG
2	B	286	LYS
2	B	292	LEU
2	B	315	ILE
2	B	321	LYS
2	B	362	PHE
2	B	442	VAL
2	B	478	VAL
3	V	7	LEU
4	C	19	THR
4	C	129	GLU
4	C	140	LYS
4	C	379	ARG
4	C	460	LEU
5	D	54	PHE
5	D	210	LEU
6	E	30	LEU
6	E	49	THR
6	E	53	ASN
8	H	36	GLU
10	J	10	ILE
12	L	8	LYS
12	L	26	PHE
14	O	76	VAL
14	O	98	CYS
14	O	107	LYS
14	O	140	LYS
14	O	141	VAL
14	O	150	LYS
14	O	151	GLU
14	O	170	VAL
14	O	185	LEU
14	O	206	LYS
14	O	215	ASP
14	O	216	ASN

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Mol	Chain	Res	Type
14	O	231	LYS
14	O	241	LYS
15	P	95	LYS
15	P	115	ASN
15	P	138	LEU
16	Q	114	VAL
16	Q	130	ARG
16	Q	146	LYS
16	Q	148	LYS
16	Q	183	LYS
18	X	65	VAL
19	Z	26	VAL
19	Z	57	LEU
20	U	106	VAL
20	U	111	LYS
21	W	60	LEU
21	W	77	ASN
21	W	96	TRP
21	W	101	LYS
21	W	102	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	113	GLN
1	A	181	ASN
1	A	187	GLN
1	A	267	ASN
1	A	304	GLN
1	A	315	ASN
1	A	337	HIS
2	B	87	ASN
2	B	114	HIS
2	B	194	ASN
2	B	274	GLN
2	B	285	GLN
2	B	289	GLN
2	B	343	HIS
2	B	455	HIS
2	B	469	HIS
4	C	106	HIS

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Mol	Chain	Res	Type
4	C	143	ASN
4	C	147	ASN
4	C	189	ASN
4	C	239	HIS
4	C	301	GLN
4	C	315	ASN
4	C	366	ASN
4	C	373	GLN
5	D	106	GLN
5	D	197	HIS
5	D	236	ASN
5	D	239	GLN
6	E	53	ASN
6	E	71	ASN
12	L	5	ASN
12	L	38	ASN
14	O	72	ASN
14	O	178	GLN
14	O	216	ASN
14	O	266	GLN
15	P	64	ASN
15	P	92	ASN
15	P	115	ASN
15	P	134	GLN
15	P	213	ASN
16	Q	117	GLN
16	Q	163	GLN
19	Z	58	ASN
21	W	66	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 66 ligands modelled in this entry, 3 are monoatomic - leaving 63 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
28	SQD	A	410	-	50,51,54	0.81	0	59,62,65	0.93	3 (5%)
25	CLA	B	512	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	17 (22%)
25	CLA	B	505	-	65,73,73	1.33	9 (13%)	76,113,113	1.97	16 (21%)
31	DGD	C	517	-	53,53,67	1.02	4 (7%)	67,67,81	1.00	3 (4%)
25	CLA	B	511	-	65,73,73	1.32	6 (9%)	76,113,113	1.99	15 (19%)
25	CLA	C	512	-	52,60,73	1.49	7 (13%)	60,97,113	2.26	17 (28%)
25	CLA	B	509	36	65,73,73	1.34	7 (10%)	76,113,113	1.94	16 (21%)
25	CLA	B	504	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
25	CLA	C	505	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	16 (21%)
27	BCR	K	101	-	41,41,41	4.79	27 (65%)	56,56,56	2.32	17 (30%)
25	CLA	B	515	-	50,58,73	1.53	7 (14%)	58,95,113	2.20	17 (29%)
25	CLA	C	510	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	17 (22%)
30	LHG	D	409	-	38,38,48	0.42	0	41,44,54	1.16	3 (7%)
25	CLA	B	514	-	51,59,73	1.50	7 (13%)	59,96,113	2.23	16 (27%)
25	CLA	H	101	-	61,69,73	1.37	8 (13%)	71,108,113	2.02	17 (23%)
30	LHG	B	521	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
25	CLA	C	506	-	50,58,73	1.51	5 (10%)	58,95,113	2.11	16 (27%)
25	CLA	B	503	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
34	PL9	D	407	-	55,55,55	0.70	1 (1%)	68,69,69	0.59	1 (1%)
25	CLA	C	502	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	20 (26%)
27	BCR	B	516	-	41,41,41	4.80	27 (65%)	56,56,56	2.28	21 (37%)
25	CLA	B	506	-	55,63,73	1.42	7 (12%)	64,101,113	2.19	17 (26%)
27	BCR	C	516	-	41,41,41	4.83	26 (63%)	56,56,56	2.50	22 (39%)
25	CLA	D	401	36	65,73,73	1.33	8 (12%)	76,113,113	1.98	17 (22%)
25	CLA	B	513	-	56,64,73	1.43	7 (12%)	65,102,113	2.13	18 (27%)
25	CLA	C	501	-	65,73,73	1.33	7 (10%)	76,113,113	1.95	17 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C	509	-	65,73,73	1.33	6 (9%)	76,113,113	1.95	19 (25%)
25	CLA	C	513	-	46,54,73	1.59	8 (17%)	53,90,113	2.23	13 (24%)
29	LMG	C	520	-	51,51,55	1.06	5 (9%)	59,59,63	1.08	2 (3%)
29	LMG	B	520	-	48,48,55	1.00	5 (10%)	56,56,63	1.11	2 (3%)
30	LHG	B	519	-	43,43,48	0.40	0	46,49,54	1.11	3 (6%)
27	BCR	D	406	-	41,41,41	4.78	27 (65%)	56,56,56	2.46	21 (37%)
29	LMG	D	410	-	36,36,55	0.58	1 (2%)	44,44,63	1.04	3 (6%)
29	LMG	B	518	-	43,43,55	0.88	2 (4%)	51,51,63	1.10	3 (5%)
31	DGD	C	519	-	55,55,67	0.94	3 (5%)	69,69,81	1.00	3 (4%)
25	CLA	C	511	4	65,73,73	1.33	8 (12%)	76,113,113	2.04	17 (22%)
35	HEM	F	101	6,7	41,50,50	1.34	5 (12%)	45,82,82	1.80	8 (17%)
27	BCR	C	514	-	41,41,41	4.81	27 (65%)	56,56,56	2.27	22 (39%)
32	LMU	C	521	-	36,36,36	0.35	0	47,47,47	0.81	1 (2%)
25	CLA	C	504	36	56,64,73	1.43	7 (12%)	65,102,113	2.14	16 (24%)
25	CLA	D	405	-	56,64,73	1.43	7 (12%)	65,102,113	2.15	16 (24%)
30	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
25	CLA	C	507	36	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
25	CLA	A	408	-	60,68,73	1.38	8 (13%)	70,107,113	2.09	15 (21%)
26	PHO	A	407	-	51,69,69	0.54	0	47,99,99	0.59	0
25	CLA	B	501	-	65,73,73	1.34	8 (12%)	76,113,113	1.97	16 (21%)
27	BCR	B	517	-	41,41,41	4.79	27 (65%)	56,56,56	2.26	18 (32%)
33	BCT	D	403	23	2,3,3	0.98	0	2,3,3	1.67	1 (50%)
25	CLA	A	405	-	65,73,73	1.32	7 (10%)	76,113,113	2.00	19 (25%)
25	CLA	A	406	36	49,57,73	1.52	7 (14%)	55,93,113	2.27	15 (27%)
25	CLA	C	503	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
25	CLA	B	508	-	65,73,73	1.33	8 (12%)	76,113,113	1.96	16 (21%)
25	CLA	B	507	36	65,73,73	1.33	7 (10%)	76,113,113	2.01	16 (21%)
25	CLA	C	508	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	19 (25%)
31	DGD	C	518	-	55,55,67	0.99	4 (7%)	69,69,81	0.95	2 (2%)
27	BCR	A	409	-	41,41,41	4.77	27 (65%)	56,56,56	2.36	21 (37%)
26	PHO	D	402	-	51,69,69	0.54	0	47,99,99	0.63	0
25	CLA	B	502	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	19 (25%)
25	CLA	B	510	-	65,73,73	1.33	7 (10%)	76,113,113	2.02	18 (23%)
29	LMG	W	201	-	48,48,55	0.99	5 (10%)	56,56,63	1.15	4 (7%)
22	OEX	A	401	1,4	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	D	404	-	65,73,73	1.32	8 (12%)	76,113,113	1.98	17 (22%)
27	BCR	C	515	-	41,41,41	4.80	27 (65%)	56,56,56	2.46	20 (35%)

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
28	SQD	A	410	-	-	7/46/66/69	0/1/1/1
25	CLA	B	512	-	1/1/15/20	12/37/115/115	-
25	CLA	B	505	-	1/1/15/20	15/37/115/115	-
31	DGD	C	517	-	-	7/41/81/95	0/2/2/2
25	CLA	B	511	-	1/1/15/20	16/37/115/115	-
25	CLA	C	512	-	1/1/12/20	11/22/100/115	-
25	CLA	B	509	36	1/1/15/20	11/37/115/115	-
25	CLA	B	504	-	1/1/15/20	17/37/115/115	-
25	CLA	C	505	-	1/1/15/20	17/37/115/115	-
27	BCR	K	101	-	-	13/29/63/63	0/2/2/2
25	CLA	B	515	-	1/1/12/20	7/19/97/115	-
25	CLA	C	510	-	1/1/15/20	21/37/115/115	-
30	LHG	D	409	-	-	29/43/43/53	-
25	CLA	B	514	-	1/1/12/20	8/21/99/115	-
25	CLA	H	101	-	1/1/14/20	14/33/111/115	-
30	LHG	B	521	-	-	33/53/53/53	-
25	CLA	C	506	-	1/1/12/20	12/19/97/115	-
25	CLA	B	503	-	1/1/15/20	16/37/115/115	-
34	PL9	D	407	-	-	7/53/73/73	0/1/1/1
25	CLA	C	502	-	1/1/15/20	17/37/115/115	-
27	BCR	B	516	-	-	15/29/63/63	0/2/2/2
25	CLA	B	506	-	1/1/13/20	13/25/103/115	-
27	BCR	C	516	-	-	9/29/63/63	0/2/2/2
25	CLA	D	401	36	1/1/15/20	18/37/115/115	-
25	CLA	B	513	-	1/1/13/20	12/27/105/115	-
25	CLA	C	501	-	1/1/15/20	20/37/115/115	-
25	CLA	C	509	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	513	-	1/1/11/20	9/15/93/115	-
29	LMG	C	520	-	-	11/46/66/70	0/1/1/1
29	LMG	B	520	-	-	7/43/63/70	0/1/1/1
30	LHG	B	519	-	-	28/48/48/53	-
27	BCR	D	406	-	-	9/29/63/63	0/2/2/2
29	LMG	D	410	-	-	7/31/51/70	0/1/1/1
29	LMG	B	518	-	-	12/38/58/70	0/1/1/1
31	DGD	C	519	-	-	7/43/83/95	0/2/2/2
25	CLA	C	511	4	1/1/15/20	17/37/115/115	-
35	HEM	F	101	6,7	-	5/12/54/54	-
27	BCR	C	514	-	-	13/29/63/63	0/2/2/2
32	LMU	C	521	-	-	10/21/61/61	0/2/2/2
25	CLA	C	504	36	1/1/13/20	19/27/105/115	-
25	CLA	D	405	-	1/1/13/20	15/27/105/115	-
30	LHG	D	408	-	-	31/53/53/53	-
25	CLA	C	507	36	1/1/15/20	17/37/115/115	-
25	CLA	A	408	-	1/1/14/20	15/31/109/115	-
26	PHO	A	407	-	-	3/37/103/103	0/5/6/6
25	CLA	B	501	-	1/1/15/20	18/37/115/115	-
27	BCR	B	517	-	-	13/29/63/63	0/2/2/2
25	CLA	A	405	-	1/1/15/20	13/37/115/115	-
25	CLA	A	406	36	1/1/11/20	8/18/96/115	-
25	CLA	C	503	-	1/1/15/20	15/37/115/115	-
25	CLA	B	508	-	1/1/15/20	14/37/115/115	-
25	CLA	B	507	36	1/1/15/20	22/37/115/115	-
25	CLA	C	508	-	1/1/15/20	16/37/115/115	-
31	DGD	C	518	-	-	12/43/83/95	0/2/2/2
27	BCR	A	409	-	-	14/29/63/63	0/2/2/2
26	PHO	D	402	-	-	6/37/103/103	0/5/6/6
25	CLA	B	502	-	1/1/15/20	17/37/115/115	-
25	CLA	B	510	-	1/1/15/20	17/37/115/115	-
29	LMG	W	201	-	-	7/43/63/70	0/1/1/1
25	CLA	D	404	-	1/1/15/20	11/37/115/115	-
27	BCR	C	515	-	-	13/29/63/63	0/2/2/2

All (505) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	516	BCR	C26-C25	15.69	1.61	1.34
27	C	514	BCR	C26-C25	15.55	1.61	1.34
27	B	517	BCR	C26-C25	15.54	1.61	1.34
27	C	515	BCR	C26-C25	15.46	1.61	1.34
27	K	101	BCR	C26-C25	15.29	1.60	1.34
27	B	516	BCR	C26-C25	15.29	1.60	1.34
27	A	409	BCR	C26-C25	15.18	1.60	1.34
27	D	406	BCR	C26-C25	15.07	1.60	1.34
27	D	406	BCR	C5-C6	14.05	1.58	1.34
27	A	409	BCR	C5-C6	14.04	1.58	1.34
27	K	101	BCR	C5-C6	13.98	1.58	1.34
27	C	514	BCR	C5-C6	13.96	1.58	1.34
27	B	517	BCR	C5-C6	13.94	1.58	1.34
27	C	516	BCR	C5-C6	13.91	1.58	1.34
27	C	515	BCR	C5-C6	13.87	1.58	1.34
27	B	516	BCR	C5-C6	13.86	1.58	1.34
27	D	406	BCR	C30-C25	-7.01	1.44	1.53
27	A	409	BCR	C30-C25	-6.90	1.44	1.53
27	C	516	BCR	C30-C25	-6.88	1.44	1.53
27	K	101	BCR	C30-C25	-6.88	1.44	1.53
27	B	516	BCR	C30-C25	-6.86	1.44	1.53
27	B	516	BCR	C1-C6	-6.76	1.44	1.53
27	K	101	BCR	C1-C6	-6.73	1.44	1.53
27	B	517	BCR	C30-C25	-6.71	1.44	1.53
27	A	409	BCR	C2-C3	-6.64	1.36	1.52
27	C	514	BCR	C1-C6	-6.63	1.44	1.53
27	C	514	BCR	C2-C3	-6.60	1.36	1.52
27	D	406	BCR	C2-C3	-6.59	1.36	1.52
27	C	515	BCR	C1-C6	-6.59	1.44	1.53
27	C	516	BCR	C2-C3	-6.57	1.36	1.52
27	D	406	BCR	C1-C6	-6.57	1.44	1.53
27	K	101	BCR	C2-C3	-6.56	1.36	1.52
27	B	516	BCR	C2-C3	-6.54	1.36	1.52
27	C	515	BCR	C2-C3	-6.54	1.36	1.52
27	B	517	BCR	C2-C3	-6.53	1.36	1.52
27	C	515	BCR	C30-C25	-6.53	1.44	1.53
27	C	514	BCR	C30-C25	-6.52	1.44	1.53
27	C	516	BCR	C1-C6	-6.50	1.44	1.53
27	B	517	BCR	C1-C6	-6.44	1.44	1.53
27	C	514	BCR	C29-C28	-6.42	1.36	1.52
27	C	516	BCR	C29-C28	-6.38	1.36	1.52
25	C	506	CLA	MG-NA	6.36	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	409	BCR	C1-C6	-6.34	1.45	1.53
27	C	515	BCR	C29-C28	-6.32	1.37	1.52
25	B	504	CLA	MG-NA	6.30	2.21	2.06
25	B	507	CLA	MG-NA	6.30	2.21	2.06
27	B	517	BCR	C29-C28	-6.29	1.37	1.52
25	C	511	CLA	MG-NA	6.29	2.21	2.06
25	B	502	CLA	MG-NA	6.28	2.21	2.06
25	B	509	CLA	MG-NA	6.28	2.21	2.06
25	C	503	CLA	MG-NA	6.27	2.21	2.06
25	B	512	CLA	MG-NA	6.27	2.21	2.06
25	C	512	CLA	MG-NA	6.26	2.21	2.06
25	C	509	CLA	MG-NA	6.25	2.21	2.06
25	C	507	CLA	MG-NA	6.25	2.21	2.06
27	A	409	BCR	C29-C28	-6.25	1.37	1.52
25	B	503	CLA	MG-NA	6.25	2.21	2.06
25	B	513	CLA	MG-NA	6.24	2.21	2.06
25	B	515	CLA	MG-NA	6.24	2.21	2.06
27	K	101	BCR	C29-C28	-6.23	1.37	1.52
25	C	510	CLA	MG-NA	6.23	2.21	2.06
25	B	514	CLA	MG-NA	6.23	2.21	2.06
25	B	511	CLA	MG-NA	6.23	2.21	2.06
25	A	408	CLA	MG-NA	6.23	2.21	2.06
27	B	516	BCR	C29-C28	-6.22	1.37	1.52
25	C	501	CLA	MG-NA	6.22	2.21	2.06
25	B	508	CLA	MG-NA	6.22	2.21	2.06
25	D	401	CLA	MG-NA	6.22	2.21	2.06
25	C	504	CLA	MG-NA	6.22	2.21	2.06
25	A	405	CLA	MG-NA	6.21	2.21	2.06
25	B	510	CLA	MG-NA	6.21	2.21	2.06
25	C	508	CLA	MG-NA	6.21	2.21	2.06
25	A	406	CLA	MG-NA	6.21	2.21	2.06
25	C	502	CLA	MG-NA	6.21	2.21	2.06
25	D	404	CLA	MG-NA	6.20	2.21	2.06
25	H	101	CLA	MG-NA	6.20	2.21	2.06
25	B	501	CLA	MG-NA	6.18	2.21	2.06
25	B	505	CLA	MG-NA	6.18	2.21	2.06
25	C	505	CLA	MG-NA	6.15	2.20	2.06
25	D	405	CLA	MG-NA	6.15	2.20	2.06
25	C	513	CLA	MG-NA	6.13	2.20	2.06
27	D	406	BCR	C29-C28	-6.12	1.37	1.52
25	B	506	CLA	MG-NA	6.08	2.20	2.06
27	C	515	BCR	C12-C13	5.85	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	516	BCR	C12-C13	5.79	1.58	1.45
27	C	516	BCR	C12-C13	5.78	1.58	1.45
27	K	101	BCR	C12-C13	5.75	1.58	1.45
27	C	514	BCR	C12-C13	5.75	1.58	1.45
27	D	406	BCR	C12-C13	5.75	1.58	1.45
27	A	409	BCR	C12-C13	5.68	1.58	1.45
27	B	517	BCR	C12-C13	5.65	1.58	1.45
27	B	516	BCR	C8-C9	5.49	1.57	1.45
27	C	514	BCR	C8-C9	5.49	1.57	1.45
27	C	515	BCR	C8-C9	5.49	1.57	1.45
27	C	516	BCR	C8-C9	5.43	1.57	1.45
27	K	101	BCR	C8-C9	5.42	1.57	1.45
27	B	517	BCR	C8-C9	5.40	1.57	1.45
27	D	406	BCR	C8-C9	5.38	1.57	1.45
27	A	409	BCR	C8-C9	5.34	1.57	1.45
27	C	515	BCR	C23-C22	5.31	1.57	1.45
27	C	514	BCR	C23-C22	5.30	1.57	1.45
27	C	516	BCR	C23-C22	5.29	1.57	1.45
27	A	409	BCR	C29-C30	5.27	1.66	1.54
27	K	101	BCR	C29-C30	5.25	1.66	1.54
27	B	516	BCR	C23-C22	5.25	1.57	1.45
27	D	406	BCR	C23-C22	5.24	1.57	1.45
27	B	516	BCR	C29-C30	5.23	1.66	1.54
27	A	409	BCR	C23-C22	5.20	1.57	1.45
27	B	517	BCR	C29-C30	5.19	1.66	1.54
27	K	101	BCR	C23-C22	5.17	1.57	1.45
27	B	517	BCR	C23-C22	5.17	1.57	1.45
27	C	515	BCR	C29-C30	5.17	1.66	1.54
27	D	406	BCR	C29-C30	5.13	1.66	1.54
27	C	516	BCR	C29-C30	5.08	1.65	1.54
27	C	514	BCR	C29-C30	5.06	1.65	1.54
27	C	514	BCR	C15-C14	4.80	1.58	1.43
27	C	515	BCR	C15-C14	4.79	1.58	1.43
27	C	516	BCR	C15-C14	4.78	1.58	1.43
27	B	516	BCR	C15-C14	4.77	1.58	1.43
27	K	101	BCR	C15-C14	4.77	1.58	1.43
27	C	516	BCR	C19-C18	4.74	1.56	1.45
27	D	406	BCR	C15-C14	4.72	1.58	1.43
27	A	409	BCR	C15-C14	4.71	1.58	1.43
27	B	517	BCR	C15-C14	4.67	1.57	1.43
27	C	515	BCR	C19-C18	4.66	1.56	1.45
27	C	514	BCR	C19-C18	4.66	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	516	BCR	C19-C18	4.66	1.55	1.45
27	C	516	BCR	C2-C1	4.62	1.64	1.54
27	B	517	BCR	C2-C1	4.62	1.64	1.54
27	D	406	BCR	C2-C1	4.60	1.64	1.54
34	D	407	PL9	C3-C4	-4.60	1.42	1.49
27	C	514	BCR	C2-C1	4.58	1.64	1.54
27	D	406	BCR	C19-C18	4.58	1.55	1.45
27	B	516	BCR	C2-C1	4.56	1.64	1.54
27	B	517	BCR	C19-C18	4.55	1.55	1.45
27	A	409	BCR	C19-C18	4.55	1.55	1.45
27	C	515	BCR	C2-C1	4.50	1.64	1.54
27	K	101	BCR	C19-C18	4.49	1.55	1.45
27	K	101	BCR	C2-C1	4.48	1.64	1.54
27	A	409	BCR	C2-C1	4.48	1.64	1.54
27	D	406	BCR	C28-C27	4.38	1.66	1.52
27	C	516	BCR	C20-C21	4.32	1.56	1.43
27	C	514	BCR	C20-C21	4.32	1.56	1.43
27	C	515	BCR	C20-C21	4.32	1.56	1.43
27	B	516	BCR	C20-C21	4.28	1.56	1.43
31	C	517	DGD	O1G-C1A	4.25	1.45	1.33
27	A	409	BCR	C20-C21	4.24	1.56	1.43
27	D	406	BCR	C20-C21	4.24	1.56	1.43
27	B	517	BCR	C20-C21	4.24	1.56	1.43
27	B	516	BCR	C28-C27	4.20	1.65	1.52
27	K	101	BCR	C28-C27	4.20	1.65	1.52
31	C	518	DGD	O1G-C1A	4.20	1.45	1.33
27	K	101	BCR	C20-C21	4.19	1.56	1.43
27	C	515	BCR	C28-C27	4.19	1.65	1.52
27	C	514	BCR	C28-C27	4.18	1.65	1.52
27	A	409	BCR	C28-C27	4.17	1.65	1.52
27	C	516	BCR	C28-C27	4.17	1.65	1.52
31	C	519	DGD	O1G-C1A	4.16	1.45	1.33
27	B	517	BCR	C28-C27	4.14	1.65	1.52
27	B	517	BCR	C3-C4	3.93	1.64	1.52
27	C	515	BCR	C3-C4	3.92	1.64	1.52
27	B	516	BCR	C3-C4	3.91	1.64	1.52
27	K	101	BCR	C3-C4	3.90	1.64	1.52
27	D	406	BCR	C3-C4	3.87	1.64	1.52
27	C	514	BCR	C3-C4	3.85	1.64	1.52
27	C	516	BCR	C3-C4	3.84	1.64	1.52
27	C	516	BCR	C16-C17	3.84	1.55	1.43
27	A	409	BCR	C3-C4	3.81	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	515	BCR	C16-C17	3.79	1.55	1.43
27	B	516	BCR	C11-C10	3.78	1.55	1.43
27	B	516	BCR	C16-C17	3.77	1.55	1.43
27	C	515	BCR	C11-C10	3.75	1.55	1.43
27	C	514	BCR	C16-C17	3.75	1.55	1.43
27	K	101	BCR	C11-C10	3.74	1.55	1.43
27	C	516	BCR	C11-C10	3.74	1.55	1.43
27	D	406	BCR	C16-C17	3.73	1.55	1.43
27	K	101	BCR	C16-C17	3.73	1.55	1.43
27	D	406	BCR	C11-C10	3.71	1.55	1.43
25	C	513	CLA	MG-ND	-3.71	1.98	2.05
27	C	514	BCR	C11-C10	3.70	1.54	1.43
25	C	505	CLA	MG-ND	-3.70	1.98	2.05
27	B	517	BCR	C16-C17	3.69	1.54	1.43
27	A	409	BCR	C11-C10	3.67	1.54	1.43
25	C	506	CLA	MG-ND	-3.66	1.98	2.05
27	A	409	BCR	C16-C17	3.65	1.54	1.43
25	C	512	CLA	MG-ND	-3.64	1.98	2.05
25	B	508	CLA	MG-ND	-3.63	1.98	2.05
25	C	504	CLA	MG-ND	-3.63	1.98	2.05
25	B	515	CLA	MG-ND	-3.62	1.98	2.05
25	C	507	CLA	MG-ND	-3.62	1.98	2.05
25	B	512	CLA	MG-ND	-3.61	1.98	2.05
27	C	516	BCR	C24-C25	3.60	1.57	1.45
27	C	515	BCR	C24-C25	3.59	1.57	1.45
25	C	503	CLA	MG-ND	-3.59	1.98	2.05
27	B	517	BCR	C11-C10	3.59	1.54	1.43
25	B	507	CLA	MG-ND	-3.59	1.98	2.05
27	D	406	BCR	C24-C25	3.59	1.57	1.45
25	B	513	CLA	MG-ND	-3.58	1.98	2.05
25	C	501	CLA	MG-ND	-3.58	1.98	2.05
25	B	502	CLA	MG-ND	-3.58	1.98	2.05
27	B	516	BCR	C24-C25	3.58	1.57	1.45
25	D	405	CLA	MG-ND	-3.58	1.98	2.05
25	B	511	CLA	MG-ND	-3.57	1.98	2.05
25	B	505	CLA	MG-ND	-3.57	1.98	2.05
25	B	504	CLA	MG-ND	-3.57	1.98	2.05
25	B	501	CLA	MG-ND	-3.57	1.98	2.05
25	C	510	CLA	MG-ND	-3.56	1.98	2.05
27	C	514	BCR	C24-C25	3.56	1.57	1.45
25	C	508	CLA	MG-ND	-3.54	1.98	2.05
25	C	502	CLA	MG-ND	-3.54	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	MG-ND	-3.54	1.98	2.05
27	B	517	BCR	C24-C25	3.54	1.57	1.45
25	C	509	CLA	MG-ND	-3.53	1.98	2.05
25	H	101	CLA	MG-ND	-3.53	1.98	2.05
25	B	506	CLA	MG-ND	-3.53	1.98	2.05
25	B	503	CLA	MG-ND	-3.53	1.98	2.05
25	B	510	CLA	MG-ND	-3.53	1.98	2.05
25	B	509	CLA	MG-ND	-3.53	1.98	2.05
25	D	401	CLA	MG-ND	-3.53	1.98	2.05
25	A	406	CLA	MG-ND	-3.53	1.98	2.05
25	A	405	CLA	MG-ND	-3.52	1.98	2.05
27	K	101	BCR	C24-C25	3.51	1.57	1.45
25	B	514	CLA	MG-ND	-3.51	1.98	2.05
27	A	409	BCR	C24-C25	3.51	1.57	1.45
25	A	408	CLA	MG-ND	-3.48	1.98	2.05
25	D	404	CLA	MG-ND	-3.46	1.98	2.05
35	F	101	HEM	C4D-ND	-3.41	1.34	1.40
35	F	101	HEM	C1B-NB	-3.41	1.34	1.40
27	A	409	BCR	C27-C26	-3.40	1.44	1.51
25	C	513	CLA	CBB-CAB	3.39	1.51	1.29
25	B	510	CLA	CBB-CAB	3.37	1.51	1.29
25	B	511	CLA	CBB-CAB	3.36	1.51	1.29
25	B	514	CLA	CBB-CAB	3.36	1.51	1.29
25	B	507	CLA	CBB-CAB	3.36	1.51	1.29
25	C	505	CLA	CBB-CAB	3.36	1.51	1.29
25	H	101	CLA	CBB-CAB	3.36	1.51	1.29
25	C	509	CLA	CBB-CAB	3.35	1.51	1.29
25	C	508	CLA	CBB-CAB	3.35	1.51	1.29
25	B	513	CLA	CBB-CAB	3.35	1.51	1.29
25	A	405	CLA	CBB-CAB	3.35	1.51	1.29
25	D	401	CLA	CBB-CAB	3.34	1.51	1.29
25	C	502	CLA	CBB-CAB	3.34	1.51	1.29
25	C	501	CLA	CBB-CAB	3.34	1.51	1.29
25	C	510	CLA	CBB-CAB	3.34	1.51	1.29
25	B	501	CLA	CBB-CAB	3.34	1.51	1.29
25	B	506	CLA	CBB-CAB	3.34	1.51	1.29
25	C	507	CLA	CBB-CAB	3.34	1.51	1.29
25	B	503	CLA	CBB-CAB	3.34	1.51	1.29
25	C	512	CLA	CBB-CAB	3.34	1.51	1.29
25	C	511	CLA	CBB-CAB	3.34	1.51	1.29
25	B	505	CLA	CBB-CAB	3.34	1.51	1.29
25	B	509	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	405	CLA	CBB-CAB	3.34	1.51	1.29
25	B	504	CLA	CBB-CAB	3.33	1.51	1.29
25	B	502	CLA	CBB-CAB	3.33	1.51	1.29
25	C	504	CLA	CBB-CAB	3.33	1.51	1.29
25	D	404	CLA	CBB-CAB	3.33	1.51	1.29
25	C	503	CLA	CBB-CAB	3.33	1.51	1.29
27	D	406	BCR	C4-C5	-3.33	1.44	1.51
25	B	512	CLA	CBB-CAB	3.33	1.51	1.29
25	B	508	CLA	CBB-CAB	3.33	1.51	1.29
25	A	406	CLA	CBB-CAB	3.33	1.51	1.29
25	A	408	CLA	CBB-CAB	3.32	1.51	1.29
25	C	506	CLA	CBB-CAB	3.32	1.51	1.29
27	B	516	BCR	C4-C5	-3.31	1.44	1.51
27	K	101	BCR	C27-C26	-3.30	1.44	1.51
25	B	514	CLA	C1C-NC	-3.29	1.32	1.37
29	B	518	LMG	C19-C18	-3.29	1.33	1.51
25	B	515	CLA	CBB-CAB	3.29	1.51	1.29
27	C	516	BCR	C4-C5	-3.28	1.44	1.51
29	W	201	LMG	C37-C36	-3.28	1.33	1.51
27	A	409	BCR	C4-C5	-3.28	1.44	1.51
27	B	517	BCR	C4-C5	-3.27	1.44	1.51
31	C	517	DGD	CAB-C9B	-3.27	1.33	1.51
27	B	517	BCR	C27-C26	-3.26	1.44	1.51
27	C	514	BCR	C4-C5	-3.26	1.44	1.51
31	C	517	DGD	CDB-CCB	-3.26	1.33	1.51
31	C	518	DGD	CAB-C9B	-3.26	1.33	1.51
29	B	520	LMG	C19-C18	-3.26	1.33	1.51
25	C	502	CLA	C1C-NC	-3.26	1.32	1.37
27	B	516	BCR	C27-C26	-3.26	1.44	1.51
29	C	520	LMG	C19-C18	-3.25	1.33	1.51
29	C	520	LMG	C22-C21	-3.25	1.33	1.51
29	B	518	LMG	C22-C21	-3.25	1.33	1.51
27	C	515	BCR	C4-C5	-3.25	1.44	1.51
25	C	504	CLA	C1C-NC	-3.25	1.33	1.37
29	C	520	LMG	C40-C39	-3.24	1.33	1.51
29	W	201	LMG	C40-C39	-3.24	1.33	1.51
29	B	520	LMG	C40-C39	-3.23	1.33	1.51
29	C	520	LMG	C37-C36	-3.23	1.33	1.51
25	D	401	CLA	C1C-NC	-3.23	1.33	1.37
29	B	520	LMG	C37-C36	-3.23	1.33	1.51
29	W	201	LMG	C19-C18	-3.22	1.33	1.51
31	C	519	DGD	CAA-C9A	-3.22	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	509	CLA	C1C-NC	-3.21	1.33	1.37
25	B	501	CLA	C1C-NC	-3.21	1.33	1.37
25	B	506	CLA	C1C-NC	-3.21	1.33	1.37
31	C	518	DGD	CDB-CCB	-3.21	1.33	1.51
25	C	505	CLA	C1C-NC	-3.21	1.33	1.37
25	B	510	CLA	C1C-NC	-3.21	1.33	1.37
27	C	515	BCR	C27-C26	-3.20	1.44	1.51
25	C	501	CLA	C1C-NC	-3.20	1.33	1.37
27	K	101	BCR	C4-C5	-3.19	1.44	1.51
25	C	512	CLA	C1C-NC	-3.18	1.33	1.37
25	B	504	CLA	C1C-NC	-3.17	1.33	1.37
25	B	513	CLA	C1C-NC	-3.17	1.33	1.37
25	B	505	CLA	C1C-NC	-3.17	1.33	1.37
25	C	508	CLA	C1C-NC	-3.16	1.33	1.37
27	C	514	BCR	C27-C26	-3.16	1.44	1.51
25	B	512	CLA	C1C-NC	-3.15	1.33	1.37
25	B	515	CLA	C1C-NC	-3.14	1.33	1.37
25	C	510	CLA	C1C-NC	-3.14	1.33	1.37
25	C	513	CLA	C1C-NC	-3.14	1.33	1.37
25	C	503	CLA	C1C-NC	-3.13	1.33	1.37
25	A	406	CLA	C1C-NC	-3.13	1.33	1.37
25	B	508	CLA	C1C-NC	-3.13	1.33	1.37
25	D	405	CLA	C1C-NC	-3.13	1.33	1.37
25	B	507	CLA	C1C-NC	-3.13	1.33	1.37
25	B	502	CLA	C1C-NC	-3.12	1.33	1.37
25	C	507	CLA	C1C-NC	-3.12	1.33	1.37
25	H	101	CLA	C1C-NC	-3.12	1.33	1.37
25	A	408	CLA	C1C-NC	-3.12	1.33	1.37
27	D	406	BCR	C27-C26	-3.11	1.44	1.51
27	C	516	BCR	C27-C26	-3.11	1.44	1.51
25	C	509	CLA	C1C-NC	-3.09	1.33	1.37
25	A	405	CLA	C1C-NC	-3.09	1.33	1.37
25	C	511	CLA	C1C-NC	-3.09	1.33	1.37
25	B	511	CLA	C1C-NC	-3.06	1.33	1.37
25	D	404	CLA	C1C-NC	-3.05	1.33	1.37
25	B	503	CLA	C1C-NC	-3.03	1.33	1.37
25	C	506	CLA	C1C-NC	-3.03	1.33	1.37
35	F	101	HEM	FE-NB	2.88	2.11	1.96
27	B	517	BCR	C34-C9	2.85	1.56	1.50
25	C	506	CLA	CHC-C1C	2.85	1.42	1.35
27	K	101	BCR	C34-C9	2.84	1.56	1.50
27	B	516	BCR	C34-C9	2.83	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	516	BCR	C34-C9	2.82	1.56	1.50
27	C	514	BCR	C34-C9	2.82	1.56	1.50
27	D	406	BCR	C34-C9	2.81	1.56	1.50
25	C	509	CLA	CHC-C1C	2.80	1.42	1.35
27	C	515	BCR	C34-C9	2.79	1.56	1.50
27	A	409	BCR	C34-C9	2.78	1.56	1.50
25	B	510	CLA	CHC-C1C	2.77	1.42	1.35
25	A	408	CLA	CHC-C1C	2.76	1.42	1.35
25	B	503	CLA	CHC-C1C	2.75	1.42	1.35
25	B	514	CLA	CHC-C1C	2.75	1.42	1.35
25	D	404	CLA	CHC-C1C	2.75	1.42	1.35
25	H	101	CLA	CHC-C1C	2.74	1.42	1.35
25	B	511	CLA	CHC-C1C	2.72	1.41	1.35
25	B	508	CLA	CHC-C1C	2.72	1.41	1.35
25	B	509	CLA	CHC-C1C	2.72	1.41	1.35
25	B	505	CLA	CHC-C1C	2.72	1.41	1.35
25	B	513	CLA	CHC-C1C	2.72	1.41	1.35
25	C	510	CLA	CHC-C1C	2.72	1.41	1.35
25	B	507	CLA	CHC-C1C	2.72	1.41	1.35
25	C	508	CLA	CHC-C1C	2.71	1.41	1.35
25	C	501	CLA	CHC-C1C	2.71	1.41	1.35
25	B	501	CLA	CHC-C1C	2.71	1.41	1.35
25	C	507	CLA	CHC-C1C	2.71	1.41	1.35
27	K	101	BCR	C7-C6	2.71	1.54	1.45
25	B	502	CLA	CHC-C1C	2.70	1.41	1.35
25	D	401	CLA	CHC-C1C	2.70	1.41	1.35
25	C	503	CLA	CHC-C1C	2.69	1.41	1.35
25	A	405	CLA	CHC-C1C	2.69	1.41	1.35
27	C	515	BCR	C7-C6	2.69	1.54	1.45
25	B	515	CLA	CHC-C1C	2.69	1.41	1.35
25	B	506	CLA	CHC-C1C	2.69	1.41	1.35
25	D	405	CLA	CHC-C1C	2.69	1.41	1.35
25	A	406	CLA	CHC-C1C	2.68	1.41	1.35
27	B	517	BCR	C7-C6	2.68	1.54	1.45
27	C	514	BCR	C7-C6	2.68	1.54	1.45
25	C	511	CLA	CHC-C1C	2.68	1.41	1.35
25	C	512	CLA	CHC-C1C	2.67	1.41	1.35
25	B	504	CLA	CHC-C1C	2.66	1.41	1.35
27	B	516	BCR	C7-C6	2.65	1.54	1.45
27	A	409	BCR	C7-C6	2.65	1.54	1.45
27	D	406	BCR	C7-C6	2.65	1.54	1.45
25	C	502	CLA	CHC-C1C	2.65	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	CHC-C1C	2.65	1.41	1.35
25	B	512	CLA	CHC-C1C	2.64	1.41	1.35
25	C	504	CLA	CHC-C1C	2.63	1.41	1.35
27	C	516	BCR	C7-C6	2.63	1.54	1.45
25	C	513	CLA	CHC-C1C	2.59	1.41	1.35
31	C	519	DGD	CAB-C9B	-2.57	1.33	1.51
25	B	515	CLA	C3B-C2B	-2.47	1.36	1.40
25	B	501	CLA	C3B-C2B	-2.41	1.37	1.40
25	D	404	CLA	C3B-C2B	-2.38	1.37	1.40
27	C	515	BCR	C36-C18	2.38	1.55	1.50
27	C	516	BCR	C36-C18	2.37	1.55	1.50
27	B	517	BCR	C36-C18	2.37	1.55	1.50
25	C	513	CLA	C1C-C2C	2.36	1.49	1.44
27	A	409	BCR	C36-C18	2.36	1.55	1.50
27	C	514	BCR	C36-C18	2.35	1.55	1.50
27	D	406	BCR	C36-C18	2.35	1.55	1.50
25	C	501	CLA	C3B-C2B	-2.34	1.37	1.40
25	B	509	CLA	C3B-C2B	-2.32	1.37	1.40
25	B	505	CLA	C3B-C2B	-2.31	1.37	1.40
27	B	516	BCR	C36-C18	2.31	1.55	1.50
25	C	507	CLA	C3B-C2B	-2.30	1.37	1.40
27	K	101	BCR	C36-C18	2.25	1.55	1.50
27	B	516	BCR	C39-C30	-2.24	1.49	1.53
25	D	404	CLA	C1C-C2C	2.24	1.48	1.44
25	C	504	CLA	C3B-C2B	-2.22	1.37	1.40
25	B	513	CLA	C3B-C2B	-2.22	1.37	1.40
27	C	516	BCR	C39-C30	-2.21	1.49	1.53
25	B	503	CLA	C1C-C2C	2.20	1.48	1.44
25	B	511	CLA	C1C-C2C	2.19	1.48	1.44
25	C	509	CLA	C1C-C2C	2.18	1.48	1.44
25	B	503	CLA	C3B-C2B	-2.18	1.37	1.40
25	B	502	CLA	C1C-C2C	2.18	1.48	1.44
25	C	505	CLA	C3B-C2B	-2.17	1.37	1.40
25	B	508	CLA	C1C-C2C	2.17	1.48	1.44
25	B	515	CLA	C1C-C2C	2.16	1.48	1.44
27	B	517	BCR	C39-C30	-2.16	1.49	1.53
25	C	513	CLA	C3D-C4D	-2.16	1.39	1.44
25	B	504	CLA	C3B-C2B	-2.16	1.37	1.40
27	C	515	BCR	C39-C30	-2.16	1.49	1.53
27	D	406	BCR	C39-C30	-2.16	1.49	1.53
27	K	101	BCR	C39-C30	-2.16	1.49	1.53
27	C	514	BCR	C39-C30	-2.16	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	514	BCR	C38-C26	2.16	1.54	1.50
27	A	409	BCR	C39-C30	-2.16	1.49	1.53
25	B	509	CLA	C1C-C2C	2.16	1.48	1.44
25	D	405	CLA	C3B-C2B	-2.15	1.37	1.40
25	B	502	CLA	C3B-C2B	-2.14	1.37	1.40
25	B	501	CLA	C1C-C2C	2.14	1.48	1.44
27	A	409	BCR	C37-C22	2.13	1.55	1.50
27	C	516	BCR	C38-C26	2.13	1.54	1.50
25	B	505	CLA	C1C-C2C	2.13	1.48	1.44
25	C	507	CLA	C1C-C2C	2.13	1.48	1.44
25	B	512	CLA	C3B-C2B	-2.13	1.37	1.40
25	C	508	CLA	C3B-C2B	-2.13	1.37	1.40
25	C	510	CLA	C1C-C2C	2.12	1.48	1.44
25	B	510	CLA	C1C-C2C	2.12	1.48	1.44
27	K	101	BCR	C38-C26	2.12	1.54	1.50
25	C	501	CLA	C1C-C2C	2.12	1.48	1.44
25	A	406	CLA	C3B-C2B	-2.12	1.37	1.40
25	C	511	CLA	C3B-C2B	-2.12	1.37	1.40
25	C	512	CLA	C3B-C2B	-2.12	1.37	1.40
25	C	513	CLA	C3B-C2B	-2.12	1.37	1.40
27	D	406	BCR	C38-C26	2.12	1.54	1.50
27	B	517	BCR	C38-C26	2.11	1.54	1.50
25	H	101	CLA	C1C-C2C	2.11	1.48	1.44
25	H	101	CLA	C3B-C2B	-2.11	1.37	1.40
27	B	517	BCR	C37-C22	2.10	1.55	1.50
25	B	513	CLA	C1C-C2C	2.10	1.48	1.44
25	C	512	CLA	C1C-C2C	2.10	1.48	1.44
25	C	503	CLA	C3B-C2B	-2.10	1.37	1.40
25	C	508	CLA	C1C-C2C	2.10	1.48	1.44
25	A	408	CLA	C1C-C2C	2.09	1.48	1.44
27	D	406	BCR	C37-C22	2.09	1.55	1.50
35	F	101	HEM	C1D-ND	-2.09	1.34	1.38
25	B	507	CLA	C1C-C2C	2.08	1.48	1.44
25	C	503	CLA	C1C-C2C	2.08	1.48	1.44
25	B	514	CLA	C1C-C2C	2.08	1.48	1.44
25	B	505	CLA	C3D-C4D	-2.08	1.39	1.44
25	D	405	CLA	C1C-C2C	2.08	1.48	1.44
27	C	515	BCR	C38-C26	2.08	1.54	1.50
25	D	401	CLA	C1C-C2C	2.08	1.48	1.44
27	C	515	BCR	C37-C22	2.07	1.55	1.50
25	C	504	CLA	C1C-C2C	2.07	1.48	1.44
27	K	101	BCR	C37-C22	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	508	CLA	C3B-C2B	-2.07	1.37	1.40
25	A	406	CLA	C1C-C2C	2.07	1.48	1.44
27	A	409	BCR	C38-C26	2.07	1.54	1.50
25	C	511	CLA	C1A-CHA	2.07	1.51	1.43
27	C	514	BCR	C37-C22	2.07	1.55	1.50
25	C	511	CLA	C1C-C2C	2.07	1.48	1.44
25	A	405	CLA	C3B-C2B	-2.06	1.37	1.40
25	C	505	CLA	C3D-C4D	-2.06	1.39	1.44
25	C	510	CLA	C3B-C2B	-2.06	1.37	1.40
25	A	408	CLA	C3B-C2B	-2.05	1.37	1.40
25	D	401	CLA	C3B-C2B	-2.05	1.37	1.40
25	B	504	CLA	C1C-C2C	2.05	1.48	1.44
25	B	504	CLA	C1A-CHA	2.05	1.51	1.43
25	B	507	CLA	C3B-C2B	-2.05	1.37	1.40
27	B	516	BCR	C37-C22	2.05	1.55	1.50
25	A	405	CLA	C1C-C2C	2.04	1.48	1.44
25	B	514	CLA	C3B-C2B	-2.04	1.37	1.40
25	B	508	CLA	C3D-C4D	-2.04	1.39	1.44
25	C	502	CLA	C3B-C2B	-2.04	1.37	1.40
25	B	505	CLA	C1B-NB	2.04	1.37	1.35
27	B	516	BCR	C38-C26	2.04	1.54	1.50
25	B	503	CLA	C1A-CHA	2.03	1.51	1.43
35	F	101	HEM	CHB-C1B	2.03	1.40	1.35
29	W	201	LMG	C43-C42	-2.02	1.33	1.49
25	B	506	CLA	C3D-C4D	-2.02	1.39	1.44
25	B	506	CLA	C3B-C2B	-2.02	1.37	1.40
25	B	510	CLA	C3B-C2B	-2.02	1.37	1.40
25	H	101	CLA	C3D-C4D	-2.02	1.39	1.44
29	D	410	LMG	C19-C18	-2.02	1.33	1.49
25	C	502	CLA	C1A-CHA	2.02	1.51	1.43
25	C	505	CLA	C1C-C2C	2.01	1.48	1.44
25	B	512	CLA	C3D-C4D	-2.01	1.39	1.44
31	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
25	A	408	CLA	C1A-CHA	2.01	1.51	1.43
29	C	520	LMG	C25-C24	-2.01	1.33	1.49
25	D	404	CLA	C1B-NB	2.00	1.37	1.35
31	C	517	DGD	CGB-CFB	-2.00	1.33	1.49
25	B	501	CLA	C3D-C4D	-2.00	1.39	1.44
29	W	201	LMG	C22-C21	-2.00	1.33	1.49
29	B	520	LMG	C43-C42	-2.00	1.33	1.49
25	B	512	CLA	C1C-C2C	2.00	1.48	1.44
25	D	401	CLA	C3D-C4D	-2.00	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	520	LMG	C22-C21	-2.00	1.33	1.49

All (798) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	C4A-NA-C1A	9.71	111.07	106.71
25	C	504	CLA	C4A-NA-C1A	9.19	110.84	106.71
25	B	506	CLA	C4A-NA-C1A	9.15	110.82	106.71
25	A	408	CLA	C4A-NA-C1A	9.12	110.80	106.71
25	C	510	CLA	C4A-NA-C1A	9.09	110.79	106.71
25	C	511	CLA	C4A-NA-C1A	9.08	110.79	106.71
25	C	505	CLA	C4A-NA-C1A	9.04	110.77	106.71
25	B	503	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	B	511	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	B	514	CLA	C4A-NA-C1A	8.92	110.72	106.71
25	B	508	CLA	C4A-NA-C1A	8.91	110.71	106.71
25	A	406	CLA	C4A-NA-C1A	8.89	110.70	106.71
25	B	507	CLA	C4A-NA-C1A	8.88	110.70	106.71
25	C	512	CLA	C4A-NA-C1A	8.88	110.70	106.71
25	B	510	CLA	C4A-NA-C1A	8.87	110.69	106.71
25	B	504	CLA	C4A-NA-C1A	8.86	110.69	106.71
25	A	405	CLA	C4A-NA-C1A	8.85	110.69	106.71
25	C	502	CLA	C4A-NA-C1A	8.85	110.68	106.71
25	C	509	CLA	C4A-NA-C1A	8.82	110.67	106.71
25	B	512	CLA	C4A-NA-C1A	8.81	110.67	106.71
25	H	101	CLA	C4A-NA-C1A	8.81	110.67	106.71
25	C	503	CLA	C4A-NA-C1A	8.79	110.66	106.71
25	C	501	CLA	C4A-NA-C1A	8.79	110.66	106.71
25	C	508	CLA	C4A-NA-C1A	8.76	110.64	106.71
25	B	513	CLA	C4A-NA-C1A	8.75	110.64	106.71
25	D	405	CLA	C4A-NA-C1A	8.74	110.63	106.71
25	B	502	CLA	C4A-NA-C1A	8.68	110.61	106.71
25	D	401	CLA	C4A-NA-C1A	8.58	110.56	106.71
25	C	507	CLA	C4A-NA-C1A	8.55	110.55	106.71
25	B	515	CLA	C4A-NA-C1A	8.41	110.49	106.71
25	B	501	CLA	C4A-NA-C1A	8.41	110.49	106.71
25	B	505	CLA	C4A-NA-C1A	8.37	110.47	106.71
25	D	404	CLA	C4A-NA-C1A	8.23	110.41	106.71
25	B	509	CLA	C4A-NA-C1A	8.10	110.35	106.71
27	D	406	BCR	C30-C25-C26	-7.63	111.86	122.61
25	C	506	CLA	C4A-NA-C1A	7.20	109.94	106.71
27	C	516	BCR	C20-C21-C22	-6.92	117.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	515	BCR	C15-C14-C13	-6.28	118.35	127.31
25	B	505	CLA	CMD-C2D-C1D	5.80	134.93	124.71
27	B	517	BCR	C15-C14-C13	-5.79	119.04	127.31
25	B	506	CLA	CMD-C2D-C1D	5.75	134.84	124.71
27	C	514	BCR	C20-C21-C22	-5.72	119.15	127.31
27	C	516	BCR	C16-C17-C18	-5.69	119.19	127.31
27	C	515	BCR	C16-C17-C18	-5.63	119.27	127.31
25	D	405	CLA	CMD-C2D-C1D	5.61	134.59	124.71
25	C	510	CLA	CMD-C2D-C1D	5.59	134.56	124.71
25	B	512	CLA	O2D-CGD-CBD	5.59	121.20	111.27
25	B	513	CLA	CMD-C2D-C1D	5.58	134.55	124.71
27	C	514	BCR	C16-C17-C18	-5.57	119.36	127.31
25	B	510	CLA	CMD-C2D-C1D	5.56	134.51	124.71
25	C	503	CLA	CMD-C2D-C1D	5.56	134.50	124.71
25	D	404	CLA	CMD-C2D-C1D	5.55	134.49	124.71
25	B	502	CLA	CMD-C2D-C1D	5.55	134.49	124.71
25	C	509	CLA	CMD-C2D-C1D	5.54	134.49	124.71
27	K	101	BCR	C24-C23-C22	-5.54	117.86	126.23
25	B	501	CLA	CMD-C2D-C1D	5.54	134.48	124.71
25	C	501	CLA	CMD-C2D-C1D	5.53	134.46	124.71
25	C	511	CLA	CMD-C2D-C1D	5.53	134.46	124.71
27	A	409	BCR	C11-C10-C9	-5.53	119.42	127.31
25	B	515	CLA	CMD-C2D-C1D	5.53	134.45	124.71
25	C	507	CLA	CMD-C2D-C1D	5.52	134.44	124.71
25	C	508	CLA	CMD-C2D-C1D	5.51	134.42	124.71
25	B	514	CLA	CMD-C2D-C1D	5.51	134.42	124.71
25	A	405	CLA	CMD-C2D-C1D	5.51	134.42	124.71
25	B	507	CLA	CMD-C2D-C1D	5.50	134.40	124.71
25	C	504	CLA	CMD-C2D-C1D	5.48	134.37	124.71
25	A	406	CLA	CMD-C2D-C1D	5.47	134.36	124.71
25	A	408	CLA	CMD-C2D-C1D	5.47	134.36	124.71
25	B	503	CLA	CMD-C2D-C1D	5.47	134.36	124.71
27	K	101	BCR	C16-C17-C18	-5.47	119.51	127.31
25	D	401	CLA	CMD-C2D-C1D	5.44	134.29	124.71
25	H	101	CLA	CMD-C2D-C1D	5.44	134.29	124.71
25	B	512	CLA	CMD-C2D-C1D	5.43	134.28	124.71
25	C	513	CLA	CMD-C2D-C1D	5.41	134.25	124.71
25	B	506	CLA	O2D-CGD-CBD	5.41	120.88	111.27
27	C	515	BCR	C38-C26-C25	-5.40	118.46	124.53
25	B	509	CLA	CMD-C2D-C1D	5.40	134.22	124.71
25	C	505	CLA	CMD-C2D-C1D	5.40	134.22	124.71
25	B	508	CLA	CMD-C2D-C1D	5.39	134.21	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	BCR	C16-C17-C18	-5.37	119.64	127.31
25	C	506	CLA	CMD-C2D-C1D	5.37	134.18	124.71
25	C	512	CLA	CMD-C2D-C1D	5.37	134.18	124.71
25	B	504	CLA	CMD-C2D-C1D	5.36	134.15	124.71
25	C	502	CLA	CMD-C2D-C1D	5.35	134.15	124.71
25	B	502	CLA	O2D-CGD-CBD	5.35	120.78	111.27
25	C	510	CLA	O2D-CGD-CBD	5.35	120.77	111.27
25	A	406	CLA	O2D-CGD-CBD	5.35	120.77	111.27
25	C	510	CLA	O2A-C1-C2	5.33	122.65	108.64
27	C	514	BCR	C38-C26-C25	-5.33	118.54	124.53
25	B	511	CLA	CMD-C2D-C1D	5.32	134.10	124.71
27	B	516	BCR	C15-C14-C13	-5.32	119.71	127.31
25	C	508	CLA	O2D-CGD-CBD	5.24	120.58	111.27
25	B	515	CLA	O2D-CGD-CBD	5.24	120.57	111.27
35	F	101	HEM	CHC-C4B-NB	5.22	130.10	124.43
25	C	504	CLA	O2D-CGD-CBD	5.21	120.52	111.27
25	C	509	CLA	O2D-CGD-CBD	5.19	120.50	111.27
25	D	405	CLA	O2D-CGD-CBD	5.19	120.49	111.27
25	C	506	CLA	O2D-CGD-CBD	5.18	120.48	111.27
25	C	505	CLA	O2A-C1-C2	5.18	122.25	108.64
25	B	509	CLA	O2D-CGD-CBD	5.18	120.47	111.27
25	C	507	CLA	O2D-CGD-CBD	5.16	120.43	111.27
25	B	511	CLA	O2D-CGD-CBD	5.15	120.42	111.27
25	A	408	CLA	O2D-CGD-CBD	5.13	120.38	111.27
27	D	406	BCR	C27-C26-C25	-5.12	115.29	122.73
27	K	101	BCR	C1-C6-C5	-5.11	115.41	122.61
25	D	401	CLA	O2D-CGD-CBD	5.11	120.34	111.27
25	C	501	CLA	O2D-CGD-CBD	5.09	120.31	111.27
25	C	502	CLA	O2D-CGD-CBD	5.09	120.31	111.27
27	C	514	BCR	C11-C10-C9	-5.06	120.09	127.31
25	B	507	CLA	O2D-CGD-CBD	5.05	120.24	111.27
27	C	516	BCR	C38-C26-C25	-5.04	118.86	124.53
25	B	510	CLA	O2D-CGD-CBD	5.04	120.22	111.27
25	B	513	CLA	O2D-CGD-CBD	5.03	120.21	111.27
25	C	512	CLA	O2D-CGD-CBD	5.02	120.18	111.27
25	A	406	CLA	O2A-C1-C2	5.00	120.65	108.97
25	C	512	CLA	O2A-C1-C2	5.00	121.76	108.64
25	D	405	CLA	O2A-C1-C2	4.99	121.74	108.64
25	B	508	CLA	O2D-CGD-CBD	4.98	120.12	111.27
25	C	511	CLA	O2D-CGD-CBD	4.98	120.12	111.27
25	B	507	CLA	O2A-C1-C2	4.98	121.72	108.64
25	D	404	CLA	O2D-CGD-CBD	4.97	120.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	405	CLA	O2D-CGD-CBD	4.97	120.09	111.27
25	B	514	CLA	O2D-CGD-CBD	4.95	120.06	111.27
25	C	505	CLA	O2D-CGD-CBD	4.95	120.06	111.27
25	C	507	CLA	O2A-C1-C2	4.94	121.62	108.64
25	D	404	CLA	O2A-C1-C2	4.93	121.59	108.64
25	C	513	CLA	O2D-CGD-CBD	4.93	120.02	111.27
25	B	504	CLA	O2D-CGD-CBD	4.92	120.00	111.27
25	B	510	CLA	O2A-C1-C2	4.90	121.51	108.64
27	C	516	BCR	C11-C10-C9	-4.89	120.33	127.31
25	B	503	CLA	O2A-C1-C2	4.88	121.47	108.64
25	C	511	CLA	O2A-C1-C2	4.87	121.44	108.64
25	B	501	CLA	O2D-CGD-CBD	4.87	119.92	111.27
25	B	513	CLA	O2A-C1-C2	4.87	121.42	108.64
25	B	505	CLA	O2D-CGD-CBD	4.85	119.89	111.27
27	A	409	BCR	C33-C5-C6	-4.85	119.08	124.53
25	B	501	CLA	O2A-C1-C2	4.84	121.36	108.64
27	C	515	BCR	C7-C8-C9	-4.81	118.97	126.23
25	C	503	CLA	O2D-CGD-CBD	4.80	119.80	111.27
25	B	512	CLA	O2A-C1-C2	4.79	121.23	108.64
27	B	517	BCR	C11-C10-C9	-4.78	120.49	127.31
25	B	502	CLA	O2A-C1-C2	4.76	121.16	108.64
27	C	516	BCR	C7-C8-C9	-4.76	119.05	126.23
25	B	504	CLA	O2A-C1-C2	4.75	121.12	108.64
25	H	101	CLA	O2D-CGD-CBD	4.74	119.69	111.27
25	B	503	CLA	O2D-CGD-CBD	4.73	119.67	111.27
25	B	505	CLA	O2A-C1-C2	4.71	121.02	108.64
27	B	517	BCR	C1-C6-C5	-4.71	115.98	122.61
27	C	515	BCR	C33-C5-C6	-4.68	119.27	124.53
25	H	101	CLA	O2A-C1-C2	4.67	120.90	108.64
27	C	516	BCR	C15-C14-C13	-4.65	120.67	127.31
25	C	502	CLA	O2A-C1-C2	4.65	120.86	108.64
25	A	405	CLA	O2A-C1-C2	4.64	120.84	108.64
25	C	503	CLA	O2A-C1-C2	4.62	120.77	108.64
27	B	516	BCR	C1-C6-C5	-4.61	116.11	122.61
25	C	508	CLA	O2A-C1-C2	4.59	120.71	108.64
25	C	504	CLA	O2A-C1-C2	4.59	120.70	108.64
25	B	511	CLA	O2A-C1-C2	4.59	120.69	108.64
27	D	406	BCR	C38-C26-C25	-4.58	119.39	124.53
25	D	401	CLA	O2A-C1-C2	4.57	120.66	108.64
25	A	408	CLA	O2A-C1-C2	4.57	120.65	108.64
27	C	515	BCR	C1-C6-C5	-4.56	116.19	122.61
27	C	515	BCR	C11-C10-C9	-4.55	120.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	409	BCR	C20-C21-C22	-4.54	120.83	127.31
27	A	409	BCR	C27-C26-C25	-4.52	116.17	122.73
27	B	516	BCR	C4-C5-C6	-4.50	116.19	122.73
25	C	506	CLA	O2A-C1-C2	4.50	120.45	108.64
27	A	409	BCR	C38-C26-C25	-4.44	119.55	124.53
25	B	506	CLA	O2A-C1-C2	4.43	120.27	108.64
27	B	516	BCR	C33-C5-C6	-4.42	119.56	124.53
30	D	409	LHG	O7-C7-C8	4.42	121.04	111.50
27	A	409	BCR	C15-C14-C13	-4.42	121.00	127.31
25	C	501	CLA	O2A-C1-C2	4.42	120.24	108.64
25	B	515	CLA	O2A-C1-C2	4.35	120.08	108.64
25	B	508	CLA	O2A-C1-C2	4.35	120.06	108.64
25	B	514	CLA	O2A-C1-C2	4.34	120.04	108.64
31	C	519	DGD	O2G-C1B-C2B	4.34	120.85	111.50
35	F	101	HEM	CHD-C1D-ND	4.33	129.13	124.43
27	K	101	BCR	C15-C14-C13	-4.33	121.14	127.31
25	B	512	CLA	C1-C2-C3	-4.30	118.60	126.04
25	B	509	CLA	O2A-C1-C2	4.29	119.91	108.64
27	C	516	BCR	C33-C5-C6	-4.27	119.73	124.53
27	C	515	BCR	C20-C21-C22	-4.27	121.22	127.31
27	C	516	BCR	C24-C23-C22	-4.25	119.81	126.23
27	K	101	BCR	C27-C26-C25	-4.24	116.57	122.73
27	K	101	BCR	C38-C26-C25	-4.23	119.78	124.53
27	A	409	BCR	C16-C17-C18	-4.21	121.30	127.31
27	C	515	BCR	C4-C5-C6	-4.19	116.65	122.73
29	W	201	LMG	O7-C10-C11	4.18	120.51	111.50
27	D	406	BCR	C11-C10-C9	-4.13	121.41	127.31
27	B	516	BCR	C11-C10-C9	-4.13	121.42	127.31
27	B	517	BCR	C33-C5-C6	-4.11	119.91	124.53
27	B	516	BCR	C30-C25-C26	-4.11	116.83	122.61
27	K	101	BCR	C33-C5-C6	-4.06	119.97	124.53
27	D	406	BCR	C7-C8-C9	-4.06	120.10	126.23
25	B	506	CLA	C1-C2-C3	-4.05	119.05	126.04
27	K	101	BCR	C30-C25-C26	-4.01	116.96	122.61
29	B	520	LMG	O7-C10-C11	4.00	120.13	111.50
31	C	518	DGD	O2G-C1B-C2B	4.00	120.13	111.50
30	B	519	LHG	O7-C7-C8	4.00	120.12	111.50
27	B	517	BCR	C4-C5-C6	-4.00	116.93	122.73
25	C	510	CLA	C1-C2-C3	-3.96	119.19	126.04
29	C	520	LMG	O7-C10-C11	3.96	120.03	111.50
25	C	511	CLA	C1-C2-C3	-3.95	119.21	126.04
27	B	516	BCR	C7-C8-C9	-3.94	120.29	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	515	CLA	C1-C2-C3	-3.93	120.39	126.75
27	C	516	BCR	C1-C6-C5	-3.89	117.13	122.61
29	B	518	LMG	O7-C10-C11	3.87	119.84	111.50
25	C	506	CLA	C1-C2-C3	-3.86	120.50	126.75
27	C	516	BCR	C4-C5-C6	-3.86	117.13	122.73
30	D	408	LHG	O7-C7-C8	3.84	119.78	111.50
25	B	504	CLA	C1-C2-C3	-3.83	119.42	126.04
27	D	406	BCR	C15-C14-C13	-3.82	121.86	127.31
35	F	101	HEM	C1B-NB-C4B	3.82	109.02	105.07
25	B	514	CLA	C1-C2-C3	-3.80	119.47	126.04
25	B	507	CLA	C1-C2-C3	-3.80	119.48	126.04
25	C	509	CLA	O2A-C1-C2	3.77	118.55	108.64
27	B	516	BCR	C27-C26-C25	-3.77	117.26	122.73
25	D	404	CLA	C1-C2-C3	-3.76	119.54	126.04
27	D	406	BCR	C20-C21-C22	-3.75	121.96	127.31
27	D	406	BCR	C33-C5-C6	-3.74	120.32	124.53
27	B	516	BCR	C38-C26-C25	-3.73	120.34	124.53
29	D	410	LMG	O7-C10-C11	3.72	119.53	111.50
27	B	517	BCR	C16-C17-C18	-3.72	122.00	127.31
25	A	408	CLA	C1-C2-C3	-3.68	119.67	126.04
25	C	503	CLA	C1-C2-C3	-3.67	119.69	126.04
25	B	501	CLA	C1-C2-C3	-3.67	119.70	126.04
25	C	512	CLA	C6-C5-C3	-3.64	108.66	114.62
25	D	404	CLA	C2D-C1D-ND	3.64	112.78	110.10
25	D	401	CLA	C1-C2-C3	-3.60	119.82	126.04
25	B	510	CLA	C1-C2-C3	-3.59	119.84	126.04
27	B	517	BCR	C20-C21-C22	-3.58	122.20	127.31
25	C	502	CLA	C1-C2-C3	-3.56	119.88	126.04
27	B	516	BCR	C38-C26-C27	3.56	120.45	113.62
30	B	521	LHG	O7-C7-C8	3.56	119.17	111.50
34	D	407	PL9	C7-C3-C4	3.56	119.77	116.88
27	B	517	BCR	C38-C26-C25	-3.55	120.55	124.53
27	K	101	BCR	C11-C10-C9	-3.54	122.25	127.31
27	C	515	BCR	C27-C26-C25	-3.54	117.59	122.73
28	A	410	SQD	O7-S-C6	-3.53	102.75	106.94
25	D	405	CLA	C1-C2-C3	-3.53	119.94	126.04
27	B	516	BCR	C24-C23-C22	-3.50	120.94	126.23
25	C	505	CLA	C1-C2-C3	-3.49	120.01	126.04
25	B	505	CLA	C1-C2-C3	-3.49	120.01	126.04
27	D	406	BCR	C4-C5-C6	-3.49	117.67	122.73
27	B	516	BCR	C16-C17-C18	-3.48	122.35	127.31
27	A	409	BCR	C24-C23-C22	-3.48	120.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	C2C-C1C-NC	3.48	113.23	109.97
27	C	514	BCR	C33-C5-C6	-3.47	120.64	124.53
25	A	405	CLA	C1-C2-C3	-3.46	120.05	126.04
25	C	512	CLA	C1-C2-C3	-3.46	120.05	126.04
27	A	409	BCR	C1-C6-C5	-3.46	117.75	122.61
27	C	514	BCR	C33-C5-C4	3.45	120.24	113.62
27	C	514	BCR	C4-C5-C6	-3.44	117.74	122.73
31	C	517	DGD	O2G-C1B-C2B	3.43	118.89	111.50
35	F	101	HEM	CHA-C4D-ND	3.43	128.62	124.38
25	C	508	CLA	C1-C2-C3	-3.43	120.12	126.04
35	F	101	HEM	CHB-C1B-NB	3.42	128.61	124.38
25	D	404	CLA	CHD-C1D-ND	-3.42	121.31	124.45
25	B	502	CLA	C1-C2-C3	-3.42	120.14	126.04
27	A	409	BCR	C7-C8-C9	-3.41	121.08	126.23
25	C	504	CLA	C1-C2-C3	-3.40	120.15	126.04
25	C	507	CLA	C1-C2-C3	-3.39	120.18	126.04
27	C	514	BCR	C24-C23-C22	-3.39	121.11	126.23
27	A	409	BCR	C4-C5-C6	-3.39	117.81	122.73
27	D	406	BCR	C1-C6-C5	-3.38	117.86	122.61
25	B	511	CLA	C1-C2-C3	-3.37	120.21	126.04
25	D	404	CLA	C1D-ND-C4D	-3.35	103.95	106.33
27	C	514	BCR	C1-C6-C5	-3.35	117.89	122.61
25	B	505	CLA	CHD-C1D-ND	-3.35	121.37	124.45
27	B	517	BCR	C30-C25-C26	-3.32	117.93	122.61
27	A	409	BCR	C38-C26-C27	3.31	119.97	113.62
25	B	513	CLA	C1-C2-C3	-3.30	120.33	126.04
25	B	511	CLA	C2D-C1D-ND	3.30	112.54	110.10
27	C	514	BCR	C7-C8-C9	-3.27	121.29	126.23
27	B	517	BCR	C23-C24-C25	-3.26	118.05	127.20
27	B	517	BCR	C38-C26-C27	3.26	119.88	113.62
25	B	503	CLA	C1-C2-C3	-3.26	120.41	126.04
27	A	409	BCR	C30-C25-C26	-3.25	118.03	122.61
25	C	504	CLA	C2C-C1C-NC	3.25	113.02	109.97
25	B	510	CLA	C2D-C1D-ND	3.25	112.50	110.10
27	K	101	BCR	C38-C26-C27	3.23	119.81	113.62
27	K	101	BCR	C4-C5-C6	-3.22	118.06	122.73
25	B	503	CLA	C2D-C1D-ND	3.22	112.47	110.10
27	B	517	BCR	C33-C5-C4	3.21	119.79	113.62
25	A	408	CLA	C2D-C1D-ND	3.21	112.47	110.10
25	H	101	CLA	C2D-C1D-ND	3.21	112.47	110.10
25	H	101	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	H	101	CLA	C1-C2-C3	-3.20	120.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	BCR	C38-C26-C27	3.20	119.75	113.62
25	C	512	CLA	C2C-C1C-NC	3.19	112.97	109.97
25	D	405	CLA	CHD-C1D-ND	-3.18	121.53	124.45
25	C	510	CLA	C2D-C1D-ND	3.18	112.45	110.10
25	C	511	CLA	C2C-C1C-NC	3.18	112.95	109.97
25	C	509	CLA	C2D-C1D-ND	3.16	112.44	110.10
25	B	512	CLA	C2C-C1C-NC	3.16	112.93	109.97
25	B	514	CLA	C2C-C1C-NC	3.15	112.93	109.97
25	C	507	CLA	C2D-C1D-ND	3.15	112.43	110.10
25	B	514	CLA	CHD-C1D-ND	-3.14	121.56	124.45
25	B	511	CLA	C2C-C1C-NC	3.14	112.92	109.97
27	C	516	BCR	C30-C25-C26	-3.14	118.19	122.61
27	D	406	BCR	C23-C24-C25	-3.14	118.39	127.20
25	B	502	CLA	CMA-C3A-C4A	3.14	120.20	111.77
25	B	504	CLA	C2C-C1C-NC	3.13	112.91	109.97
25	C	506	CLA	C2D-C1D-ND	3.13	112.41	110.10
25	A	405	CLA	C2D-C1D-ND	3.13	112.41	110.10
27	C	516	BCR	C33-C5-C4	3.12	119.61	113.62
25	C	509	CLA	CHD-C1D-ND	-3.12	121.59	124.45
25	C	501	CLA	C2D-C1D-ND	3.11	112.40	110.10
25	B	501	CLA	CHD-C1D-ND	-3.11	121.59	124.45
25	B	510	CLA	CHD-C1D-ND	-3.11	121.60	124.45
25	C	506	CLA	CMA-C3A-C4A	3.10	120.11	111.77
25	A	406	CLA	C2D-C1D-ND	3.10	112.39	110.10
25	C	508	CLA	C2D-C1D-ND	3.10	112.39	110.10
25	B	507	CLA	C2C-C1C-NC	3.10	112.87	109.97
25	C	502	CLA	C2C-C1C-NC	3.10	112.87	109.97
25	A	406	CLA	C2C-C1C-NC	3.10	112.87	109.97
25	C	510	CLA	CHD-C1D-ND	-3.09	121.61	124.45
25	B	502	CLA	CHD-C1D-ND	-3.09	121.61	124.45
25	B	501	CLA	C2D-C1D-ND	3.09	112.38	110.10
25	B	506	CLA	C2D-C1D-ND	3.08	112.38	110.10
25	B	506	CLA	CHD-C1D-ND	-3.08	121.62	124.45
25	B	508	CLA	C2D-C1D-ND	3.08	112.38	110.10
27	A	409	BCR	C23-C24-C25	-3.08	118.55	127.20
25	B	514	CLA	C2D-C1D-ND	3.08	112.37	110.10
27	K	101	BCR	C33-C5-C4	3.08	119.53	113.62
25	C	507	CLA	C2C-C1C-NC	3.08	112.86	109.97
25	D	401	CLA	CHD-C1D-ND	-3.07	121.64	124.45
25	C	511	CLA	C2D-C1D-ND	3.07	112.36	110.10
32	C	521	LMU	C1B-O1B-C4'	-3.07	110.38	117.96
25	C	512	CLA	C2D-C1D-ND	3.06	112.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	CHD-C1D-ND	-3.06	121.64	124.45
27	D	406	BCR	C33-C5-C4	3.06	119.49	113.62
25	A	408	CLA	CHD-C1D-ND	-3.06	121.64	124.45
25	B	509	CLA	C2C-C1C-NC	3.06	112.84	109.97
25	B	504	CLA	C2D-C1D-ND	3.05	112.35	110.10
25	B	514	CLA	CMA-C3A-C4A	3.05	119.98	111.77
25	A	405	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	C	510	CLA	C2C-C1C-NC	3.04	112.82	109.97
25	B	515	CLA	C2C-C1C-NC	3.04	112.82	109.97
25	C	504	CLA	C2D-C1D-ND	3.04	112.35	110.10
25	C	513	CLA	CHD-C1D-ND	-3.04	121.66	124.45
27	C	515	BCR	C24-C23-C22	-3.04	121.64	126.23
25	B	513	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	A	406	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	B	511	CLA	C1D-ND-C4D	-3.03	104.18	106.33
25	C	507	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	C	505	CLA	C2C-C1C-NC	3.03	112.81	109.97
25	D	401	CLA	CMA-C3A-C4A	3.03	119.92	111.77
25	B	502	CLA	C2D-C1D-ND	3.03	112.33	110.10
25	B	505	CLA	C1D-ND-C4D	-3.02	104.19	106.33
25	C	503	CLA	C2D-C1D-ND	3.02	112.33	110.10
25	D	405	CLA	C2D-C1D-ND	3.02	112.33	110.10
25	B	513	CLA	C2D-C1D-ND	3.02	112.33	110.10
27	C	514	BCR	C15-C16-C17	-3.02	117.29	123.47
25	B	509	CLA	CHD-C1D-ND	-3.02	121.68	124.45
27	C	514	BCR	C27-C26-C25	-3.01	118.36	122.73
25	B	507	CLA	C2D-C1D-ND	3.01	112.32	110.10
25	C	502	CLA	C2D-C1D-ND	3.01	112.32	110.10
25	B	508	CLA	CHD-C1D-ND	-3.01	121.69	124.45
25	C	512	CLA	CHD-C1D-ND	-3.00	121.69	124.45
25	B	509	CLA	C2D-C1D-ND	3.00	112.32	110.10
25	B	502	CLA	C2C-C1C-NC	3.00	112.78	109.97
25	D	401	CLA	C2C-C1C-NC	2.99	112.77	109.97
27	B	516	BCR	C33-C5-C4	2.99	119.36	113.62
25	B	501	CLA	C2C-C1C-NC	2.99	112.77	109.97
27	C	515	BCR	C33-C5-C4	2.99	119.35	113.62
25	C	509	CLA	C2C-C1C-NC	2.98	112.77	109.97
25	C	503	CLA	CHD-C1D-ND	-2.98	121.71	124.45
27	K	101	BCR	C8-C7-C6	-2.98	118.84	127.20
25	B	504	CLA	CMA-C3A-C4A	2.98	119.78	111.77
25	C	501	CLA	CMA-C3A-C4A	2.98	119.78	111.77
25	B	515	CLA	CHD-C1D-ND	-2.98	121.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	510	CLA	CMA-C3A-C4A	2.97	119.76	111.77
25	C	501	CLA	C1-C2-C3	-2.97	120.91	126.04
25	A	408	CLA	C1D-ND-C4D	-2.97	104.23	106.33
25	C	502	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	B	515	CLA	CMA-C3A-C4A	2.96	119.72	111.77
25	B	510	CLA	C1D-ND-C4D	-2.95	104.24	106.33
27	B	517	BCR	C8-C7-C6	-2.95	118.92	127.20
25	B	506	CLA	C2C-C1C-NC	2.95	112.73	109.97
25	C	512	CLA	CMA-C3A-C4A	2.95	119.70	111.77
25	C	503	CLA	C2C-C1C-NC	2.95	112.73	109.97
25	D	405	CLA	C2C-C1C-NC	2.95	112.73	109.97
25	B	511	CLA	CMA-C3A-C4A	2.94	119.68	111.77
25	B	509	CLA	CMA-C3A-C4A	2.94	119.68	111.77
25	B	515	CLA	C2D-C1D-ND	2.94	112.27	110.10
25	C	509	CLA	C1D-ND-C4D	-2.94	104.25	106.33
25	C	504	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	D	404	CLA	C2C-C1C-NC	2.94	112.72	109.97
25	B	507	CLA	CHD-C1D-ND	-2.94	121.76	124.45
25	C	513	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
25	C	511	CLA	CMA-C3A-C4A	2.93	119.65	111.77
25	B	506	CLA	C1D-ND-C4D	-2.93	104.25	106.33
25	B	508	CLA	CMA-C3A-C4A	2.93	119.65	111.77
25	B	505	CLA	C2C-C1C-NC	2.93	112.71	109.97
25	B	501	CLA	C1D-ND-C4D	-2.93	104.26	106.33
25	B	511	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	C	503	CLA	CMA-C3A-C4A	2.92	119.62	111.77
25	C	509	CLA	CMA-C3A-C4A	2.92	119.61	111.77
25	B	512	CLA	C2D-C1D-ND	2.92	112.25	110.10
25	D	401	CLA	C2D-C1D-ND	2.92	112.25	110.10
25	A	406	CLA	CMA-C3A-C4A	2.91	119.60	111.77
25	D	405	CLA	C1D-ND-C4D	-2.91	104.27	106.33
25	B	505	CLA	CMA-C3A-C4A	2.91	119.59	111.77
25	A	408	CLA	C2C-C1C-NC	2.90	112.69	109.97
25	H	101	CLA	C1D-ND-C4D	-2.90	104.27	106.33
25	B	501	CLA	CMA-C3A-C4A	2.90	119.58	111.77
25	B	508	CLA	C2C-C1C-NC	2.90	112.69	109.97
30	B	519	LHG	C5-O7-C7	-2.90	110.66	117.79
25	B	503	CLA	CMA-C3A-C4A	2.90	119.55	111.77
25	A	405	CLA	CMA-C3A-C4A	2.89	119.55	111.77
25	C	508	CLA	C1D-ND-C4D	-2.89	104.28	106.33
25	H	101	CLA	C2C-C1C-NC	2.89	112.68	109.97
25	C	513	CLA	CMA-C3A-C4A	2.88	119.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	505	CLA	C2D-C1D-ND	2.88	112.23	110.10
25	B	513	CLA	C2C-C1C-NC	2.88	112.67	109.97
25	B	512	CLA	CHD-C1D-ND	-2.87	121.81	124.45
25	D	405	CLA	CMA-C3A-C4A	2.87	119.49	111.77
27	B	517	BCR	C27-C26-C25	-2.87	118.57	122.73
25	C	506	CLA	C1D-ND-C4D	-2.86	104.30	106.33
25	C	501	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	B	507	CLA	CMA-C3A-C4A	2.86	119.46	111.77
25	C	501	CLA	C2C-C1C-NC	2.86	112.65	109.97
25	B	503	CLA	CHD-C1D-ND	-2.85	121.83	124.45
25	C	502	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	A	408	CLA	CMA-C3A-C4A	2.84	119.41	111.77
25	C	510	CLA	C1D-ND-C4D	-2.84	104.32	106.33
27	B	516	BCR	C15-C16-C17	-2.83	117.67	123.47
27	C	515	BCR	C23-C24-C25	-2.83	119.26	127.20
25	B	508	CLA	C1D-ND-C4D	-2.82	104.33	106.33
31	C	517	DGD	O1G-C1A-C2A	2.82	120.74	111.91
25	C	508	CLA	C2C-C1C-NC	2.81	112.61	109.97
25	C	511	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	A	409	BCR	C33-C5-C4	2.80	118.99	113.62
25	B	503	CLA	C1D-ND-C4D	-2.80	104.35	106.33
27	C	515	BCR	C30-C25-C26	-2.79	118.68	122.61
25	A	406	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
25	D	401	CLA	C1D-ND-C4D	-2.79	104.36	106.33
25	C	505	CLA	CHD-C1D-ND	-2.78	121.89	124.45
25	C	508	CLA	CMA-C3A-C4A	2.78	119.26	111.77
25	C	507	CLA	C1D-ND-C4D	-2.78	104.36	106.33
25	B	514	CLA	C1D-ND-C4D	-2.78	104.36	106.33
25	A	405	CLA	C1D-ND-C4D	-2.77	104.37	106.33
25	A	405	CLA	C2C-C1C-NC	2.77	112.56	109.97
25	C	501	CLA	C1D-ND-C4D	-2.77	104.37	106.33
25	B	503	CLA	C2C-C1C-NC	2.77	112.56	109.97
27	C	516	BCR	C37-C22-C21	-2.77	119.05	122.92
25	C	504	CLA	CMA-C3A-C4A	2.76	119.19	111.77
27	A	409	BCR	C8-C7-C6	-2.76	119.46	127.20
30	B	521	LHG	O8-C23-C24	2.75	120.55	111.91
25	C	512	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
25	C	503	CLA	C1D-ND-C4D	-2.75	104.38	106.33
25	D	404	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
30	D	409	LHG	O8-C23-C24	2.74	120.51	111.91
25	C	505	CLA	C2D-C1D-ND	2.74	112.12	110.10
25	B	510	CLA	C2C-C1C-NC	2.74	112.54	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	508	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
25	B	513	CLA	C1D-ND-C4D	-2.73	104.39	106.33
25	A	406	CLA	C1D-ND-C4D	-2.73	104.39	106.33
27	C	515	BCR	C35-C13-C14	-2.73	119.10	122.92
27	D	406	BCR	C16-C15-C14	-2.72	117.89	123.47
25	B	509	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
25	B	509	CLA	C1D-ND-C4D	-2.72	104.41	106.33
27	K	101	BCR	C16-C15-C14	-2.71	117.92	123.47
25	C	510	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
27	C	514	BCR	C8-C7-C6	-2.70	119.62	127.20
25	B	501	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
25	B	515	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
27	B	516	BCR	C8-C7-C6	-2.70	119.63	127.20
25	C	512	CLA	C1D-ND-C4D	-2.70	104.42	106.33
27	C	516	BCR	C20-C19-C18	-2.70	118.84	126.42
25	B	504	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	B	513	CLA	CMA-C3A-C4A	2.69	119.01	111.77
29	B	518	LMG	C8-O7-C10	-2.69	111.16	117.79
25	B	509	CLA	C1-C2-C3	-2.69	121.39	126.04
25	B	507	CLA	C1D-ND-C4D	-2.69	104.42	106.33
25	B	511	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
27	C	514	BCR	C23-C24-C25	-2.69	119.65	127.20
27	C	516	BCR	C27-C26-C25	-2.69	118.83	122.73
25	B	508	CLA	C1-C2-C3	-2.69	121.39	126.04
25	B	502	CLA	C1D-ND-C4D	-2.69	104.43	106.33
25	B	509	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
35	F	101	HEM	CHD-C1D-C2D	-2.68	120.79	124.98
25	C	511	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
25	B	502	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	D	409	LHG	C5-O7-C7	-2.68	111.20	117.79
25	C	506	CLA	CHD-C1D-ND	-2.67	122.00	124.45
29	W	201	LMG	C8-O7-C10	-2.66	111.23	117.79
27	B	517	BCR	C7-C8-C9	-2.66	122.21	126.23
25	B	512	CLA	CMA-C3A-C4A	2.66	118.93	111.77
25	B	512	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	B	514	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
25	C	507	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
25	B	504	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	C	501	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	C	505	CLA	C1D-ND-C4D	-2.65	104.45	106.33
25	D	405	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
27	B	517	BCR	C24-C23-C22	-2.65	122.24	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	H	101	CLA	CMA-C3A-C4A	2.64	118.88	111.77
25	C	504	CLA	C1D-ND-C4D	-2.64	104.46	106.33
25	B	511	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	C	509	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
25	C	504	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
25	C	506	CLA	CHA-C4D-ND	2.63	138.01	132.50
31	C	518	DGD	O1G-C1A-C2A	2.63	120.17	111.91
25	B	507	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
25	B	505	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
27	A	409	BCR	C20-C19-C18	-2.63	119.04	126.42
25	B	512	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
25	C	502	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	C	507	CLA	CMA-C3A-C4A	2.62	118.81	111.77
25	C	504	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
27	K	101	BCR	C20-C21-C22	-2.61	123.58	127.31
25	C	511	CLA	O2A-CGA-CBA	2.61	120.11	111.91
25	A	406	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	C	506	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	D	401	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
27	D	406	BCR	C8-C7-C6	-2.60	119.89	127.20
29	C	520	LMG	O8-C28-C29	2.60	120.07	111.91
25	H	101	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
25	D	404	CLA	CMA-C3A-C4A	2.60	118.75	111.77
27	B	516	BCR	C23-C24-C25	-2.59	119.92	127.20
30	D	408	LHG	O8-C23-C24	2.59	120.04	111.91
25	C	511	CLA	C1D-ND-C4D	-2.59	104.50	106.33
25	C	503	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
25	D	401	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
27	B	517	BCR	C16-C15-C14	-2.56	118.22	123.47
27	K	101	BCR	C7-C8-C9	-2.56	122.36	126.23
29	B	518	LMG	O8-C28-C29	2.56	119.95	111.91
27	D	406	BCR	C24-C23-C22	-2.56	122.36	126.23
25	B	507	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	504	CLA	C1D-ND-C4D	-2.55	104.52	106.33
31	C	519	DGD	O1G-C1A-C2A	2.55	119.91	111.91
25	B	503	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
25	B	506	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
25	C	507	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
25	B	504	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
31	C	519	DGD	C2G-O2G-C1B	-2.54	111.54	117.79
30	B	519	LHG	O8-C23-C24	2.54	119.87	111.91
25	B	515	CLA	O2D-CGD-O1D	-2.54	118.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	513	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
25	C	505	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
25	C	505	CLA	CHA-C4D-ND	2.53	137.80	132.50
25	B	505	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
25	C	508	CLA	O2A-CGA-CBA	2.53	119.84	111.91
25	C	505	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
25	C	501	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
25	B	504	CLA	CHA-C4D-ND	2.52	137.77	132.50
25	A	408	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
25	B	515	CLA	CHA-C4D-ND	2.51	137.76	132.50
25	C	502	CLA	C1D-ND-C4D	-2.51	104.55	106.33
25	B	503	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
27	C	516	BCR	C36-C18-C17	-2.51	119.41	122.92
25	B	512	CLA	CHA-C4D-ND	2.50	137.73	132.50
25	B	512	CLA	C1D-ND-C4D	-2.50	104.56	106.33
25	C	501	CLA	CHA-C4D-ND	2.50	137.73	132.50
25	B	515	CLA	C1D-ND-C4D	-2.50	104.56	106.33
25	B	503	CLA	CHA-C4D-ND	2.49	137.71	132.50
25	C	511	CLA	CHA-C4D-ND	2.49	137.70	132.50
25	C	510	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
25	C	508	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
25	B	507	CLA	CHA-C4D-ND	2.48	137.69	132.50
25	C	509	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	A	405	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
25	C	503	CLA	CHA-C4D-ND	2.47	137.67	132.50
25	C	502	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
25	C	512	CLA	O2A-CGA-CBA	2.47	119.66	111.91
25	B	506	CLA	CHA-C4D-ND	2.47	137.66	132.50
25	B	502	CLA	CHA-C4D-ND	2.46	137.65	132.50
25	B	513	CLA	CHA-C4D-ND	2.46	137.65	132.50
25	C	504	CLA	CHA-C4D-ND	2.46	137.65	132.50
25	B	506	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
25	A	406	CLA	CHA-C4D-ND	2.45	137.63	132.50
25	C	510	CLA	CHA-C4D-ND	2.45	137.63	132.50
25	B	514	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
25	A	405	CLA	CHA-C4D-ND	2.45	137.62	132.50
25	C	510	CLA	CMA-C3A-C4A	2.44	118.33	111.77
25	B	505	CLA	CHA-C4D-ND	2.44	137.60	132.50
25	A	408	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	C	508	CLA	CHA-C4D-ND	2.44	137.59	132.50
27	B	516	BCR	C30-C25-C24	2.44	122.67	115.78
27	C	515	BCR	C38-C26-C27	2.44	118.29	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	506	CLA	CMA-C3A-C4A	2.43	118.30	111.77
25	B	508	CLA	CHA-C4D-ND	2.43	137.58	132.50
25	C	502	CLA	CHA-C4D-ND	2.43	137.58	132.50
25	C	505	CLA	CMA-C3A-C4A	2.43	118.30	111.77
25	C	506	CLA	CAC-C3C-C4C	2.42	127.95	124.81
25	C	507	CLA	CHA-C4D-ND	2.42	137.56	132.50
25	B	506	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
25	C	512	CLA	CHA-C4D-ND	2.42	137.55	132.50
25	B	510	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
25	B	502	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
25	B	509	CLA	CHA-C4D-ND	2.40	137.53	132.50
25	C	509	CLA	CHA-C4D-ND	2.40	137.52	132.50
25	B	501	CLA	CHA-C4D-ND	2.40	137.52	132.50
25	D	405	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	B	520	LMG	O8-C28-C29	2.40	119.43	111.91
25	D	405	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	B	510	CLA	CHA-C4D-ND	2.39	137.51	132.50
25	H	101	CLA	CHA-C4D-ND	2.39	137.51	132.50
25	B	514	CLA	CHA-C4D-ND	2.39	137.50	132.50
25	C	508	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
25	A	408	CLA	CHA-C4D-ND	2.38	137.49	132.50
25	B	501	CLA	O2A-CGA-CBA	2.38	119.38	111.91
25	D	401	CLA	CHA-C4D-ND	2.38	137.48	132.50
25	B	510	CLA	O2A-CGA-CBA	2.38	119.37	111.91
25	B	503	CLA	O2A-CGA-CBA	2.38	119.37	111.91
25	B	509	CLA	O2A-CGA-CBA	2.38	119.36	111.91
29	D	410	LMG	O8-C28-C29	2.38	119.36	111.91
25	D	401	CLA	O2A-CGA-CBA	2.37	119.34	111.91
25	B	512	CLA	O2A-CGA-CBA	2.37	119.34	111.91
25	A	408	CLA	O2A-CGA-CBA	2.36	119.33	111.91
25	B	513	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
27	C	516	BCR	C8-C7-C6	-2.35	120.60	127.20
25	B	511	CLA	CHA-C4D-ND	2.35	137.41	132.50
25	D	405	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
25	B	510	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
25	C	511	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	C	506	CLA	O2A-CGA-CBA	2.33	119.22	111.91
27	C	514	BCR	C21-C20-C19	-2.33	115.95	123.22
25	B	508	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
25	D	405	CLA	O2A-CGA-CBA	2.33	119.20	111.91
25	A	405	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
27	C	515	BCR	C36-C18-C17	-2.32	119.67	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	514	BCR	C15-C14-C13	-2.32	124.00	127.31
27	B	516	BCR	C20-C21-C22	-2.32	124.00	127.31
25	D	404	CLA	CHA-C4D-ND	2.31	137.32	132.50
27	C	514	BCR	C36-C18-C17	-2.30	119.70	122.92
25	C	505	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
35	F	101	HEM	C4D-ND-C1D	2.29	107.44	105.07
25	C	512	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
27	C	514	BCR	C38-C26-C27	2.29	118.02	113.62
25	B	513	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
27	K	101	BCR	C23-C24-C25	-2.28	120.80	127.20
25	D	404	CLA	O2A-CGA-CBA	2.28	119.06	111.91
27	D	406	BCR	C20-C19-C18	-2.28	120.01	126.42
25	C	513	CLA	CHA-C1A-NA	-2.28	121.18	126.40
29	W	201	LMG	O8-C28-C29	2.28	119.05	111.91
27	C	514	BCR	C37-C22-C21	-2.27	119.74	122.92
25	B	505	CLA	O2A-CGA-CBA	2.27	119.04	111.91
25	C	502	CLA	O2A-CGA-CBA	2.27	119.04	111.91
25	B	501	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
25	C	513	CLA	CHA-C4D-ND	2.27	137.25	132.50
28	A	410	SQD	O3-C3-C2	-2.27	105.11	110.35
27	D	406	BCR	C24-C25-C26	-2.26	115.98	121.46
25	B	507	CLA	O2A-CGA-CBA	2.26	119.00	111.91
27	B	517	BCR	C29-C30-C25	2.26	113.95	110.48
25	C	509	CLA	O2A-CGA-CBA	2.26	118.99	111.91
25	C	503	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
25	C	509	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
25	B	504	CLA	O2A-CGA-CBA	2.25	118.97	111.91
25	C	510	CLA	O2A-CGA-CBA	2.25	118.97	111.91
25	C	510	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
25	C	505	CLA	O2A-CGA-CBA	2.25	118.95	111.91
25	B	506	CLA	O2A-CGA-CBA	2.24	118.95	111.91
25	B	515	CLA	O2A-CGA-CBA	2.24	118.94	111.91
25	B	514	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
25	C	513	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
25	C	511	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
27	B	516	BCR	C11-C12-C13	-2.24	120.12	126.42
25	B	502	CLA	CHA-C1A-NA	-2.24	121.27	126.40
25	C	513	CLA	C2D-C1D-ND	2.24	111.75	110.10
25	B	507	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
25	B	502	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
25	C	508	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
25	C	513	CLA	O2D-CGD-O1D	-2.23	119.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	501	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
25	C	507	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
25	B	502	CLA	O2A-CGA-CBA	2.23	118.89	111.91
25	C	507	CLA	O2A-CGA-CBA	2.22	118.87	111.91
25	D	401	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
25	C	509	CLA	C1-C2-C3	-2.21	122.21	126.04
25	H	101	CLA	O2A-CGA-CBA	2.21	118.85	111.91
25	A	405	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
25	A	408	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
25	B	510	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
27	C	516	BCR	C23-C22-C21	2.20	122.32	118.94
25	B	515	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
25	C	504	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
27	B	516	BCR	C35-C13-C14	-2.20	119.84	122.92
30	B	521	LHG	C5-O7-C7	-2.20	112.38	117.79
25	B	508	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
25	C	501	CLA	O2A-CGA-CBA	2.20	118.80	111.91
25	A	406	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
25	B	501	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
33	D	403	BCT	O2-C-O1	2.19	125.23	119.55
25	B	508	CLA	CMB-C2B-C3B	2.19	128.78	124.68
25	C	503	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
25	A	405	CLA	O2A-CGA-CBA	2.19	118.78	111.91
25	D	404	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
25	D	401	CLA	C6-C5-C3	-2.18	107.73	113.45
25	A	406	CLA	O2A-CGA-CBA	2.18	118.75	111.91
25	B	513	CLA	CHA-C1A-NA	-2.18	121.41	126.40
25	C	506	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
25	B	512	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
27	A	409	BCR	C34-C9-C10	-2.17	119.88	122.92
25	B	502	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
27	C	514	BCR	C29-C30-C25	2.17	113.83	110.48
25	C	506	CLA	C2C-C1C-NC	2.17	112.00	109.97
27	C	516	BCR	C2-C1-C6	2.16	113.80	110.48
25	B	503	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
27	C	515	BCR	C11-C12-C13	-2.16	120.36	126.42
27	C	516	BCR	C11-C12-C13	-2.15	120.37	126.42
25	B	509	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
25	B	506	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
25	B	514	CLA	CHA-C1A-NA	-2.15	121.48	126.40
25	B	502	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
25	B	514	CLA	O2A-CGA-CBA	2.15	118.65	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	509	CLA	CHA-C1A-NA	-2.14	121.49	126.40
31	C	517	DGD	O6D-C5D-C6D	2.14	110.99	106.67
25	C	509	CLA	C6-C5-C3	-2.14	107.84	113.45
25	H	101	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
25	C	509	CLA	CHA-C1A-NA	-2.14	121.50	126.40
25	B	515	CLA	CHA-C1A-NA	-2.13	121.51	126.40
25	D	404	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
25	C	512	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
27	B	516	BCR	C21-C20-C19	-2.13	116.58	123.22
25	C	506	CLA	CMB-C2B-C3B	2.13	128.66	124.68
25	D	404	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
25	B	503	CLA	CHA-C1A-NA	-2.13	121.53	126.40
25	H	101	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
27	C	514	BCR	C34-C9-C10	-2.12	119.95	122.92
27	A	409	BCR	C11-C12-C13	-2.12	120.45	126.42
25	C	507	CLA	CHA-C1A-NA	-2.12	121.54	126.40
25	B	510	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
25	C	503	CLA	O2A-CGA-CBA	2.12	118.56	111.91
25	B	512	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
25	H	101	CLA	CHA-C1A-NA	-2.11	121.58	126.40
25	B	504	CLA	CHA-C1A-NA	-2.11	121.58	126.40
25	C	511	CLA	CHA-C1A-NA	-2.11	121.58	126.40
25	C	503	CLA	CHA-C1A-NA	-2.10	121.58	126.40
25	C	513	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	C	502	CLA	CHA-C1A-NA	-2.10	121.60	126.40
25	B	513	CLA	C6-C5-C3	-2.10	107.96	113.45
25	B	505	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
25	H	101	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
35	F	101	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
25	D	404	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
25	C	502	CLA	C16-C15-C13	-2.09	109.17	115.92
27	C	514	BCR	C30-C25-C26	-2.09	119.67	122.61
25	C	502	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
25	B	504	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
25	B	503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
25	A	405	CLA	CHA-C1A-NA	-2.08	121.63	126.40
27	A	409	BCR	C15-C16-C17	-2.08	119.21	123.47
25	C	512	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	D	408	LHG	C5-O7-C7	-2.08	112.68	117.79
25	B	511	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
25	C	510	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
25	A	405	CLA	CMB-C2B-C3B	2.07	128.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	515	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
25	C	508	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
25	C	510	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
25	C	509	CLA	CMB-C2B-C3B	2.07	128.55	124.68
25	C	508	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
25	B	508	CLA	O2A-CGA-CBA	2.06	118.39	111.91
29	D	410	LMG	C8-O7-C10	-2.06	112.71	117.79
25	B	507	CLA	CHA-C1A-NA	-2.06	121.68	126.40
27	A	409	BCR	C30-C25-C24	2.05	121.59	115.78
25	D	401	CLA	CHA-C1A-NA	-2.05	121.69	126.40
25	B	504	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
25	B	510	CLA	CMB-C2B-C3B	2.05	128.52	124.68
25	C	504	CLA	O2A-CGA-CBA	2.05	118.33	111.91
25	C	502	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
25	B	502	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
27	D	406	BCR	C2-C1-C6	2.04	113.63	110.48
25	C	502	CLA	CMB-C2B-C3B	2.04	128.50	124.68
25	C	501	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
25	B	501	CLA	CHA-C1A-NA	-2.04	121.73	126.40
25	A	405	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
27	C	515	BCR	C8-C7-C6	-2.03	121.50	127.20
25	B	511	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
25	C	505	CLA	CHA-C1A-NA	-2.03	121.76	126.40
25	C	507	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
25	C	503	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	B	510	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	A	406	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	C	502	CLA	C11-C12-C13	-2.02	109.39	115.92
25	C	501	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	A	405	CLA	C6-C7-C8	-2.02	109.40	115.92
25	D	405	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
25	C	504	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	C	511	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
25	B	513	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
25	C	509	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
27	C	516	BCR	C35-C13-C14	-2.01	120.10	122.92
25	B	505	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
27	C	516	BCR	C23-C24-C25	-2.01	121.56	127.20
25	B	513	CLA	C6-C7-C8	-2.01	109.43	115.92
25	C	508	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
25	C	508	CLA	CHA-C1A-NA	-2.01	121.80	126.40
27	D	406	BCR	C36-C18-C17	-2.01	120.11	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	515	BCR	C1-C6-C7	2.01	121.45	115.78
28	A	410	SQD	O8-S-C6	-2.00	102.55	105.74
25	B	512	CLA	CHA-C1A-NA	-2.00	121.81	126.40
25	B	506	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
29	W	201	LMG	C7-O1-C1	-2.00	109.83	113.74

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	408	CLA	ND
25	B	501	CLA	ND
25	B	502	CLA	ND
25	B	503	CLA	ND
25	B	504	CLA	ND
25	B	505	CLA	ND
25	B	506	CLA	ND
25	B	507	CLA	ND
25	B	508	CLA	ND
25	B	509	CLA	ND
25	B	510	CLA	ND
25	B	511	CLA	ND
25	B	512	CLA	ND
25	B	513	CLA	ND
25	B	514	CLA	ND
25	B	515	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	401	CLA	ND
25	D	404	CLA	ND

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Mol	Chain	Res	Type	Atom
25	D	405	CLA	ND
25	H	101	CLA	ND

All (843) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	406	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	O1A-CGA-O2A-C1
25	A	406	CLA	CHA-CBD-CGD-O2D
25	A	408	CLA	C3A-C2A-CAA-CBA
25	A	408	CLA	C2-C1-O2A-CGA
25	A	408	CLA	CHA-CBD-CGD-O1D
25	A	408	CLA	CHA-CBD-CGD-O2D
25	B	501	CLA	CHA-CBD-CGD-O1D
25	B	501	CLA	CHA-CBD-CGD-O2D
25	B	502	CLA	CBD-CGD-O2D-CED
25	B	503	CLA	C1A-C2A-CAA-CBA
25	B	503	CLA	CAD-CBD-CGD-O1D
25	B	503	CLA	CBD-CGD-O2D-CED
25	B	504	CLA	CAD-CBD-CGD-O1D
25	B	504	CLA	C6-C7-C8-C9
25	B	505	CLA	C1A-C2A-CAA-CBA
25	B	505	CLA	C3A-C2A-CAA-CBA
25	B	505	CLA	CBD-CGD-O2D-CED
25	B	506	CLA	C1A-C2A-CAA-CBA
25	B	506	CLA	C3A-C2A-CAA-CBA
25	B	506	CLA	CHA-CBD-CGD-O1D
25	B	506	CLA	CHA-CBD-CGD-O2D
25	B	507	CLA	C1A-C2A-CAA-CBA
25	B	507	CLA	C3A-C2A-CAA-CBA
25	B	507	CLA	CAD-CBD-CGD-O1D
25	B	507	CLA	CAD-CBD-CGD-O2D
25	B	509	CLA	CHA-CBD-CGD-O1D
25	B	509	CLA	CHA-CBD-CGD-O2D
25	B	509	CLA	CAD-CBD-CGD-O1D
25	B	509	CLA	CAD-CBD-CGD-O2D
25	B	509	CLA	CBD-CGD-O2D-CED
25	B	511	CLA	C1A-C2A-CAA-CBA
25	B	511	CLA	C3A-C2A-CAA-CBA
25	B	511	CLA	CBA-CGA-O2A-C1
25	B	511	CLA	O1A-CGA-O2A-C1
25	B	511	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	511	CLA	CHA-CBD-CGD-O2D
25	B	511	CLA	CAD-CBD-CGD-O1D
25	B	511	CLA	CAD-CBD-CGD-O2D
25	B	511	CLA	CBD-CGD-O2D-CED
25	B	512	CLA	CBA-CGA-O2A-C1
25	B	512	CLA	O1A-CGA-O2A-C1
25	B	512	CLA	CHA-CBD-CGD-O1D
25	B	512	CLA	CHA-CBD-CGD-O2D
25	B	513	CLA	C1A-C2A-CAA-CBA
25	B	513	CLA	C3A-C2A-CAA-CBA
25	B	513	CLA	CBD-CGD-O2D-CED
25	B	514	CLA	C1A-C2A-CAA-CBA
25	B	515	CLA	C2-C1-O2A-CGA
25	B	515	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C3A-C2A-CAA-CBA
25	C	501	CLA	C2-C1-O2A-CGA
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C3A-C2A-CAA-CBA
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	C1A-C2A-CAA-CBA
25	C	505	CLA	C3A-C2A-CAA-CBA
25	C	505	CLA	C2-C1-O2A-CGA
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	C11-C12-C13-C14
25	C	506	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C3A-C2A-CAA-CBA
25	C	506	CLA	C2-C1-O2A-CGA
25	C	506	CLA	CHA-CBD-CGD-O1D
25	C	506	CLA	CHA-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C3A-C2A-CAA-CBA
25	C	508	CLA	C2-C1-O2A-CGA
25	C	509	CLA	C2-C1-O2A-CGA
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	C1A-C2A-CAA-CBA
25	C	510	CLA	C3A-C2A-CAA-CBA
25	C	510	CLA	C2A-CAA-CBA-CGA
25	C	510	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	C1A-C2A-CAA-CBA
25	C	511	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	CHA-CBD-CGD-O1D
25	C	511	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	CAD-CBD-CGD-O1D
25	C	511	CLA	CAD-CBD-CGD-O2D
25	C	512	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	C3-C5-C6-C7
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	401	CLA	C1A-C2A-CAA-CBA
25	D	401	CLA	C3A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C3A-C2A-CAA-CBA
25	D	405	CLA	C1A-C2A-CAA-CBA
25	D	405	CLA	C3A-C2A-CAA-CBA
25	H	101	CLA	C1A-C2A-CAA-CBA
25	H	101	CLA	C3A-C2A-CAA-CBA
26	A	407	PHO	O2A-C1-C2-C3
27	A	409	BCR	C1-C6-C7-C8
27	A	409	BCR	C17-C18-C19-C20
27	A	409	BCR	C21-C22-C23-C24
27	A	409	BCR	C37-C22-C23-C24
27	B	516	BCR	C9-C10-C11-C12
27	B	516	BCR	C21-C22-C23-C24
27	B	516	BCR	C37-C22-C23-C24
27	B	517	BCR	C1-C6-C7-C8
27	B	517	BCR	C9-C10-C11-C12
27	C	514	BCR	C7-C8-C9-C34
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
27	C	514	BCR	C13-C14-C15-C16
27	C	514	BCR	C15-C16-C17-C18
27	C	514	BCR	C21-C22-C23-C24
27	C	514	BCR	C37-C22-C23-C24
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C15-C16-C17-C18
27	C	516	BCR	C7-C8-C9-C10
27	C	516	BCR	C7-C8-C9-C34
27	C	516	BCR	C17-C18-C19-C20
27	C	516	BCR	C21-C22-C23-C24
27	C	516	BCR	C37-C22-C23-C24
27	D	406	BCR	C21-C22-C23-C24
27	D	406	BCR	C37-C22-C23-C24
27	D	406	BCR	C23-C24-C25-C30
27	K	101	BCR	C9-C10-C11-C12
28	A	410	SQD	O5-C5-C6-S
29	C	520	LMG	C2-C1-O1-C7
29	C	520	LMG	O6-C1-O1-C7
30	B	519	LHG	O1-C1-C2-C3
30	B	519	LHG	C3-O3-P-O4
30	B	519	LHG	C3-O3-P-O5
30	B	519	LHG	C3-O3-P-O6
30	B	521	LHG	O1-C1-C2-C3
30	B	521	LHG	C3-O3-P-O4
30	B	521	LHG	C3-O3-P-O5
30	B	521	LHG	C4-O6-P-O4
30	B	521	LHG	C4-O6-P-O5
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C1-C2-C3-O3
30	D	408	LHG	C4-O6-P-O3
30	D	408	LHG	C4-O6-P-O4
30	D	408	LHG	C4-O6-P-O5
30	D	409	LHG	C3-O3-P-O4
30	D	409	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O5
31	C	519	DGD	C2A-C1A-O1G-C1G
31	C	519	DGD	O1A-C1A-O1G-C1G
25	A	405	CLA	O1D-CGD-O2D-CED
25	B	515	CLA	O1D-CGD-O2D-CED
25	A	405	CLA	CBD-CGD-O2D-CED
25	A	406	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	408	CLA	CBD-CGD-O2D-CED
25	B	507	CLA	CBD-CGD-O2D-CED
25	B	508	CLA	CBD-CGD-O2D-CED
25	B	510	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	D	401	CLA	CBD-CGD-O2D-CED
25	D	405	CLA	CBD-CGD-O2D-CED
25	B	515	CLA	O1A-CGA-O2A-C1
25	H	101	CLA	O1A-CGA-O2A-C1
29	B	518	LMG	O10-C28-O8-C9
25	C	506	CLA	O1D-CGD-O2D-CED
25	B	502	CLA	O1D-CGD-O2D-CED
25	B	503	CLA	O1D-CGD-O2D-CED
25	B	511	CLA	O1D-CGD-O2D-CED
25	B	513	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	O1D-CGD-O2D-CED
25	B	515	CLA	CBA-CGA-O2A-C1
25	H	101	CLA	CBA-CGA-O2A-C1
29	B	518	LMG	C29-C28-O8-C9
25	B	501	CLA	CBD-CGD-O2D-CED
25	B	506	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	B	504	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	D	401	CLA	O1A-CGA-O2A-C1
25	B	505	CLA	O1D-CGD-O2D-CED
25	B	509	CLA	O1D-CGD-O2D-CED
25	C	507	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	O1D-CGD-O2D-CED
25	B	512	CLA	CBD-CGD-O2D-CED
29	W	201	LMG	O9-C10-O7-C8
25	A	408	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	A	405	CLA	C3-C5-C6-C7
25	B	503	CLA	C3-C5-C6-C7
25	B	505	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	508	CLA	C3-C5-C6-C7
25	C	507	CLA	C3-C5-C6-C7
25	C	510	CLA	C3-C5-C6-C7
25	B	504	CLA	CBA-CGA-O2A-C1
29	W	201	LMG	C11-C10-O7-C8
25	B	508	CLA	O1D-CGD-O2D-CED
25	C	501	CLA	C4-C3-C5-C6
25	A	406	CLA	C2A-CAA-CBA-CGA
25	D	401	CLA	O1D-CGD-O2D-CED
29	B	518	LMG	C17-C18-C19-C20
29	B	520	LMG	C38-C39-C40-C41
29	C	520	LMG	C17-C18-C19-C20
29	C	520	LMG	C35-C36-C37-C38
29	W	201	LMG	C17-C18-C19-C20
30	B	519	LHG	C28-C29-C30-C31
31	C	517	DGD	C8B-C9B-CAB-CBB
31	C	518	DGD	CBB-CCB-CDB-CEB
25	B	507	CLA	C3-C5-C6-C7
25	D	401	CLA	C3-C5-C6-C7
25	A	408	CLA	CBA-CGA-O2A-C1
25	B	507	CLA	CBA-CGA-O2A-C1
25	C	501	CLA	CBA-CGA-O2A-C1
25	C	509	CLA	CBA-CGA-O2A-C1
25	D	401	CLA	CBA-CGA-O2A-C1
30	B	519	LHG	C24-C23-O8-C6
25	B	507	CLA	O1D-CGD-O2D-CED
25	B	510	CLA	O1D-CGD-O2D-CED
25	A	408	CLA	O1D-CGD-O2D-CED
25	B	507	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	O1A-CGA-O2A-C1
25	C	503	CLA	O1A-CGA-O2A-C1
25	C	506	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	O1D-CGD-O2D-CED
27	A	409	BCR	C19-C20-C21-C22
27	B	516	BCR	C15-C16-C17-C18
27	K	101	BCR	C13-C14-C15-C16
25	D	405	CLA	O1D-CGD-O2D-CED
30	B	521	LHG	O2-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3
30	D	409	LHG	O2-C2-C3-O3
25	B	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	B	511	CLA	C3-C5-C6-C7
25	H	101	CLA	C3-C5-C6-C7
25	B	501	CLA	CBA-CGA-O2A-C1
25	B	506	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	CBA-CGA-O2A-C1
25	C	504	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	D	405	CLA	CBA-CGA-O2A-C1
25	C	504	CLA	O1A-CGA-O2A-C1
32	C	521	LMU	O5B-C5B-C6B-O6B
25	A	406	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
25	B	501	CLA	O1A-CGA-O2A-C1
30	D	408	LHG	C13-C14-C15-C16
25	C	509	CLA	O1D-CGD-O2D-CED
32	C	521	LMU	C1-C2-C3-C4
25	B	503	CLA	C8-C10-C11-C12
25	B	504	CLA	C3-C5-C6-C7
25	C	503	CLA	CBA-CGA-O2A-C1
25	C	506	CLA	CBA-CGA-O2A-C1
30	B	519	LHG	O10-C23-O8-C6
30	B	521	LHG	C5-C6-O8-C23
25	B	506	CLA	O1A-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
25	B	514	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	O1A-CGA-O2A-C1
25	D	405	CLA	O1A-CGA-O2A-C1
25	B	506	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
30	B	521	LHG	C1-C2-C3-O3
30	D	409	LHG	C1-C2-C3-O3
25	B	506	CLA	C3-C5-C6-C7
25	A	405	CLA	CBA-CGA-O2A-C1
25	B	502	CLA	CBA-CGA-O2A-C1
25	B	510	CLA	CBA-CGA-O2A-C1
25	B	514	CLA	CBA-CGA-O2A-C1
30	D	408	LHG	C24-C23-O8-C6
25	B	501	CLA	O1D-CGD-O2D-CED
30	D	409	LHG	O6-C4-C5-O7
25	B	503	CLA	C4-C3-C5-C6
25	C	501	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	501	CLA	C11-C10-C8-C9
25	B	503	CLA	C6-C7-C8-C9
25	B	504	CLA	C11-C10-C8-C9
25	B	507	CLA	C6-C7-C8-C9
25	B	507	CLA	C11-C10-C8-C9
25	B	508	CLA	C6-C7-C8-C9
25	C	501	CLA	C11-C12-C13-C14
25	C	502	CLA	C6-C7-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	508	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	510	CLA	C11-C12-C13-C14
25	D	401	CLA	C6-C7-C8-C9
25	H	101	CLA	C6-C7-C8-C9
27	A	409	BCR	C7-C8-C9-C34
27	A	409	BCR	C11-C12-C13-C35
27	A	409	BCR	C36-C18-C19-C20
27	B	516	BCR	C7-C8-C9-C34
27	B	517	BCR	C7-C8-C9-C34
27	B	517	BCR	C11-C12-C13-C35
27	B	517	BCR	C36-C18-C19-C20
27	C	514	BCR	C36-C18-C19-C20
27	C	516	BCR	C36-C18-C19-C20
27	D	406	BCR	C36-C18-C19-C20
27	K	101	BCR	C11-C12-C13-C35
27	K	101	BCR	C36-C18-C19-C20
27	B	516	BCR	C7-C8-C9-C10
27	B	516	BCR	C11-C12-C13-C14
27	B	517	BCR	C7-C8-C9-C10
27	B	517	BCR	C11-C12-C13-C14
27	C	514	BCR	C7-C8-C9-C10
27	C	514	BCR	C17-C18-C19-C20
27	C	515	BCR	C7-C8-C9-C10
27	D	406	BCR	C17-C18-C19-C20
27	K	101	BCR	C7-C8-C9-C10
27	K	101	BCR	C11-C12-C13-C14
27	K	101	BCR	C17-C18-C19-C20
30	D	409	LHG	C23-C24-C25-C26
25	A	405	CLA	O1A-CGA-O2A-C1
25	B	502	CLA	O1A-CGA-O2A-C1
25	B	510	CLA	O1A-CGA-O2A-C1
25	B	514	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	C	521	LMU	C4B-C5B-C6B-O6B
30	D	409	LHG	C7-C8-C9-C10
25	B	502	CLA	C8-C10-C11-C12
25	C	507	CLA	C13-C15-C16-C17
25	B	510	CLA	C5-C6-C7-C8
25	B	509	CLA	C3-C5-C6-C7
25	B	502	CLA	C2-C1-O2A-CGA
25	D	401	CLA	C2-C1-O2A-CGA
30	B	519	LHG	C7-C8-C9-C10
25	C	505	CLA	C8-C10-C11-C12
25	A	405	CLA	C11-C10-C8-C7
25	A	408	CLA	C6-C7-C8-C10
25	B	502	CLA	C11-C12-C13-C15
25	C	501	CLA	C11-C12-C13-C15
25	C	510	CLA	C11-C12-C13-C15
25	C	508	CLA	O1A-CGA-O2A-C1
27	B	516	BCR	C13-C14-C15-C16
27	B	517	BCR	C13-C14-C15-C16
27	B	517	BCR	C15-C16-C17-C18
27	C	514	BCR	C19-C20-C21-C22
27	C	515	BCR	C19-C20-C21-C22
27	D	406	BCR	C15-C16-C17-C18
25	B	512	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C8-C10-C11-C12
30	B	519	LHG	O2-C2-C3-O3
25	B	512	CLA	O1D-CGD-O2D-CED
30	D	408	LHG	O10-C23-O8-C6
25	C	505	CLA	CBD-CGD-O2D-CED
29	C	520	LMG	C11-C10-O7-C8
25	A	408	CLA	C5-C6-C7-C8
25	B	511	CLA	C5-C6-C7-C8
30	B	521	LHG	C3-O3-P-O6
30	B	521	LHG	C4-O6-P-O3
30	D	408	LHG	C3-O3-P-O6
30	D	409	LHG	C3-O3-P-O6
31	C	518	DGD	C2A-C1A-O1G-C1G
30	B	519	LHG	C1-C2-C3-O3
25	B	502	CLA	C2A-CAA-CBA-CGA
25	B	502	CLA	C3-C5-C6-C7
25	C	504	CLA	C3-C5-C6-C7
27	A	409	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	B	517	BCR	C19-C20-C21-C22
27	C	515	BCR	C13-C14-C15-C16
27	D	406	BCR	C19-C20-C21-C22
27	K	101	BCR	C15-C16-C17-C18
29	B	520	LMG	C11-C10-O7-C8
30	D	408	LHG	C11-C12-C13-C14
30	B	521	LHG	C28-C29-C30-C31
29	B	520	LMG	O9-C10-O7-C8
29	C	520	LMG	O9-C10-O7-C8
29	D	410	LMG	O9-C10-O7-C8
30	D	409	LHG	C2-C3-O3-P
30	B	519	LHG	C13-C14-C15-C16
30	B	521	LHG	C13-C14-C15-C16
25	C	509	CLA	C6-C7-C8-C9
30	B	519	LHG	C23-C24-C25-C26
30	D	408	LHG	C28-C29-C30-C31
27	B	516	BCR	C11-C12-C13-C35
27	B	516	BCR	C36-C18-C19-C20
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C12-C13-C35
27	C	515	BCR	C36-C18-C19-C20
27	K	101	BCR	C7-C8-C9-C34
30	D	409	LHG	O1-C1-C2-C3
27	A	409	BCR	C7-C8-C9-C10
27	A	409	BCR	C11-C12-C13-C14
27	B	516	BCR	C17-C18-C19-C20
27	B	517	BCR	C17-C18-C19-C20
27	C	515	BCR	C11-C12-C13-C14
27	C	515	BCR	C17-C18-C19-C20
25	B	512	CLA	C3-C5-C6-C7
29	B	518	LMG	O9-C10-O7-C8
29	B	518	LMG	C11-C10-O7-C8
29	D	410	LMG	C11-C10-O7-C8
30	B	519	LHG	C11-C12-C13-C14
30	D	408	LHG	C7-C8-C9-C10
30	D	408	LHG	C23-C24-C25-C26
25	B	506	CLA	C6-C7-C8-C10
25	C	503	CLA	C15-C16-C17-C18
31	C	518	DGD	C3B-C4B-C5B-C6B
32	C	521	LMU	C6-C7-C8-C9
30	B	521	LHG	C23-C24-C25-C26
25	A	405	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	502	CLA	C3A-C2A-CAA-CBA
25	B	514	CLA	C3A-C2A-CAA-CBA
25	C	512	CLA	C3A-C2A-CAA-CBA
31	C	518	DGD	O1A-C1A-O1G-C1G
30	B	521	LHG	C11-C12-C13-C14
30	D	408	LHG	C4-C5-C6-O8
30	B	521	LHG	C26-C27-C28-C29
30	B	519	LHG	O1-C1-C2-O2
30	D	408	LHG	O1-C1-C2-O2
30	D	409	LHG	O1-C1-C2-O2
30	B	521	LHG	C31-C32-C33-C34
29	B	518	LMG	C14-C15-C16-C17
25	B	503	CLA	C2-C1-O2A-CGA
25	C	504	CLA	C2-C1-O2A-CGA
25	C	507	CLA	C2-C1-O2A-CGA
25	C	510	CLA	C2-C1-O2A-CGA
25	D	405	CLA	C2-C1-O2A-CGA
26	D	402	PHO	C2-C1-O2A-CGA
30	D	409	LHG	C33-C34-C35-C36
32	C	521	LMU	O1'-C1-C2-C3
25	C	510	CLA	C15-C16-C17-C18
25	C	501	CLA	C3-C5-C6-C7
27	A	409	BCR	C5-C6-C7-C8
27	B	516	BCR	C5-C6-C7-C8
27	B	516	BCR	C23-C24-C25-C26
27	B	516	BCR	C23-C24-C25-C30
27	B	517	BCR	C5-C6-C7-C8
27	B	517	BCR	C23-C24-C25-C30
27	C	515	BCR	C5-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
30	B	519	LHG	C33-C34-C35-C36
30	B	521	LHG	C24-C23-O8-C6
31	C	517	DGD	C2A-C1A-O1G-C1G
25	B	505	CLA	C4-C3-C5-C6
25	B	507	CLA	C4-C3-C5-C6
25	B	501	CLA	C11-C10-C8-C7
25	B	502	CLA	C6-C7-C8-C10
25	B	507	CLA	C11-C10-C8-C7
25	B	507	CLA	C11-C12-C13-C15
25	B	511	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	B	512	CLA	C11-C10-C8-C7
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C11-C12-C13-C15
25	C	509	CLA	C6-C7-C8-C10
25	C	511	CLA	C11-C12-C13-C15
25	C	503	CLA	C3-C5-C6-C7
31	C	517	DGD	O1A-C1A-O1G-C1G
30	B	519	LHG	C34-C35-C36-C37
30	B	519	LHG	C35-C36-C37-C38
26	D	402	PHO	CBA-CGA-O2A-C1
30	B	521	LHG	C35-C36-C37-C38
25	D	405	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	C31-C32-C33-C34
25	B	507	CLA	C5-C6-C7-C8
25	A	408	CLA	C3-C5-C6-C7
25	B	514	CLA	O1D-CGD-O2D-CED
29	D	410	LMG	C11-C12-C13-C14
30	B	521	LHG	C9-C10-C11-C12
30	B	521	LHG	C27-C28-C29-C30
25	D	405	CLA	C3-C5-C6-C7
30	B	519	LHG	O7-C5-C6-O8
30	D	408	LHG	O7-C5-C6-O8
31	C	517	DGD	O6E-C5E-C6E-O5E
25	B	503	CLA	C2-C3-C5-C6
34	D	407	PL9	C4-C3-C7-C8
25	A	405	CLA	C11-C10-C8-C9
25	A	408	CLA	C6-C7-C8-C9
25	B	502	CLA	C6-C7-C8-C9
25	B	510	CLA	C6-C7-C8-C9
25	C	502	CLA	C11-C10-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	D	405	CLA	C6-C7-C8-C9
30	D	409	LHG	C24-C25-C26-C27
29	D	410	LMG	O6-C5-C6-O5
31	C	518	DGD	O6E-C5E-C6E-O5E
31	C	519	DGD	O6E-C5E-C6E-O5E
30	D	408	LHG	C10-C11-C12-C13
30	B	521	LHG	O10-C23-O8-C6
25	A	405	CLA	C1A-C2A-CAA-CBA
25	A	408	CLA	C1A-C2A-CAA-CBA
25	B	501	CLA	C1A-C2A-CAA-CBA
25	B	502	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	508	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	B	509	CLA	C5-C6-C7-C8
25	B	511	CLA	C8-C10-C11-C12
30	D	409	LHG	C9-C10-C11-C12
25	B	503	CLA	CBA-CGA-O2A-C1
30	D	409	LHG	O6-C4-C5-C6
31	C	518	DGD	C2G-C1G-O1G-C1A
25	C	511	CLA	C3-C5-C6-C7
30	B	521	LHG	C25-C26-C27-C28
30	D	409	LHG	C4-C5-C6-O8
31	C	518	DGD	C2G-C3G-O3G-C1D
25	D	404	CLA	C8-C10-C11-C12
26	D	402	PHO	O1A-CGA-O2A-C1
25	C	504	CLA	C5-C6-C7-C8
30	B	519	LHG	C11-C10-C9-C8
25	C	505	CLA	O1D-CGD-O2D-CED
30	B	519	LHG	O6-C4-C5-O7
30	D	408	LHG	C31-C32-C33-C34
30	B	519	LHG	C9-C10-C11-C12
25	B	505	CLA	C5-C6-C7-C8
25	B	503	CLA	O1A-CGA-O2A-C1
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
25	B	501	CLA	C6-C7-C8-C10
25	B	501	CLA	C12-C13-C15-C16
25	B	504	CLA	C6-C7-C8-C10
25	B	504	CLA	C11-C10-C8-C7
25	B	510	CLA	C6-C7-C8-C10
25	B	513	CLA	C6-C7-C8-C10
25	C	501	CLA	C6-C7-C8-C10
25	C	504	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
25	D	401	CLA	C11-C12-C13-C15
25	D	405	CLA	C6-C7-C8-C10
29	B	520	LMG	O7-C10-C11-C12
25	A	405	CLA	C6-C7-C8-C9
25	B	501	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	509	CLA	C6-C7-C8-C9
25	C	501	CLA	C6-C7-C8-C9
25	C	504	CLA	C6-C7-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	D	404	CLA	C6-C7-C8-C9
25	C	505	CLA	C5-C6-C7-C8
25	B	504	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	C28-C29-C30-C31
25	B	508	CLA	C8-C10-C11-C12
25	C	501	CLA	C8-C10-C11-C12
30	B	521	LHG	O6-C4-C5-C6
25	B	501	CLA	C5-C6-C7-C8
25	B	505	CLA	C8-C10-C11-C12
32	C	521	LMU	C2-C3-C4-C5
25	D	404	CLA	CBA-CGA-O2A-C1
25	B	506	CLA	CAA-CBA-CGA-O2A
31	C	519	DGD	O6D-C5D-C6D-O5D
30	B	521	LHG	C7-C8-C9-C10
25	B	508	CLA	C3A-C2A-CAA-CBA
26	D	402	PHO	C3A-C2A-CAA-CBA
27	C	514	BCR	C9-C10-C11-C12
25	B	507	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
30	B	519	LHG	C4-C5-C6-O8
30	D	409	LHG	C25-C26-C27-C28
30	D	409	LHG	C26-C27-C28-C29
25	B	502	CLA	O2A-C1-C2-C3
25	C	513	CLA	CAA-CBA-CGA-O2A
25	B	501	CLA	C3-C5-C6-C7
25	B	512	CLA	C5-C6-C7-C8
30	B	521	LHG	O7-C5-C6-O8
25	B	510	CLA	C8-C10-C11-C12
25	B	511	CLA	C2-C1-O2A-CGA
25	C	511	CLA	C8-C10-C11-C12
25	B	513	CLA	C6-C7-C8-C9
25	C	507	CLA	C6-C7-C8-C9
25	C	507	CLA	C16-C17-C18-C20
27	C	515	BCR	C23-C24-C25-C26
27	D	406	BCR	C23-C24-C25-C26
25	C	508	CLA	C8-C10-C11-C12
25	C	511	CLA	C5-C6-C7-C8
31	C	517	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
25	B	506	CLA	C6-C7-C8-C9
30	B	519	LHG	O6-C4-C5-C6
30	D	408	LHG	O6-C4-C5-C6
25	A	405	CLA	C6-C7-C8-C10
25	B	503	CLA	C6-C7-C8-C10
25	B	509	CLA	C6-C7-C8-C10
25	B	510	CLA	C11-C10-C8-C7
25	C	507	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	D	401	CLA	C6-C7-C8-C10
25	H	101	CLA	C6-C7-C8-C10
25	C	510	CLA	C8-C10-C11-C12
25	D	401	CLA	C5-C6-C7-C8
25	B	503	CLA	C5-C6-C7-C8
25	B	504	CLA	C10-C11-C12-C13
25	C	507	CLA	CBA-CGA-O2A-C1
25	A	408	CLA	C8-C10-C11-C12
25	B	503	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
35	F	101	HEM	C2B-C3B-CAB-CBB
29	B	518	LMG	O6-C1-O1-C7
30	B	521	LHG	C2-C3-O3-P
25	C	507	CLA	O1A-CGA-O2A-C1
30	B	521	LHG	O6-C4-C5-O7
25	B	501	CLA	CAA-CBA-CGA-O2A
25	C	505	CLA	CAA-CBA-CGA-O2A
25	A	406	CLA	CHA-CBD-CGD-O1D
25	B	510	CLA	CHA-CBD-CGD-O1D
25	B	510	CLA	CHA-CBD-CGD-O2D
25	B	514	CLA	CHA-CBD-CGD-O1D
25	B	514	CLA	CHA-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	C	513	CLA	CHA-CBD-CGD-O1D
25	C	513	CLA	CHA-CBD-CGD-O2D
25	H	101	CLA	CHA-CBD-CGD-O1D
25	H	101	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	O1A-CGA-O2A-C1
28	A	410	SQD	O47-C45-C46-O48
30	B	521	LHG	O1-C1-C2-O2
29	B	518	LMG	C12-C13-C14-C15
25	C	502	CLA	C5-C6-C7-C8
25	B	503	CLA	C13-C15-C16-C17
27	K	101	BCR	C37-C22-C23-C24
25	B	501	CLA	C8-C10-C11-C12
27	K	101	BCR	C21-C22-C23-C24
25	B	504	CLA	C1A-C2A-CAA-CBA
25	A	408	CLA	C11-C12-C13-C15
30	D	408	LHG	C30-C31-C32-C33
30	D	409	LHG	C30-C31-C32-C33
25	C	508	CLA	C3-C5-C6-C7
30	B	519	LHG	C5-C4-O6-P
25	B	505	CLA	C2-C3-C5-C6
25	B	507	CLA	C2-C3-C5-C6
30	D	408	LHG	C3-O3-P-O5
29	B	518	LMG	C11-C12-C13-C14
31	C	519	DGD	C1B-C2B-C3B-C4B
25	B	505	CLA	CBA-CGA-O2A-C1
25	B	504	CLA	C11-C12-C13-C15
25	B	508	CLA	C6-C7-C8-C10
25	B	515	CLA	C3A-C2A-CAA-CBA
25	C	502	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C12-C13-C15
25	C	508	CLA	C11-C10-C8-C7
30	D	408	LHG	O6-C4-C5-O7
30	B	519	LHG	C31-C32-C33-C34
25	H	101	CLA	C8-C10-C11-C12
28	A	410	SQD	C44-C45-C46-O48
35	F	101	HEM	C1A-C2A-CAA-CBA
35	F	101	HEM	C3A-C2A-CAA-CBA
25	B	508	CLA	C5-C6-C7-C8
25	A	405	CLA	O2A-C1-C2-C3
31	C	518	DGD	C5D-C6D-O5D-C1E
25	C	507	CLA	C16-C17-C18-C19
25	C	508	CLA	C5-C6-C7-C8
25	B	510	CLA	C11-C10-C8-C9
25	C	503	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	511	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	A	409	BCR	C15-C16-C17-C18
25	B	505	CLA	O1A-CGA-O2A-C1
30	D	408	LHG	C35-C36-C37-C38
34	D	407	PL9	C40-C39-C41-C42
30	D	408	LHG	C29-C30-C31-C32
25	B	513	CLA	C5-C6-C7-C8
25	A	406	CLA	C1-C2-C3-C4
29	C	520	LMG	C7-C8-O7-C10
31	C	519	DGD	O1B-C1B-O2G-C2G
25	B	510	CLA	C13-C15-C16-C17
30	B	519	LHG	C26-C27-C28-C29
30	D	409	LHG	C5-C4-O6-P
27	C	514	BCR	C23-C24-C25-C26
29	B	520	LMG	C30-C31-C32-C33
31	C	519	DGD	C2B-C1B-O2G-C2G
34	D	407	PL9	C16-C17-C18-C19
30	D	409	LHG	O7-C5-C6-O8
25	B	513	CLA	C11-C10-C8-C9
30	B	521	LHG	C4-C5-C6-O8
25	B	508	CLA	C11-C12-C13-C15
25	C	502	CLA	C11-C10-C8-C7
25	C	503	CLA	C6-C7-C8-C10
25	D	401	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C10-C8-C7
27	C	516	BCR	C15-C16-C17-C18
27	C	516	BCR	C19-C20-C21-C22
27	D	406	BCR	C13-C14-C15-C16
30	D	408	LHG	C25-C26-C27-C28
25	C	509	CLA	C3-C5-C6-C7
25	B	513	CLA	C11-C10-C8-C7
31	C	518	DGD	O6E-C1E-O5D-C6D
27	B	516	BCR	C19-C20-C21-C22
35	F	101	HEM	C4B-C3B-CAB-CBB
25	B	505	CLA	C2-C1-O2A-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	H	101	CLA	C2A-CAA-CBA-CGA
25	B	510	CLA	C3A-C2A-CAA-CBA
30	D	409	LHG	C34-C35-C36-C37
30	D	408	LHG	C9-C10-C11-C12
25	B	502	CLA	C11-C12-C13-C14
25	B	504	CLA	C11-C12-C13-C14
25	B	510	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	B	521	LHG	C34-C35-C36-C37
29	B	518	LMG	C9-C8-O7-C10
29	B	520	LMG	O9-C10-C11-C12
25	B	515	CLA	C1A-C2A-CAA-CBA
25	C	509	CLA	C1A-C2A-CAA-CBA
25	B	505	CLA	C11-C12-C13-C15
25	B	507	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
29	W	201	LMG	C13-C14-C15-C16
31	C	517	DGD	C2B-C3B-C4B-C5B
25	B	513	CLA	CAA-CBA-CGA-O2A
25	D	401	CLA	C2A-CAA-CBA-CGA
32	C	521	LMU	C5'-C4'-O1B-C1B
29	W	201	LMG	C29-C30-C31-C32
25	C	511	CLA	C2-C1-O2A-CGA
34	D	407	PL9	C38-C39-C41-C42
25	C	506	CLA	CAA-CBA-CGA-O2A
25	B	506	CLA	CAA-CBA-CGA-O1A
29	C	520	LMG	C7-C8-C9-O8
30	D	408	LHG	C34-C35-C36-C37
31	C	518	DGD	C1A-C2A-C3A-C4A
29	B	518	LMG	C13-C14-C15-C16
25	C	510	CLA	CAA-CBA-CGA-O2A
25	C	504	CLA	C11-C10-C8-C9
29	B	518	LMG	C31-C32-C33-C34
25	B	512	CLA	C4-C3-C5-C6
25	B	509	CLA	C12-C13-C15-C16
25	C	508	CLA	C6-C7-C8-C10
25	C	509	CLA	C13-C15-C16-C17
32	C	521	LMU	C4-C5-C6-C7
26	A	407	PHO	C1-C2-C3-C4
31	C	518	DGD	C2E-C1E-O5D-C6D
34	D	407	PL9	C2-C3-C7-C8
28	A	410	SQD	C32-C33-C34-C35
25	C	504	CLA	C11-C10-C8-C7
25	D	405	CLA	C11-C10-C8-C7
25	B	511	CLA	C6-C7-C8-C9
25	C	502	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	D	404	CLA	C3-C5-C6-C7
25	C	507	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C3A-C2A-CAA-CBA
26	A	407	PHO	C3A-C2A-CAA-CBA
32	C	521	LMU	C3'-C4'-O1B-C1B
25	B	505	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
29	C	520	LMG	C9-C8-O7-C10
29	W	201	LMG	O6-C5-C6-O5
25	B	505	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	CAA-CBA-CGA-O2A
25	C	504	CLA	CAA-CBA-CGA-O2A
29	D	410	LMG	O7-C10-C11-C12
28	A	410	SQD	O47-C7-C8-C9
30	D	408	LHG	C5-C4-O6-P
30	D	409	LHG	O9-C7-O7-C5
25	C	505	CLA	O1A-CGA-O2A-C1
25	B	504	CLA	O2A-C1-C2-C3
25	C	504	CLA	O2A-C1-C2-C3
25	C	513	CLA	CAA-CBA-CGA-O1A
31	C	517	DGD	O1A-C1A-C2A-C3A
25	B	502	CLA	CHA-CBD-CGD-O1D
25	B	502	CLA	CHA-CBD-CGD-O2D
25	B	507	CLA	CHA-CBD-CGD-O1D
25	B	507	CLA	CHA-CBD-CGD-O2D
25	B	508	CLA	CHA-CBD-CGD-O1D
25	B	508	CLA	CHA-CBD-CGD-O2D
25	B	513	CLA	CHA-CBD-CGD-O2D
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	D	401	CLA	CHA-CBD-CGD-O1D
25	D	401	CLA	CHA-CBD-CGD-O2D
25	D	404	CLA	CHA-CBD-CGD-O1D
25	D	404	CLA	CHA-CBD-CGD-O2D
28	A	410	SQD	C27-C28-C29-C30
30	B	519	LHG	C30-C31-C32-C33
30	D	408	LHG	C15-C16-C17-C18
25	C	512	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
29	D	410	LMG	C16-C17-C18-C19
25	H	101	CLA	C11-C10-C8-C7
25	D	401	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	B	508	CLA	C11-C12-C13-C14
25	D	401	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C10-C8-C9
25	H	101	CLA	C11-C10-C8-C9
30	D	409	LHG	C8-C7-O7-C5
25	B	507	CLA	C2A-CAA-CBA-CGA
25	C	504	CLA	C2A-CAA-CBA-CGA
34	D	407	PL9	C11-C12-C13-C14
25	D	405	CLA	C11-C10-C8-C9
25	C	505	CLA	CBA-CGA-O2A-C1
30	B	521	LHG	C33-C34-C35-C36
30	B	519	LHG	C29-C30-C31-C32
25	B	510	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C1A-C2A-CAA-CBA
28	A	410	SQD	O49-C7-C8-C9
30	B	521	LHG	C11-C10-C9-C8
31	C	518	DGD	C7B-C8B-C9B-CAB
25	C	504	CLA	CAA-CBA-CGA-O1A
29	D	410	LMG	O9-C10-C11-C12
27	A	409	BCR	C23-C24-C25-C26
30	B	521	LHG	C24-C25-C26-C27
25	C	503	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	C13-C15-C16-C17
34	D	407	PL9	C31-C32-C33-C34
25	A	405	CLA	CAD-CBD-CGD-O1D
25	B	513	CLA	CAD-CBD-CGD-O1D
25	B	501	CLA	C14-C13-C15-C16
25	B	512	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C10-C8-C9
25	C	511	CLA	C11-C12-C13-C14
25	B	507	CLA	CAA-CBA-CGA-O2A
29	B	520	LMG	C11-C12-C13-C14
25	B	504	CLA	CAA-CBA-CGA-O2A
25	B	508	CLA	CAA-CBA-CGA-O2A
25	D	405	CLA	CAA-CBA-CGA-O2A
25	H	101	CLA	CAA-CBA-CGA-O2A
29	W	201	LMG	O7-C10-C11-C12
30	D	408	LHG	O8-C23-C24-C25
29	C	520	LMG	O9-C10-C11-C12
25	C	510	CLA	C11-C10-C8-C7
25	C	511	CLA	C3A-C2A-CAA-CBA
35	F	101	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	CAA-CBA-CGA-O1A
25	C	512	CLA	CAA-CBA-CGA-O1A
25	D	405	CLA	CAA-CBA-CGA-O1A
27	C	516	BCR	C11-C12-C13-C14
25	B	504	CLA	C5-C6-C7-C8
25	B	501	CLA	CAA-CBA-CGA-O1A
32	C	521	LMU	C4'-C5'-C6'-O6'
30	D	409	LHG	C29-C30-C31-C32
25	B	504	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

62 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	410	SQD	15	0
25	B	512	CLA	20	0
25	B	505	CLA	17	0
31	C	517	DGD	11	0
25	B	511	CLA	15	0
25	C	512	CLA	7	0
25	B	509	CLA	23	0
25	B	504	CLA	14	0
25	C	505	CLA	11	0
27	K	101	BCR	12	0
25	B	515	CLA	4	0
25	C	510	CLA	17	0
30	D	409	LHG	6	0
25	B	514	CLA	14	0
25	H	101	CLA	12	0
30	B	521	LHG	7	0
25	C	506	CLA	15	0
25	B	503	CLA	23	0
34	D	407	PL9	6	0
25	C	502	CLA	7	0
27	B	516	BCR	11	0
25	B	506	CLA	12	0
27	C	516	BCR	8	0
25	D	401	CLA	13	0
25	B	513	CLA	10	0
25	C	501	CLA	20	0
25	C	509	CLA	9	0
25	C	513	CLA	5	0

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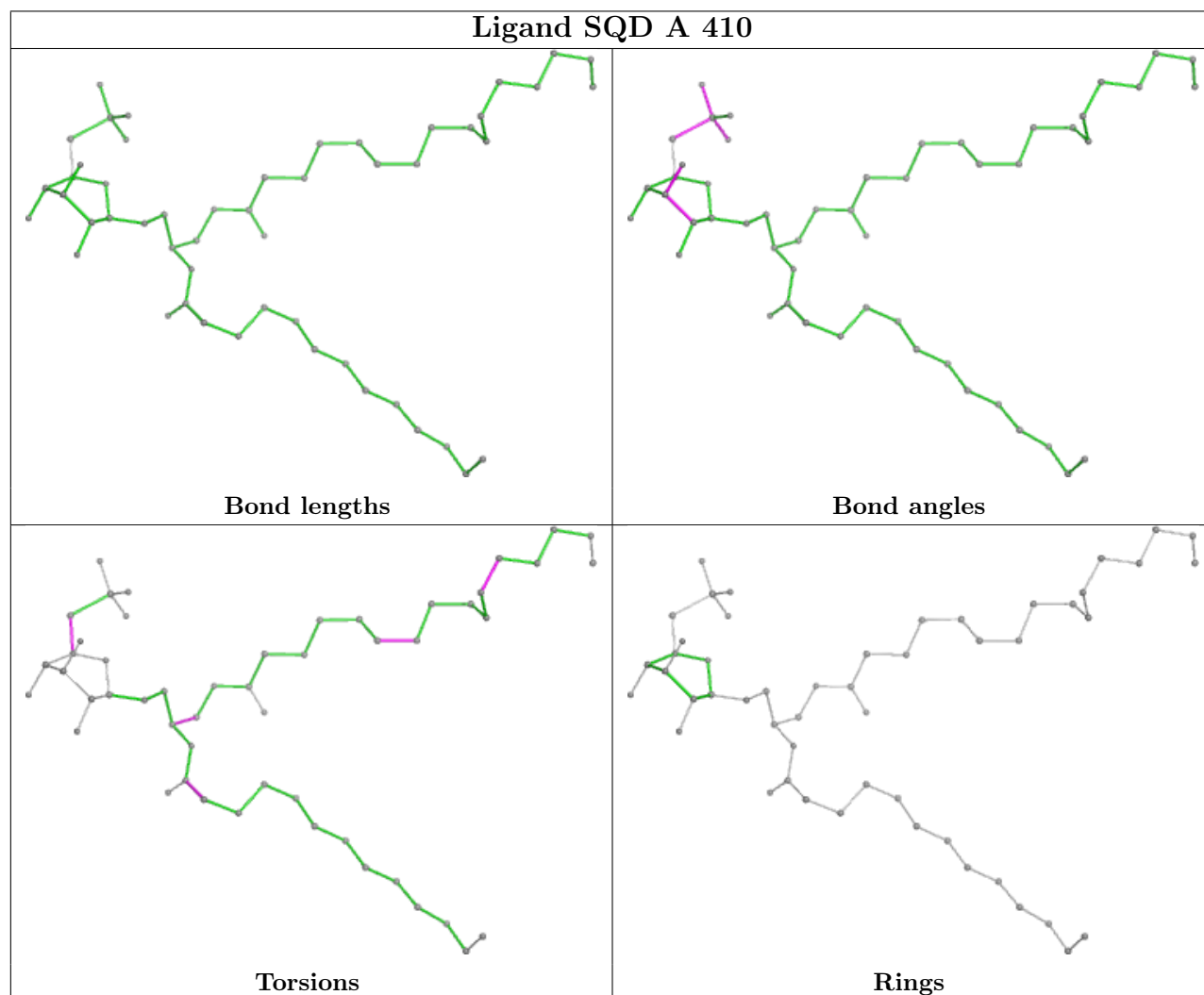


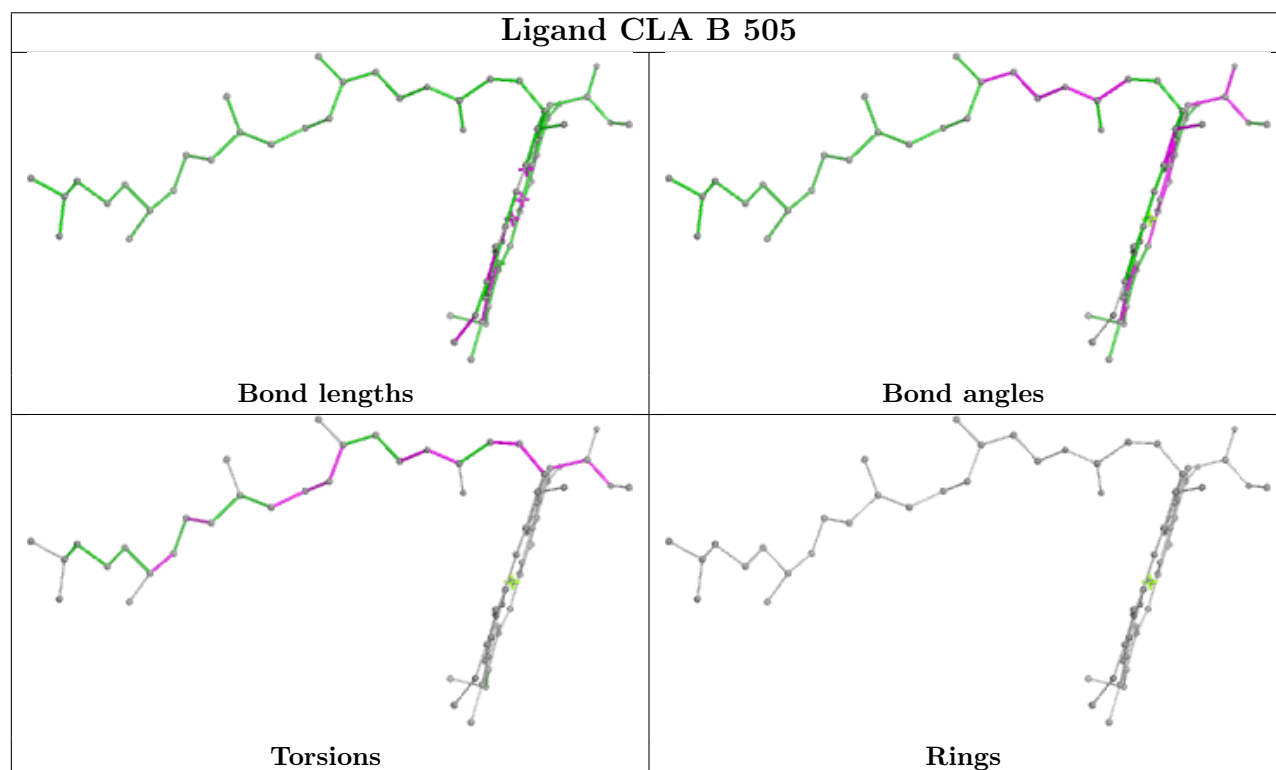
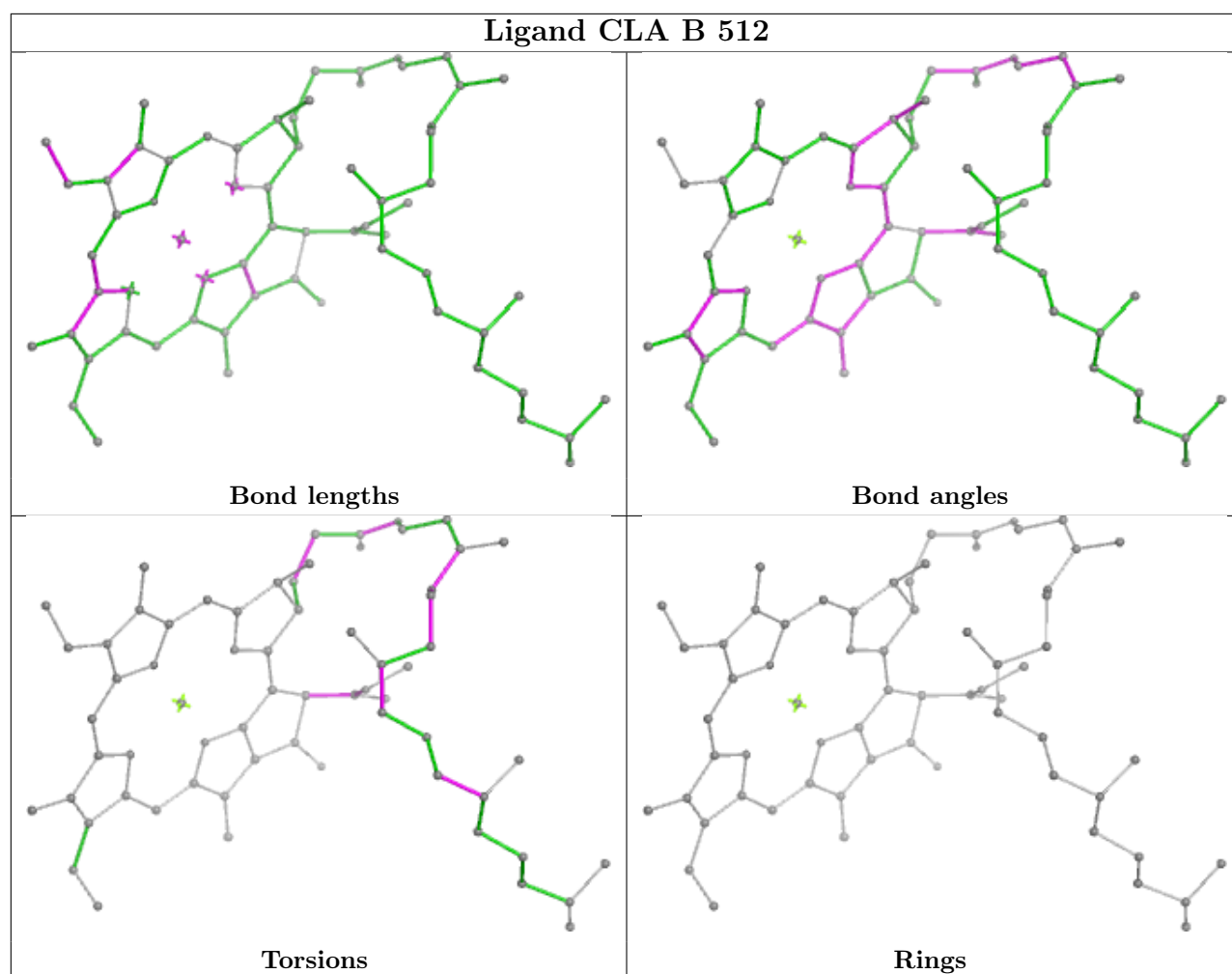
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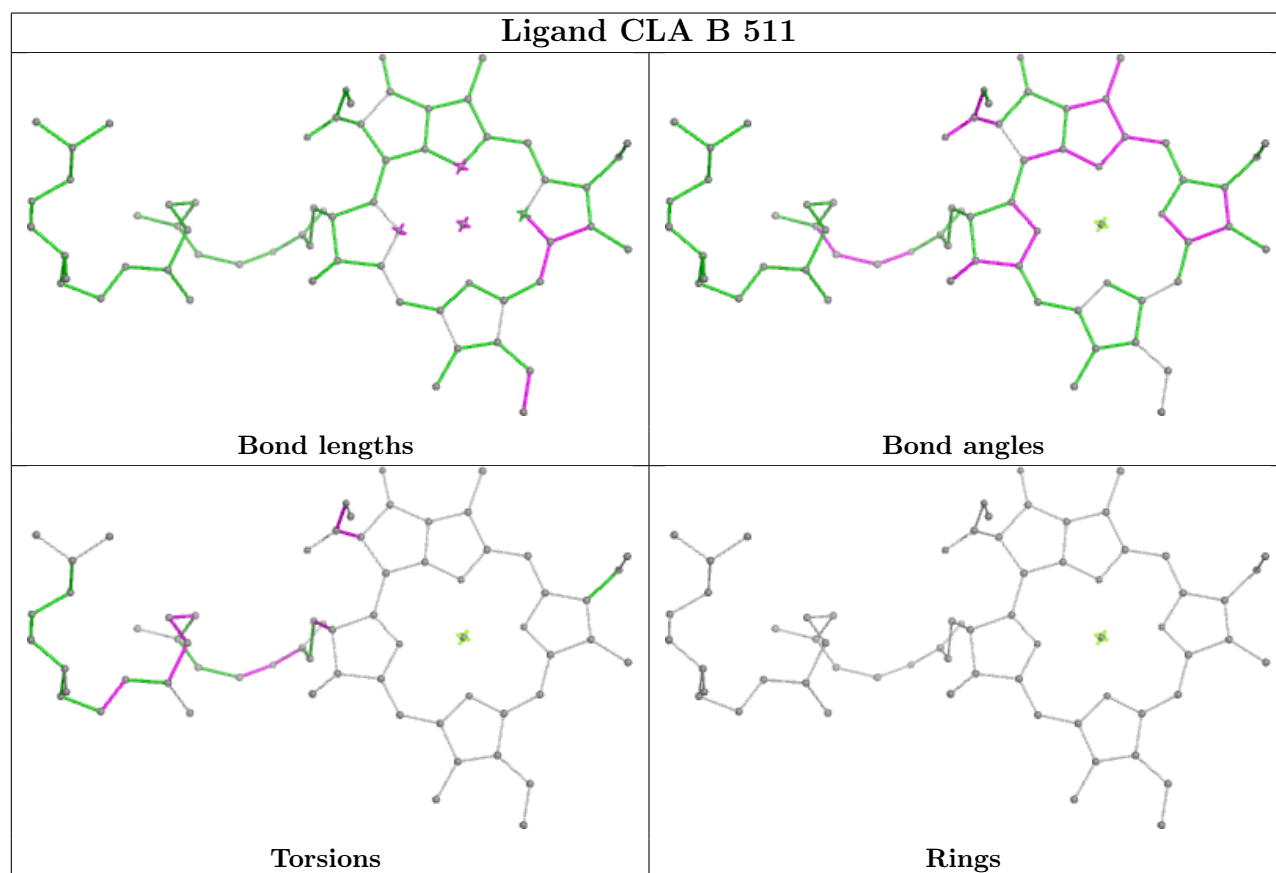
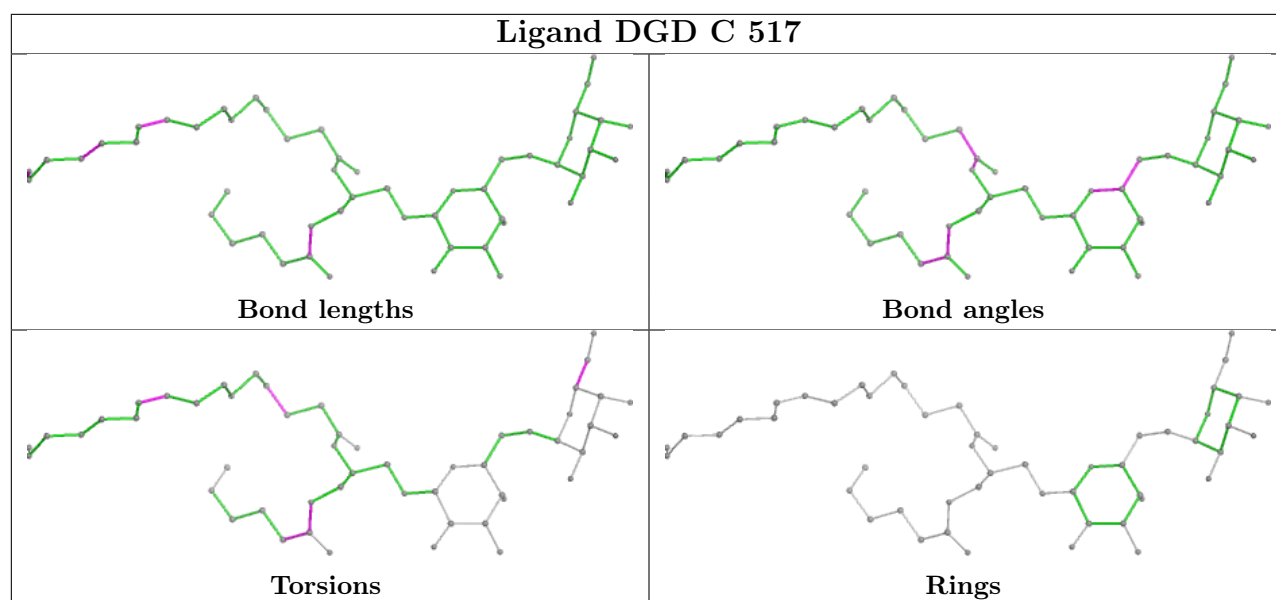
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	520	LMG	12	0
29	B	520	LMG	3	0
30	B	519	LHG	8	0
27	D	406	BCR	9	0
29	D	410	LMG	6	0
29	B	518	LMG	16	0
31	C	519	DGD	9	0
25	C	511	CLA	9	0
35	F	101	HEM	6	0
27	C	514	BCR	10	0
32	C	521	LMU	5	0
25	C	504	CLA	13	0
25	D	405	CLA	6	0
30	D	408	LHG	9	0
25	C	507	CLA	27	0
25	A	408	CLA	19	0
26	A	407	PHO	6	0
25	B	501	CLA	12	0
27	B	517	BCR	10	0
33	D	403	BCT	1	0
25	A	405	CLA	14	0
25	A	406	CLA	9	0
25	C	503	CLA	6	0
25	B	508	CLA	20	0
25	B	507	CLA	18	0
25	C	508	CLA	11	0
31	C	518	DGD	15	0
27	A	409	BCR	19	0
26	D	402	PHO	12	0
25	B	502	CLA	6	0
25	B	510	CLA	20	0
29	W	201	LMG	23	0
25	D	404	CLA	10	0
27	C	515	BCR	16	0

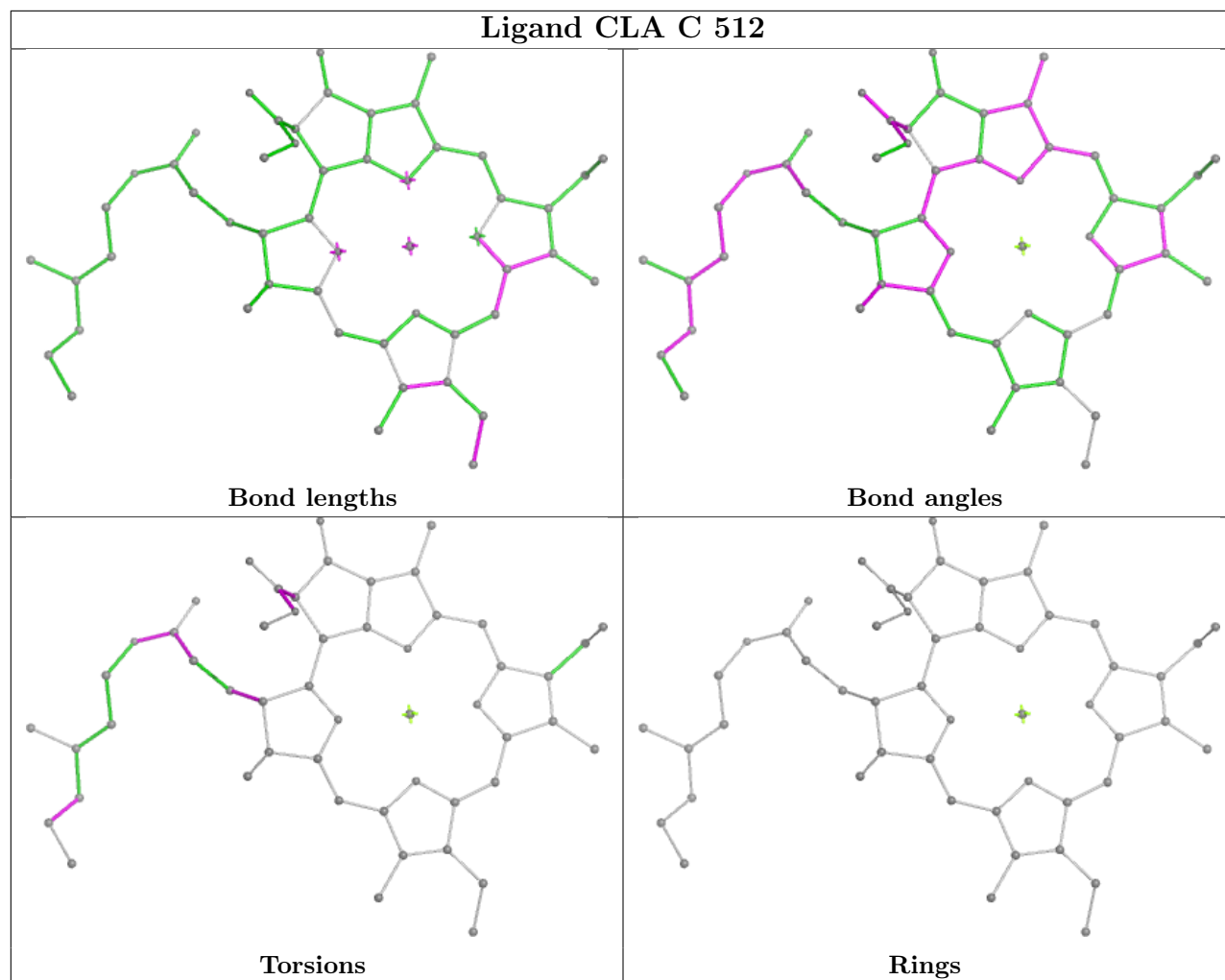
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

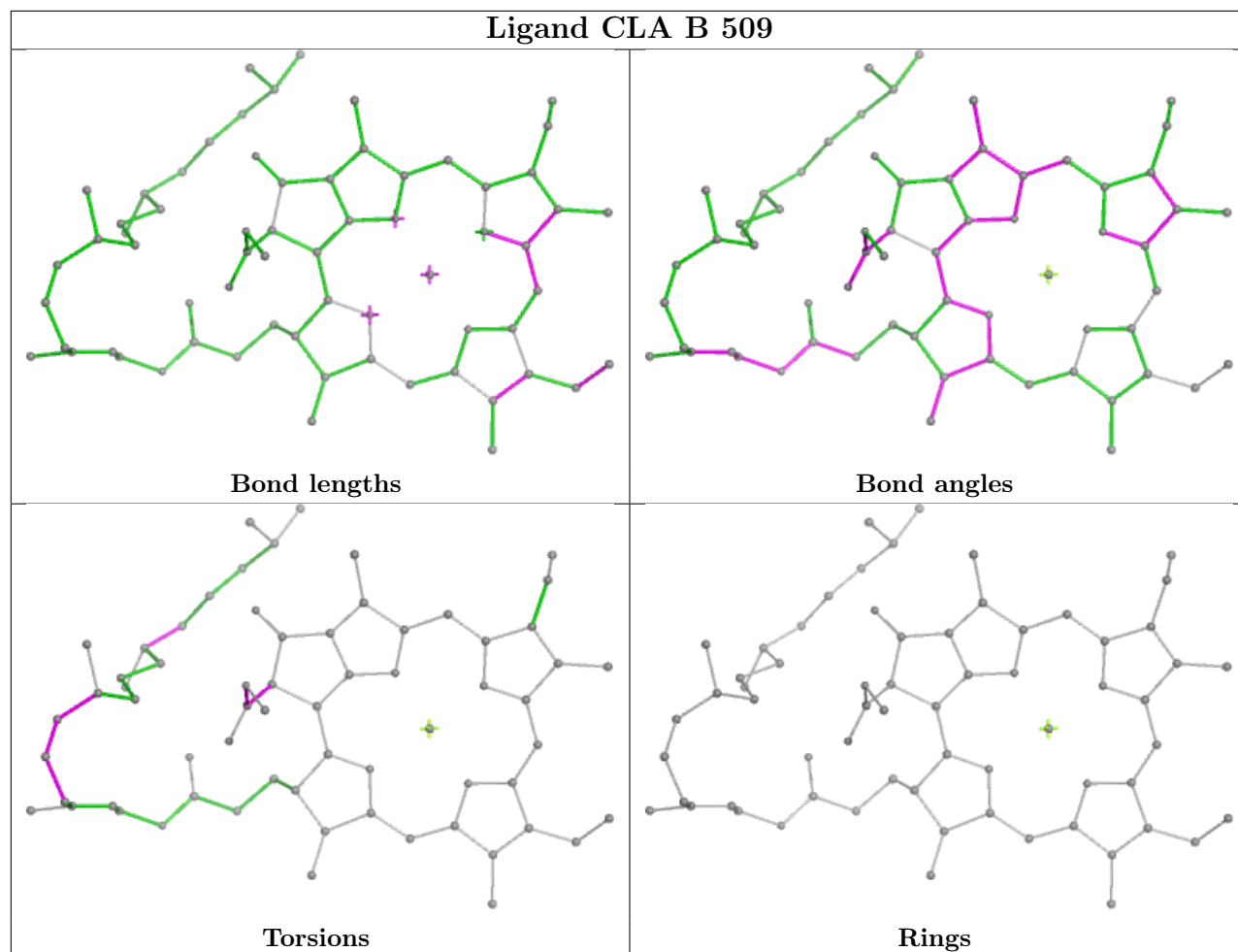




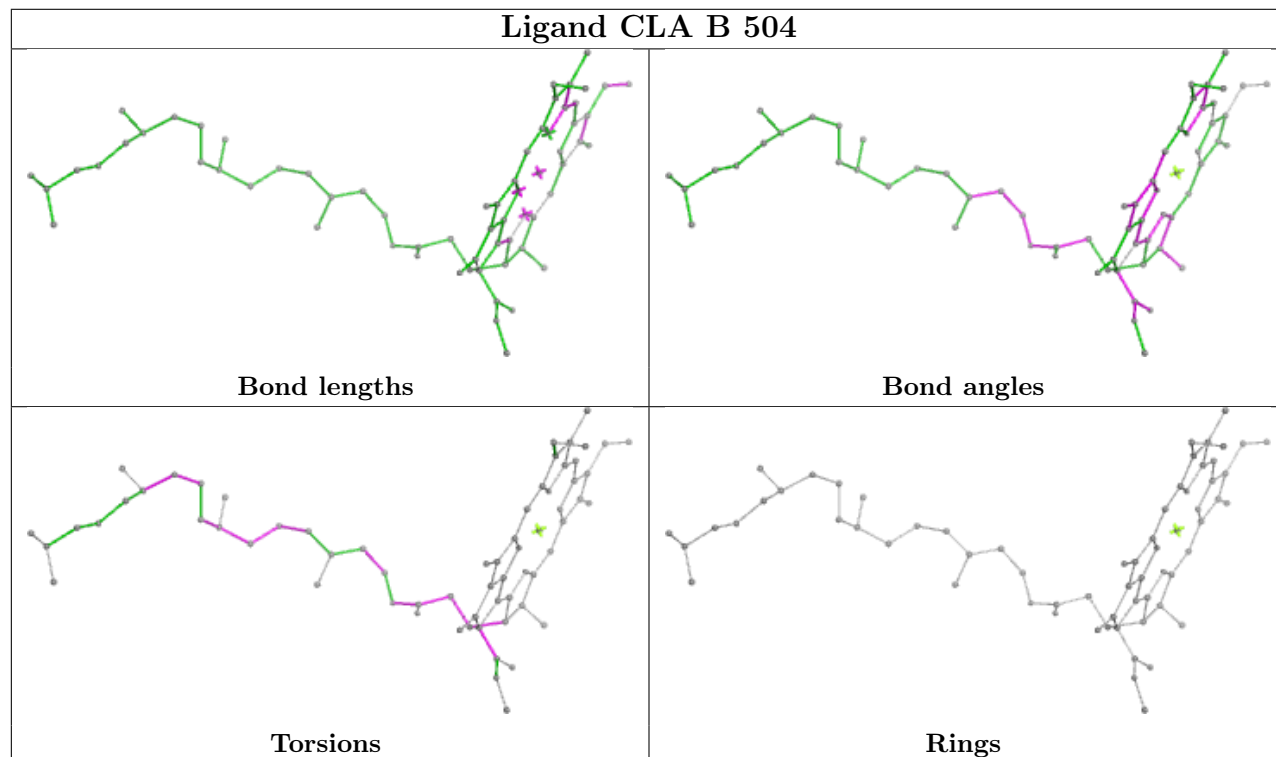


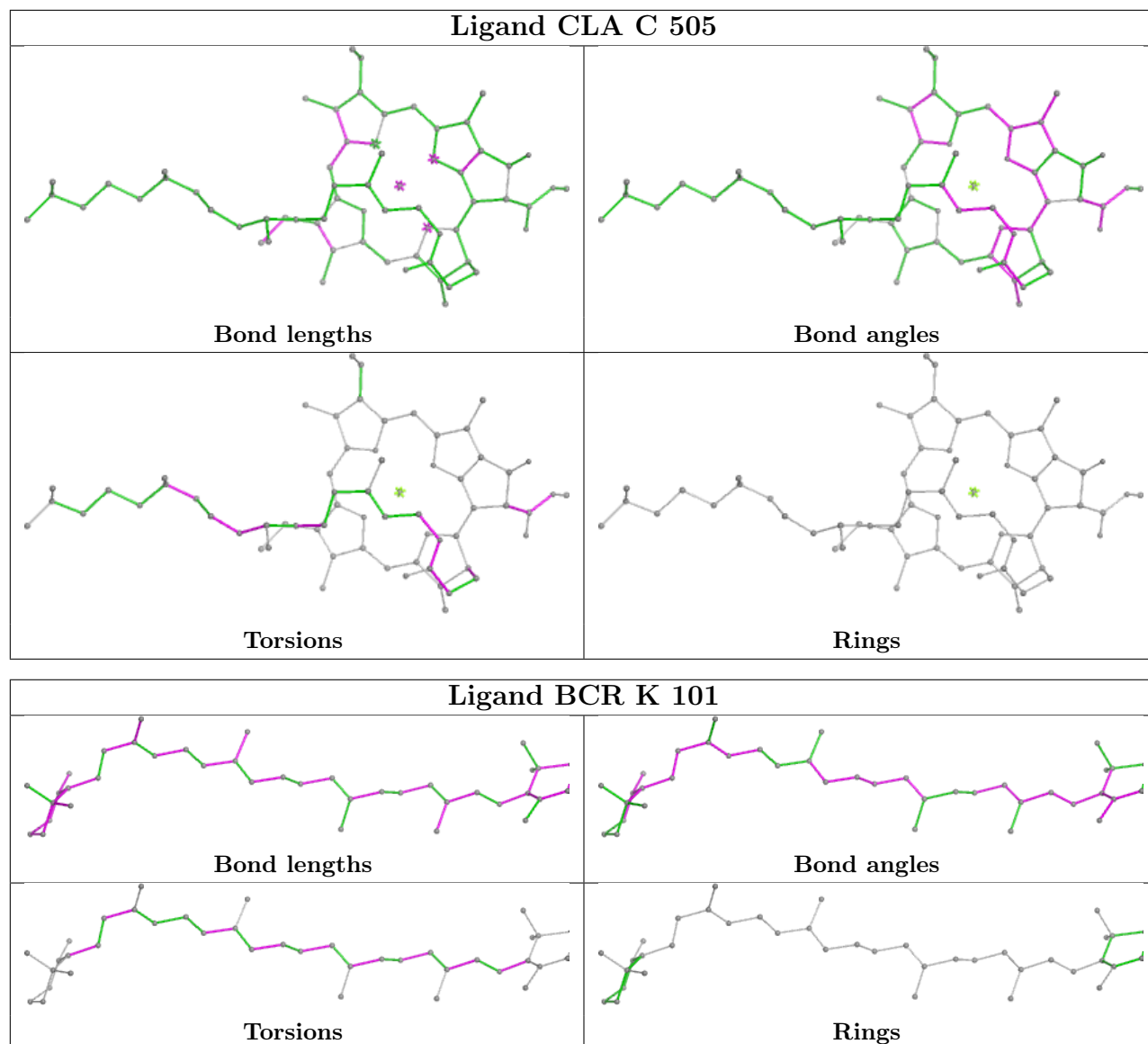


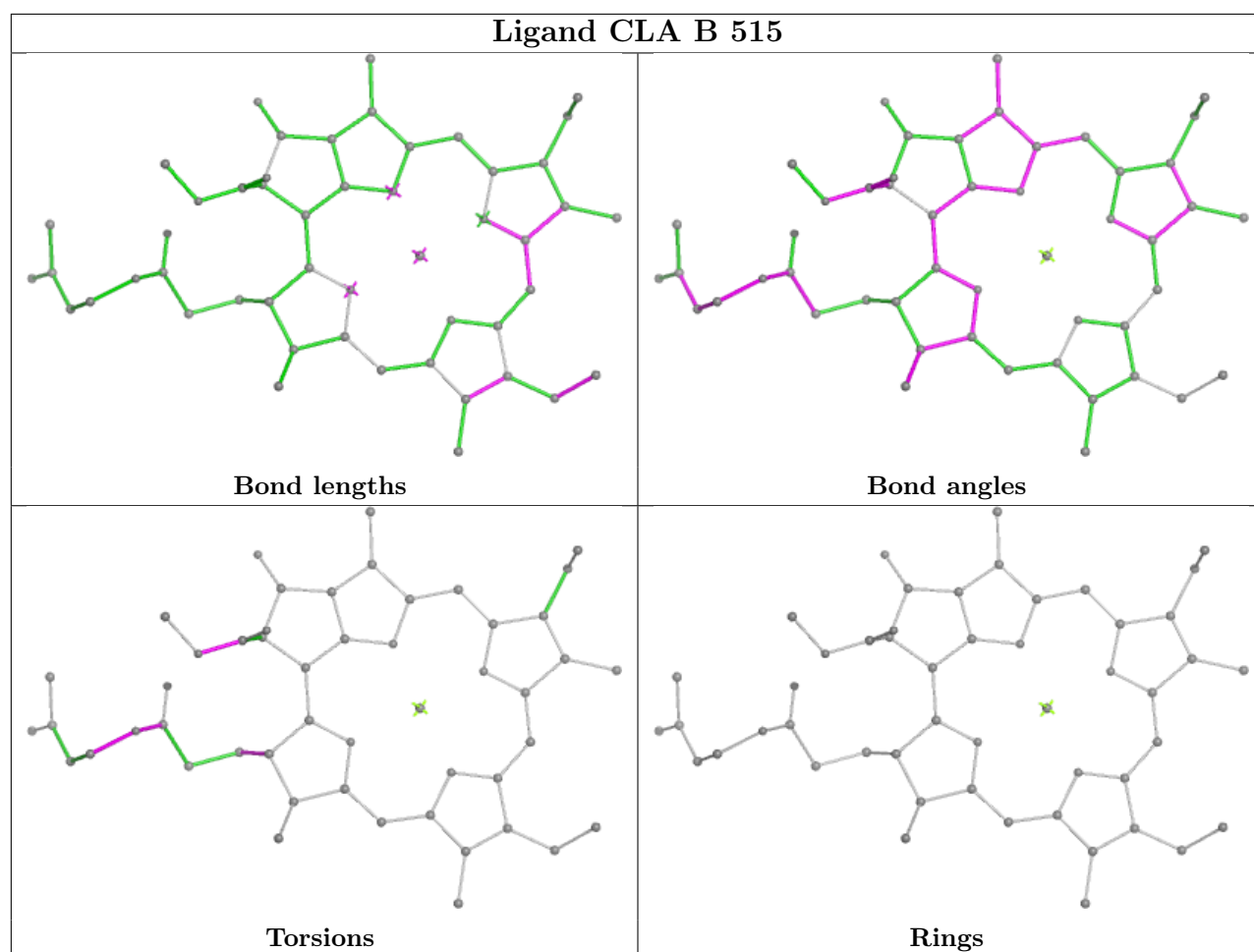
## Ligand CLA B 509



## Ligand CLA B 504

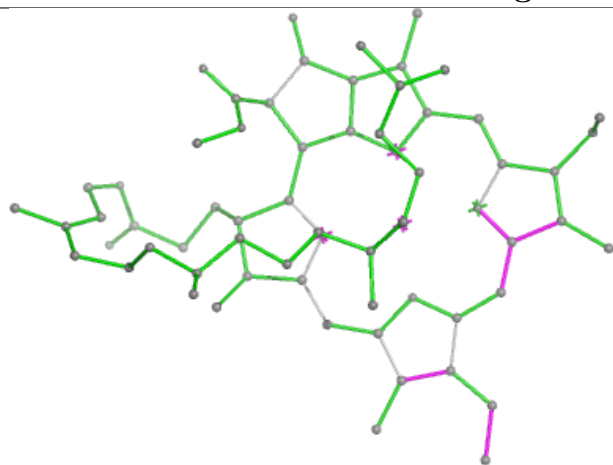




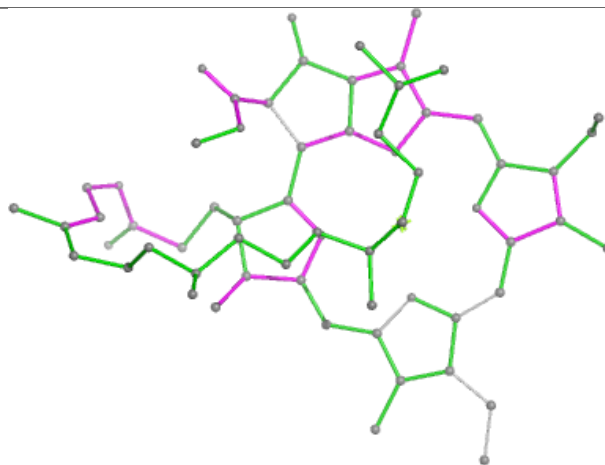




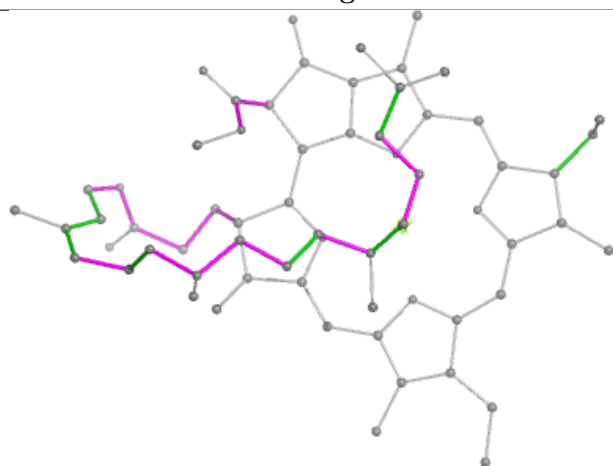
## Ligand CLA C 510



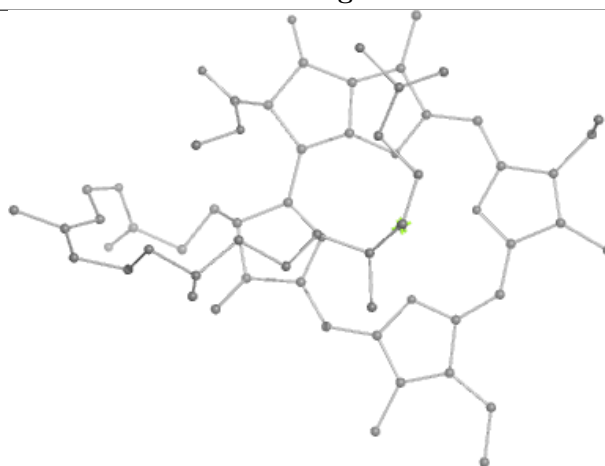
Bond lengths



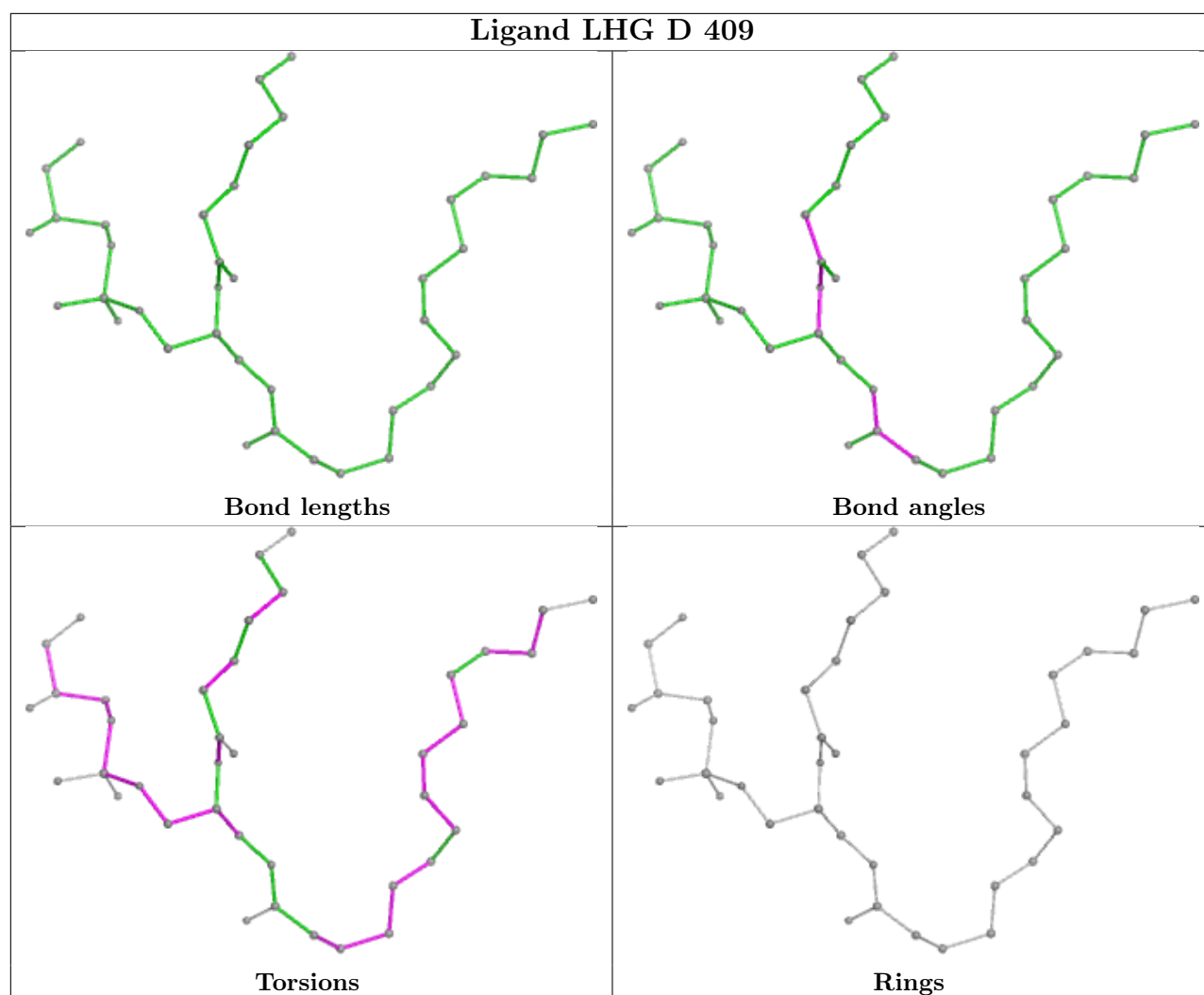
Bond angles



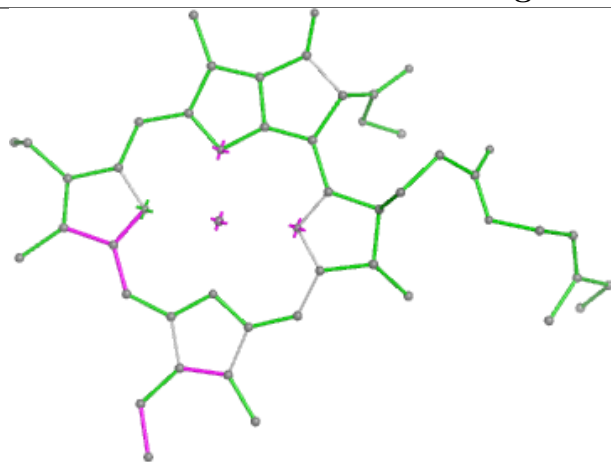
Torsions



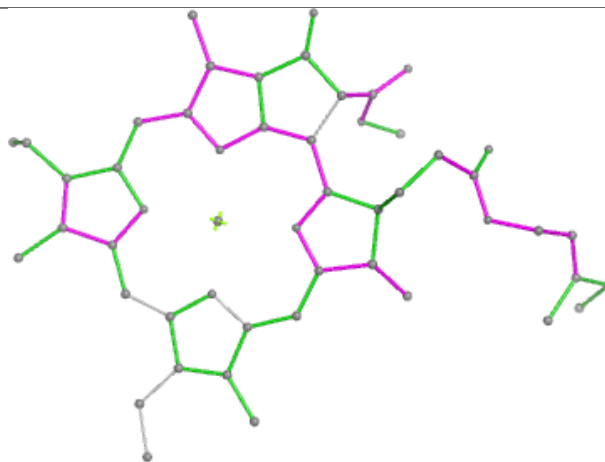
Rings



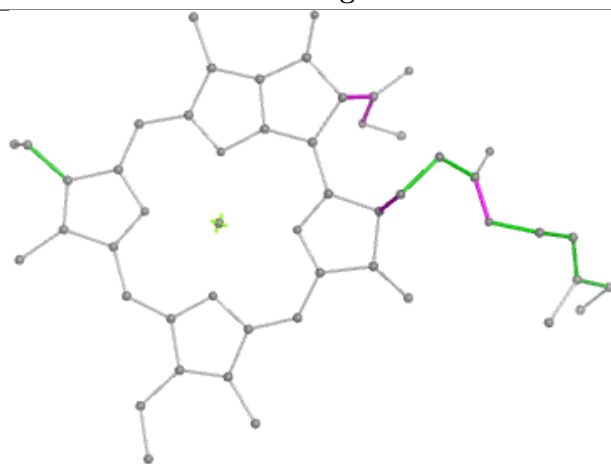
## Ligand CLA B 514



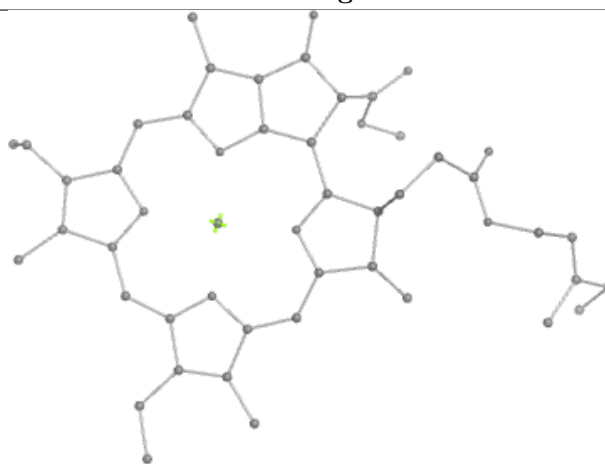
Bond lengths



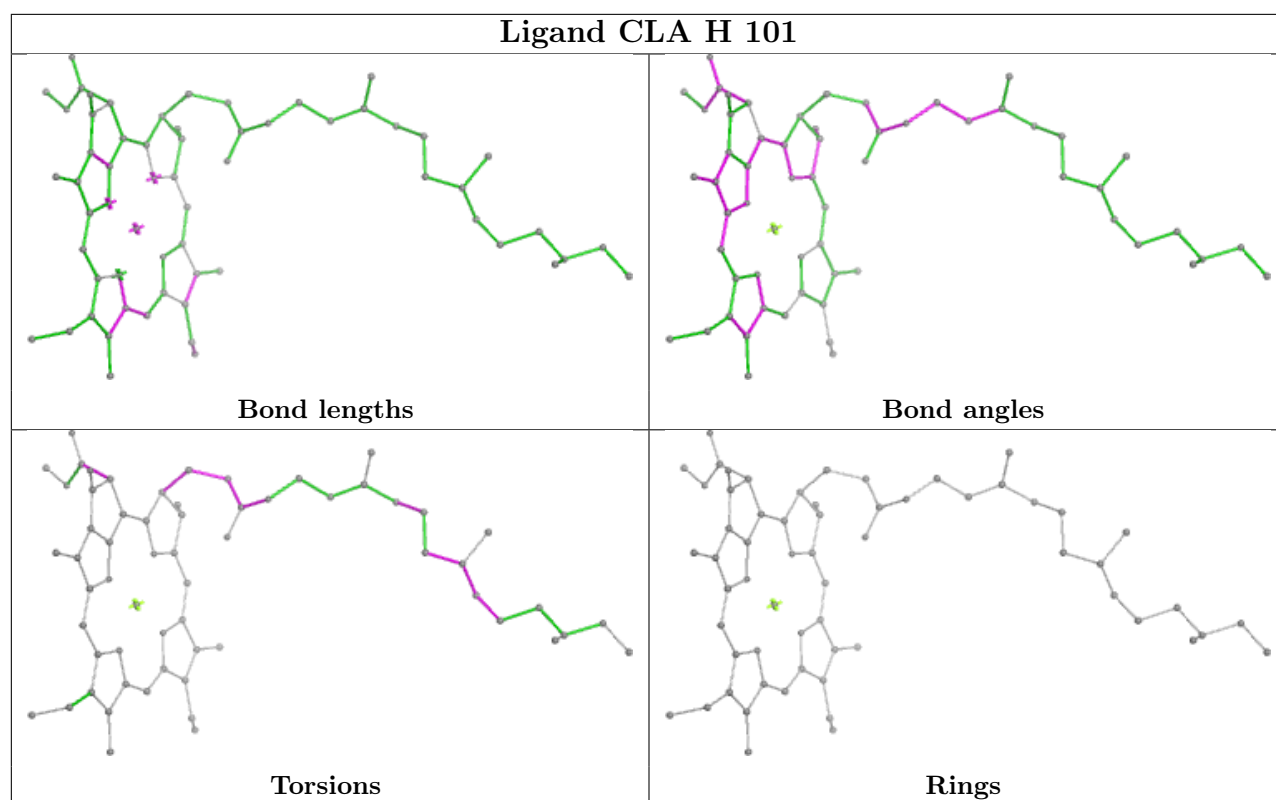
Bond angles

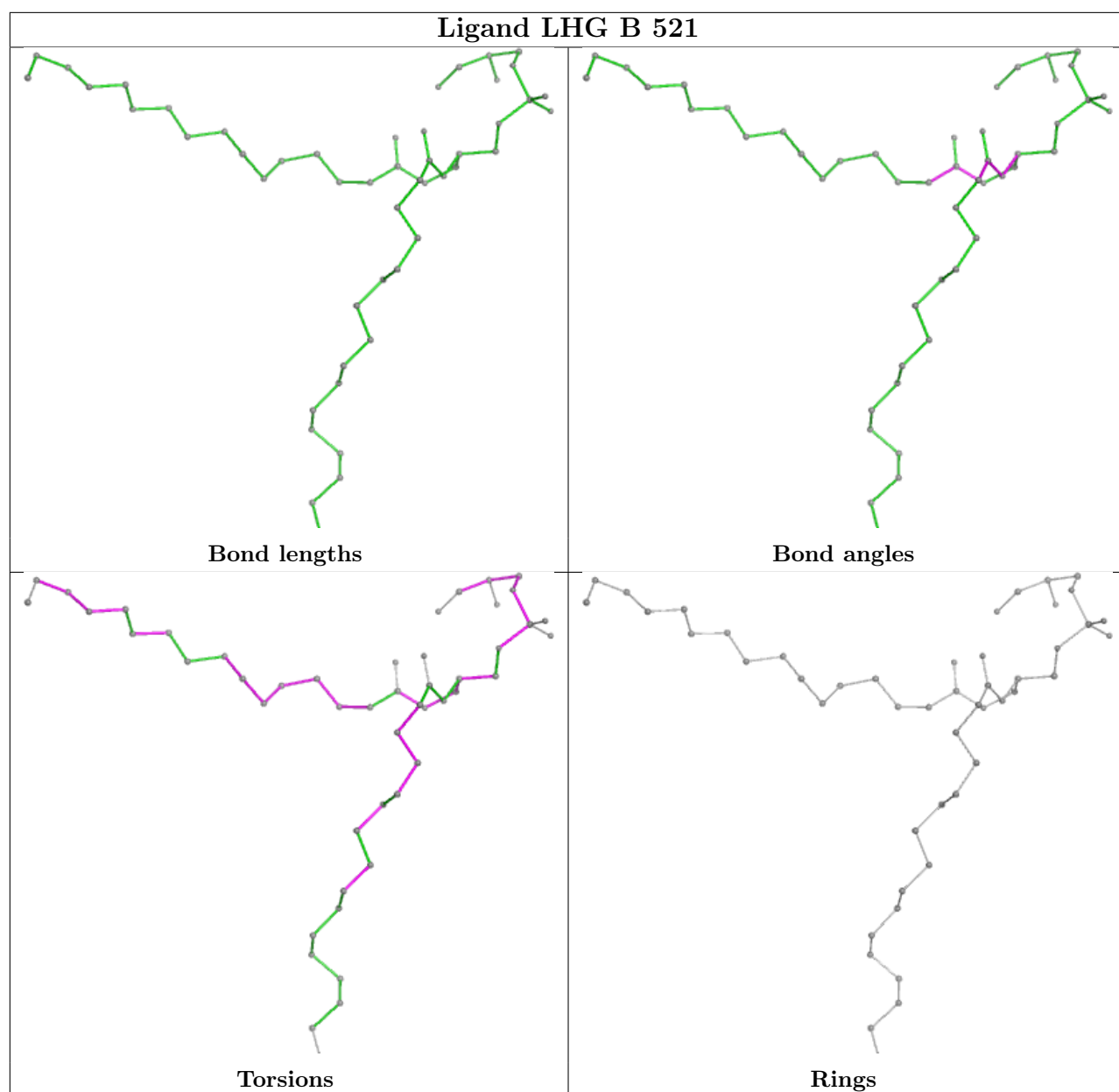


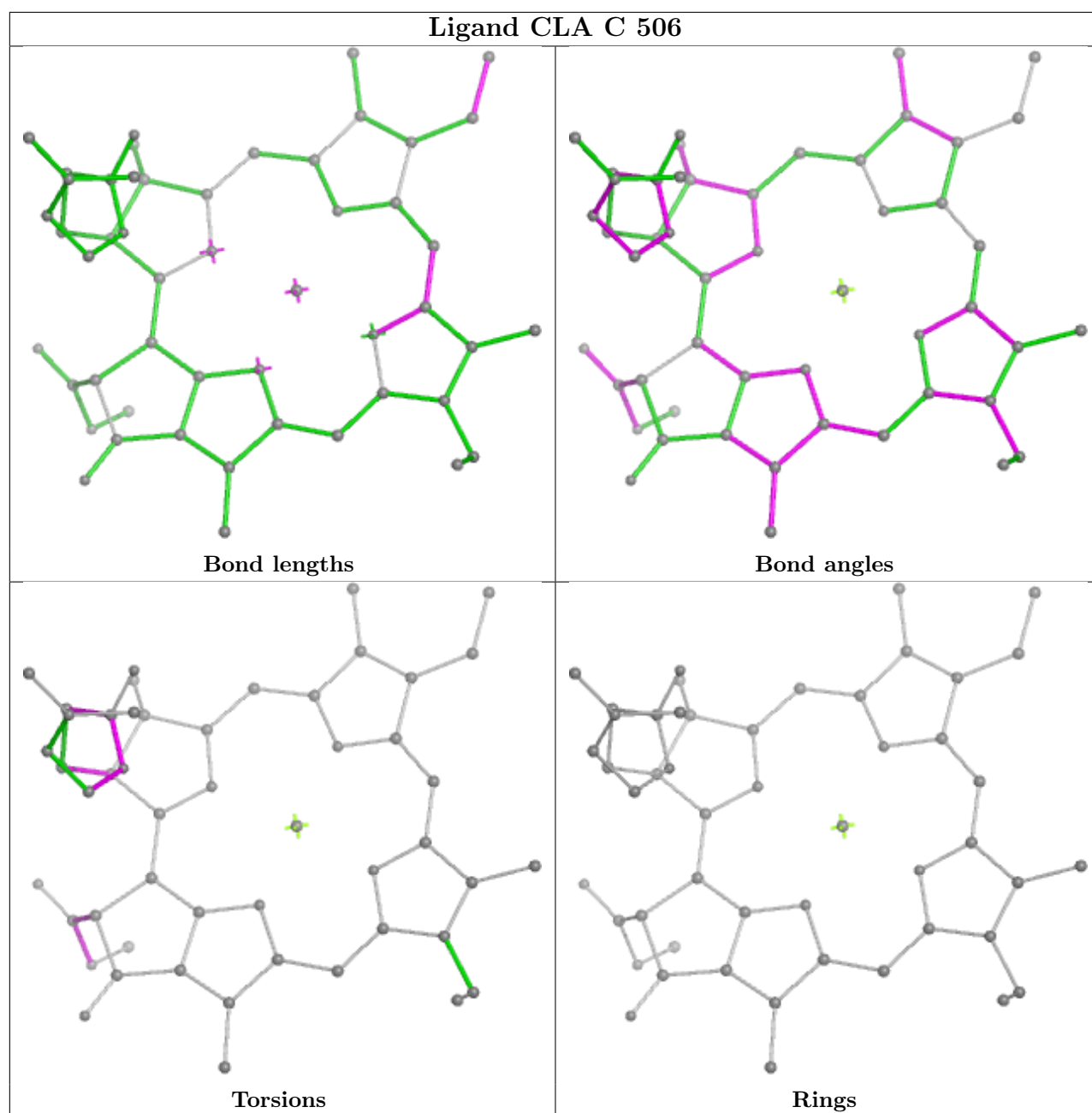
Torsions

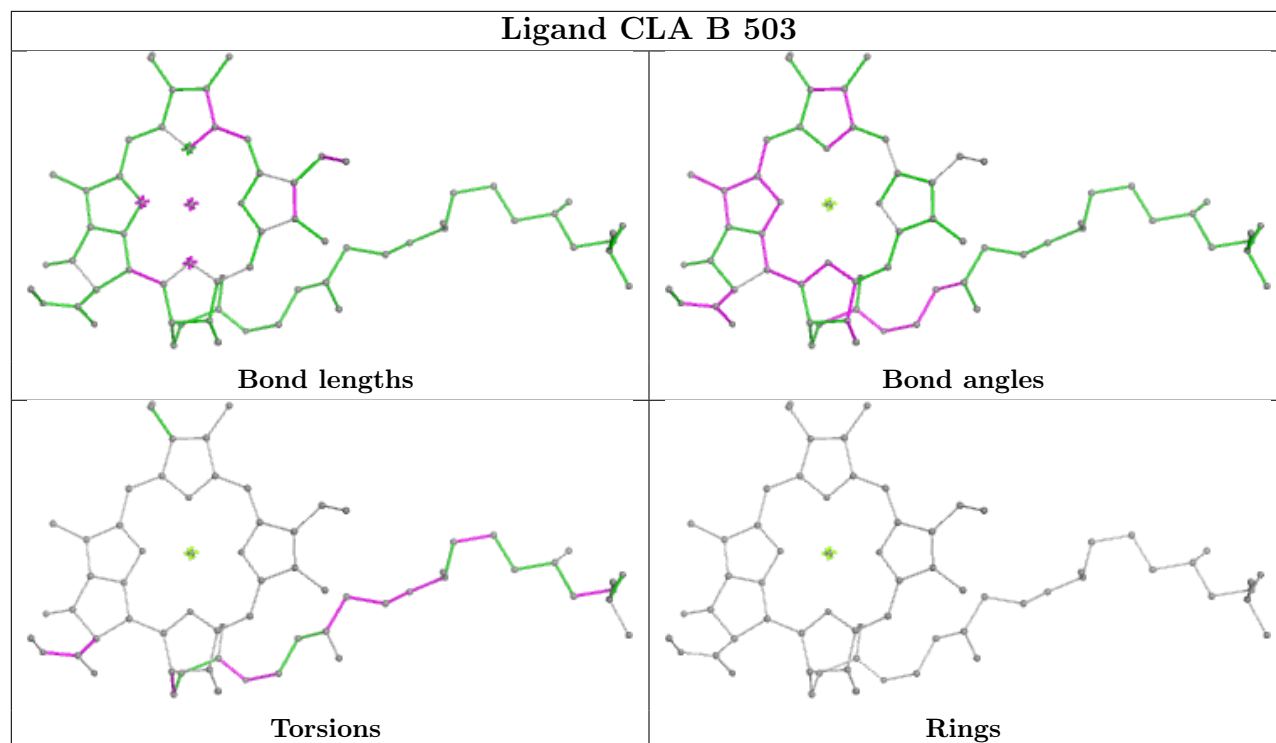
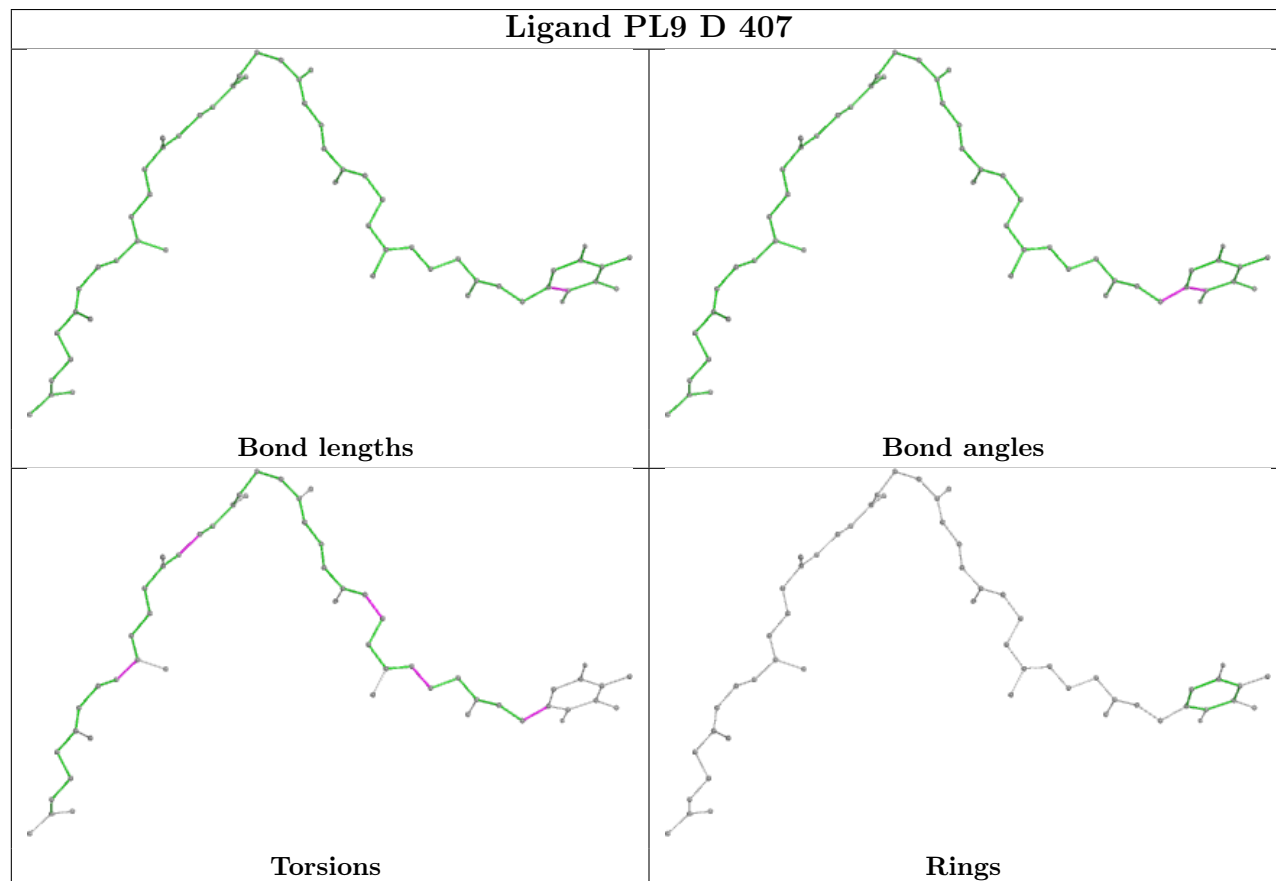


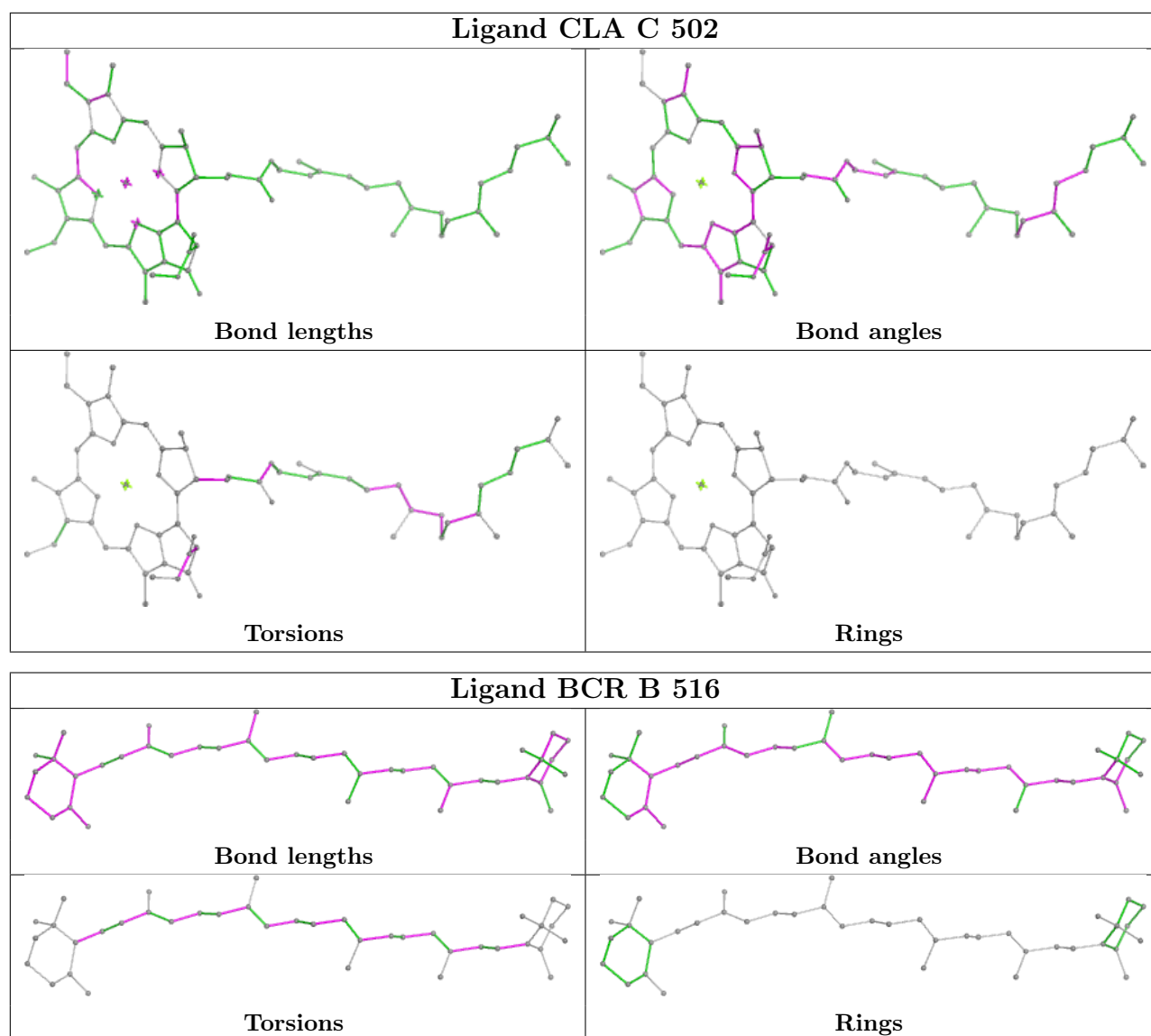
Rings



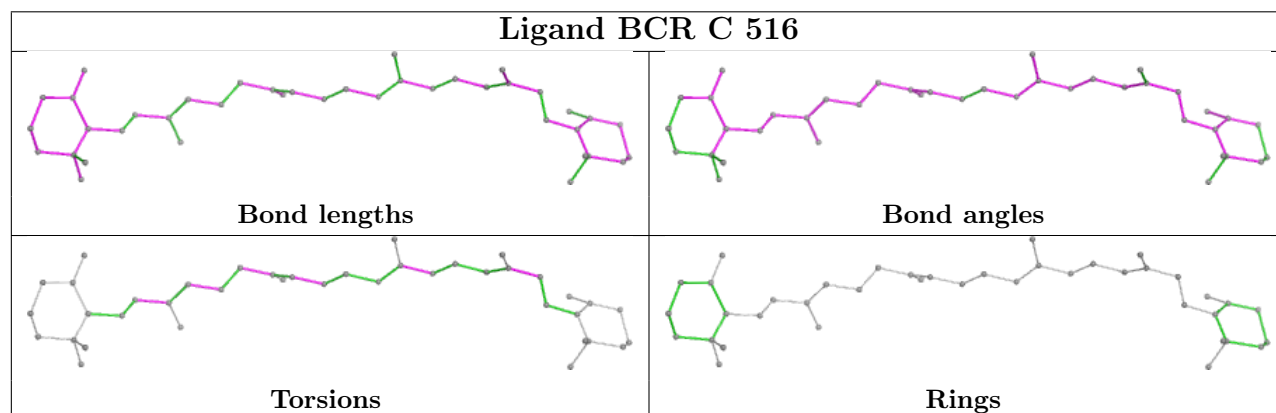
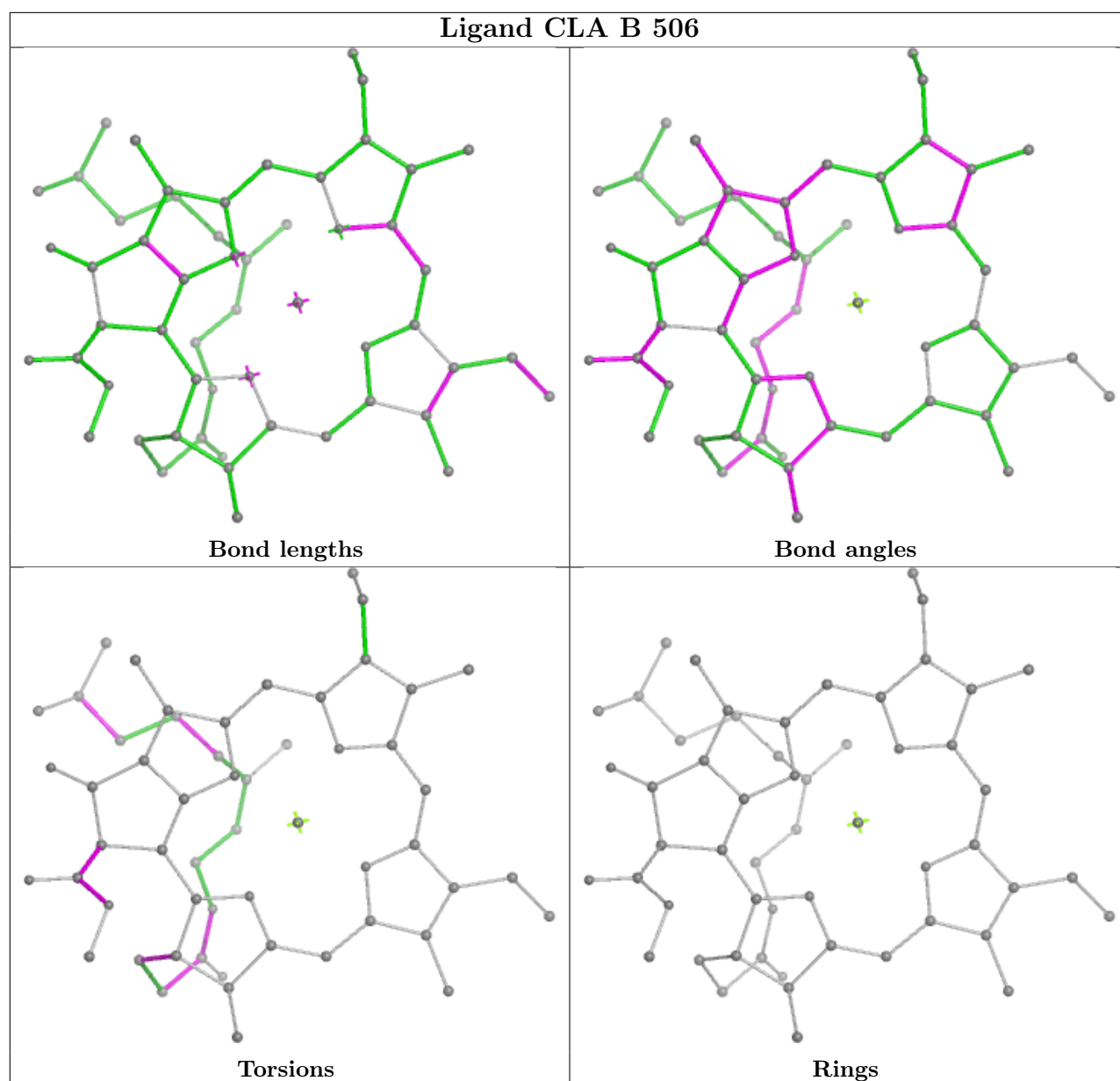


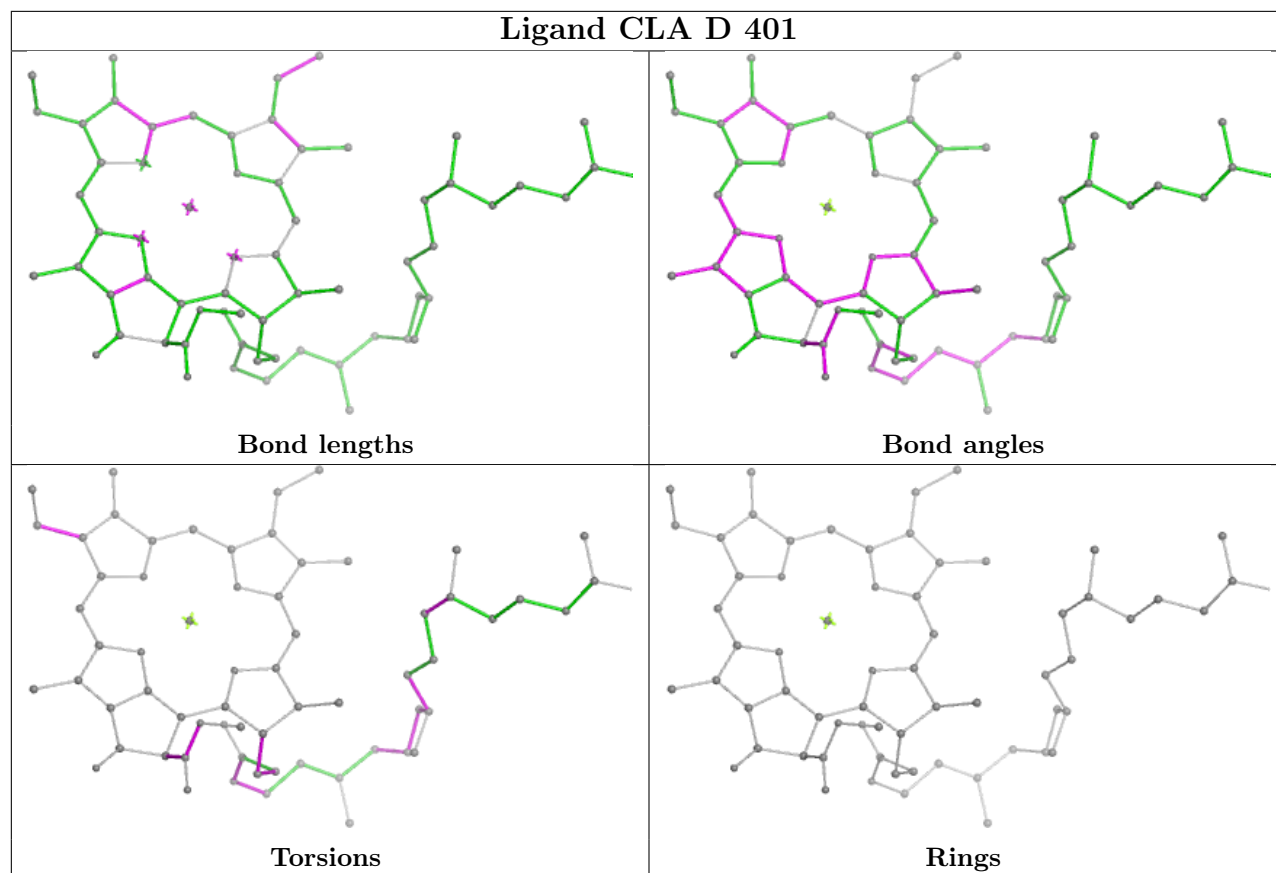


**Ligand CLA B 503****Ligand PL9 D 407**

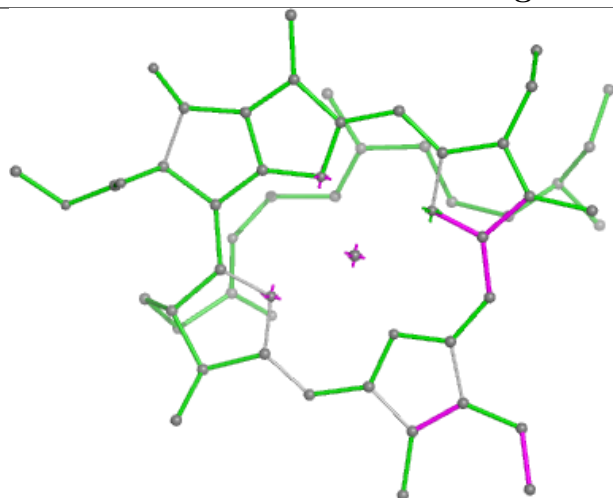




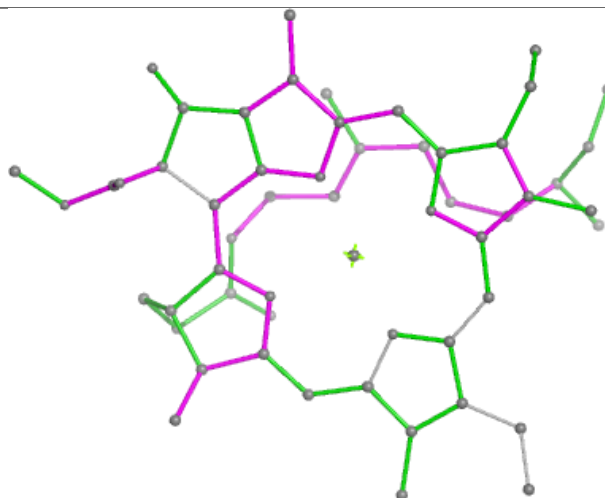




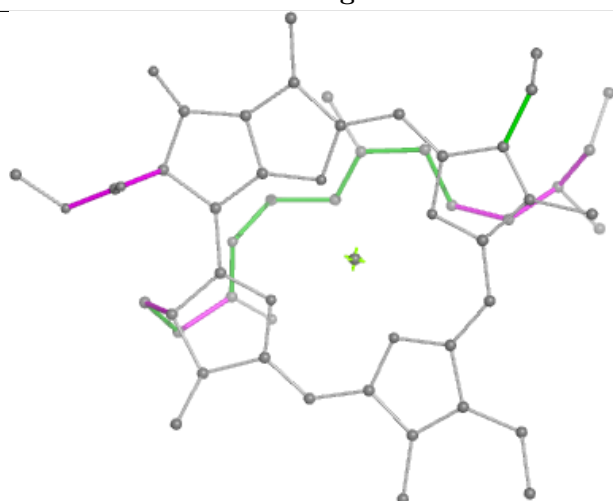
## Ligand CLA B 513



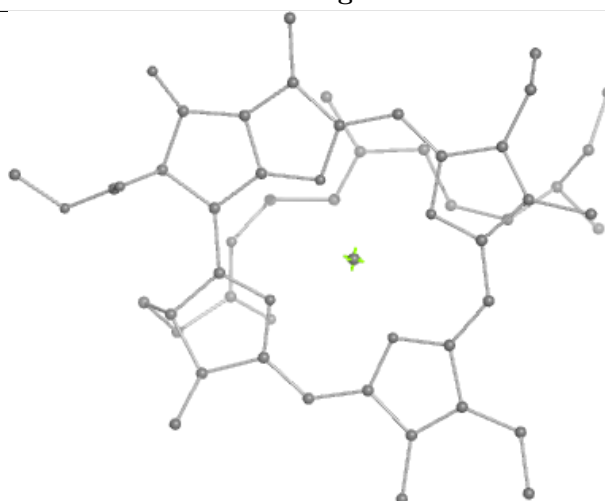
Bond lengths



Bond angles

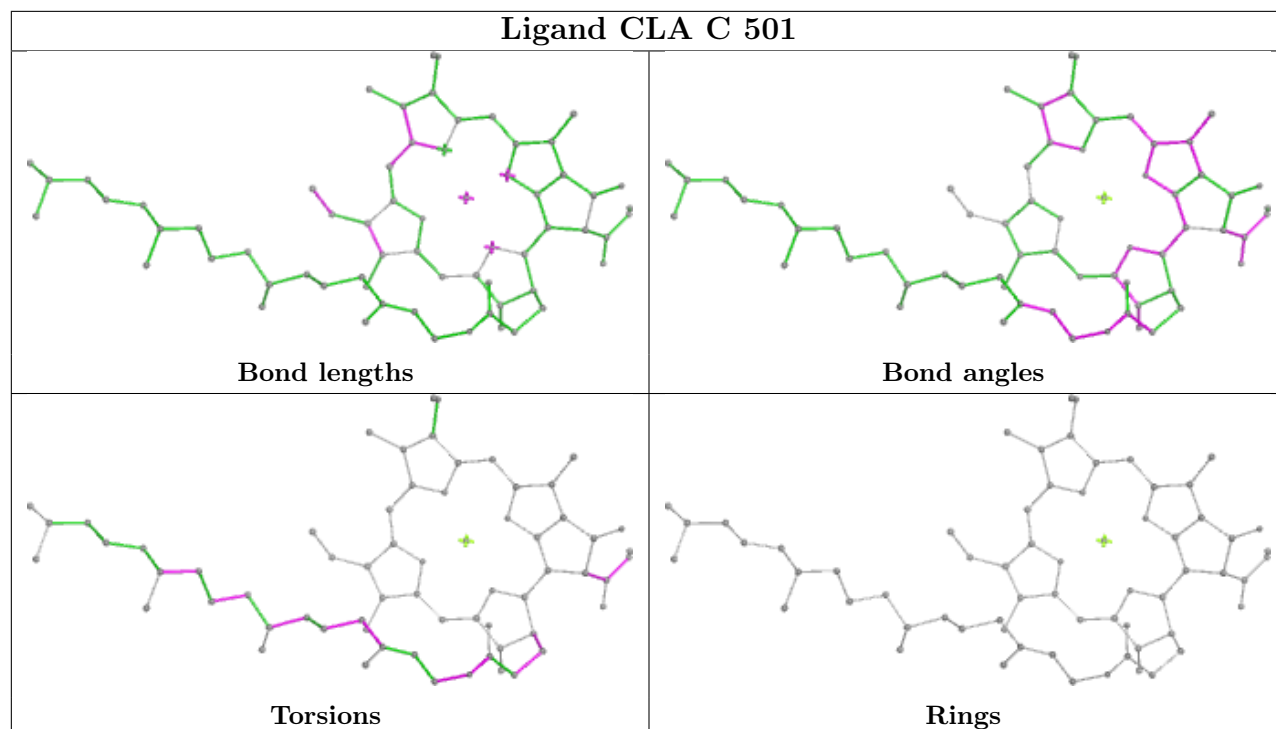


Torsions

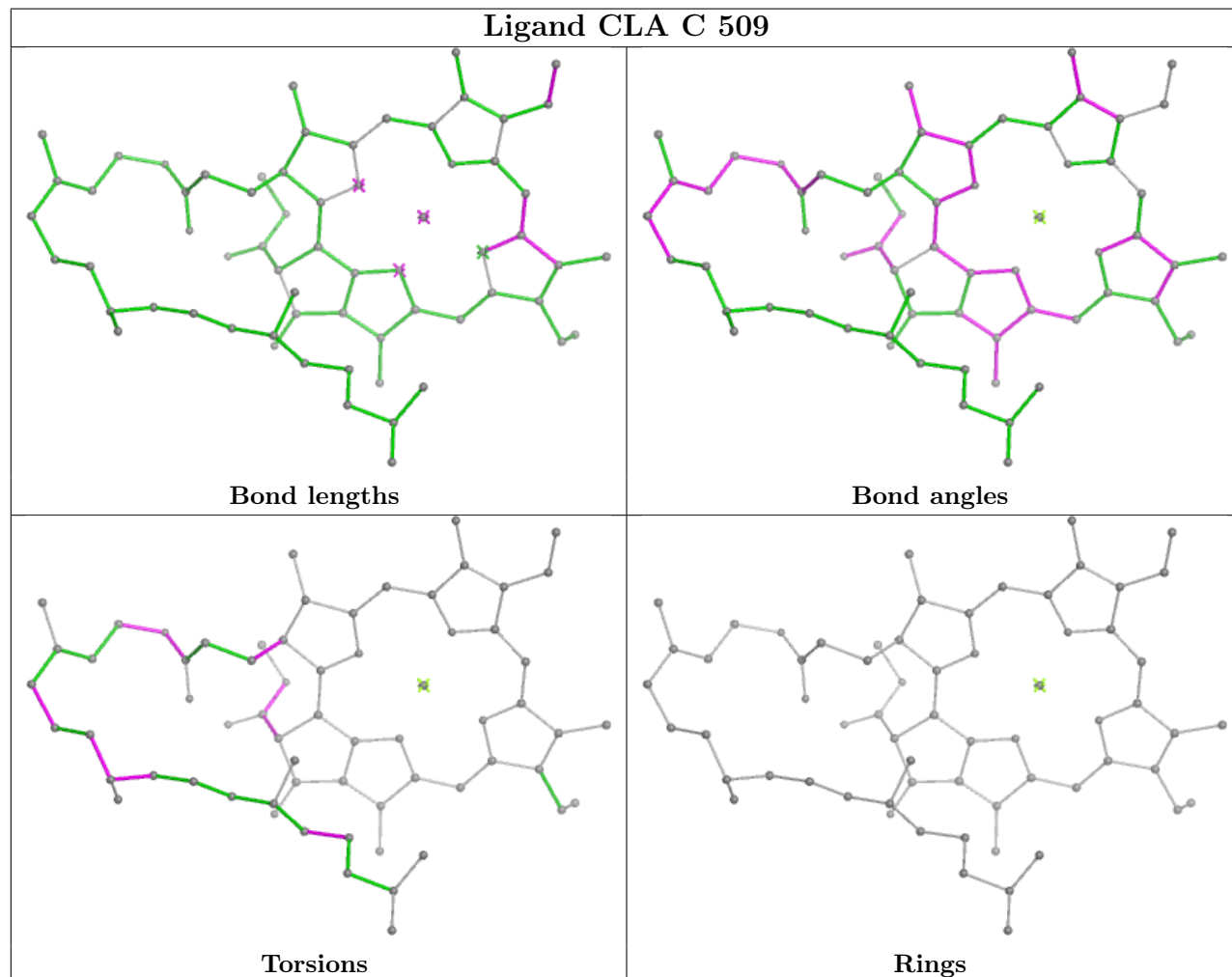


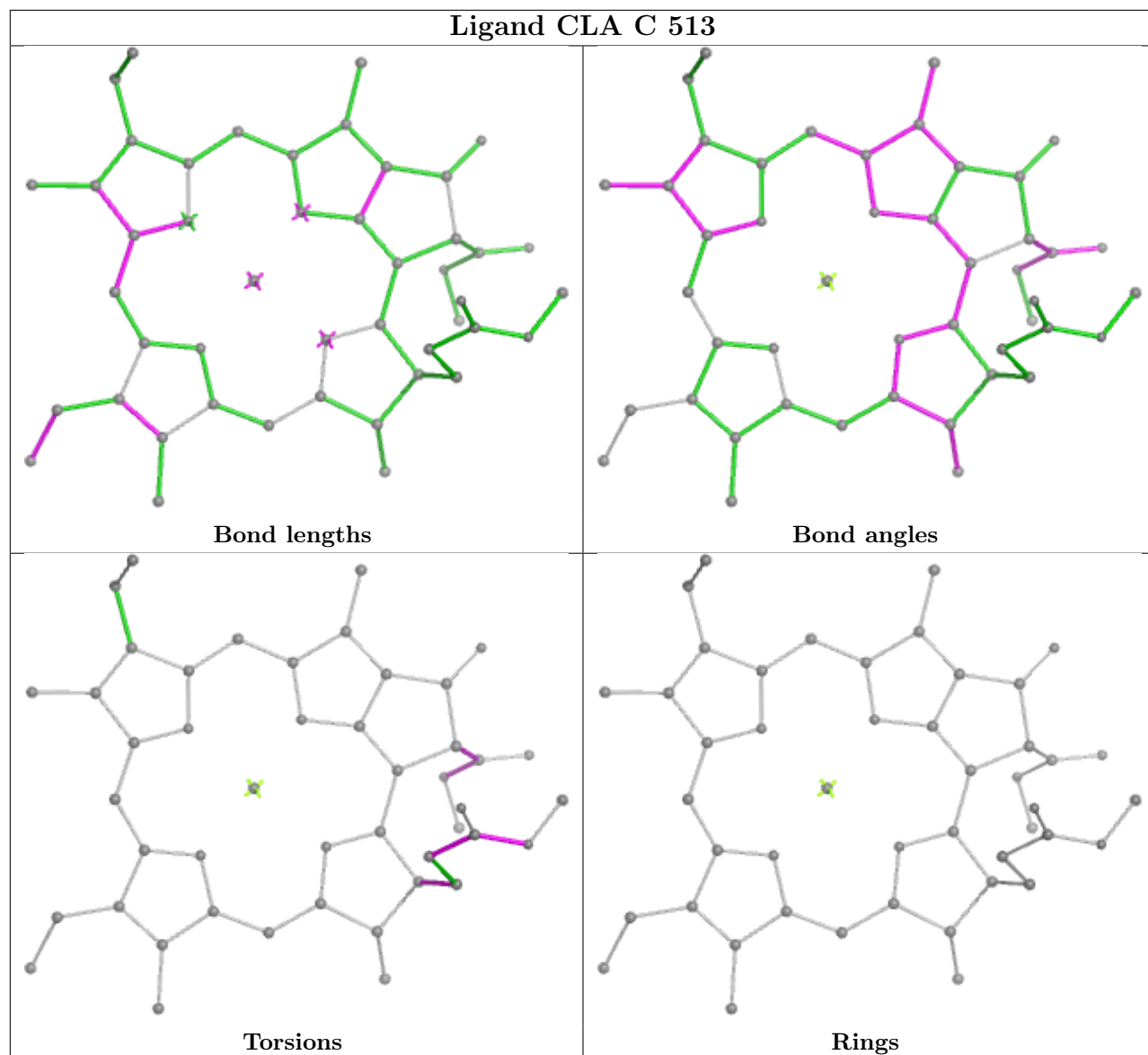
Rings

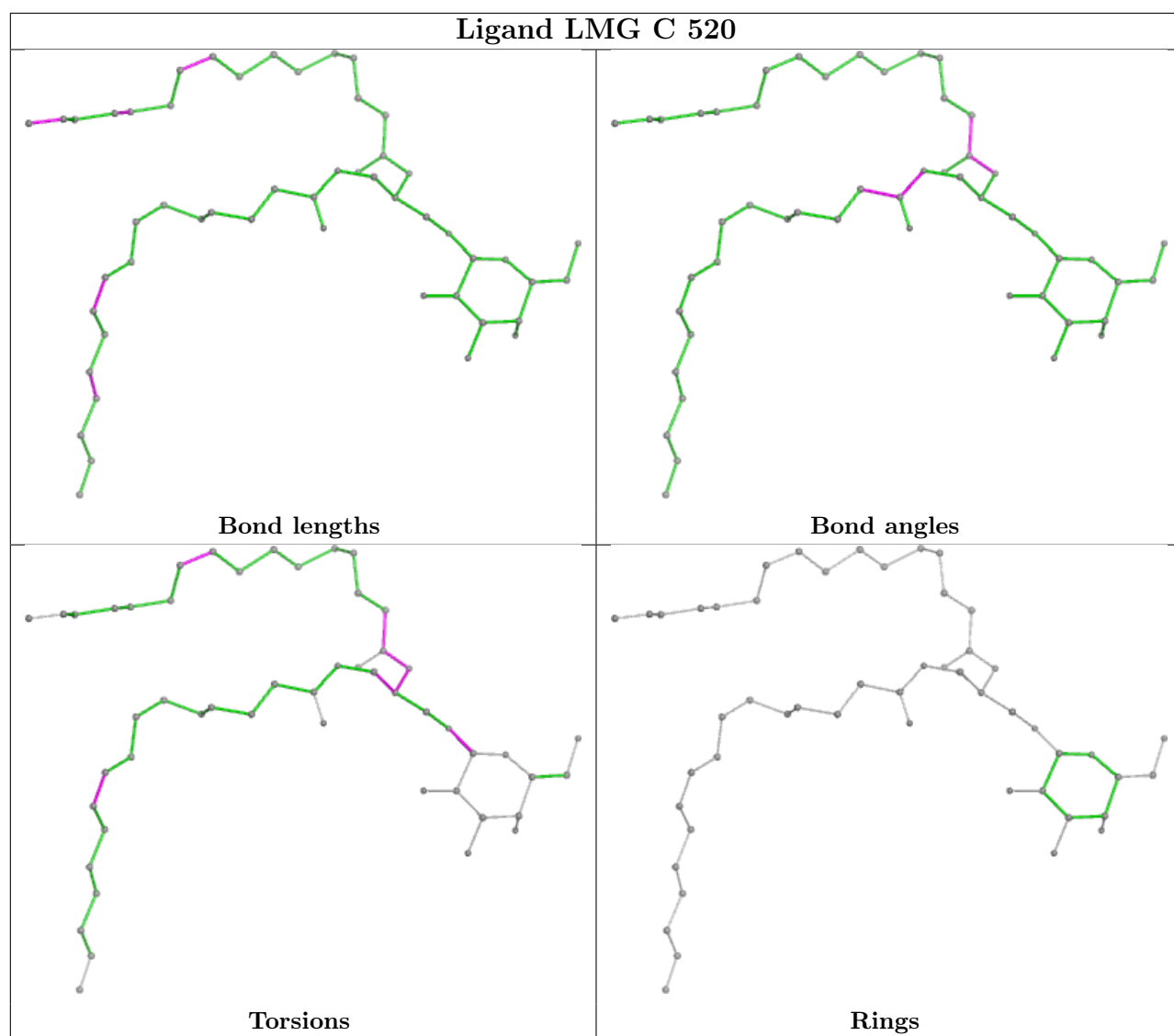
## Ligand CLA C 501

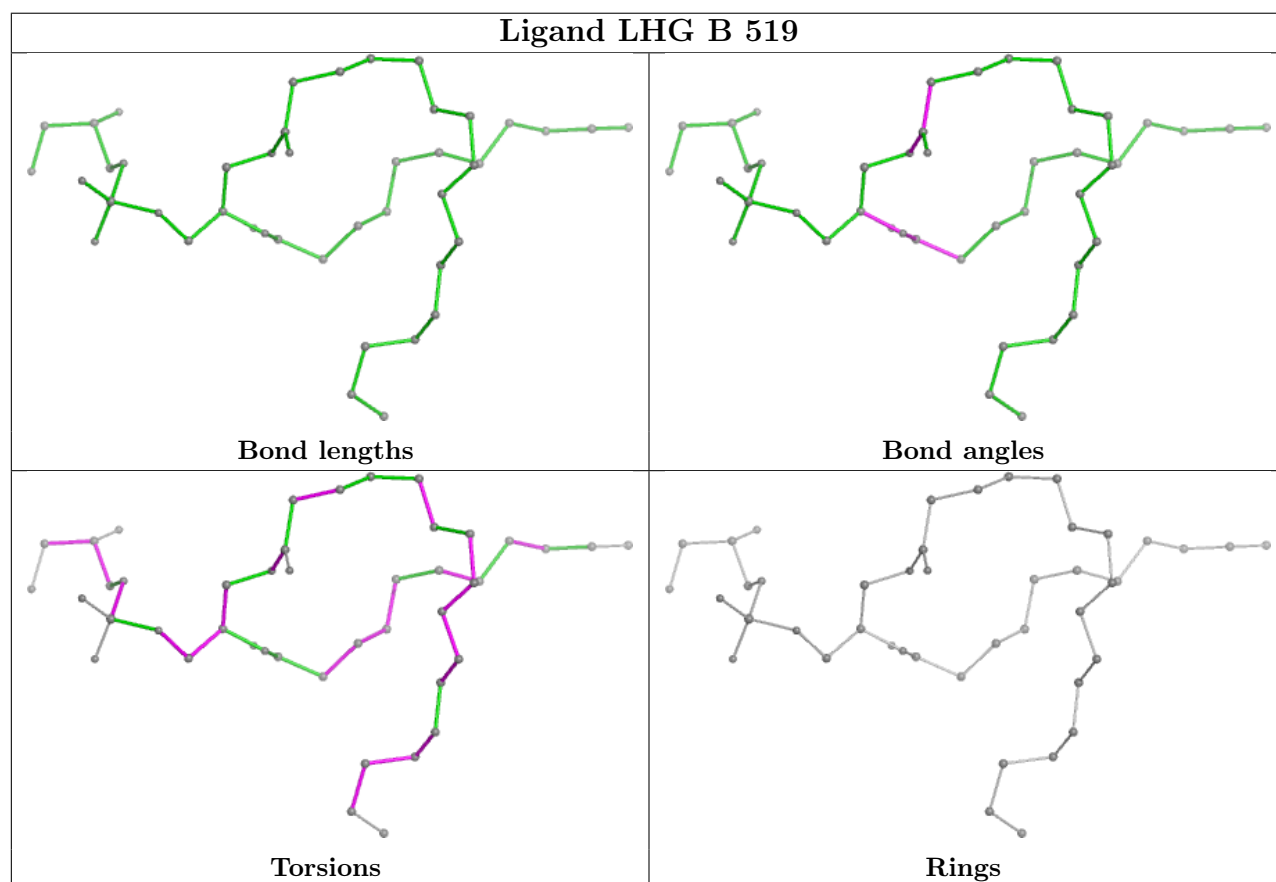
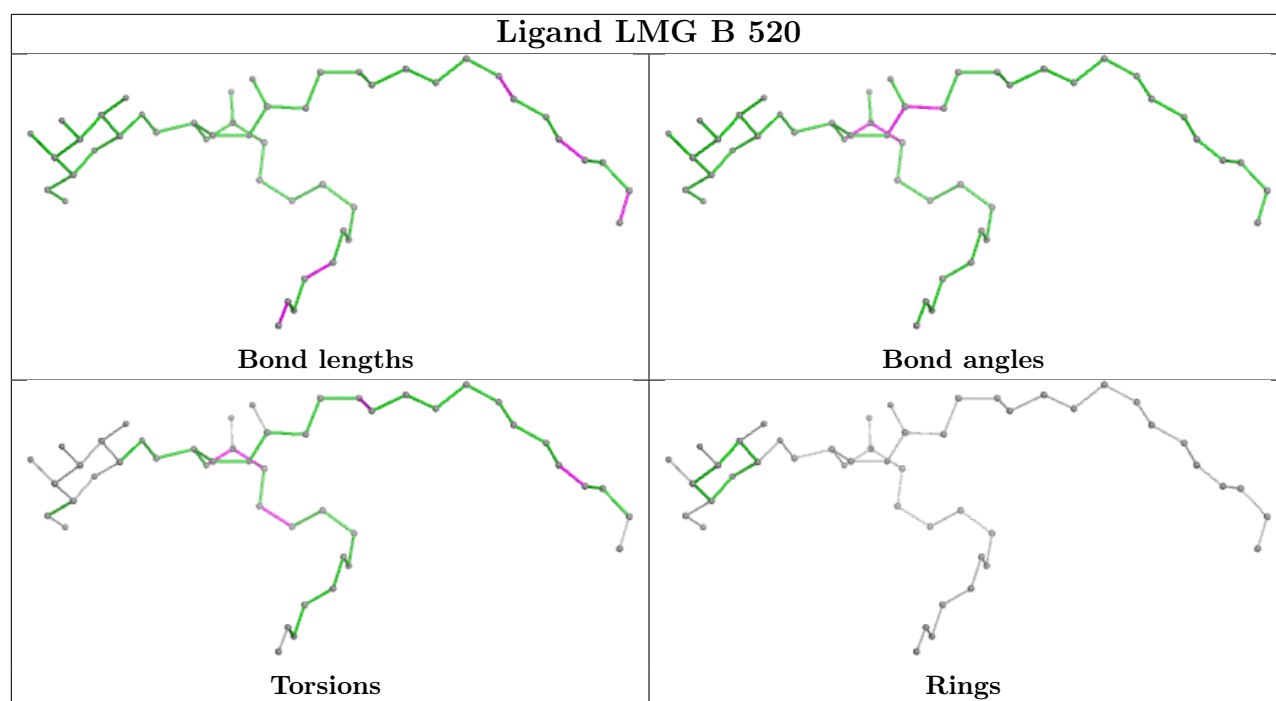


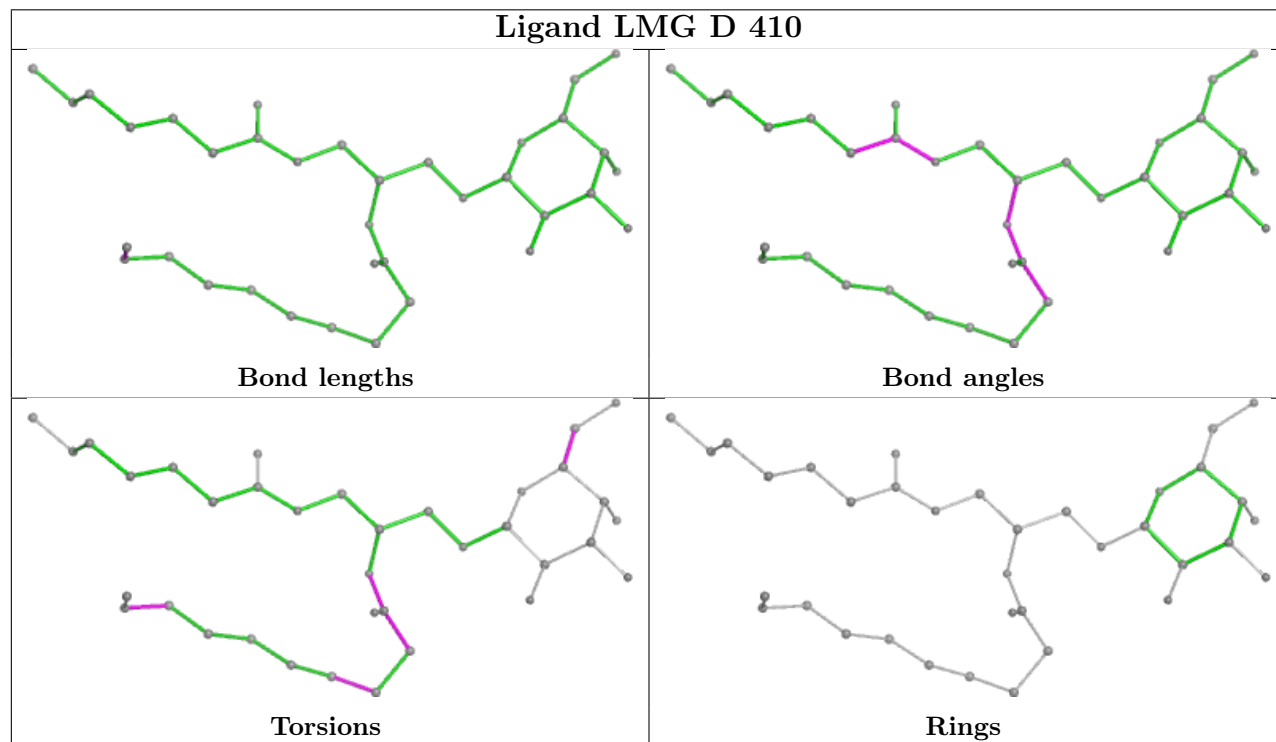
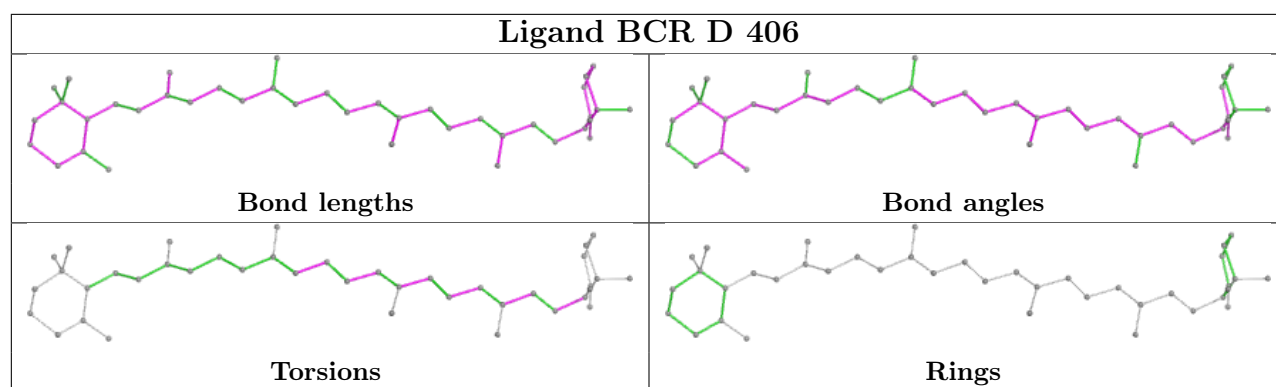
## Ligand CLA C 509



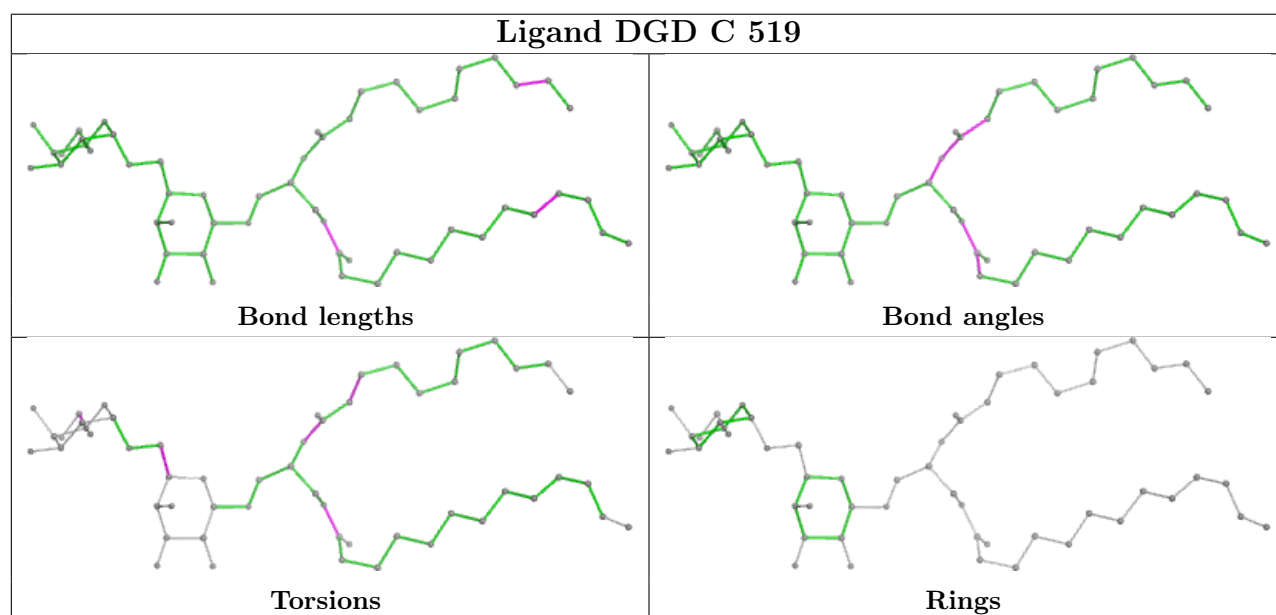
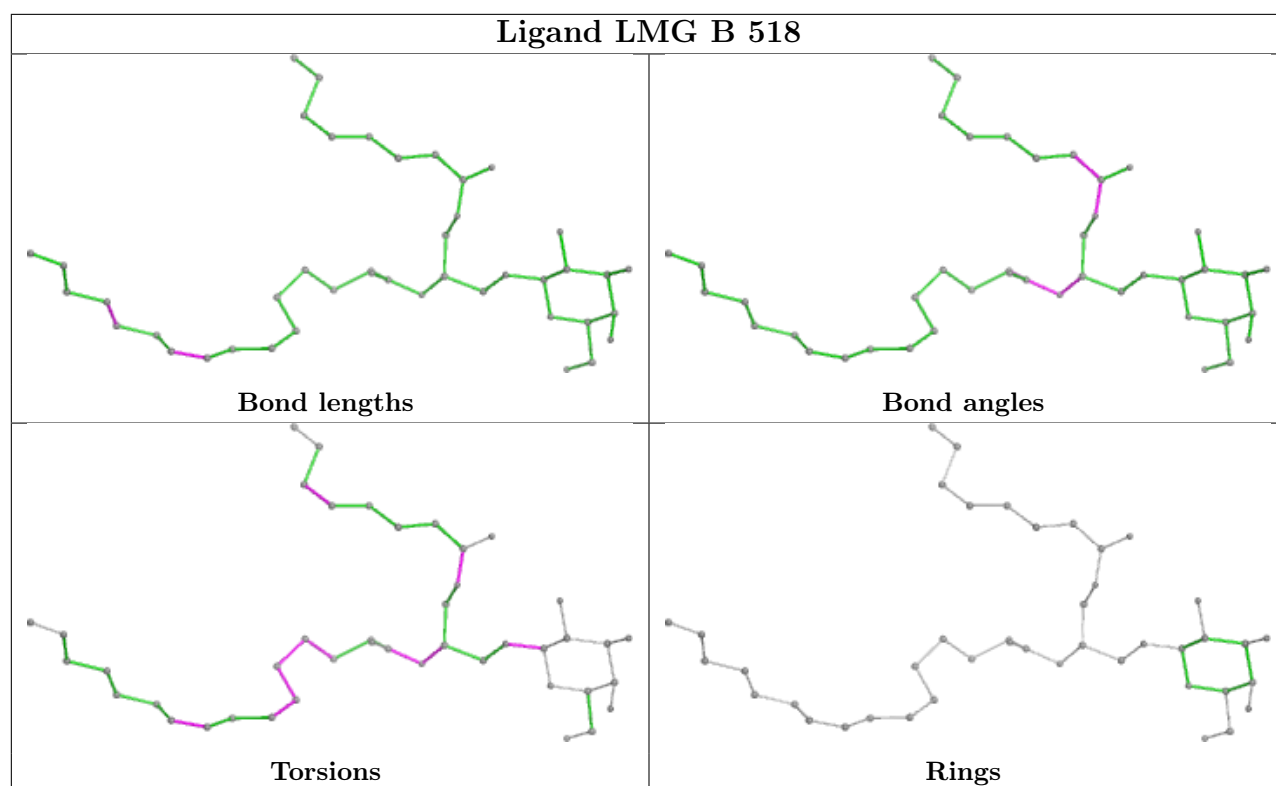


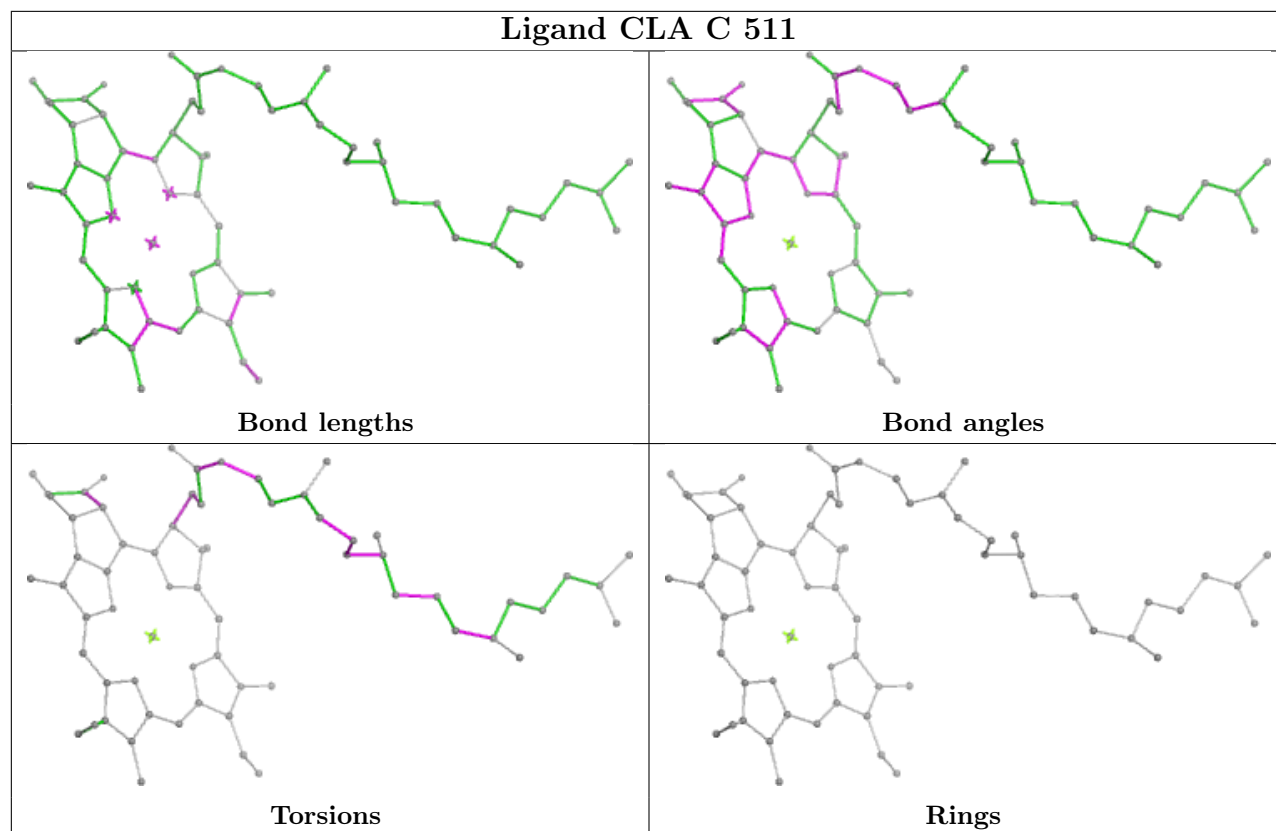


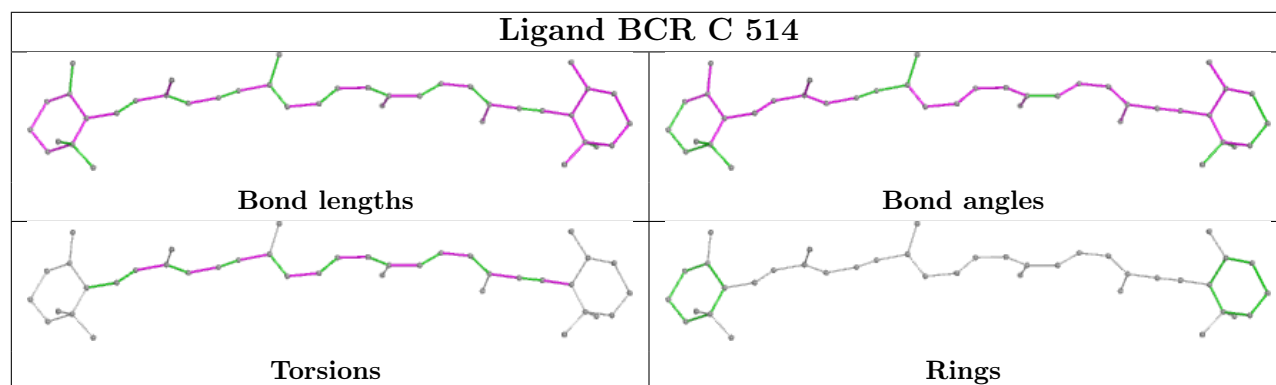
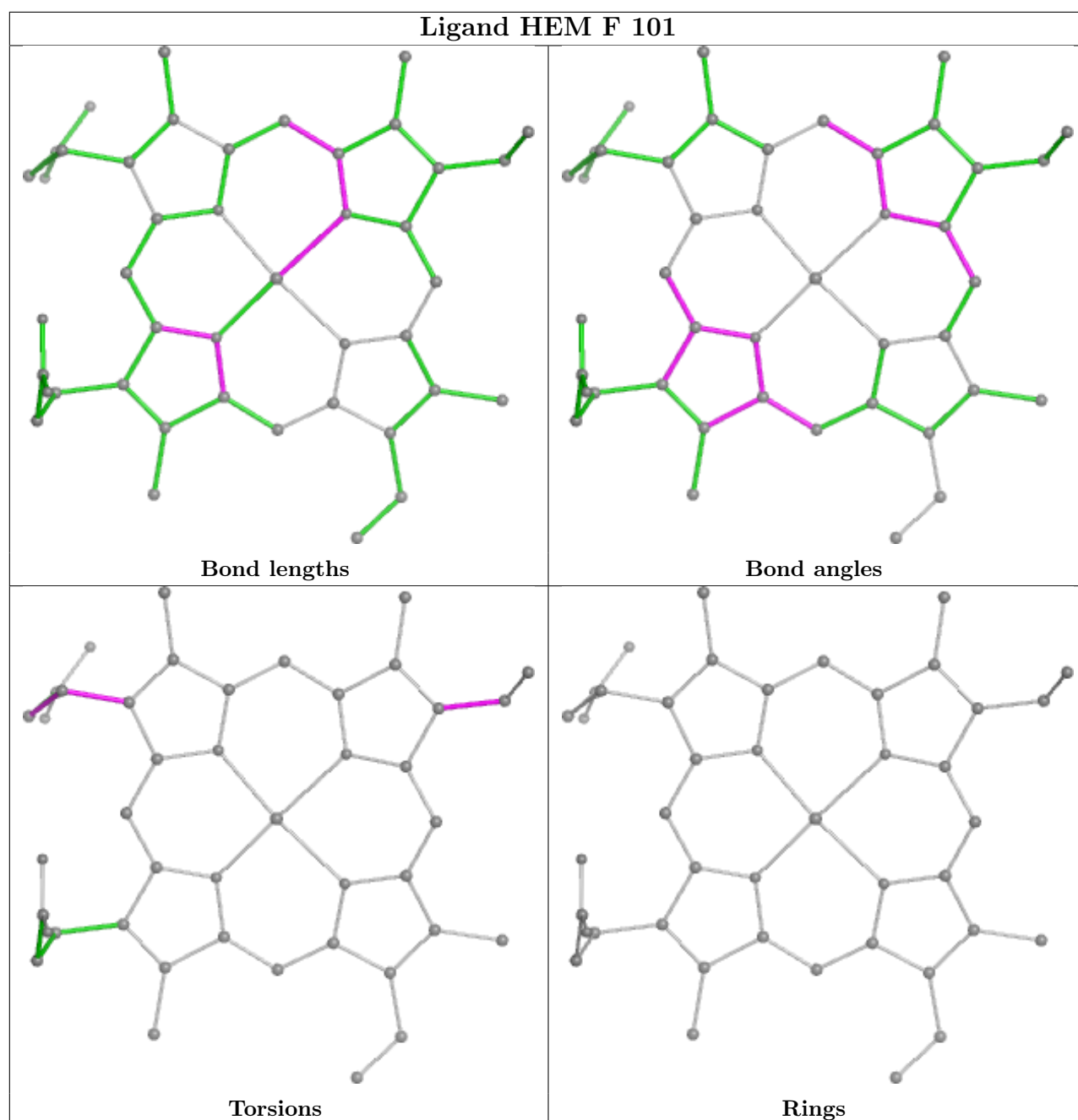


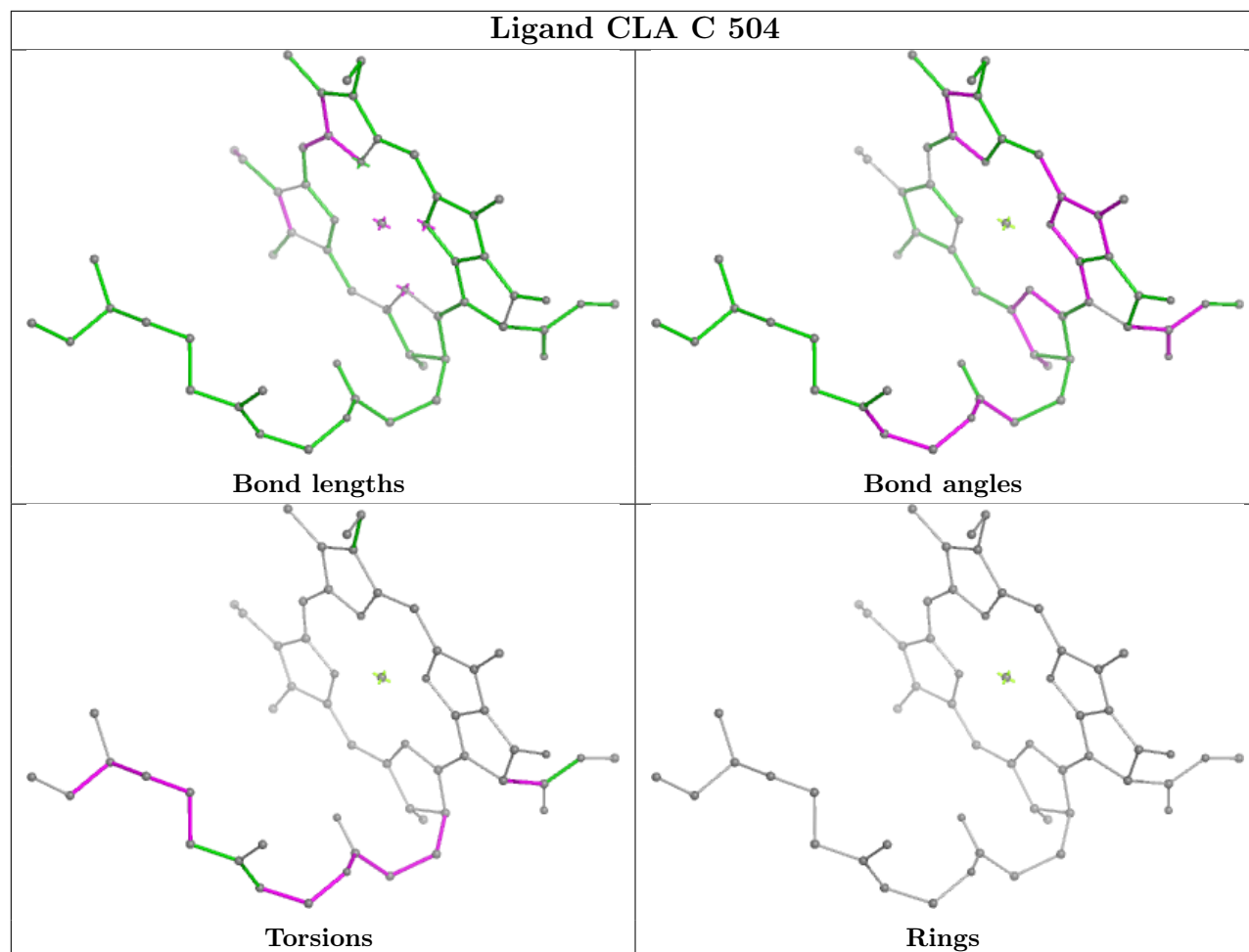
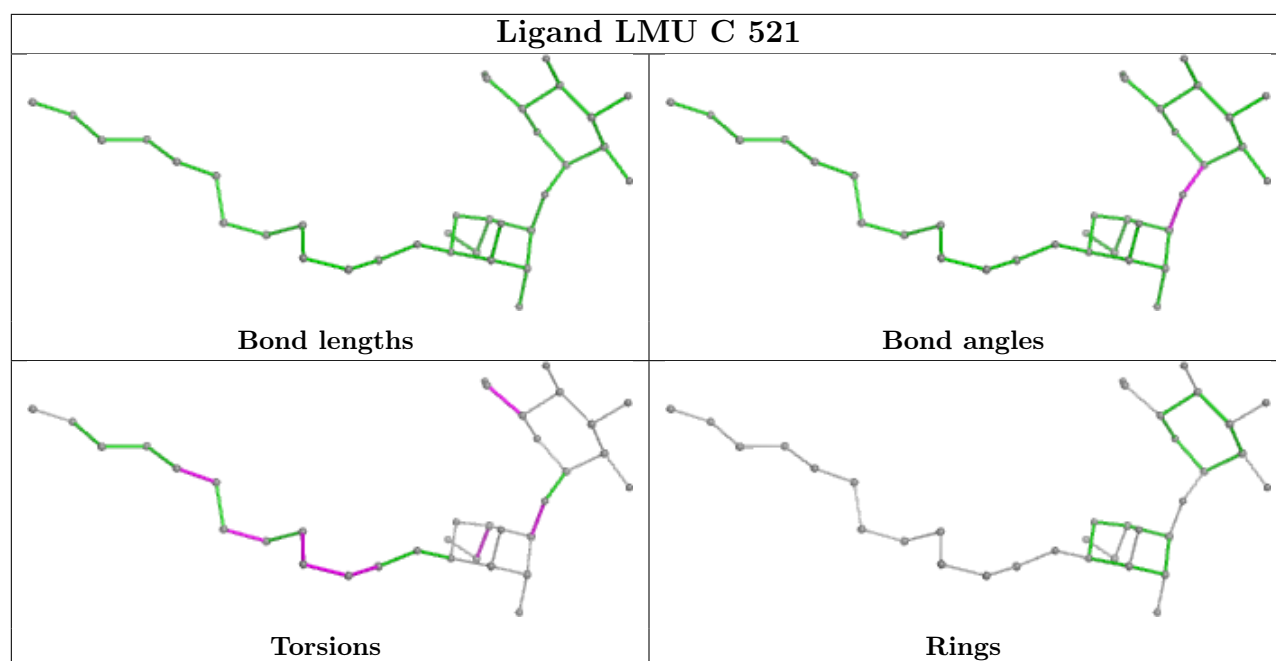


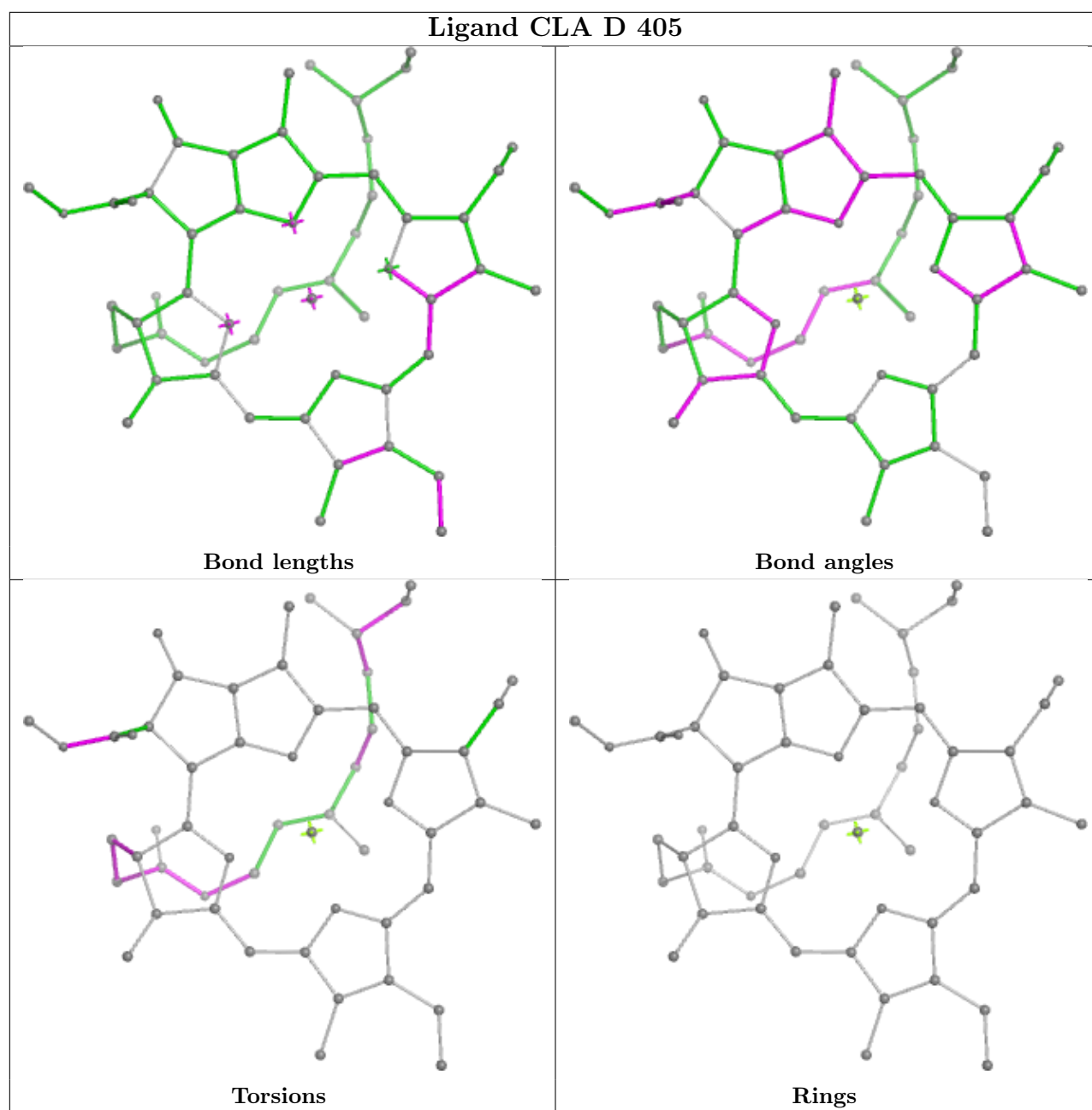


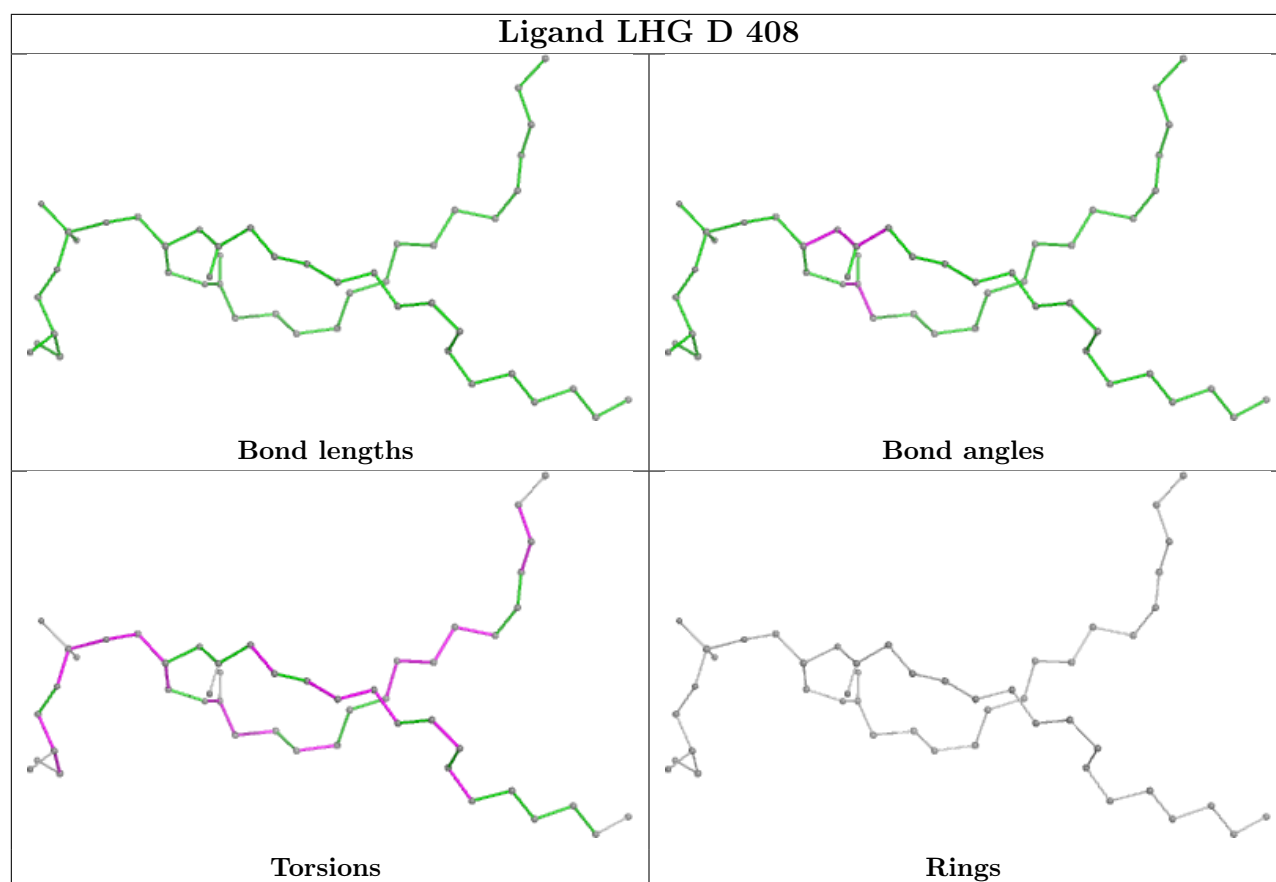


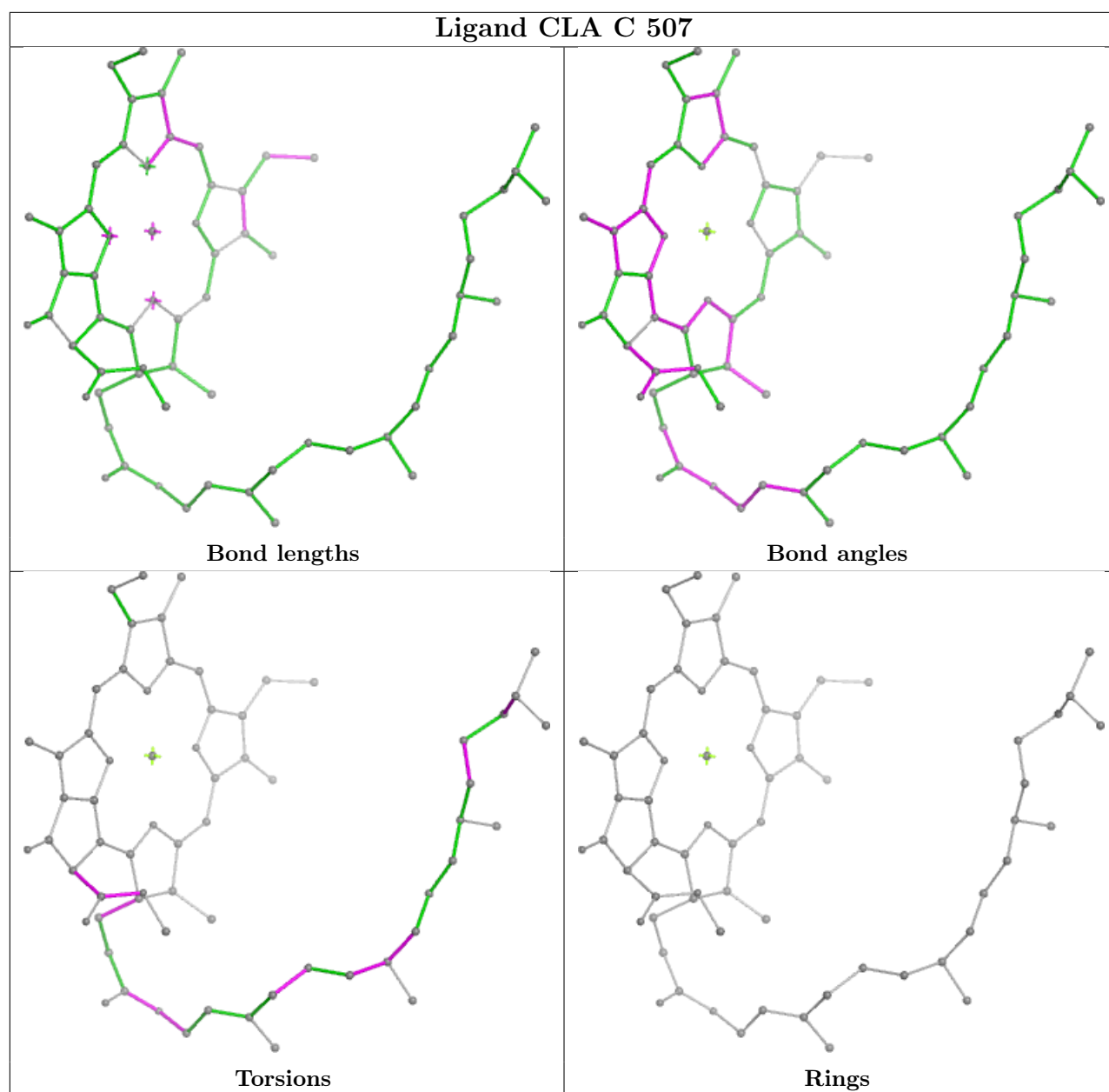




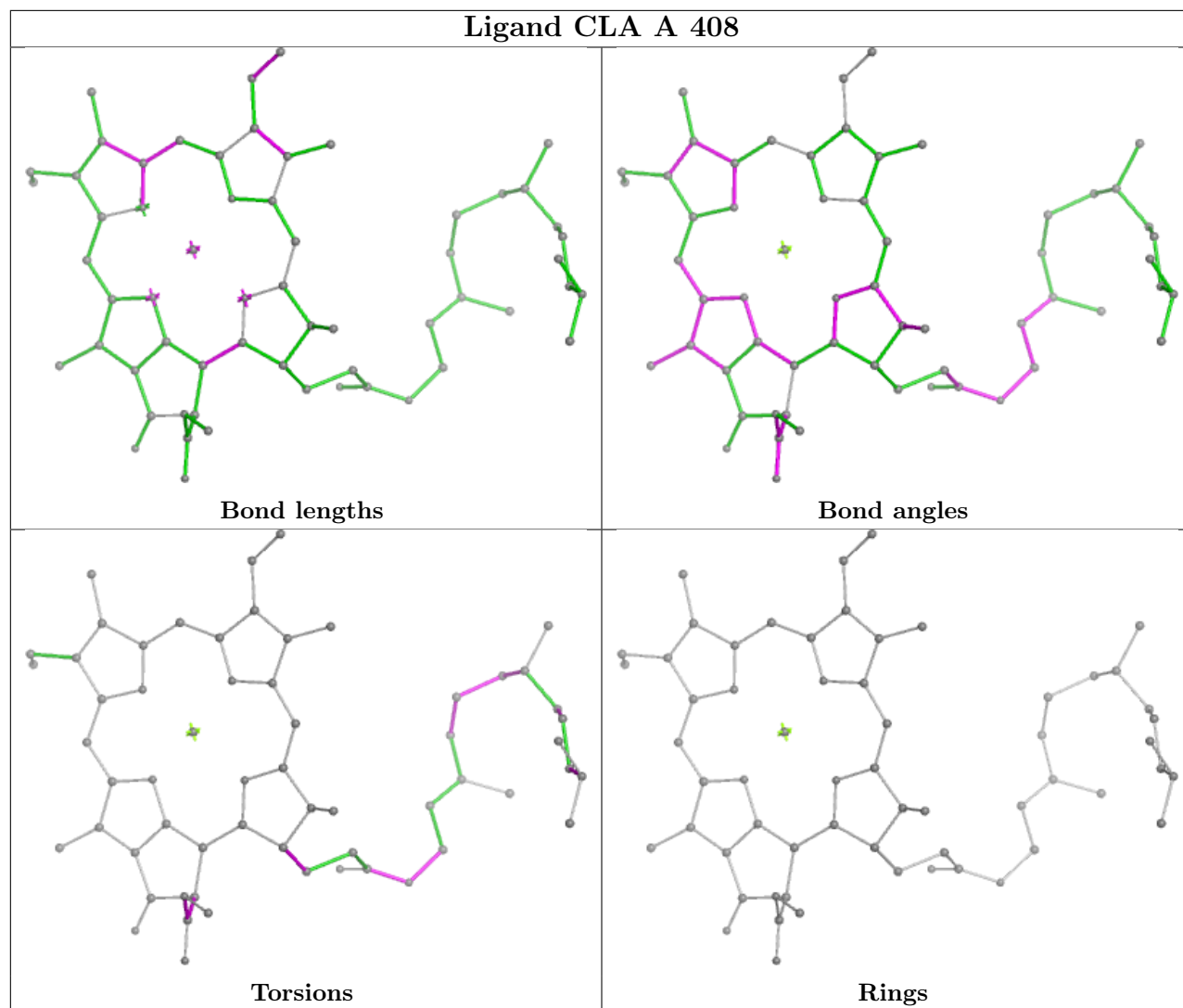




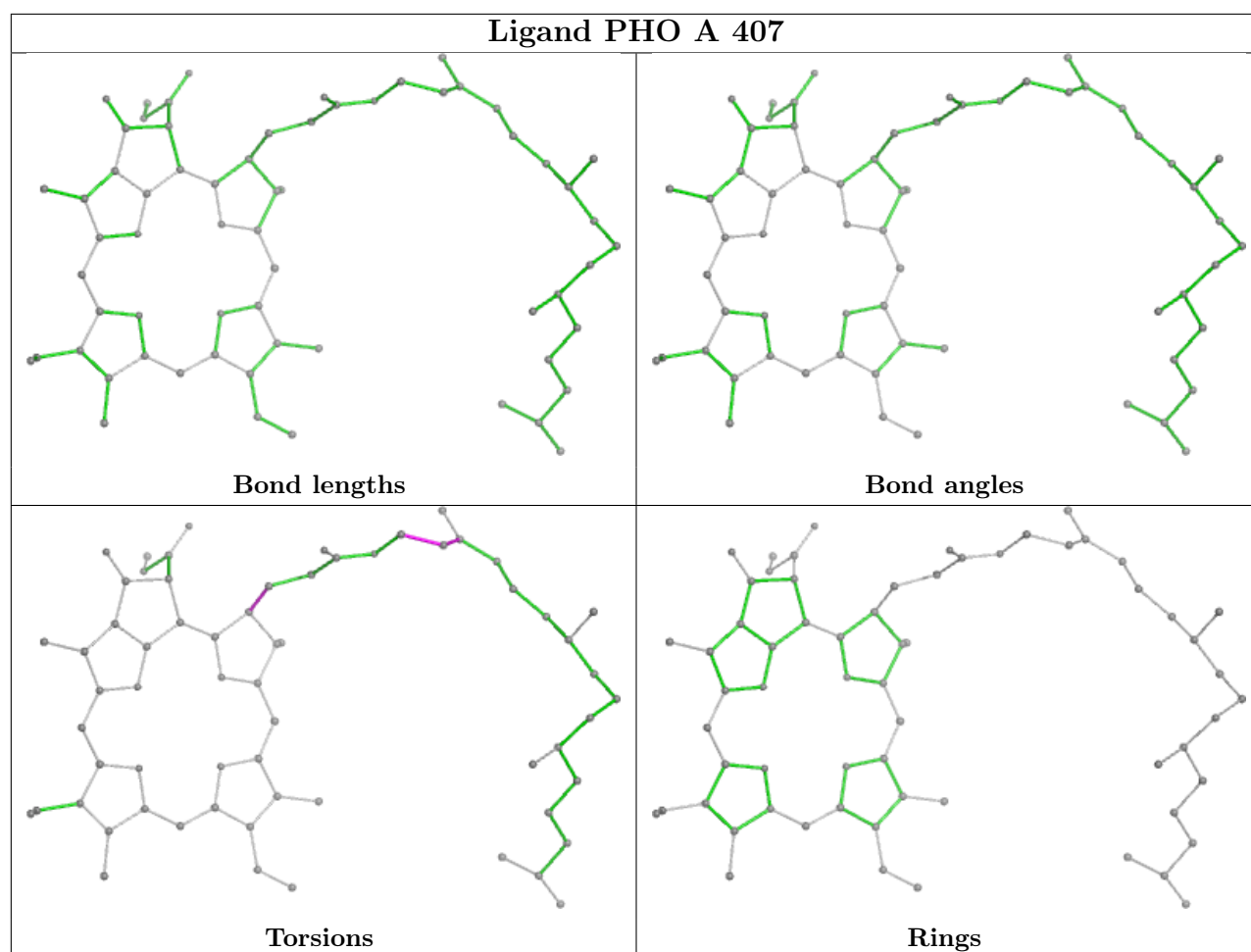


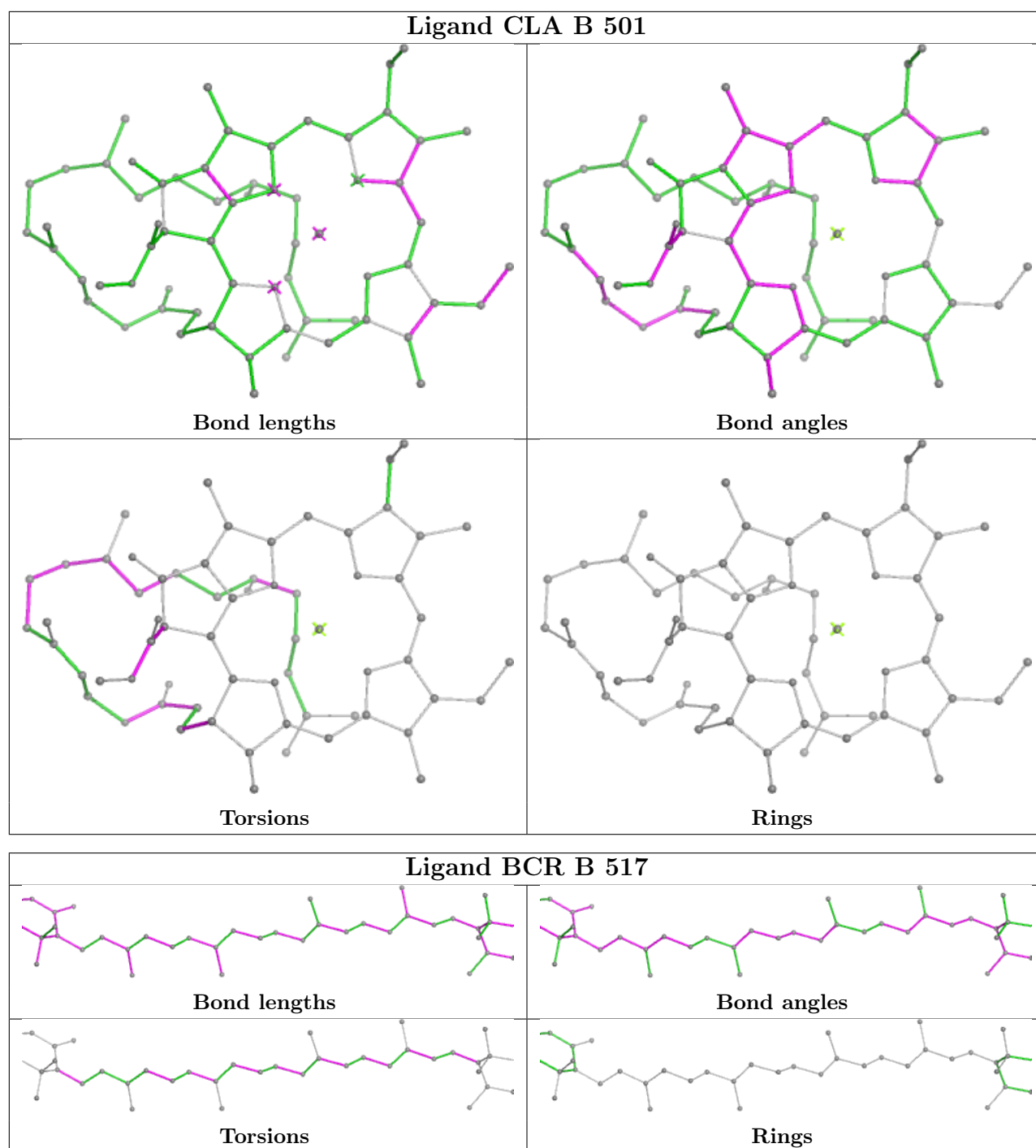


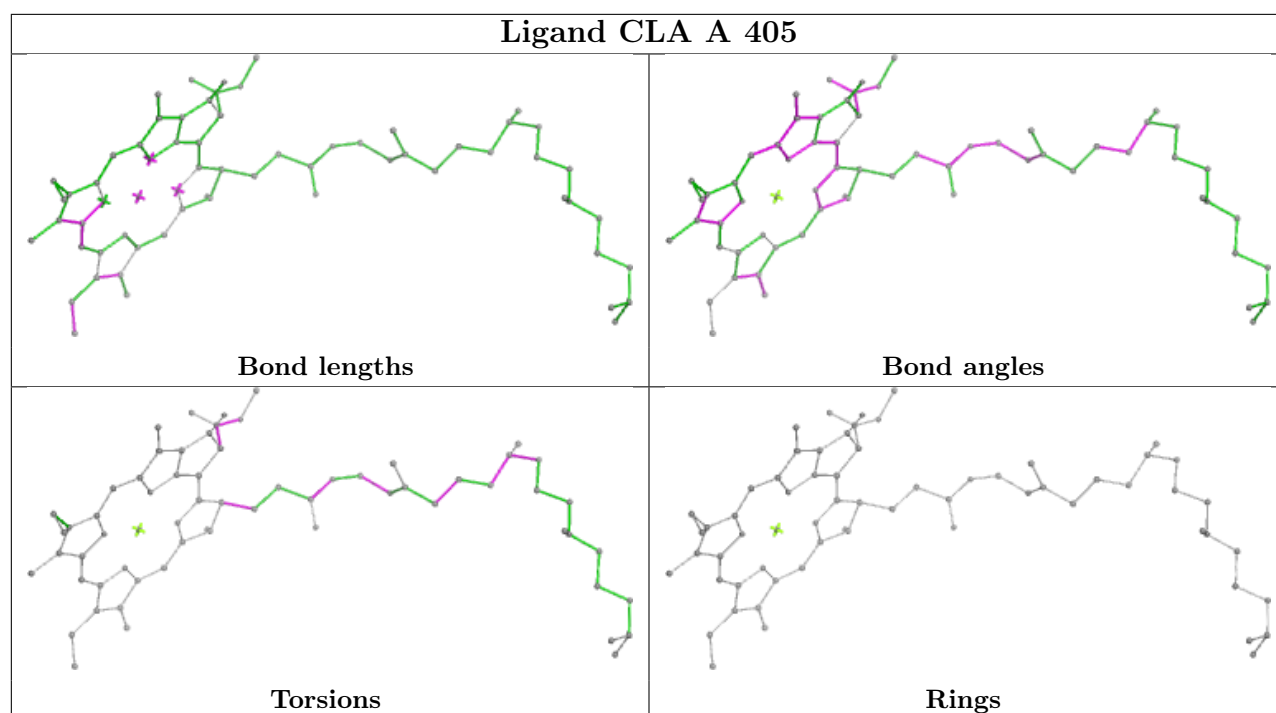
## Ligand CLA A 408

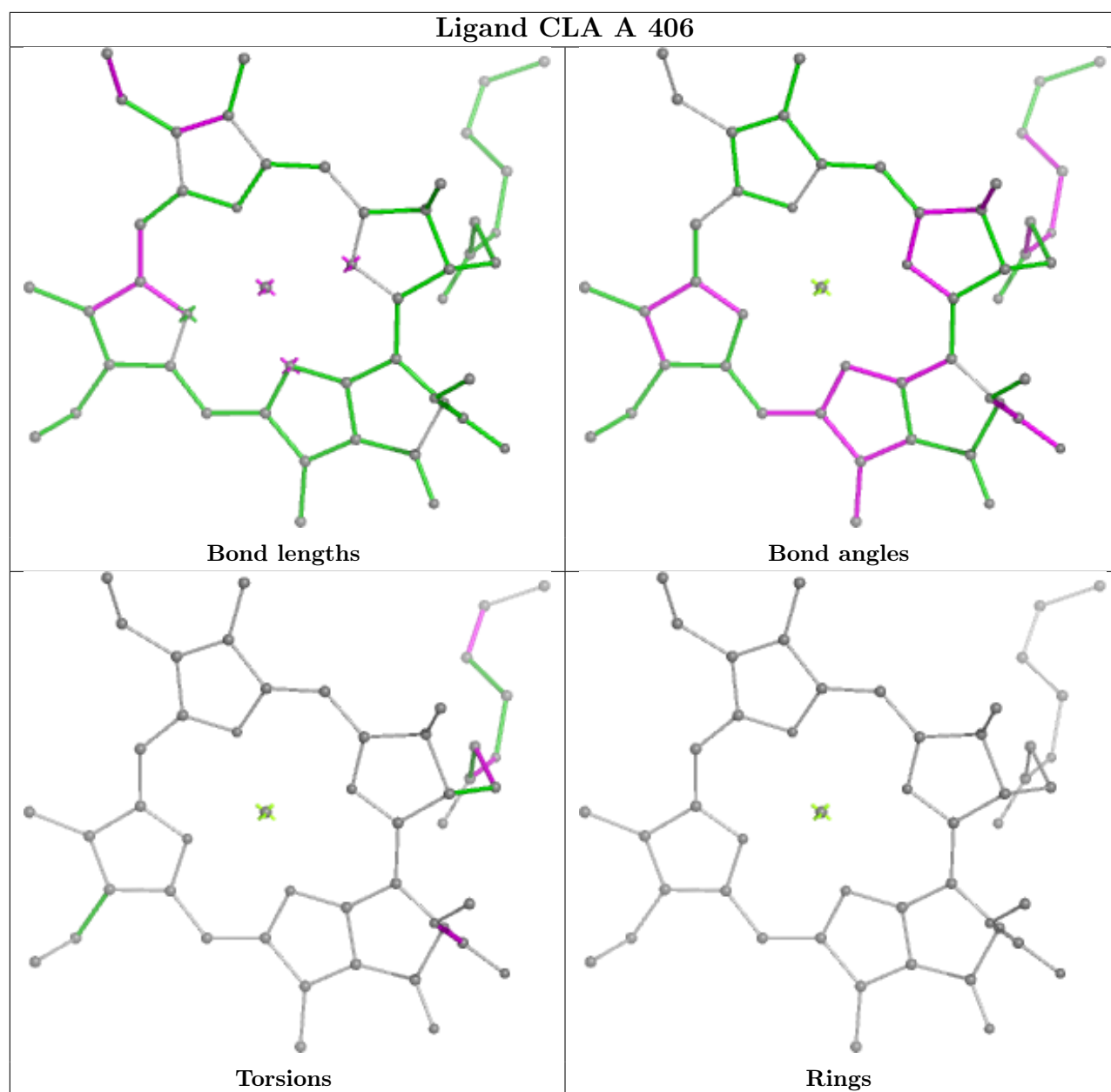




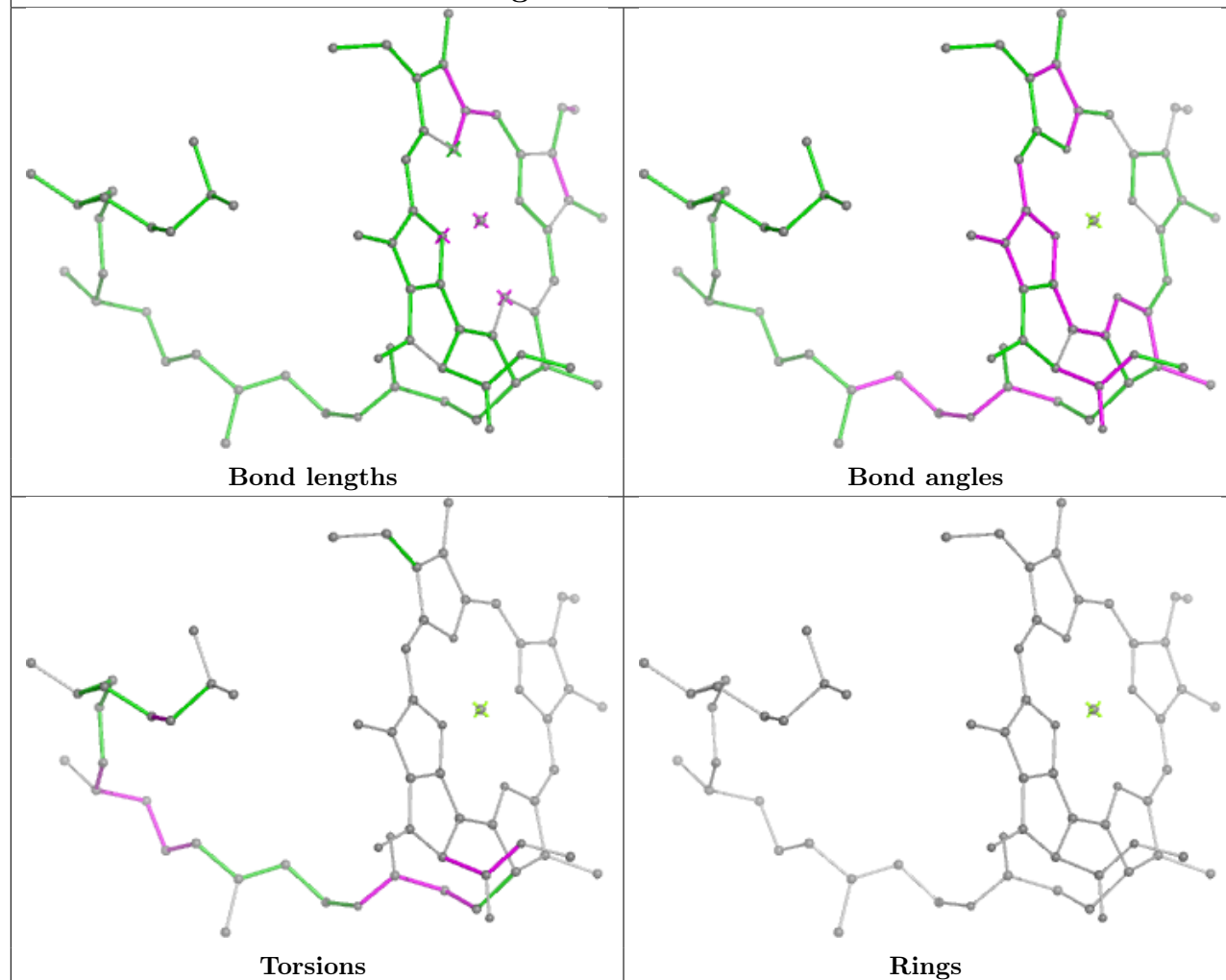




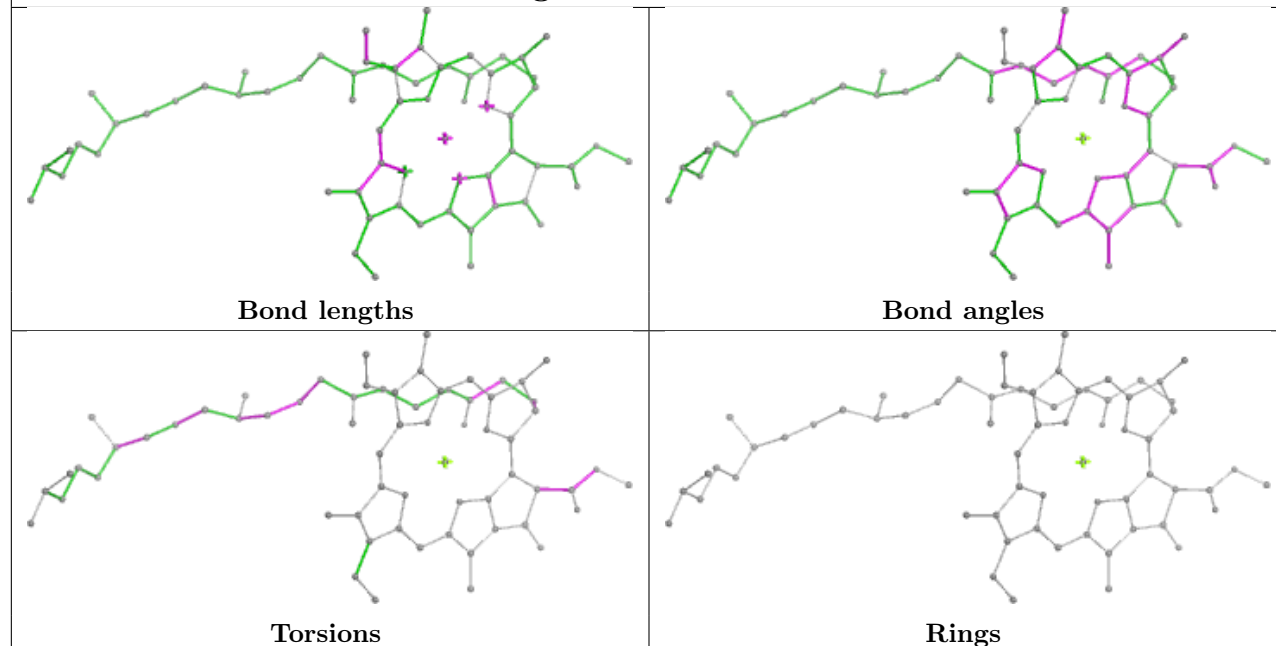


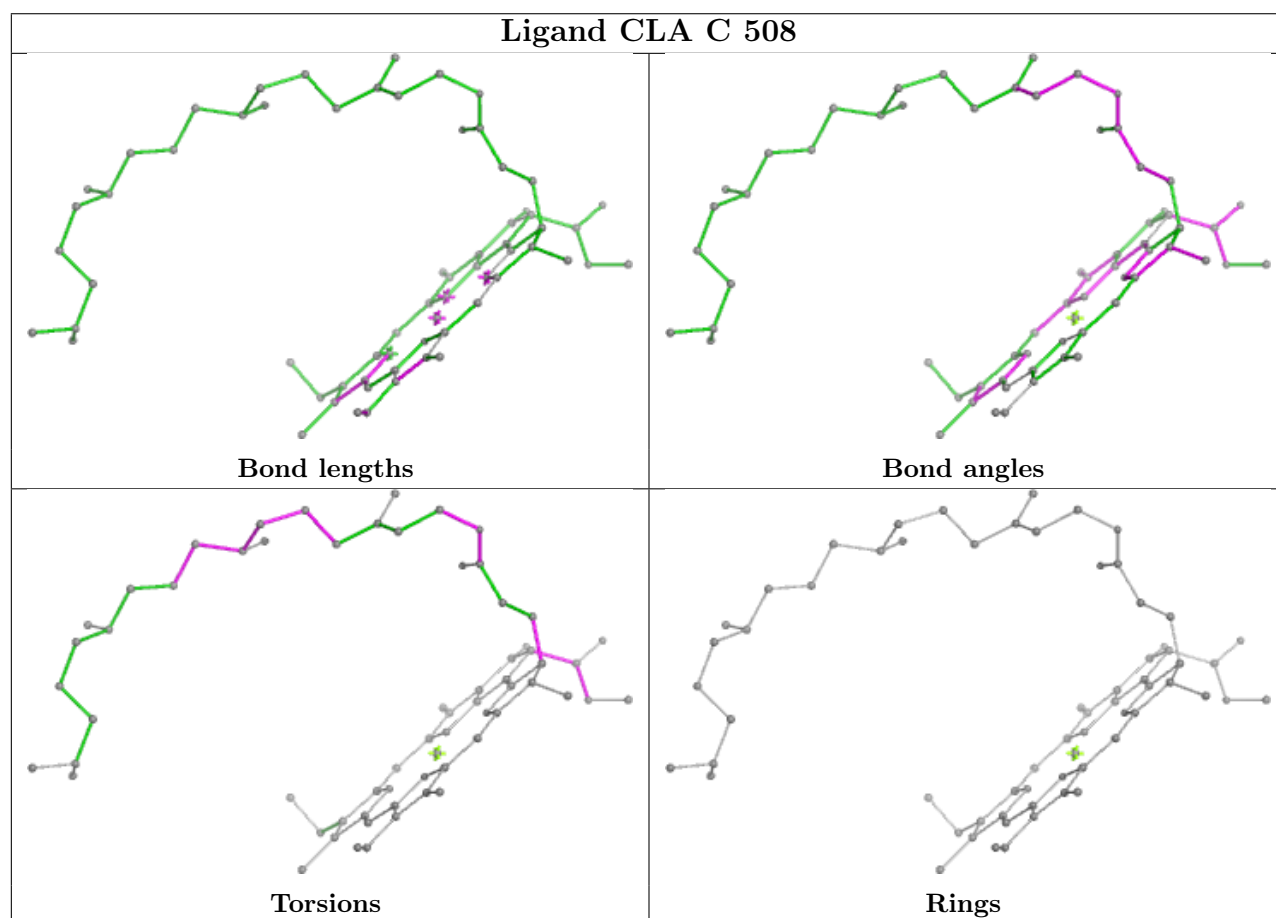
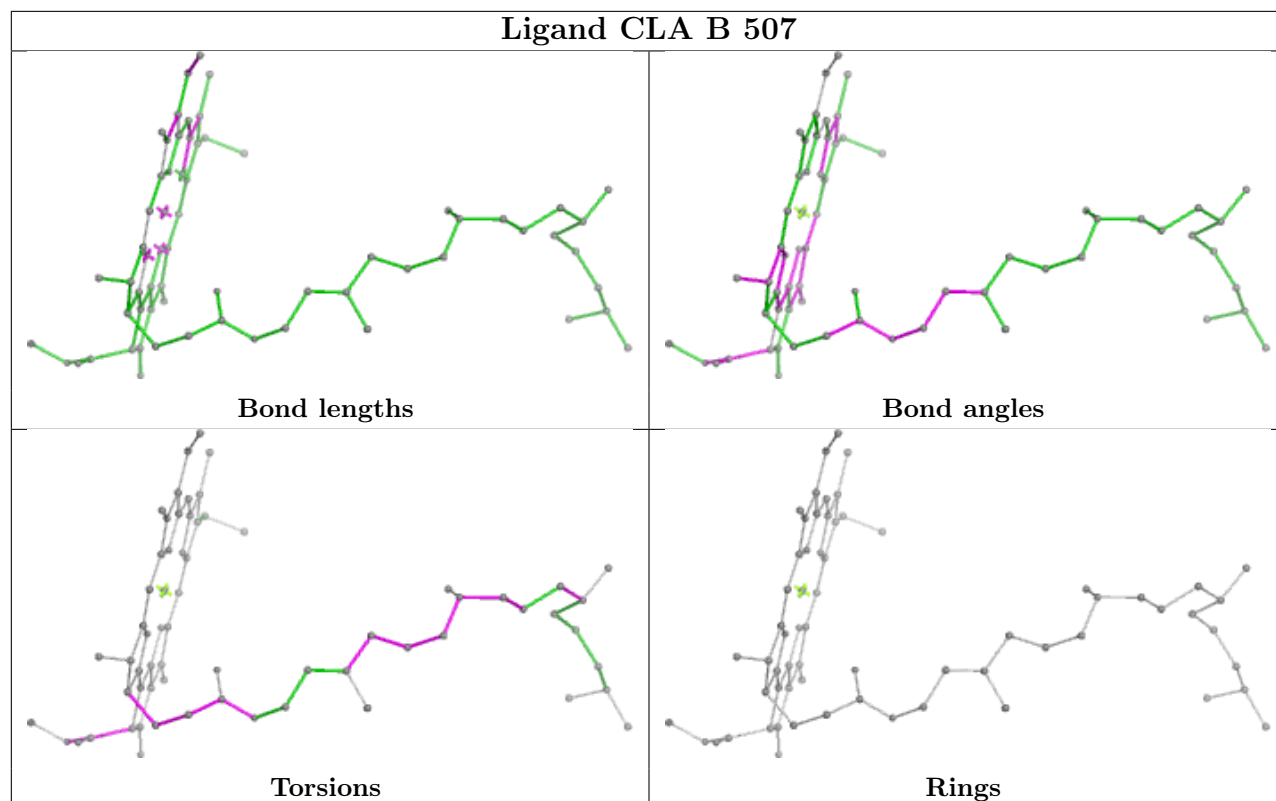


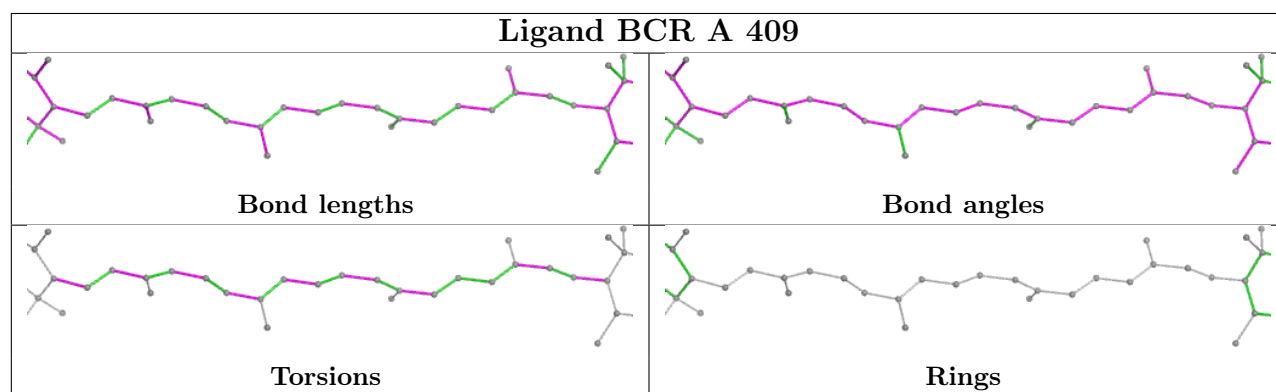
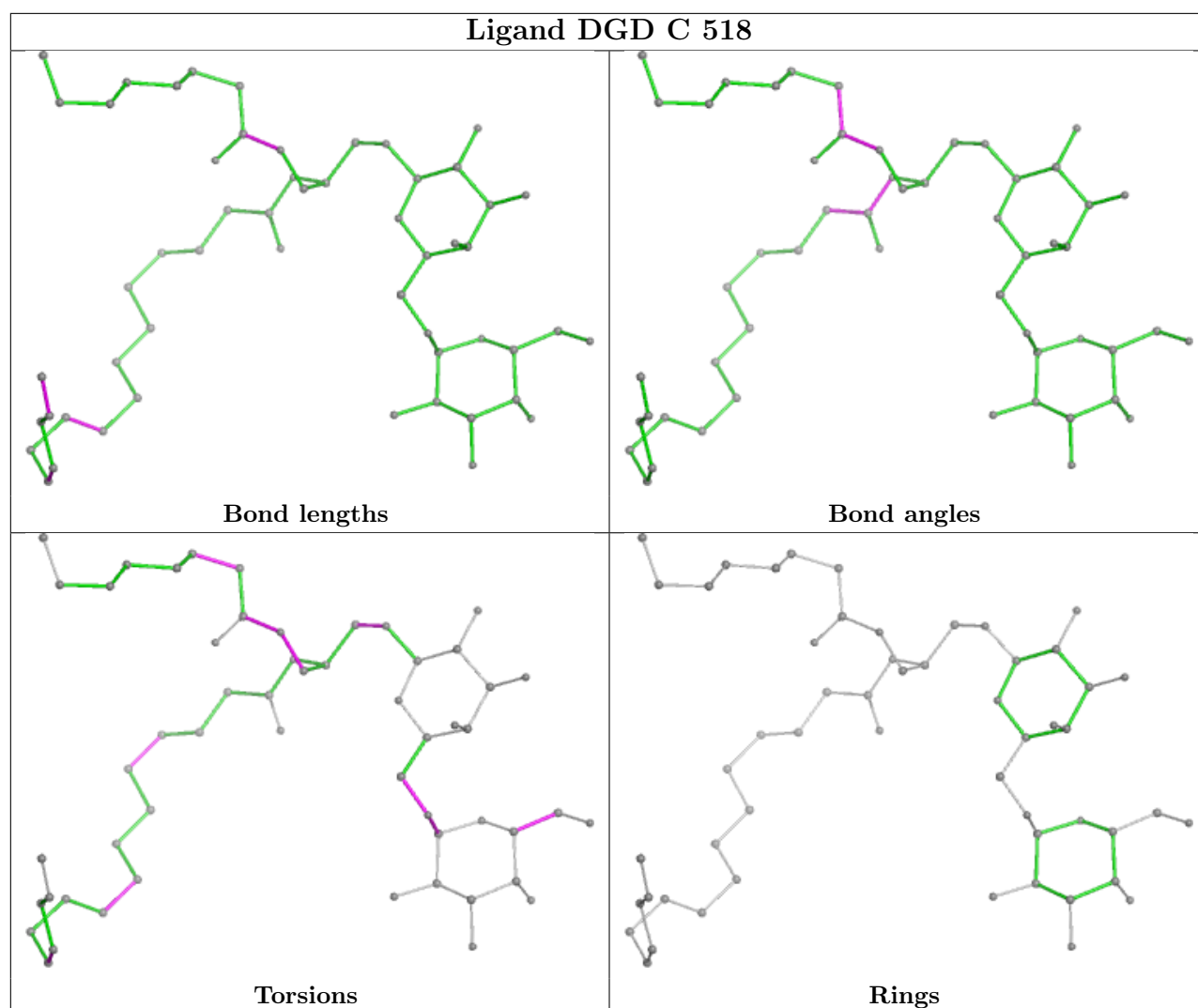
## Ligand CLA C 503

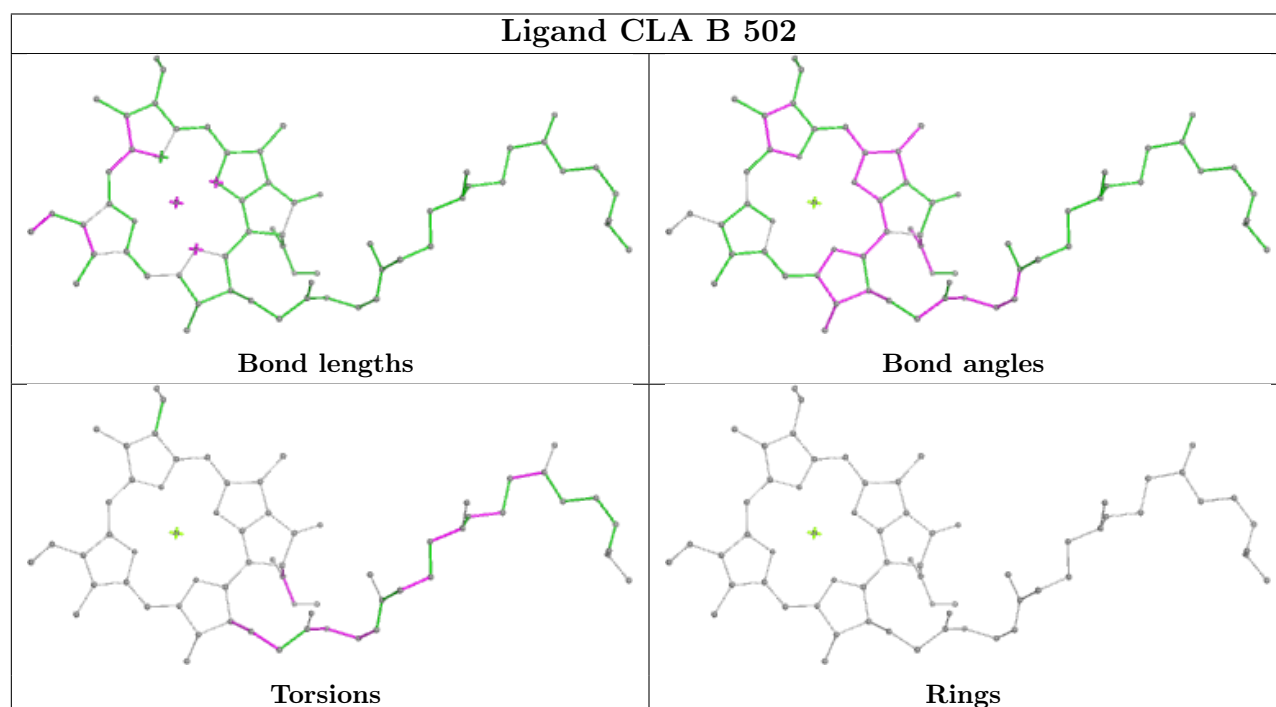
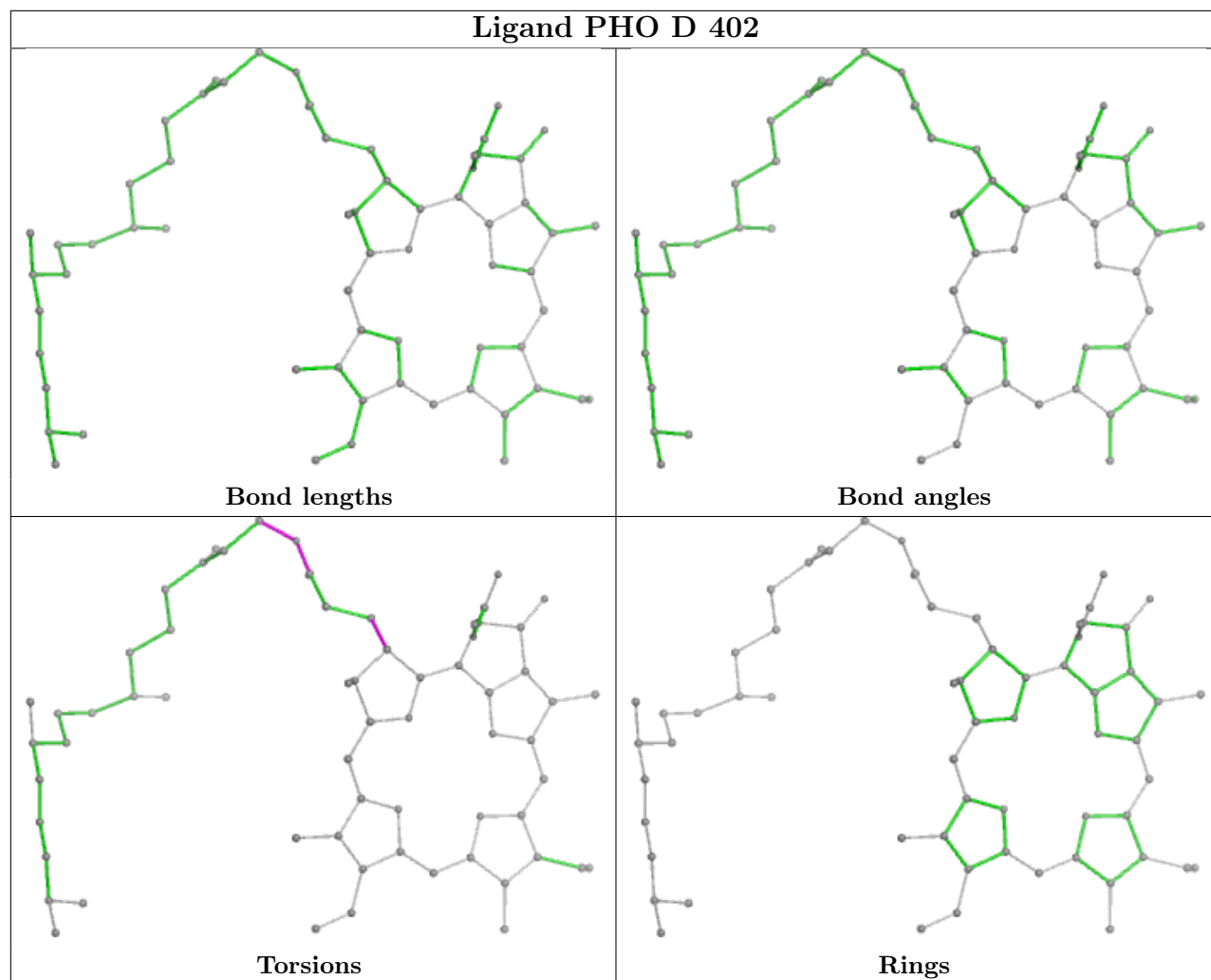


## Ligand CLA B 508

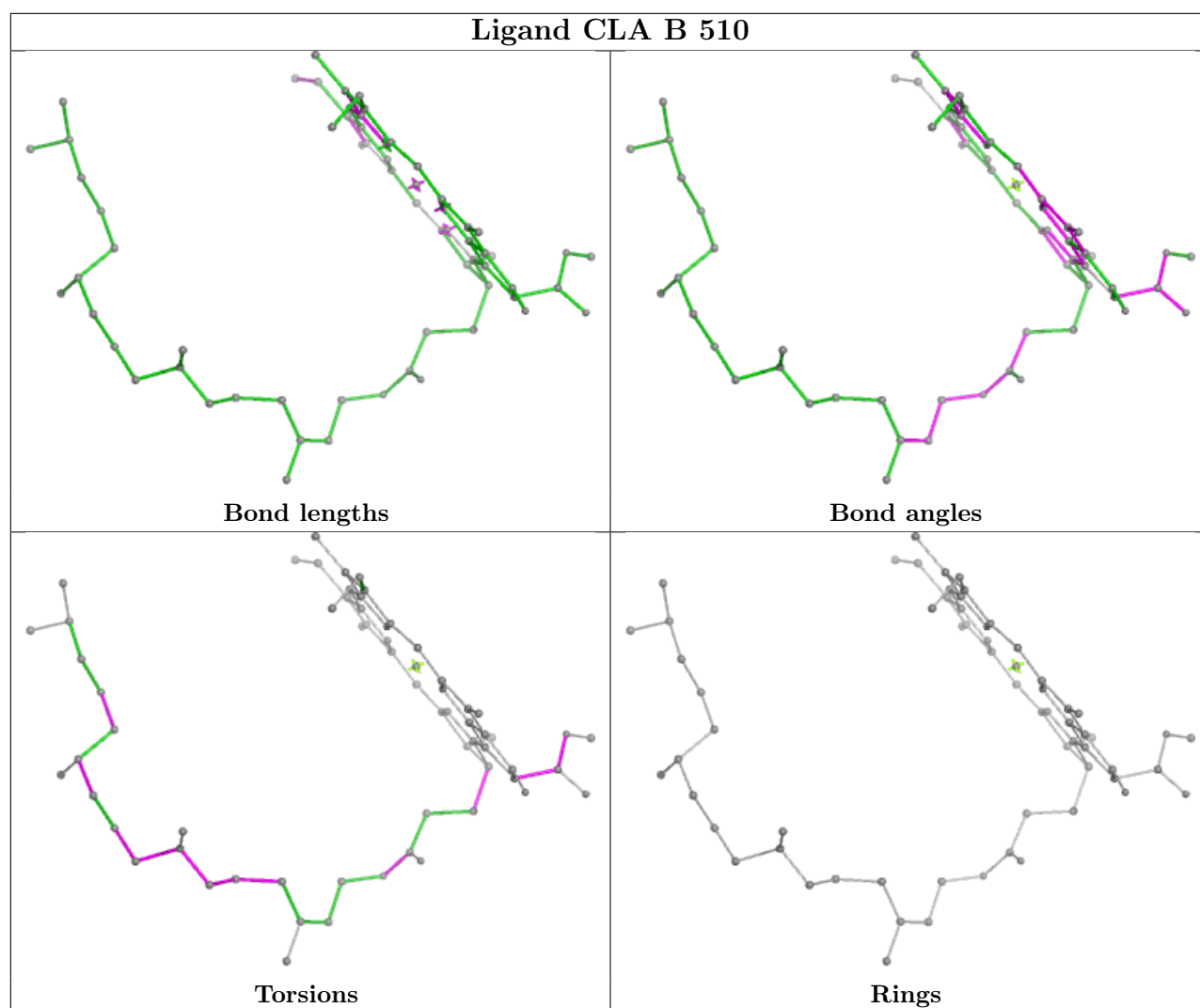


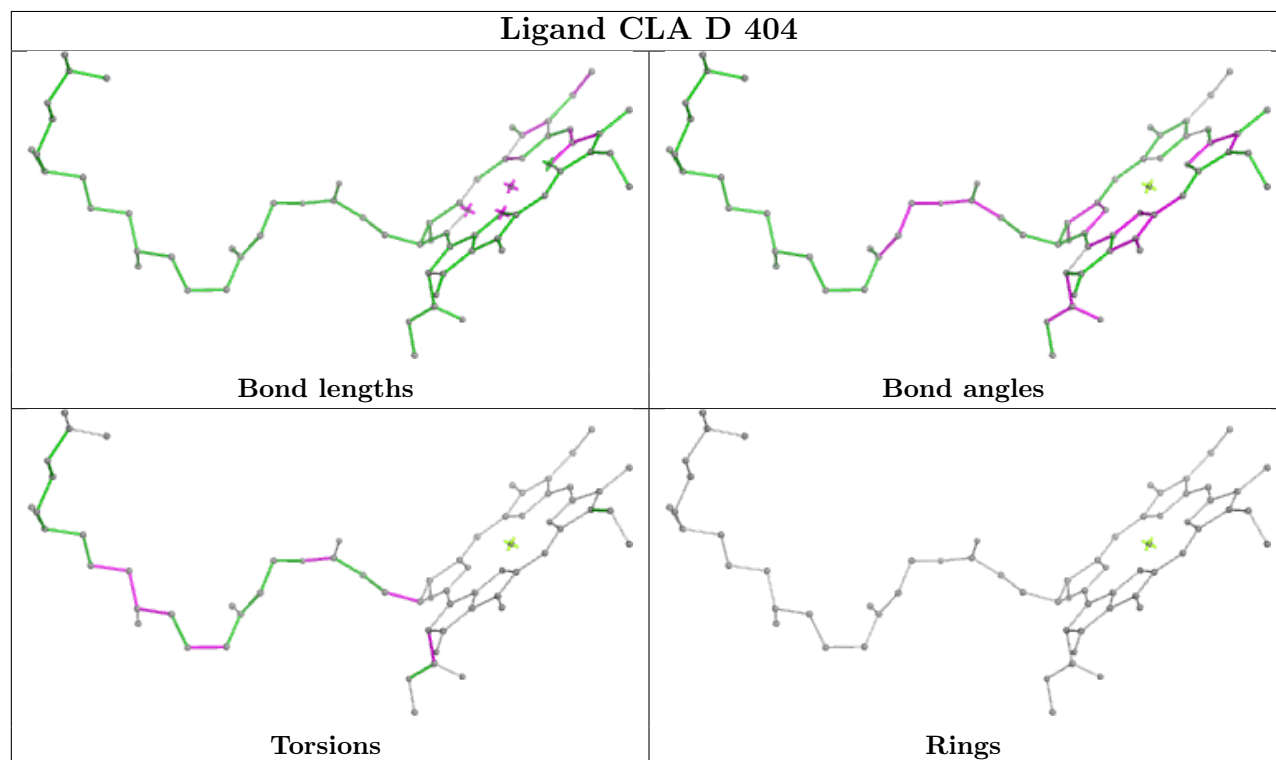
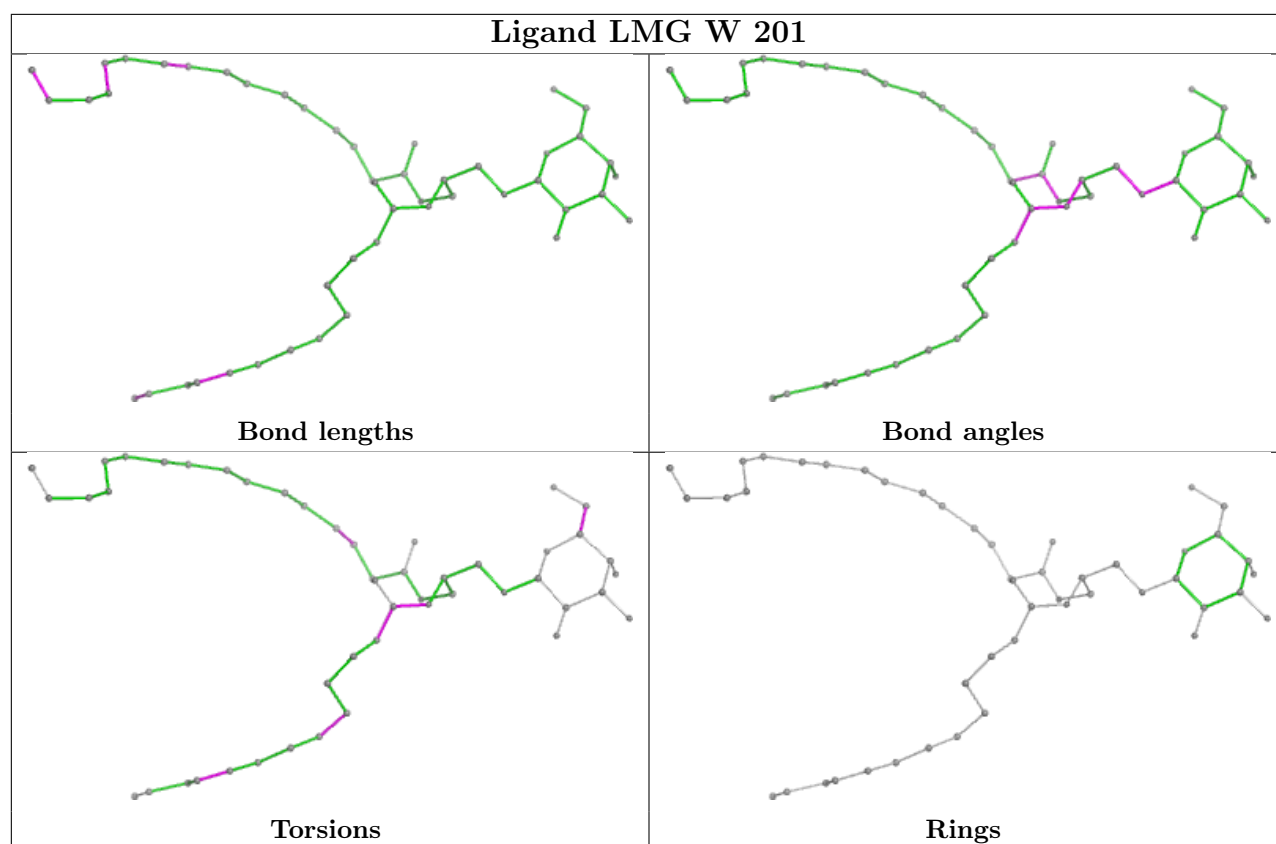


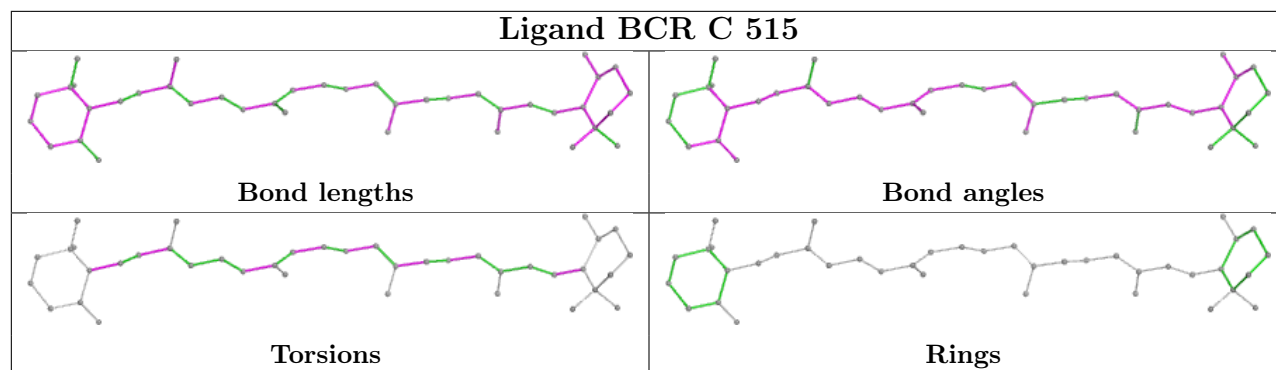












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

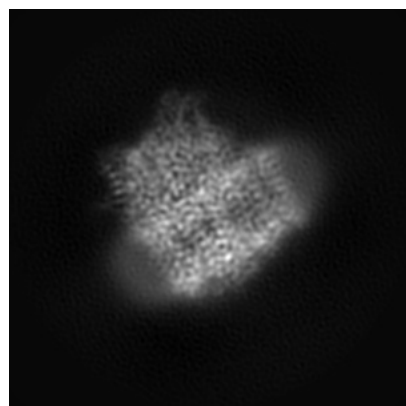
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52077. These allow visual inspection of the internal detail of the map and identification of artifacts.

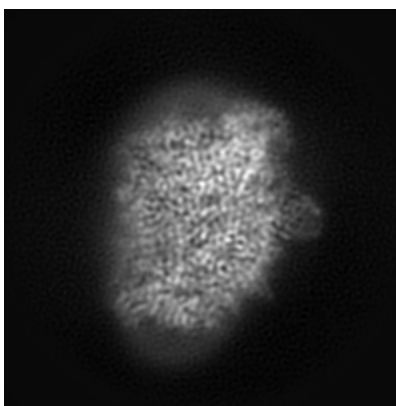
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

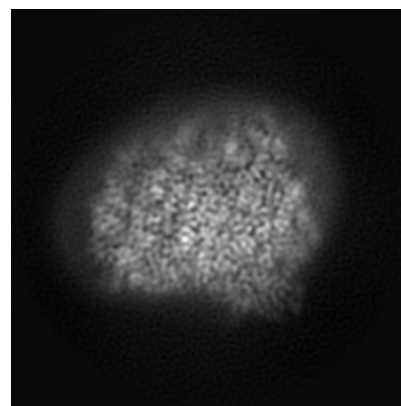
#### 6.1.1 Primary map



X

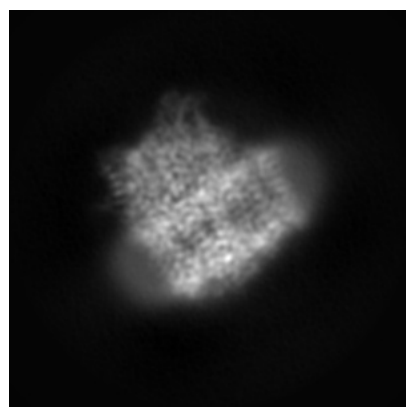


Y

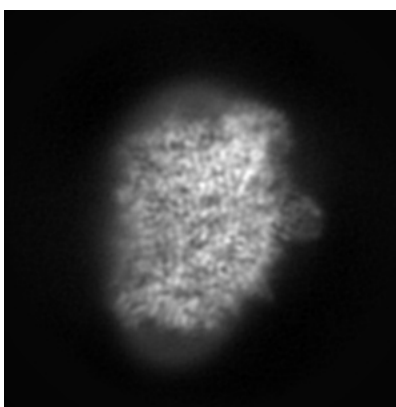


Z

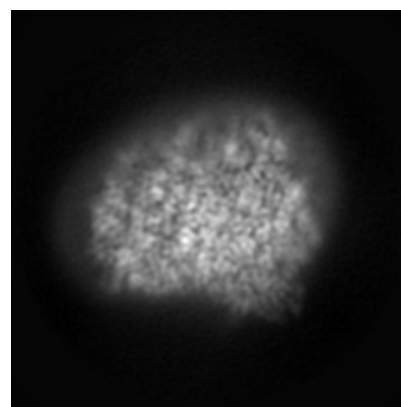
#### 6.1.2 Raw map



X



Y

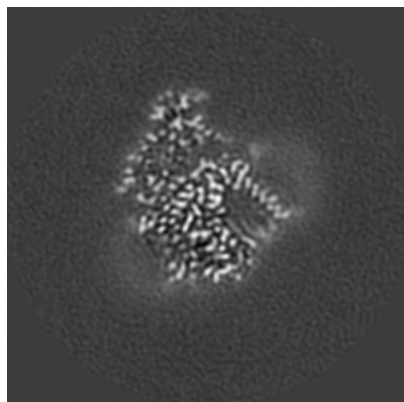


Z

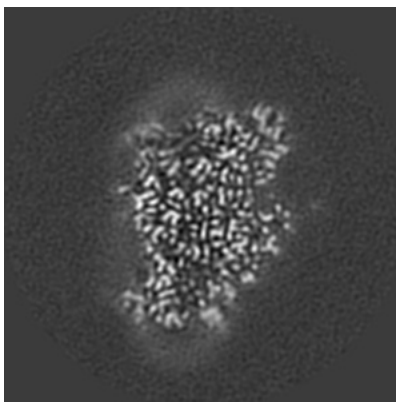
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

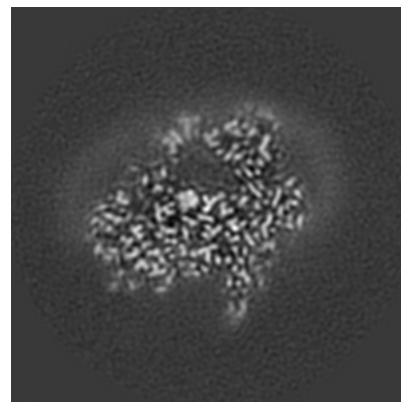
### 6.2.1 Primary map



X Index: 125

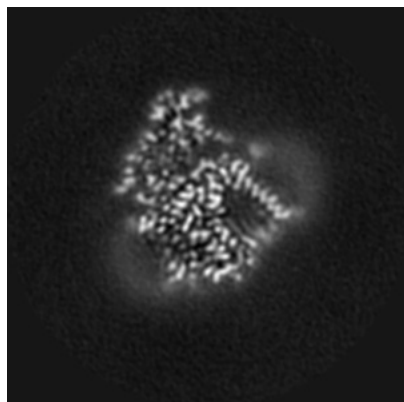


Y Index: 125

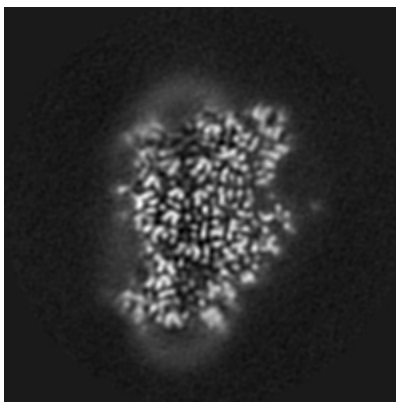


Z Index: 125

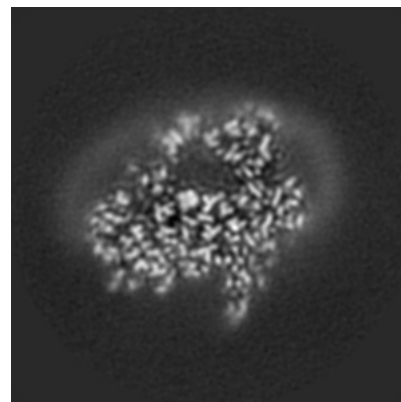
### 6.2.2 Raw map



X Index: 125



Y Index: 125

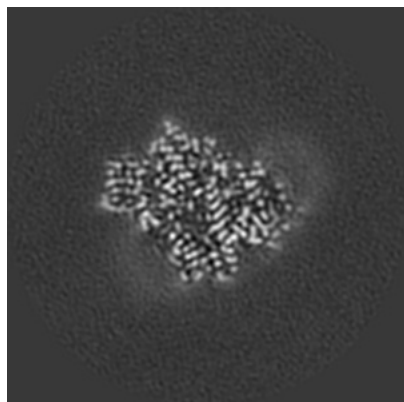


Z Index: 125

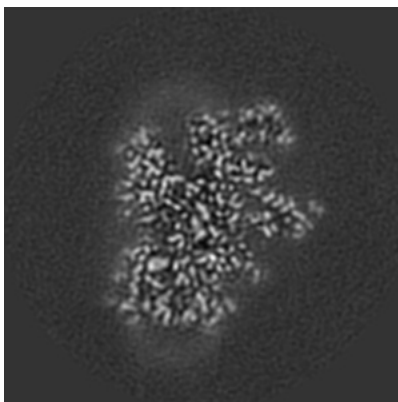
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

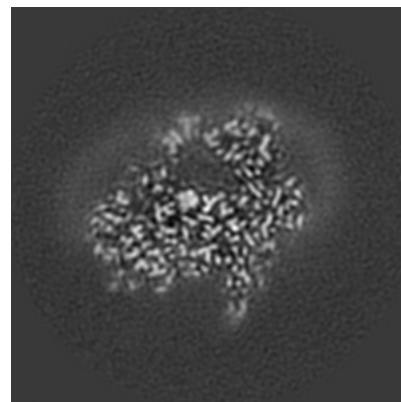
### 6.3.1 Primary map



X Index: 145

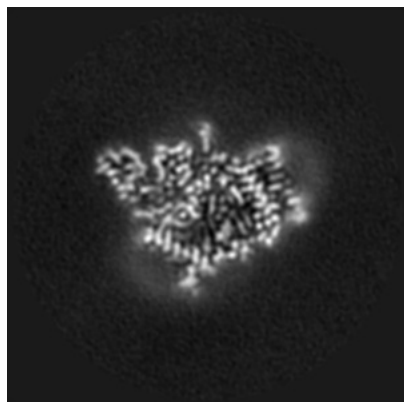


Y Index: 118

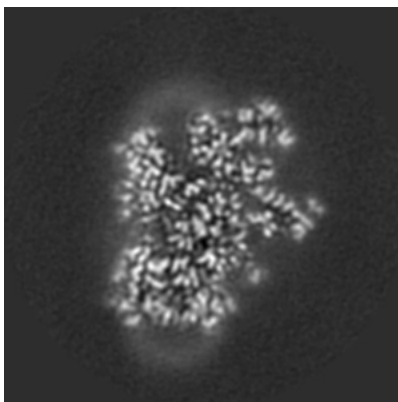


Z Index: 125

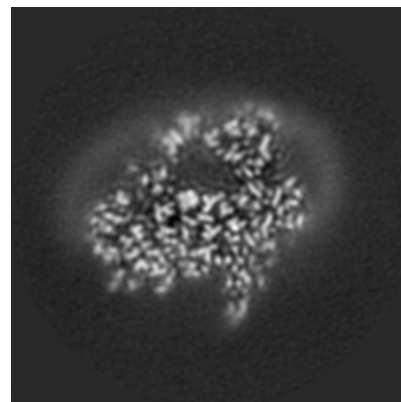
### 6.3.2 Raw map



X Index: 159



Y Index: 117

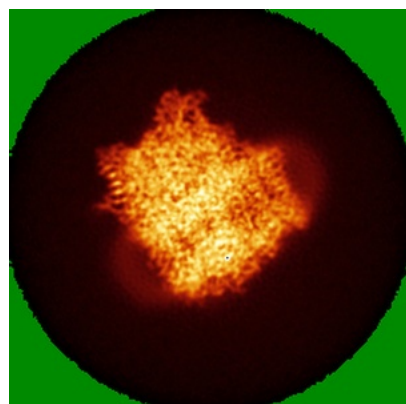


Z Index: 125

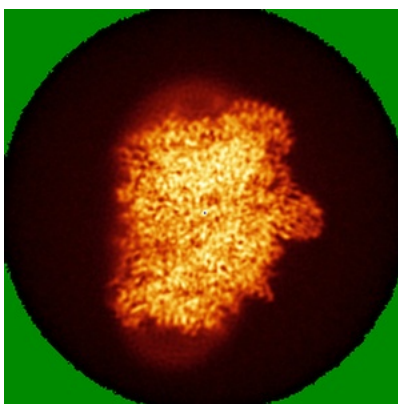
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

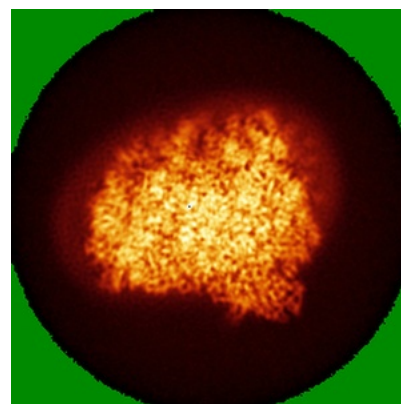
### 6.4.1 Primary map



X

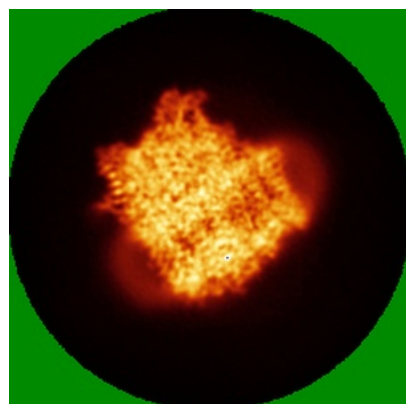


Y

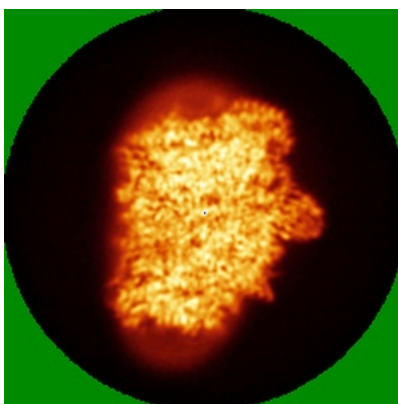


Z

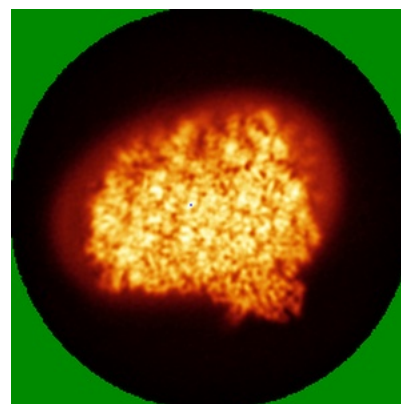
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



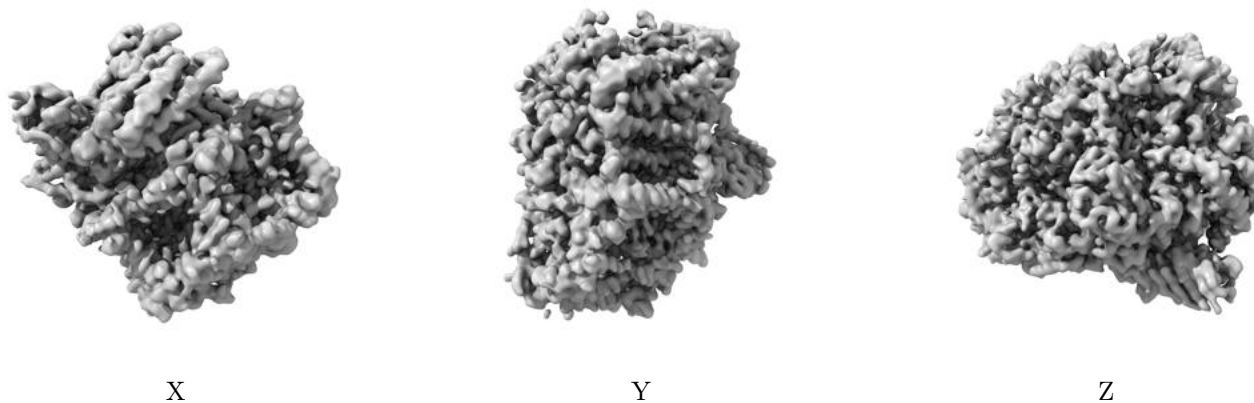
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

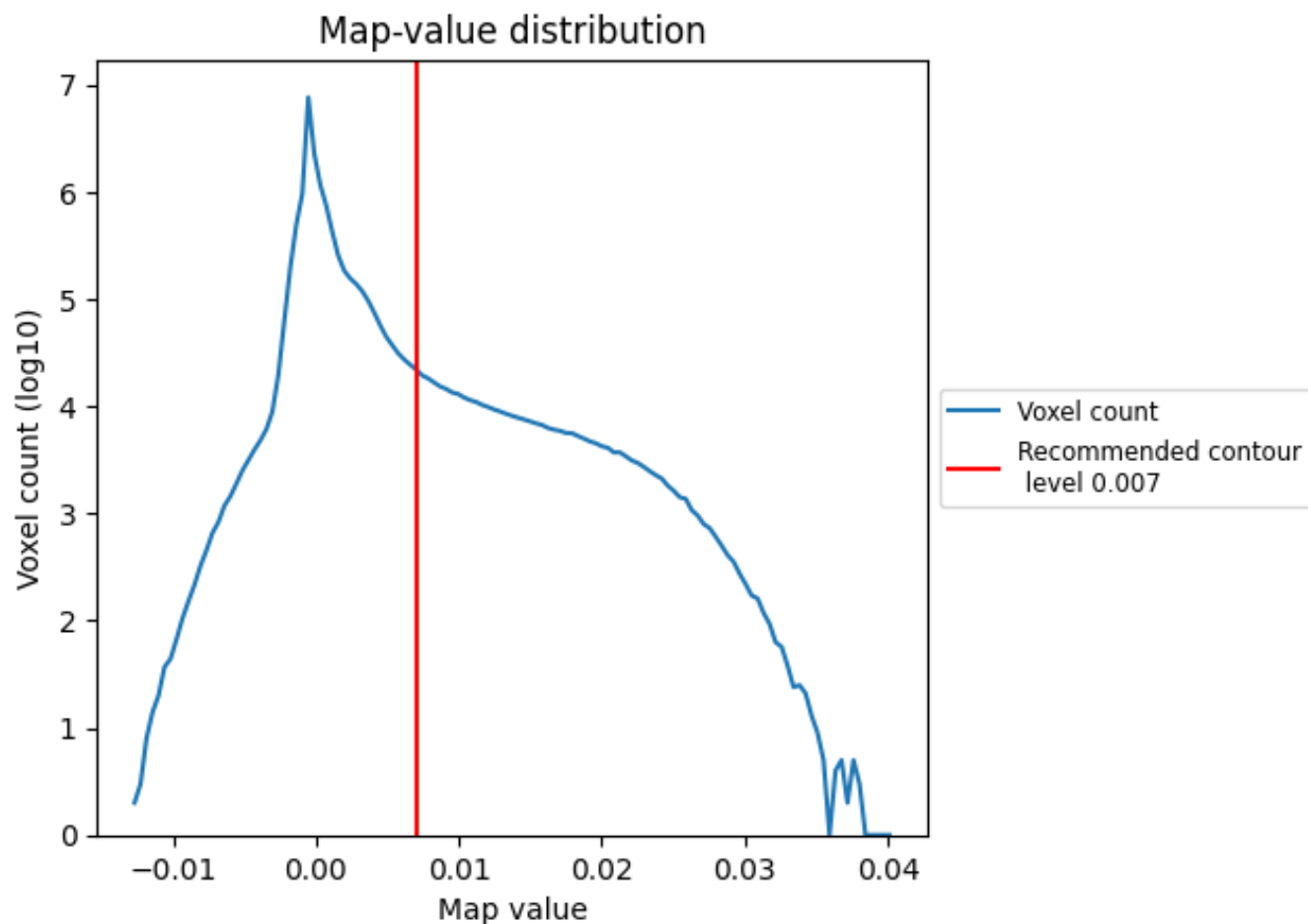
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

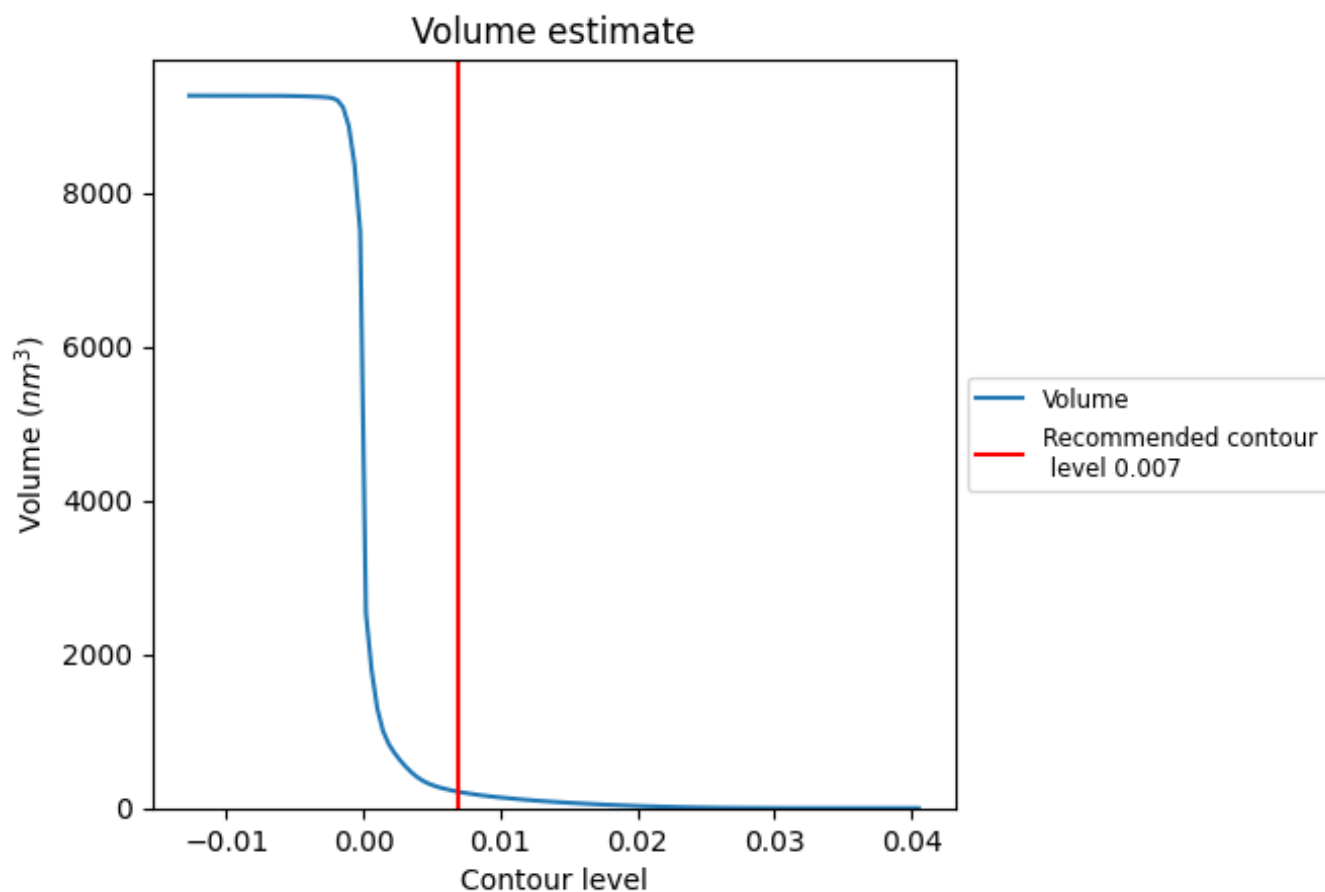
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

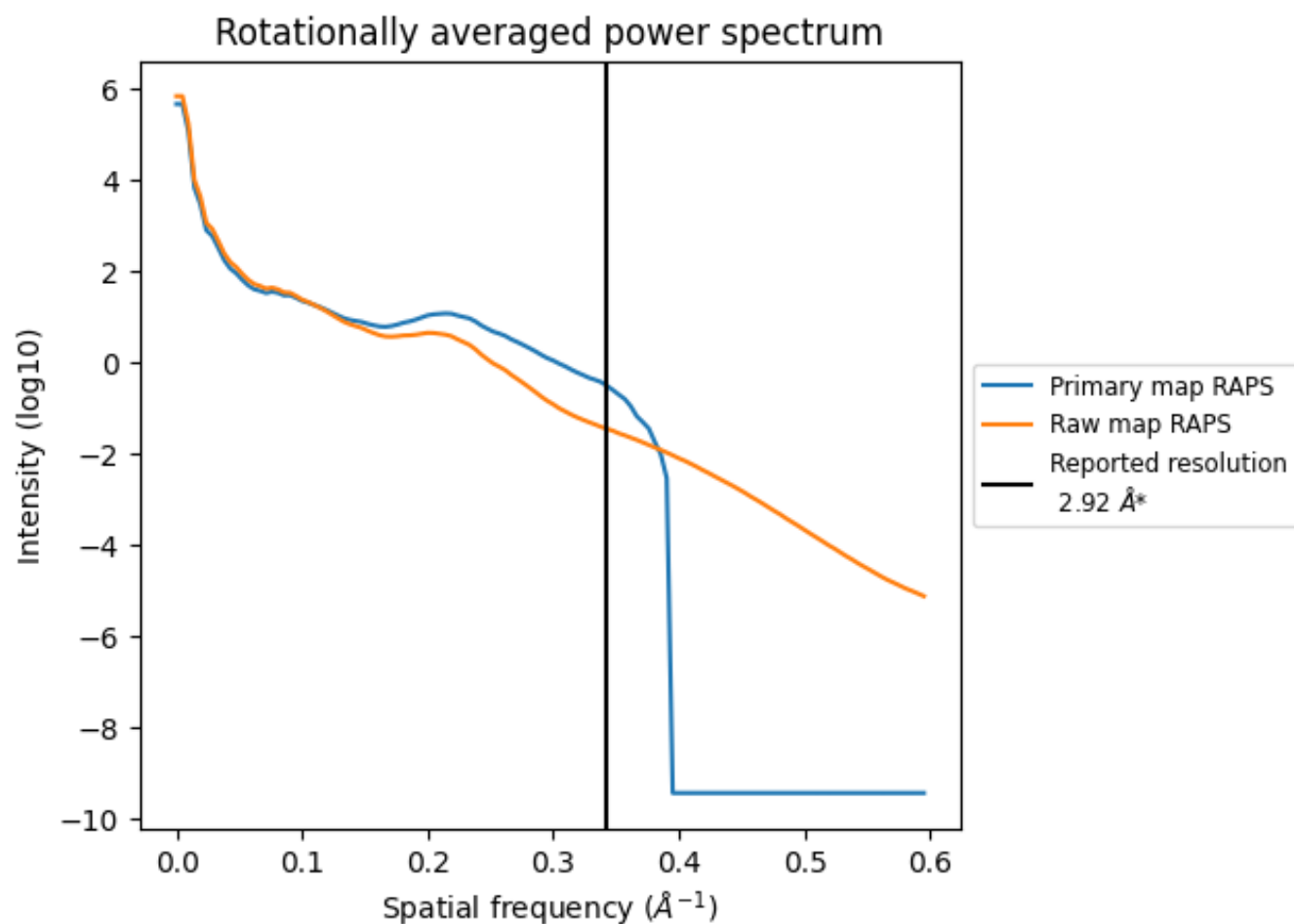
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm<sup>3</sup>; this corresponds to an approximate mass of 191 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

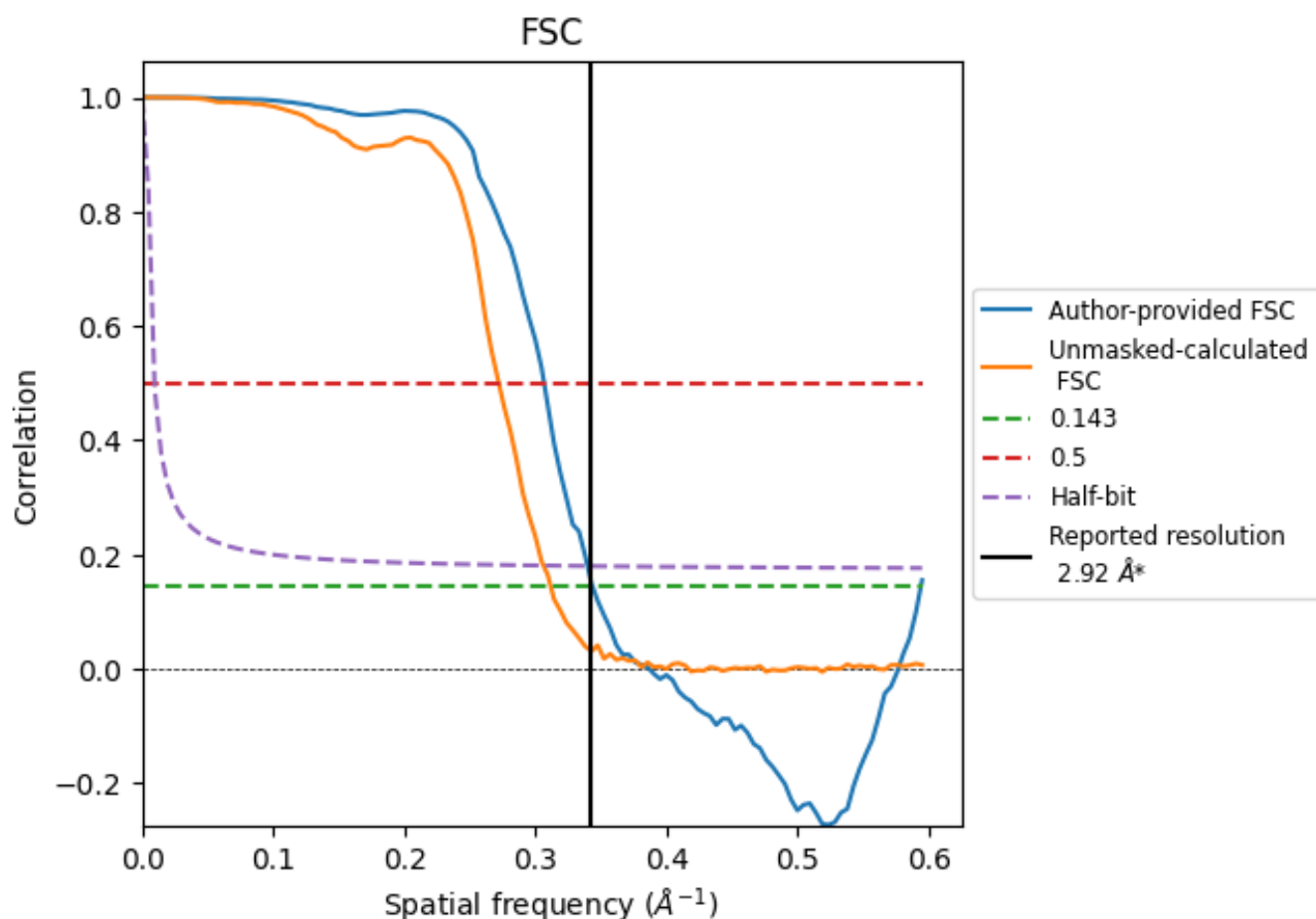


\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.342  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

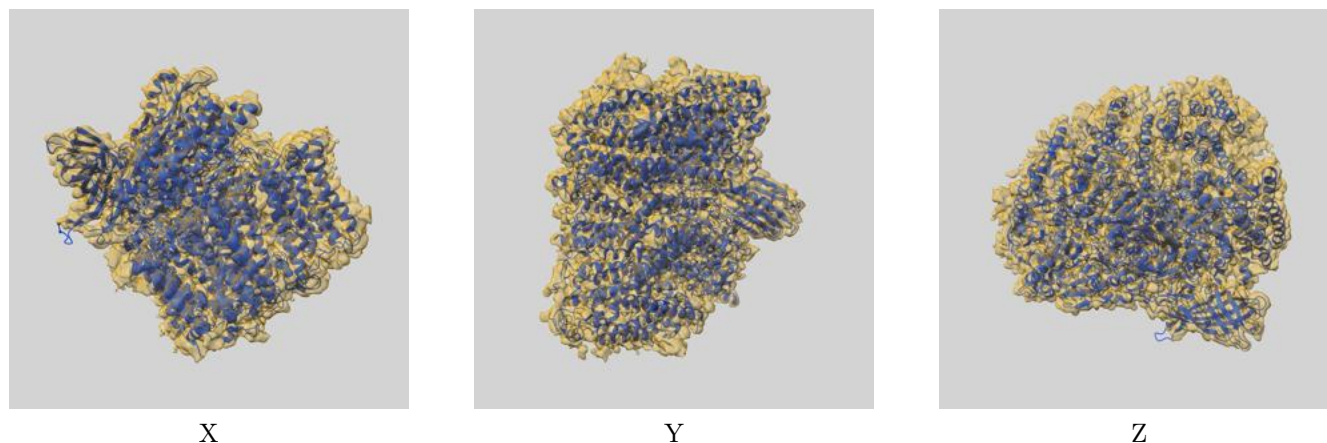
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.91	3.26	2.94
Unmasked-calculated*	3.21	3.68	3.27

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

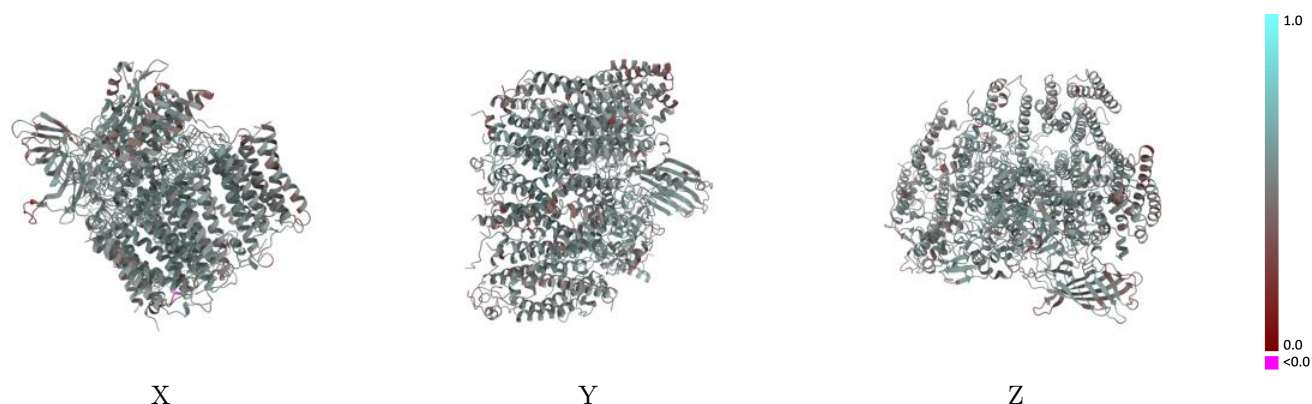
This section contains information regarding the fit between EMDB map EMD-52077 and PDB model 9HEI. Per-residue inclusion information can be found in section [3](#) on page [18](#).

### 9.1 Map-model overlay [i](#)



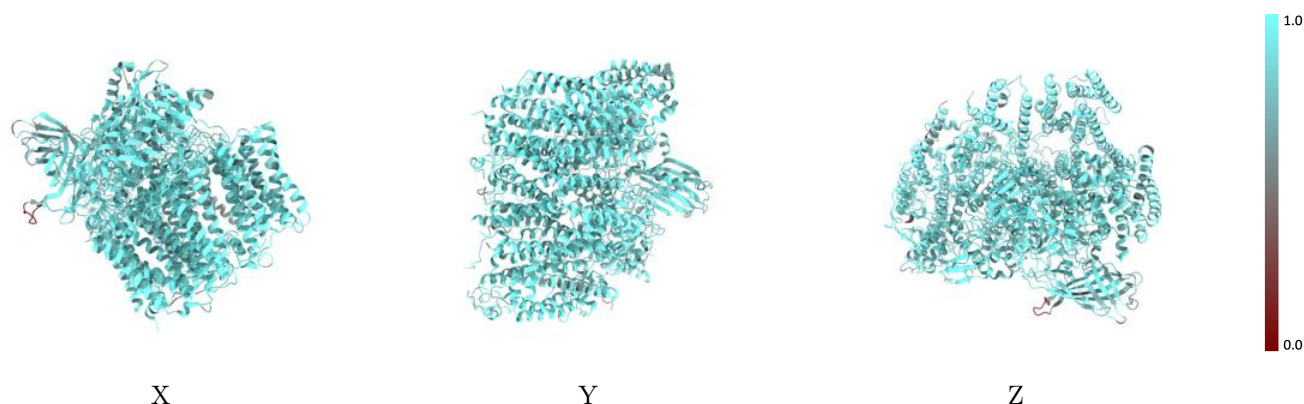
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



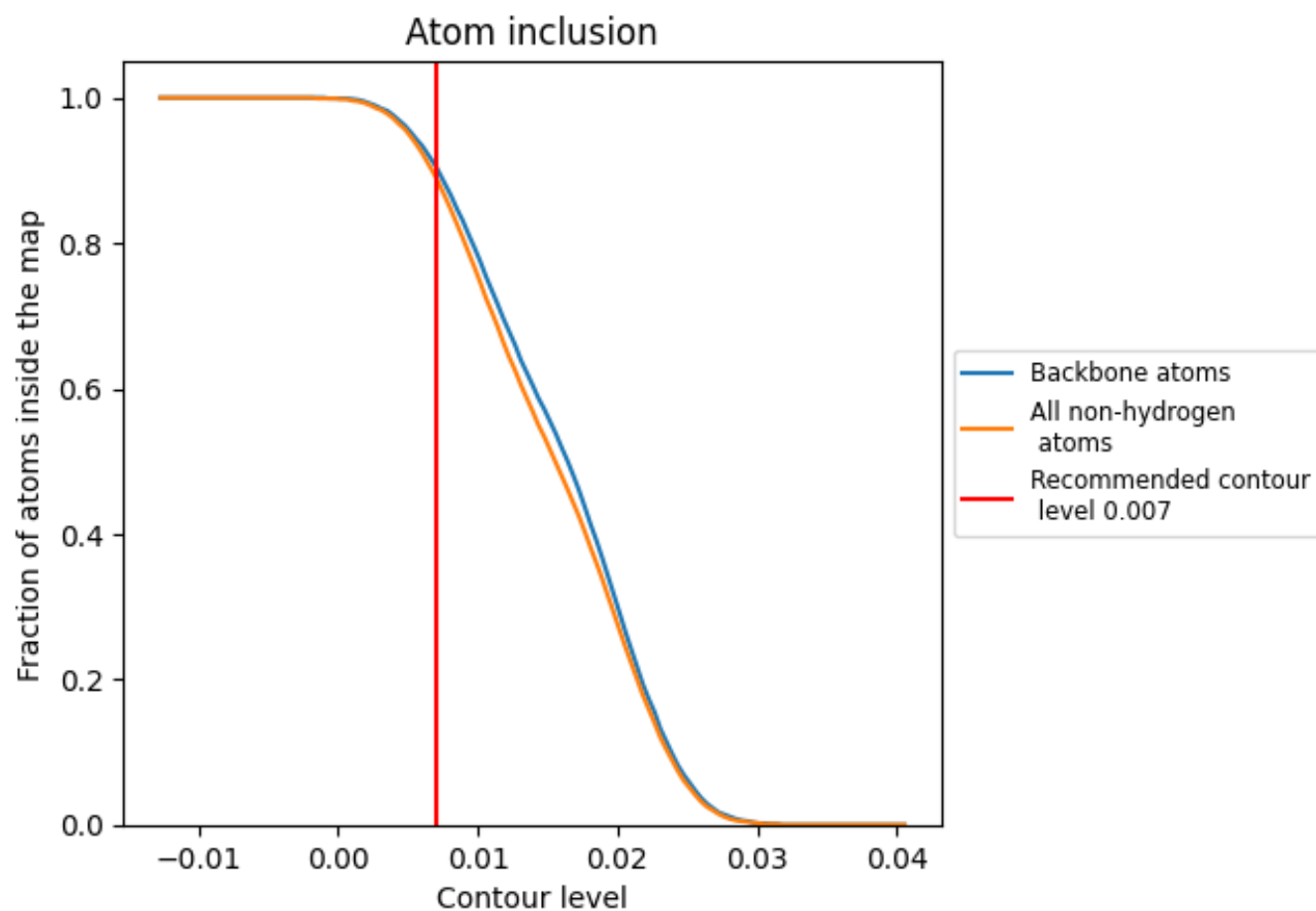
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

## 9.4 Atom inclusion [i](#)















































At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5100
A	 0.9240	 0.5290
B	 0.9020	 0.5140
C	 0.9010	 0.5220
D	 0.9240	 0.5440
E	 0.9160	 0.4760
F	 0.9020	 0.4870
H	 0.8590	 0.4820
I	 0.9230	 0.5160
J	 0.8910	 0.4990
K	 0.9280	 0.5190
L	 0.9370	 0.5200
M	 0.8370	 0.4570
O	 0.8160	 0.4860
P	 0.8800	 0.5130
Q	 0.8690	 0.4660
T	 0.8550	 0.4900
U	 0.7130	 0.4130
V	 0.9140	 0.4700
W	 0.8620	 0.4490
X	 0.7590	 0.4610
Z	 0.9060	 0.4630

