



Full wwPDB EM Validation Report ⓘ

Oct 6, 2025 – 10:57 am BST

PDB ID : 9IHP / pdb_00009ihp
EMDB ID : EMD-52876
Title : Open state without NUQM and with flavoprotein (classification state 3) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2025-02-21
Resolution : 3.34 Å(reported)
Based on initial model : 9ihr

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

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

A user guide is available at

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

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

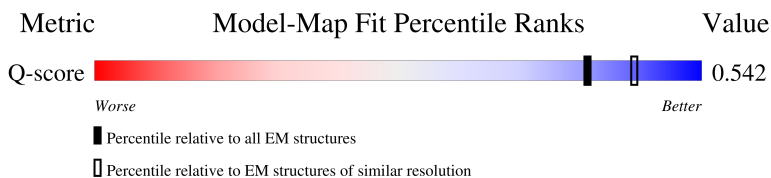
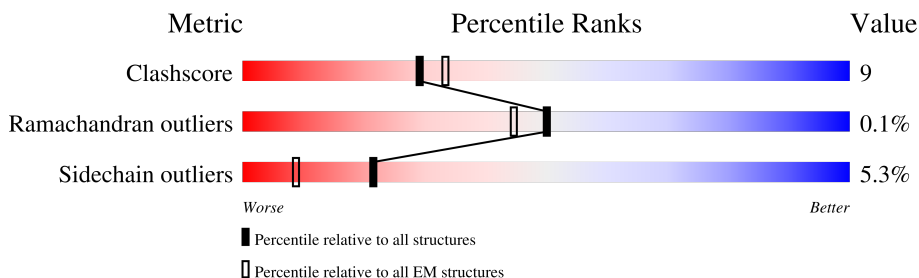
EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up 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 3.34 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.





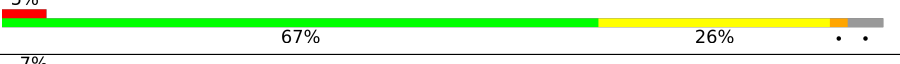
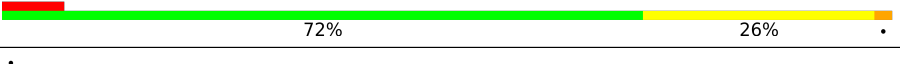
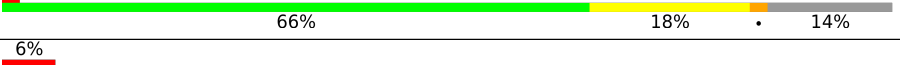
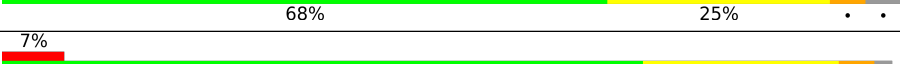
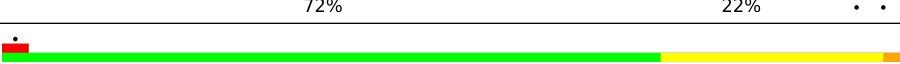
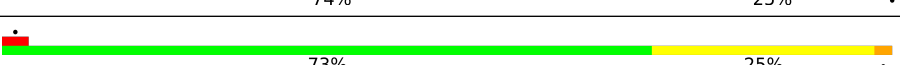
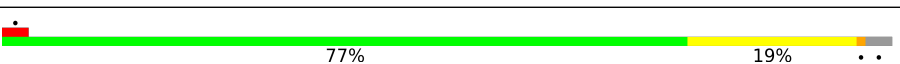

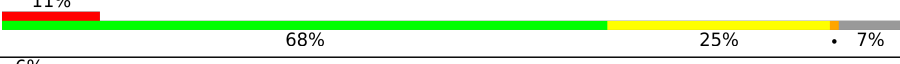
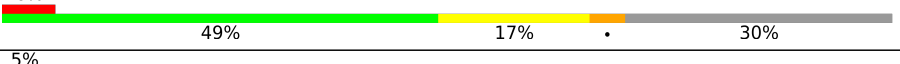


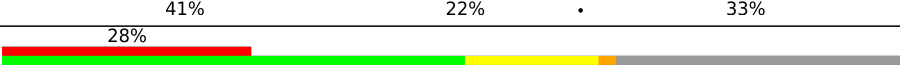
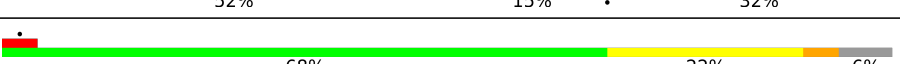
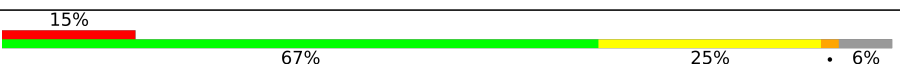
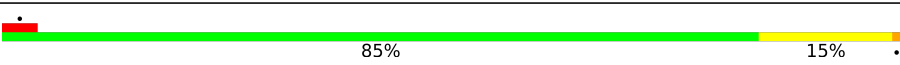


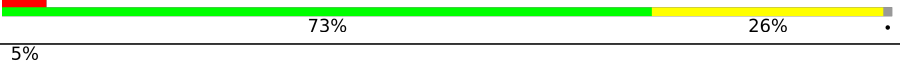

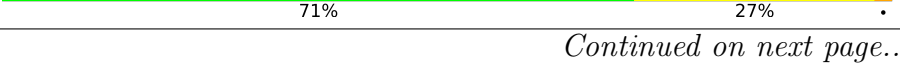


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14446 (2.84 - 3.84)

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 ≥ 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	141	
2	B	204	
3	C	289	
4	D	482	

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Mol	Chain	Length	Quality of chain
5	E	241	
6	F	473	
7	G	726	
8	H	353	
9	I	222	
10	J	161	
11	K	82	
12	L	642	
13	M	491	
14	N	523	
15	O	193	
16	P	384	
17	Q	159	
18	R	139	
19	S	90	
20	T	138	
21	U	130	
22	V	134	
23	W	122	
24	X	184	
25	Y	216	
26	Z	147	
27	a	150	
28	b	79	
29	c	182	

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Mol	Chain	Length	Quality of chain
30	d	78	
31	e	106	
32	f	86	
33	g	239	
34	h	182	
35	i	74	
36	j	59	
37	k	61	
38	l	156	
39	m	81	
40	n	111	
41	o	87	
42	p	92	
43	q	140	

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
44	SF4	F	501	-	-	X	-
44	SF4	I	302	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 68464 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	137	Total	C	N	O	S	0	0
			1099	745	159	191	4		

- Molecule 2 is a protein called BA75_00622T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	175	Total	C	N	O	S	0	0
			1407	901	241	249	16		

- Molecule 3 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	240	Total	C	N	O	S	0	0
			1970	1273	331	361	5		

- Molecule 4 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	440	Total	C	N	O	S	0	0
			3536	2259	602	657	18		

- Molecule 5 is a protein called NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	183	Total	C	N	O	S	0	0
			1446	920	239	273	14		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	453	Total	C	N	O	S	0	0
			3500	2213	612	654	21		

- Molecule 7 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	696	Total	C	N	O	S	0	0
			5344	3345	939	1037	23		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	353	Total	C	N	O	S	0	0
			2809	1903	414	478	14		

- Molecule 9 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	192	Total	C	N	O	S	0	0
			1556	988	259	299	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	155	Total	C	N	O	S	0	0
			1250	836	174	237	3		

- Molecule 11 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	80	Total	C	N	O	S	0	0
			617	400	93	118	6		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	642	Total	C	N	O	S	0	0
			5115	3454	766	866	29		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	491	Total	C	N	O	S	0	0
			3868	2597	593	663	15		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	506	Total	C	N	O	S	0	0
			4045	2723	594	714	14		

- Molecule 15 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	193	Total	C	N	O	S	0	0
			1575	1019	257	294	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	acetylation	UNP E1UWB9

- Molecule 16 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	359	Total	C	N	O	S	0	0
			2851	1821	496	531	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			924	585	161	176	2		

- Molecule 18 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	124	Total	C	N	O	S	0	0
			978	610	179	186	3		

- Molecule 19 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	90	Total	C	N	O	0	0
			697	454	117	126		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	ACE	-	acetylation	UNP E1UWD3

- Molecule 20 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	93	Total	C	N	O	S	0	0
			730	459	116	154	1		

- Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	88	Total	C	N	O	0	0
			681	427	102	152		

- Molecule 22 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	126	Total	C	N	O	S	0	0
			1025	658	165	201	1		

- Molecule 23 is a protein called BA75_04796T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	115	Total	C	N	O	S	0	0
			979	626	177	171	5		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	184	Total	C	N	O	S	0	0
			1450	905	253	282	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	0	ACE	-	acetylation	UNP E1UWB8

- Molecule 25 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	205	Total	C	N	O	S	0	0
			1578	1012	274	289	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	142	Total	C	N	O	S	0	0
			1176	758	212	202	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ACE	-	acetylation	UNP E1UWD8

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	149	Total	C	N	O	S	0	0
			1215	756	228	225	6		

- Molecule 28 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	78	Total	C	N	O	S	0	0
			641	419	111	109	2		

- Molecule 29 is a protein called BA75_00589T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	182	Total	C	N	O	S	0	0
			1418	902	248	266	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	1	ACE	-	acetylation	UNP E1UWC1

- Molecule 30 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	75	Total	C	N	O	S	0	0
			616	406	106	103	1		

- Molecule 31 is a protein called BA75_05084T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	105	Total	C	N	O	S	0	0
			848	531	154	157	6		

- Molecule 32 is a protein called NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	78	Total	C	N	O	S	0	0
			642	428	113	101			

- Molecule 33 is a protein called NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	158	Total	C	N	O	S	0	0
			1280	815	210	252	3		

- Molecule 34 is a protein called NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	131	Total	C	N	O	S	0	0
			1078	699	183	196			

- Molecule 35 is a protein called NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	69	Total	C	N	O	S	0	0
			552	358	95	97	2		

- Molecule 36 is a protein called Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	53	Total	C	N	O	S	0	0
			460	319	76	64	1		

- Molecule 37 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	45	Total	C	N	O	S	0	0
			368	240	71	56	1		

- Molecule 38 is a protein called NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	132	Total	C	N	O	S	0	0
			1082	706	175	200	1		

- Molecule 39 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	77	Total	C	N	O	0	0
			642	418	116	108		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	105	Total	C	N	O	S	0	0
			861	550	155	155	1		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	80	Total	C	N	O	S	0	0
			682	428	126	122	6		

- Molecule 42 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	90	Total	C	N	O	S	0	0
			740	457	135	144	4		

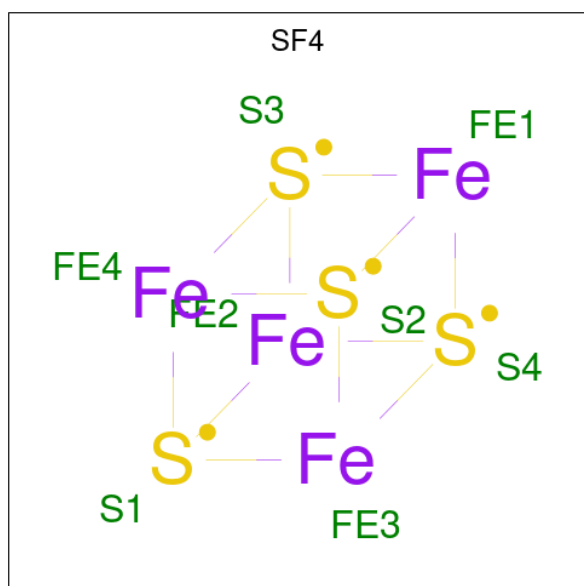
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	140	Total	C	N	O	S	0	0
			1156	741	201	211	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	0	ACE	-	acetylation	UNP E1UWE0

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



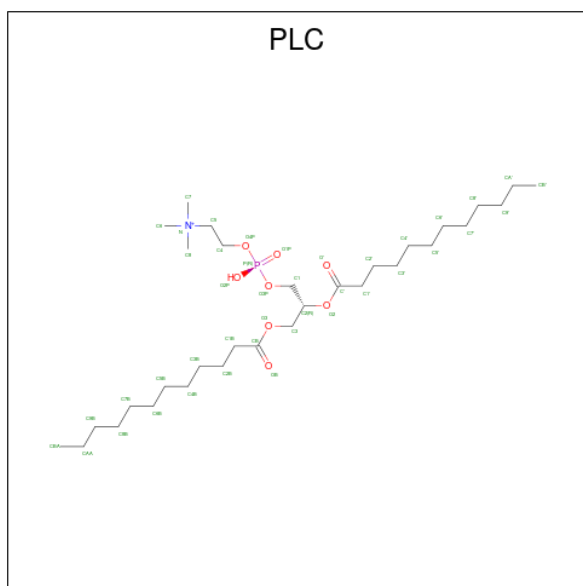
Mol	Chain	Residues	Atoms			AltConf
44	B	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
44	F	1	Total	Fe	S	0
			8	4	4	
44	G	1	Total	Fe	S	0
			8	4	4	
44	G	1	Total	Fe	S	0
			8	4	4	
44	I	1	Total	Fe	S	0
			8	4	4	
44	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 45 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	H	1	Total	C	N	O	P	0
			24	14	1	8	1	
45	I	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	

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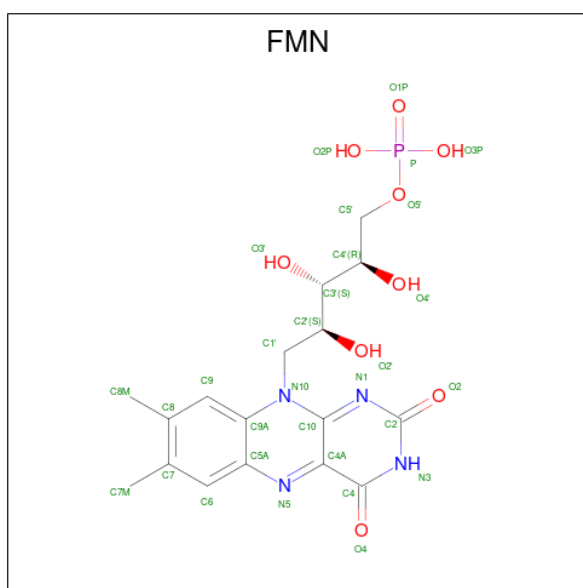
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Z	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	a	1	Total	C	N	O	P	0
			22	12	1	8	1	
45	b	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	h	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	l	1	Total	C	N	O	P	0
			32	22	1	8	1	
45	m	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	q	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	q	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

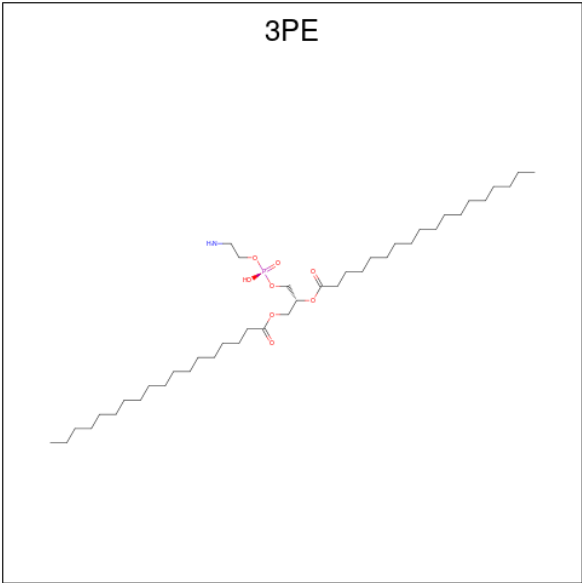


Mol	Chain	Residues	Atoms					AltConf
47	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
48	G	1	Total	K	0
			1	1	

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



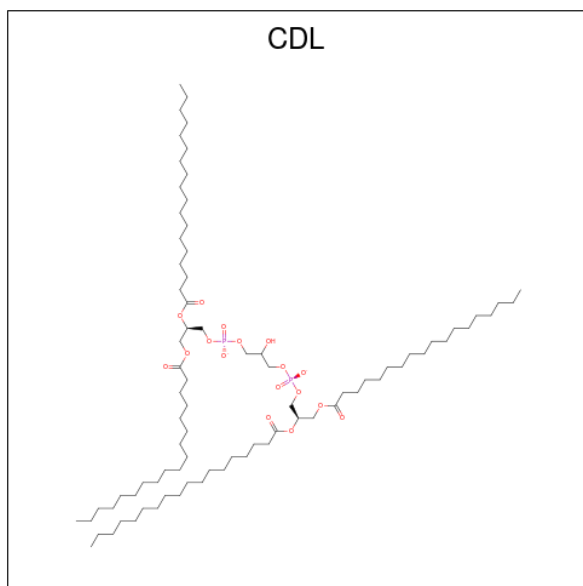
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
49	H	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
49	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	O	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
49	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	g	1	Total	C	N	O	P	0
			46	36	1	8	1	
49	j	1	Total	C	N	O	P	0
			27	17	1	8	1	
49	l	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	m	1	Total	C	N	O	P	0
			29	19	1	8	1	
49	m	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



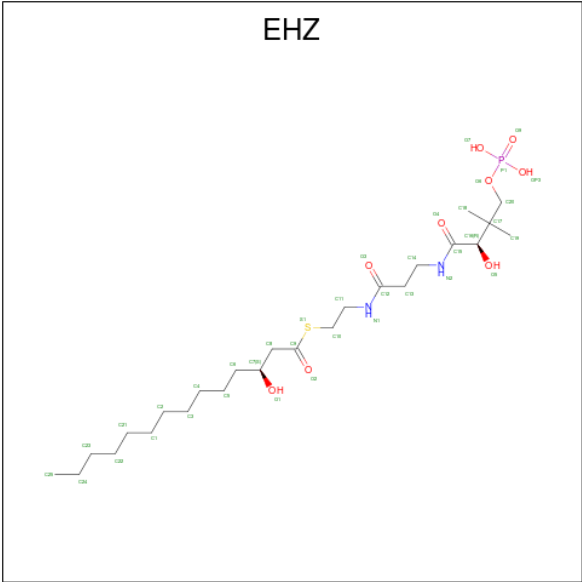
Mol	Chain	Residues	Atoms				AltConf
50	O	1	Total	C	O	P	0
			75	56	17	2	
50	Z	1	Total	C	O	P	0
			49	30	17	2	

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Mol	Chain	Residues	Atoms				AltConf
50	a	1	Total 60	C 41	O 17	P 2	0
50	b	1	Total 59	C 40	O 17	P 2	0

- # NDP

- Molecule 53 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

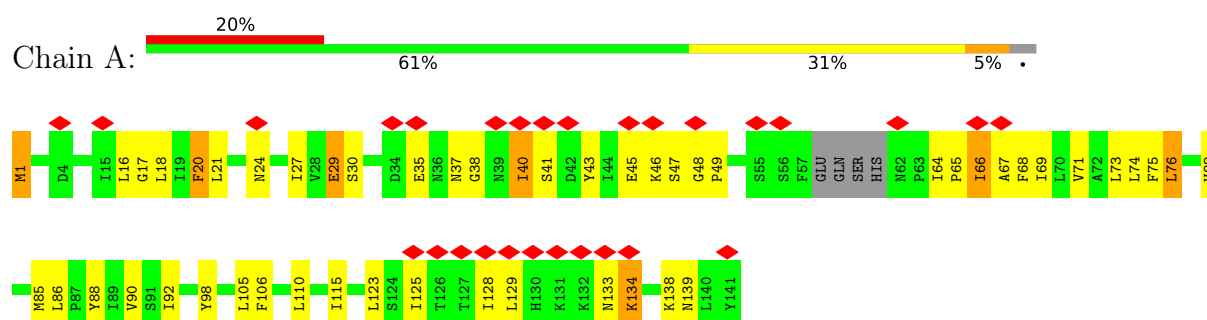


Mol	Chain	Residues	Atoms						AltConf
53	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
53	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

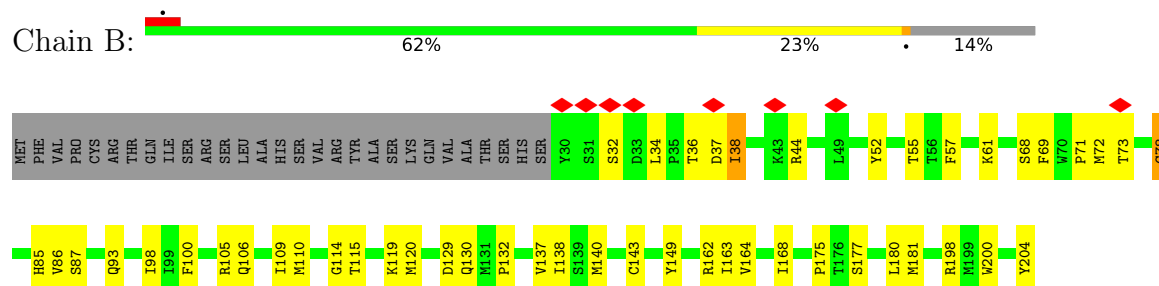
3 Residue-property plots

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.

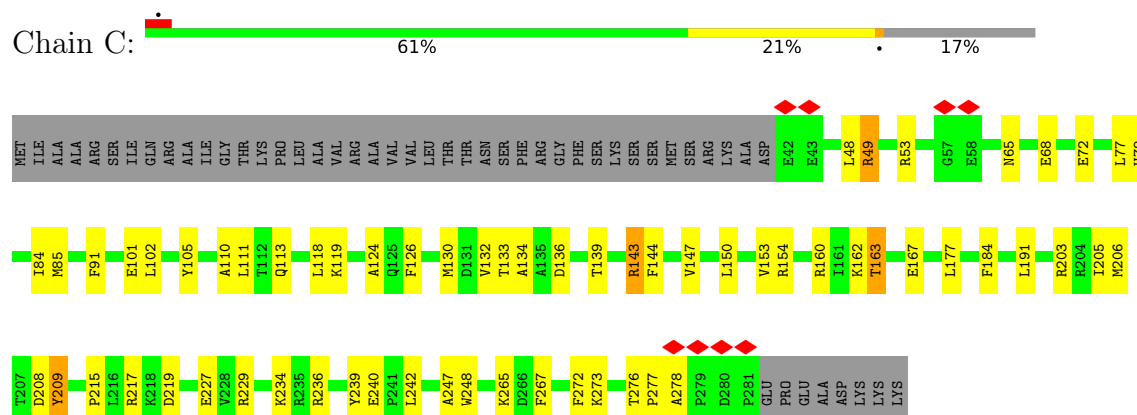
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3



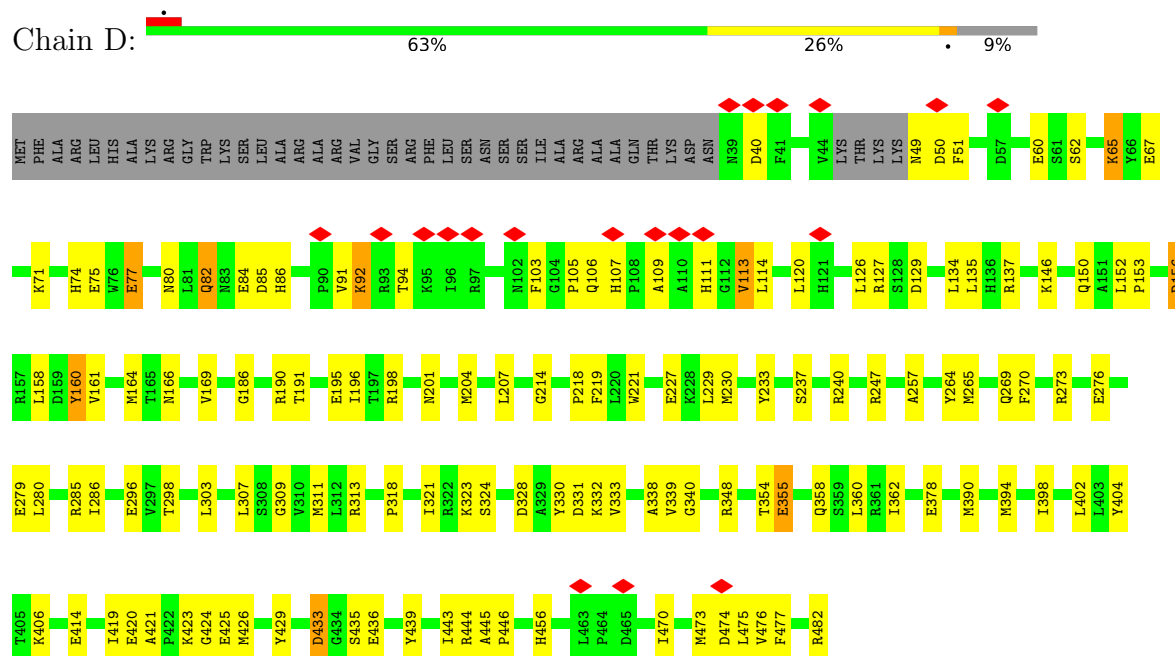
• Molecule 2: BA75_00622T0



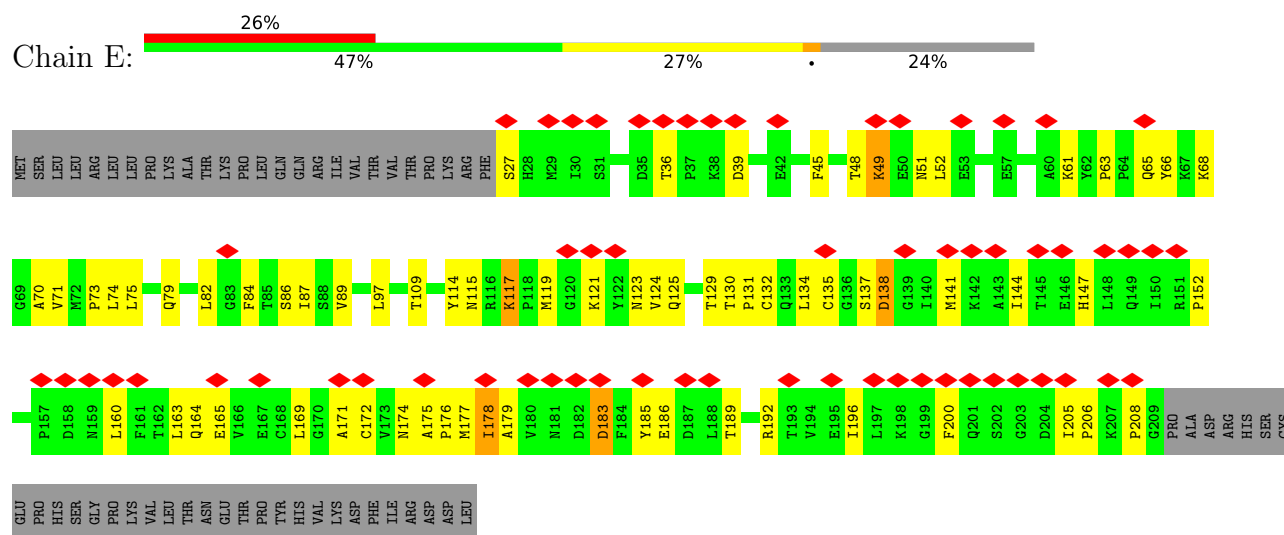
• Molecule 3: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



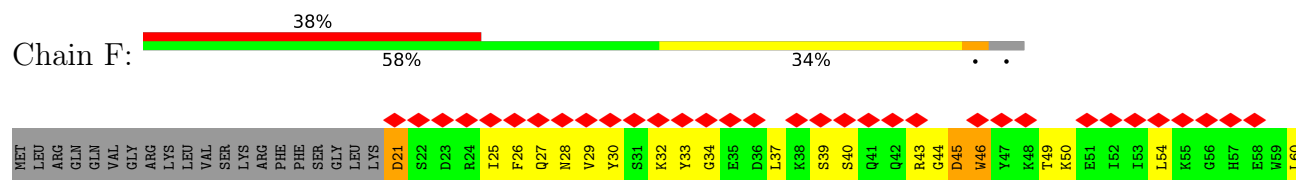
- Molecule 4: NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

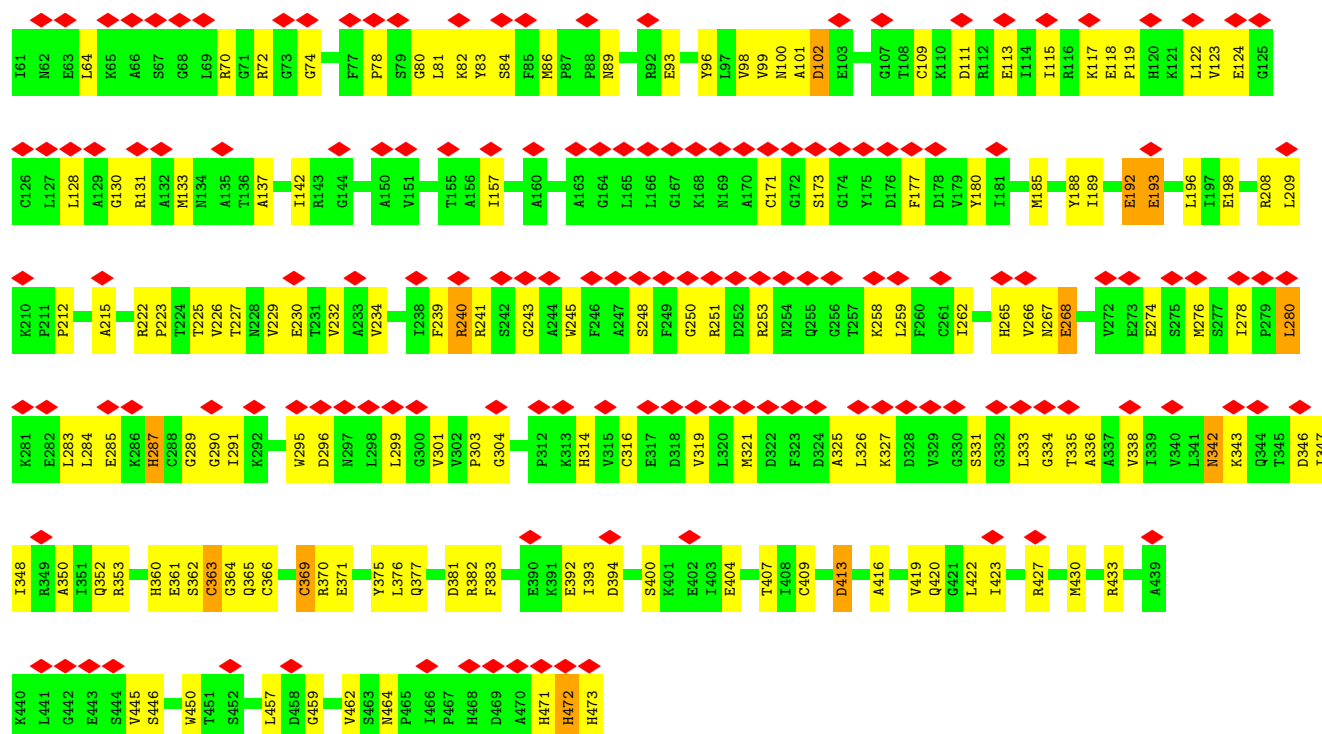


- Molecule 5: NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

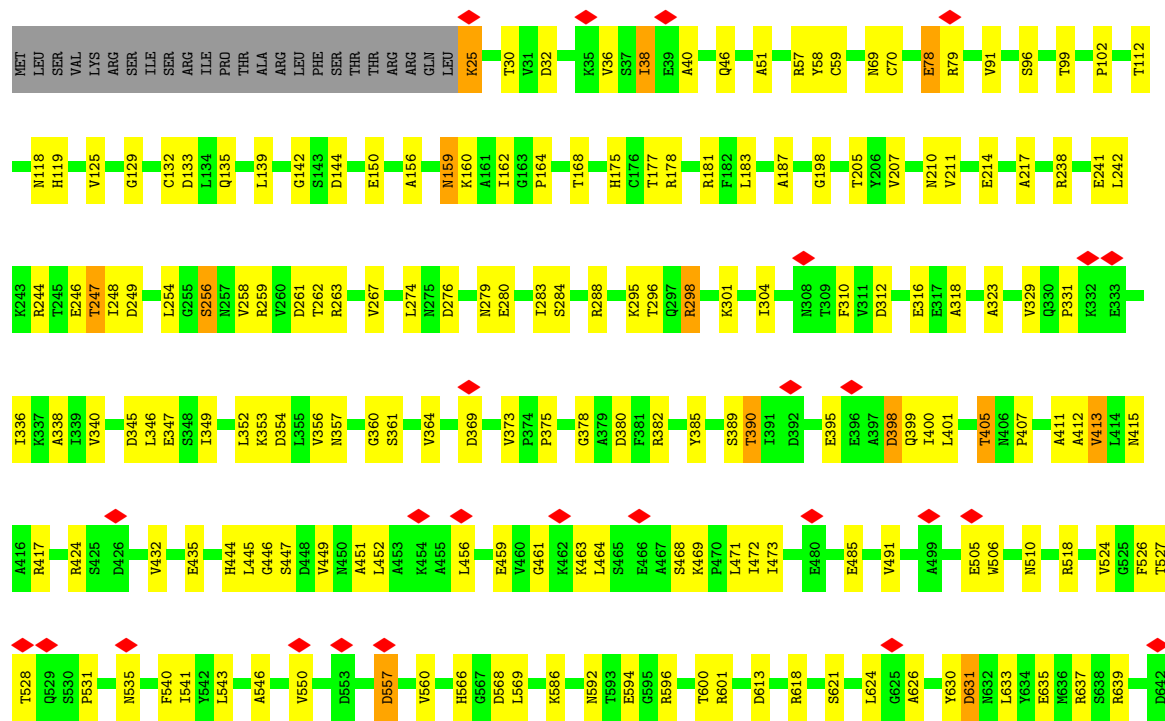


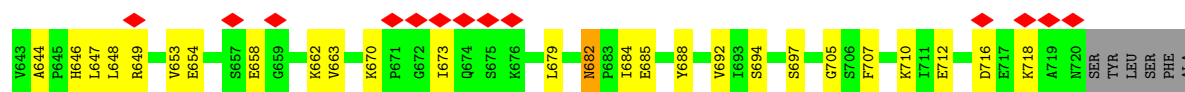
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



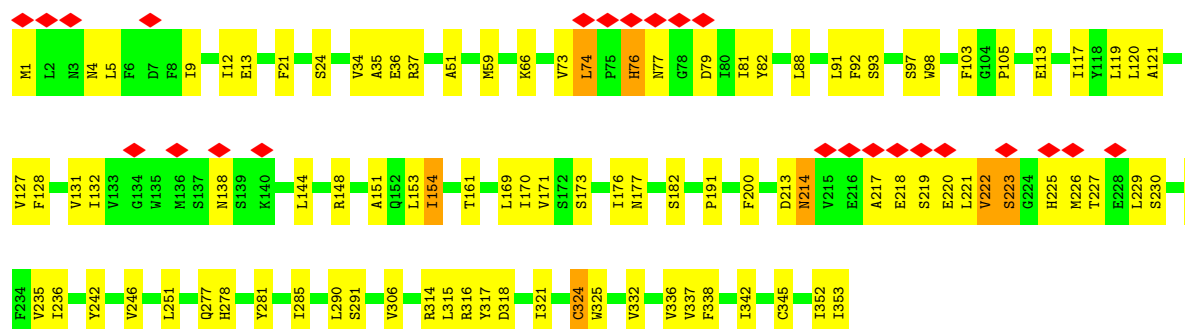


- Molecule 7: NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

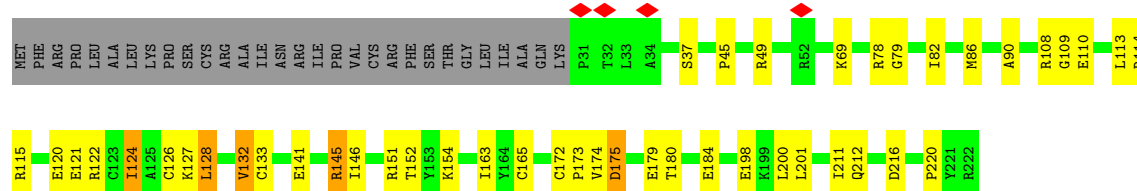




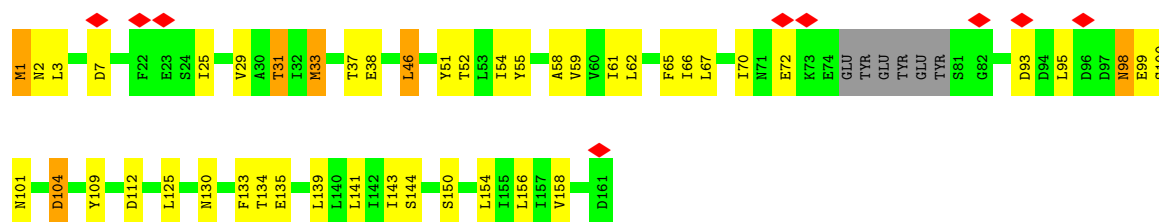
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



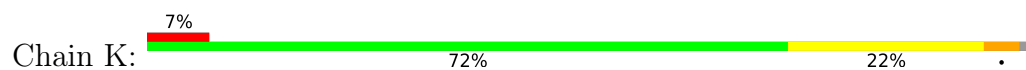
• Molecule 9: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



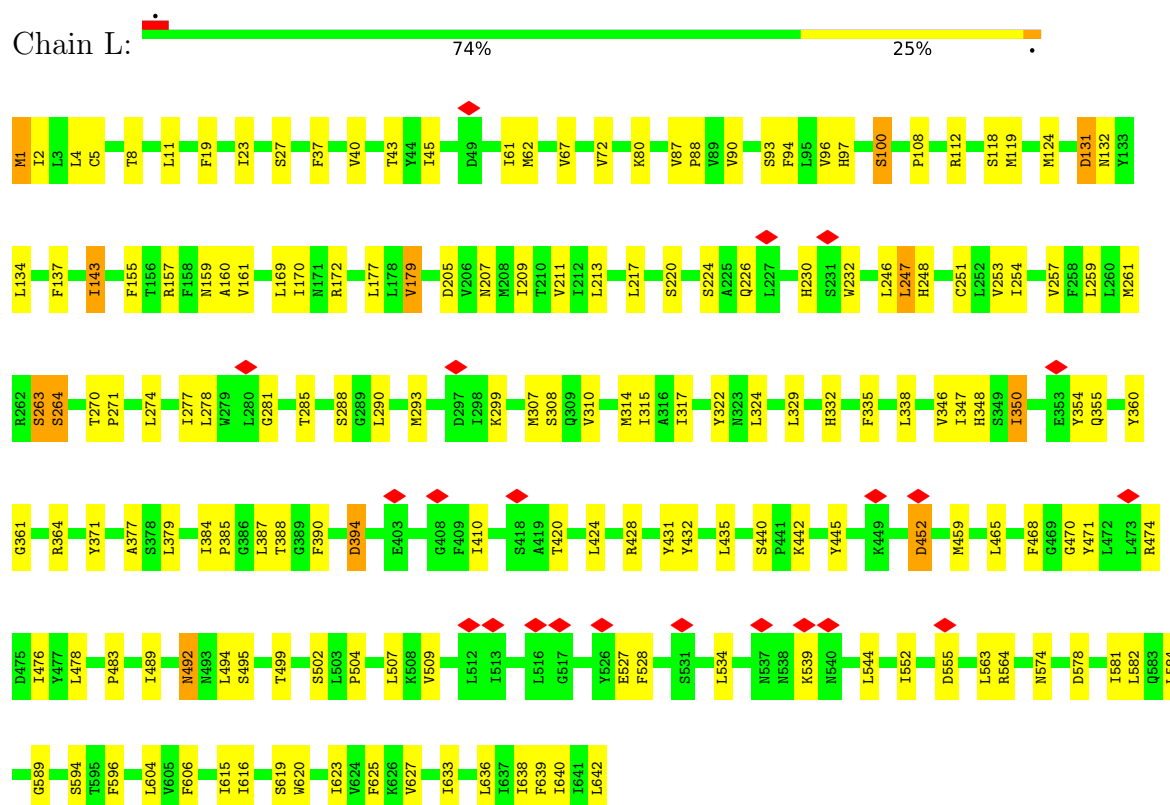
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



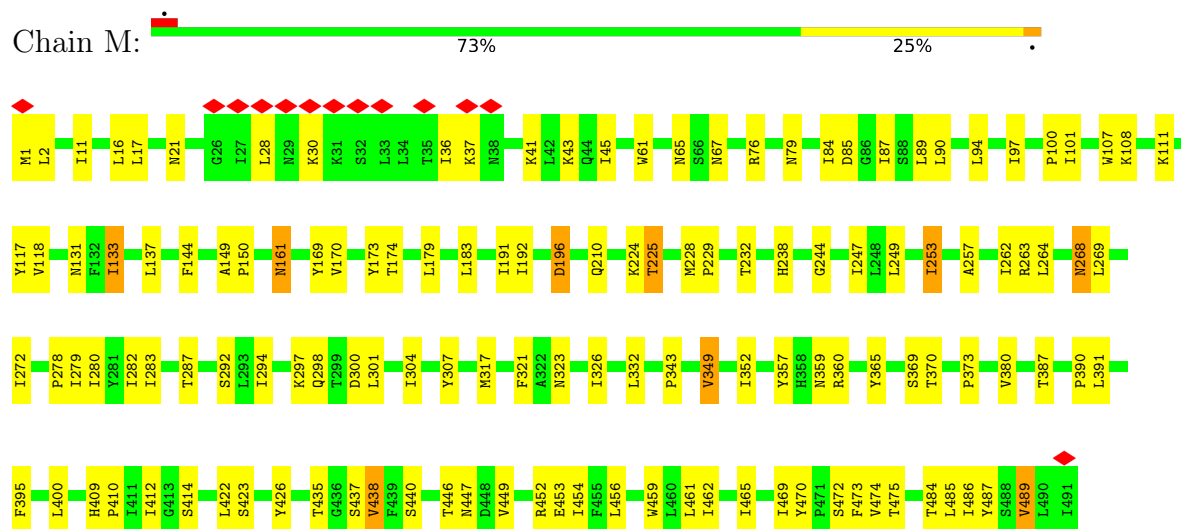
• Molecule 11: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



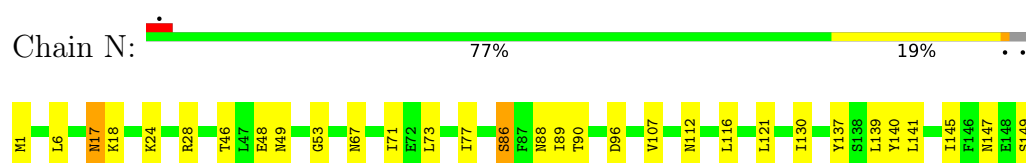
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

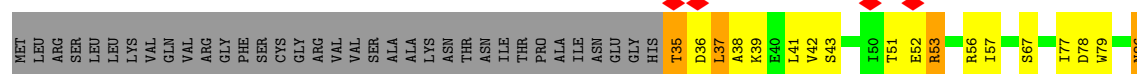


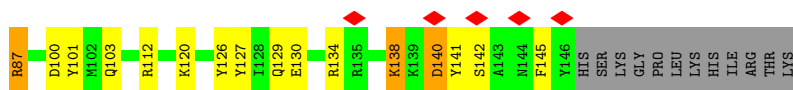
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



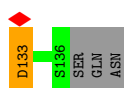
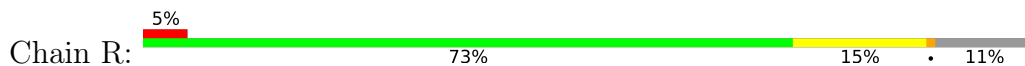
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



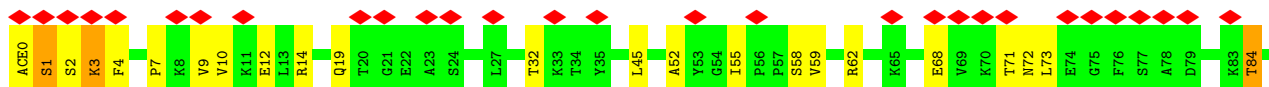




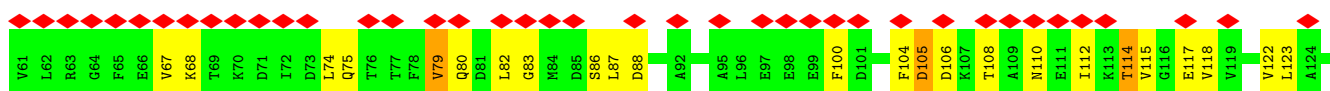
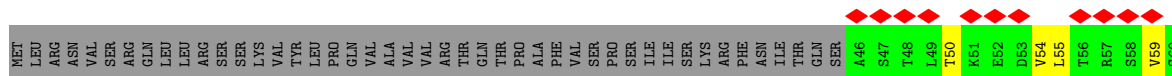
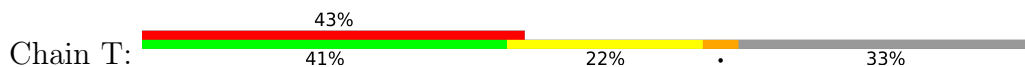
- Molecule 18: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



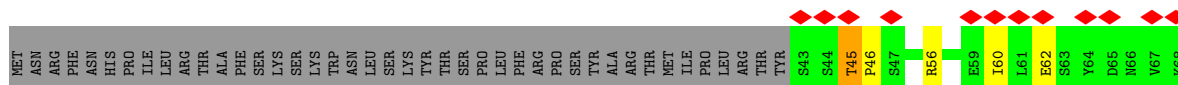
- Molecule 19: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

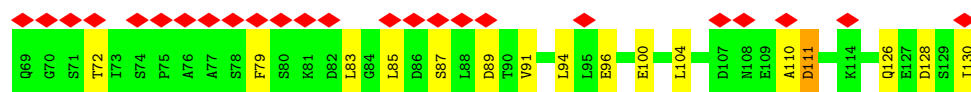


- Molecule 20: Acyl carrier protein

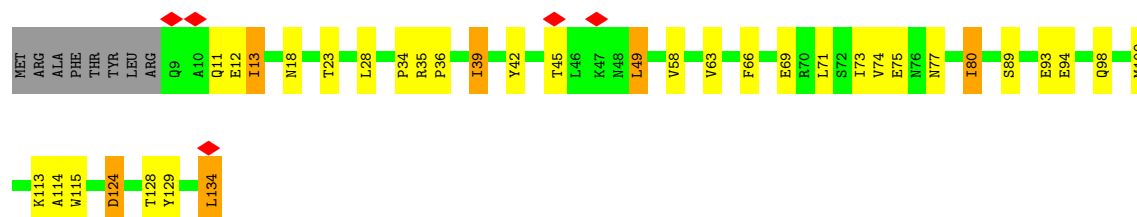


- Molecule 21: Acyl carrier protein

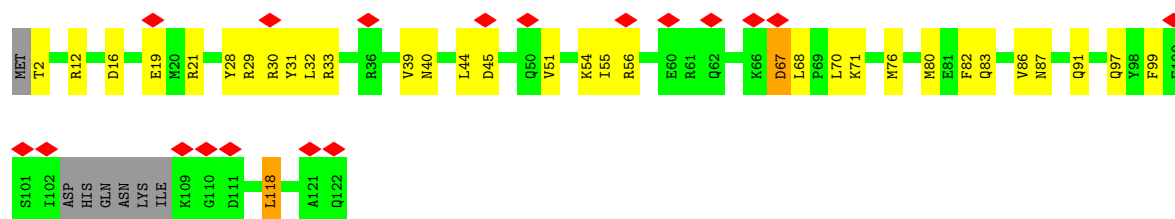




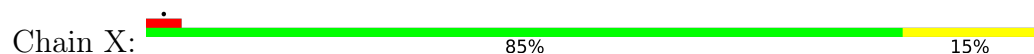
- Molecule 22: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



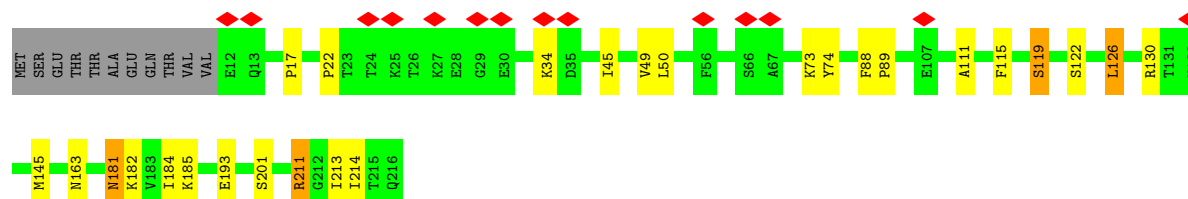
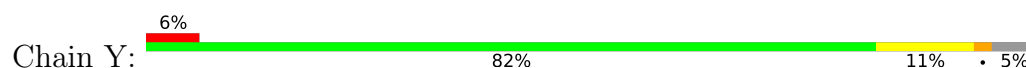
- Molecule 23: BA75_04796T0



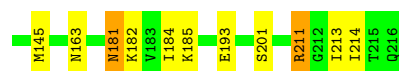
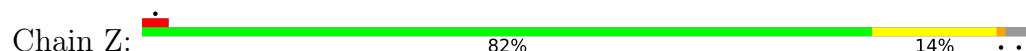
- Molecule 24: NADH-ubiquinone oxidoreductase



- Molecule 25: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

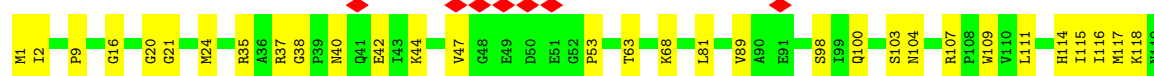
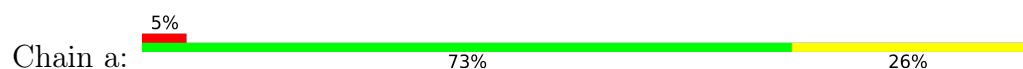


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

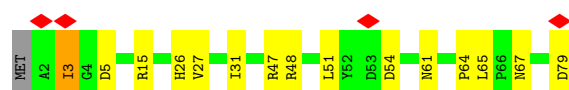
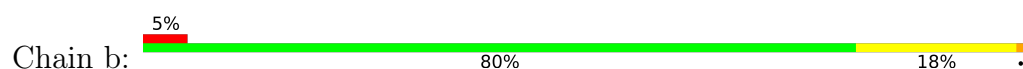




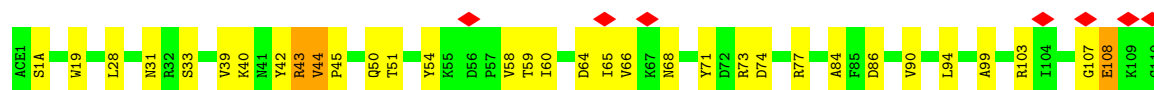
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



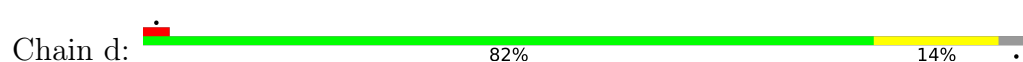
- Molecule 28: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



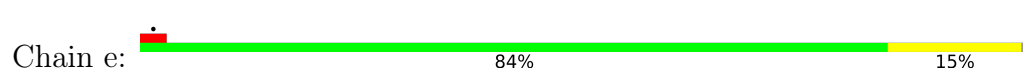
- Molecule 29: BA75_00589T0



- Molecule 30: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM



- Molecule 31: BA75_05084T0



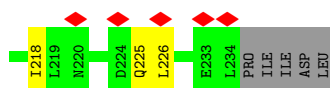
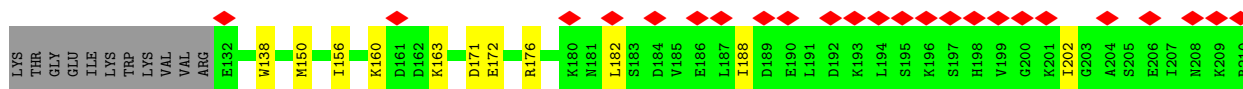
- Molecule 32: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain f: 



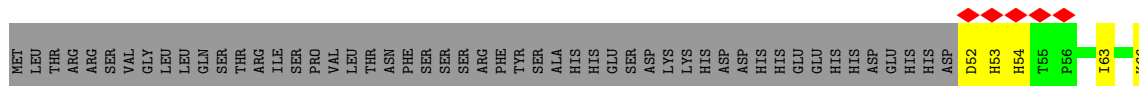
- Molecule 33: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain g: 




- Molecule 34: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain h: 

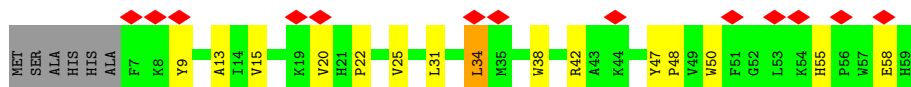


- Molecule 35: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

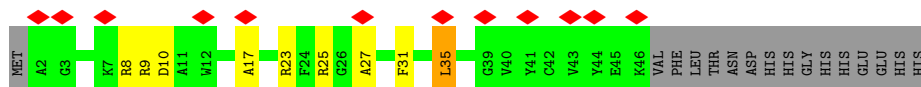
Chain i: 



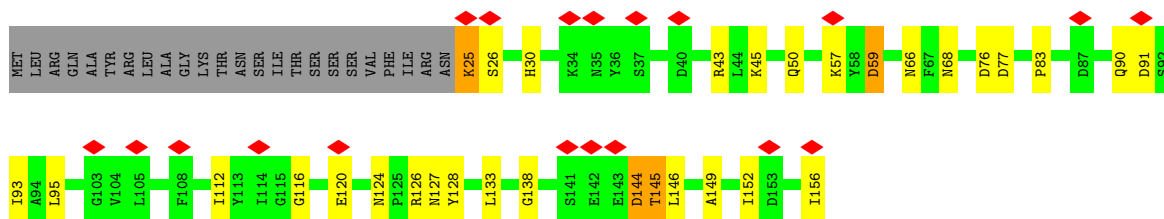
- Molecule 36: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



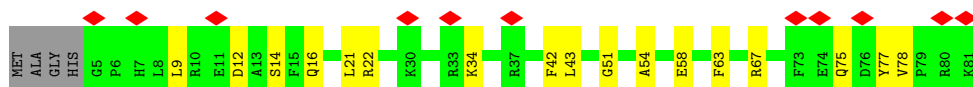
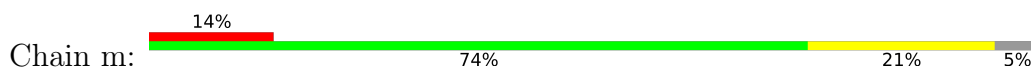
- Molecule 37: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



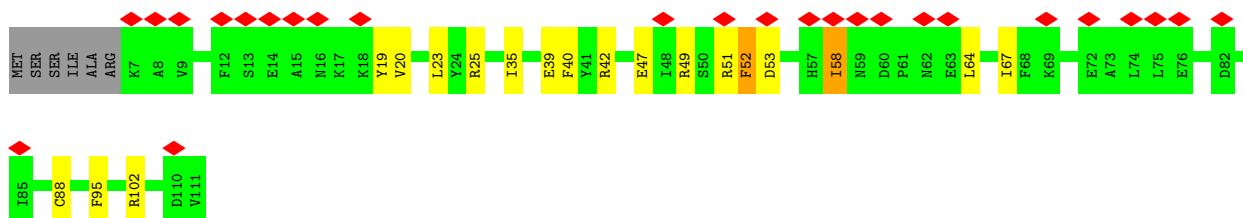
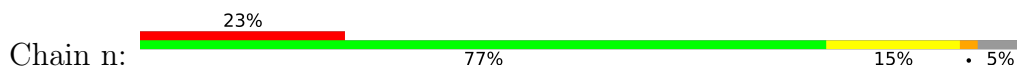
- Molecule 38: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 39: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

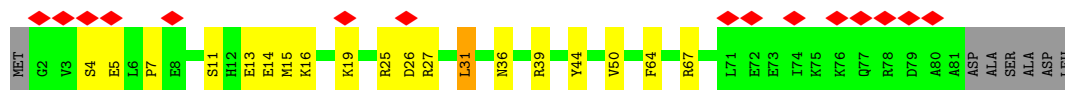


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

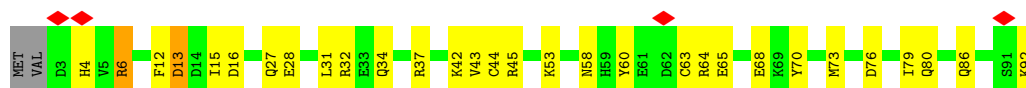


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

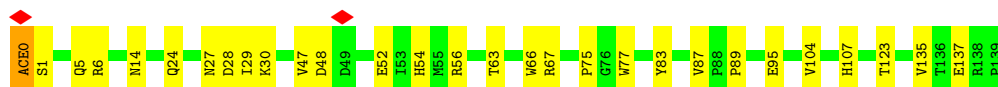
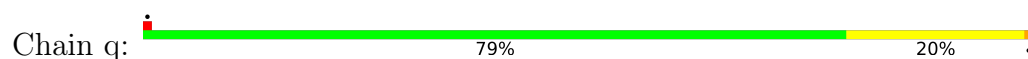




- Molecule 42: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25125	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 ($e^-/\text{\AA}^2$)	47.79	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	501.66, 501.66, 501.66	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.929, 0.929, 0.929	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, EH2, FMN, PLC, ACE, CDL, SF4, ZN, FES, K, FME, NDP, 3PE

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	0.24	0/1115	0.34	0/1514
2	B	0.30	0/1450	0.33	0/1969
3	C	0.26	0/2033	0.31	0/2770
4	D	0.29	0/3612	0.33	0/4892
5	E	0.18	0/1480	0.35	0/2008
6	F	0.17	0/3579	0.32	0/4832
7	G	0.23	0/5436	0.32	0/7370
8	H	0.28	0/2880	0.33	0/3939
9	I	0.33	0/1596	0.35	0/2164
10	J	0.28	0/1262	0.35	0/1723
11	K	0.27	0/610	0.28	0/828
12	L	0.25	0/5236	0.31	0/7128
13	M	0.29	0/3940	0.31	0/5379
14	N	0.30	0/4110	0.31	0/5609
15	O	0.30	1/1621 (0.1%)	0.32	0/2199
16	P	0.21	0/2911	0.32	0/3932
17	Q	0.23	0/945	0.28	0/1273
18	R	0.24	0/998	0.29	0/1350
19	S	0.28	1/710 (0.1%)	0.31	0/961
20	T	0.14	0/737	0.29	0/1001
21	U	0.16	0/688	0.28	0/936
22	V	0.21	0/1044	0.31	0/1411
23	W	0.19	0/999	0.30	0/1340
24	X	0.29	1/1475 (0.1%)	0.31	0/1990
25	Y	0.22	0/1615	0.29	0/2175
26	Z	0.32	1/1210 (0.1%)	0.27	0/1639
27	a	0.26	0/1241	0.29	0/1670
28	b	0.22	0/666	0.27	0/911
29	c	0.26	0/1448	0.35	0/1964
30	d	0.24	0/633	0.26	0/854
31	e	0.27	0/865	0.30	0/1158
32	f	0.20	0/663	0.27	0/896

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.18	0/1293	0.30	0/1735
34	h	0.23	0/1114	0.29	0/1516
35	i	0.20	0/571	0.31	0/777
36	j	0.17	0/484	0.29	0/658
37	k	0.20	0/382	0.29	0/514
38	l	0.19	0/1119	0.32	0/1520
39	m	0.23	0/661	0.28	0/893
40	n	0.17	0/884	0.27	0/1197
41	o	0.18	0/696	0.32	0/933
42	p	0.25	0/756	0.29	0/1020
43	q	0.31	1/1192 (0.1%)	0.32	0/1620
All	All	0.25	5/67960 (0.0%)	0.31	0/92168

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	0	ACE	C-N	6.15	1.45	1.33
19	S	0	ACE	C-N	6.05	1.45	1.33
24	X	0	ACE	C-N	6.05	1.45	1.33
15	O	0	ACE	C-N	5.99	1.45	1.33
43	q	0	ACE	C-N	5.91	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1099	0	1140	44	0
2	B	1407	0	1372	42	0
3	C	1970	0	1905	52	0
4	D	3536	0	3436	96	0
5	E	1446	0	1435	43	0
6	F	3500	0	3459	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	5344	0	5332	123	0
8	H	2809	0	2880	62	0
9	I	1556	0	1499	34	0
10	J	1250	0	1274	36	0
11	K	617	0	657	19	0
12	L	5115	0	5338	110	0
13	M	3868	0	4127	93	0
14	N	4045	0	4327	64	0
15	O	1575	0	1523	12	0
16	P	2851	0	2848	62	0
17	Q	924	0	891	26	0
18	R	978	0	964	15	0
19	S	697	0	736	14	0
20	T	730	0	721	20	0
21	U	681	0	664	12	0
22	V	1025	0	1035	20	0
23	W	979	0	980	26	0
24	X	1450	0	1422	20	0
25	Y	1578	0	1567	20	0
26	Z	1176	0	1165	19	0
27	a	1215	0	1197	41	0
28	b	641	0	620	17	0
29	c	1418	0	1452	42	0
30	d	616	0	624	8	0
31	e	848	0	830	16	0
32	f	642	0	640	12	0
33	g	1280	0	1302	21	0
34	h	1078	0	1036	21	0
35	i	552	0	540	11	0
36	j	460	0	455	12	0
37	k	368	0	348	8	0
38	l	1082	0	1033	21	0
39	m	642	0	635	15	0
40	n	861	0	866	14	0
41	o	682	0	677	13	0
42	p	740	0	700	26	0
43	q	1156	0	1115	24	0
44	B	8	0	0	1	0
44	F	8	0	0	3	0
44	G	16	0	0	1	0
44	I	16	0	0	3	0
45	B	62	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	H	24	0	22	0	0
45	I	42	0	64	3	0
45	L	77	0	108	3	0
45	M	84	0	128	3	0
45	N	84	0	128	2	0
45	P	31	0	36	1	0
45	Y	36	0	49	1	0
45	Z	42	0	64	2	0
45	a	22	0	18	0	0
45	b	39	0	55	3	0
45	h	39	0	55	6	0
45	i	42	0	64	9	0
45	l	32	0	38	0	0
45	m	36	0	49	1	0
45	q	78	0	113	7	0
46	E	4	0	0	0	0
46	G	4	0	0	1	0
47	F	31	0	19	2	0
48	G	1	0	0	0	0
49	H	67	0	82	2	0
49	J	51	0	82	3	0
49	L	188	0	290	13	0
49	M	97	0	151	10	0
49	N	40	0	57	1	0
49	O	66	0	80	0	0
49	b	40	0	57	0	0
49	d	35	0	44	1	0
49	g	46	0	69	1	0
49	j	27	0	28	0	0
49	l	42	0	58	2	0
49	m	54	0	56	1	0
50	O	75	0	97	3	0
50	Z	49	0	42	1	0
50	a	60	0	64	8	0
50	b	59	0	62	1	0
51	P	48	0	25	4	0
52	R	1	0	0	0	0
53	T	37	0	0	1	0
53	U	37	0	0	1	0
All	All	68464	0	69193	1258	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 9.

All (1258) 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)
18:R:103:HIS:CD2	18:R:121:CYS:SG	2.60	0.93
10:J:31:THR:HG1	27:a:114:HIS:HE2	1.06	0.91
43:q:47:VAL:HG11	43:q:52:GLU:HG3	1.60	0.84
13:M:440:SER:O	40:n:102:ARG:NH2	2.15	0.80
4:D:279:GLU:HB3	9:I:82:ILE:HD13	1.64	0.78
2:B:163:ILE:HG22	2:B:164:VAL:HG13	1.67	0.77
6:F:44:GLY:O	6:F:240:ARG:NH2	2.19	0.76
3:C:239:TYR:HB2	23:W:97:GLN:HE22	1.51	0.74
29:c:94:LEU:O	29:c:103:ARG:NH2	2.19	0.74
5:E:189:THR:H	5:E:192:ARG:HB2	1.54	0.73
10:J:67:LEU:HD11	11:K:16:ILE:HG12	1.68	0.73
3:C:147:VAL:HG22	3:C:162:LYS:HG2	1.70	0.73
23:W:83:GLN:O	23:W:87:ASN:ND2	2.21	0.73
38:l:126:ARG:NH2	41:o:26:ASP:OD2	2.21	0.73
15:O:190:ASN:HD21	28:b:65:LEU:H	1.35	0.73
38:l:25:LYS:HD3	38:l:26:SER:H	1.51	0.73
7:G:246:GLU:OE1	17:Q:129:GLN:NE2	2.18	0.73
7:G:705:GLY:HA3	7:G:718:LYS:HD2	1.69	0.73
12:L:476:ILE:HG12	41:o:44:TYR:HB2	1.71	0.72
21:U:96:GLU:OE2	40:n:42:ARG:NH2	2.16	0.72
5:E:125:GLN:HB2	5:E:179:ALA:HB3	1.71	0.71
1:A:1:FME:HCN	27:a:68:LYS:HG2	1.71	0.71
9:I:212:GLN:NE2	9:I:216:ASP:OD1	2.22	0.71
1:A:48:GLY:O	2:B:105:ARG:NH2	2.24	0.71
12:L:257:VAL:HG13	12:L:317:ILE:HD11	1.73	0.71
28:b:47:ARG:NH2	28:b:54:ASP:OD1	2.24	0.71
4:D:80:ASN:O	14:N:287:ARG:NH2	2.19	0.70
10:J:101:ASN:ND2	27:a:126:ARG:O	2.24	0.70
12:L:23:ILE:O	12:L:27:SER:OG	2.08	0.70
8:H:37:ARG:HH22	8:H:59:MET:HE2	1.56	0.70
9:I:220:PRO:HB2	29:c:54:TYR:HB3	1.71	0.70
12:L:527:GLU:OE1	37:k:23:ARG:NH2	2.24	0.70
5:E:171:ALA:HB3	5:E:177:MET:HE2	1.72	0.70
14:N:71:ILE:HD11	14:N:121:LEU:HD21	1.73	0.70
4:D:313:ARG:NH2	4:D:355:GLU:OE2	2.23	0.69
7:G:59:CYS:HB3	7:G:70:CYS:HB3	1.73	0.69
38:l:144:ASP:O	38:l:146:LEU:N	2.25	0.69
9:I:115:ARG:NH2	18:R:72:TYR:O	2.24	0.69
16:P:173:GLU:OE2	16:P:188:ARG:NE	2.23	0.69
35:i:72:LYS:HB2	42:p:65:GLU:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:59:LEU:HD11	34:h:131:ILE:HD11	1.73	0.69
19:S:12:GLU:OE2	19:S:14:ARG:NH1	2.24	0.69
8:H:226:MET:HG2	8:H:229:LEU:HD12	1.75	0.69
16:P:125:SER:OG	16:P:128:ASP:OD2	2.09	0.69
6:F:274:GLU:OE2	6:F:287:HIS:NE2	2.26	0.68
22:V:23:THR:OG1	22:V:28:LEU:O	2.09	0.68
12:L:324:LEU:HD23	12:L:478:LEU:HD22	1.75	0.68
16:P:303:PRO:HA	45:P:502:PLC:H82	1.75	0.68
6:F:251:ARG:HH12	6:F:325:ALA:HB2	1.55	0.68
3:C:49:ARG:NH2	29:c:51:THR:OG1	2.25	0.68
4:D:230:MET:HE2	4:D:240:ARG:HE	1.59	0.68
8:H:345:CYS:O	28:b:47:ARG:NH1	2.27	0.68
21:U:56:ARG:NE	21:U:100:GLU:OE1	2.27	0.68
9:I:163:ILE:HG13	9:I:165:CYS:HB3	1.76	0.67
27:a:37:ARG:HH12	27:a:47:VAL:HG22	1.58	0.67
3:C:101:GLU:OE1	3:C:160:ARG:NH2	2.24	0.67
4:D:84:GLU:OE1	14:N:154:LYS:NZ	2.28	0.67
8:H:81:ILE:HD12	32:f:18:ARG:HD3	1.77	0.67
38:l:59:ASP:OD1	38:l:66:ASN:ND2	2.27	0.67
5:E:178:ILE:HG22	5:E:185:TYR:HB2	1.76	0.67
7:G:649:ARG:NH1	7:G:654:GLU:OE2	2.26	0.67
7:G:274:LEU:HD21	17:Q:134:ARG:HB2	1.75	0.67
8:H:316:ARG:NH1	8:H:318:ASP:OD1	2.28	0.67
7:G:618:ARG:NH2	7:G:631:ASP:OD1	2.27	0.67
2:B:34:LEU:O	16:P:136:ARG:NH2	2.28	0.66
13:M:36:ILE:HG22	13:M:37:LYS:HG3	1.78	0.66
4:D:191:THR:OG1	4:D:328:ASP:O	2.12	0.66
13:M:43:LYS:NZ	13:M:107:TRP:O	2.28	0.66
43:q:30:LYS:NZ	43:q:56:ARG:O	2.28	0.66
4:D:75:GLU:OE1	25:Y:73:LYS:NZ	2.29	0.66
1:A:67:ALA:HB3	1:A:125:ILE:HD13	1.77	0.66
6:F:346:ASP:OD2	6:F:433:ARG:NH2	2.28	0.66
7:G:32:ASP:OD2	7:G:99:THR:OG1	2.13	0.66
10:J:135:GLU:OE2	15:O:127:ARG:NH2	2.28	0.66
16:P:252:ARG:O	16:P:369:ARG:NH2	2.28	0.66
2:B:85:HIS:ND1	4:D:227:GLU:OE2	2.28	0.66
12:L:124:MET:HE2	12:L:143:ILE:HD11	1.76	0.66
33:g:82:ASP:N	33:g:82:ASP:OD1	2.29	0.66
7:G:210:ASN:ND2	7:G:716:ASP:OD1	2.28	0.66
7:G:329:VAL:HG23	7:G:331:PRO:HD3	1.77	0.66
13:M:179:LEU:HB3	14:N:436:ILE:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:115:PHE:O	25:Y:119:SER:OG	2.14	0.65
2:B:86:VAL:HG21	2:B:180:LEU:HD23	1.78	0.65
2:B:140:MET:HG2	2:B:175:PRO:HG2	1.77	0.65
3:C:65:ASN:HB3	3:C:68:GLU:HG2	1.78	0.65
10:J:112:ASP:O	27:a:100:GLN:NE2	2.29	0.65
13:M:484:THR:HG22	42:p:31:LEU:HD11	1.78	0.65
26:Z:81:ARG:NH2	27:a:98:SER:O	2.28	0.65
5:E:132:CYS:HA	5:E:175:ALA:HB1	1.77	0.65
6:F:192:GLU:OE1	6:F:193:GLU:N	2.28	0.65
27:a:115:ILE:HG23	27:a:116:ILE:HG13	1.78	0.65
2:B:106:GLN:NE2	8:H:226:MET:O	2.29	0.65
10:J:93:ASP:OD1	27:a:118:LYS:NZ	2.27	0.65
13:M:76:ARG:NH2	13:M:79:ASN:OD1	2.30	0.65
49:H:402:3PE:H2B2	26:Z:39:GLY:HA2	1.78	0.65
12:L:492:ASN:OD1	12:L:492:ASN:N	2.29	0.65
23:W:31:TYR:HB3	23:W:55:ILE:HD13	1.78	0.65
10:J:33:MET:HB3	32:f:4:LEU:HD13	1.78	0.64
8:H:148:ARG:HH12	8:H:214:ASN:HB3	1.62	0.64
12:L:96:VAL:O	12:L:100:SER:OG	2.14	0.64
3:C:154:ARG:NH2	22:V:94:GLU:OE1	2.31	0.64
4:D:273:ARG:NH2	4:D:276:GLU:OE2	2.28	0.64
4:D:470:ILE:HG23	4:D:475:LEU:HD12	1.80	0.64
14:N:89:ILE:HD12	14:N:337:LEU:HB3	1.78	0.64
20:T:104:PHE:HZ	20:T:118:VAL:HG13	1.63	0.64
21:U:62:GLU:O	37:k:8:ARG:NH2	2.26	0.64
6:F:30:TYR:HB2	6:F:32:LYS:HE2	1.80	0.63
12:L:124:MET:HE3	12:L:251:CYS:HA	1.79	0.63
16:P:254:SER:HB3	16:P:257:GLU:HG3	1.80	0.63
13:M:170:VAL:O	13:M:174:THR:OG1	2.14	0.63
3:C:208:ASP:OD1	3:C:209:TYR:N	2.31	0.63
12:L:4:LEU:O	12:L:8:THR:OG1	2.13	0.63
12:L:604:LEU:HD13	49:L:703:3PE:H352	1.81	0.63
17:Q:140:ASP:OD1	17:Q:140:ASP:N	2.32	0.63
22:V:34:PRO:HG2	22:V:80:ILE:HD11	1.79	0.63
6:F:50:LYS:HE2	6:F:173:SER:HB3	1.81	0.63
6:F:101:ALA:HB1	6:F:115:ILE:HD11	1.80	0.63
7:G:346:LEU:HD21	7:G:647:LEU:HD13	1.79	0.63
24:X:19:LYS:HB3	27:a:103:SER:HB2	1.82	0.62
29:c:68:ASN:OD1	29:c:73:ARG:NH1	2.32	0.62
9:I:120:GLU:OE2	9:I:145:ARG:NH2	2.28	0.62
13:M:247:ILE:HG23	13:M:343:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:172:ASP:OD2	27:a:120:SER:OG	2.17	0.62
21:U:111:ASP:OD1	21:U:111:ASP:N	2.33	0.62
22:V:66:PHE:HA	22:V:69:GLU:HB2	1.82	0.62
13:M:279:ILE:HA	13:M:282:ILE:HD12	1.82	0.62
21:U:94:LEU:HD13	21:U:110:ALA:HB1	1.81	0.62
45:B:302:PLC:O2P	16:P:302:GLN:NE2	2.33	0.62
17:Q:35:THR:OG1	17:Q:36:ASP:N	2.32	0.62
11:K:51:ILE:HD13	14:N:130:ILE:HD11	1.81	0.62
4:D:158:LEU:HD11	4:D:443:ILE:HD13	1.81	0.62
18:R:21:ARG:O	18:R:40:ARG:NH2	2.32	0.62
3:C:229:ARG:NE	3:C:240:GLU:OE2	2.29	0.61
13:M:268:ASN:OD1	13:M:268:ASN:N	2.31	0.61
13:M:300:ASP:OD2	13:M:360:ARG:NH1	2.32	0.61
6:F:70:ARG:O	6:F:72:ARG:NH1	2.32	0.61
7:G:177:THR:N	44:G:804:SF4:S4	2.70	0.61
8:H:76:HIS:ND1	8:H:79:ASP:OD1	2.32	0.61
12:L:371:TYR:OH	37:k:27:ALA:O	2.14	0.61
17:Q:53:ARG:NH2	17:Q:100:ASP:OD1	2.31	0.61
24:X:73:LYS:NZ	34:h:165:THR:O	2.25	0.61
28:b:47:ARG:HG3	28:b:51:LEU:HD12	1.82	0.61
6:F:29:VAL:O	6:F:117:LYS:NZ	2.20	0.61
6:F:303:PRO:HA	6:F:338:VAL:HA	1.82	0.61
17:Q:56:ARG:HH21	17:Q:127:TYR:HE2	1.48	0.61
12:L:217:LEU:HD13	12:L:277:ILE:HG12	1.82	0.61
13:M:191:ILE:HG13	13:M:192:ILE:HG13	1.81	0.61
16:P:310:LEU:O	16:P:313:SER:OG	2.16	0.61
4:D:161:VAL:HG11	4:D:204:MET:HG2	1.83	0.61
7:G:301:LYS:HD2	16:P:25:THR:HG21	1.82	0.61
15:O:185:TYR:O	28:b:67:ASN:ND2	2.34	0.61
3:C:72:GLU:OE2	29:c:154:LYS:NZ	2.34	0.61
6:F:86:MET:HG3	6:F:133:MET:HG2	1.83	0.61
8:H:213:ASP:HB3	8:H:314:ARG:HD3	1.83	0.61
31:e:21:GLN:NE2	34:h:150:PRO:O	2.34	0.60
4:D:156:ASP:N	4:D:156:ASP:OD1	2.33	0.60
40:n:64:LEU:HD12	40:n:67:ILE:HD12	1.82	0.60
43:q:67:ARG:NH2	45:q:402:PLC:O1P	2.34	0.60
16:P:156:ASN:HD21	16:P:317:GLN:HA	1.66	0.60
7:G:144:ASP:OD1	29:c:73:ARG:NH2	2.34	0.60
4:D:433:ASP:OD1	4:D:433:ASP:N	2.34	0.60
28:b:5:ASP:O	28:b:15:ARG:NH2	2.35	0.60
6:F:267:ASN:HB2	6:F:290:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:126:ARG:NH1	38:l:128:TYR:OH	2.34	0.60
4:D:92:LYS:HB2	20:T:127:LEU:HB2	1.84	0.60
13:M:437:SER:OG	13:M:438:VAL:N	2.35	0.60
50:a:201:CDL:OB3	43:q:5:GLN:NE2	2.34	0.60
7:G:684:ILE:O	7:G:710:LYS:NZ	2.33	0.60
49:L:706:3PE:H392	25:Y:50:LEU:HG	1.83	0.60
17:Q:112:ARG:NH2	17:Q:130:GLU:OE2	2.32	0.60
43:q:28:ASP:OD2	43:q:56:ARG:NH2	2.35	0.60
1:A:74:LEU:HD23	10:J:154:LEU:HD12	1.83	0.59
6:F:382:ARG:NH2	6:F:392:GLU:OE1	2.34	0.59
6:F:413:ASP:OD1	6:F:413:ASP:N	2.34	0.59
12:L:172:ARG:NH2	13:M:387:THR:O	2.35	0.59
27:a:38:GLY:O	27:a:44:LYS:NZ	2.34	0.59
6:F:86:MET:SD	6:F:225:THR:OG1	2.59	0.59
6:F:347:ILE:HD12	6:F:350:ALA:HB3	1.82	0.59
4:D:311:MET:HG2	4:D:348:ARG:HD3	1.84	0.59
4:D:323:LYS:O	29:c:153:ASN:ND2	2.33	0.59
6:F:78:PRO:HB2	6:F:81:LEU:HB3	1.83	0.59
8:H:9:ILE:HA	8:H:12:ILE:HG22	1.85	0.59
12:L:347:ILE:HD13	12:L:355:GLN:HG2	1.84	0.59
3:C:132:VAL:HB	3:C:184:PHE:HB3	1.85	0.59
16:P:120:PHE:HB2	16:P:125:SER:HA	1.84	0.59
4:D:233:TYR:O	4:D:237:SER:OG	2.21	0.59
7:G:432:VAL:HG11	7:G:452:LEU:HB2	1.85	0.59
12:L:1:FME:HE2	12:L:45:ILE:HG21	1.84	0.59
24:X:70:LYS:HE2	28:b:65:LEU:HD13	1.84	0.59
5:E:131:PRO:HA	5:E:134:LEU:HD12	1.85	0.59
7:G:262:THR:HG22	7:G:267:VAL:HG22	1.83	0.59
12:L:642:LEU:HD21	49:L:704:3PE:H242	1.85	0.59
14:N:183:LEU:HD13	14:N:188:TYR:HB3	1.84	0.59
16:P:118:GLU:OE1	16:P:312:ARG:NH1	2.36	0.59
22:V:124:ASP:N	22:V:124:ASP:OD1	2.34	0.59
10:J:104:ASP:OD1	32:f:63:LYS:NZ	2.36	0.59
14:N:53:GLY:O	34:h:145:ARG:NH1	2.36	0.59
16:P:110:ILE:HD13	16:P:235:ALA:HB1	1.85	0.59
20:T:68:LYS:HE2	20:T:83:GLY:HA3	1.85	0.59
16:P:205:GLN:O	16:P:259:ARG:NH1	2.26	0.58
22:V:35:ARG:NH2	22:V:74:VAL:O	2.33	0.58
43:q:95:GLU:N	43:q:95:GLU:OE1	2.35	0.58
27:a:1:MET:HG3	43:q:0:ACE:H1	1.84	0.58
1:A:30:SER:OG	16:P:302:GLN:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:118:GLU:OE1	16:P:309:GLN:NE2	2.37	0.58
18:R:29:ASP:O	18:R:35:GLN:NE2	2.36	0.58
25:Y:184:ILE:HG21	42:p:92:LYS:HG3	1.85	0.58
1:A:49:PRO:O	2:B:130:GLN:NE2	2.36	0.58
3:C:91:PHE:HB3	3:C:110:ALA:HB1	1.84	0.58
18:R:82:PRO:O	18:R:84:ARG:NH1	2.35	0.58
3:C:49:ARG:HD2	29:c:45:PRO:HG3	1.85	0.58
45:B:303:PLC:H31	45:q:402:PLC:H1'2	1.85	0.58
9:I:114:ARG:HD3	9:I:211:ILE:HG21	1.84	0.58
38:l:76:ASP:OD2	39:m:22:ARG:NH1	2.26	0.58
25:Y:211:ARG:NH1	39:m:58:GLU:OE2	2.36	0.58
7:G:354:ASP:OD1	7:G:639:ARG:NH2	2.37	0.58
13:M:196:ASP:OD1	34:h:117:TYR:OH	2.17	0.58
43:q:1:SER:HA	43:q:6:ARG:HD3	1.85	0.58
3:C:119:LYS:NZ	3:C:177:LEU:O	2.37	0.57
12:L:452:ASP:OD1	12:L:452:ASP:N	2.36	0.57
20:T:55:LEU:HD22	20:T:74:LEU:HG	1.86	0.57
3:C:53:ARG:NH1	26:Z:5:LEU:O	2.37	0.57
43:q:6:ARG:NH1	43:q:52:GLU:OE2	2.38	0.57
23:W:76:MET:HG2	23:W:80:MET:HE3	1.86	0.57
16:P:226:GLN:NE2	16:P:332:VAL:O	2.36	0.57
22:V:89:SER:OG	22:V:98:GLN:NE2	2.36	0.57
4:D:443:ILE:HB	4:D:482:ARG:HD3	1.86	0.57
12:L:534:LEU:HD22	40:n:35:ILE:HG12	1.87	0.57
5:E:48:THR:OG1	5:E:51:ASN:ND2	2.32	0.57
6:F:189:ILE:HG12	6:F:363:CYS:HB3	1.86	0.57
7:G:356:VAL:HG12	7:G:361:SER:HB3	1.86	0.57
4:D:196:ILE:HG23	4:D:229:LEU:HD22	1.87	0.57
12:L:220:SER:O	12:L:224:SER:OG	2.22	0.57
13:M:85:ASP:CG	13:M:263:ARG:HH22	2.13	0.57
9:I:90:ALA:HB2	27:a:1:MET:HE1	1.87	0.57
12:L:616:ILE:O	12:L:619:SER:OG	2.23	0.57
13:M:370:THR:HA	45:i:101:PLC:H71	1.86	0.57
13:M:486:ILE:HD12	42:p:79:ILE:HG22	1.87	0.56
19:S:7:PRO:HB2	19:S:9:VAL:HG22	1.86	0.56
7:G:531:PRO:O	7:G:535:ASN:ND2	2.32	0.56
1:A:45:GLU:HB3	2:B:129:ASP:HB3	1.85	0.56
2:B:37:ASP:OD1	2:B:37:ASP:N	2.38	0.56
12:L:361:GLY:O	12:L:445:TYR:OH	2.13	0.56
13:M:297:LYS:O	39:m:22:ARG:NH2	2.38	0.56
13:M:301:LEU:HB3	13:M:349:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:223:HIS:HE2	16:P:343:TYR:HH	1.49	0.56
4:D:60:GLU:HG2	4:D:65:LYS:HB3	1.87	0.56
42:p:34:GLN:NE2	42:p:80:GLN:OE1	2.38	0.56
12:L:169:LEU:HD12	49:l:201:3PE:H222	1.87	0.56
14:N:90:THR:OG1	14:N:96:ASP:OD1	2.22	0.56
15:O:21:ARG:NH2	15:O:93:GLU:OE2	2.38	0.56
10:J:109:TYR:CE1	27:a:104:ASN:HB3	2.40	0.56
12:L:93:SER:O	12:L:97:HIS:ND1	2.36	0.56
33:g:76:ARG:HH22	33:g:97:ASN:HB2	1.69	0.56
34:h:66:LYS:HG2	45:h:201:PLC:H81	1.87	0.56
2:B:162:ARG:NH2	3:C:227:GLU:OE2	2.36	0.56
27:a:114:HIS:HB3	27:a:117:MET:HB2	1.87	0.56
5:E:134:LEU:O	6:F:265:HIS:NE2	2.39	0.56
8:H:93:SER:O	8:H:97:SER:OG	2.21	0.56
10:J:143:ILE:HD11	11:K:51:ILE:HG12	1.88	0.56
11:K:40:ASP:OD2	31:e:49:ARG:NH2	2.27	0.56
23:W:16:ASP:OD2	23:W:19:GLU:N	2.33	0.56
24:X:142:LYS:NZ	26:Z:58:GLU:OE2	2.29	0.56
1:A:1:FME:HE2	27:a:63:THR:H	1.71	0.55
7:G:557:ASP:OD1	7:G:557:ASP:N	2.39	0.55
12:L:379:LEU:HD22	12:L:384:ILE:HG13	1.87	0.55
14:N:312:ASN:ND2	34:h:133:PHE:O	2.37	0.55
33:g:156:ILE:HG23	33:g:160:LYS:HD2	1.88	0.55
41:o:36:ASN:OD1	41:o:39:ARG:NH2	2.39	0.55
14:N:210:ILE:O	14:N:220:TYR:OH	2.17	0.55
49:M:504:3PE:H3I2	45:h:201:PLC:H2A2	1.87	0.55
3:C:144:PHE:HZ	3:C:217:ARG:HE	1.54	0.55
4:D:198:ARG:NH2	4:D:420:GLU:O	2.33	0.55
9:I:69:LYS:HE2	45:Z:201:PLC:H12	1.88	0.55
11:K:74:ARG:NH2	20:T:136:THR:OG1	2.38	0.55
13:M:87:ILE:HD13	13:M:262:ILE:HD13	1.87	0.55
1:A:46:LYS:HD3	2:B:132:PRO:HA	1.88	0.55
8:H:36:GLU:OE1	8:H:242:TYR:OH	2.23	0.55
12:L:61:ILE:HG22	12:L:62:MET:HG2	1.87	0.55
13:M:90:LEU:HD13	13:M:474:VAL:HG13	1.88	0.55
38:l:120:GLU:OE2	39:m:77:TYR:OH	2.19	0.55
14:N:24:LYS:NZ	14:N:88:ASN:OD1	2.39	0.55
14:N:291:LEU:HD11	14:N:445:TYR:CD1	2.41	0.55
19:S:2:SER:OG	19:S:3:LYS:N	2.38	0.55
7:G:162:ILE:HB	7:G:211:VAL:HG23	1.89	0.55
7:G:164:PRO:HD2	7:G:707:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:256:SER:HB3	7:G:279:ASN:HB3	1.88	0.55
7:G:316:GLU:HG2	23:W:118:LEU:HD11	1.88	0.55
16:P:111:VAL:HG23	16:P:146:VAL:HG11	1.89	0.55
29:c:65:ILE:HG13	29:c:66:VAL:HG13	1.88	0.55
38:l:59:ASP:OD1	38:l:59:ASP:N	2.39	0.55
2:B:110:MET:HB3	2:B:137:VAL:HG22	1.88	0.55
15:O:127:ARG:NH1	31:e:2:ALA:O	2.40	0.55
16:P:345:LYS:NZ	23:W:45:ASP:OD1	2.30	0.55
38:l:152:ILE:HG13	39:m:75:GLN:HE22	1.72	0.55
39:m:51:GLY:HA3	45:m:702:PLC:H2A2	1.89	0.55
10:J:95:LEU:O	32:f:44:ARG:NH1	2.40	0.54
13:M:459:TRP:NE1	45:h:201:PLC:O2P	2.38	0.54
6:F:37:LEU:HD11	6:F:46:TRP:HE1	1.72	0.54
7:G:36:VAL:HG22	7:G:51:ALA:HB2	1.89	0.54
12:L:108:PRO:HB2	35:i:19:TRP:HA	1.89	0.54
24:X:150:ASP:OD1	24:X:150:ASP:N	2.28	0.54
5:E:138:ASP:OD1	5:E:138:ASP:N	2.38	0.54
12:L:293:MET:O	12:L:428:ARG:NH1	2.40	0.54
13:M:283:ILE:O	13:M:287:THR:OG1	2.24	0.54
14:N:390:ASN:HB3	14:N:393:ILE:HG22	1.88	0.54
16:P:210:GLY:HA3	16:P:289:LEU:HD11	1.88	0.54
18:R:51:ARG:NH2	18:R:69:PRO:O	2.28	0.54
33:g:172:GLU:OE1	42:p:6:ARG:NH2	2.39	0.54
36:j:47:TYR:CD2	36:j:48:PRO:HD3	2.42	0.54
6:F:50:LYS:NZ	6:F:171:CYS:O	2.32	0.54
7:G:353:LYS:NZ	7:G:524:VAL:O	2.31	0.54
4:D:285:ARG:NH1	45:I:303:PLC:OB	2.41	0.54
7:G:276:ASP:O	7:G:417:ARG:NH2	2.40	0.54
8:H:324:CYS:HG	8:H:325:TRP:CD1	2.25	0.54
25:Y:181:ASN:HD21	42:p:16:ASP:HA	1.73	0.54
27:a:35:ARG:HA	27:a:44:LYS:HD3	1.88	0.54
4:D:152:LEU:HD22	4:D:247:ARG:HG2	1.88	0.54
6:F:34:GLY:O	6:F:43:ARG:NH2	2.41	0.54
6:F:407:THR:HB	44:F:501:SF4:S1	2.48	0.54
11:K:28:GLY:HA2	27:a:117:MET:HE3	1.88	0.54
20:T:105:ASP:N	20:T:105:ASP:OD1	2.38	0.54
7:G:214:GLU:HG3	7:G:412:ALA:HB1	1.89	0.54
10:J:99:GLU:HG3	27:a:107:ARG:HD2	1.90	0.54
20:T:86:SER:OG	23:W:21:ARG:NH2	2.40	0.54
22:V:134:LEU:HD12	29:c:84:ALA:HB2	1.90	0.54
7:G:400:ILE:HG12	7:G:471:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:87:LEU:HD13	23:W:56:ARG:HG3	1.89	0.54
6:F:296:ASP:O	6:F:343:LYS:NZ	2.31	0.54
6:F:304:GLY:O	6:F:335:THR:OG1	2.15	0.54
7:G:58:TYR:O	7:G:178:ARG:NH2	2.34	0.54
7:G:280:GLU:HB2	7:G:417:ARG:HH12	1.73	0.54
12:L:288:SER:OG	12:L:307:MET:SD	2.66	0.54
8:H:217:ALA:HB3	8:H:220:GLU:HB2	1.90	0.53
16:P:218:GLU:OE1	16:P:316:ASN:ND2	2.40	0.53
28:b:3:ILE:HD13	28:b:3:ILE:H	1.72	0.53
7:G:688:TYR:O	7:G:694:SER:HB3	2.08	0.53
9:I:141:GLU:HB2	9:I:154:LYS:HB3	1.90	0.53
12:L:155:PHE:HZ	45:i:101:PLC:H61	1.73	0.53
12:L:574:ASN:OD1	13:M:298:GLN:NE2	2.41	0.53
24:X:178:GLN:O	24:X:182:SER:OG	2.26	0.53
35:i:16:THR:OG1	45:i:101:PLC:O2P	2.27	0.53
6:F:122:LEU:HD13	6:F:229:VAL:HG23	1.91	0.53
7:G:373:VAL:HG11	7:G:531:PRO:HA	1.91	0.53
10:J:54:ILE:O	10:J:58:ALA:HB3	2.09	0.53
12:L:72:VAL:HG21	12:L:134:LEU:HD12	1.90	0.53
16:P:220:TYR:N	16:P:317:GLN:OE1	2.40	0.53
7:G:338:ALA:HB3	7:G:364:VAL:HG12	1.90	0.53
13:M:410:PRO:O	13:M:414:SER:OG	2.26	0.53
22:V:42:TYR:HB2	22:V:71:LEU:HD13	1.90	0.53
2:B:38:ILE:HD12	16:P:96:ARG:HD2	1.90	0.53
13:M:278:PRO:HG3	39:m:58:GLU:HG3	1.91	0.53
23:W:28:TYR:CZ	23:W:32:LEU:HD11	2.44	0.53
7:G:247:THR:OG1	7:G:248:ILE:N	2.39	0.53
14:N:498:LEU:HD12	30:d:15:VAL:HG22	1.90	0.53
27:a:2:ILE:HD12	50:a:201:CDL:HB4	1.90	0.53
5:E:175:ALA:O	5:E:177:MET:N	2.42	0.53
9:I:78:ARG:HG2	9:I:82:ILE:HD11	1.90	0.53
14:N:491:TYR:O	14:N:495:SER:OG	2.26	0.53
2:B:119:LYS:HE3	3:C:209:TYR:CZ	2.43	0.53
3:C:48:LEU:O	3:C:53:ARG:NH2	2.42	0.53
13:M:161:ASN:N	13:M:161:ASN:OD1	2.42	0.53
1:A:69:ILE:HD13	10:J:65:PHE:HE1	1.74	0.53
4:D:107:HIS:HD2	4:D:109:ALA:H	1.55	0.53
5:E:63:PRO:HG2	5:E:66:TYR:HB2	1.90	0.53
7:G:312:ASP:OD2	16:P:25:THR:OG1	2.25	0.53
13:M:85:ASP:OD1	13:M:263:ARG:NH2	2.40	0.53
13:M:297:LYS:NZ	38:l:77:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LYS:HD2	3:C:208:ASP:HA	1.91	0.53
7:G:241:GLU:OE1	7:G:263:ARG:NH1	2.41	0.53
12:L:271:PRO:HA	12:L:274:LEU:HD12	1.90	0.53
13:M:469:ILE:HD12	49:M:504:3PE:H3A1	1.91	0.53
1:A:40:ILE:HD12	1:A:47:SER:HB3	1.92	0.52
6:F:383:PHE:HZ	6:F:393:ILE:HA	1.74	0.52
7:G:59:CYS:O	7:G:181:ARG:NH2	2.33	0.52
14:N:46:THR:OG1	14:N:49:ASN:OD1	2.27	0.52
17:Q:53:ARG:HH12	17:Q:79:TRP:HB3	1.75	0.52
18:R:133:ASP:OD1	18:R:133:ASP:N	2.40	0.52
3:C:113:GLN:OE1	3:C:113:GLN:N	2.42	0.52
4:D:286:ILE:HG23	8:H:315:LEU:HD13	1.90	0.52
12:L:564:ARG:NH2	38:l:83:PRO:O	2.42	0.52
16:P:21:LYS:HG2	16:P:147:SER:HB2	1.91	0.52
25:Y:185:LYS:NZ	25:Y:193:GLU:OE2	2.42	0.52
1:A:115:ILE:HG23	45:b:102:PLC:H2'1	1.91	0.52
6:F:457:LEU:HD12	6:F:462:VAL:HG21	1.91	0.52
16:P:188:ARG:NH1	16:P:246:GLU:OE2	2.37	0.52
33:g:226:LEU:HD22	42:p:37:ARG:HD2	1.90	0.52
38:l:90:GLN:HB2	38:l:93:ILE:HD13	1.91	0.52
4:D:421:ALA:HB2	4:D:426:MET:HE2	1.90	0.52
5:E:196:ILE:HG12	5:E:206:PRO:HG3	1.91	0.52
7:G:279:ASN:HA	7:G:413:VAL:HG11	1.91	0.52
13:M:373:PRO:HG2	35:i:14:PRO:HG3	1.91	0.52
3:C:143:ARG:HD2	3:C:167:GLU:HG2	1.91	0.52
8:H:24:SER:OG	27:a:16:GLY:O	2.20	0.52
12:L:388:THR:HG22	12:L:470:GLY:H	1.72	0.52
4:D:307:LEU:HD13	4:D:311:MET:HE2	1.92	0.52
4:D:398:ILE:HG23	7:G:135:GLN:HG2	1.92	0.52
49:L:704:3PE:H341	49:L:705:3PE:H242	1.91	0.52
13:M:137:LEU:HD22	13:M:264:LEU:HD22	1.92	0.52
16:P:69:PRO:HA	16:P:91:VAL:O	2.10	0.52
23:W:54:LYS:HD3	23:W:99:PHE:HD1	1.74	0.52
2:B:115:THR:HA	2:B:143:CYS:HB3	1.91	0.52
4:D:456:HIS:HB2	23:W:2:THR:HG23	1.92	0.52
6:F:21:ASP:OD1	6:F:21:ASP:N	2.42	0.52
6:F:188:TYR:HB3	6:F:361:GLU:HB3	1.92	0.52
42:p:44:CYS:SG	42:p:73:MET:HE1	2.49	0.52
2:B:57:PHE:HB3	45:B:302:PLC:H3A1	1.92	0.52
4:D:338:ALA:HB2	4:D:354:THR:HG21	1.91	0.52
7:G:38:ILE:HD11	7:G:91:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:121:GLU:O	9:I:151:ARG:NH1	2.43	0.52
21:U:60:ILE:HG12	37:k:9:ARG:NH2	2.26	0.52
4:D:107:HIS:NE2	8:H:219:SER:O	2.34	0.51
16:P:175:VAL:O	16:P:179:ASN:ND2	2.33	0.51
22:V:49:LEU:HD11	22:V:63:VAL:HB	1.91	0.51
36:j:55:HIS:N	36:j:58:GLU:OE1	2.43	0.51
5:E:49:LYS:HA	5:E:52:LEU:HD12	1.92	0.51
5:E:71:VAL:HG22	5:E:97:LEU:HD12	1.91	0.51
2:B:71:PRO:HA	2:B:109:ILE:HB	1.92	0.51
7:G:382:ARG:HA	7:G:385:TYR:CE2	2.45	0.51
8:H:191:PRO:HB3	26:Z:41:GLY:HA3	1.93	0.51
14:N:477:ASN:ND2	14:N:480:GLU:OE2	2.43	0.51
5:E:79:GLN:NE2	5:E:115:ASN:OD1	2.43	0.51
8:H:34:VAL:HG22	8:H:59:MET:HB3	1.91	0.51
11:K:77:GLU:HG3	11:K:78:GLU:H	1.76	0.51
25:Y:181:ASN:ND2	42:p:15:ILE:O	2.43	0.51
41:o:7:PRO:HG3	41:o:31:LEU:HD12	1.91	0.51
43:q:75:PRO:HD3	43:q:107:HIS:CE1	2.46	0.51
3:C:124:ALA:HB1	3:C:126:PHE:HE2	1.76	0.51
12:L:131:ASP:OD1	12:L:132:ASN:ND2	2.39	0.51
17:Q:37:LEU:HD12	17:Q:37:LEU:H	1.75	0.51
29:c:43:ARG:NH2	43:q:83:TYR:O	2.43	0.51
4:D:82:GLN:OE1	14:N:368:ASN:ND2	2.43	0.51
6:F:404:GLU:OE2	6:F:420:GLN:NE2	2.31	0.51
13:M:65:ASN:ND2	34:h:105:LYS:O	2.40	0.51
26:Z:100:GLU:HB2	27:a:147:MET:HE2	1.91	0.51
34:h:74:TRP:O	34:h:78:THR:OG1	2.26	0.51
7:G:354:ASP:OD2	7:G:630:TYR:OH	2.28	0.51
7:G:446:GLY:HA3	7:G:451:ALA:HB1	1.93	0.51
12:L:254:ILE:HD12	12:L:329:LEU:HD11	1.93	0.51
20:T:75:GLN:OE1	20:T:75:GLN:N	2.43	0.51
2:B:78:CYS:HB3	4:D:160:TYR:HB3	1.92	0.51
4:D:257:ALA:O	29:c:50:GLN:NE2	2.43	0.51
6:F:280:LEU:HD22	6:F:316:CYS:HB3	1.93	0.51
10:J:156:LEU:HD13	14:N:145:ILE:HD12	1.93	0.51
22:V:73:ILE:O	22:V:77:ASN:ND2	2.36	0.51
4:D:321:ILE:HB	4:D:420:GLU:HB2	1.93	0.51
26:Z:26:ARG:HH21	50:Z:202:CDL:HA31	1.76	0.51
39:m:42:PHE:HE1	49:m:701:3PE:H352	1.76	0.51
6:F:301:VAL:HG12	6:F:303:PRO:HD3	1.93	0.51
7:G:586:LYS:NZ	7:G:613:ASP:OD1	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:139:LEU:HD22	14:N:130:ILE:HD12	1.93	0.51
14:N:169:ILE:HG23	27:a:121:PRO:HG2	1.93	0.51
14:N:208:LEU:HD22	14:N:244:ILE:HG23	1.93	0.51
45:N:603:PLC:O1P	30:d:23:ARG:NH1	2.37	0.51
7:G:395:GLU:HB3	7:G:424:ARG:NH2	2.26	0.50
2:B:93:GLN:HE22	2:B:100:PHE:HD2	1.57	0.50
3:C:273:LYS:O	29:c:99:ALA:N	2.44	0.50
6:F:371:GLU:OE1	7:G:118:ASN:ND2	2.44	0.50
6:F:382:ARG:NH1	7:G:150:GLU:OE1	2.44	0.50
16:P:47:GLY:HA2	16:P:52:GLY:HA3	1.93	0.50
19:S:12:GLU:OE1	19:S:62:ARG:NH2	2.34	0.50
28:b:65:LEU:HD11	34:h:162:PHE:HE1	1.75	0.50
31:e:31:LYS:NZ	34:h:172:GLU:OE2	2.41	0.50
12:L:209:ILE:HG22	12:L:213:LEU:HD12	1.93	0.50
12:L:640:ILE:HG13	49:L:703:3PE:H221	1.92	0.50
39:m:12:ASP:O	39:m:16:GLN:HG2	2.11	0.50
6:F:362:SER:HB2	6:F:369:CYS:SG	2.50	0.50
13:M:390:PRO:HA	13:M:395:PHE:CG	2.46	0.50
24:X:105:GLU:OE1	24:X:105:GLU:N	2.37	0.50
31:e:19:GLU:CD	31:e:22:ARG:HH21	2.19	0.50
6:F:28:ASN:HB3	6:F:118:GLU:HG2	1.94	0.50
6:F:46:TRP:H	6:F:46:TRP:CD1	2.29	0.50
6:F:274:GLU:HB3	6:F:278:ILE:HG13	1.93	0.50
7:G:183:LEU:HA	7:G:187:ALA:HB3	1.93	0.50
7:G:242:LEU:HB3	7:G:261:ASP:HB3	1.93	0.50
49:g:301:3PE:H3A1	34:h:75:LEU:HD23	1.92	0.50
11:K:1:FME:O	11:K:4:ILE:HG12	2.12	0.50
6:F:304:GLY:HA2	6:F:336:ALA:N	2.26	0.50
7:G:242:LEU:O	7:G:244:ARG:NH1	2.45	0.50
9:I:122:ARG:NH1	9:I:174:VAL:O	2.43	0.50
14:N:313:GLU:HA	14:N:316:ILE:HD12	1.93	0.50
15:O:103:LYS:O	15:O:106:SER:OG	2.24	0.50
16:P:356:ASN:OD1	23:W:40:ASN:ND2	2.43	0.50
6:F:400:SER:HB2	6:F:416:ALA:HB1	1.94	0.50
22:V:39:ILE:HD11	22:V:75:GLU:HG2	1.93	0.50
36:j:22:PRO:HA	36:j:25:VAL:HB	1.94	0.50
1:A:105:LEU:HD13	50:O:201:CDL:H802	1.93	0.50
7:G:407:PRO:HB2	7:G:415:ASN:HB2	1.94	0.50
8:H:21:PHE:HE1	8:H:103:PHE:HE1	1.58	0.50
10:J:158:VAL:O	11:K:72:ARG:NH1	2.45	0.50
12:L:19:PHE:HE2	45:M:501:PLC:HEA3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:46:SER:O	26:Z:50:ARG:HG3	2.12	0.50
26:Z:121:LYS:HG2	31:e:73:GLU:HB3	1.94	0.50
4:D:105:PRO:HB3	4:D:113:VAL:HG12	1.94	0.49
6:F:342:ASN:HD22	6:F:342:ASN:H	1.60	0.49
34:h:138:ASP:N	34:h:138:ASP:OD1	2.44	0.49
2:B:73:THR:O	4:D:106:GLN:NE2	2.38	0.49
3:C:91:PHE:CZ	3:C:113:GLN:HG2	2.47	0.49
4:D:313:ARG:O	4:D:340:GLY:N	2.39	0.49
7:G:601:ARG:HH22	17:Q:78:ASP:CG	2.18	0.49
12:L:636:LEU:HD22	49:L:706:3PE:H2B1	1.94	0.49
27:a:140:LYS:HD3	31:e:56:TYR:HB2	1.93	0.49
29:c:42:TYR:HD2	43:q:54:HIS:CE1	2.30	0.49
6:F:284:LEU:HD13	6:F:291:ILE:HD11	1.93	0.49
6:F:348:ILE:HD12	6:F:433:ARG:HG3	1.94	0.49
7:G:79:ARG:NH2	7:G:96:SER:H	2.10	0.49
9:I:79:GLY:HA2	9:I:82:ILE:HD12	1.93	0.49
11:K:15:ILE:HG21	14:N:157:LEU:HD21	1.94	0.49
33:g:79:SER:OG	33:g:82:ASP:OD1	2.26	0.49
3:C:105:TYR:CE2	3:C:162:LYS:HD2	2.48	0.49
6:F:33:TYR:HB3	6:F:43:ARG:HE	1.77	0.49
9:I:175:ASP:N	9:I:175:ASP:OD1	2.45	0.49
14:N:311:SER:H	14:N:314:SER:HB2	1.78	0.49
19:S:1:SER:HB3	19:S:4:PHE:HD2	1.77	0.49
50:a:201:CDL:H122	50:a:201:CDL:HA62	1.94	0.49
32:f:68:LYS:NZ	32:f:71:ASP:OD2	2.39	0.49
2:B:86:VAL:HG12	2:B:93:GLN:HB3	1.94	0.49
4:D:358:GLN:HE21	29:c:168:MET:HE3	1.78	0.49
6:F:366:CYS:N	44:F:501:SF4:S3	2.85	0.49
7:G:310:PHE:CE2	43:q:135:VAL:HG22	2.47	0.49
2:B:114:GLY:HA2	44:B:301:SF4:S2	2.52	0.49
7:G:401:LEU:HD23	7:G:472:ILE:HG12	1.94	0.49
12:L:442:LYS:NZ	36:j:13:ALA:O	2.36	0.49
13:M:144:PHE:CZ	13:M:224:LYS:HG3	2.47	0.49
22:V:113:LYS:HA	22:V:115:TRP:CH2	2.47	0.49
2:B:87:SER:HA	2:B:93:GLN:HG2	1.93	0.49
3:C:126:PHE:HB3	3:C:150:LEU:HB3	1.95	0.49
4:D:435:SER:OG	4:D:436:GLU:N	2.45	0.49
6:F:102:ASP:N	6:F:102:ASP:OD1	2.43	0.49
6:F:230:GLU:OE2	6:F:258:LYS:NZ	2.46	0.49
6:F:363:CYS:SG	6:F:364:GLY:N	2.85	0.49
7:G:682:ASN:OD1	7:G:682:ASN:N	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:157:ARG:NH1	40:n:95:PHE:O	2.44	0.49
13:M:84:ILE:HG12	13:M:133:ILE:HG22	1.95	0.49
1:A:29:GLU:OE1	2:B:61:LYS:NZ	2.44	0.49
6:F:209:LEU:HD13	17:Q:141:TYR:CE1	2.48	0.49
6:F:365:GLN:N	44:F:501:SF4:S3	2.80	0.49
7:G:244:ARG:HB3	7:G:259:ARG:HD2	1.94	0.49
7:G:469:LYS:HB3	7:G:506:TRP:CE2	2.47	0.49
13:M:412:ILE:HD12	39:m:54:ALA:HB2	1.95	0.49
38:l:133:LEU:HD11	41:o:25:ARG:HB2	1.95	0.49
6:F:99:VAL:HG13	6:F:232:VAL:HG21	1.93	0.49
6:F:230:GLU:O	6:F:234:VAL:HG23	2.12	0.49
6:F:377:GLN:NE2	6:F:381:ASP:OD2	2.46	0.49
12:L:205:ASP:O	12:L:209:ILE:HG13	2.12	0.49
19:S:19:GLN:OE1	19:S:19:GLN:N	2.45	0.49
4:D:423:LYS:HD2	4:D:474:ASP:HB3	1.94	0.49
6:F:93:GLU:OE1	6:F:222:ARG:NH2	2.46	0.49
8:H:291:SER:OG	27:a:21:GLY:HA3	2.12	0.49
17:Q:57:ILE:HG12	17:Q:77:ILE:HG12	1.95	0.49
4:D:169:VAL:HG23	4:D:419:ILE:HG23	1.94	0.48
6:F:250:GLY:HA3	6:F:276:MET:HB2	1.95	0.48
12:L:226:GLN:HE22	12:L:310:VAL:HG12	1.77	0.48
4:D:214:GLY:HA3	8:H:314:ARG:H	1.77	0.48
10:J:66:ILE:O	10:J:70:ILE:HG12	2.14	0.48
12:L:346:VAL:O	12:L:350:ILE:HG22	2.13	0.48
13:M:21:ASN:ND2	45:M:502:PLC:O2P	2.36	0.48
15:O:5:GLU:O	15:O:90:ASN:ND2	2.46	0.48
3:C:53:ARG:HG3	26:Z:0:ACE:H2	1.95	0.48
13:M:249:LEU:HD12	13:M:253:ILE:HD12	1.96	0.48
16:P:191:PRO:HA	51:P:501:NDP:H41N	1.95	0.48
41:o:15:MET:O	41:o:19:LYS:N	2.46	0.48
4:D:309:GLY:HA3	4:D:424:GLY:HA2	1.95	0.48
6:F:327:LYS:HA	6:F:331:SER:O	2.13	0.48
7:G:594:GLU:OE2	7:G:596:ARG:NH2	2.37	0.48
49:J:201:3PE:H3A1	32:f:11:VAL:HG23	1.94	0.48
3:C:133:THR:OG1	3:C:134:ALA:N	2.46	0.48
7:G:345:ASP:OD1	7:G:345:ASP:N	2.46	0.48
7:G:432:VAL:HG22	7:G:445:LEU:HB2	1.95	0.48
25:Y:182:LYS:NZ	42:p:13:ASP:O	2.44	0.48
1:A:133:ASN:OD1	1:A:134:LYS:N	2.46	0.48
7:G:568:ASP:OD1	7:G:569:LEU:N	2.44	0.48
12:L:638:ILE:HG22	25:Y:145:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:37:ARG:HH22	27:a:47:VAL:HG13	1.79	0.48
33:g:176:ARG:NH1	33:g:225:GLN:OE1	2.47	0.48
4:D:340:GLY:HA2	29:c:175:ILE:HG22	1.96	0.48
21:U:79:PHE:HD1	21:U:83:LEU:HD12	1.78	0.48
3:C:203:ARG:NH2	4:D:129:ASP:OD1	2.41	0.48
4:D:311:MET:HE2	4:D:311:MET:HB3	1.78	0.48
12:L:388:THR:CG2	12:L:470:GLY:H	2.27	0.48
40:n:39:GLU:HG2	40:n:40:PHE:HD1	1.78	0.48
41:o:11:SER:N	41:o:14:GLU:OE1	2.42	0.48
4:D:186:GLY:O	4:D:190:ARG:HG3	2.14	0.48
12:L:385:PRO:HB2	36:j:50:TRP:CZ3	2.49	0.48
14:N:485:ILE:HD12	30:d:22:ILE:HG22	1.95	0.48
24:X:107:ARG:HA	24:X:110:TRP:NE1	2.28	0.48
26:Z:136:ASN:ND2	26:Z:138:PHE:O	2.41	0.48
33:g:29:GLN:HA	33:g:32:LYS:HG2	1.96	0.48
39:m:12:ASP:OD1	39:m:14:SER:N	2.46	0.48
2:B:73:THR:HG22	2:B:100:PHE:HB3	1.95	0.48
7:G:125:VAL:HG12	9:I:124:ILE:HG13	1.94	0.48
14:N:89:ILE:HG13	14:N:90:THR:HG23	1.96	0.48
16:P:192:MET:H	51:P:501:NDP:H71N	1.61	0.48
17:Q:120:LYS:NZ	17:Q:126:TYR:OH	2.47	0.48
40:n:47:GLU:OE2	40:n:51:ARG:NH2	2.47	0.48
6:F:240:ARG:HH11	6:F:240:ARG:HB2	1.79	0.47
7:G:57:ARG:HB2	46:G:801:FES:S2	2.54	0.47
12:L:207:ASN:O	12:L:211:VAL:HG23	2.13	0.47
19:S:3:LYS:O	19:S:3:LYS:NZ	2.26	0.47
42:p:27:GLN:NE2	42:p:86:GLN:OE1	2.42	0.47
11:K:73:ILE:HD11	14:N:147:ASN:O	2.13	0.47
13:M:323:ASN:ND2	13:M:487:TYR:O	2.44	0.47
13:M:414:SER:HB2	49:M:503:3PE:H3A1	1.96	0.47
23:W:12:ARG:NH2	23:W:19:GLU:OE2	2.29	0.47
50:a:201:CDL:H522	50:a:201:CDL:HB32	1.96	0.47
35:i:14:PRO:HD2	35:i:17:GLY:O	2.14	0.47
9:I:37:SER:O	9:I:37:SER:OG	2.29	0.47
12:L:290:LEU:HA	12:L:293:MET:HE2	1.96	0.47
22:V:129:TYR:HD2	22:V:134:LEU:HD23	1.79	0.47
4:D:378:GLU:OE1	29:c:59:THR:OG1	2.31	0.47
7:G:352:LEU:O	7:G:356:VAL:HG23	2.15	0.47
4:D:67:GLU:CD	4:D:67:GLU:H	2.22	0.47
4:D:273:ARG:NH2	29:c:33:SER:O	2.44	0.47
6:F:100:ASN:N	6:F:227:THR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:447:SER:HB2	7:G:679:LEU:HD13	1.97	0.47
10:J:150:SER:O	10:J:154:LEU:HG	2.14	0.47
12:L:119:MET:HE2	45:i:101:PLC:H9A2	1.96	0.47
16:P:120:PHE:HB3	16:P:126:ILE:HG13	1.97	0.47
27:a:142:ASP:OD1	27:a:145:ARG:NH1	2.47	0.47
8:H:223:SER:HB2	8:H:227:THR:N	2.29	0.47
10:J:1:FME:HCN	32:f:37:ARG:HH21	1.78	0.47
29:c:39:VAL:HG22	43:q:54:HIS:HA	1.96	0.47
35:i:16:THR:OG1	45:i:101:PLC:OB	2.27	0.47
4:D:221:TRP:CZ2	9:I:86:MET:HG3	2.50	0.47
4:D:404:TYR:O	9:I:132:VAL:HG22	2.14	0.47
6:F:124:GLU:O	6:F:128:LEU:HG	2.15	0.47
6:F:241:ARG:O	6:F:243:GLY:N	2.47	0.47
7:G:456:LEU:O	7:G:461:GLY:HA3	2.15	0.47
10:J:134:THR:HB	15:O:124:MET:HE2	1.97	0.47
49:L:706:3PE:H3I1	32:f:51:LYS:HB2	1.97	0.47
14:N:368:ASN:HD21	14:N:370:MET:HE3	1.80	0.47
16:P:297:GLN:HE22	16:P:306:ASN:HB2	1.80	0.47
29:c:60:ILE:O	29:c:64:ASP:HB2	2.15	0.47
38:l:30:HIS:NE2	38:l:91:ASP:OD2	2.48	0.47
15:O:191:TYR:CE1	28:b:61:ASN:HB2	2.50	0.47
28:b:47:ARG:HG2	28:b:51:LEU:HB2	1.97	0.47
2:B:44:ARG:O	2:B:198:ARG:NH2	2.42	0.47
4:D:65:LYS:HB3	4:D:65:LYS:HE2	1.77	0.47
4:D:103:PHE:HE2	4:D:109:ALA:HB3	1.79	0.47
5:E:183:ASP:HB3	5:E:208:PRO:HB3	1.97	0.47
7:G:79:ARG:HH22	7:G:96:SER:H	1.62	0.47
8:H:98:TRP:HZ2	8:H:246:VAL:HG12	1.79	0.47
8:H:230:SER:O	8:H:233:PRO:HD2	2.15	0.47
12:L:390:PHE:O	12:L:394:ASP:HB3	2.14	0.47
14:N:506:GLN:OE1	14:N:509:ASN:ND2	2.46	0.47
5:E:65:GLN:CD	5:E:65:GLN:H	2.23	0.47
7:G:389:SER:O	7:G:390:THR:OG1	2.26	0.47
8:H:120:LEU:HD13	8:H:161:THR:HG23	1.96	0.47
13:M:380:VAL:HG11	45:i:101:PLC:H5'1	1.97	0.47
14:N:17:ASN:OD1	14:N:17:ASN:N	2.32	0.47
16:P:94:ASP:OD2	16:P:96:ARG:NH2	2.32	0.47
29:c:131:ASP:HB3	29:c:134:VAL:HG23	1.97	0.47
33:g:218:ILE:HD12	42:p:43:VAL:HG11	1.96	0.47
3:C:217:ARG:HH12	17:Q:43:SER:HA	1.79	0.46
4:D:49:ASN:OD1	4:D:50:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:120:GLU:HA	18:R:74:ALA:HB1	1.96	0.46
10:J:104:ASP:OD1	10:J:104:ASP:N	2.47	0.46
12:L:1:FME:HCN	35:i:48:GLY:HA3	1.95	0.46
12:L:495:SER:O	12:L:499:THR:OG1	2.30	0.46
13:M:423:SER:HA	13:M:426:TYR:CE2	2.49	0.46
23:W:29:ARG:O	23:W:33:ARG:N	2.43	0.46
2:B:69:PHE:O	2:B:71:PRO:HD3	2.15	0.46
4:D:40:ASP:OD2	23:W:30:ARG:NH2	2.44	0.46
14:N:235:TYR:CZ	14:N:239:MET:HG3	2.51	0.46
16:P:344:VAL:O	16:P:348:ILE:HG13	2.15	0.46
5:E:135:CYS:HB3	5:E:176:PRO:HG3	1.97	0.46
7:G:459:GLU:HG3	7:G:463:LYS:HE3	1.97	0.46
11:K:70:TYR:OH	11:K:74:ARG:NH2	2.49	0.46
12:L:388:THR:HG21	12:L:465:LEU:O	2.15	0.46
13:M:461:LEU:HD23	49:M:504:3PE:H3I1	1.97	0.46
16:P:68:VAL:HG11	16:P:79:LEU:HD13	1.97	0.46
19:S:14:ARG:HH22	19:S:68:GLU:CD	2.23	0.46
4:D:107:HIS:HE2	8:H:219:SER:C	2.21	0.46
6:F:89:ASN:OD1	6:F:93:GLU:N	2.45	0.46
8:H:12:ILE:HD11	49:H:403:3PE:H292	1.98	0.46
8:H:35:ALA:HB2	27:a:9:PRO:HB2	1.96	0.46
9:I:141:GLU:HG3	9:I:154:LYS:HD3	1.95	0.46
12:L:502:SER:HB3	41:o:64:PHE:CZ	2.50	0.46
12:L:581:ILE:HG21	39:m:43:LEU:HD11	1.97	0.46
14:N:387:PHE:CD1	14:N:454:SER:HB3	2.51	0.46
25:Y:22:PRO:HG2	25:Y:163:ASN:HB3	1.97	0.46
34:h:53:HIS:O	34:h:54:HIS:ND1	2.48	0.46
37:k:25:ARG:HA	37:k:25:ARG:HD2	1.66	0.46
7:G:471:LEU:HD22	7:G:510:ASN:ND2	2.31	0.46
19:S:59:VAL:O	19:S:71:THR:N	2.46	0.46
24:X:49:SER:HG	24:X:109:HIS:HD1	1.60	0.46
1:A:69:ILE:HG21	11:K:68:VAL:HG11	1.97	0.46
5:E:124:VAL:HG11	5:E:144:ILE:HD13	1.97	0.46
6:F:119:PRO:O	6:F:123:VAL:HG23	2.16	0.46
8:H:338:PHE:O	8:H:342:ILE:HG12	2.15	0.46
10:J:46:LEU:HD11	10:J:125:LEU:HD13	1.98	0.46
16:P:265:ILE:HG23	16:P:360:TYR:HE2	1.80	0.46
27:a:40:ASN:HA	31:e:97:ASP:HB2	1.98	0.46
1:A:65:PRO:HD2	1:A:68:PHE:HD2	1.80	0.46
2:B:34:LEU:HD21	16:P:128:ASP:HB3	1.97	0.46
5:E:68:LYS:O	5:E:71:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:GLU:O	9:I:180:THR:N	2.48	0.46
10:J:38:GLU:OE2	27:a:109:TRP:N	2.34	0.46
13:M:61:TRP:CD1	13:M:89:LEU:HD21	2.50	0.46
23:W:82:PHE:O	23:W:86:VAL:HG23	2.15	0.46
24:X:10:ASN:O	31:e:83:ARG:NH2	2.36	0.46
24:X:26:GLU:O	26:Z:80:ARG:NH1	2.41	0.46
38:l:138:GLY:N	42:p:60:TYR:HB3	2.31	0.46
42:p:64:ARG:HH12	42:p:68:GLU:HB2	1.81	0.46
2:B:138:ILE:HG23	2:B:168:ILE:HG23	1.98	0.46
5:E:39:ASP:OD1	5:E:87:ILE:HG22	2.16	0.46
47:F:502:FMN:H4'	47:F:502:FMN:H1'2	1.61	0.46
4:D:49:ASN:ND2	4:D:51:PHE:O	2.49	0.46
5:E:70:ALA:C	5:E:73:PRO:HD2	2.41	0.46
6:F:70:ARG:NH1	6:F:253:ARG:O	2.48	0.46
6:F:376:LEU:HD13	6:F:419:VAL:HG21	1.98	0.46
7:G:631:ASP:N	7:G:635:GLU:OE1	2.49	0.46
29:c:123:LEU:HD12	29:c:126:THR:HB	1.97	0.46
29:c:162:GLU:OE1	29:c:162:GLU:N	2.49	0.46
2:B:177:SER:O	2:B:181:MET:HG3	2.16	0.46
4:D:201:ASN:OD1	4:D:423:LYS:HE3	2.16	0.46
5:E:152:PRO:HB3	5:E:165:GLU:HG3	1.96	0.46
6:F:40:SER:O	6:F:45:ASP:HB2	2.16	0.46
12:L:67:VAL:HG11	13:M:326:ILE:HA	1.97	0.46
16:P:221:PRO:HB3	16:P:336:LEU:HD22	1.97	0.46
21:U:56:ARG:HG3	36:j:9:TYR:CE2	2.51	0.46
33:g:88:ALA:O	33:g:92:ALA:N	2.49	0.46
42:p:76:ASP:OD1	42:p:76:ASP:N	2.47	0.46
4:D:264:TYR:CE1	26:Z:11:TYR:HB3	2.51	0.45
5:E:27:SER:OG	6:F:360:HIS:NE2	2.42	0.45
6:F:364:GLY:HA3	7:G:198:GLY:HA2	1.96	0.45
7:G:336:ILE:HG23	7:G:540:PHE:HD2	1.81	0.45
25:Y:213:ILE:HG22	25:Y:214:ILE:HG12	1.97	0.45
41:o:39:ARG:HB3	41:o:44:TYR:CD1	2.50	0.45
3:C:124:ALA:HB1	3:C:126:PHE:CE2	2.50	0.45
12:L:170:ILE:HD12	12:L:232:TRP:HB3	1.98	0.45
20:T:67:VAL:HG11	20:T:82:LEU:HD22	1.97	0.45
1:A:40:ILE:HD13	1:A:40:ILE:HA	1.84	0.45
6:F:25:ILE:O	6:F:27:GLN:NE2	2.48	0.45
14:N:139:LEU:HD11	14:N:240:PRO:HG3	1.98	0.45
41:o:26:ASP:OD1	41:o:26:ASP:N	2.48	0.45
5:E:163:LEU:HD12	5:E:164:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:CYS:O	6:F:113:GLU:HG2	2.17	0.45
12:L:157:ARG:HG2	12:L:160:ALA:H	1.82	0.45
12:L:259:LEU:O	12:L:263:SER:OG	2.34	0.45
12:L:261:MET:O	12:L:264:SER:OG	2.21	0.45
14:N:197:GLU:OE1	27:a:135:ARG:NH1	2.39	0.45
15:O:101:VAL:HG13	15:O:111:PRO:HB3	1.99	0.45
26:Z:121:LYS:NZ	26:Z:136:ASN:O	2.41	0.45
29:c:86:ASP:OD1	29:c:86:ASP:N	2.37	0.45
43:q:27:ASN:OD1	45:q:401:PLC:H61	2.17	0.45
1:A:35:GLU:OE2	16:P:77:ARG:NH2	2.46	0.45
5:E:45:PHE:CD1	5:E:82:LEU:HD12	2.52	0.45
6:F:26:PHE:HD2	6:F:259:LEU:HD21	1.80	0.45
6:F:98:VAL:HG11	6:F:196:LEU:HD22	1.97	0.45
14:N:496:LEU:HD21	49:N:601:3PE:H2D2	1.99	0.45
20:T:55:LEU:O	20:T:59:VAL:N	2.41	0.45
3:C:205:ILE:HG23	3:C:206:MET:HG2	1.97	0.45
7:G:133:ASP:OD2	17:Q:67:SER:OG	2.34	0.45
8:H:173:SER:HB2	8:H:352:ILE:HG12	1.98	0.45
12:L:338:LEU:HD23	12:L:377:ALA:HB2	1.97	0.45
12:L:384:ILE:HB	12:L:387:LEU:HD12	1.98	0.45
42:p:12:PHE:CZ	42:p:86:GLN:HB2	2.51	0.45
1:A:40:ILE:HG13	8:H:73:VAL:HA	1.99	0.45
1:A:75:PHE:CD1	8:H:154:ILE:HG23	2.52	0.45
6:F:365:GLN:O	7:G:69:ASN:HB2	2.17	0.45
8:H:119:LEU:HD21	8:H:251:LEU:HD21	1.98	0.45
9:I:78:ARG:HE	29:c:28:LEU:HD13	1.80	0.45
10:J:99:GLU:OE1	10:J:99:GLU:N	2.49	0.45
12:L:431:TYR:CD1	12:L:435:LEU:HB2	2.52	0.45
12:L:584:LEU:O	12:L:589:GLY:HA3	2.17	0.45
13:M:326:ILE:HG23	13:M:400:LEU:HD22	1.99	0.45
43:q:6:ARG:HH22	43:q:28:ASP:CG	2.25	0.45
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.78	0.45
6:F:99:VAL:HG11	6:F:122:LEU:HD11	1.97	0.45
21:U:45:THR:HA	21:U:46:PRO:HD3	1.82	0.45
4:D:324:SER:O	29:c:153:ASN:HB2	2.17	0.45
6:F:198:GLU:HG2	6:F:208:ARG:HE	1.82	0.45
7:G:644:ALA:HB1	7:G:646:HIS:NE2	2.32	0.45
9:I:127:LYS:N	44:I:302:SF4:S1	2.86	0.45
13:M:262:ILE:HG23	13:M:485:LEU:HD11	1.98	0.45
18:R:132:GLU:CD	18:R:132:GLU:H	2.25	0.45
19:S:72:ASN:O	19:S:73:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ASP:O	4:D:439:TYR:OH	2.25	0.45
4:D:166:ASN:O	4:D:169:VAL:HG12	2.16	0.45
6:F:192:GLU:O	6:F:196:LEU:HB2	2.17	0.45
8:H:82:TYR:CE2	49:J:201:3PE:H222	2.51	0.45
13:M:228:MET:HE3	13:M:228:MET:HB2	1.87	0.45
5:E:119:MET:HE1	5:E:123:ASN:HB2	1.99	0.44
6:F:60:LEU:HB3	6:F:239:PHE:CZ	2.52	0.44
12:L:332:HIS:HA	12:L:335:PHE:CZ	2.52	0.44
16:P:218:GLU:HG2	16:P:254:SER:HB2	1.99	0.44
22:V:35:ARG:HB2	22:V:36:PRO:HD3	1.99	0.44
27:a:81:LEU:HD11	31:e:103:VAL:HG12	1.98	0.44
30:d:16:ARG:O	30:d:20:GLN:HG2	2.16	0.44
34:h:93:ASP:OD1	34:h:93:ASP:N	2.49	0.44
3:C:234:LYS:HB3	3:C:236:ARG:NH1	2.33	0.44
12:L:594:SER:HB3	14:N:283:LEU:HD13	1.98	0.44
24:X:26:GLU:OE2	26:Z:88:ARG:NH2	2.34	0.44
31:e:36:GLU:HG2	34:h:140:HIS:CE1	2.52	0.44
2:B:120:MET:SD	4:D:134:LEU:HD23	2.58	0.44
12:L:468:PHE:HZ	36:j:34:LEU:HD22	1.82	0.44
12:L:639:PHE:HB3	25:Y:88:PHE:CE1	2.52	0.44
13:M:449:VAL:HG13	13:M:453:GLU:HB2	1.99	0.44
13:M:489:VAL:O	25:Y:214:ILE:N	2.50	0.44
49:M:503:3PE:H2	39:m:63:PHE:HZ	1.81	0.44
50:a:201:CDL:H131	50:a:201:CDL:H161	1.59	0.44
2:B:36:THR:HB	16:P:98:LEU:HB2	1.99	0.44
6:F:81:LEU:O	6:F:84:SER:OG	2.35	0.44
7:G:258:VAL:HG12	7:G:283:ILE:HG21	1.98	0.44
12:L:40:VAL:HG23	12:L:90:VAL:HG12	2.00	0.44
12:L:137:PHE:CZ	12:L:179:VAL:HG23	2.52	0.44
12:L:582:LEU:HD21	13:M:229:PRO:HB2	1.98	0.44
14:N:73:LEU:O	14:N:77:ILE:HG12	2.18	0.44
33:g:97:ASN:O	33:g:101:LEU:HB2	2.17	0.44
33:g:150:MET:HE3	45:h:201:PLC:H8'1	1.99	0.44
4:D:85:ASP:OD2	14:N:149:SER:OG	2.25	0.44
5:E:84:PHE:HB2	5:E:115:ASN:O	2.18	0.44
12:L:625:PHE:HD2	12:L:633:ILE:HD11	1.82	0.44
13:M:301:LEU:HD23	13:M:301:LEU:HA	1.83	0.44
14:N:249:TYR:HD2	14:N:307:ILE:HG12	1.83	0.44
14:N:487:ASN:OD1	30:d:19:GLN:NE2	2.46	0.44
16:P:216:LYS:NZ	16:P:314:HIS:HA	2.32	0.44
26:Z:132:ALA:HB2	31:e:85:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:16:THR:OG1	45:i:101:PLC:H11	2.16	0.44
1:A:38:GLY:HA2	16:P:196:ASN:HD21	1.82	0.44
1:A:73:LEU:HB3	10:J:154:LEU:HD13	1.99	0.44
6:F:74:GLY:HA2	6:F:334:GLY:HA2	1.98	0.44
6:F:83:TYR:HB3	6:F:133:MET:HG3	1.99	0.44
8:H:151:ALA:HB3	8:H:317:TYR:OH	2.17	0.44
49:L:703:3PE:H261	49:L:703:3PE:H232	1.74	0.44
43:q:77:TRP:CE2	43:q:89:PRO:HG2	2.51	0.44
7:G:129:GLY:HA3	7:G:238:ARG:NH1	2.33	0.44
13:M:292:SER:HB3	13:M:422:LEU:HB3	2.00	0.44
50:a:201:CDL:HB21	29:c:19:TRP:CE2	2.53	0.44
40:n:20:VAL:HG13	40:n:52:PHE:HE1	1.82	0.44
1:A:17:GLY:HA3	8:H:92:PHE:HZ	1.83	0.44
4:D:135:LEU:HD12	4:D:135:LEU:HA	1.83	0.44
5:E:169:LEU:HD12	5:E:177:MET:SD	2.58	0.44
6:F:262:ILE:HD11	6:F:283:LEU:HD21	1.99	0.44
8:H:251:LEU:HD23	8:H:251:LEU:HA	1.79	0.44
10:J:141:LEU:HD23	10:J:141:LEU:HA	1.80	0.44
12:L:563:LEU:HD21	49:l:201:3PE:H242	1.99	0.44
13:M:225:THR:HG22	13:M:257:ALA:HB1	1.99	0.44
16:P:297:GLN:HE21	16:P:297:GLN:HB2	1.67	0.44
40:n:58:ILE:HD12	40:n:64:LEU:HD13	2.00	0.44
4:D:333:VAL:HG21	4:D:362:ILE:HG23	2.00	0.44
4:D:390:MET:HE1	9:I:173:PRO:HA	2.00	0.44
6:F:28:ASN:ND2	6:F:117:LYS:O	2.48	0.44
7:G:398:ASP:OD2	7:G:468:SER:OG	2.33	0.44
8:H:277:GLN:NE2	24:X:166:LEU:O	2.42	0.44
12:L:62:MET:HE2	49:M:504:3PE:H2C2	1.99	0.44
13:M:352:ILE:HD13	13:M:449:VAL:HG22	2.00	0.44
14:N:149:SER:HB3	14:N:152:SER:HB3	2.00	0.44
20:T:106:ASP:O	20:T:110:ASN:ND2	2.50	0.44
1:A:71:VAL:HG22	1:A:123:LEU:HD13	2.00	0.43
4:D:414:GLU:OE1	4:D:429:TYR:OH	2.31	0.43
6:F:423:ILE:HG12	6:F:430:MET:HE1	1.99	0.43
12:L:442:LYS:NZ	36:j:13:ALA:H	2.15	0.43
53:U:201:EHZ:O2	53:U:201:EHZ:O1	2.32	0.43
22:V:109:MET:HE1	22:V:114:ALA:HB3	2.00	0.43
23:W:31:TYR:CZ	23:W:82:PHE:HB2	2.52	0.43
33:g:27:ASN:CG	33:g:30:LEU:HB2	2.44	0.43
43:q:14:ASN:ND2	43:q:30:LYS:O	2.35	0.43
3:C:84:ILE:HD13	3:C:118:LEU:HD21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ASN:ND2	4:D:426:MET:SD	2.90	0.43
7:G:25:LYS:O	7:G:40:ALA:HB2	2.17	0.43
8:H:121:ALA:HB1	10:J:52:THR:HB	1.99	0.43
9:I:172:CYS:HA	44:I:302:SF4:S2	2.58	0.43
12:L:317:ILE:HG23	12:L:322:TYR:HE1	1.84	0.43
35:i:58:LYS:HD3	35:i:58:LYS:HA	1.86	0.43
3:C:239:TYR:HB2	23:W:97:GLN:NE2	2.27	0.43
8:H:113:GLU:OE1	8:H:113:GLU:N	2.47	0.43
13:M:183:LEU:HD22	14:N:424:LEU:HD11	1.99	0.43
16:P:43:THR:OG1	16:P:108:SER:OG	2.18	0.43
21:U:128:ASP:OD1	21:U:128:ASP:N	2.49	0.43
24:X:36:ASP:OD1	24:X:37:VAL:N	2.51	0.43
4:D:445:ALA:HB3	4:D:482:ARG:HH21	1.83	0.43
5:E:61:LYS:HG2	6:F:180:TYR:HD2	1.83	0.43
5:E:86:SER:HB3	5:E:89:VAL:HG23	2.00	0.43
5:E:200:PHE:CE1	5:E:206:PRO:HD2	2.54	0.43
6:F:33:TYR:O	6:F:39:SER:OG	2.26	0.43
6:F:262:ILE:HG12	6:F:338:VAL:HB	1.99	0.43
6:F:471:HIS:O	6:F:473:HIS:N	2.51	0.43
7:G:345:ASP:O	7:G:349:ILE:HG13	2.18	0.43
8:H:278:HIS:ND1	27:a:53:PRO:HB2	2.34	0.43
12:L:226:GLN:O	12:L:230:HIS:HB3	2.17	0.43
13:M:294:ILE:HG22	13:M:298:GLN:HE21	1.83	0.43
14:N:451:LYS:HG3	14:N:455:PHE:CD2	2.53	0.43
53:T:201:EHZ:P1	23:W:21:ARG:HH21	2.41	0.43
23:W:51:VAL:O	23:W:55:ILE:HG13	2.17	0.43
40:n:67:ILE:H	40:n:67:ILE:HG13	1.62	0.43
1:A:92:ILE:HD12	8:H:169:LEU:HD11	2.00	0.43
3:C:111:LEU:HD13	3:C:163:THR:HG21	2.00	0.43
4:D:92:LYS:NZ	20:T:127:LEU:O	2.52	0.43
5:E:74:LEU:HD12	5:E:97:LEU:HD11	2.00	0.43
5:E:117:LYS:HE3	5:E:117:LYS:HB3	1.65	0.43
9:I:201:LEU:HD23	9:I:201:LEU:HA	1.80	0.43
12:L:37:PHE:HB2	12:L:94:PHE:CE1	2.54	0.43
45:L:702:PLC:H62	45:L:702:PLC:H41	1.87	0.43
13:M:117:TYR:OH	13:M:244:GLY:HA3	2.18	0.43
21:U:91:VAL:HG13	40:n:25:ARG:HE	1.82	0.43
26:Z:118:LEU:HD11	31:e:61:MET:HE3	1.99	0.43
31:e:45:TYR:CZ	31:e:49:ARG:HD2	2.53	0.43
34:h:107:LYS:NZ	42:p:28:GLU:OE1	2.42	0.43
35:i:45:TYR:O	35:i:49:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:GLU:OE2	4:D:330:TYR:OH	2.31	0.43
6:F:46:TRP:HB3	6:F:49:THR:HG21	2.01	0.43
6:F:268:GLU:OE2	6:F:289:GLY:N	2.52	0.43
6:F:304:GLY:HA2	6:F:336:ALA:H	1.84	0.43
7:G:295:LYS:HB2	7:G:295:LYS:HE3	1.73	0.43
10:J:98:ASN:ND2	10:J:100:SER:O	2.46	0.43
12:L:620:TRP:CE2	27:a:121:PRO:HG3	2.53	0.43
13:M:470:TYR:CE2	13:M:472:SER:HB2	2.54	0.43
20:T:132:SER:OG	20:T:135:HIS:ND1	2.51	0.43
27:a:142:ASP:HA	27:a:145:ARG:HB2	1.99	0.43
5:E:75:LEU:HB3	5:E:114:TYR:CE1	2.54	0.43
6:F:89:ASN:ND2	6:F:93:GLU:O	2.39	0.43
7:G:347:GLU:OE1	7:G:347:GLU:N	2.52	0.43
10:J:1:FME:O	10:J:3:LEU:N	2.51	0.43
10:J:37:THR:OG1	32:f:4:LEU:HB2	2.19	0.43
14:N:67:ASN:OD1	14:N:250:ILE:HD11	2.19	0.43
14:N:137:TYR:O	14:N:141:LEU:HG	2.18	0.43
16:P:71:ARG:NH2	51:P:501:NDP:O2X	2.44	0.43
16:P:180:PHE:HD2	16:P:184:ALA:HB2	1.84	0.43
27:a:1:MET:HA	50:a:201:CDL:OB4	2.19	0.43
29:c:169:TYR:HB3	29:c:173:TYR:CD2	2.53	0.43
43:q:6:ARG:NH2	43:q:28:ASP:OD1	2.52	0.43
5:E:177:MET:HB3	5:E:177:MET:HE3	1.73	0.43
8:H:127:VAL:HG13	8:H:153:LEU:HD13	2.00	0.43
13:M:272:ILE:HD11	25:Y:17:PRO:HB3	2.01	0.43
19:S:84:THR:O	19:S:87:SER:OG	2.33	0.43
29:c:141:ALA:O	29:c:145:SER:N	2.50	0.43
33:g:182:LEU:HA	33:g:188:ILE:HD11	2.00	0.43
2:B:200:TRP:HA	2:B:204:TYR:HB2	2.01	0.43
47:F:502:FMN:HM73	47:F:502:FMN:HM81	1.40	0.43
11:K:12:GLY:HA3	11:K:17:ASP:OD2	2.19	0.43
12:L:420:THR:O	12:L:424:LEU:HG	2.18	0.43
16:P:138:ALA:HB1	16:P:180:PHE:HB2	2.01	0.43
45:q:401:PLC:H32	45:q:401:PLC:H41	1.99	0.43
4:D:273:ARG:HH21	4:D:276:GLU:CD	2.21	0.43
7:G:375:PRO:O	7:G:378:GLY:N	2.48	0.43
9:I:128:LEU:O	9:I:132:VAL:HG23	2.18	0.43
12:L:155:PHE:CZ	45:i:101:PLC:H61	2.52	0.43
14:N:112:ASN:HD22	14:N:235:TYR:HE1	1.65	0.43
16:P:113:ASN:HD21	16:P:134:ALA:HA	1.84	0.43
25:Y:111:ALA:HB3	45:Y:301:PLC:H11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:122:SER:O	25:Y:126:LEU:HB2	2.19	0.43
28:b:26:HIS:CD2	28:b:27:VAL:HG23	2.54	0.43
43:q:66:TRP:CZ2	45:q:402:PLC:H2'2	2.53	0.43
7:G:159:ASN:OD1	7:G:159:ASN:N	2.50	0.42
7:G:399:GLN:HB2	7:G:464:LEU:HD23	2.01	0.42
9:I:49:ARG:NH1	22:V:93:GLU:OE2	2.40	0.42
12:L:471:TYR:OH	36:j:42:ARG:NH2	2.52	0.42
13:M:149:ALA:HB3	13:M:150:PRO:HD3	1.99	0.42
51:P:501:NDP:H2N	51:P:501:NDP:H2D	1.85	0.42
17:Q:51:THR:OG1	17:Q:52:GLU:HG3	2.19	0.42
19:S:52:ALA:HB3	19:S:55:ILE:HD13	2.01	0.42
25:Y:45:ILE:O	25:Y:49:VAL:HG23	2.18	0.42
29:c:74:ASP:OD2	29:c:77:ARG:HD2	2.18	0.42
37:k:9:ARG:HG2	37:k:10:ASP:OD1	2.19	0.42
43:q:24:GLN:C	45:q:401:PLC:H63	2.44	0.42
7:G:78:GLU:HB2	7:G:79:ARG:HH21	1.84	0.42
7:G:102:PRO:HB3	29:c:71:TYR:CE2	2.55	0.42
7:G:670:LYS:HB2	7:G:673:ILE:HD11	2.00	0.42
12:L:596:PHE:HB2	49:L:704:3PE:H11	2.01	0.42
45:L:701:PLC:H63	45:L:701:PLC:H42	1.77	0.42
13:M:101:ILE:HG23	13:M:456:LEU:HD22	2.00	0.42
13:M:210:GLN:HB3	13:M:272:ILE:HB	2.00	0.42
13:M:465:ILE:HD13	45:M:501:PLC:H8'1	1.99	0.42
14:N:6:LEU:HD11	14:N:107:VAL:HG13	2.01	0.42
14:N:140:TYR:OH	14:N:163:GLY:HA3	2.19	0.42
18:R:63:LYS:HD3	18:R:63:LYS:HA	1.80	0.42
18:R:103:HIS:ND1	18:R:104:PRO:O	2.46	0.42
29:c:60:ILE:HD13	29:c:60:ILE:HA	1.78	0.42
40:n:19:TYR:O	40:n:23:LEU:HG	2.19	0.42
2:B:72:MET:HE2	2:B:72:MET:HB3	1.82	0.42
3:C:248:TRP:HB3	17:Q:103:GLN:HE22	1.83	0.42
3:C:265:LYS:HD3	3:C:267:PHE:CE2	2.54	0.42
6:F:342:ASN:HD22	6:F:342:ASN:N	2.17	0.42
8:H:51:ALA:HA	43:q:27:ASN:OD1	2.20	0.42
8:H:144:LEU:HD13	8:H:221:LEU:HD22	2.00	0.42
11:K:40:ASP:OD1	11:K:40:ASP:N	2.51	0.42
12:L:281:GLY:HA3	12:L:314:MET:HB2	2.00	0.42
12:L:527:GLU:HG3	12:L:528:PHE:CD1	2.54	0.42
13:M:17:LEU:HD21	13:M:45:ILE:HB	2.00	0.42
16:P:99:LYS:HE2	16:P:103:ASP:OD1	2.19	0.42
16:P:251:GLU:HB2	16:P:253:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:58:VAL:HG21	29:c:139:LEU:HD23	2.02	0.42
29:c:31:ASN:ND2	29:c:31:ASN:O	2.51	0.42
43:q:137:GLU:N	43:q:137:GLU:OE1	2.52	0.42
1:A:40:ILE:HG21	8:H:74:LEU:HD12	2.02	0.42
3:C:85:MET:SD	29:c:90:VAL:HG21	2.59	0.42
4:D:318:PRO:HB3	4:D:339:VAL:HG21	2.02	0.42
6:F:130:GLY:HA3	6:F:177:PHE:HE1	1.83	0.42
7:G:592:ASN:HD21	7:G:594:GLU:HG2	1.85	0.42
9:I:133:CYS:HA	44:I:301:SF4:S4	2.59	0.42
12:L:285:THR:HG22	12:L:308:SER:O	2.19	0.42
13:M:97:ILE:O	13:M:100:PRO:HD2	2.19	0.42
13:M:111:LYS:HE2	14:N:458:LEU:HB3	2.01	0.42
17:Q:86:ASN:O	17:Q:87:ARG:HG2	2.20	0.42
36:j:31:LEU:HD23	36:j:31:LEU:HA	1.91	0.42
1:A:66:ILE:H	1:A:66:ILE:HD12	1.84	0.42
1:A:82:VAL:HA	1:A:85:MET:HE2	2.01	0.42
5:E:132:CYS:O	5:E:137:SER:HB2	2.19	0.42
6:F:96:TYR:HD1	6:F:137:ALA:HB3	1.85	0.42
6:F:326:LEU:HD12	6:F:333:LEU:HB2	2.01	0.42
7:G:298:ARG:HD3	7:G:566:HIS:CE1	2.54	0.42
8:H:91:LEU:HD22	8:H:236:ILE:HG23	2.00	0.42
8:H:148:ARG:NH2	8:H:214:ASN:HD22	2.17	0.42
9:I:113:LEU:HD12	9:I:200:LEU:HB2	2.02	0.42
11:K:71:ASN:HB2	20:T:133:ILE:HD12	2.01	0.42
12:L:247:LEU:HG	12:L:248:HIS:ND1	2.34	0.42
12:L:544:LEU:HG	45:L:701:PLC:H2'1	2.02	0.42
49:L:704:3PE:H371	49:L:704:3PE:H342	1.77	0.42
13:M:462:ILE:HG21	45:h:201:PLC:H4'1	2.00	0.42
40:n:49:ARG:O	40:n:53:ASP:N	2.52	0.42
1:A:138:LYS:HD3	1:A:139:ASN:H	1.84	0.42
1:A:138:LYS:HB3	22:V:13:ILE:HG13	2.02	0.42
3:C:153:VAL:HG21	4:D:303:LEU:HD21	2.01	0.42
3:C:278:ALA:O	29:c:107:GLY:N	2.43	0.42
4:D:74:HIS:CE1	4:D:75:GLU:HG2	2.55	0.42
4:D:164:MET:HG3	4:D:233:TYR:CZ	2.55	0.42
5:E:152:PRO:HA	5:E:163:LEU:HG	2.01	0.42
6:F:212:PRO:HD3	17:Q:142:SER:HB3	2.02	0.42
6:F:291:ILE:HG13	6:F:295:TRP:HA	2.00	0.42
7:G:217:ALA:HB3	7:G:288:ARG:HD3	2.01	0.42
13:M:357:TYR:HB3	39:m:9:LEU:HD12	2.02	0.42
13:M:462:ILE:HD11	45:h:201:PLC:H2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:28:ARG:HG2	14:N:86:SER:OG	2.19	0.42
14:N:334:SER:HB3	14:N:489:ILE:HD11	2.02	0.42
28:b:65:LEU:HD11	34:h:162:PHE:CE1	2.53	0.42
34:h:152:LYS:HG2	34:h:153:HIS:CD2	2.54	0.42
42:p:28:GLU:O	42:p:32:ARG:HG3	2.20	0.42
1:A:20:PHE:HB3	8:H:236:ILE:HD11	2.01	0.42
1:A:21:LEU:HD21	8:H:88:LEU:HD21	2.02	0.42
1:A:88:TYR:HB2	10:J:133:PHE:CZ	2.55	0.42
5:E:114:TYR:CZ	6:F:185:MET:HG3	2.55	0.42
7:G:543:LEU:HD22	7:G:546:ALA:HB3	2.01	0.42
7:G:648:LEU:HD23	7:G:648:LEU:HA	1.88	0.42
49:J:201:3PE:H321	49:J:201:3PE:H32	1.90	0.42
12:L:246:LEU:O	12:L:251:CYS:HB2	2.19	0.42
13:M:452:ARG:HA	33:g:138:TRP:CZ2	2.55	0.42
50:O:201:CDL:H832	50:O:201:CDL:H801	1.73	0.42
24:X:16:ASP:OD2	31:e:83:ARG:HD2	2.19	0.42
27:a:2:ILE:HD11	50:a:201:CDL:H711	2.01	0.42
4:D:311:MET:SD	4:D:473:MET:HG2	2.60	0.42
5:E:174:ASN:HB3	5:E:186:GLU:HB3	2.02	0.42
7:G:112:THR:HG21	7:G:142:GLY:HA3	2.01	0.42
7:G:435:GLU:HG2	7:G:444:HIS:NE2	2.35	0.42
12:L:5:CYS:SG	12:L:43:THR:OG1	2.77	0.42
14:N:510:ILE:HD11	45:N:602:PLC:H9'2	2.02	0.42
16:P:38:THR:OG1	16:P:64:THR:OG1	2.22	0.42
22:V:18:ASN:OD1	22:V:18:ASN:N	2.52	0.42
2:B:52:TYR:HE1	45:B:303:PLC:H63	1.84	0.42
7:G:633:LEU:HD21	7:G:637:ARG:HE	1.85	0.42
7:G:658:GLU:HG2	7:G:662:LYS:HE3	2.00	0.42
8:H:281:TYR:O	8:H:285:ILE:HG12	2.20	0.42
32:f:15:PHE:HZ	32:f:26:LEU:HD12	1.85	0.42
36:j:38:TRP:CZ2	36:j:42:ARG:HD3	2.55	0.42
38:l:112:ILE:O	38:l:116:GLY:N	2.53	0.42
38:l:145:THR:O	38:l:149:ALA:N	2.50	0.42
1:A:18:LEU:HD21	32:f:10:ALA:HA	2.01	0.42
1:A:27:ILE:HD12	45:B:302:PLC:H2A2	2.01	0.42
3:C:277:PRO:HD3	29:c:114:LEU:HD12	2.02	0.42
4:D:77:GLU:HG2	12:L:606:PHE:HA	2.02	0.42
4:D:265:MET:HE1	29:c:42:TYR:HA	2.02	0.42
5:E:200:PHE:HE1	5:E:206:PRO:HD2	1.85	0.42
6:F:64:LEU:HB3	6:F:80:GLY:HA3	2.02	0.42
6:F:446:SER:OG	6:F:450:TRP:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:PRO:HD3	8:H:290:LEU:HD13	2.02	0.42
12:L:564:ARG:HH22	38:I:50:GLN:HE22	1.68	0.42
49:L:704:3PE:H2C1	49:L:704:3PE:H2F2	1.82	0.42
13:M:67:ASN:HB2	33:g:163:LYS:O	2.20	0.42
17:Q:38:ALA:H	23:W:70:LEU:HD11	1.84	0.42
2:B:149:TYR:HE2	4:D:153:PRO:HB2	1.85	0.41
3:C:191:LEU:HA	3:C:215:PRO:HD2	2.01	0.41
8:H:200:PHE:HD2	45:I:303:PLC:H9'2	1.83	0.41
24:X:19:LYS:HB3	27:a:103:SER:CB	2.49	0.41
24:X:38:GLU:HB3	27:a:89:VAL:HG13	2.01	0.41
42:p:53:LYS:HD3	42:p:53:LYS:HA	1.69	0.41
1:A:35:GLU:O	16:P:53:ARG:NH2	2.43	0.41
6:F:353:ARG:HA	6:F:353:ARG:HD2	1.81	0.41
7:G:156:ALA:HB1	18:R:109:ASN:HB2	2.02	0.41
7:G:621:SER:HB2	7:G:626:ALA:O	2.20	0.41
8:H:128:PHE:CZ	10:J:29:VAL:HG21	2.55	0.41
13:M:41:LYS:HA	13:M:41:LYS:HD3	1.76	0.41
23:W:67:ASP:O	23:W:71:LYS:HG3	2.20	0.41
27:a:20:GLY:O	27:a:24:MET:HG3	2.19	0.41
33:g:100:ASP:O	33:g:103:GLU:HB3	2.20	0.41
45:q:401:PLC:H82	45:q:401:PLC:H42	1.79	0.41
1:A:65:PRO:HD2	1:A:68:PHE:CD2	2.55	0.41
2:B:69:PHE:HB3	2:B:98:ILE:HG12	2.02	0.41
4:D:190:ARG:NH2	4:D:328:ASP:OD2	2.52	0.41
7:G:541:ILE:HB	7:G:560:VAL:HG22	2.02	0.41
8:H:182:SER:OG	26:Z:52:LYS:NZ	2.53	0.41
8:H:218:GLU:HA	8:H:222:VAL:O	2.20	0.41
12:L:87:VAL:HB	12:L:88:PRO:HD3	2.02	0.41
12:L:494:LEU:HD23	38:I:126:ARG:NH1	2.34	0.41
49:L:706:3PE:H272	49:L:706:3PE:H2A1	1.68	0.41
13:M:262:ILE:HD11	13:M:332:LEU:HD21	2.01	0.41
14:N:518:LEU:HD22	14:N:521:ASN:HB2	2.02	0.41
27:a:37:ARG:HH22	27:a:47:VAL:HG22	1.86	0.41
29:c:108:GLU:O	29:c:112:LYS:HG3	2.19	0.41
2:B:105:ARG:HH12	2:B:130:GLN:HB3	1.84	0.41
4:D:207:LEU:HB3	4:D:219:PHE:HA	2.01	0.41
4:D:402:LEU:HD13	7:G:139:LEU:HD22	2.01	0.41
6:F:394:ASP:OD1	6:F:427:ARG:NH2	2.53	0.41
6:F:459:GLY:HA2	18:R:93:VAL:O	2.20	0.41
7:G:46:GLN:HE22	17:Q:138:LYS:HA	1.85	0.41
7:G:205:THR:O	7:G:207:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:254:LEU:HD11	7:G:411:ALA:HB1	2.01	0.41
7:G:518:ARG:HD3	7:G:518:ARG:HA	1.90	0.41
12:L:11:LEU:HD11	35:i:37:PHE:HD1	1.85	0.41
14:N:309:SER:OG	14:N:314:SER:OG	2.38	0.41
36:j:15:VAL:O	37:k:17:ALA:N	2.48	0.41
41:o:16:LYS:HE3	42:p:58:ASN:HB3	2.03	0.41
3:C:130:MET:HE3	4:D:444:ARG:HH21	1.85	0.41
3:C:227:GLU:OE1	3:C:242:LEU:HD12	2.20	0.41
6:F:299:LEU:HB2	6:F:343:LYS:HA	2.03	0.41
8:H:9:ILE:O	8:H:13:GLU:N	2.52	0.41
11:K:27:MET:HE2	11:K:27:MET:HB2	1.70	0.41
12:L:278:LEU:HD12	12:L:315:ILE:HA	2.02	0.41
13:M:169:TYR:O	13:M:173:TYR:HB2	2.20	0.41
13:M:391:LEU:HD23	13:M:391:LEU:HA	1.91	0.41
18:R:35:GLN:HG2	18:R:41:ILE:HG12	2.01	0.41
37:k:31:PHE:O	37:k:35:LEU:HB2	2.21	0.41
1:A:115:ILE:HG12	45:b:102:PLC:H4'2	2.01	0.41
2:B:68:SER:HB3	8:H:66:LYS:HG3	2.01	0.41
7:G:248:ILE:HG12	7:G:600:THR:HG22	2.03	0.41
7:G:304:ILE:HD11	7:G:318:ALA:HA	2.03	0.41
9:I:45:PRO:HB3	29:c:158:PHE:O	2.20	0.41
12:L:299:LYS:NZ	12:L:355:GLN:HE22	2.18	0.41
12:L:623:ILE:HD13	14:N:203:CYS:SG	2.60	0.41
13:M:300:ASP:O	13:M:304:ILE:HG13	2.21	0.41
16:P:153:SER:O	16:P:189:PRO:HD2	2.20	0.41
38:l:156:ILE:HA	41:o:27:ARG:NH2	2.35	0.41
3:C:85:MET:HG2	29:c:123:LEU:HD23	2.02	0.41
6:F:54:LEU:HD23	6:F:54:LEU:HA	1.91	0.41
6:F:245:TRP:O	6:F:248:SER:OG	2.30	0.41
45:I:303:PLC:H5A1	45:I:303:PLC:H2A2	1.88	0.41
14:N:311:SER:OG	14:N:313:GLU:OE1	2.28	0.41
16:P:217:LYS:HB2	16:P:313:SER:HA	2.02	0.41
32:f:43:ILE:H	32:f:43:ILE:HG13	1.73	0.41
33:g:34:ILE:HG21	33:g:97:ASN:HB3	2.02	0.41
33:g:76:ARG:NH2	33:g:97:ASN:HB2	2.34	0.41
1:A:98:TYR:CE2	50:O:201:CDL:H722	2.55	0.41
4:D:270:PHE:HD2	4:D:360:LEU:HD13	1.86	0.41
6:F:82:LYS:HD3	6:F:225:THR:HG23	2.03	0.41
6:F:100:ASN:O	6:F:229:VAL:N	2.53	0.41
6:F:321:MET:SD	6:F:326:LEU:HD11	2.61	0.41
7:G:353:LYS:HB2	7:G:526:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:62:LEU:HD23	10:J:62:LEU:HA	1.81	0.41
13:M:369:SER:HB3	13:M:435:THR:HB	2.02	0.41
13:M:446:THR:OG1	13:M:447:ASN:N	2.54	0.41
14:N:285:VAL:HG21	14:N:291:LEU:HD13	2.02	0.41
20:T:108:THR:O	20:T:112:ILE:HG13	2.20	0.41
21:U:85:LEU:HD22	21:U:89:ASP:HB3	2.03	0.41
34:h:75:LEU:O	34:h:79:VAL:HG23	2.21	0.41
3:C:247:ALA:HB1	17:Q:87:ARG:HH21	1.85	0.41
4:D:86:HIS:CG	14:N:370:MET:HB3	2.56	0.41
4:D:425:GLU:C	4:D:446:PRO:HG3	2.46	0.41
7:G:405:THR:HG21	7:G:473:ILE:HG22	2.03	0.41
7:G:601:ARG:HD2	17:Q:56:ARG:NH1	2.36	0.41
11:K:2:ASP:OD1	11:K:2:ASP:N	2.38	0.41
12:L:112:ARG:HD3	45:i:101:PLC:H2	2.03	0.41
12:L:317:ILE:HG23	12:L:322:TYR:CE1	2.55	0.41
12:L:324:LEU:CD2	12:L:478:LEU:HD22	2.48	0.41
12:L:354:TYR:O	12:L:360:TYR:OH	2.37	0.41
12:L:504:PRO:HD2	12:L:507:LEU:HD12	2.03	0.41
12:L:539:LYS:HB2	12:L:539:LYS:HE3	1.86	0.41
13:M:11:ILE:HD11	49:d:101:3PE:H291	2.02	0.41
13:M:449:VAL:HG12	13:M:454:ILE:HG13	2.02	0.41
14:N:116:LEU:HD11	14:N:239:MET:HB3	2.02	0.41
16:P:156:ASN:HB2	16:P:166:TYR:CE1	2.56	0.41
17:Q:41:LEU:HD23	17:Q:41:LEU:HA	1.90	0.41
20:T:79:VAL:HG23	20:T:80:GLN:CD	2.46	0.41
20:T:100:PHE:CD2	20:T:122:VAL:HG21	2.55	0.41
23:W:39:VAL:HG13	23:W:44:LEU:HB2	2.02	0.41
25:Y:88:PHE:HB2	25:Y:89:PRO:HD3	2.03	0.41
26:Z:61:TRP:CH2	28:b:64:PRO:HG2	2.56	0.41
33:g:84:LEU:HD23	33:g:84:LEU:HA	1.91	0.41
33:g:171:ASP:HB2	42:p:4:HIS:CE1	2.56	0.41
40:n:64:LEU:HD12	40:n:64:LEU:HA	1.86	0.41
42:p:42:LYS:HG2	42:p:45:ARG:HH21	1.85	0.41
4:D:146:LYS:HB3	4:D:150:GLN:HB2	2.03	0.41
5:E:121:LYS:HB2	5:E:160:LEU:O	2.21	0.41
5:E:141:MET:SD	5:E:152:PRO:HG3	2.60	0.41
7:G:323:ALA:HA	7:G:624:LEU:HD21	2.03	0.41
13:M:409:HIS:CE1	13:M:412:ILE:HG22	2.56	0.41
50:b:103:CDL:H111	50:b:103:CDL:H142	1.73	0.41
39:m:67:ARG:HH12	42:p:68:GLU:CD	2.28	0.41
43:q:28:ASP:OD1	43:q:29:ILE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:CD1	10:J:144:SER:HB3	2.56	0.40
4:D:218:PRO:HG3	4:D:280:LEU:HD12	2.01	0.40
6:F:215:ALA:O	6:F:223:PRO:HB3	2.21	0.40
6:F:348:ILE:HA	6:F:422:LEU:HD11	2.02	0.40
6:F:370:ARG:CZ	7:G:175:HIS:HB2	2.51	0.40
8:H:36:GLU:HG3	8:H:306:VAL:HG22	2.03	0.40
49:L:706:3PE:H331	49:L:706:3PE:H361	1.51	0.40
13:M:472:SER:HA	13:M:475:THR:HB	2.03	0.40
49:M:503:3PE:H3H1	49:M:503:3PE:H3E1	1.82	0.40
16:P:261:MET:O	16:P:368:LEU:HD21	2.21	0.40
25:Y:126:LEU:HD23	25:Y:130:ARG:HB2	2.03	0.40
1:A:41:SER:HB3	8:H:77:ASN:HB3	2.04	0.40
4:D:114:LEU:HD22	4:D:477:PHE:HZ	1.87	0.40
4:D:394:MET:HE2	7:G:119:HIS:HD2	1.85	0.40
6:F:100:ASN:HB2	6:F:226:VAL:HG13	2.03	0.40
7:G:624:LEU:HD23	7:G:624:LEU:HA	1.92	0.40
7:G:663:VAL:HG22	19:S:32:THR:HG23	2.03	0.40
9:I:108:ARG:HB3	9:I:179:GLU:OE1	2.21	0.40
9:I:109:GLY:H	9:I:179:GLU:HB3	1.87	0.40
13:M:269:LEU:HB3	13:M:272:ILE:HG22	2.03	0.40
13:M:359:ASN:O	13:M:365:TYR:OH	2.18	0.40
13:M:473:PHE:HZ	49:M:504:3PE:H331	1.86	0.40
49:M:504:3PE:H321	49:M:504:3PE:H351	1.91	0.40
14:N:202:LEU:HD22	14:N:263:LEU:HD13	2.04	0.40
17:Q:39:LYS:O	17:Q:42:VAL:HG22	2.21	0.40
23:W:54:LYS:HD3	23:W:99:PHE:CD1	2.56	0.40
24:X:5:THR:HG22	31:e:9:ARG:NH2	2.36	0.40
45:Z:201:PLC:HT'1	45:Z:201:PLC:H7'2	1.82	0.40
42:p:45:ARG:HB2	42:p:70:TYR:CE1	2.57	0.40
1:A:76:LEU:HA	1:A:76:LEU:HD22	1.72	0.40
3:C:77:LEU:HD22	3:C:102:LEU:HB2	2.02	0.40
3:C:143:ARG:H	3:C:143:ARG:HG3	1.54	0.40
7:G:284:SER:HB3	7:G:412:ALA:HB3	2.04	0.40
7:G:380:ASP:N	7:G:380:ASP:OD1	2.53	0.40
8:H:220:GLU:O	8:H:221:LEU:HD23	2.20	0.40
13:M:272:ILE:HD12	13:M:272:ILE:HA	1.84	0.40
13:M:409:HIS:ND1	13:M:412:ILE:HG22	2.36	0.40
15:O:98:ARG:NE	15:O:164:GLU:OE2	2.51	0.40
19:S:10:VAL:HG12	19:S:45:LEU:HD11	2.04	0.40
24:X:89:ARG:NH2	28:b:79:ASP:OD1	2.53	0.40
30:d:4:SER:OG	30:d:49:ASN:ND2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:291:ILE:H	6:F:291:ILE:HG12	1.65	0.40
6:F:366:CYS:HA	7:G:69:ASN:O	2.21	0.40
7:G:357:ASN:C	7:G:360:GLY:H	2.29	0.40
12:L:578:ASP:OD2	13:M:307:TYR:OH	2.29	0.40
13:M:280:ILE:HG21	13:M:321:PHE:CD2	2.56	0.40
13:M:292:SER:HB2	13:M:422:LEU:HD13	2.04	0.40
49:M:504:3PE:H2C2	49:M:504:3PE:H292	1.82	0.40
15:O:164:GLU:HG2	15:O:167:TRP:CH2	2.57	0.40
18:R:93:VAL:HG22	18:R:107:TYR:CD2	2.56	0.40
20:T:114:THR:OG1	20:T:117:GLU:HG3	2.21	0.40
23:W:68:LEU:O	23:W:71:LYS:N	2.52	0.40
24:X:113:LEU:HD23	24:X:113:LEU:HA	1.88	0.40
30:d:41:TRP:O	30:d:45:GLY:N	2.43	0.40
34:h:101:LEU:HD23	34:h:101:LEU:HA	1.90	0.40
38:l:124:ASN:O	41:o:67:ARG:HD2	2.22	0.40
2:B:32:SER:HB2	16:P:128:ASP:HA	2.02	0.40
3:C:78:HIS:HB3	3:C:272:PHE:CZ	2.57	0.40
3:C:242:LEU:HD23	17:Q:101:TYR:HB3	2.03	0.40
4:D:114:LEU:HD22	4:D:477:PHE:CZ	2.56	0.40
7:G:160:LYS:O	7:G:168:THR:OG1	2.29	0.40
11:K:74:ARG:NE	20:T:133:ILE:HA	2.36	0.40
12:L:80:LYS:NZ	12:L:483:PRO:O	2.37	0.40
12:L:96:VAL:HG11	12:L:246:LEU:HB2	2.03	0.40
14:N:218:TYR:HD2	14:N:222:ILE:HD13	1.87	0.40
16:P:297:GLN:HB3	16:P:298:TYR:CE1	2.55	0.40
28:b:31:ILE:HD12	45:b:102:PLC:H4A1	2.04	0.40
28:b:48:ARG:NH1	28:b:54:ASP:OD2	2.54	0.40
29:c:40:LYS:C	29:c:44:VAL:HG21	2.46	0.40
42:p:64:ARG:HA	42:p:64:ARG:HD2	1.88	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	133/141 (94%)	124 (93%)	9 (7%)	0	100	100
2	B	173/204 (85%)	163 (94%)	10 (6%)	0	100	100
3	C	238/289 (82%)	229 (96%)	9 (4%)	0	100	100
4	D	435/482 (90%)	413 (95%)	22 (5%)	0	100	100
5	E	181/241 (75%)	172 (95%)	9 (5%)	0	100	100
6	F	451/473 (95%)	419 (93%)	31 (7%)	1 (0%)	44	72
7	G	694/726 (96%)	664 (96%)	29 (4%)	1 (0%)	48	76
8	H	351/353 (99%)	333 (95%)	17 (5%)	1 (0%)	37	66
9	I	190/222 (86%)	183 (96%)	7 (4%)	0	100	100
10	J	151/161 (94%)	142 (94%)	8 (5%)	1 (1%)	19	50
11	K	78/82 (95%)	76 (97%)	2 (3%)	0	100	100
12	L	640/642 (100%)	617 (96%)	22 (3%)	1 (0%)	44	72
13	M	489/491 (100%)	471 (96%)	17 (4%)	1 (0%)	44	72
14	N	502/523 (96%)	484 (96%)	17 (3%)	1 (0%)	44	72
15	O	191/193 (99%)	185 (97%)	6 (3%)	0	100	100
16	P	353/384 (92%)	342 (97%)	11 (3%)	0	100	100
17	Q	110/159 (69%)	107 (97%)	3 (3%)	0	100	100
18	R	122/139 (88%)	116 (95%)	6 (5%)	0	100	100
19	S	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
20	T	91/138 (66%)	86 (94%)	5 (6%)	0	100	100
21	U	86/130 (66%)	77 (90%)	9 (10%)	0	100	100
22	V	124/134 (92%)	118 (95%)	6 (5%)	0	100	100
23	W	111/122 (91%)	108 (97%)	3 (3%)	0	100	100
24	X	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
25	Y	203/216 (94%)	190 (94%)	13 (6%)	0	100	100
26	Z	140/147 (95%)	133 (95%)	6 (4%)	1 (1%)	19	50
27	a	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
28	b	76/79 (96%)	71 (93%)	5 (7%)	0	100	100
29	c	180/182 (99%)	170 (94%)	10 (6%)	0	100	100
30	d	73/78 (94%)	71 (97%)	2 (3%)	0	100	100
31	e	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
32	f	76/86 (88%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	g	152/239 (64%)	148 (97%)	4 (3%)	0	100	100
34	h	129/182 (71%)	122 (95%)	7 (5%)	0	100	100
35	i	67/74 (90%)	63 (94%)	4 (6%)	0	100	100
36	j	51/59 (86%)	45 (88%)	6 (12%)	0	100	100
37	k	43/61 (70%)	41 (95%)	2 (5%)	0	100	100
38	l	130/156 (83%)	123 (95%)	6 (5%)	1 (1%)	16	47
39	m	75/81 (93%)	70 (93%)	5 (7%)	0	100	100
40	n	103/111 (93%)	101 (98%)	2 (2%)	0	100	100
41	o	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
42	p	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
43	q	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
All	All	8216/9029 (91%)	7853 (96%)	354 (4%)	9 (0%)	50	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	2	ASN
38	l	145	THR
6	F	472	HIS
26	Z	1	ALA
13	M	2	LEU
7	G	390	THR
8	H	222	VAL
14	N	522	TRP
12	L	552	ILE

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	124/128 (97%)	109 (88%)	15 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	154/180 (86%)	151 (98%)	3 (2%)	52	72
3	C	214/254 (84%)	207 (97%)	7 (3%)	33	60
4	D	375/408 (92%)	351 (94%)	24 (6%)	14	41
5	E	163/218 (75%)	151 (93%)	12 (7%)	11	36
6	F	369/387 (95%)	341 (92%)	28 (8%)	11	35
7	G	582/610 (95%)	551 (95%)	31 (5%)	19	47
8	H	307/307 (100%)	284 (92%)	23 (8%)	11	35
9	I	166/192 (86%)	156 (94%)	10 (6%)	16	43
10	J	143/149 (96%)	130 (91%)	13 (9%)	7	28
11	K	70/72 (97%)	66 (94%)	4 (6%)	17	45
12	L	576/576 (100%)	546 (95%)	30 (5%)	19	48
13	M	439/439 (100%)	420 (96%)	19 (4%)	25	53
14	N	474/489 (97%)	458 (97%)	16 (3%)	32	59
15	O	169/169 (100%)	161 (95%)	8 (5%)	22	51
16	P	309/332 (93%)	296 (96%)	13 (4%)	25	54
17	Q	95/135 (70%)	87 (92%)	8 (8%)	9	32
18	R	104/118 (88%)	101 (97%)	3 (3%)	37	63
19	S	77/77 (100%)	73 (95%)	4 (5%)	19	48
20	T	85/128 (66%)	72 (85%)	13 (15%)	2	10
21	U	80/120 (67%)	73 (91%)	7 (9%)	8	30
22	V	112/119 (94%)	102 (91%)	10 (9%)	8	29
23	W	107/114 (94%)	104 (97%)	3 (3%)	38	64
24	X	165/165 (100%)	159 (96%)	6 (4%)	30	57
25	Y	163/173 (94%)	156 (96%)	7 (4%)	25	53
26	Z	123/128 (96%)	122 (99%)	1 (1%)	79	87
27	a	128/129 (99%)	126 (98%)	2 (2%)	58	75
28	b	66/67 (98%)	65 (98%)	1 (2%)	60	77
29	c	159/159 (100%)	150 (94%)	9 (6%)	17	45
30	d	62/65 (95%)	62 (100%)	0	100	100
31	e	91/92 (99%)	91 (100%)	0	100	100
32	f	64/71 (90%)	62 (97%)	2 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	143/215 (66%)	134 (94%)	9 (6%)	15	42
34	h	118/167 (71%)	109 (92%)	9 (8%)	11	35
35	i	59/63 (94%)	56 (95%)	3 (5%)	20	49
36	j	46/50 (92%)	44 (96%)	2 (4%)	25	53
37	k	32/47 (68%)	31 (97%)	1 (3%)	35	62
38	l	116/137 (85%)	107 (92%)	9 (8%)	10	34
39	m	64/66 (97%)	61 (95%)	3 (5%)	22	51
40	n	95/100 (95%)	92 (97%)	3 (3%)	34	61
41	o	74/79 (94%)	69 (93%)	5 (7%)	13	39
42	p	83/85 (98%)	80 (96%)	3 (4%)	30	57
43	q	125/125 (100%)	120 (96%)	5 (4%)	27	54
All	All	7270/7904 (92%)	6886 (95%)	384 (5%)	21	47

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	20	PHE
1	A	24	ASN
1	A	29	GLU
1	A	37	ASN
1	A	40	ILE
1	A	43	TYR
1	A	64	ILE
1	A	66	ILE
1	A	76	LEU
1	A	90	VAL
1	A	110	LEU
1	A	128	ILE
1	A	129	LEU
1	A	134	LYS
2	B	38	ILE
2	B	55	THR
2	B	78	CYS
3	C	49	ARG
3	C	139	THR
3	C	143	ARG
3	C	163	THR

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Mol	Chain	Res	Type
3	C	209	TYR
3	C	219	ASP
3	C	276	THR
4	D	62	SER
4	D	65	LYS
4	D	71	LYS
4	D	77	GLU
4	D	82	GLN
4	D	91	VAL
4	D	92	LYS
4	D	94	THR
4	D	111	HIS
4	D	113	VAL
4	D	120	LEU
4	D	126	LEU
4	D	127	ARG
4	D	156	ASP
4	D	160	TYR
4	D	269	GLN
4	D	296	GLU
4	D	298	THR
4	D	331	ASP
4	D	332	LYS
4	D	355	GLU
4	D	406	LYS
4	D	433	ASP
4	D	476	VAL
5	E	36	THR
5	E	49	LYS
5	E	109	THR
5	E	117	LYS
5	E	129	THR
5	E	130	THR
5	E	138	ASP
5	E	147	HIS
5	E	172	CYS
5	E	178	ILE
5	E	183	ASP
5	E	205	ILE
6	F	21	ASP
6	F	45	ASP
6	F	46	TRP

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Mol	Chain	Res	Type
6	F	102	ASP
6	F	111	ASP
6	F	131	ARG
6	F	142	ILE
6	F	157	ILE
6	F	192	GLU
6	F	193	GLU
6	F	240	ARG
6	F	266	VAL
6	F	268	GLU
6	F	280	LEU
6	F	285	GLU
6	F	287	HIS
6	F	314	HIS
6	F	319	VAL
6	F	342	ASN
6	F	352	GLN
6	F	363	CYS
6	F	369	CYS
6	F	375	TYR
6	F	409	CYS
6	F	413	ASP
6	F	445	VAL
6	F	464	ASN
6	F	472	HIS
7	G	25	LYS
7	G	30	THR
7	G	38	ILE
7	G	78	GLU
7	G	132	CYS
7	G	159	ASN
7	G	247	THR
7	G	249	ASP
7	G	256	SER
7	G	296	THR
7	G	298	ARG
7	G	340	VAL
7	G	369	ASP
7	G	398	ASP
7	G	405	THR
7	G	413	VAL
7	G	449	VAL

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Mol	Chain	Res	Type
7	G	485	GLU
7	G	491	VAL
7	G	505	GLU
7	G	527	THR
7	G	528	THR
7	G	550	VAL
7	G	557	ASP
7	G	631	ASP
7	G	653	VAL
7	G	682	ASN
7	G	685	GLU
7	G	692	VAL
7	G	697	SER
7	G	712	GLU
8	H	4	ASN
8	H	5	LEU
8	H	74	LEU
8	H	76	HIS
8	H	117	ILE
8	H	131	VAL
8	H	132	ILE
8	H	138	ASN
8	H	154	ILE
8	H	170	ILE
8	H	171	VAL
8	H	176	ILE
8	H	177	ASN
8	H	214	ASN
8	H	223	SER
8	H	225	HIS
8	H	235	VAL
8	H	321	ILE
8	H	324	CYS
8	H	332	VAL
8	H	336	VAL
8	H	337	VAL
8	H	353	ILE
9	I	124	ILE
9	I	126	CYS
9	I	128	LEU
9	I	132	VAL
9	I	145	ARG

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Mol	Chain	Res	Type
9	I	146	ILE
9	I	152	THR
9	I	175	ASP
9	I	184	GLU
9	I	198	GLU
10	J	7	ASP
10	J	25	ILE
10	J	31	THR
10	J	33	MET
10	J	46	LEU
10	J	51	TYR
10	J	55	TYR
10	J	59	VAL
10	J	61	ILE
10	J	72	GLU
10	J	98	ASN
10	J	104	ASP
10	J	130	ASN
11	K	5	LEU
11	K	27	MET
11	K	73	ILE
11	K	80	GLU
12	L	2	ILE
12	L	100	SER
12	L	118	SER
12	L	131	ASP
12	L	143	ILE
12	L	159	ASN
12	L	161	VAL
12	L	177	LEU
12	L	179	VAL
12	L	247	LEU
12	L	253	VAL
12	L	263	SER
12	L	264	SER
12	L	270	THR
12	L	348	HIS
12	L	350	ILE
12	L	364	ARG
12	L	394	ASP
12	L	410	ILE
12	L	432	TYR

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Mol	Chain	Res	Type
12	L	440	SER
12	L	452	ASP
12	L	459	MET
12	L	474	ARG
12	L	489	ILE
12	L	492	ASN
12	L	509	VAL
12	L	555	ASP
12	L	615	ILE
12	L	627	VAL
13	M	16	LEU
13	M	28	LEU
13	M	30	LYS
13	M	94	LEU
13	M	108	LYS
13	M	118	VAL
13	M	131	ASN
13	M	133	ILE
13	M	161	ASN
13	M	196	ASP
13	M	225	THR
13	M	232	THR
13	M	238	HIS
13	M	253	ILE
13	M	268	ASN
13	M	317	MET
13	M	349	VAL
13	M	438	VAL
13	M	489	VAL
14	N	17	ASN
14	N	18	LYS
14	N	48	GLU
14	N	86	SER
14	N	221	SER
14	N	263	LEU
14	N	273	ILE
14	N	372	THR
14	N	377	ILE
14	N	384	LYS
14	N	387	PHE
14	N	435	LEU
14	N	436	ILE

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Mol	Chain	Res	Type
14	N	463	ILE
14	N	466	ASN
14	N	511	VAL
15	O	1	MET
15	O	3	THR
15	O	54	LYS
15	O	93	GLU
15	O	116	LEU
15	O	127	ARG
15	O	165	GLU
15	O	175	ASP
16	P	10	THR
16	P	57	SER
16	P	93	PHE
16	P	118	GLU
16	P	127	GLU
16	P	152	VAL
16	P	256	LYS
16	P	262	ILE
16	P	297	GLN
16	P	299	ILE
16	P	337	SER
16	P	364	ASP
16	P	365	ILE
17	Q	35	THR
17	Q	37	LEU
17	Q	53	ARG
17	Q	86	ASN
17	Q	87	ARG
17	Q	138	LYS
17	Q	140	ASP
17	Q	145	PHE
18	R	75	ILE
18	R	118	CYS
18	R	133	ASP
19	S	1	SER
19	S	3	LYS
19	S	58	SER
19	S	84	THR
20	T	50	THR
20	T	54	VAL
20	T	79	VAL

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Mol	Chain	Res	Type
20	T	88	ASP
20	T	105	ASP
20	T	114	THR
20	T	115	VAL
20	T	123	LEU
20	T	130	GLU
20	T	133	ILE
20	T	136	THR
20	T	137	ILE
20	T	138	ARG
21	U	45	THR
21	U	72	THR
21	U	87	SER
21	U	104	LEU
21	U	111	ASP
21	U	126	GLN
21	U	130	ILE
22	V	11	GLN
22	V	12	GLU
22	V	13	ILE
22	V	39	ILE
22	V	45	THR
22	V	49	LEU
22	V	80	ILE
22	V	124	ASP
22	V	128	THR
22	V	134	LEU
23	W	67	ASP
23	W	91	GLN
23	W	118	LEU
24	X	12	SER
24	X	33	GLU
24	X	82	LYS
24	X	150	ASP
24	X	180	GLU
24	X	183	ILE
25	Y	34	LYS
25	Y	74	TYR
25	Y	119	SER
25	Y	126	LEU
25	Y	181	ASN
25	Y	201	SER

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Mol	Chain	Res	Type
25	Y	211	ARG
26	Z	51	GLU
27	a	42	GLU
27	a	111	LEU
28	b	3	ILE
29	c	1(A)	SER
29	c	43	ARG
29	c	44	VAL
29	c	58	VAL
29	c	108	GLU
29	c	114	LEU
29	c	118	ASP
29	c	133	LYS
29	c	160	LEU
32	f	36	ASP
32	f	38	HIS
33	g	30	LEU
33	g	32	LYS
33	g	43	LYS
33	g	74	THR
33	g	75	ASN
33	g	82	ASP
33	g	95	VAL
33	g	101	LEU
33	g	202	ILE
34	h	52	ASP
34	h	63	ILE
34	h	75	LEU
34	h	93	ASP
34	h	119	THR
34	h	121	VAL
34	h	156	THR
34	h	159	THR
34	h	167	ASP
35	i	7	HIS
35	i	20	ASN
35	i	34	LEU
36	j	20	VAL
36	j	34	LEU
37	k	35	LEU
38	l	25	LYS
38	l	43	ARG

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Mol	Chain	Res	Type
38	l	45	LYS
38	l	57	LYS
38	l	59	ASP
38	l	68	ASN
38	l	95	LEU
38	l	127	ASN
38	l	144	ASP
39	m	21	LEU
39	m	34	LYS
39	m	78	VAL
40	n	52	PHE
40	n	58	ILE
40	n	88	CYS
41	o	4	SER
41	o	5	GLU
41	o	13	GLU
41	o	31	LEU
41	o	50	VAL
42	p	6	ARG
42	p	13	ASP
42	p	63	CYS
43	q	48	ASP
43	q	63	THR
43	q	87	VAL
43	q	104	VAL
43	q	123	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	93	GLN
2	B	118	ASN
4	D	74	HIS
4	D	102	ASN
4	D	121	HIS
4	D	358	GLN
5	E	28	HIS
5	E	33	HIS
5	E	51	ASN
5	E	79	GLN
6	F	27	GLN

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Mol	Chain	Res	Type
6	F	134	ASN
6	F	254	ASN
6	F	342	ASN
6	F	344	GLN
7	G	393	ASN
7	G	415	ASN
7	G	430	HIS
7	G	443	ASN
8	H	214	ASN
8	H	265	ASN
9	I	44	HIS
9	I	209	GLN
10	J	45	GLN
10	J	106	ASN
10	J	130	ASN
12	L	355	GLN
13	M	5	ASN
13	M	329	ASN
13	M	359	ASN
13	M	386	ASN
14	N	310	ASN
14	N	368	ASN
14	N	381	ASN
14	N	390	ASN
14	N	466	ASN
14	N	471	ASN
14	N	478	ASN
14	N	521	ASN
15	O	168	ASN
15	O	190	ASN
16	P	113	ASN
16	P	196	ASN
16	P	297	GLN
16	P	302	GLN
17	Q	59	GLN
18	R	34	GLN
18	R	48	GLN
18	R	55	GLN
18	R	109	ASN
20	T	134	ASN
21	U	118	GLN
23	W	3	ASN

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Mol	Chain	Res	Type
23	W	97	GLN
24	X	122	ASN
25	Y	15	HIS
25	Y	163	ASN
26	Z	65	HIS
26	Z	74	GLN
26	Z	77	ASN
27	a	41	GLN
29	c	31	ASN
29	c	41	ASN
33	g	133	ASN
33	g	198	HIS
34	h	53	HIS
34	h	118	GLN
34	h	140	HIS
34	h	153	HIS
34	h	170	ASN
37	k	4	ASN
37	k	22	ASN
38	l	124	ASN
39	m	75	GLN
42	p	24	HIS
42	p	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
14	FME	N	1	14	8,9,10	1.47	1 (12%)	7,9,11	1.41	1 (14%)
4	2MR	D	137	4	10,12,13	2.32	2 (20%)	5,13,15	2.32	1 (20%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.66	1 (14%)
12	FME	L	1	12	8,9,10	1.48	1 (12%)	7,9,11	1.74	2 (28%)
13	FME	M	1	13	8,9,10	1.53	1 (12%)	7,9,11	1.93	3 (42%)
11	FME	K	1	11	8,9,10	1.47	1 (12%)	7,9,11	1.66	3 (42%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.68	1 (14%)
10	FME	J	1	10	8,9,10	1.48	1 (12%)	7,9,11	1.72	2 (28%)

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
14	FME	N	1	14	-	0/7/9/11	-
4	2MR	D	137	4	-	0/10/13/15	-
8	FME	H	1	8	-	3/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	137	2MR	CZ-NH2	5.08	1.44	1.33
4	D	137	2MR	CZ-NE	4.75	1.44	1.34
13	M	1	FME	CN-N	3.68	1.45	1.33
1	A	1	FME	CN-N	3.67	1.45	1.33
8	H	1	FME	CN-N	3.63	1.45	1.33
12	L	1	FME	CN-N	3.54	1.45	1.33
10	J	1	FME	CN-N	3.53	1.45	1.33
11	K	1	FME	CN-N	3.48	1.44	1.33
14	N	1	FME	CN-N	3.46	1.44	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	2MR	CD-NE-CZ	-4.24	115.46	123.41
13	M	1	FME	CA-N-CN	-2.79	118.54	122.82
8	H	1	FME	CE-SD-CG	2.76	109.88	100.40
1	A	1	FME	CE-SD-CG	2.67	109.56	100.40
10	J	1	FME	CE-SD-CG	2.62	109.40	100.40
13	M	1	FME	CE-SD-CG	2.53	109.08	100.40
12	L	1	FME	CE-SD-CG	2.45	108.82	100.40
12	L	1	FME	CA-N-CN	-2.44	119.07	122.82
14	N	1	FME	CE-SD-CG	2.36	108.49	100.40
10	J	1	FME	O1-CN-N	-2.36	119.06	125.27
11	K	1	FME	O1-CN-N	-2.22	119.42	125.27
11	K	1	FME	CE-SD-CG	2.20	107.97	100.40
13	M	1	FME	O-C-CA	-2.19	119.05	124.78
11	K	1	FME	CA-N-CN	-2.17	119.49	122.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
13	M	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0
1	A	1	FME	2	0
10	J	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 2 are monoatomic - leaving 56 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	$\# Z > 2$
49	3PE	m	701	-	28,28,50	1.12	4 (14%)	31,33,55	1.12	2 (6%)
45	PLC	B	303	-	30,30,41	0.58	0	36,38,49	0.62	0
45	PLC	N	602	-	41,41,41	0.54	0	47,49,49	0.51	0
49	3PE	L	706	-	50,50,50	0.85	3 (6%)	53,55,55	1.07	2 (3%)
50	CDL	a	201	-	59,59,99	1.12	8 (13%)	65,71,111	1.20	4 (6%)
44	SF4	G	803	7	0,12,12	-	-	-	-	-
44	SF4	I	302	9	0,12,12	-	-	-	-	-
49	3PE	O	202	-	30,30,50	1.09	4 (13%)	33,35,55	1.19	2 (6%)
45	PLC	Y	301	-	35,35,41	0.53	0	41,43,49	0.61	0
44	SF4	F	501	6	0,12,12	-	-	-	-	-
45	PLC	L	702	-	41,41,41	0.53	0	47,49,49	0.57	1 (2%)
49	3PE	M	503	-	45,45,50	0.90	4 (8%)	48,50,55	1.04	2 (4%)
44	SF4	B	301	2	0,12,12	-	-	-	-	-
46	FES	E	301	5	0,4,4	-	-	-	-	-
50	CDL	Z	202	-	48,48,99	1.23	8 (16%)	54,60,111	1.27	4 (7%)
45	PLC	q	401	-	35,35,41	0.56	0	41,43,49	0.60	0
53	EHZ	U	201	21	29,36,37	1.66	5 (17%)	35,44,47	1.63	7 (20%)
44	SF4	G	804	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	3PE	H	403	-	30,30,50	1.10	4 (13%)	33,35,55	1.17	2 (6%)
49	3PE	b	101	-	39,39,50	0.95	4 (10%)	42,44,55	1.17	2 (4%)
50	CDL	O	201	-	74,74,99	0.98	6 (8%)	80,86,111	1.17	4 (5%)
45	PLC	i	101	-	41,41,41	0.53	0	47,49,49	0.55	0
49	3PE	N	601	-	39,39,50	0.98	4 (10%)	42,44,55	1.14	2 (4%)
49	3PE	H	402	-	35,35,50	1.01	4 (11%)	38,40,55	1.04	2 (5%)
49	3PE	L	705	-	34,34,50	1.02	4 (11%)	37,39,55	1.10	2 (5%)
51	NDP	P	501	-	45,52,52	4.25	22 (48%)	53,80,80	2.14	6 (11%)
49	3PE	J	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.12	2 (3%)
45	PLC	b	102	-	38,38,41	0.54	0	44,46,49	0.59	0
53	EHZ	T	201	20	29,36,37	1.72	5 (17%)	35,44,47	1.58	5 (14%)
45	PLC	H	401	-	23,23,41	0.65	0	29,31,49	0.67	0
45	PLC	I	303	-	41,41,41	0.52	0	47,49,49	0.59	0
45	PLC	a	202	-	21,21,41	0.69	0	27,29,49	0.77	1 (3%)
49	3PE	O	203	-	34,34,50	1.02	4 (11%)	37,39,55	1.15	2 (5%)
45	PLC	m	702	-	35,35,41	0.56	0	41,43,49	0.59	1 (2%)
49	3PE	L	703	-	50,50,50	0.85	4 (8%)	53,55,55	1.11	2 (3%)
45	PLC	l	202	-	31,31,41	0.55	0	37,39,49	0.56	0
49	3PE	d	101	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
47	FMN	F	502	-	33,33,33	2.72	10 (30%)	48,50,50	1.90	14 (29%)
49	3PE	g	301	-	45,45,50	0.90	4 (8%)	48,50,55	1.06	2 (4%)
46	FES	G	801	7	0,4,4	-	-	-	-	-
45	PLC	M	501	-	41,41,41	0.52	0	47,49,49	0.58	1 (2%)
44	SF4	I	301	9	0,12,12	-	-	-	-	-
45	PLC	N	603	-	41,41,41	0.53	0	47,49,49	0.55	1 (2%)
45	PLC	h	201	-	38,38,41	0.54	0	44,46,49	0.55	0
49	3PE	M	504	-	50,50,50	0.85	3 (6%)	53,55,55	1.14	2 (3%)
45	PLC	L	701	-	34,34,41	0.58	0	40,42,49	0.60	0
49	3PE	L	704	-	50,50,50	0.85	4 (8%)	53,55,55	1.16	2 (3%)
49	3PE	m	703	-	24,24,50	1.20	4 (16%)	27,29,55	1.42	2 (7%)
45	PLC	M	502	-	41,41,41	0.50	0	47,49,49	0.53	0
49	3PE	l	201	-	41,41,50	0.95	3 (7%)	44,46,55	1.20	2 (4%)
45	PLC	B	302	-	30,30,41	0.60	0	36,38,49	0.53	0
45	PLC	P	502	-	30,30,41	0.57	0	36,38,49	0.66	0
45	PLC	q	402	-	41,41,41	0.49	0	47,49,49	0.71	1 (2%)
45	PLC	Z	201	-	41,41,41	0.52	0	47,49,49	0.57	0
49	3PE	j	101	-	26,26,50	1.16	4 (15%)	29,31,55	1.22	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CDL	b	103	-	58,58,99	1.12	7 (12%)	64,70,111	1.25	4 (6%)

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
49	3PE	m	701	-	-	11/32/32/54	-
45	PLC	B	303	-	-	11/34/34/45	-
45	PLC	N	602	-	-	15/45/45/45	-
49	3PE	L	706	-	-	31/54/54/54	-
50	CDL	a	201	-	-	37/70/70/110	-
49	3PE	O	202	-	-	20/34/34/54	-
44	SF4	G	803	7	-	-	0/6/5/5
44	SF4	I	302	9	-	-	0/6/5/5
45	PLC	Y	301	-	-	14/39/39/45	-
44	SF4	F	501	6	-	-	0/6/5/5
45	PLC	L	702	-	-	15/45/45/45	-
49	3PE	M	503	-	-	26/49/49/54	-
44	SF4	B	301	2	-	-	0/6/5/5
46	FES	E	301	5	-	-	0/1/1/1
50	CDL	Z	202	-	-	29/58/58/110	-
45	PLC	q	401	-	-	21/39/39/45	-
53	EHZ	U	201	21	-	20/42/44/45	-
50	CDL	O	201	-	-	42/85/85/110	-
49	3PE	H	403	-	-	17/34/34/54	-
49	3PE	b	101	-	-	22/43/43/54	-
44	SF4	G	804	7	-	-	0/6/5/5
45	PLC	i	101	-	-	13/45/45/45	-
49	3PE	N	601	-	-	23/43/43/54	-
49	3PE	H	402	-	-	17/39/39/54	-
49	3PE	L	705	-	-	19/38/38/54	-
51	NDP	P	501	-	-	12/30/77/77	0/5/5/5
49	3PE	J	201	-	-	24/54/54/54	-
45	PLC	b	102	-	-	9/42/42/45	-
53	EHZ	T	201	20	-	18/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PLC	H	401	-	-	11/26/26/45	-
45	PLC	I	303	-	-	15/45/45/45	-
45	PLC	a	202	-	-	11/23/23/45	-
49	3PE	O	203	-	-	24/38/38/54	-
45	PLC	m	702	-	-	19/39/39/45	-
49	3PE	L	703	-	-	22/54/54/54	-
45	PLC	l	202	-	-	14/35/35/45	-
49	3PE	d	101	-	-	19/38/38/54	-
47	FMN	F	502	-	-	9/18/18/18	0/3/3/3
49	3PE	g	301	-	-	26/49/49/54	-
46	FES	G	801	7	-	-	0/1/1/1
45	PLC	M	501	-	-	18/45/45/45	-
44	SF4	I	301	9	-	-	0/6/5/5
45	PLC	N	603	-	-	19/45/45/45	-
45	PLC	h	201	-	-	11/42/42/45	-
49	3PE	M	504	-	-	17/54/54/54	-
45	PLC	L	701	-	-	19/38/38/45	-
49	3PE	L	704	-	-	28/54/54/54	-
49	3PE	m	703	-	-	15/27/27/54	-
45	PLC	M	502	-	-	22/45/45/45	-
49	3PE	l	201	-	-	21/45/45/54	-
45	PLC	B	302	-	-	17/34/34/45	-
45	PLC	P	502	-	-	13/34/34/45	-
45	PLC	q	402	-	-	22/45/45/45	-
45	PLC	Z	201	-	-	17/45/45/45	-
49	3PE	j	101	-	-	14/30/30/54	-
50	CDL	b	103	-	-	30/69/69/110	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	P	501	NDP	O4B-C1B	14.53	1.61	1.41
51	P	501	NDP	C6N-C5N	12.10	1.54	1.33
51	P	501	NDP	C7N-N7N	8.26	1.55	1.33
51	P	501	NDP	O4D-C1D	8.03	1.61	1.42
51	P	501	NDP	C2D-C1D	-7.42	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	F	502	FMN	C4A-N5	7.12	1.44	1.30
51	P	501	NDP	O4D-C4D	-6.48	1.30	1.45
47	F	502	FMN	C10-N1	6.33	1.46	1.33
53	T	201	EHZ	C15-N2	5.53	1.45	1.33
51	P	501	NDP	P2B-O2B	5.41	1.69	1.59
53	T	201	EHZ	C12-N1	5.38	1.45	1.33
51	P	501	NDP	O4B-C4B	-5.24	1.33	1.45
53	U	201	EHZ	C15-N2	5.23	1.45	1.33
47	F	502	FMN	C5A-N5	5.13	1.49	1.39
53	U	201	EHZ	C12-N1	5.11	1.45	1.33
51	P	501	NDP	C2N-C3N	4.79	1.48	1.34
47	F	502	FMN	C9A-N10	4.66	1.49	1.41
47	F	502	FMN	C2-N1	4.61	1.47	1.36
47	F	502	FMN	C2-N3	4.37	1.49	1.39
51	P	501	NDP	O7N-C7N	-4.04	1.14	1.24
47	F	502	FMN	C4-N3	3.92	1.46	1.38
51	P	501	NDP	C6A-N6A	3.83	1.48	1.34
51	P	501	NDP	C5A-C4A	-3.78	1.30	1.40
51	P	501	NDP	O2D-C2D	3.73	1.51	1.43
47	F	502	FMN	C10-N10	3.46	1.44	1.37
51	P	501	NDP	C4N-C3N	3.34	1.56	1.49
47	F	502	FMN	O2-C2	-3.19	1.18	1.24
51	P	501	NDP	C2A-N3A	2.82	1.36	1.32
50	O	201	CDL	OB6-CB4	-2.81	1.39	1.46
49	M	504	3PE	O21-C2	-2.75	1.39	1.46
50	a	201	CDL	OB6-CB4	-2.75	1.39	1.46
51	P	501	NDP	O3B-C3B	-2.74	1.36	1.43
51	P	501	NDP	C4N-C5N	2.73	1.56	1.48
50	b	103	CDL	OB6-CB4	-2.71	1.39	1.46
49	l	201	3PE	O21-C2	-2.68	1.39	1.46
47	F	502	FMN	O4-C4	-2.68	1.18	1.23
50	Z	202	CDL	OB6-CB4	-2.66	1.39	1.46
50	b	103	CDL	OA6-CA4	-2.65	1.40	1.46
49	L	703	3PE	O21-C2	-2.65	1.40	1.46
49	N	601	3PE	O21-C2	-2.63	1.40	1.46
49	L	706	3PE	O21-C2	-2.61	1.40	1.46
49	j	101	3PE	O21-C2	-2.60	1.40	1.46
49	g	301	3PE	O21-C2	-2.60	1.40	1.46
50	Z	202	CDL	OA6-CA5	2.59	1.41	1.35
51	P	501	NDP	O3D-C3D	-2.58	1.36	1.43
49	L	704	3PE	O21-C2	-2.55	1.40	1.46
49	H	402	3PE	O21-C2	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	201	3PE	O21-C2	-2.51	1.40	1.46
49	L	705	3PE	O21-C2	-2.50	1.40	1.46
50	a	201	CDL	OA6-CA4	-2.48	1.40	1.46
50	O	201	CDL	OA8-CA7	2.48	1.40	1.33
49	m	703	3PE	O21-C21	2.48	1.40	1.35
50	a	201	CDL	OB8-CB7	2.46	1.40	1.33
49	m	701	3PE	O21-C2	-2.46	1.40	1.46
49	J	201	3PE	O31-C3	-2.44	1.39	1.45
51	P	501	NDP	C7N-C3N	2.44	1.53	1.48
50	b	103	CDL	OA8-CA7	2.43	1.40	1.33
50	b	103	CDL	OB8-CB7	2.42	1.40	1.33
49	l	201	3PE	O31-C31	2.41	1.40	1.33
49	O	202	3PE	O31-C31	2.41	1.40	1.33
49	b	101	3PE	O21-C2	-2.41	1.40	1.46
53	U	201	EHZ	O4-C15	-2.40	1.18	1.23
49	O	202	3PE	O21-C2	-2.39	1.40	1.46
49	L	705	3PE	O31-C31	2.39	1.40	1.33
49	L	703	3PE	O31-C3	-2.39	1.39	1.45
49	H	403	3PE	O31-C31	2.38	1.40	1.33
53	U	201	EHZ	O3-C12	-2.38	1.18	1.23
49	g	301	3PE	O31-C31	2.38	1.40	1.33
50	Z	202	CDL	OA8-CA7	2.37	1.40	1.33
49	H	403	3PE	O21-C2	-2.36	1.40	1.46
49	b	101	3PE	O31-C3	-2.35	1.39	1.45
49	d	101	3PE	O31-C3	-2.34	1.39	1.45
49	H	402	3PE	O31-C31	2.34	1.40	1.33
49	d	101	3PE	O21-C21	2.33	1.40	1.34
49	N	601	3PE	O31-C31	2.33	1.40	1.33
53	U	201	EHZ	C9-S1	2.32	1.81	1.76
49	m	701	3PE	O31-C31	2.32	1.40	1.33
49	N	601	3PE	O31-C3	-2.32	1.39	1.45
49	m	703	3PE	O31-C31	2.31	1.40	1.33
51	P	501	NDP	C6N-N1N	2.31	1.43	1.37
53	T	201	EHZ	C9-S1	2.31	1.81	1.76
49	O	203	3PE	O21-C2	-2.31	1.40	1.46
50	Z	202	CDL	OB8-CB6	-2.31	1.39	1.45
49	j	101	3PE	O31-C31	2.29	1.40	1.33
49	M	503	3PE	O21-C21	2.29	1.40	1.34
49	d	101	3PE	O31-C31	2.29	1.40	1.33
49	L	706	3PE	O31-C31	2.28	1.40	1.33
50	Z	202	CDL	OB8-CB7	2.28	1.40	1.33
53	T	201	EHZ	O3-C12	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	d	101	3PE	O21-C2	-2.26	1.40	1.46
50	a	201	CDL	OA8-CA7	2.26	1.39	1.33
50	O	201	CDL	OA6-CA5	2.26	1.40	1.34
49	O	203	3PE	O21-C21	2.26	1.40	1.34
49	O	203	3PE	O31-C31	2.26	1.39	1.33
49	L	704	3PE	O31-C3	-2.26	1.40	1.45
49	O	203	3PE	O31-C3	-2.26	1.40	1.45
49	M	504	3PE	O31-C3	-2.25	1.40	1.45
49	H	403	3PE	O21-C21	2.25	1.40	1.34
50	a	201	CDL	OA8-CA6	-2.25	1.40	1.45
51	P	501	NDP	PA-O5B	2.25	1.68	1.59
49	M	503	3PE	O31-C3	-2.25	1.40	1.45
49	M	503	3PE	O31-C31	2.24	1.39	1.33
50	O	201	CDL	OB8-CB7	2.24	1.39	1.33
49	L	704	3PE	O31-C31	2.24	1.39	1.33
50	O	201	CDL	OB8-CB6	-2.23	1.40	1.45
49	J	201	3PE	O21-C21	2.23	1.40	1.34
50	a	201	CDL	OB8-CB6	-2.23	1.40	1.45
49	L	706	3PE	O31-C3	-2.22	1.40	1.45
53	T	201	EHZ	O4-C15	-2.22	1.19	1.23
51	P	501	NDP	P2B-O1X	2.21	1.57	1.50
49	M	504	3PE	O31-C31	2.21	1.39	1.33
49	m	703	3PE	O21-C2	-2.20	1.41	1.46
49	m	701	3PE	O31-C3	-2.20	1.40	1.45
50	Z	202	CDL	OA6-CA4	-2.19	1.41	1.46
50	b	103	CDL	OB8-CB6	-2.19	1.40	1.45
49	M	503	3PE	O21-C2	-2.18	1.41	1.46
49	J	201	3PE	O31-C31	2.18	1.39	1.33
49	H	403	3PE	O31-C3	-2.17	1.40	1.45
49	m	701	3PE	O21-C21	2.17	1.40	1.34
50	a	201	CDL	OA6-CA5	2.17	1.40	1.34
49	l	201	3PE	O31-C3	-2.17	1.40	1.45
49	b	101	3PE	O21-C21	2.16	1.40	1.34
49	O	202	3PE	O21-C21	2.15	1.40	1.34
49	b	101	3PE	O31-C31	2.15	1.39	1.33
49	g	301	3PE	O31-C3	-2.14	1.40	1.45
49	H	402	3PE	O31-C3	-2.14	1.40	1.45
49	j	101	3PE	O31-C3	-2.14	1.40	1.45
50	O	201	CDL	OA6-CA4	-2.14	1.41	1.46
50	b	103	CDL	OA8-CA6	-2.13	1.40	1.45
49	L	704	3PE	O21-C21	2.11	1.40	1.34
49	m	703	3PE	O31-C3	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	L	703	3PE	O21-C21	2.10	1.40	1.34
49	L	705	3PE	O31-C3	-2.10	1.40	1.45
50	Z	202	CDL	OB6-CB5	2.09	1.40	1.34
49	L	703	3PE	O31-C31	2.08	1.39	1.33
49	H	402	3PE	O21-C21	2.08	1.40	1.34
49	L	705	3PE	O21-C21	2.07	1.40	1.34
49	j	101	3PE	O21-C21	2.06	1.40	1.34
49	O	202	3PE	O31-C3	-2.05	1.40	1.45
49	N	601	3PE	O21-C21	2.05	1.40	1.34
50	a	201	CDL	OB6-CB5	2.04	1.40	1.34
50	b	103	CDL	OB6-CB5	2.04	1.40	1.34
50	Z	202	CDL	OA8-CA6	-2.02	1.40	1.45
49	g	301	3PE	O21-C21	2.02	1.40	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	P	501	NDP	C5A-C6A-N6A	8.79	133.71	120.35
51	P	501	NDP	C1B-N9A-C4A	-7.35	113.73	126.64
51	P	501	NDP	N6A-C6A-N1A	-6.41	105.27	118.57
53	T	201	EHZ	C8-C9-S1	5.73	120.71	113.63
49	m	703	3PE	O21-C21-C22	5.37	120.96	111.09
51	P	501	NDP	N3A-C2A-N1A	-5.32	120.36	128.68
47	F	502	FMN	C7M-C7-C6	5.21	129.12	119.49
53	U	201	EHZ	C8-C9-S1	5.18	120.04	113.63
47	F	502	FMN	C9-C8-C7	5.12	127.01	119.67
50	Z	202	CDL	OA6-CA5-C11	5.06	120.40	111.09
49	N	601	3PE	O21-C21-C22	4.28	120.73	111.50
49	b	101	3PE	O21-C21-C22	4.27	120.70	111.50
49	O	203	3PE	O21-C21-C22	4.25	120.67	111.50
49	O	202	3PE	O21-C21-C22	4.25	120.67	111.50
49	H	403	3PE	O21-C21-C22	4.20	120.56	111.50
50	a	201	CDL	OB6-CB5-C51	4.18	120.52	111.50
47	F	502	FMN	C8M-C8-C7	-4.14	112.25	120.74
49	L	704	3PE	O21-C21-C22	4.14	120.42	111.50
50	b	103	CDL	OA6-CA5-C11	4.11	120.36	111.50
49	d	101	3PE	O21-C21-C22	4.06	120.25	111.50
50	O	201	CDL	OA6-CA5-C11	4.04	120.22	111.50
49	j	101	3PE	O21-C21-C22	4.04	120.21	111.50
49	l	201	3PE	O21-C21-C22	4.01	120.14	111.50
50	O	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
49	L	706	3PE	O21-C21-C22	3.94	119.99	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g	301	3PE	O21-C21-C22	3.93	119.97	111.50
49	M	504	3PE	O21-C21-C22	3.91	119.92	111.50
49	M	503	3PE	O21-C21-C22	3.90	119.91	111.50
49	J	201	3PE	O21-C21-C22	3.87	119.83	111.50
50	b	103	CDL	OB6-CB5-C51	3.82	119.74	111.50
50	Z	202	CDL	OB6-CB5-C51	3.77	119.62	111.50
49	L	703	3PE	O21-C21-C22	3.74	119.55	111.50
50	b	103	CDL	OB8-CB7-C71	3.69	121.06	111.38
51	P	501	NDP	PN-O3-PA	-3.64	120.34	132.83
49	H	402	3PE	O21-C21-C22	3.63	119.33	111.50
49	L	705	3PE	O21-C21-C22	3.56	119.17	111.50
49	m	701	3PE	O21-C21-C22	3.56	119.17	111.50
50	a	201	CDL	OA6-CA5-C11	3.50	119.05	111.50
47	F	502	FMN	C4-N3-C2	-3.40	119.36	125.64
49	l	201	3PE	O31-C31-C32	3.20	121.96	111.91
47	F	502	FMN	C7M-C7-C8	-3.15	114.28	120.74
50	O	201	CDL	OB8-CB7-C71	3.01	121.36	111.91
50	a	201	CDL	OB8-CB7-C71	2.96	121.19	111.91
50	a	201	CDL	OA8-CA7-C31	2.91	121.05	111.91
47	F	502	FMN	C4A-C10-N10	2.83	120.62	116.48
53	T	201	EHZ	C10-S1-C9	2.82	110.64	101.87
49	O	202	3PE	O31-C31-C32	2.75	120.55	111.91
50	b	103	CDL	OA8-CA7-C31	2.71	120.40	111.91
49	M	504	3PE	O31-C31-C32	2.70	120.40	111.91
49	N	601	3PE	O31-C31-C32	2.69	120.34	111.91
49	L	705	3PE	O31-C31-C32	2.68	120.33	111.91
53	T	201	EHZ	C7-C8-C9	-2.66	107.82	113.89
49	m	703	3PE	O31-C31-C32	2.65	120.21	111.91
50	O	201	CDL	OA8-CA7-C31	2.61	120.08	111.91
49	m	701	3PE	O31-C31-C32	2.60	120.07	111.91
49	d	101	3PE	O31-C31-C32	2.59	120.05	111.91
49	j	101	3PE	O31-C31-C32	2.58	120.00	111.91
50	Z	202	CDL	OA8-CA7-C31	2.58	120.00	111.91
49	L	704	3PE	O31-C31-C32	2.58	119.99	111.91
53	U	201	EHZ	C14-C13-C12	-2.56	108.09	112.36
49	O	203	3PE	O31-C31-C32	2.55	119.92	111.91
49	L	703	3PE	O31-C31-C32	2.55	119.90	111.91
47	F	502	FMN	O4-C4-C4A	-2.54	119.87	126.60
50	Z	202	CDL	OB8-CB7-C71	2.53	119.85	111.91
45	L	702	PLC	C3-C2-C1	2.53	117.77	111.79
53	U	201	EHZ	C7-C8-C9	-2.51	108.17	113.89
47	F	502	FMN	C4A-C4-N3	2.50	119.55	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	T	201	EHZ	C13-C12-N1	2.49	120.62	116.42
49	H	402	3PE	O31-C31-C32	2.49	119.72	111.91
49	g	301	3PE	O31-C31-C32	2.47	119.67	111.91
49	M	503	3PE	O31-C31-C32	2.46	119.61	111.91
49	H	403	3PE	O31-C31-C32	2.45	119.58	111.91
45	q	402	PLC	C2-O2-C'	2.41	123.72	117.79
47	F	502	FMN	C9A-C5A-N5	-2.41	119.82	122.43
49	J	201	3PE	O31-C31-C32	2.38	119.37	111.91
49	b	101	3PE	O31-C31-C32	2.32	119.19	111.91
49	L	706	3PE	O31-C31-C32	2.32	119.17	111.91
47	F	502	FMN	C5A-C9A-N10	2.27	120.30	117.95
47	F	502	FMN	C10-C4A-N5	-2.22	120.14	124.86
45	m	702	PLC	C3-C2-C1	2.18	116.94	111.79
47	F	502	FMN	C6-C5A-C9A	2.17	122.00	118.94
47	F	502	FMN	C6-C7-C8	-2.15	116.59	119.67
53	T	201	EHZ	O2-C9-S1	-2.12	119.86	122.61
45	M	501	PLC	C3-C2-C1	2.10	116.77	111.79
53	U	201	EHZ	O2-C9-S1	-2.05	119.95	122.61
47	F	502	FMN	C4-C4A-C10	2.05	120.23	116.79
53	U	201	EHZ	C11-N1-C12	-2.04	119.05	122.84
45	N	603	PLC	C3-C2-C1	2.04	116.61	111.79
53	U	201	EHZ	C5-C6-C7	-2.03	109.00	114.85
45	a	202	PLC	C3-C2-C1	2.02	116.57	111.79
51	P	501	NDP	C5B-C4B-C3B	-2.02	107.62	115.18
53	U	201	EHZ	C13-C12-N1	2.01	119.80	116.42

There are no chirality outliers.

All (919) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	303	PLC	O4P-C4-C5-N
45	B	303	PLC	C5-C4-O4P-P
45	B	303	PLC	C1'-C'-O2-C2
45	B	303	PLC	O'-C'-O2-C2
45	B	303	PLC	C1-O3P-P-O2P
45	B	303	PLC	C4-O4P-P-O1P
45	B	303	PLC	C4-O4P-P-O3P
45	I	303	PLC	C1'-C'-O2-C2
45	L	701	PLC	O4P-C4-C5-N
45	L	701	PLC	C1-O3P-P-O1P
45	L	701	PLC	C1-O3P-P-O2P
45	L	702	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
45	L	702	PLC	C1-O3P-P-O1P
45	L	702	PLC	C1-O3P-P-O2P
45	L	702	PLC	C1-O3P-P-O4P
45	M	501	PLC	C1'-C'-O2-C2
45	M	501	PLC	O'-C'-O2-C2
45	M	502	PLC	C4-O4P-P-O1P
45	N	602	PLC	O4P-C4-C5-N
45	N	602	PLC	C4-O4P-P-O2P
45	N	603	PLC	O4P-C4-C5-N
45	N	603	PLC	C1-O3P-P-O1P
45	N	603	PLC	C4-O4P-P-O1P
45	N	603	PLC	C4-O4P-P-O2P
45	P	502	PLC	O2-C2-C3-O3
45	Y	301	PLC	C2-C3-O3-CB
45	Y	301	PLC	C5-C4-O4P-P
45	Y	301	PLC	C1'-C'-O2-C2
45	Y	301	PLC	O'-C'-O2-C2
45	Z	201	PLC	C1-O3P-P-O1P
45	Z	201	PLC	C1-O3P-P-O2P
45	a	202	PLC	C4-O4P-P-O1P
45	h	201	PLC	O4P-C4-C5-N
45	h	201	PLC	C1'-C'-O2-C2
45	h	201	PLC	O'-C'-O2-C2
45	h	201	PLC	C4-O4P-P-O2P
45	i	101	PLC	C1'-C'-O2-C2
45	i	101	PLC	C1-O3P-P-O1P
45	i	101	PLC	C1-O3P-P-O4P
45	l	202	PLC	O4P-C4-C5-N
45	l	202	PLC	C1'-C'-O2-C2
45	l	202	PLC	C1-O3P-P-O2P
45	m	702	PLC	O4P-C4-C5-N
45	m	702	PLC	C1'-C'-O2-C2
45	m	702	PLC	C1-O3P-P-O1P
45	m	702	PLC	C1-O3P-P-O2P
45	q	401	PLC	O4P-C4-C5-N
45	q	401	PLC	C1'-C'-O2-C2
45	q	401	PLC	C4-O4P-P-O1P
45	q	401	PLC	C4-O4P-P-O3P
45	q	402	PLC	C1-O3P-P-O1P
47	F	502	FMN	N10-C1'-C2'-O2'
47	F	502	FMN	N10-C1'-C2'-C3'
47	F	502	FMN	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
47	F	502	FMN	C1'-C2'-C3'-C4'
47	F	502	FMN	O2'-C2'-C3'-O3'
47	F	502	FMN	C3'-C4'-C5'-O5'
47	F	502	FMN	O4'-C4'-C5'-O5'
49	H	402	3PE	C11-O13-P-O12
49	H	403	3PE	C1-O11-P-O12
49	H	403	3PE	C11-O13-P-O12
49	H	403	3PE	C11-O13-P-O14
49	H	403	3PE	O22-C21-O21-C2
49	J	201	3PE	C1-O11-P-O12
49	J	201	3PE	C12-C11-O13-P
49	J	201	3PE	O13-C11-C12-N
49	J	201	3PE	O22-C21-O21-C2
49	L	704	3PE	C1-O11-P-O12
49	L	704	3PE	C11-O13-P-O14
49	L	704	3PE	O13-C11-C12-N
49	L	705	3PE	O21-C2-C3-O31
49	L	706	3PE	C11-O13-P-O11
49	L	706	3PE	C11-O13-P-O14
49	L	706	3PE	O21-C2-C3-O31
49	L	706	3PE	O22-C21-O21-C2
49	M	503	3PE	C1-O11-P-O13
49	M	503	3PE	C1-O11-P-O14
49	M	503	3PE	C11-O13-P-O12
49	M	503	3PE	C11-O13-P-O14
49	M	503	3PE	C22-C21-O21-C2
49	M	504	3PE	C1-O11-P-O14
49	M	504	3PE	C11-O13-P-O11
49	M	504	3PE	C11-O13-P-O12
49	M	504	3PE	C11-O13-P-O14
49	M	504	3PE	O22-C21-O21-C2
49	M	504	3PE	C22-C21-O21-C2
49	N	601	3PE	C1-O11-P-O12
49	N	601	3PE	C1-O11-P-O14
49	N	601	3PE	C11-O13-P-O11
49	N	601	3PE	C11-O13-P-O12
49	N	601	3PE	C11-O13-P-O14
49	N	601	3PE	O13-C11-C12-N
49	N	601	3PE	O22-C21-O21-C2
49	N	601	3PE	C22-C21-O21-C2
49	O	202	3PE	C11-O13-P-O11
49	O	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
49	O	203	3PE	C1-O11-P-O12
49	O	203	3PE	C1-O11-P-O13
49	O	203	3PE	C1-O11-P-O14
49	O	203	3PE	C11-O13-P-O11
49	O	203	3PE	C11-O13-P-O12
49	O	203	3PE	C11-O13-P-O14
49	O	203	3PE	O22-C21-O21-C2
49	b	101	3PE	C1-O11-P-O12
49	b	101	3PE	C11-O13-P-O11
49	b	101	3PE	C11-O13-P-O14
49	b	101	3PE	C22-C21-O21-C2
49	d	101	3PE	C1-O11-P-O12
49	d	101	3PE	C11-O13-P-O14
49	d	101	3PE	O13-C11-C12-N
49	g	301	3PE	C11-O13-P-O12
49	g	301	3PE	C11-O13-P-O14
49	g	301	3PE	O13-C11-C12-N
49	l	201	3PE	O11-C1-C2-O21
49	m	701	3PE	C1-O11-P-O12
49	m	701	3PE	C1-O11-P-O13
49	m	701	3PE	C1-O11-P-O14
49	m	703	3PE	C11-O13-P-O11
49	m	703	3PE	C11-O13-P-O14
49	m	703	3PE	O13-C11-C12-N
49	m	703	3PE	C22-C21-O21-C2
50	O	201	CDL	CA2-OA2-PA1-OA3
50	O	201	CDL	CA2-OA2-PA1-OA4
50	O	201	CDL	CA3-OA5-PA1-OA2
50	O	201	CDL	CA3-OA5-PA1-OA3
50	O	201	CDL	CA3-OA5-PA1-OA4
50	O	201	CDL	C11-CA5-OA6-CA4
50	O	201	CDL	CB2-OB2-PB2-OB3
50	O	201	CDL	C51-CB5-OB6-CB4
50	Z	202	CDL	CA3-OA5-PA1-OA2
50	Z	202	CDL	CA3-OA5-PA1-OA3
50	Z	202	CDL	C11-CA5-OA6-CA4
50	Z	202	CDL	CB3-OB5-PB2-OB3
50	Z	202	CDL	CB3-OB5-PB2-OB4
50	Z	202	CDL	OB7-CB5-OB6-CB4
50	a	201	CDL	CA2-OA2-PA1-OA4
50	a	201	CDL	OA9-CA7-OA8-CA6
50	a	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
50	a	201	CDL	CB3-OB5-PB2-OB3
50	a	201	CDL	CB3-OB5-PB2-OB4
50	a	201	CDL	C51-CB5-OB6-CB4
50	a	201	CDL	OB9-CB7-OB8-CB6
50	b	103	CDL	CA2-C1-CB2-OB2
50	b	103	CDL	CB3-OB5-PB2-OB4
50	b	103	CDL	OB5-CB3-CB4-OB6
50	b	103	CDL	OB9-CB7-OB8-CB6
50	b	103	CDL	C71-CB7-OB8-CB6
51	P	501	NDP	C5B-O5B-PA-O3
53	T	201	EHZ	C5-C6-C7-C8
53	T	201	EHZ	S1-C10-C11-N1
53	T	201	EHZ	O2-C9-S1-C10
53	T	201	EHZ	C8-C9-S1-C10
53	U	201	EHZ	N2-C15-C16-C17
53	U	201	EHZ	N2-C15-C16-O5
53	U	201	EHZ	O4-C15-C16-C17
53	U	201	EHZ	C15-C16-C17-C19
53	U	201	EHZ	C15-C16-C17-C20
53	U	201	EHZ	O2-C9-S1-C10
53	U	201	EHZ	C8-C9-S1-C10
45	H	401	PLC	C1'-C'-O2-C2
49	m	703	3PE	O22-C21-O21-C2
50	Z	202	CDL	OA7-CA5-OA6-CA4
45	M	501	PLC	OB-CB-O3-C3
49	N	601	3PE	O32-C31-O31-C3
49	j	101	3PE	O32-C31-O31-C3
45	H	401	PLC	O'-C'-O2-C2
49	N	601	3PE	C32-C31-O31-C3
50	a	201	CDL	C31-CA7-OA8-CA6
45	H	401	PLC	OB-CB-O3-C3
49	J	201	3PE	O32-C31-O31-C3
49	L	704	3PE	O32-C31-O31-C3
49	L	706	3PE	O32-C31-O31-C3
49	b	101	3PE	O32-C31-O31-C3
49	l	201	3PE	O32-C31-O31-C3
49	m	703	3PE	O32-C31-O31-C3
50	O	201	CDL	OA9-CA7-OA8-CA6
45	I	303	PLC	O'-C'-O2-C2
45	i	101	PLC	O'-C'-O2-C2
45	m	702	PLC	O'-C'-O2-C2
45	q	401	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
49	M	503	3PE	O22-C21-O21-C2
49	b	101	3PE	O22-C21-O21-C2
50	O	201	CDL	OA7-CA5-OA6-CA4
50	b	103	CDL	OA7-CA5-OA6-CA4
45	Y	301	PLC	OB-CB-O3-C3
45	M	501	PLC	C1B-CB-O3-C3
49	J	201	3PE	C32-C31-O31-C3
49	b	101	3PE	C32-C31-O31-C3
49	j	101	3PE	C32-C31-O31-C3
49	l	201	3PE	C32-C31-O31-C3
49	m	703	3PE	C32-C31-O31-C3
50	O	201	CDL	C31-CA7-OA8-CA6
50	a	201	CDL	C71-CB7-OB8-CB6
49	H	403	3PE	C22-C21-O21-C2
49	J	201	3PE	C22-C21-O21-C2
49	L	706	3PE	C22-C21-O21-C2
49	O	203	3PE	C22-C21-O21-C2
50	Z	202	CDL	C51-CB5-OB6-CB4
50	b	103	CDL	C11-CA5-OA6-CA4
45	H	401	PLC	C1B-CB-O3-C3
49	L	704	3PE	C32-C31-O31-C3
49	L	706	3PE	C32-C31-O31-C3
49	O	202	3PE	C32-C31-O31-C3
50	Z	202	CDL	C31-CA7-OA8-CA6
45	l	202	PLC	O'-C'-O2-C2
50	O	201	CDL	OB7-CB5-OB6-CB4
50	a	201	CDL	OB7-CB5-OB6-CB4
49	O	202	3PE	O32-C31-O31-C3
50	Z	202	CDL	OA9-CA7-OA8-CA6
49	l	201	3PE	C2-C3-O31-C31
45	Y	301	PLC	C1B-CB-O3-C3
49	O	202	3PE	C22-C21-O21-C2
49	d	101	3PE	C32-C31-O31-C3
49	d	101	3PE	O32-C31-O31-C3
49	O	202	3PE	O22-C21-O21-C2
45	H	401	PLC	C4-C5-N-C7
45	H	401	PLC	C4-C5-N-C8
45	L	701	PLC	C1B-CB-O3-C3
45	M	502	PLC	C1B-CB-O3-C3
45	q	401	PLC	O3P-C1-C2-O2
49	J	201	3PE	O21-C2-C3-O31
45	M	501	PLC	CB-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
45	b	102	PLC	CB-C1B-C2B-C3B
49	L	705	3PE	C21-C22-C23-C24
49	d	101	3PE	C21-C22-C23-C24
45	M	502	PLC	OB-CB-O3-C3
45	B	302	PLC	CB-C1B-C2B-C3B
45	Y	301	PLC	C'-C1'-C2'-C3'
45	q	401	PLC	CB-C1B-C2B-C3B
49	H	403	3PE	C21-C22-C23-C24
49	L	704	3PE	C31-C32-C33-C34
49	L	705	3PE	C31-C32-C33-C34
49	m	703	3PE	C31-C32-C33-C34
53	T	201	EHZ	C5-C6-C7-O1
45	a	202	PLC	C1'-C'-O2-C2
45	B	302	PLC	C4-C5-N-C8
45	q	402	PLC	C4-C5-N-C6
45	M	502	PLC	CB-C1B-C2B-C3B
45	N	602	PLC	C'-C1'-C2'-C3'
50	a	201	CDL	CA5-C11-C12-C13
49	L	706	3PE	C33-C34-C35-C36
45	L	701	PLC	OB-CB-O3-C3
49	g	301	3PE	C21-C22-C23-C24
45	B	302	PLC	C1-O3P-P-O4P
45	L	701	PLC	C1-O3P-P-O4P
45	L	701	PLC	C4-O4P-P-O3P
45	M	502	PLC	C1-O3P-P-O4P
45	N	603	PLC	C1-O3P-P-O4P
45	N	603	PLC	C4-O4P-P-O3P
45	Z	201	PLC	C1-O3P-P-O4P
45	h	201	PLC	C4-O4P-P-O3P
45	l	202	PLC	C1-O3P-P-O4P
45	m	702	PLC	C1-O3P-P-O4P
45	q	402	PLC	C4-O4P-P-O3P
49	H	403	3PE	C11-O13-P-O11
49	J	201	3PE	C1-O11-P-O13
49	L	704	3PE	C1-O11-P-O13
49	L	705	3PE	C11-O13-P-O11
49	M	503	3PE	C11-O13-P-O11
49	M	504	3PE	C1-O11-P-O13
49	N	601	3PE	C1-O11-P-O13
49	b	101	3PE	C1-O11-P-O13
49	d	101	3PE	C1-O11-P-O13
49	d	101	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	g	301	3PE	C11-O13-P-O11
49	j	101	3PE	C1-O11-P-O13
50	O	201	CDL	CA2-OA2-PA1-OA5
50	O	201	CDL	CB2-OB2-PB2-OB5
50	Z	202	CDL	CB3-OB5-PB2-OB2
50	a	201	CDL	CA2-OA2-PA1-OA5
50	a	201	CDL	CB3-OB5-PB2-OB2
50	b	103	CDL	CB3-OB5-PB2-OB2
45	P	502	PLC	CB-C1B-C2B-C3B
45	B	303	PLC	C1B-C2B-C3B-C4B
53	T	201	EHZ	C4-C5-C6-C7
45	N	602	PLC	C4'-C5'-C6'-C7'
45	N	603	PLC	C2B-C3B-C4B-C5B
49	H	402	3PE	C32-C33-C34-C35
49	L	706	3PE	C39-C3A-C3B-C3C
49	L	706	3PE	C3A-C3B-C3C-C3D
49	M	504	3PE	C2E-C2F-C2G-C2H
49	O	202	3PE	C26-C27-C28-C29
45	I	303	PLC	C5B-C6B-C7B-C8B
49	J	201	3PE	C33-C34-C35-C36
49	J	201	3PE	C38-C39-C3A-C3B
49	N	601	3PE	C25-C26-C27-C28
45	I	303	PLC	C3-C2-O2-C'
50	a	201	CDL	OA7-CA5-OA6-CA4
47	F	502	FMN	O2'-C2'-C3'-C4'
45	q	401	PLC	C6'-C7'-C8'-C9'
49	H	402	3PE	C27-C28-C29-C2A
49	J	201	3PE	C35-C36-C37-C38
49	L	704	3PE	C35-C36-C37-C38
49	L	706	3PE	C37-C38-C39-C3A
49	L	706	3PE	C23-C24-C25-C26
49	L	706	3PE	C29-C2A-C2B-C2C
49	N	601	3PE	C26-C27-C28-C29
50	Z	202	CDL	C72-C73-C74-C75
45	P	502	PLC	O3P-C1-C2-O2
45	h	201	PLC	C4'-C5'-C6'-C7'
45	q	402	PLC	C2B-C3B-C4B-C5B
49	L	706	3PE	C24-C25-C26-C27
49	L	706	3PE	C2B-C2C-C2D-C2E
50	O	201	CDL	C31-C32-C33-C34
50	b	103	CDL	O1-C1-CB2-OB2
50	O	201	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
45	i	101	PLC	C6'-C7'-C8'-C9'
45	q	402	PLC	C3B-C4B-C5B-C6B
49	M	503	3PE	C32-C33-C34-C35
49	m	701	3PE	C32-C33-C34-C35
45	Z	201	PLC	C4'-C5'-C6'-C7'
49	M	503	3PE	C3A-C3B-C3C-C3D
49	g	301	3PE	C32-C33-C34-C35
50	O	201	CDL	C52-C53-C54-C55
45	M	501	PLC	C6'-C7'-C8'-C9'
45	M	502	PLC	C4B-C5B-C6B-C7B
45	q	401	PLC	C4'-C5'-C6'-C7'
49	L	705	3PE	C25-C26-C27-C28
49	M	504	3PE	C35-C36-C37-C38
49	O	202	3PE	C24-C25-C26-C27
50	a	201	CDL	C51-C52-C53-C54
45	M	502	PLC	C3B-C4B-C5B-C6B
50	a	201	CDL	C11-CA5-OA6-CA4
45	B	302	PLC	C1B-C2B-C3B-C4B
49	L	703	3PE	C25-C26-C27-C28
49	M	503	3PE	C34-C35-C36-C37
49	d	101	3PE	C22-C23-C24-C25
53	T	201	EHZ	C1-C2-C3-C4
45	Y	301	PLC	C1'-C2'-C3'-C4'
45	b	102	PLC	C3B-C4B-C5B-C6B
49	L	703	3PE	C2D-C2E-C2F-C2G
49	L	704	3PE	C37-C38-C39-C3A
50	O	201	CDL	C77-C78-C79-C80
53	U	201	EHZ	C1-C21-C22-C23
45	B	302	PLC	C4-C5-N-C6
45	M	502	PLC	C7B-C8B-C9B-CAA
49	L	703	3PE	O13-C11-C12-N
49	O	202	3PE	O13-C11-C12-N
45	I	303	PLC	C5'-C6'-C7'-C8'
45	L	701	PLC	C1'-C2'-C3'-C4'
45	L	702	PLC	C3B-C4B-C5B-C6B
49	J	201	3PE	C3A-C3B-C3C-C3D
49	L	704	3PE	C28-C29-C2A-C2B
49	g	301	3PE	C35-C36-C37-C38
50	O	201	CDL	C54-C55-C56-C57
53	T	201	EHZ	C21-C1-C2-C3
49	H	402	3PE	C32-C31-O31-C3
49	L	704	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	b	101	3PE	C38-C39-C3A-C3B
49	m	701	3PE	C34-C35-C36-C37
45	B	302	PLC	C2B-C3B-C4B-C5B
45	m	702	PLC	C6B-C7B-C8B-C9B
49	O	202	3PE	C23-C24-C25-C26
49	d	101	3PE	C2A-C2B-C2C-C2D
49	g	301	3PE	C37-C38-C39-C3A
50	Z	202	CDL	C71-C72-C73-C74
50	O	201	CDL	C73-C74-C75-C76
50	a	201	CDL	C31-C32-C33-C34
50	b	103	CDL	C51-C52-C53-C54
45	q	402	PLC	C5B-C6B-C7B-C8B
45	M	502	PLC	C1'-C'-O2-C2
49	l	201	3PE	C22-C21-O21-C2
49	L	703	3PE	C36-C37-C38-C39
49	O	203	3PE	C33-C34-C35-C36
49	g	301	3PE	C34-C35-C36-C37
51	P	501	NDP	C3B-C4B-C5B-O5B
45	q	401	PLC	C1B-C2B-C3B-C4B
53	U	201	EHZ	C1-C2-C3-C4
45	M	502	PLC	O'-C'-O2-C2
49	l	201	3PE	O22-C21-O21-C2
49	H	402	3PE	O32-C31-O31-C3
50	b	103	CDL	C11-C12-C13-C14
45	H	401	PLC	C4-C5-N-C6
45	a	202	PLC	C4-C5-N-C8
49	L	704	3PE	C21-C22-C23-C24
49	l	201	3PE	C21-C22-C23-C24
45	N	602	PLC	C5B-C6B-C7B-C8B
49	O	202	3PE	C25-C26-C27-C28
45	i	101	PLC	C1B-CB-O3-C3
45	q	402	PLC	C1'-C'-O2-C2
49	l	201	3PE	C31-C32-C33-C34
50	O	201	CDL	C35-C36-C37-C38
45	N	603	PLC	C1'-C2'-C3'-C4'
49	H	403	3PE	C22-C23-C24-C25
49	l	201	3PE	C26-C27-C28-C29
45	L	701	PLC	O'-C'-O2-C2
45	Z	201	PLC	CB-C1B-C2B-C3B
49	O	203	3PE	C32-C31-O31-C3
45	N	602	PLC	C1'-C2'-C3'-C4'
45	q	401	PLC	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
49	L	706	3PE	C28-C29-C2A-C2B
50	O	201	CDL	C78-C79-C80-C81
45	N	603	PLC	C3B-C4B-C5B-C6B
49	L	703	3PE	C34-C35-C36-C37
49	g	301	3PE	C36-C37-C38-C39
50	O	201	CDL	C12-C13-C14-C15
50	Z	202	CDL	C73-C74-C75-C76
50	b	103	CDL	C58-C59-C60-C61
49	b	101	3PE	C23-C24-C25-C26
49	g	301	3PE	C25-C26-C27-C28
50	b	103	CDL	C12-C13-C14-C15
45	L	701	PLC	C'-C1'-C2'-C3'
49	O	203	3PE	C31-C32-C33-C34
45	L	701	PLC	C1'-C'-O2-C2
45	P	502	PLC	C1'-C'-O2-C2
49	L	703	3PE	C22-C21-O21-C2
50	b	103	CDL	C51-CB5-OB6-CB4
45	M	501	PLC	O3P-C1-C2-O2
49	L	705	3PE	C22-C23-C24-C25
50	O	201	CDL	C79-C80-C81-C82
49	M	503	3PE	C21-C22-C23-C24
45	h	201	PLC	C2'-C3'-C4'-C5'
45	b	102	PLC	C2'-C3'-C4'-C5'
49	b	101	3PE	C3A-C3B-C3C-C3D
45	B	302	PLC	C4-C5-N-C7
45	q	402	PLC	C4-C5-N-C7
45	h	201	PLC	C3'-C4'-C5'-C6'
49	l	201	3PE	C39-C3A-C3B-C3C
53	T	201	EHZ	C2-C3-C4-C5
45	Z	201	PLC	C1B-C2B-C3B-C4B
50	O	201	CDL	C13-C14-C15-C16
49	M	504	3PE	C39-C3A-C3B-C3C
45	B	302	PLC	C5B-C6B-C7B-C8B
45	i	101	PLC	OB-CB-O3-C3
45	q	402	PLC	O'-C'-O2-C2
49	M	503	3PE	C3D-C3E-C3F-C3G
49	M	504	3PE	C3A-C3B-C3C-C3D
49	d	101	3PE	C26-C27-C28-C29
45	N	602	PLC	C4-O4P-P-O3P
45	q	402	PLC	C1-O3P-P-O4P
49	L	704	3PE	C11-O13-P-O11
49	j	101	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	M	501	PLC	C1B-C2B-C3B-C4B
45	M	502	PLC	C3'-C4'-C5'-C6'
49	O	203	3PE	O32-C31-O31-C3
45	P	502	PLC	O3P-C1-C2-C3
49	L	704	3PE	O11-C1-C2-C3
50	Z	202	CDL	OA5-CA3-CA4-CA6
50	b	103	CDL	OB5-CB3-CB4-CB6
45	M	502	PLC	C2'-C3'-C4'-C5'
45	Y	301	PLC	C1B-C2B-C3B-C4B
53	T	201	EHZ	O3-C12-C13-C14
49	J	201	3PE	C36-C37-C38-C39
45	B	303	PLC	C1-C2-C3-O3
45	M	502	PLC	C1-C2-C3-O3
45	m	702	PLC	C1-C2-C3-O3
49	J	201	3PE	C1-C2-C3-O31
49	L	706	3PE	C1-C2-C3-O31
49	g	301	3PE	C1-C2-C3-O31
49	j	101	3PE	C1-C2-C3-O31
50	a	201	CDL	CB3-CB4-CB6-OB8
50	b	103	CDL	CB3-CB4-CB6-OB8
45	N	603	PLC	C4'-C5'-C6'-C7'
45	N	602	PLC	C8'-C9'-CA'-CB'
49	N	601	3PE	C28-C29-C2A-C2B
45	a	202	PLC	O'-C'-O2-C2
50	b	103	CDL	C16-C17-C18-C19
45	P	502	PLC	O'-C'-O2-C2
45	q	402	PLC	C8'-C9'-CA'-CB'
49	N	601	3PE	C2C-C2D-C2E-C2F
53	U	201	EHZ	O4-C15-C16-O5
49	J	201	3PE	C25-C26-C27-C28
49	g	301	3PE	C24-C25-C26-C27
45	m	702	PLC	C2B-C3B-C4B-C5B
49	L	703	3PE	C21-C22-C23-C24
45	i	101	PLC	C6B-C7B-C8B-C9B
49	l	201	3PE	C3A-C3B-C3C-C3D
51	P	501	NDP	O4B-C4B-C5B-O5B
53	U	201	EHZ	C18-C17-C20-O6
53	U	201	EHZ	C19-C17-C20-O6
49	N	601	3PE	C21-C22-C23-C24
45	q	402	PLC	C2-C3-O3-CB
45	i	101	PLC	C3-C2-O2-C'
49	m	703	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
50	Z	202	CDL	CA3-CA4-OA6-CA5
45	M	501	PLC	C5'-C6'-C7'-C8'
50	b	103	CDL	C13-C14-C15-C16
49	m	701	3PE	C2-C1-O11-P
49	L	704	3PE	C29-C2A-C2B-C2C
45	L	702	PLC	O3P-C1-C2-O2
45	q	402	PLC	C4-C5-N-C8
45	q	402	PLC	C1B-C2B-C3B-C4B
45	I	303	PLC	O2-C2-C3-O3
49	N	601	3PE	O21-C2-C3-O31
49	b	101	3PE	O21-C2-C3-O31
50	a	201	CDL	OB6-CB4-CB6-OB8
45	b	102	PLC	C8'-C9'-CA'-CB'
49	g	301	3PE	C38-C39-C3A-C3B
49	l	201	3PE	C23-C24-C25-C26
49	L	703	3PE	O22-C21-O21-C2
53	U	201	EHZ	O5-C16-C17-C18
53	U	201	EHZ	O5-C16-C17-C19
49	l	201	3PE	C24-C25-C26-C27
45	l	202	PLC	C3B-C4B-C5B-C6B
49	b	101	3PE	C22-C23-C24-C25
50	a	201	CDL	C15-C16-C17-C18
50	b	103	CDL	OB7-CB5-OB6-CB4
45	N	603	PLC	C8'-C9'-CA'-CB'
50	b	103	CDL	CB5-C51-C52-C53
45	M	501	PLC	O3P-C1-C2-C3
49	H	403	3PE	O11-C1-C2-C3
49	L	705	3PE	O11-C1-C2-C3
49	M	503	3PE	O11-C1-C2-C3
49	O	202	3PE	O11-C1-C2-C3
49	l	201	3PE	O11-C1-C2-C3
49	L	705	3PE	O13-C11-C12-N
49	O	202	3PE	C28-C29-C2A-C2B
49	L	706	3PE	C3E-C3F-C3G-C3H
45	L	702	PLC	C1B-C2B-C3B-C4B
49	H	402	3PE	O21-C21-C22-C23
49	O	202	3PE	O21-C21-C22-C23
50	O	201	CDL	C76-C77-C78-C79
50	a	201	CDL	C1-CB2-OB2-PB2
49	L	706	3PE	C22-C23-C24-C25
45	Y	301	PLC	C6'-C7'-C8'-C9'
45	N	603	PLC	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
45	L	702	PLC	C1-C2-C3-O3
45	P	502	PLC	C1-C2-C3-O3
45	i	101	PLC	C1-C2-C3-O3
49	L	703	3PE	C1-C2-C3-O31
49	L	704	3PE	C1-C2-C3-O31
49	N	601	3PE	C1-C2-C3-O31
49	l	201	3PE	C1-C2-C3-O31
45	b	102	PLC	C4B-C5B-C6B-C7B
49	O	203	3PE	C34-C35-C36-C37
53	T	201	EHZ	N2-C15-C16-C17
49	J	201	3PE	C22-C23-C24-C25
49	H	402	3PE	C11-O13-P-O11
49	H	403	3PE	C1-O11-P-O13
49	L	703	3PE	C39-C3A-C3B-C3C
45	h	201	PLC	C1'-C2'-C3'-C4'
45	B	302	PLC	O3P-C1-C2-O2
49	L	704	3PE	O11-C1-C2-O21
49	M	503	3PE	O11-C1-C2-O21
49	j	101	3PE	O11-C1-C2-O21
50	O	201	CDL	OA5-CA3-CA4-OA6
50	a	201	CDL	CB7-C71-C72-C73
49	L	706	3PE	C31-C32-C33-C34
49	O	202	3PE	C31-C32-C33-C34
49	L	705	3PE	C33-C34-C35-C36
45	M	502	PLC	O2-C2-C3-O3
45	i	101	PLC	O2-C2-C3-O3
49	M	503	3PE	C3E-C3F-C3G-C3H
50	O	201	CDL	C74-C75-C76-C77
49	g	301	3PE	C2D-C2E-C2F-C2G
45	L	702	PLC	C2-C1-O3P-P
49	L	705	3PE	C2-C1-O11-P
50	a	201	CDL	C33-C34-C35-C36
45	a	202	PLC	C4-C5-N-C6
45	q	402	PLC	C1'-C2'-C3'-C4'
50	O	201	CDL	CA5-C11-C12-C13
51	P	501	NDP	PN-O3-PA-O5B
51	P	501	NDP	PA-O3-PN-O5D
49	L	705	3PE	C26-C27-C28-C29
45	q	401	PLC	O3P-C1-C2-C3
49	O	203	3PE	O11-C1-C2-C3
49	j	101	3PE	O11-C1-C2-C3
49	L	706	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
49	L	705	3PE	O21-C21-C22-C23
49	O	203	3PE	C32-C33-C34-C35
49	L	706	3PE	C2C-C2D-C2E-C2F
49	H	403	3PE	C32-C31-O31-C3
45	L	701	PLC	C5'-C6'-C7'-C8'
50	a	201	CDL	C57-C58-C59-C60
49	M	503	3PE	C3-C2-O21-C21
50	O	201	CDL	CA6-CA4-OA6-CA5
50	a	201	CDL	CA6-CA4-OA6-CA5
49	J	201	3PE	C28-C29-C2A-C2B
45	m	702	PLC	C'-C1'-C2'-C3'
49	J	201	3PE	C2B-C2C-C2D-C2E
50	b	103	CDL	C31-C32-C33-C34
45	h	201	PLC	C2B-C3B-C4B-C5B
50	O	201	CDL	C36-C37-C38-C39
45	P	502	PLC	C2-C1-O3P-P
45	Z	201	PLC	C1-C2-C3-O3
45	l	202	PLC	C1-C2-C3-O3
49	d	101	3PE	C2-C1-O11-P
49	g	301	3PE	C2-C1-O11-P
45	a	202	PLC	O3P-C1-C2-O2
49	H	402	3PE	O11-C1-C2-O21
49	H	403	3PE	O11-C1-C2-O21
49	L	703	3PE	O11-C1-C2-O21
49	L	705	3PE	O11-C1-C2-O21
49	L	706	3PE	O11-C1-C2-O21
49	O	202	3PE	O11-C1-C2-O21
49	O	203	3PE	O11-C1-C2-O21
50	Z	202	CDL	OB5-CB3-CB4-OB6
49	L	703	3PE	C27-C28-C29-C2A
53	U	201	EHZ	O1-C7-C8-C9
45	N	602	PLC	C3'-C4'-C5'-C6'
49	l	201	3PE	C37-C38-C39-C3A
49	j	101	3PE	O21-C2-C3-O31
50	b	103	CDL	OA6-CA4-CA6-OA8
49	L	704	3PE	C25-C26-C27-C28
45	H	401	PLC	CB-C1B-C2B-C3B
49	N	601	3PE	C2D-C2E-C2F-C2G
49	d	101	3PE	C24-C25-C26-C27
49	M	503	3PE	C38-C39-C3A-C3B
45	M	501	PLC	C7'-C8'-C9'-CA'
49	M	503	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
49	O	203	3PE	C28-C29-C2A-C2B
50	Z	202	CDL	C71-CB7-OB8-CB6
53	T	201	EHZ	C3-C4-C5-C6
45	H	401	PLC	C4-O4P-P-O3P
45	I	303	PLC	C1-O3P-P-O4P
45	M	502	PLC	C4-O4P-P-O3P
45	Y	301	PLC	C4-O4P-P-O3P
49	L	706	3PE	C1-O11-P-O13
49	g	301	3PE	C1-O11-P-O13
49	l	201	3PE	C11-O13-P-O11
50	a	201	CDL	CA3-OA5-PA1-OA2
45	B	303	PLC	C3B-C4B-C5B-C6B
50	a	201	CDL	CA7-C31-C32-C33
45	L	701	PLC	C2-C1-O3P-P
45	l	202	PLC	C2-C1-O3P-P
49	m	703	3PE	C2-C1-O11-P
50	Z	202	CDL	C1-CA2-OA2-PA1
45	B	302	PLC	C1-O3P-P-O1P
45	L	701	PLC	C4-O4P-P-O1P
45	L	701	PLC	C4-O4P-P-O2P
45	M	502	PLC	C1-O3P-P-O1P
45	N	602	PLC	C4-O4P-P-O1P
45	q	402	PLC	C1-O3P-P-O2P
45	q	402	PLC	C4-O4P-P-O1P
45	q	402	PLC	C4-O4P-P-O2P
49	H	402	3PE	C11-O13-P-O14
49	H	403	3PE	C1-O11-P-O14
49	J	201	3PE	C1-O11-P-O14
49	L	703	3PE	C11-O13-P-O12
49	L	704	3PE	C1-O11-P-O14
49	L	704	3PE	C11-O13-P-O12
49	L	705	3PE	C11-O13-P-O14
49	M	503	3PE	C1-O11-P-O12
49	M	504	3PE	C1-O11-P-O12
49	b	101	3PE	C1-O11-P-O14
49	d	101	3PE	C1-O11-P-O14
49	d	101	3PE	C11-O13-P-O12
49	g	301	3PE	C1-O11-P-O14
49	j	101	3PE	C1-O11-P-O12
49	j	101	3PE	C11-O13-P-O12
50	O	201	CDL	CB2-OB2-PB2-OB4
50	O	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
50	a	201	CDL	CA2-OA2-PA1-OA3
50	b	103	CDL	CB3-OB5-PB2-OB3
51	P	501	NDP	C5B-O5B-PA-O2A
53	U	201	EHZ	C6-C7-C8-C9
45	P	502	PLC	C1B-CB-O3-C3
45	B	302	PLC	O3P-C1-C2-C3
45	I	303	PLC	O3P-C1-C2-C3
45	L	701	PLC	O3P-C1-C2-C3
45	L	702	PLC	O3P-C1-C2-C3
45	a	202	PLC	O3P-C1-C2-C3
49	H	402	3PE	O11-C1-C2-C3
49	L	703	3PE	O11-C1-C2-C3
49	L	706	3PE	O11-C1-C2-C3
49	b	101	3PE	O11-C1-C2-C3
49	d	101	3PE	O11-C1-C2-C3
50	O	201	CDL	OA5-CA3-CA4-CA6
50	Z	202	CDL	OB5-CB3-CB4-CB6
45	l	202	PLC	C2B-C1B-CB-O3
45	L	702	PLC	C1'-C2'-C3'-C4'
49	L	705	3PE	C24-C25-C26-C27
45	I	303	PLC	C5-C4-O4P-P
45	L	702	PLC	C5-C4-O4P-P
45	N	602	PLC	C5-C4-O4P-P
45	N	603	PLC	C5-C4-O4P-P
49	L	706	3PE	C12-C11-O13-P
49	O	202	3PE	C12-C11-O13-P
49	O	203	3PE	C12-C11-O13-P
49	d	101	3PE	C12-C11-O13-P
49	j	101	3PE	C12-C11-O13-P
49	H	403	3PE	O32-C31-O31-C3
45	b	102	PLC	C2B-C3B-C4B-C5B
45	I	303	PLC	O3P-C1-C2-O2
49	b	101	3PE	O11-C1-C2-O21
49	b	101	3PE	C31-C32-C33-C34
49	d	101	3PE	O11-C1-C2-O21
49	m	703	3PE	O11-C1-C2-O21
50	Z	202	CDL	OA5-CA3-CA4-OA6
50	a	201	CDL	C12-C13-C14-C15
45	P	502	PLC	OB-CB-O3-C3
45	M	502	PLC	C4-C5-N-C7
45	N	603	PLC	C4-C5-N-C7
45	N	603	PLC	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
45	m	702	PLC	C4-C5-N-C6
53	T	201	EHZ	N1-C12-C13-C14
45	M	501	PLC	O4P-C4-C5-N
45	Y	301	PLC	O4P-C4-C5-N
45	a	202	PLC	O4P-C4-C5-N
49	L	705	3PE	C1-C2-C3-O31
49	b	101	3PE	C1-C2-C3-O31
53	U	201	EHZ	O5-C16-C17-C20
45	l	202	PLC	O2-C2-C3-O3
45	m	702	PLC	O2-C2-C3-O3
49	L	703	3PE	O21-C2-C3-O31
49	L	704	3PE	O21-C2-C3-O31
49	g	301	3PE	O21-C2-C3-O31
49	l	201	3PE	O21-C2-C3-O31
50	O	201	CDL	OB6-CB4-CB6-OB8
50	b	103	CDL	OB6-CB4-CB6-OB8
45	I	303	PLC	C4'-C5'-C6'-C7'
49	L	704	3PE	C3A-C3B-C3C-C3D
45	Z	201	PLC	C7'-C8'-C9'-CA'
45	q	401	PLC	C2'-C3'-C4'-C5'
45	b	102	PLC	C1B-C2B-C3B-C4B
50	b	103	CDL	C1-CA2-OA2-PA1
49	H	403	3PE	C23-C24-C25-C26
50	Z	202	CDL	OB9-CB7-OB8-CB6
45	i	101	PLC	C5B-C6B-C7B-C8B
45	Z	201	PLC	C2B-C1B-CB-O3
49	b	101	3PE	O21-C21-C22-C23
45	a	202	PLC	C4-C5-N-C7
45	q	401	PLC	C4-C5-N-C8
45	N	602	PLC	C1B-C2B-C3B-C4B
49	L	705	3PE	C32-C33-C34-C35
50	a	201	CDL	C14-C15-C16-C17
45	I	303	PLC	CB-C1B-C2B-C3B
50	Z	202	CDL	C72-C71-CB7-OB8
49	H	402	3PE	C33-C34-C35-C36
45	q	402	PLC	C3-C2-O2-C'
49	N	601	3PE	O11-C1-C2-C3
45	N	603	PLC	C3'-C4'-C5'-C6'
45	I	303	PLC	C7'-C8'-C9'-CA'
49	M	504	3PE	C2-C1-O11-P
45	L	701	PLC	O3P-C1-C2-O2
45	M	502	PLC	C4-C5-N-C6

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Mol	Chain	Res	Type	Atoms
45	Z	201	PLC	C4-C5-N-C8
49	O	202	3PE	C22-C23-C24-C25
49	m	701	3PE	C33-C34-C35-C36
49	M	503	3PE	C25-C26-C27-C28
49	M	504	3PE	C3B-C3C-C3D-C3E
50	a	201	CDL	C11-C12-C13-C14
45	B	302	PLC	C4-O4P-P-O3P
45	H	401	PLC	C1-O3P-P-O4P
45	L	702	PLC	C4-O4P-P-O3P
45	M	501	PLC	C4-O4P-P-O3P
45	P	502	PLC	C4-O4P-P-O3P
45	Z	201	PLC	C4-O4P-P-O3P
45	a	202	PLC	C4-O4P-P-O3P
45	m	702	PLC	C4-O4P-P-O3P
49	H	402	3PE	C1-O11-P-O13
49	L	703	3PE	C1-O11-P-O13
49	m	701	3PE	C11-O13-P-O11
50	b	103	CDL	CB2-OB2-PB2-OB5
51	P	501	NDP	C2D-C1D-N1N-C6N
50	O	201	CDL	CB3-CB4-CB6-OB8
49	m	701	3PE	C35-C36-C37-C38
49	M	503	3PE	C3C-C3D-C3E-C3F
51	P	501	NDP	O4D-C1D-N1N-C6N
45	B	302	PLC	C2-C1-O3P-P
45	q	401	PLC	C2-C1-O3P-P
50	Z	202	CDL	CA2-C1-CB2-OB2
45	b	102	PLC	O'-C'-O2-C2
50	O	201	CDL	C71-C72-C73-C74
49	O	203	3PE	O13-C11-C12-N
45	l	202	PLC	O3P-C1-C2-O2
49	N	601	3PE	O11-C1-C2-O21
49	O	202	3PE	C27-C28-C29-C2A
49	l	201	3PE	C34-C35-C36-C37
49	L	706	3PE	C26-C27-C28-C29
49	L	706	3PE	C34-C35-C36-C37
45	M	501	PLC	C5B-C6B-C7B-C8B
49	b	101	3PE	C37-C38-C39-C3A
49	L	704	3PE	C3B-C3C-C3D-C3E
45	q	402	PLC	C6B-C7B-C8B-C9B
49	j	101	3PE	C22-C23-C24-C25
49	j	101	3PE	C33-C34-C35-C36
50	O	201	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
45	N	603	PLC	C1-C2-C3-O3
45	q	402	PLC	C1-C2-C3-O3
49	M	504	3PE	C33-C34-C35-C36
53	T	201	EHZ	C18-C17-C20-O6
45	L	702	PLC	C1B-CB-O3-C3
45	m	702	PLC	C4-C5-N-C7
45	L	702	PLC	OB-CB-O3-C3
49	g	301	3PE	C39-C3A-C3B-C3C
49	L	703	3PE	C11-O13-P-O11
49	l	201	3PE	C36-C37-C38-C39
49	g	301	3PE	C2A-C2B-C2C-C2D
50	O	201	CDL	C75-C76-C77-C78
49	H	402	3PE	O22-C21-O21-C2
45	Z	201	PLC	C6'-C7'-C8'-C9'
49	N	601	3PE	C27-C28-C29-C2A
49	l	201	3PE	C33-C34-C35-C36
45	m	702	PLC	C1B-C2B-C3B-C4B
53	T	201	EHZ	C11-C10-S1-C9
53	U	201	EHZ	C11-C10-S1-C9
49	L	704	3PE	C22-C23-C24-C25
50	b	103	CDL	C59-C60-C61-C62
49	m	703	3PE	C35-C36-C37-C38
49	b	101	3PE	C32-C33-C34-C35
45	b	102	PLC	C1'-C'-O2-C2
50	a	201	CDL	CA2-C1-CB2-OB2
49	H	403	3PE	C2-C1-O11-P
49	L	703	3PE	C24-C25-C26-C27
45	M	502	PLC	C5'-C6'-C7'-C8'
49	H	402	3PE	C25-C26-C27-C28
51	P	501	NDP	C3B-C2B-O2B-P2B
45	q	402	PLC	C5'-C6'-C7'-C8'
45	M	502	PLC	O3P-C1-C2-O2
49	O	202	3PE	O22-C21-C22-C23
45	m	702	PLC	C7B-C8B-C9B-CAA
45	l	202	PLC	O3P-C1-C2-C3
49	m	703	3PE	O11-C1-C2-C3
45	M	501	PLC	C3'-C4'-C5'-C6'
49	M	503	3PE	C23-C24-C25-C26
50	Z	202	CDL	OA6-CA4-CA6-OA8
50	a	201	CDL	C52-C51-CB5-OB6
45	Z	201	PLC	C3'-C4'-C5'-C6'
47	F	502	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
49	L	703	3PE	C38-C39-C3A-C3B
53	T	201	EHZ	C19-C17-C20-O6
50	Z	202	CDL	CB7-C71-C72-C73
45	m	702	PLC	C4-C5-N-C8
45	N	602	PLC	C7'-C8'-C9'-CA'
50	Z	202	CDL	C32-C31-CA7-OA8
45	B	302	PLC	C3B-C4B-C5B-C6B
45	B	302	PLC	O'-C'-O2-C2
45	B	303	PLC	C1'-C2'-C3'-C4'
49	M	503	3PE	O31-C31-C32-C33
49	g	301	3PE	O31-C31-C32-C33
49	H	402	3PE	O22-C21-C22-C23
49	j	101	3PE	C34-C35-C36-C37
49	L	704	3PE	O21-C21-C22-C23
45	I	303	PLC	C1-C2-C3-O3
50	b	103	CDL	CA3-CA4-CA6-OA8
45	M	502	PLC	C4-C5-N-C8
45	N	603	PLC	C4-C5-N-C6
49	d	101	3PE	C23-C24-C25-C26
53	U	201	EHZ	C15-C16-C17-C18
45	q	401	PLC	O2-C'-C1'-C2'
45	M	501	PLC	C2'-C3'-C4'-C5'
50	O	201	CDL	C33-C34-C35-C36
50	a	201	CDL	C54-C55-C56-C57
49	O	203	3PE	O21-C21-C22-C23
45	m	702	PLC	OB-CB-O3-C3
45	L	701	PLC	O2-C'-C1'-C2'
45	N	602	PLC	C4-C5-N-C7
45	q	401	PLC	C4-C5-N-C6
51	P	501	NDP	C5D-O5D-PN-O3
45	m	702	PLC	C1B-CB-O3-C3
49	H	402	3PE	C22-C21-O21-C2
49	L	703	3PE	O31-C31-C32-C33
49	g	301	3PE	C33-C34-C35-C36
49	H	403	3PE	C28-C29-C2A-C2B
49	L	704	3PE	C2E-C2F-C2G-C2H
49	L	706	3PE	C36-C37-C38-C39
51	P	501	NDP	C2D-C1D-N1N-C2N
49	O	203	3PE	O31-C31-C32-C33
51	P	501	NDP	PN-O3-PA-O2A
49	g	301	3PE	C2F-C2G-C2H-C2I
49	L	706	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
45	l	202	PLC	C'-C1'-C2'-C3'
49	L	704	3PE	O22-C21-C22-C23
53	T	201	EHZ	C22-C23-C24-C25
49	M	503	3PE	O32-C31-C32-C33
45	I	303	PLC	C8B-C9B-CAA-CBA
45	B	302	PLC	C1'-C'-O2-C2
50	a	201	CDL	C13-C14-C15-C16
45	q	401	PLC	O'-C'-C1'-C2'
49	g	301	3PE	O32-C31-C32-C33
45	Z	201	PLC	C5'-C6'-C7'-C8'
50	O	201	CDL	C32-C31-CA7-OA8
45	i	101	PLC	C4B-C5B-C6B-C7B
50	a	201	CDL	C52-C51-CB5-OB7
49	g	301	3PE	C26-C27-C28-C29
49	O	203	3PE	O32-C31-C32-C33
45	Y	301	PLC	C7'-C8'-C9'-CA'
45	B	302	PLC	C4-O4P-P-O1P
45	H	401	PLC	C4-O4P-P-O2P
45	M	501	PLC	C4-O4P-P-O1P
45	M	502	PLC	C4-O4P-P-O2P
45	P	502	PLC	C4-O4P-P-O1P
45	Y	301	PLC	C4-O4P-P-O2P
45	Z	201	PLC	C4-O4P-P-O1P
45	a	202	PLC	C1-O3P-P-O2P
45	q	401	PLC	C4-O4P-P-O2P
49	m	701	3PE	C11-O13-P-O14
50	a	201	CDL	CA3-OA5-PA1-OA3
50	b	103	CDL	CA3-OA5-PA1-OA3
50	b	103	CDL	CB2-OB2-PB2-OB3
50	Z	202	CDL	C32-C31-CA7-OA9
49	M	504	3PE	O13-C11-C12-N
45	q	401	PLC	C7'-C8'-C9'-CA'
49	O	203	3PE	O22-C21-C22-C23
49	L	703	3PE	C22-C23-C24-C25
49	M	503	3PE	C27-C28-C29-C2A
49	b	101	3PE	C35-C36-C37-C38
45	P	502	PLC	C5-C4-O4P-P
45	h	201	PLC	C5-C4-O4P-P
49	H	402	3PE	C12-C11-O13-P
49	M	503	3PE	C12-C11-O13-P
49	N	601	3PE	C12-C11-O13-P
49	m	701	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
53	T	201	EHZ	O4-C15-C16-C17
49	L	703	3PE	O32-C31-C32-C33
49	J	201	3PE	C24-C25-C26-C27
49	L	706	3PE	C3B-C3C-C3D-C3E
49	M	504	3PE	C38-C39-C3A-C3B
49	L	705	3PE	O22-C21-C22-C23
45	Z	201	PLC	C4-C5-N-C7
45	q	401	PLC	C4-C5-N-C7
49	m	703	3PE	O31-C31-C32-C33
49	J	201	3PE	C34-C35-C36-C37
49	L	705	3PE	C23-C24-C25-C26
50	O	201	CDL	C32-C31-CA7-OA9
49	J	201	3PE	C39-C3A-C3B-C3C
45	Z	201	PLC	O'-C'-O2-C2
45	M	501	PLC	C8'-C9'-CA'-CB'
49	J	201	3PE	C2-C1-O11-P
49	O	203	3PE	C2-C1-O11-P
53	U	201	EHZ	S1-C10-C11-N1
45	L	701	PLC	O'-C'-C1'-C2'
49	L	704	3PE	C34-C35-C36-C37
50	Z	202	CDL	O1-C1-CB2-OB2
45	N	603	PLC	C2B-C1B-CB-O3
45	N	602	PLC	C4-C5-N-C8
45	l	202	PLC	CB-C1B-C2B-C3B
49	m	703	3PE	O32-C31-C32-C33

There are no ring outliers.

46 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	m	701	3PE	1	0
45	B	303	PLC	2	0
45	N	602	PLC	1	0
49	L	706	3PE	5	0
50	a	201	CDL	8	0
44	I	302	SF4	2	0
45	Y	301	PLC	1	0
44	F	501	SF4	3	0
45	L	702	PLC	1	0
49	M	503	3PE	3	0
44	B	301	SF4	1	0
50	Z	202	CDL	1	0

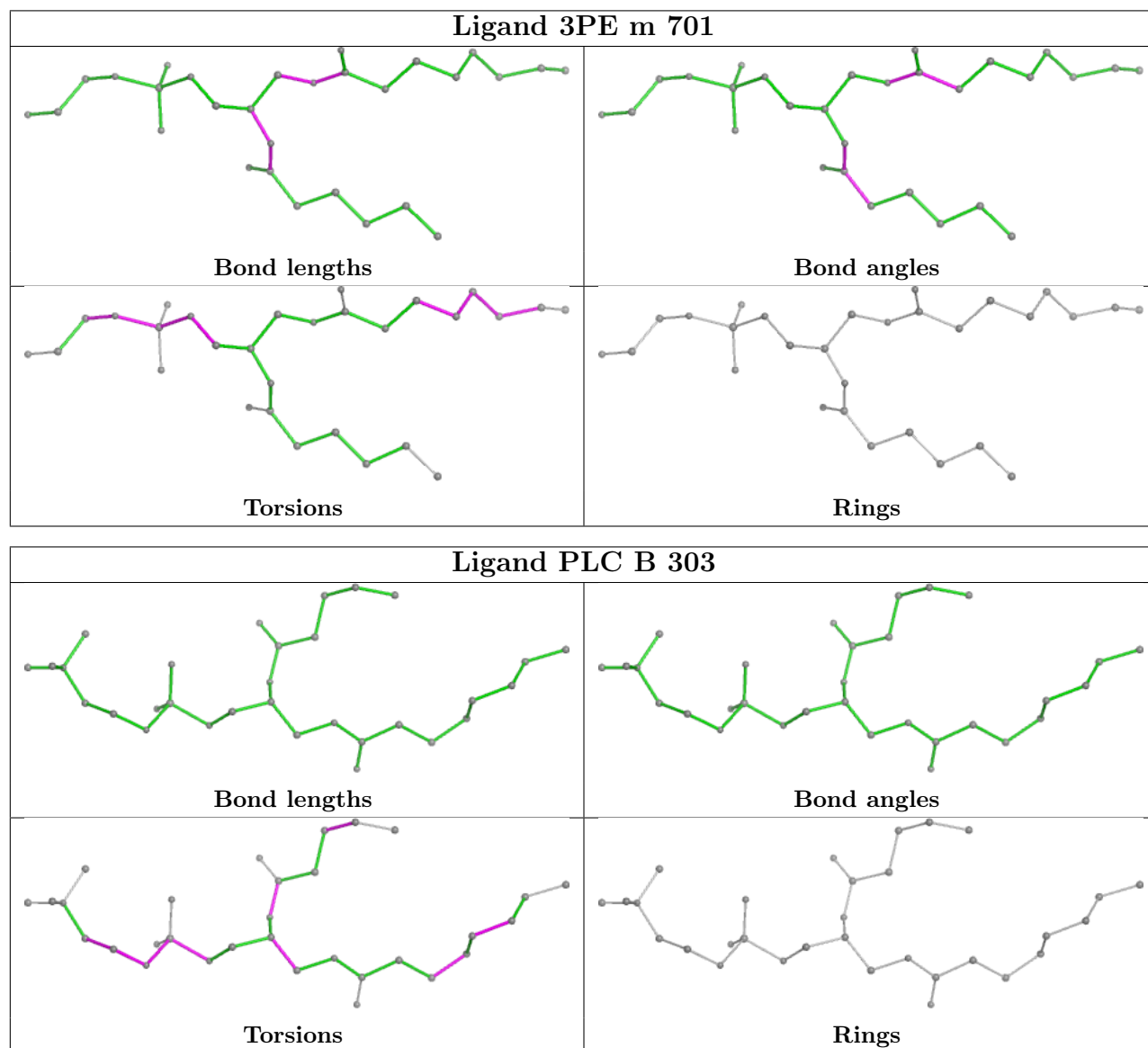
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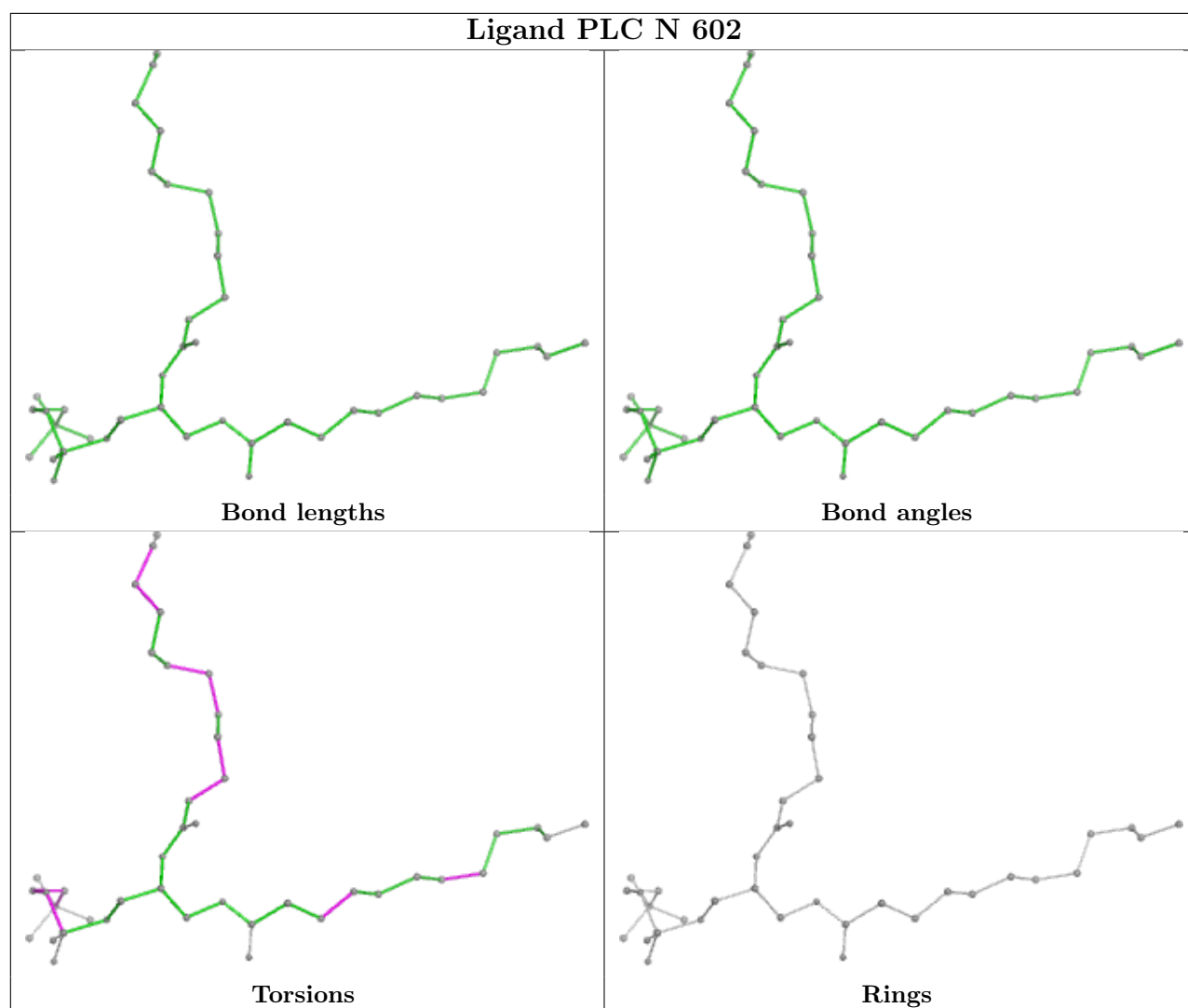
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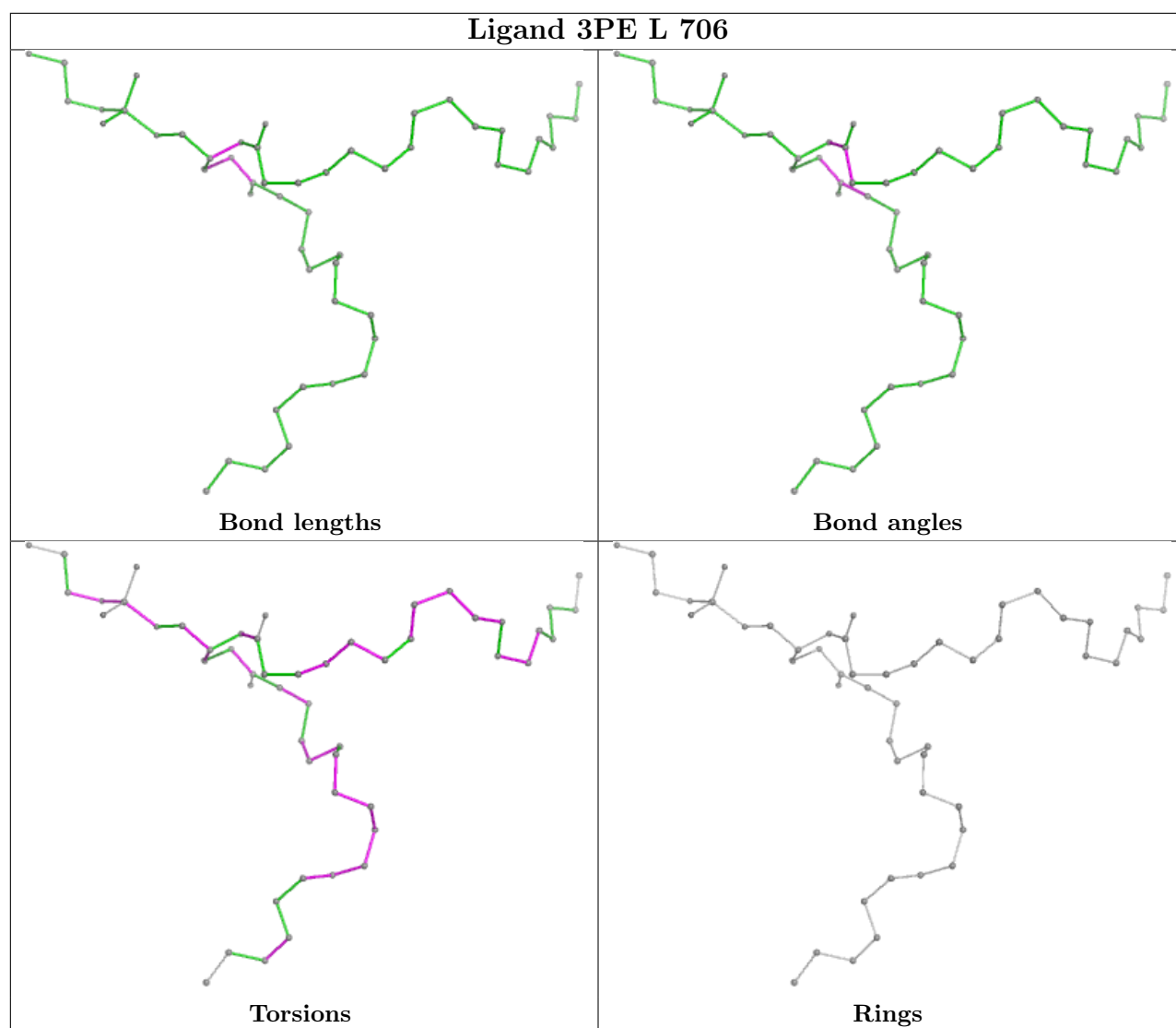
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	q	401	PLC	4	0
53	U	201	EHZ	1	0
44	G	804	SF4	1	0
49	H	403	3PE	1	0
50	O	201	CDL	3	0
45	i	101	PLC	9	0
49	N	601	3PE	1	0
49	H	402	3PE	1	0
49	L	705	3PE	1	0
51	P	501	NDP	4	0
49	J	201	3PE	3	0
45	b	102	PLC	3	0
53	T	201	EHZ	1	0
45	I	303	PLC	3	0
45	m	702	PLC	1	0
49	L	703	3PE	3	0
49	d	101	3PE	1	0
47	F	502	FMN	2	0
49	g	301	3PE	1	0
46	G	801	FES	1	0
45	M	501	PLC	2	0
44	I	301	SF4	1	0
45	N	603	PLC	1	0
45	h	201	PLC	6	0
49	M	504	3PE	7	0
45	L	701	PLC	2	0
49	L	704	3PE	5	0
45	M	502	PLC	1	0
49	l	201	3PE	2	0
45	B	302	PLC	3	0
45	P	502	PLC	1	0
45	q	402	PLC	3	0
45	Z	201	PLC	2	0
50	b	103	CDL	1	0

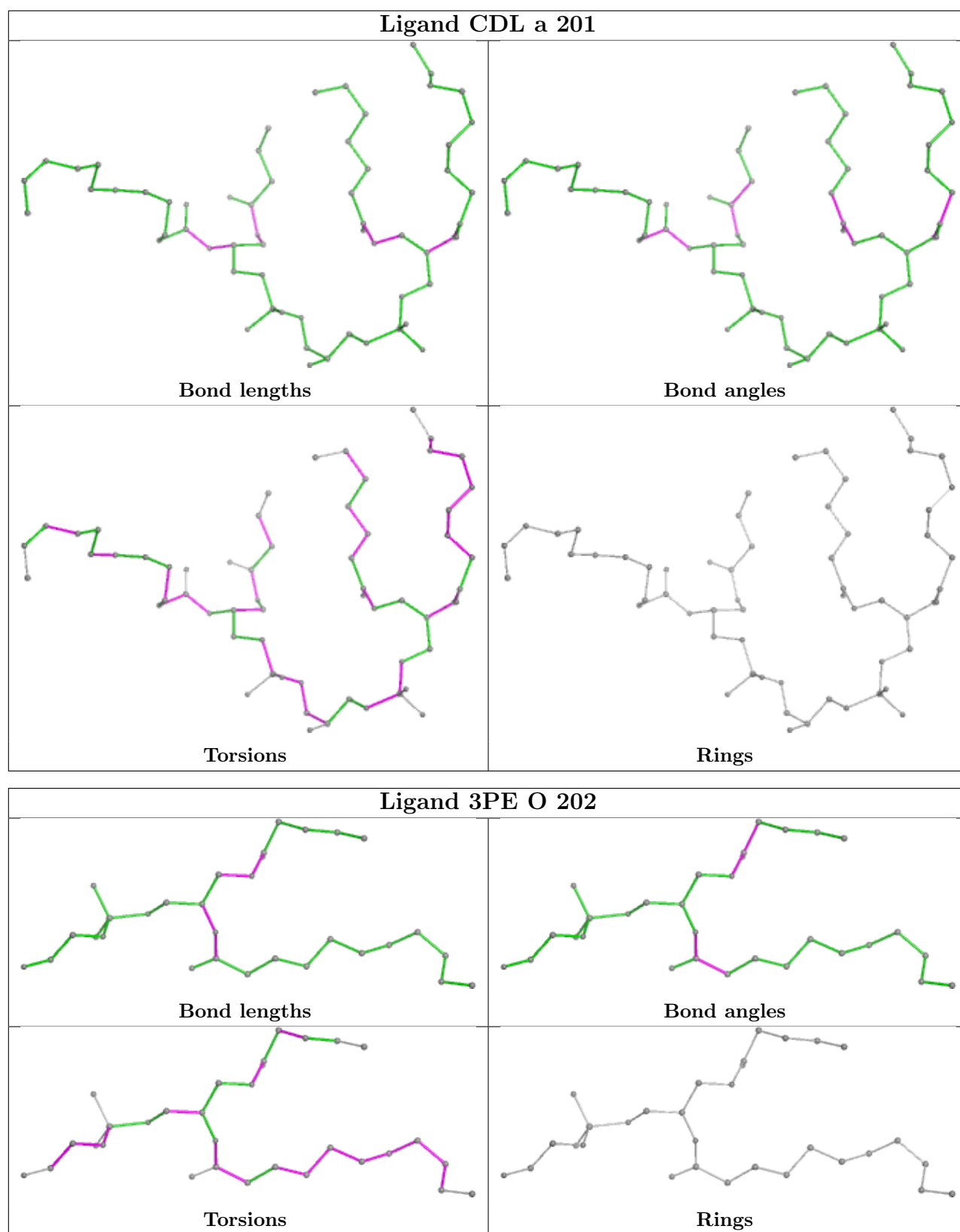
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

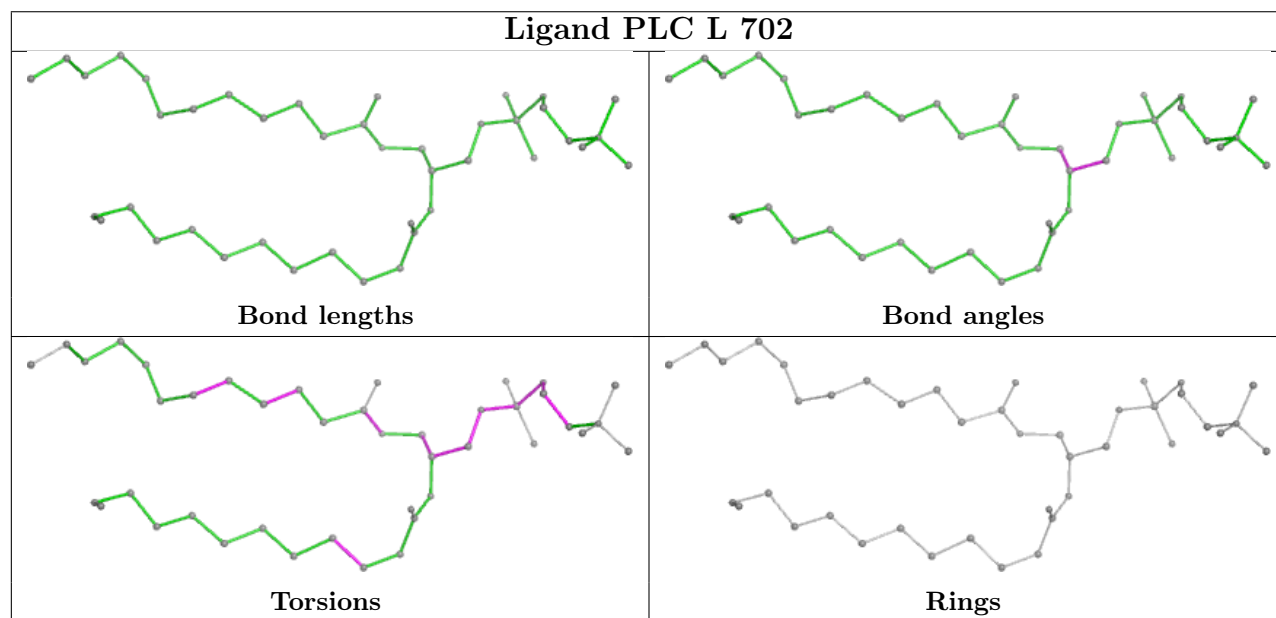
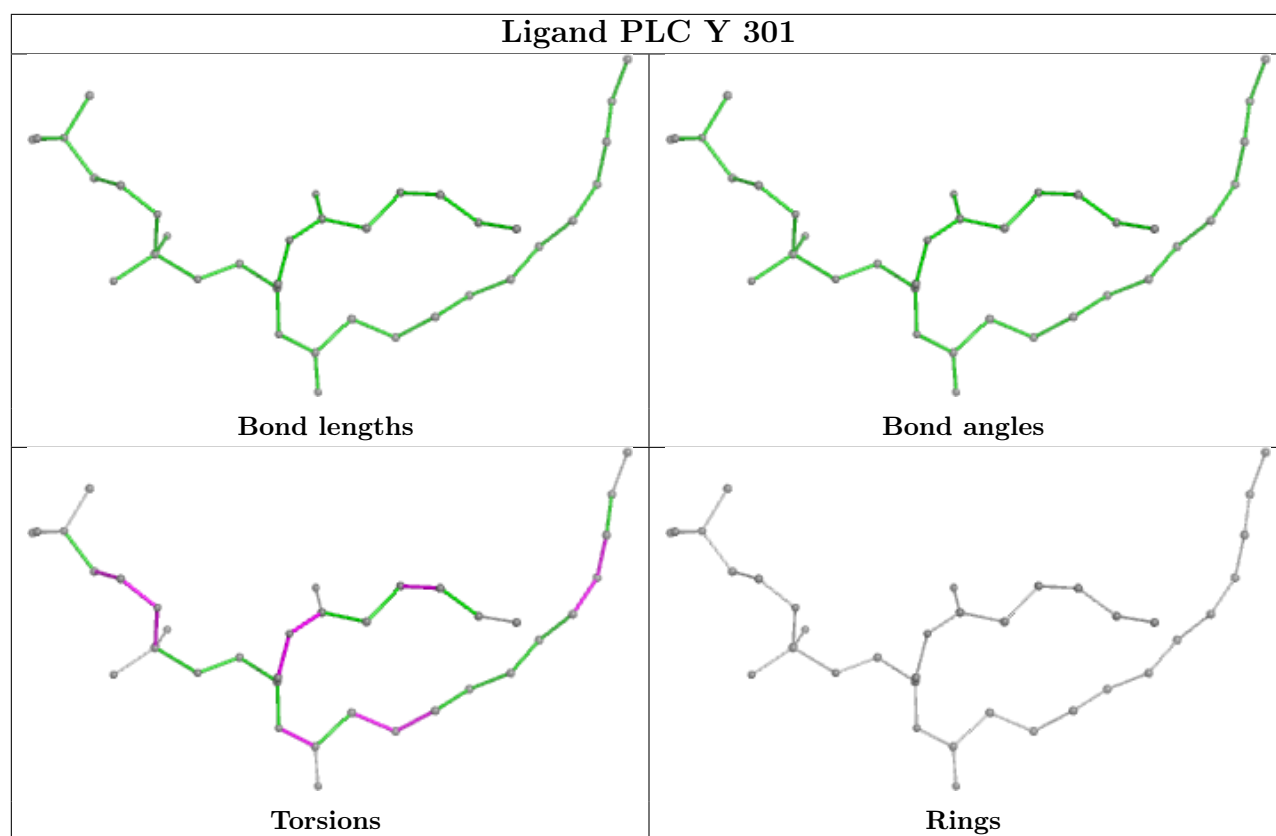
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

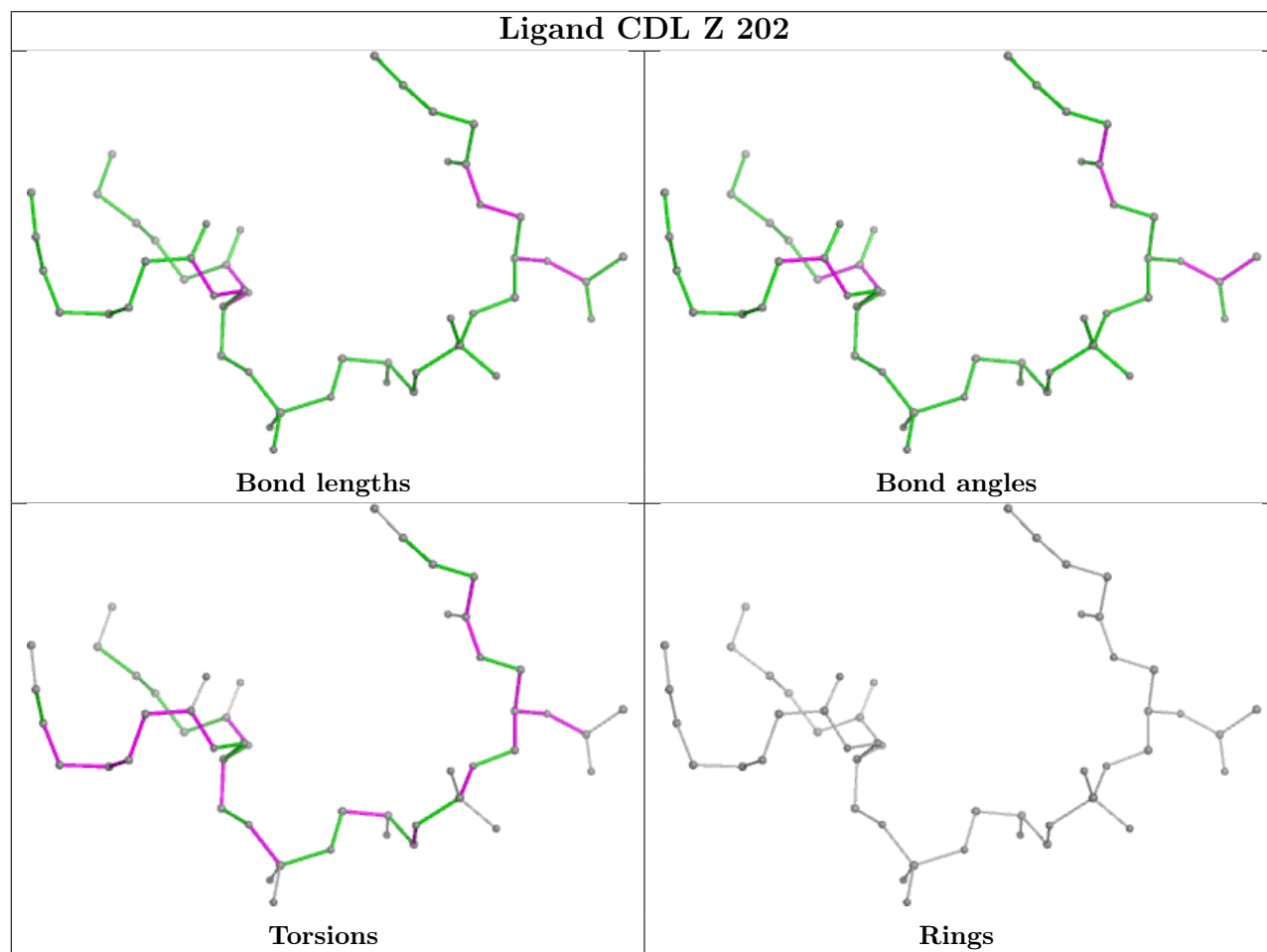
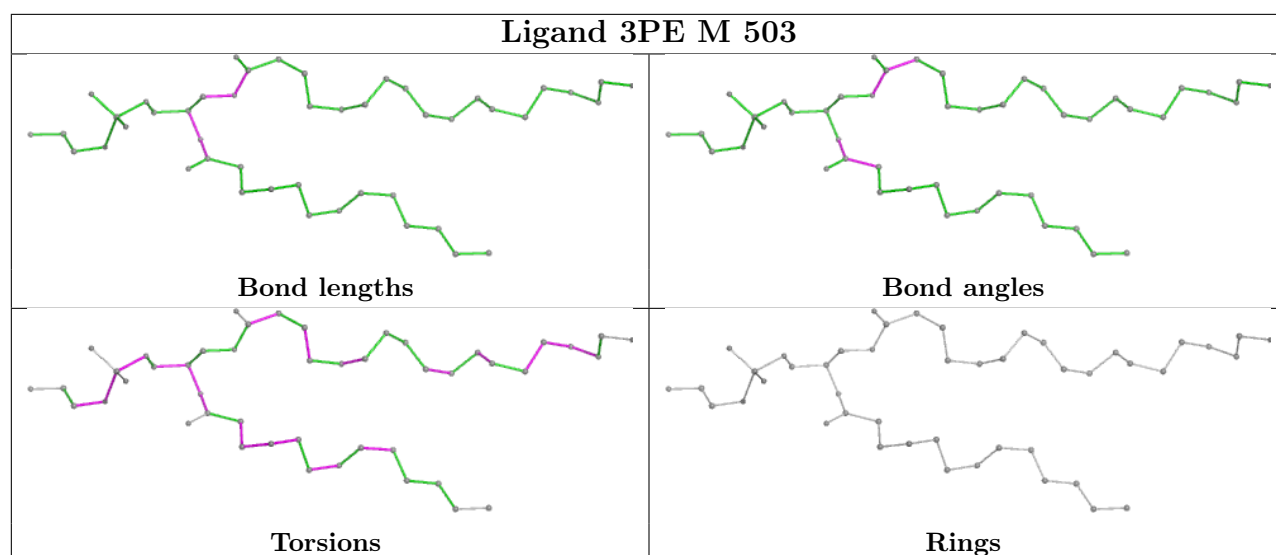


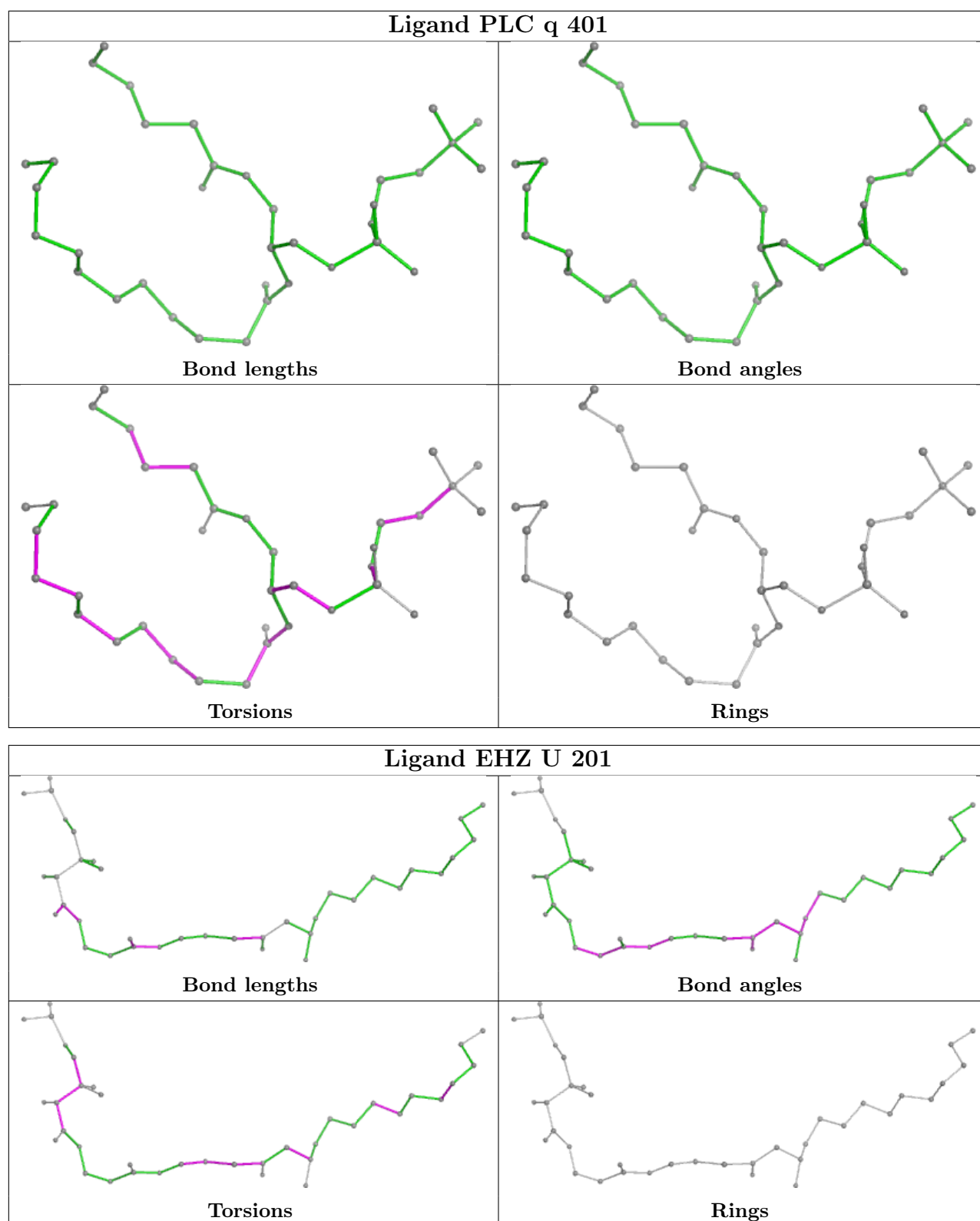


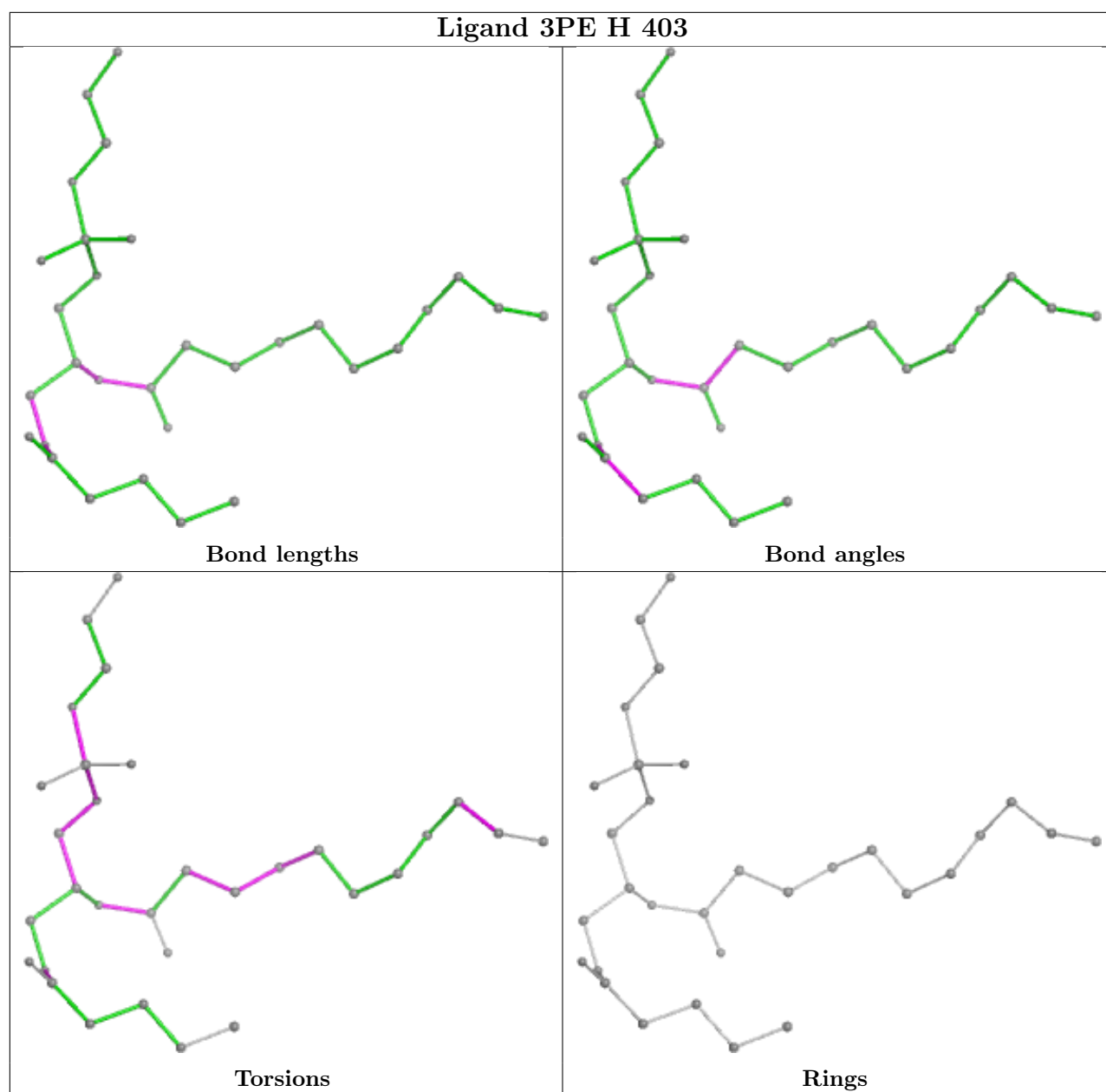


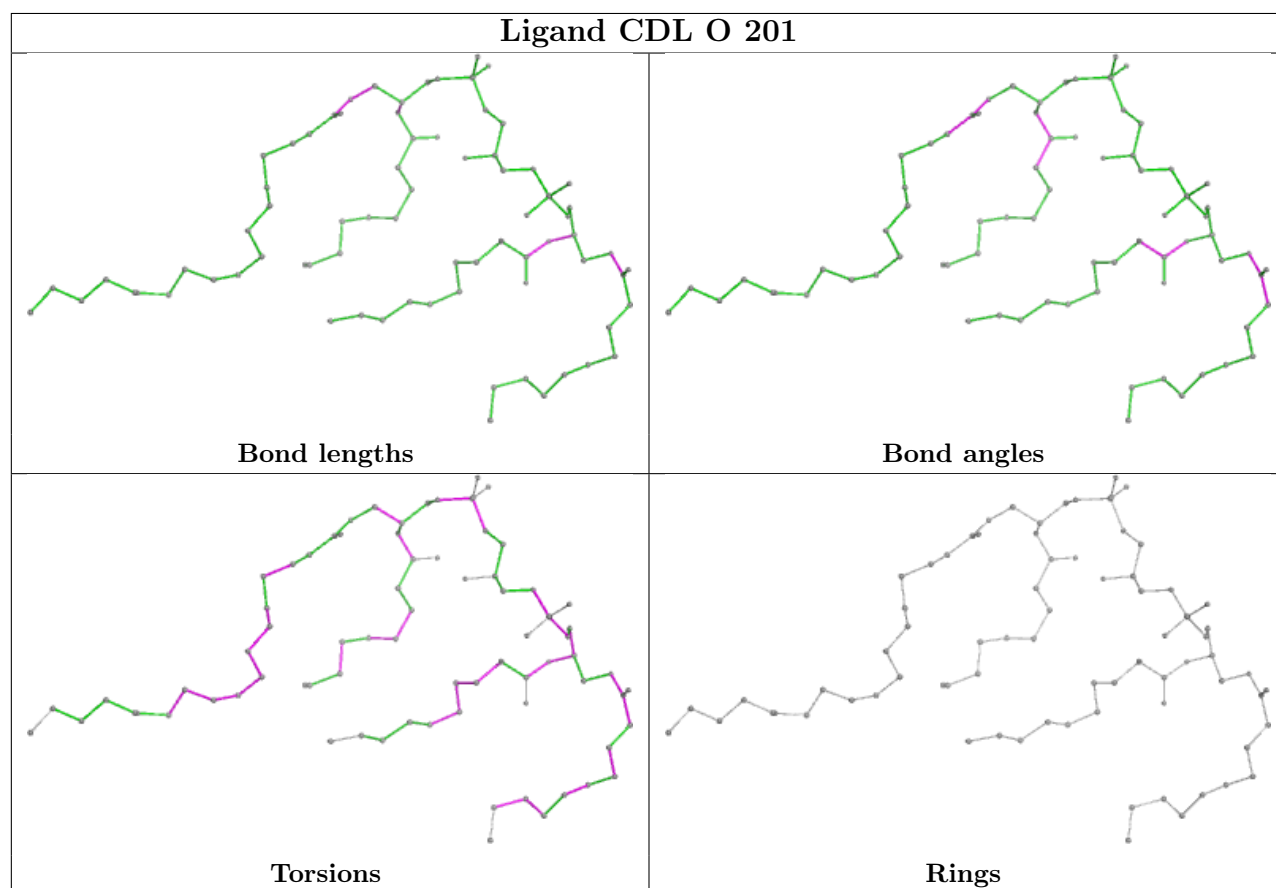
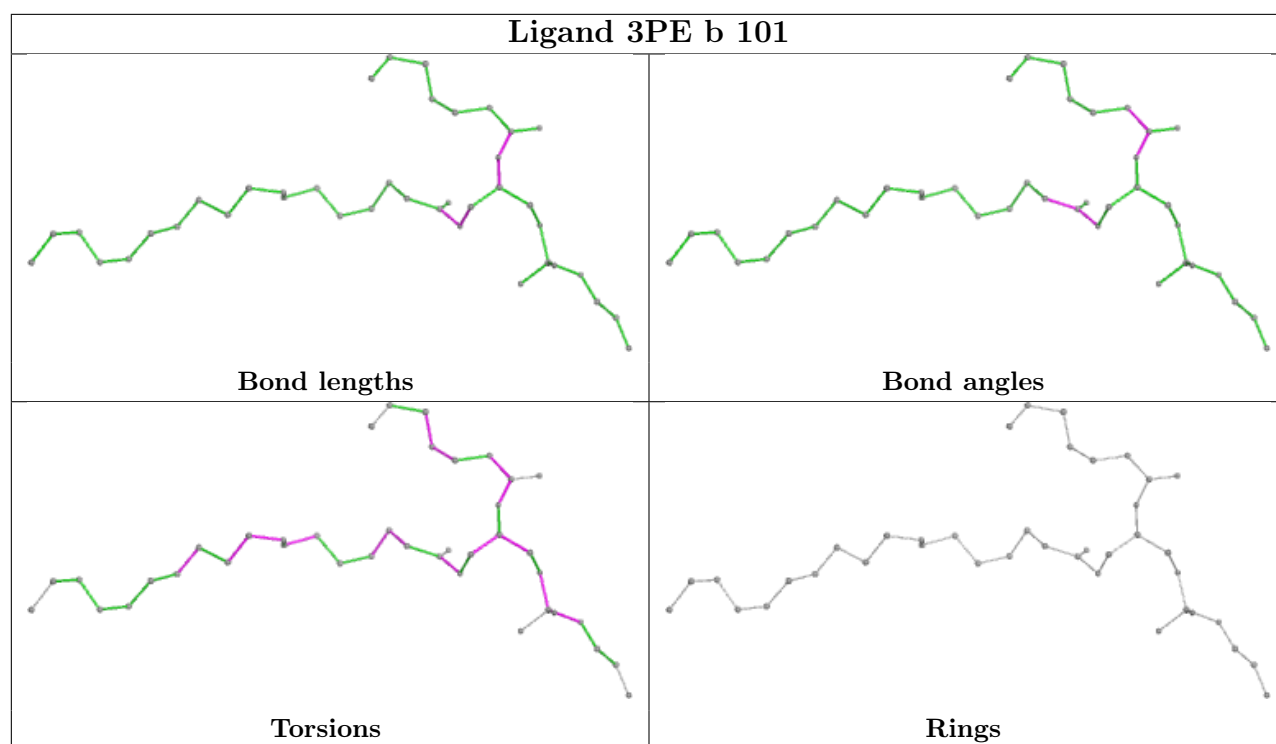


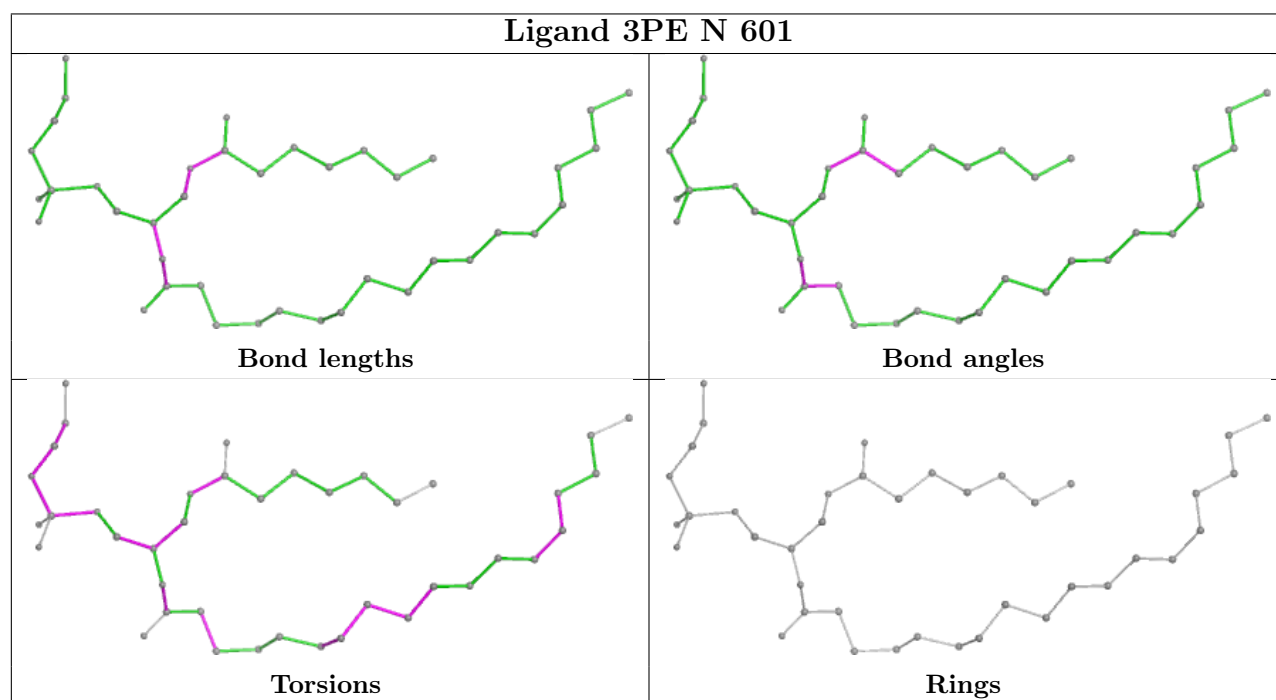
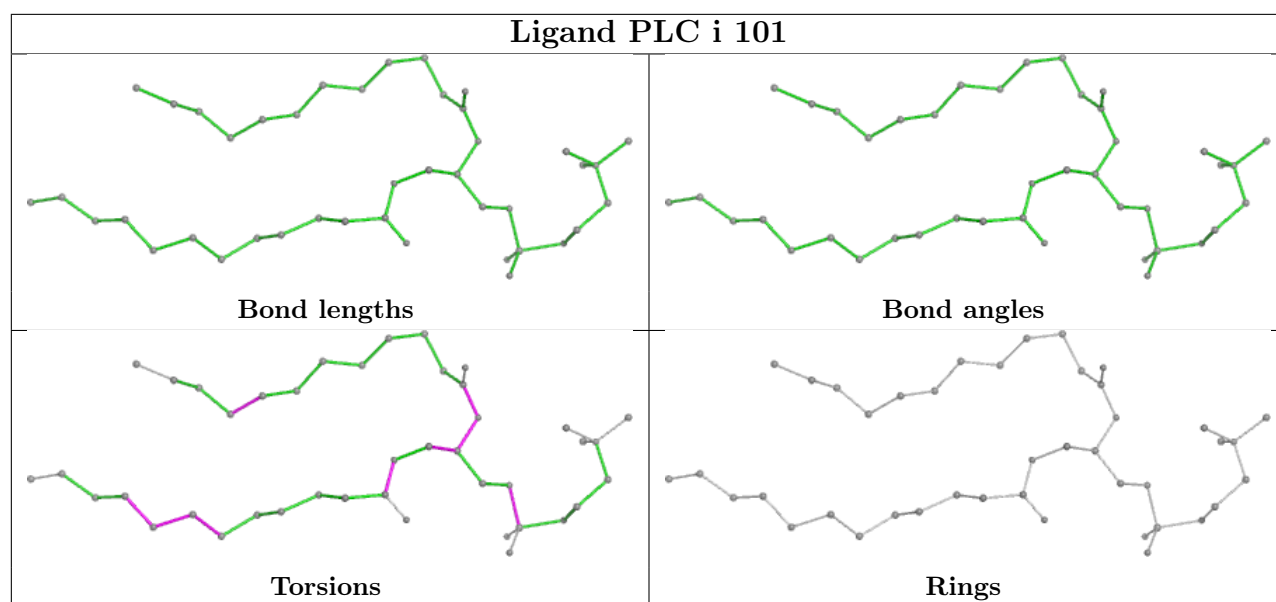


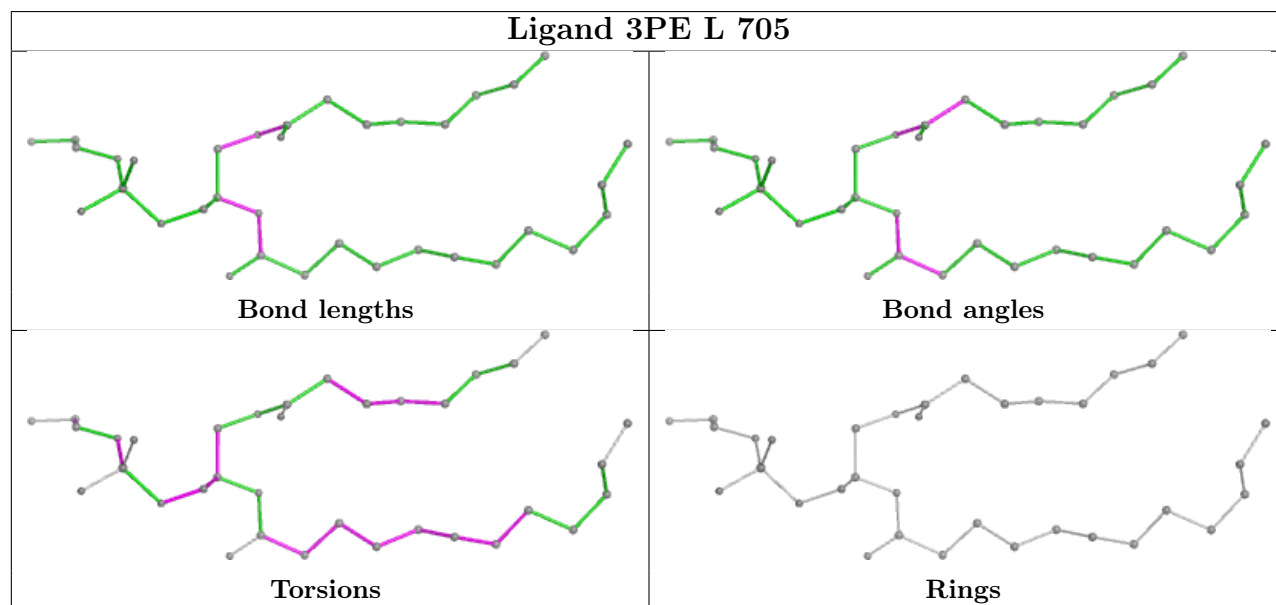
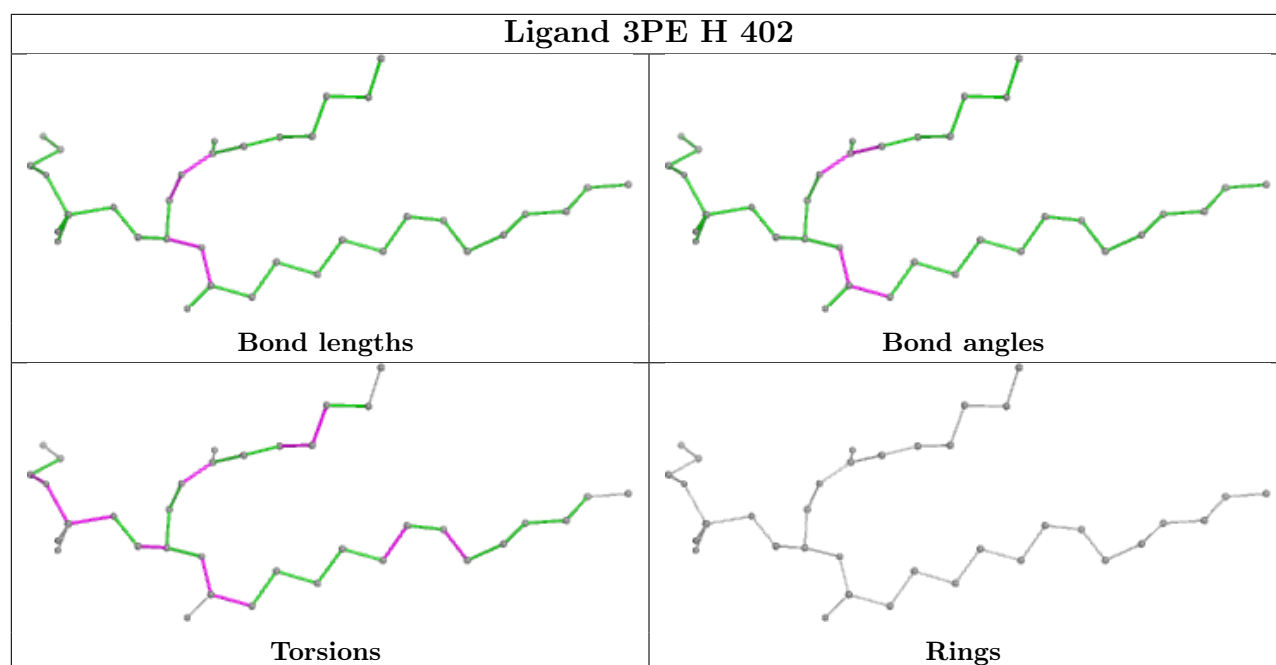


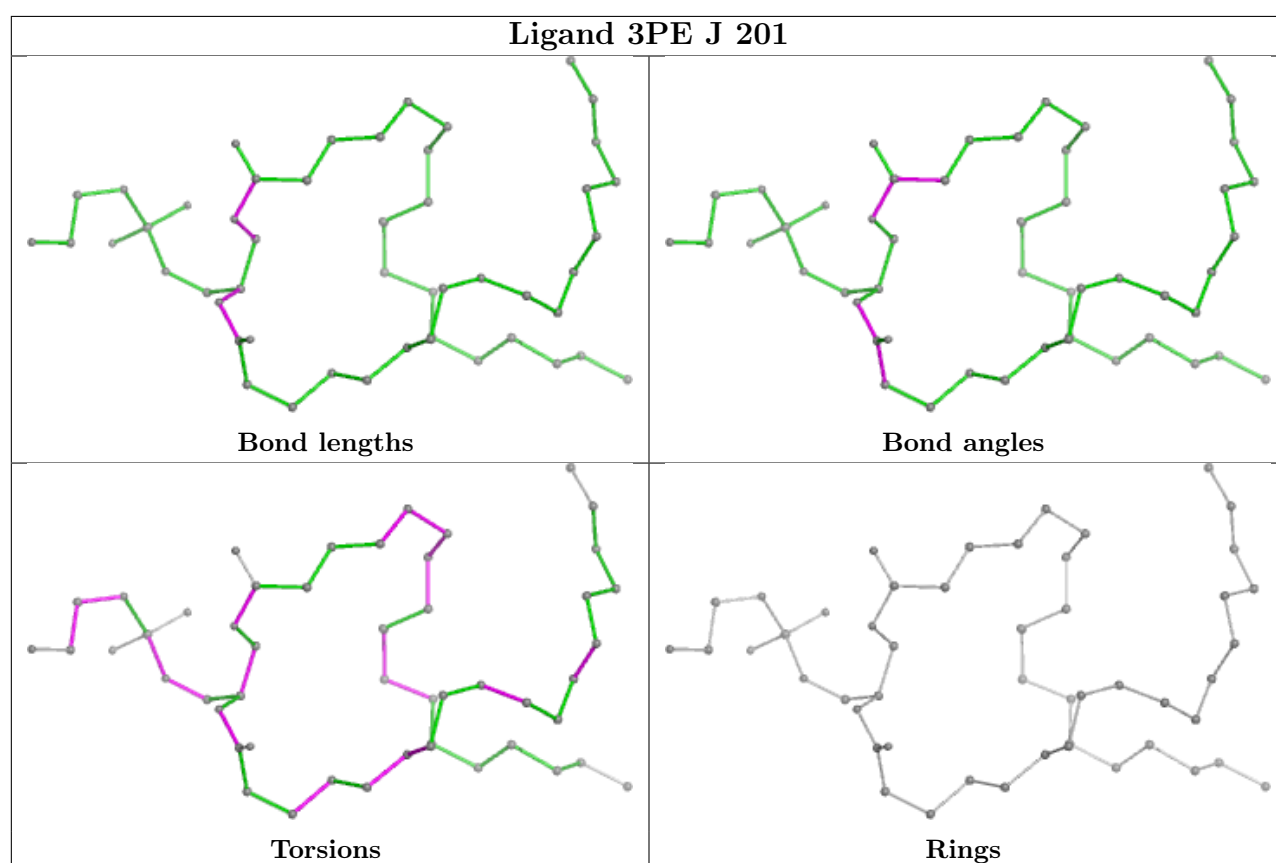
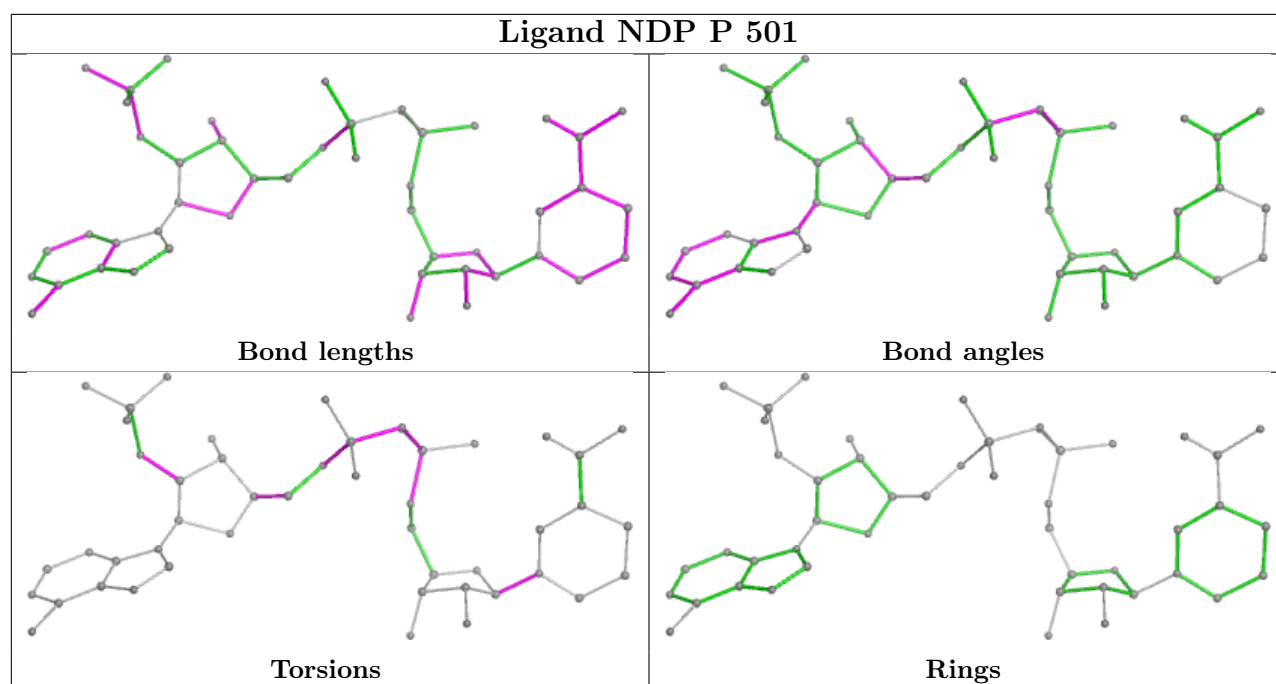


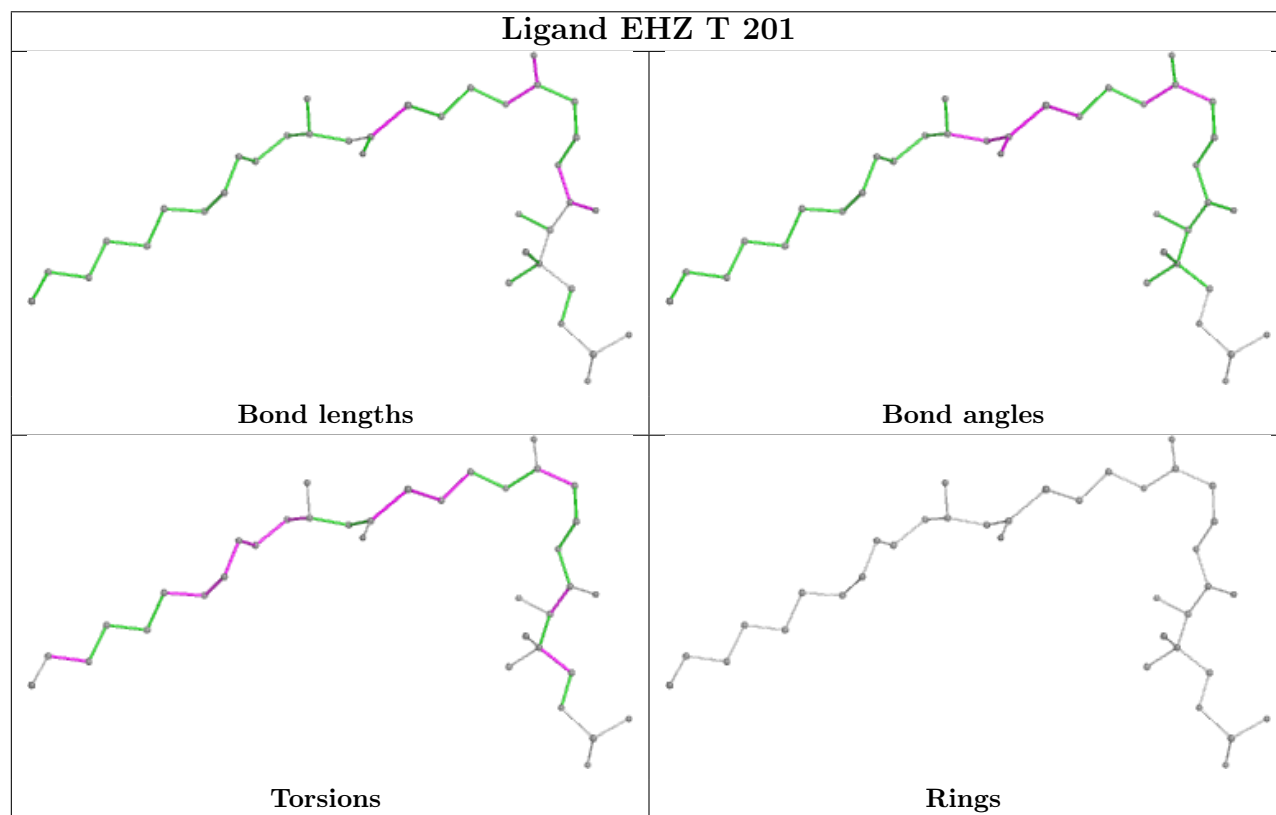
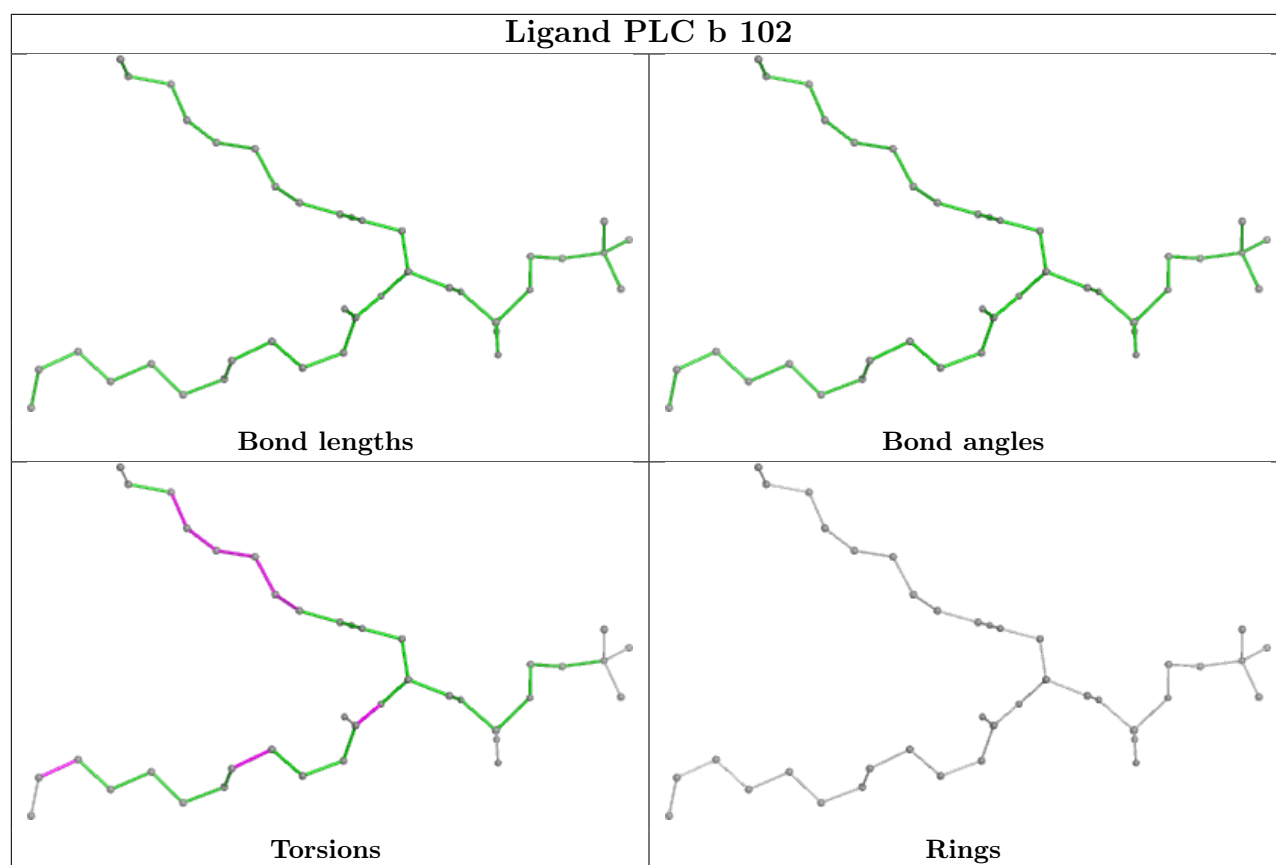


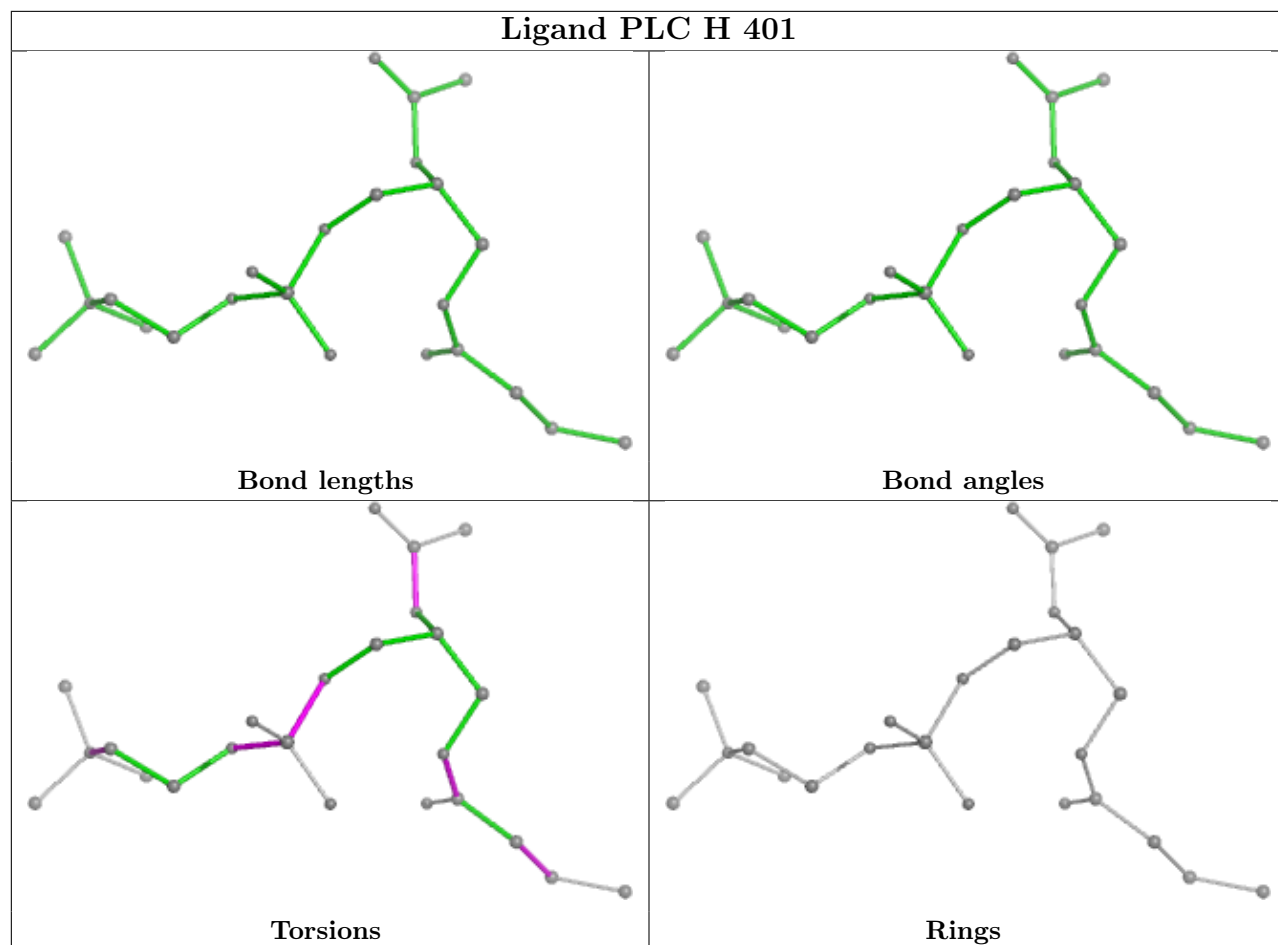


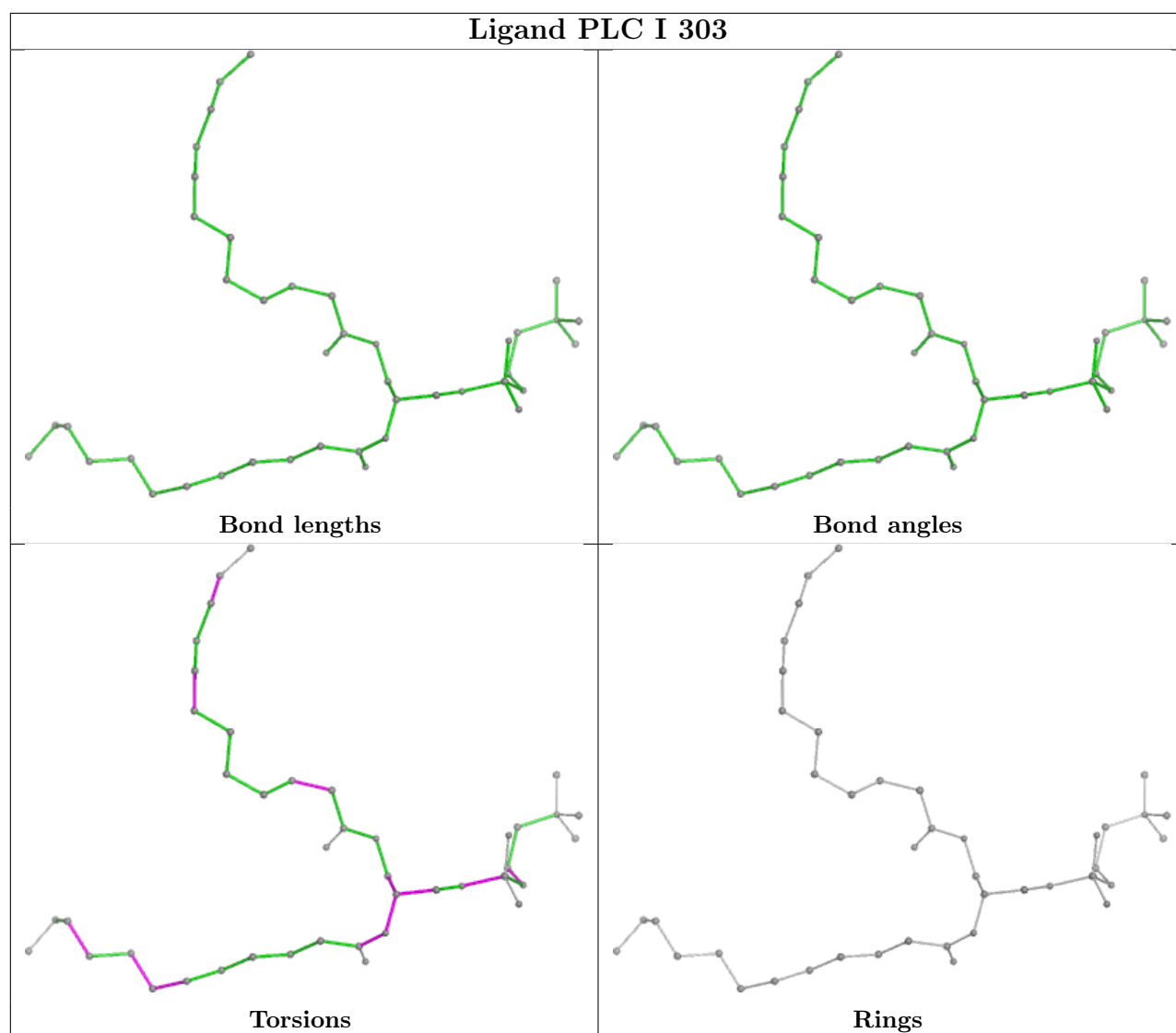


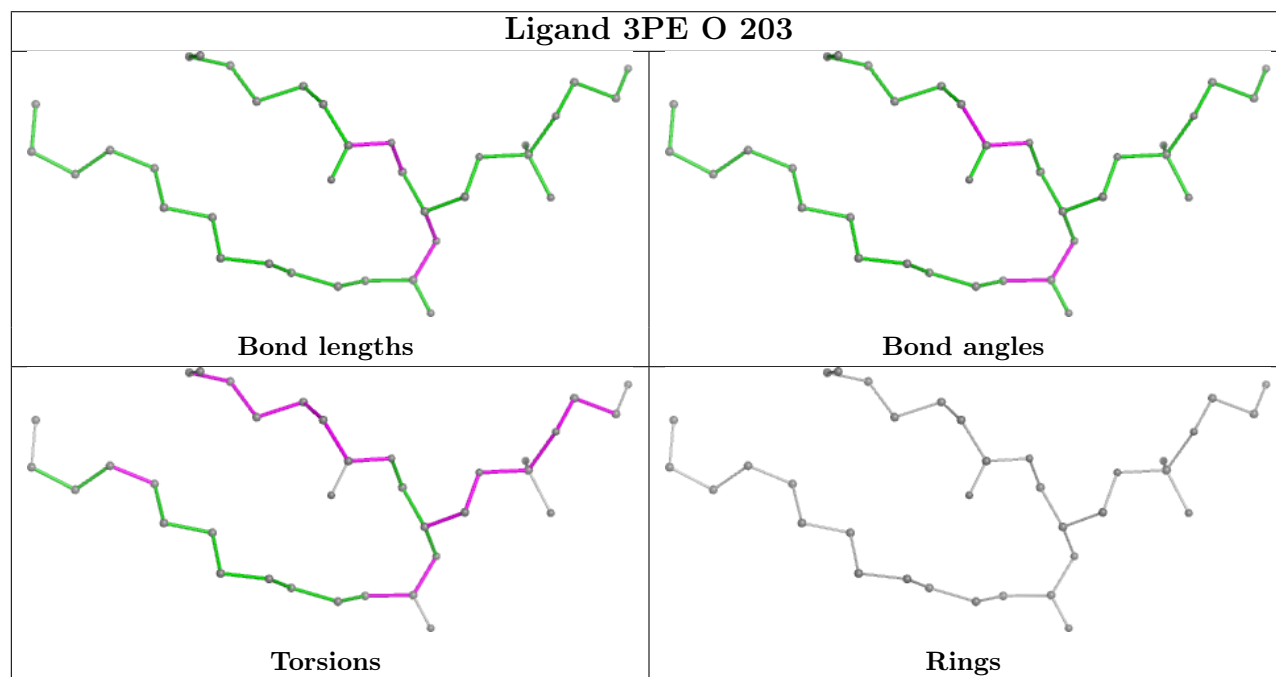
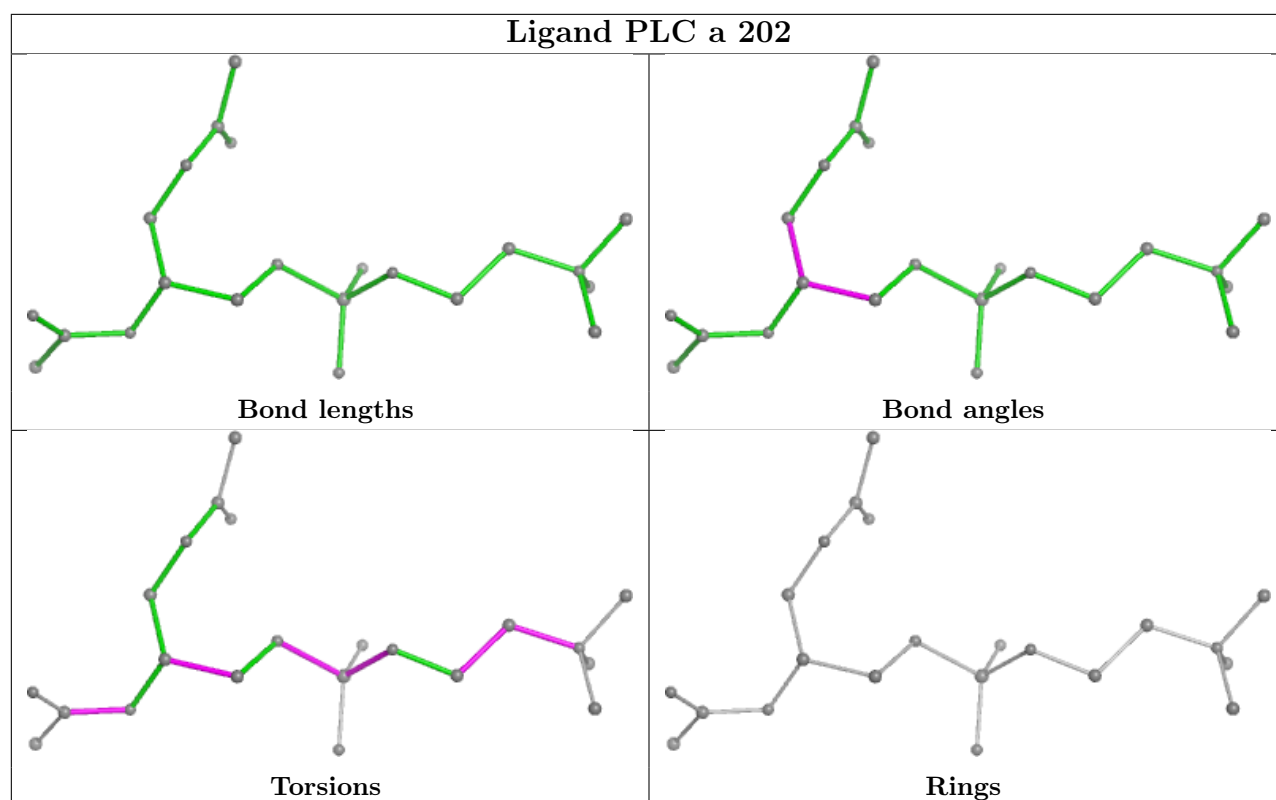


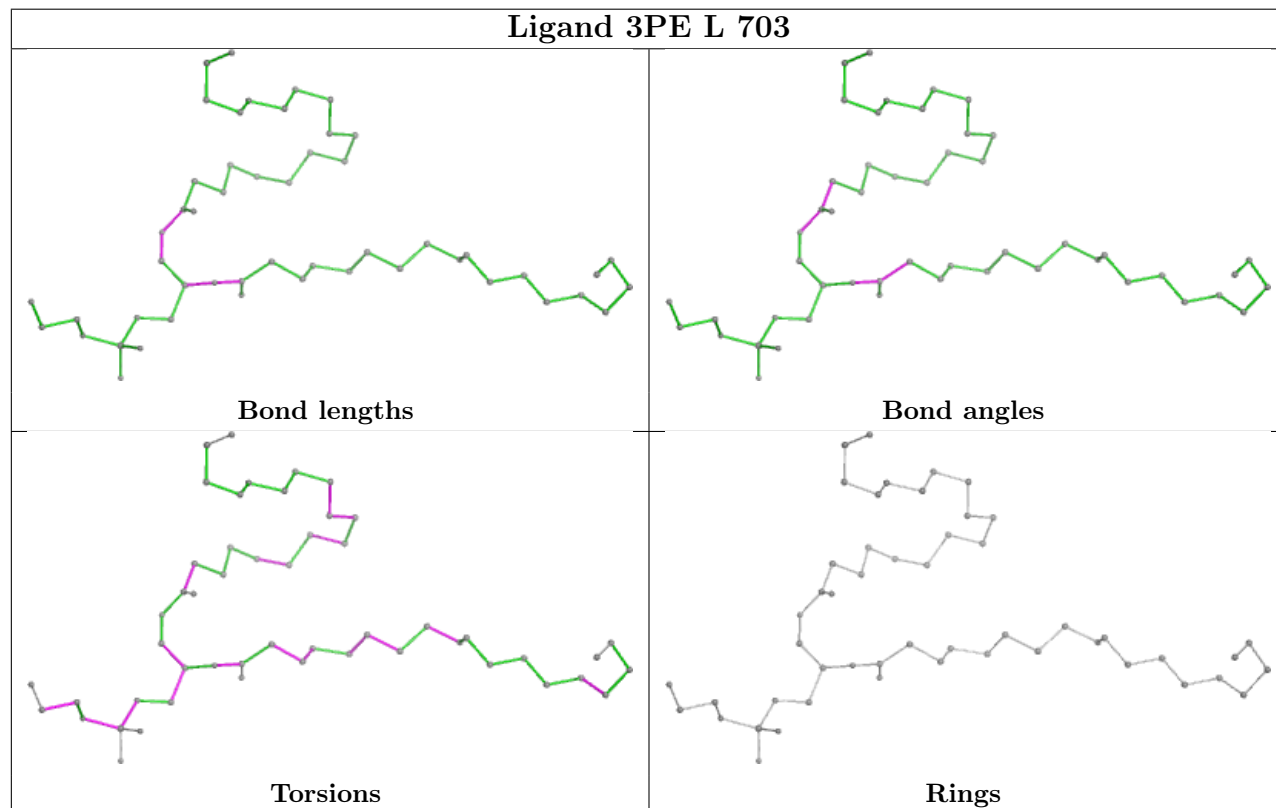
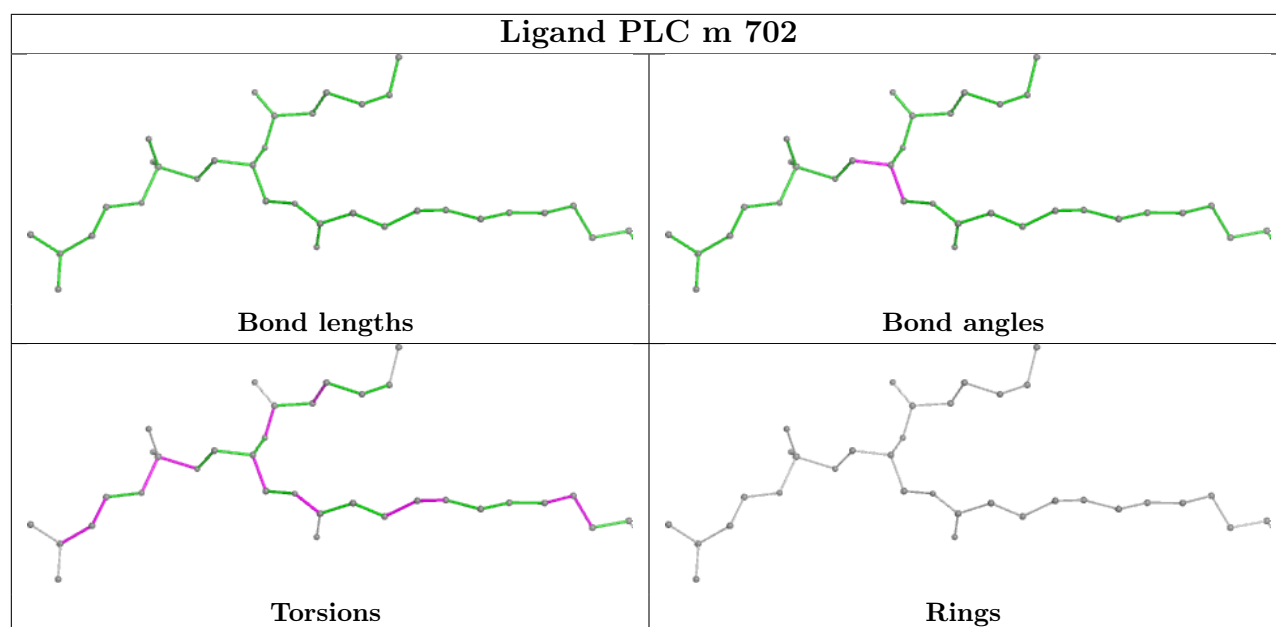


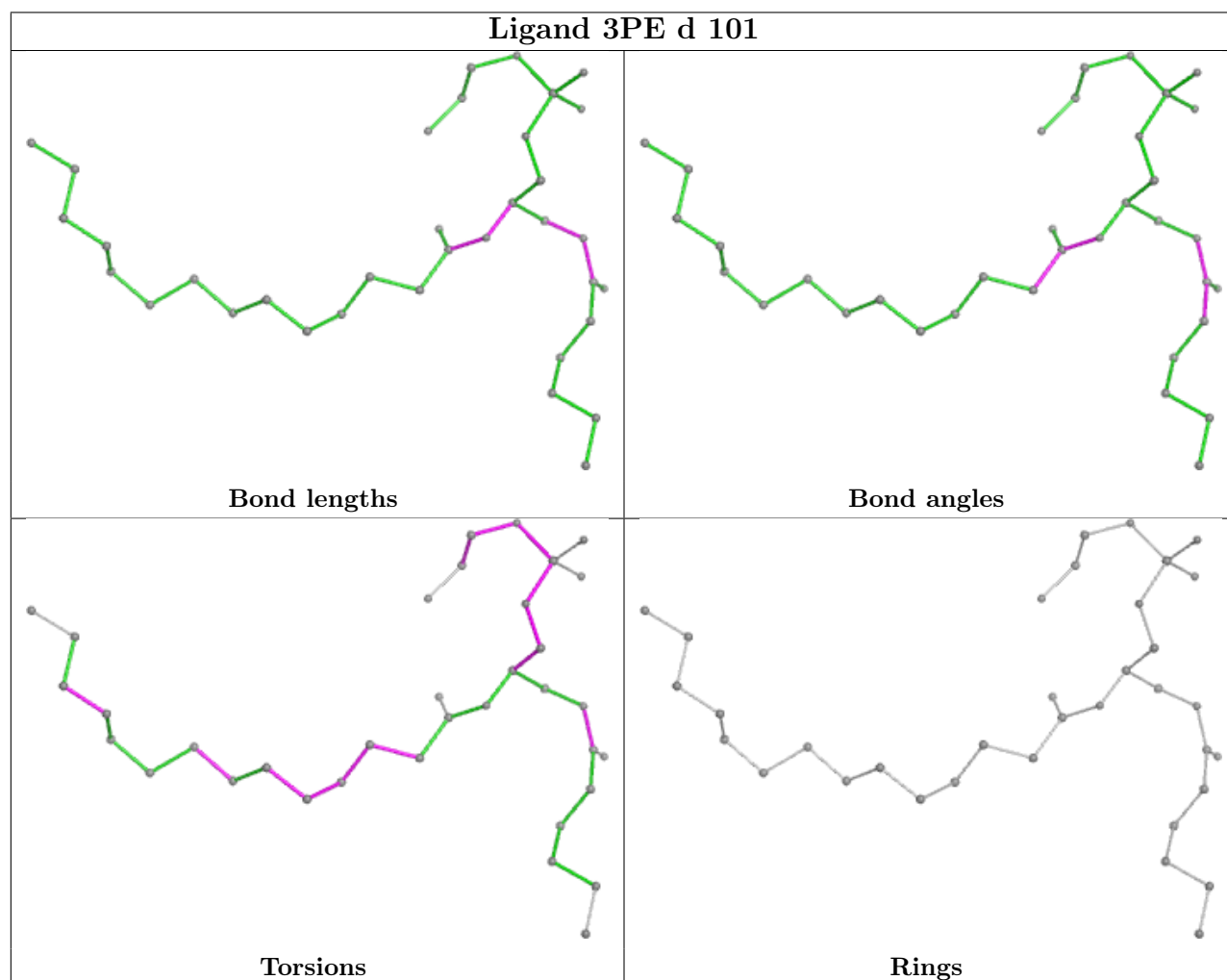
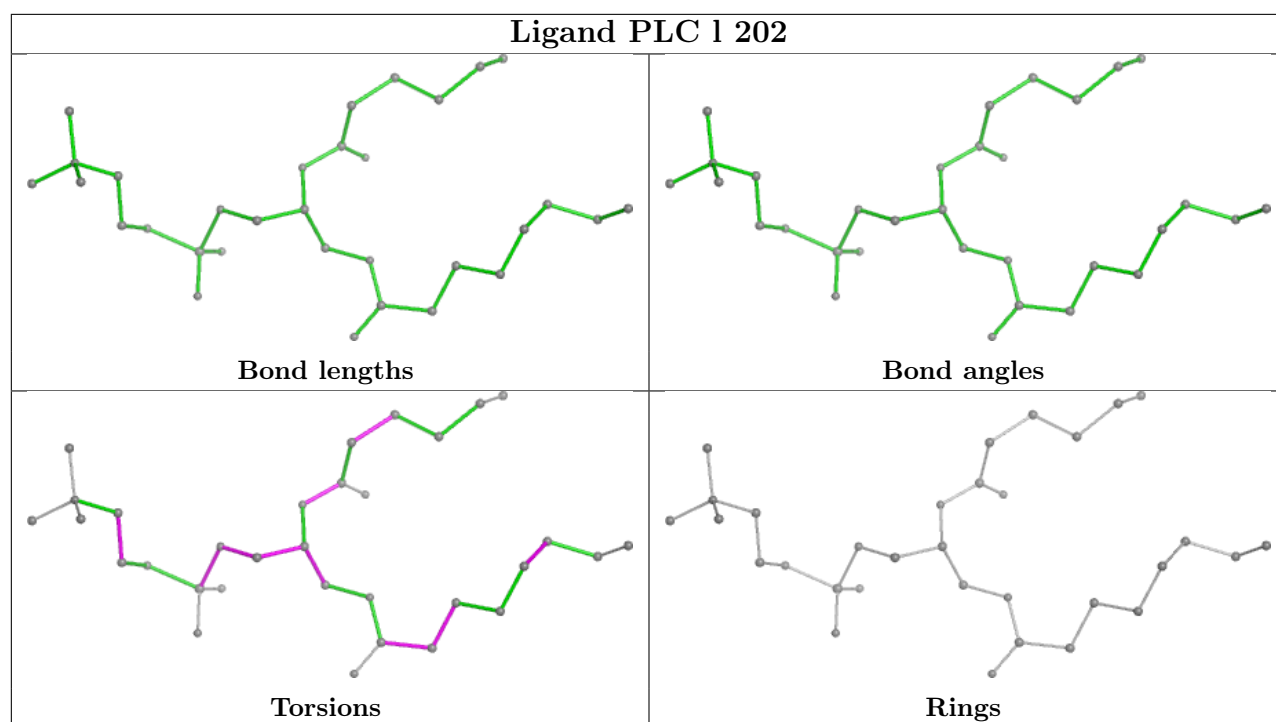


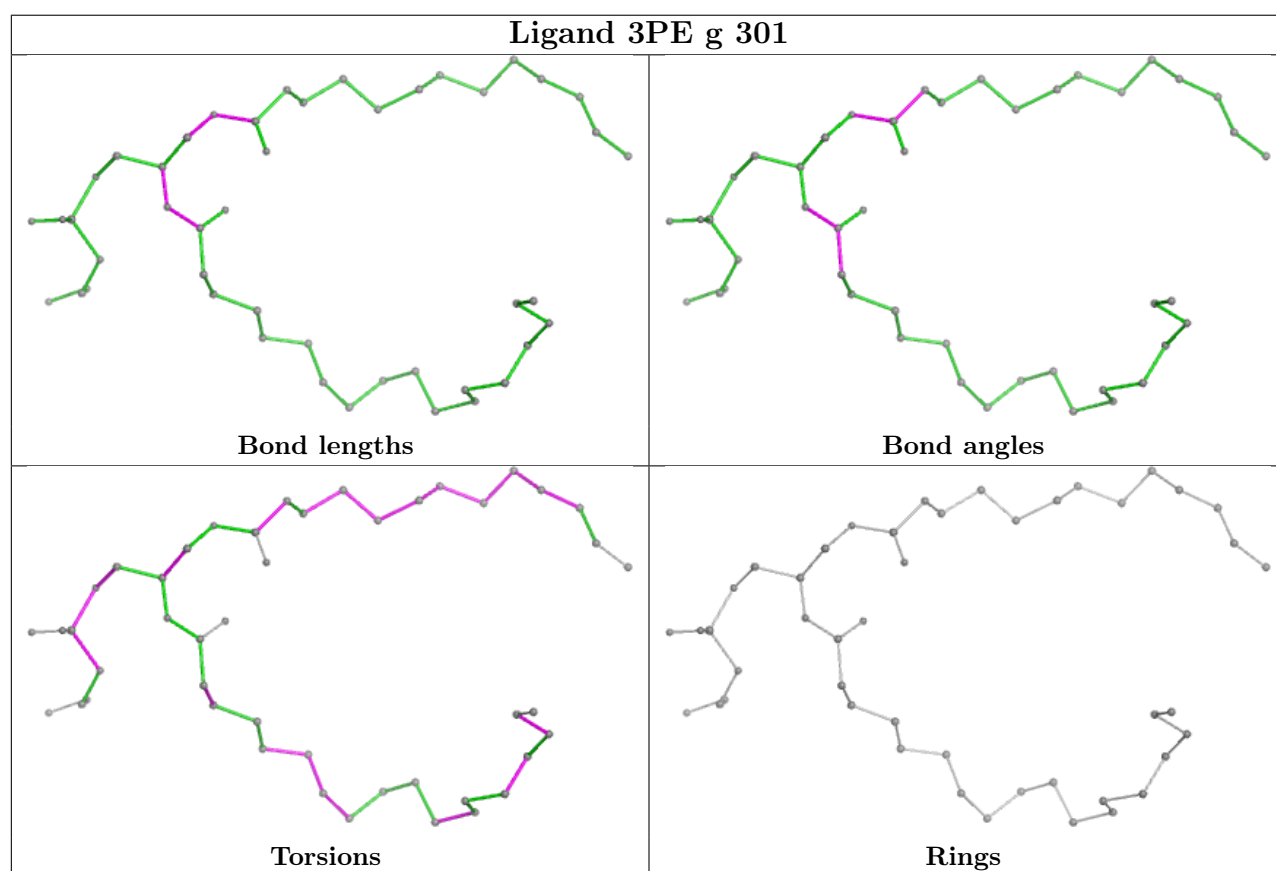
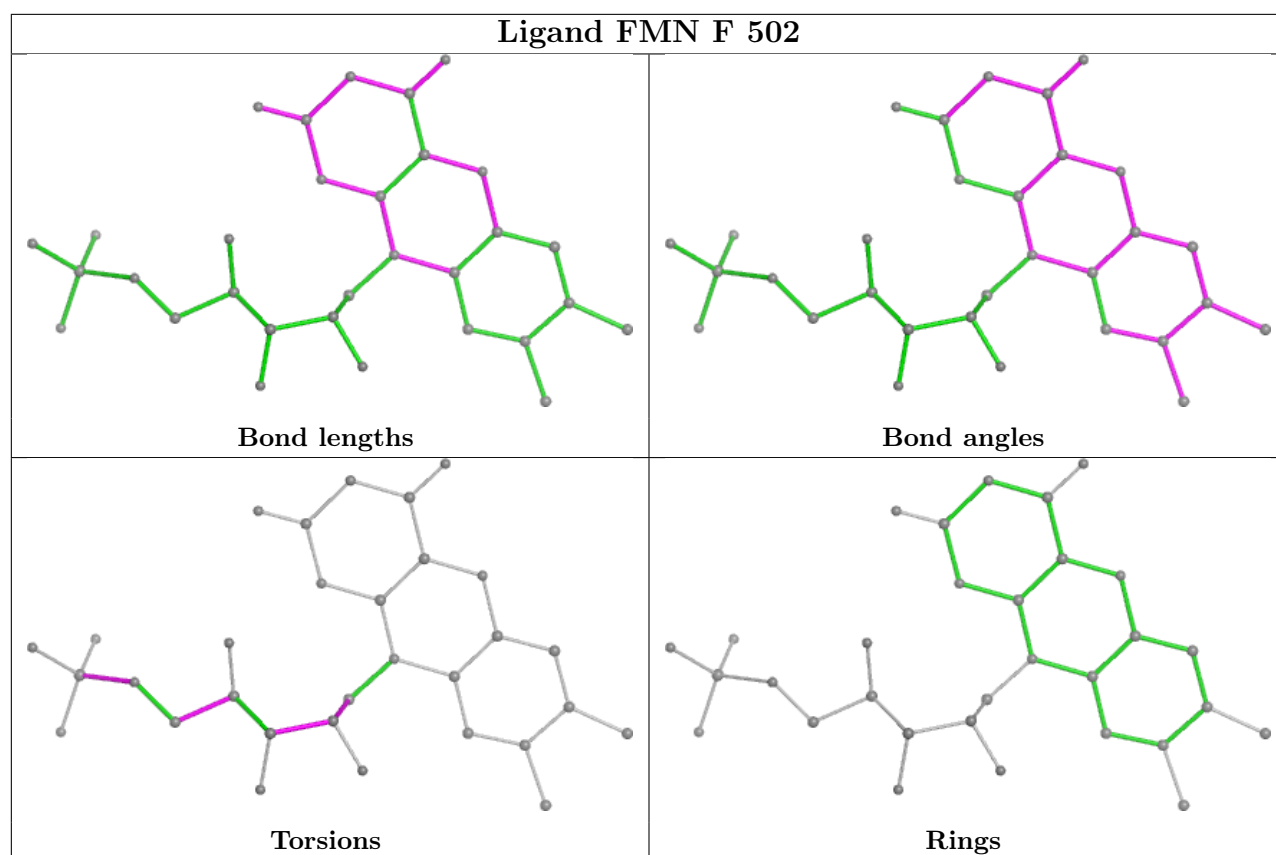


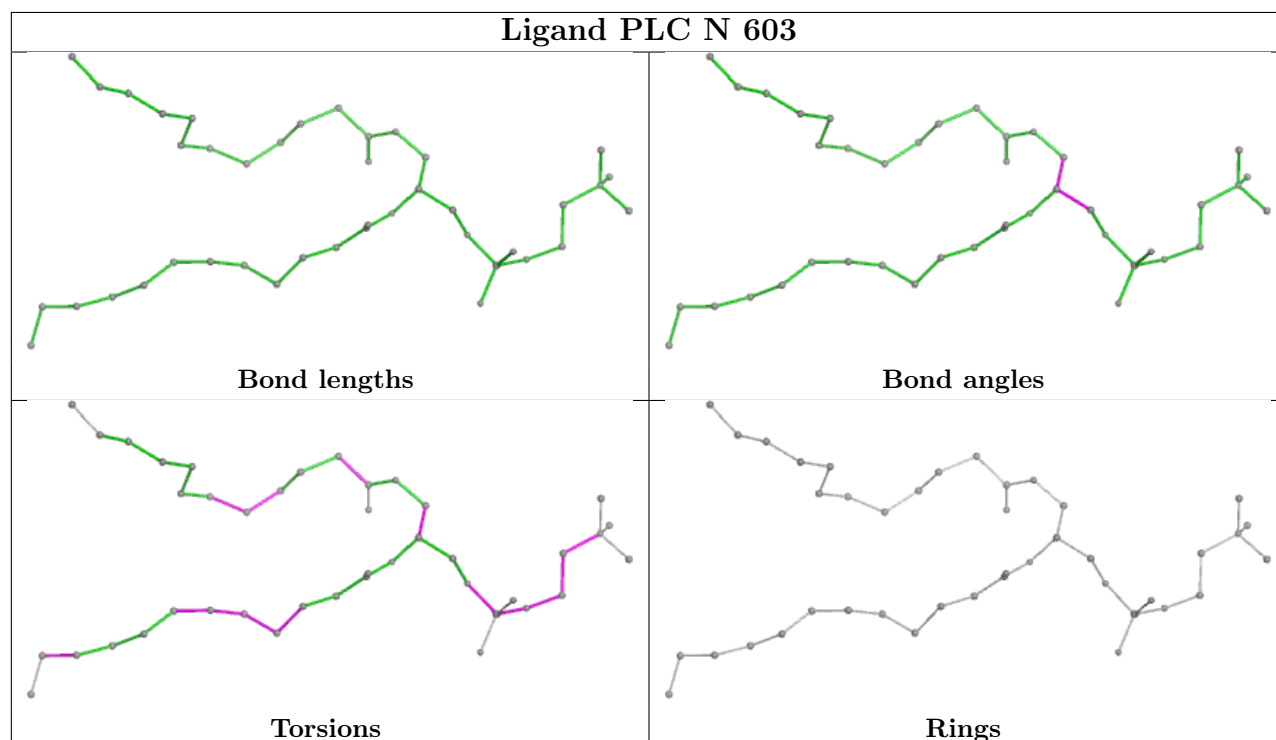
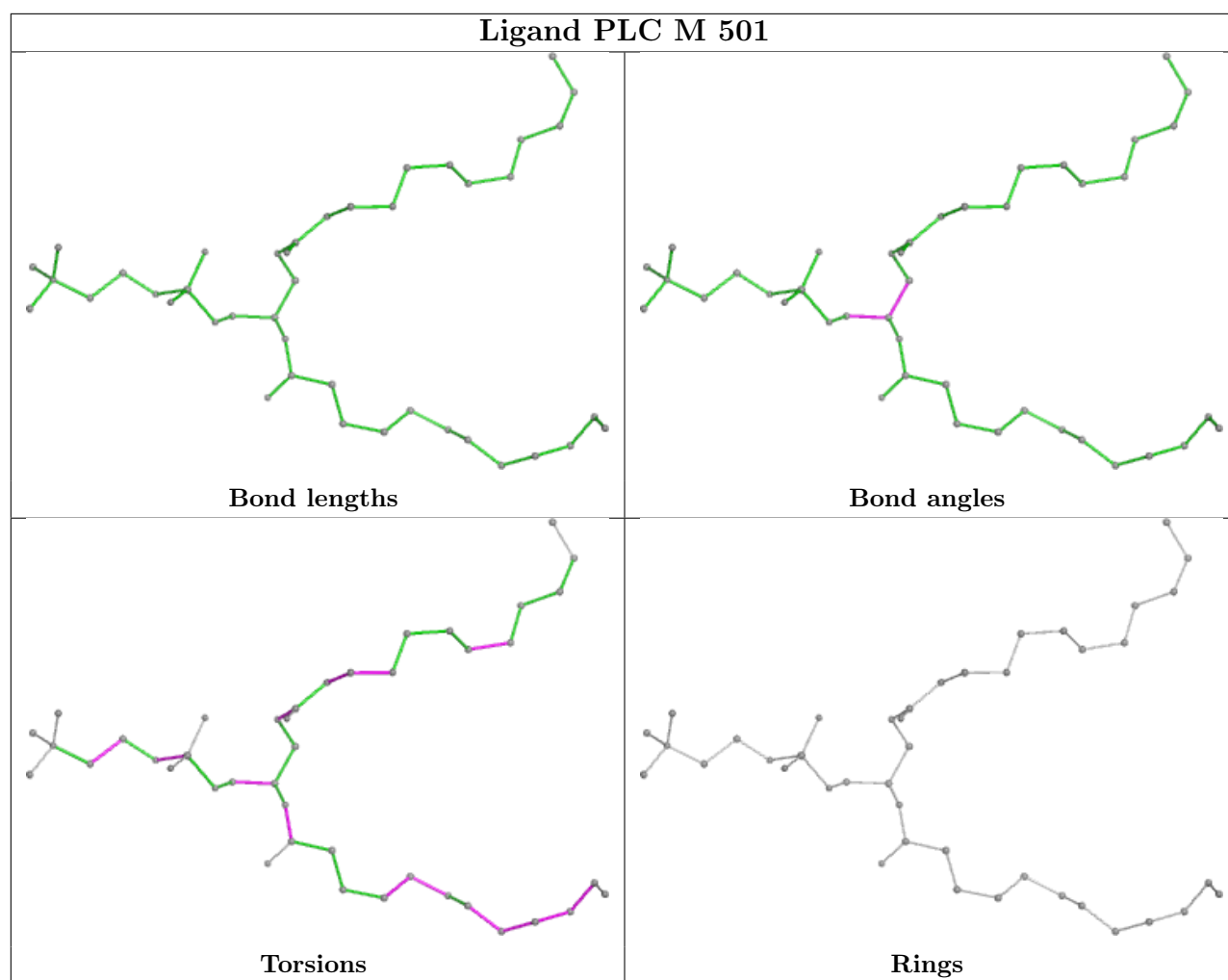


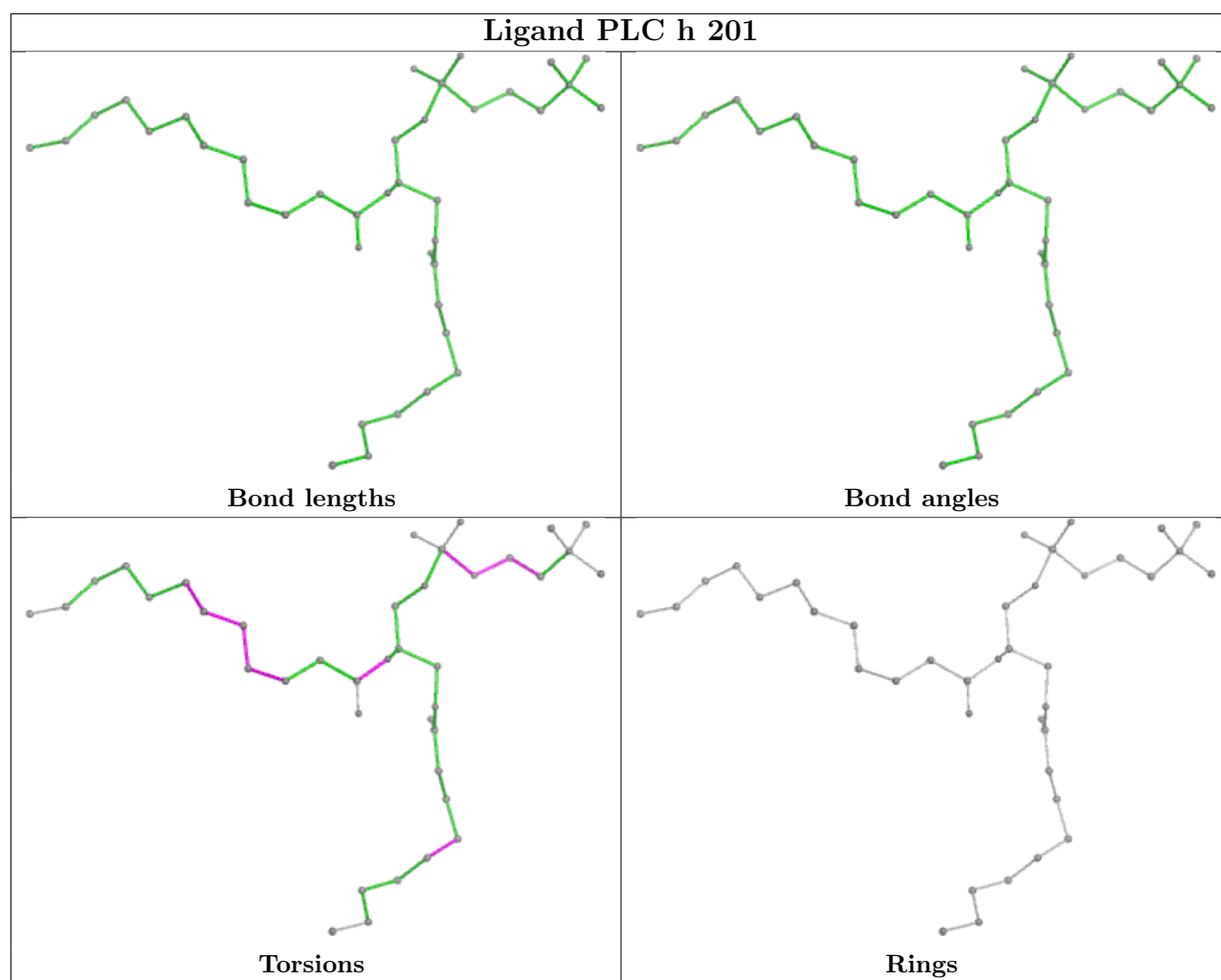


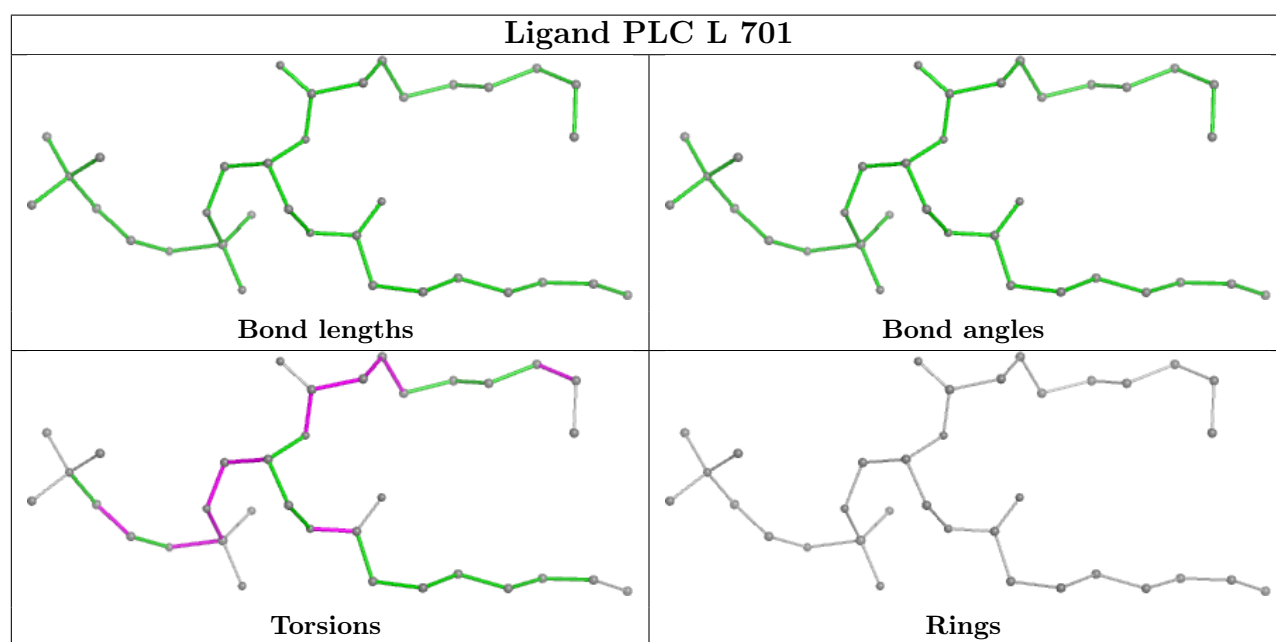
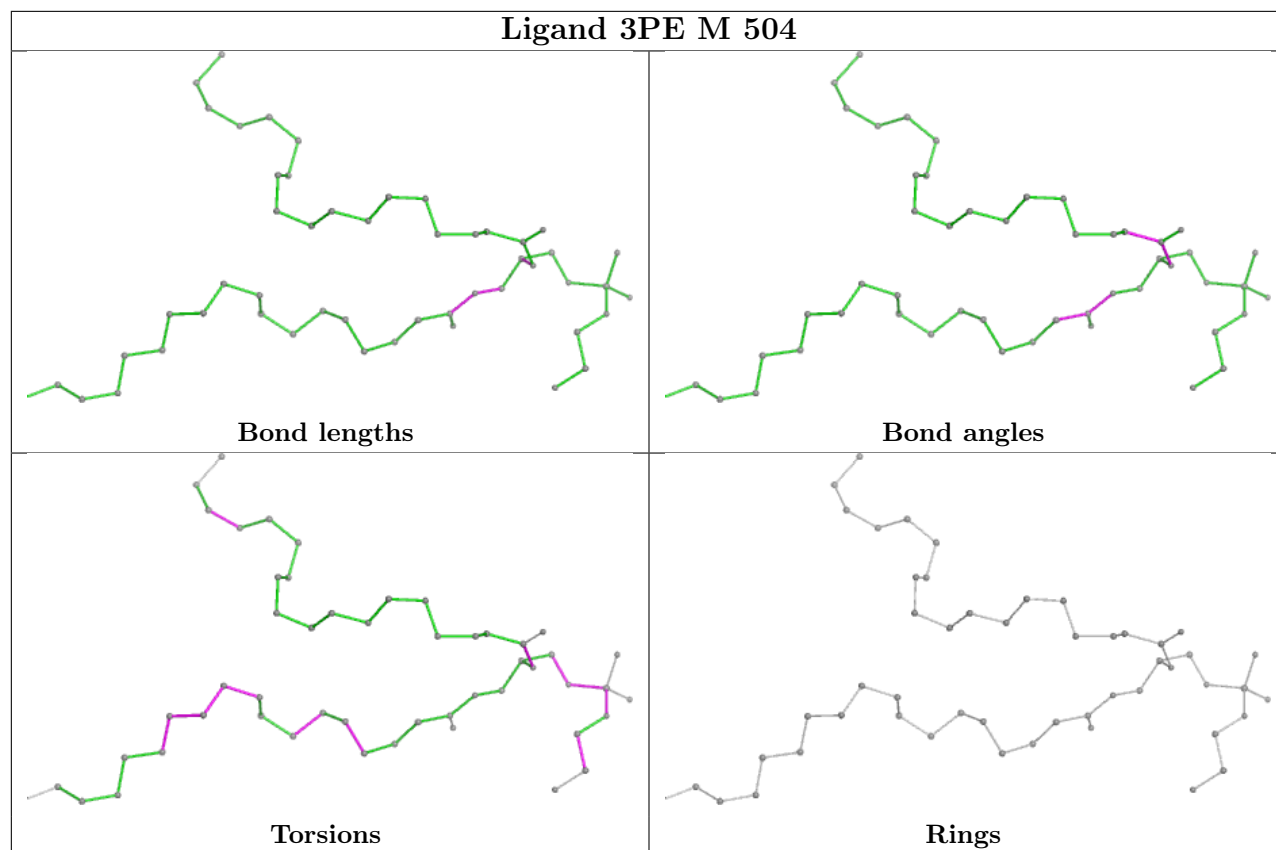


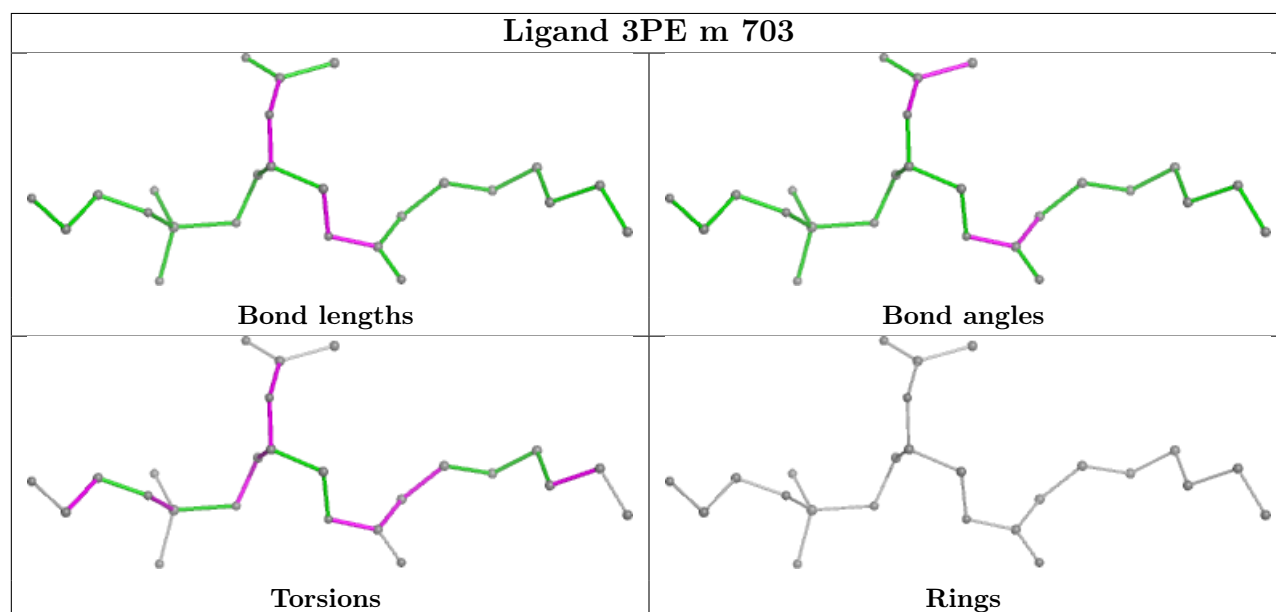
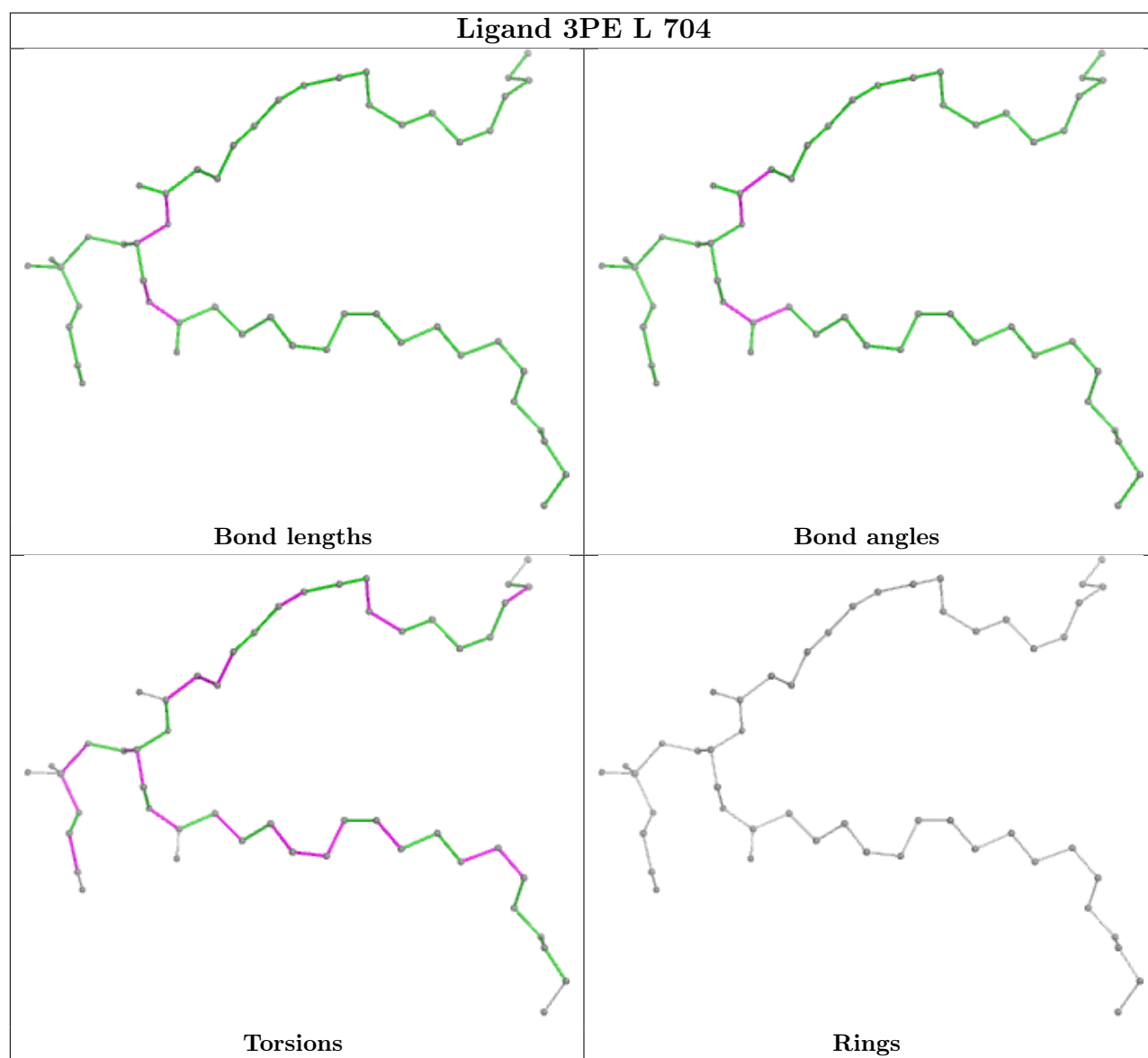


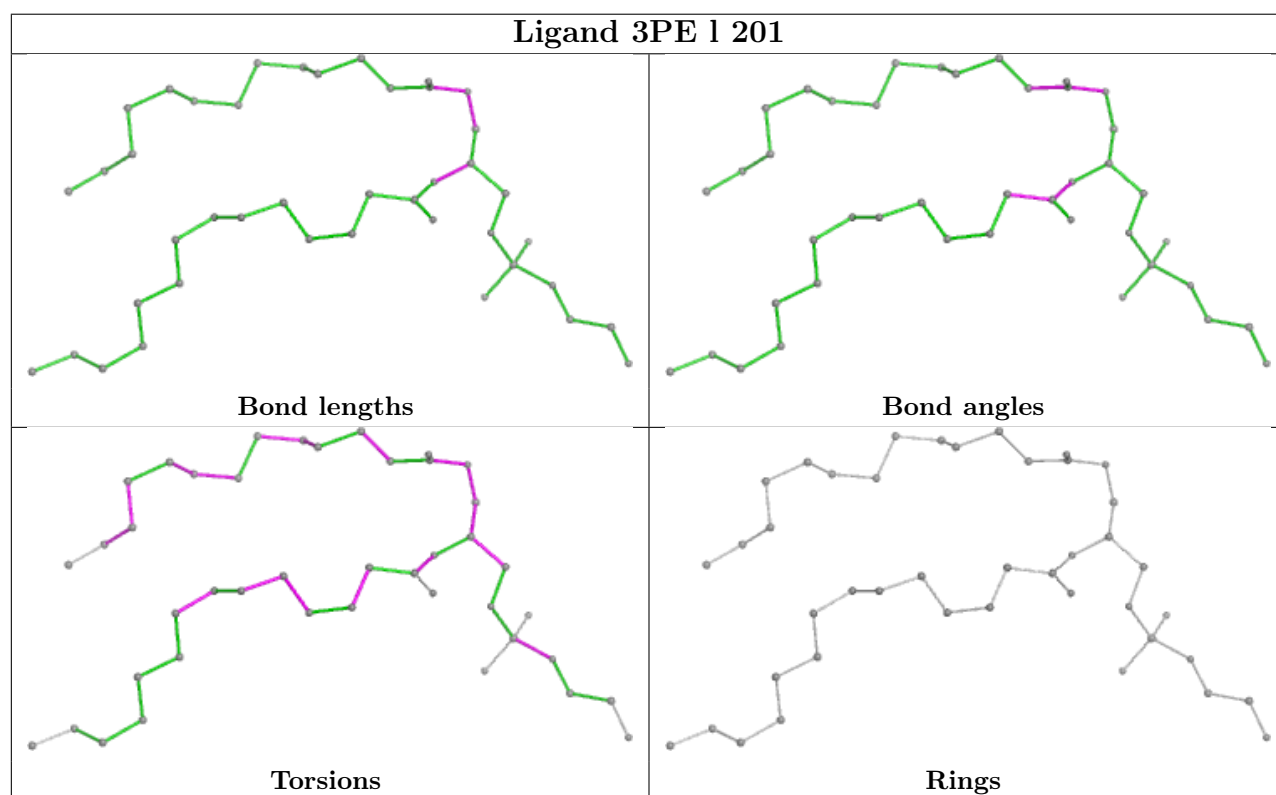
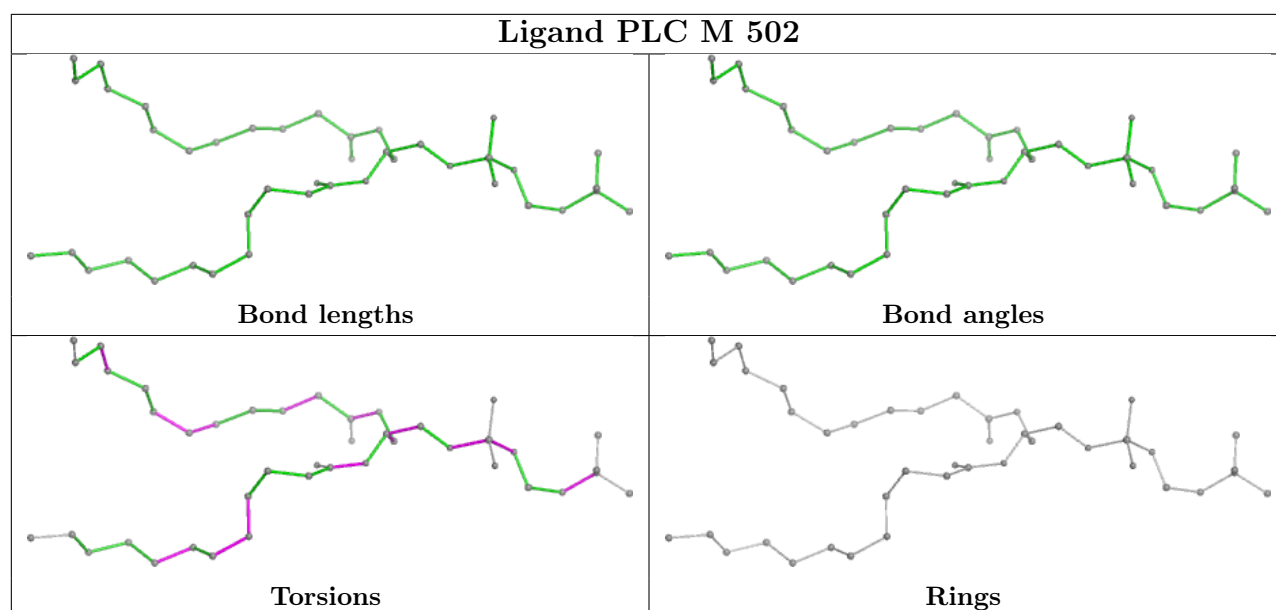




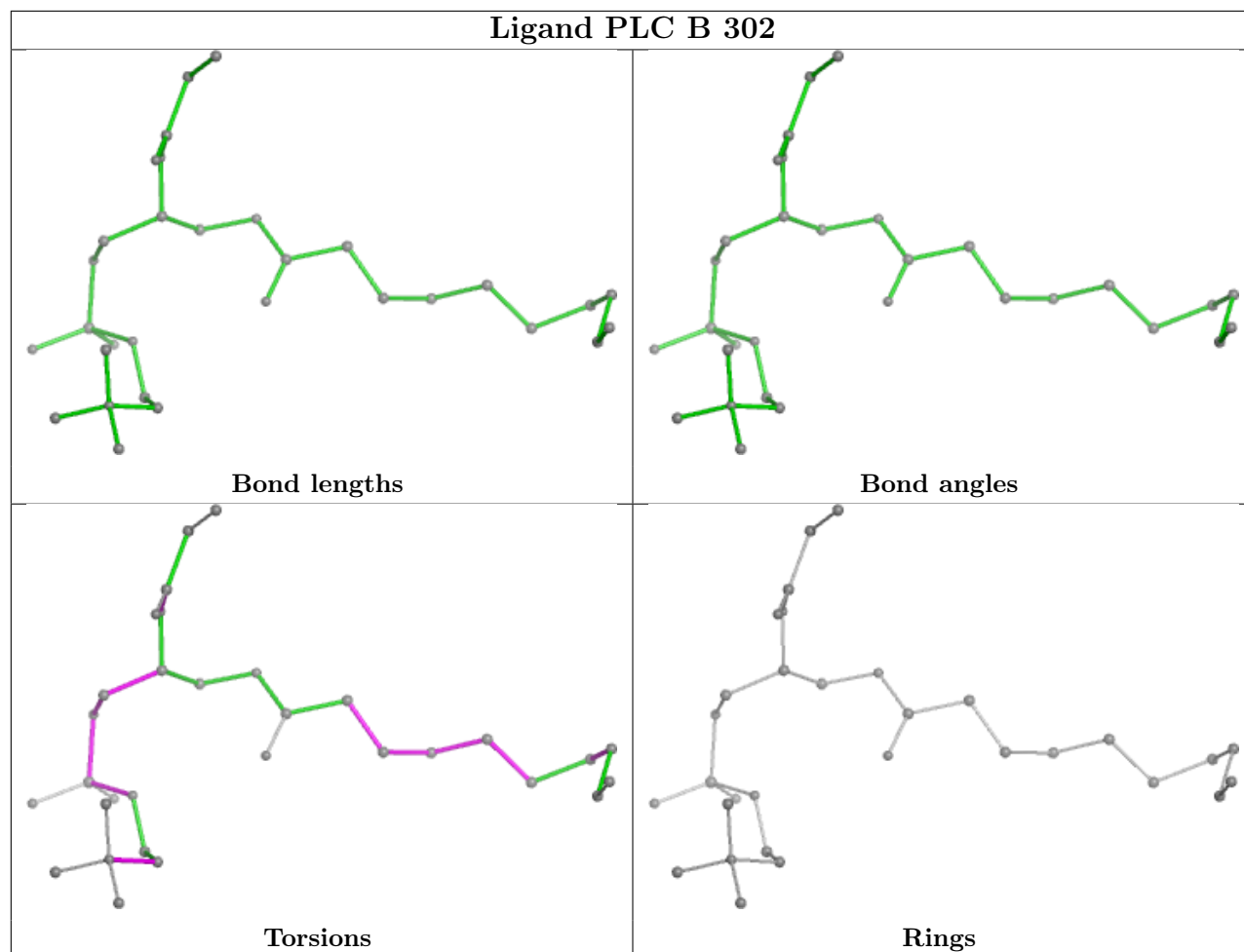




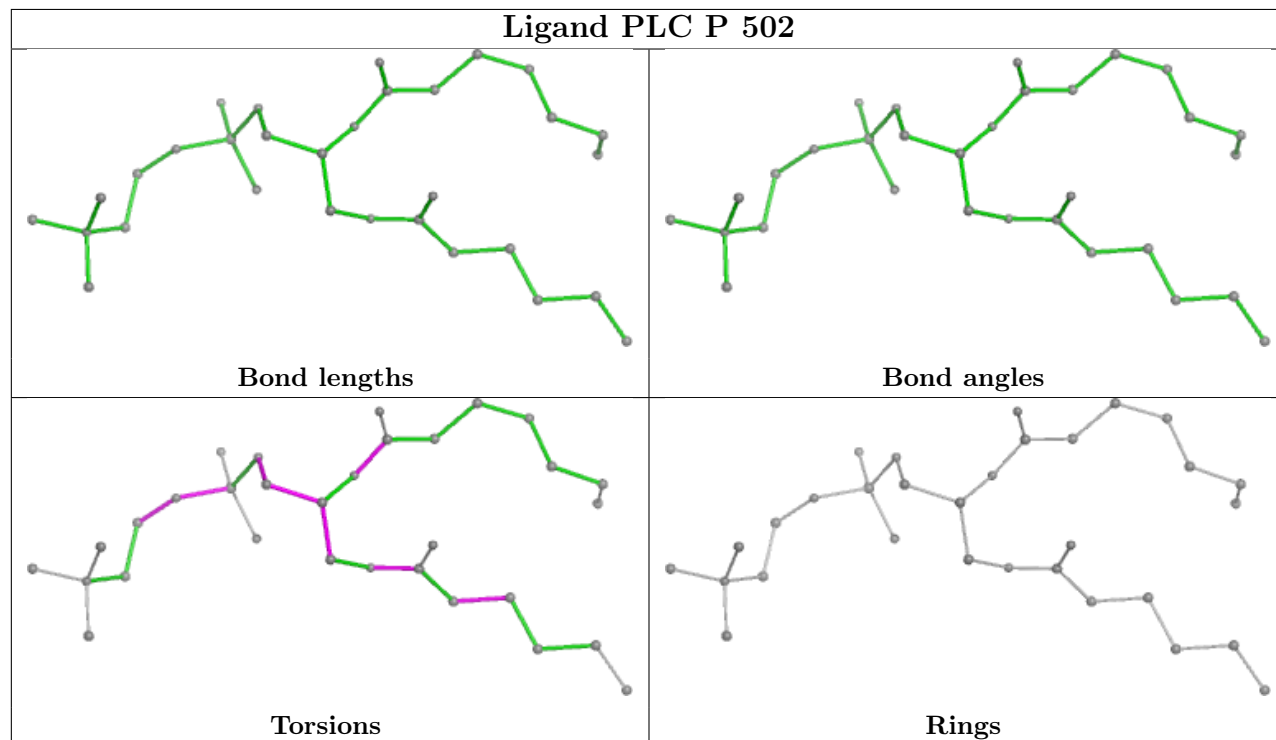


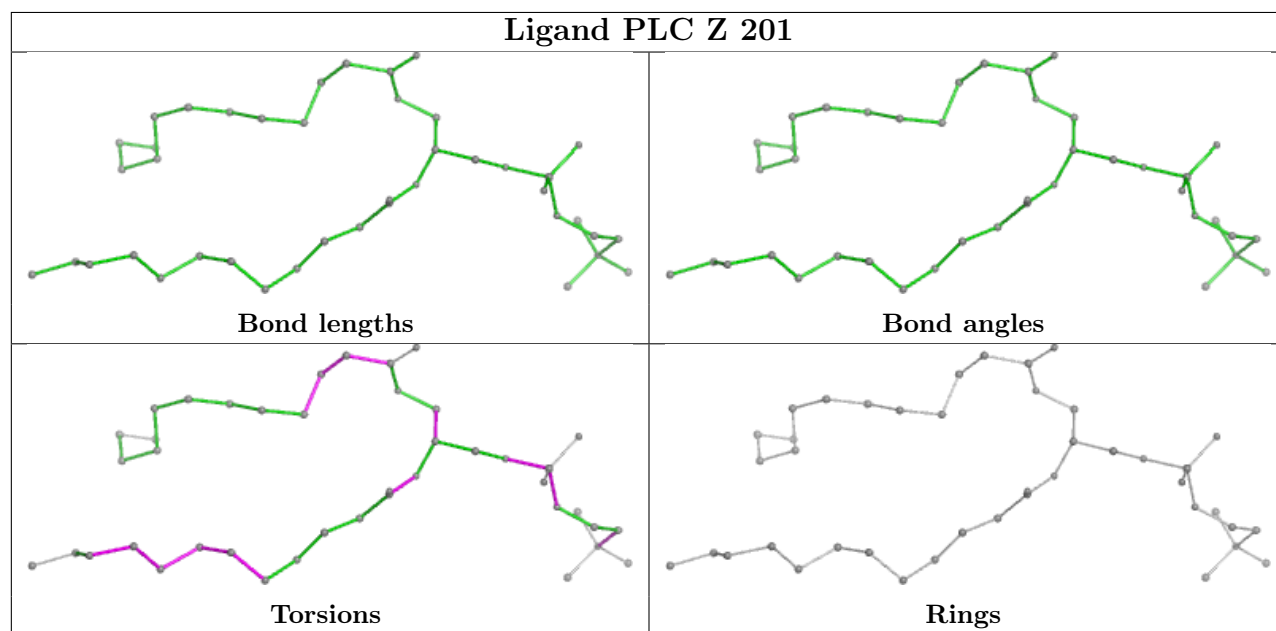
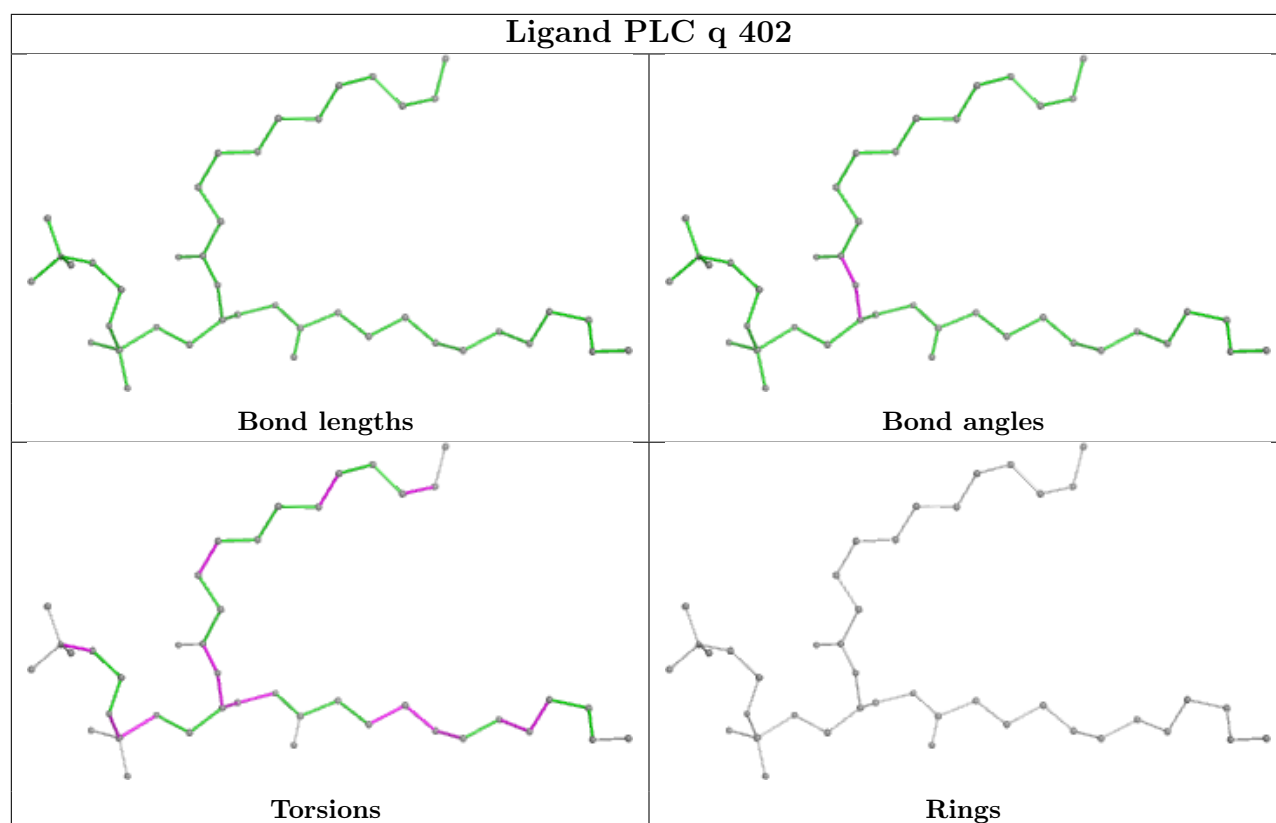


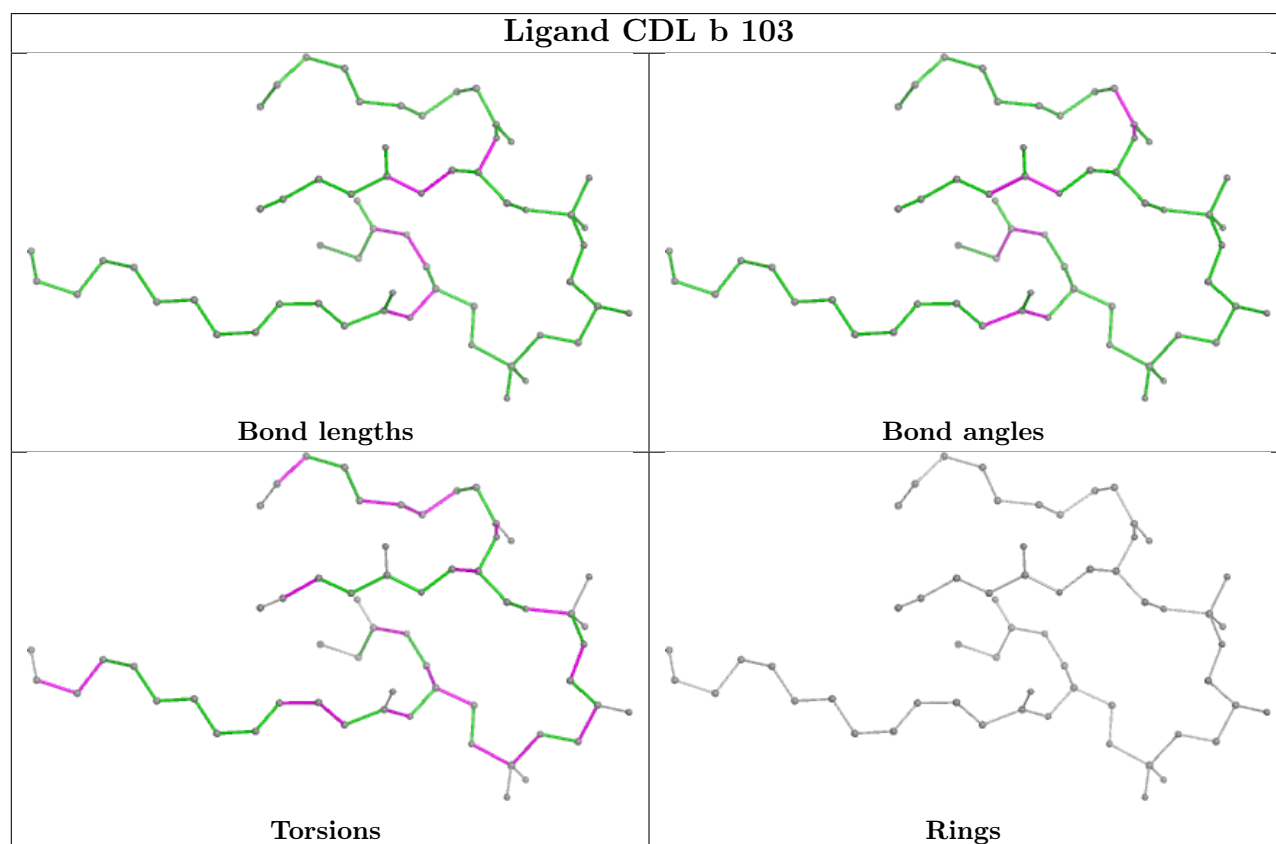
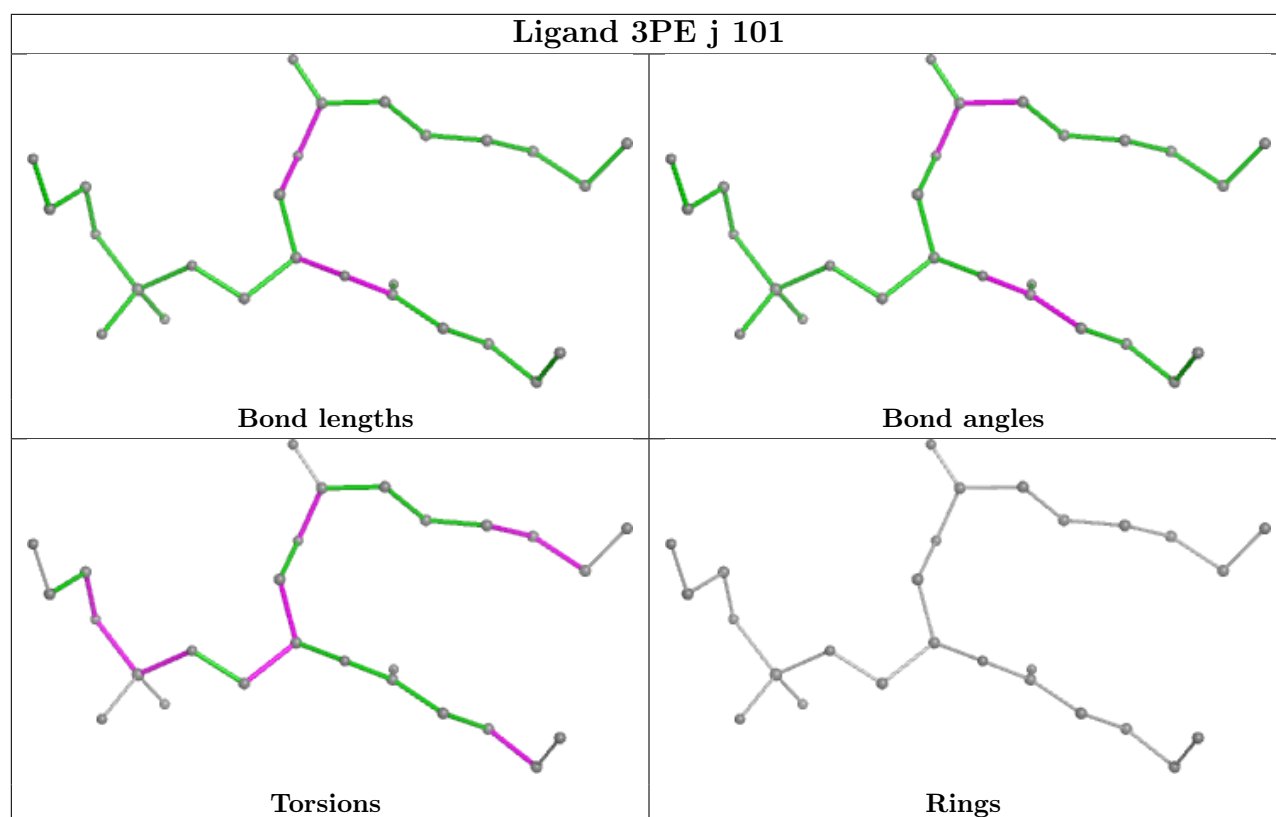
Ligand PLC B 302



Ligand PLC P 502







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.

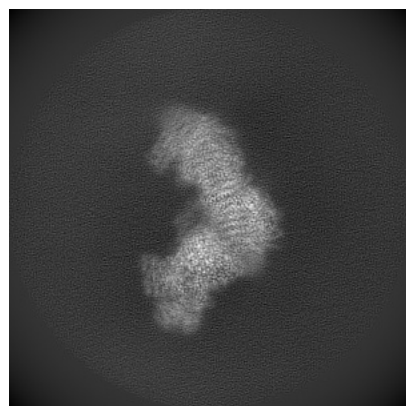
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52876. These allow visual inspection of the internal detail of the map and identification of artifacts.

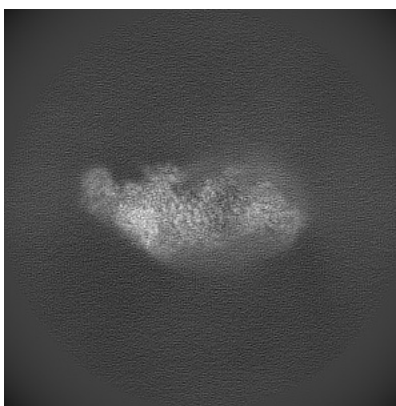
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

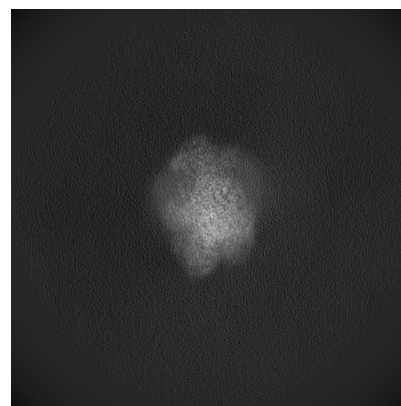
6.1.1 Primary map



X

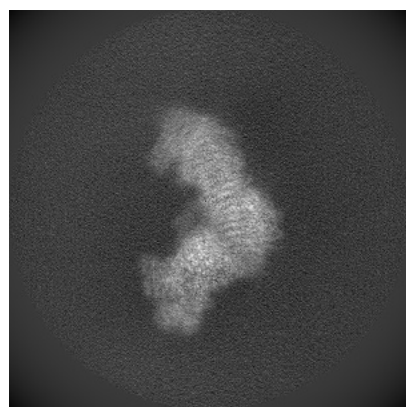


Y

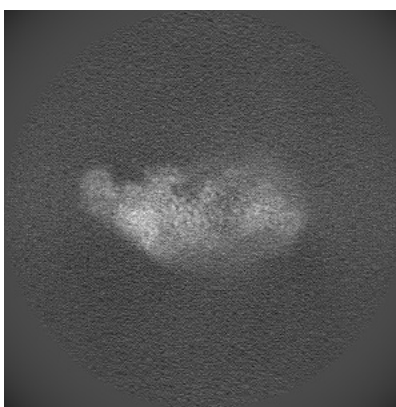


Z

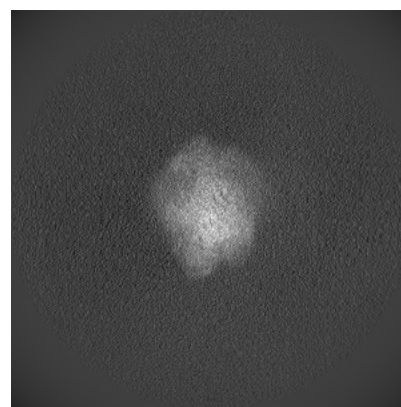
6.1.2 Raw map



X



Y

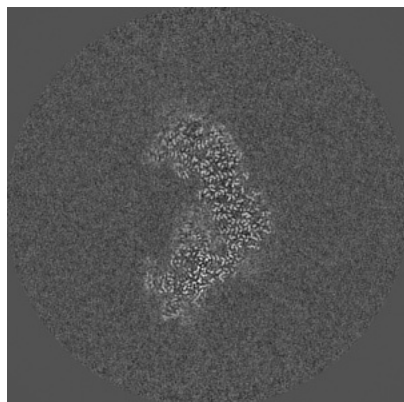


Z

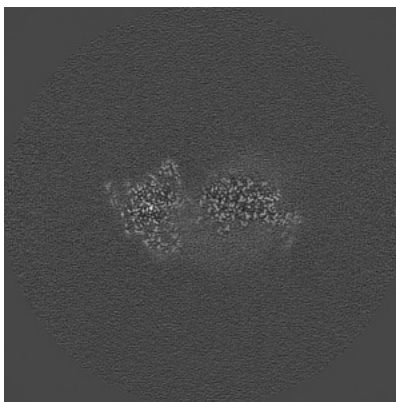
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

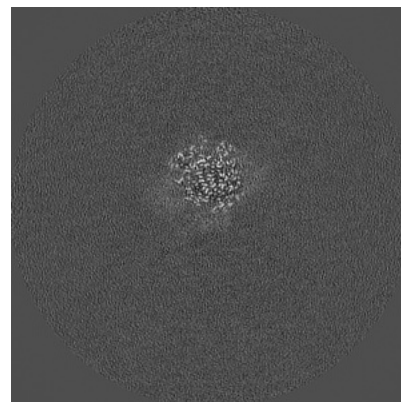
6.2.1 Primary map



X Index: 270

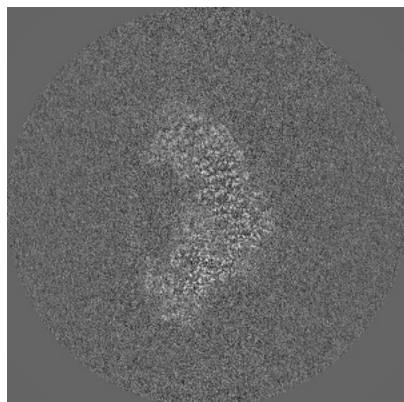


Y Index: 270

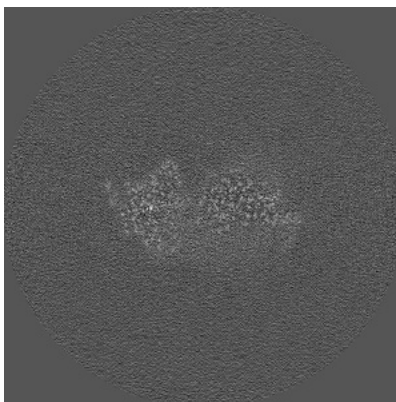


Z Index: 270

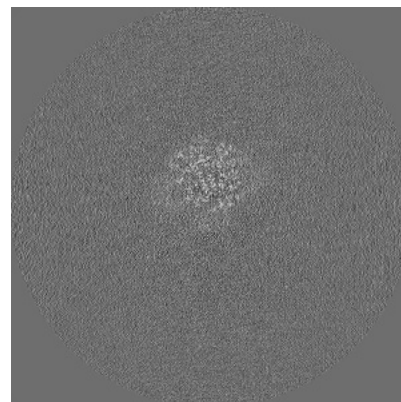
6.2.2 Raw map



X Index: 270



Y Index: 270

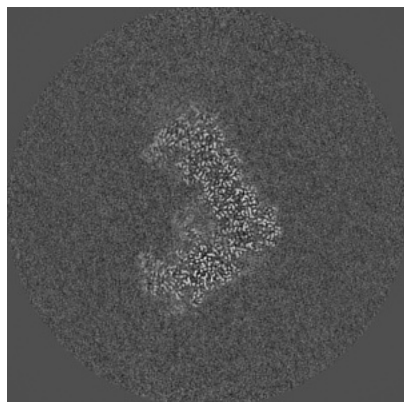


Z Index: 270

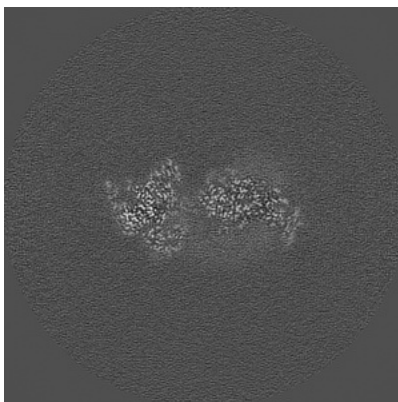
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

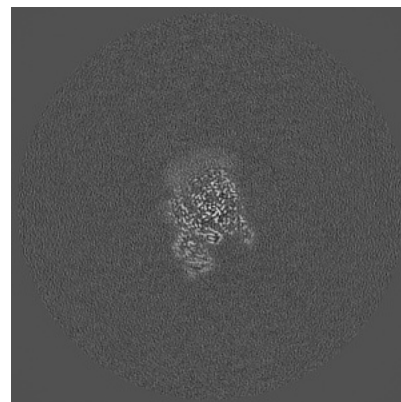
6.3.1 Primary map



X Index: 259

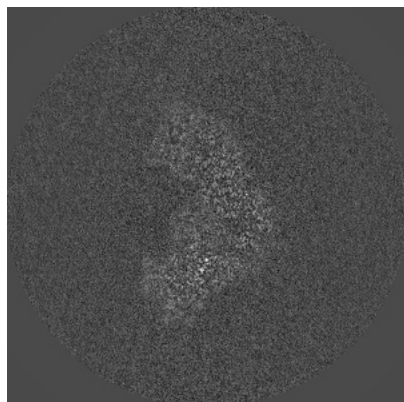


Y Index: 267

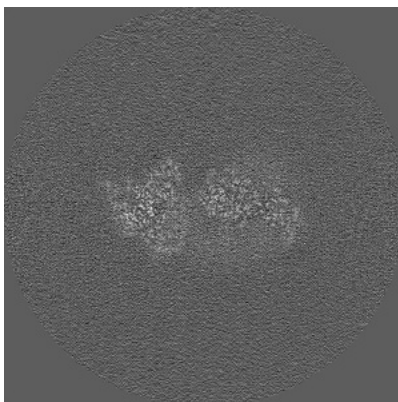


Z Index: 196

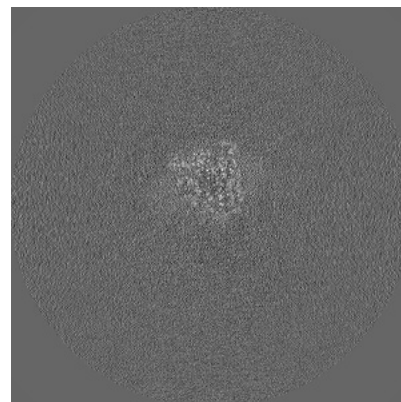
6.3.2 Raw map



X Index: 267



Y Index: 267

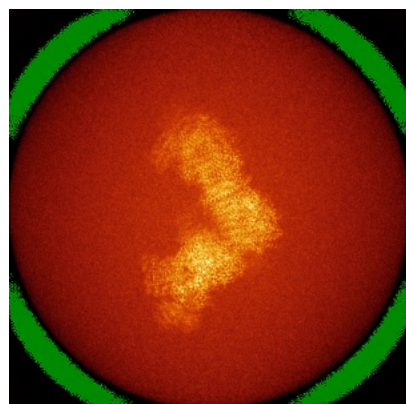


Z Index: 275

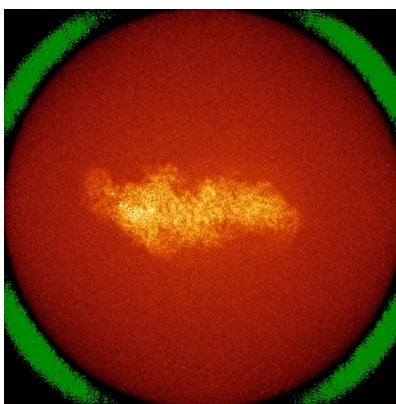
The images above show the largest variance slices of the map in three orthogonal directions.

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

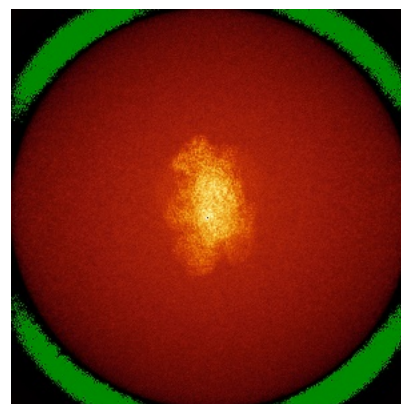
6.4.1 Primary map



X

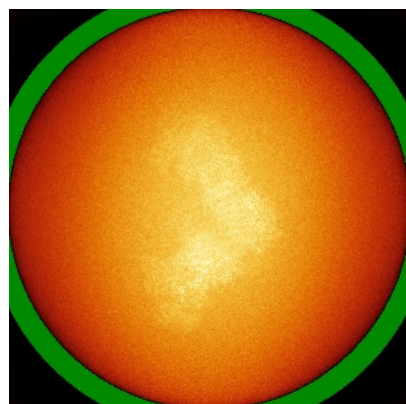


Y

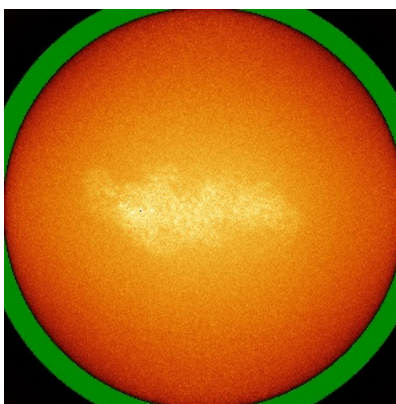


Z

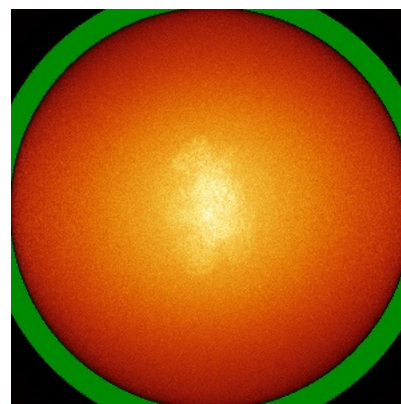
6.4.2 Raw map



X



Y

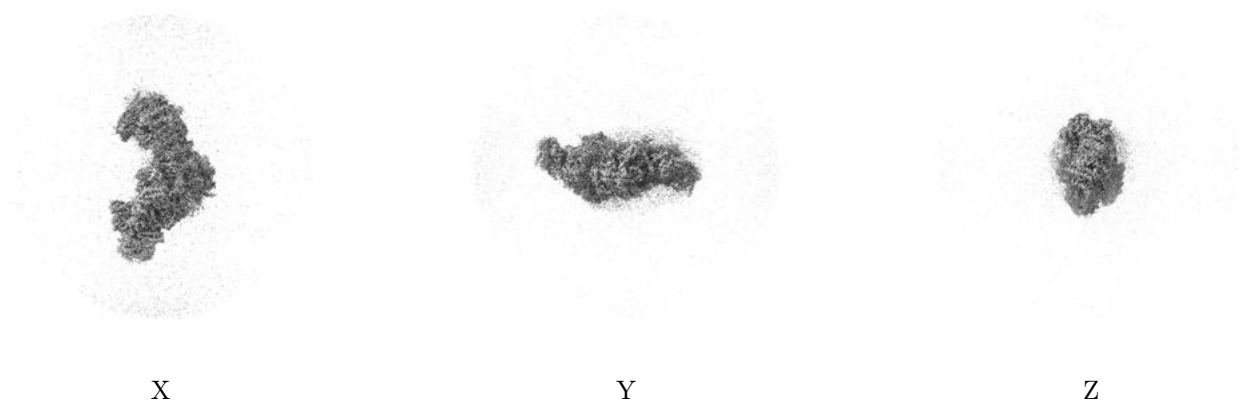


Z

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.

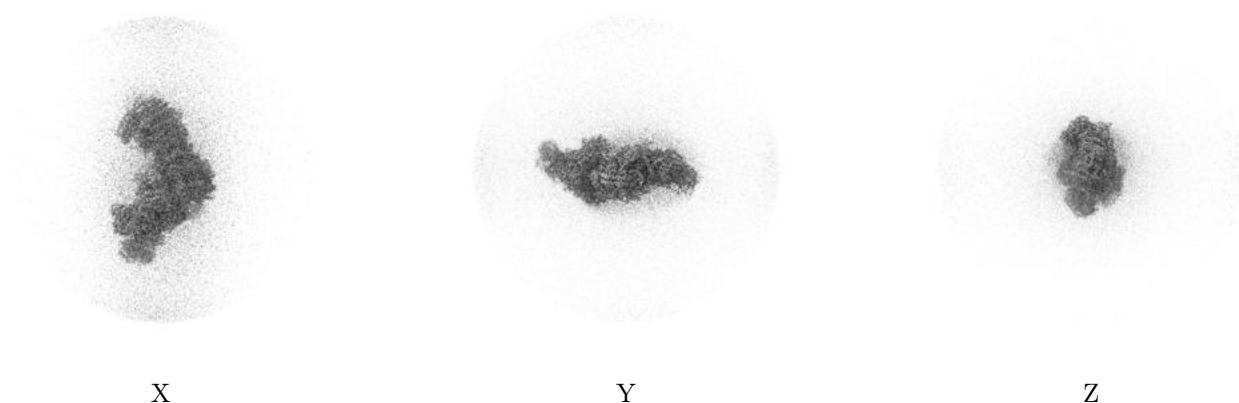
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

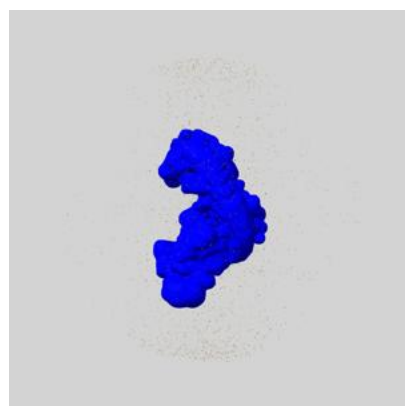
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

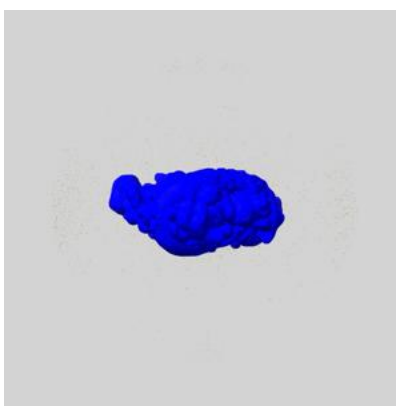
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

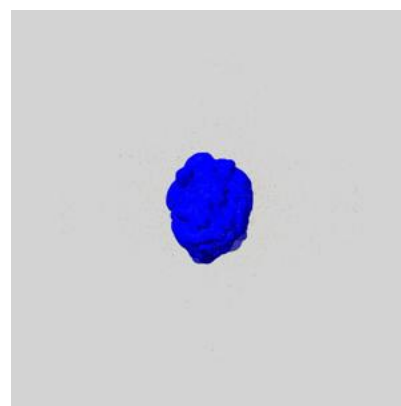
6.6.1 emd_52876_msk_1.map [i](#)



X



Y

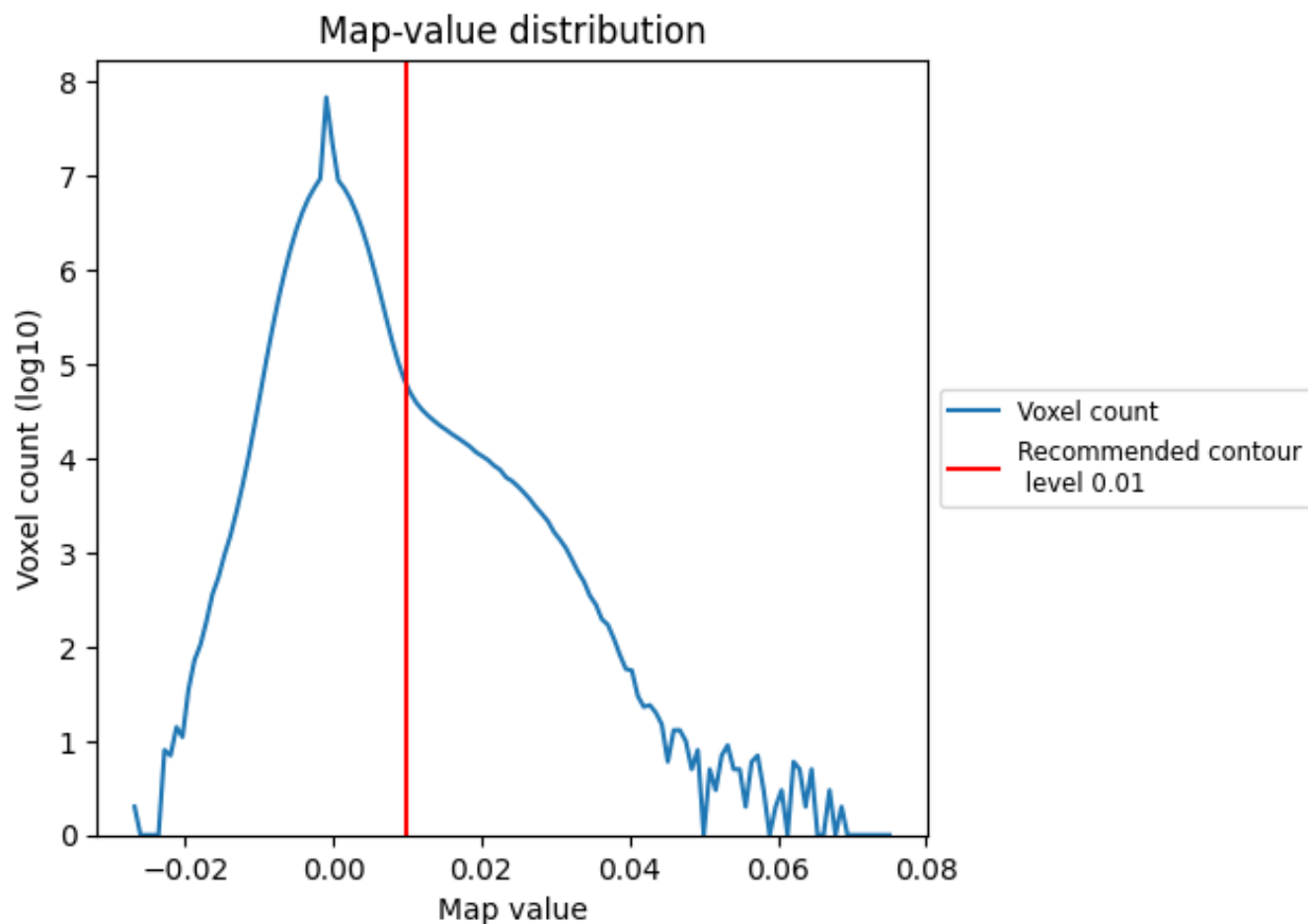


Z

7 Map analysis [i](#)

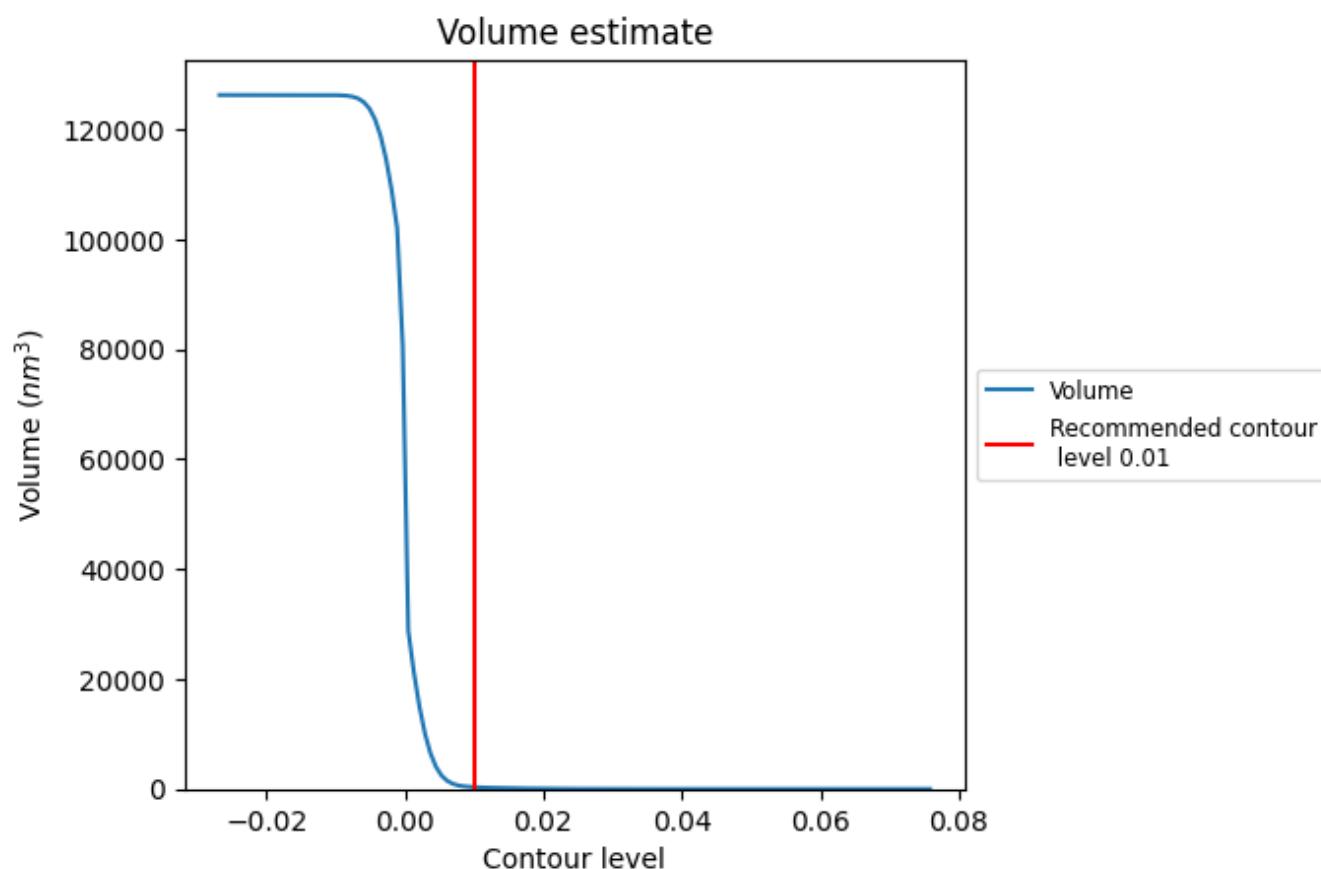
This section contains the results of statistical analysis of the map.

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.

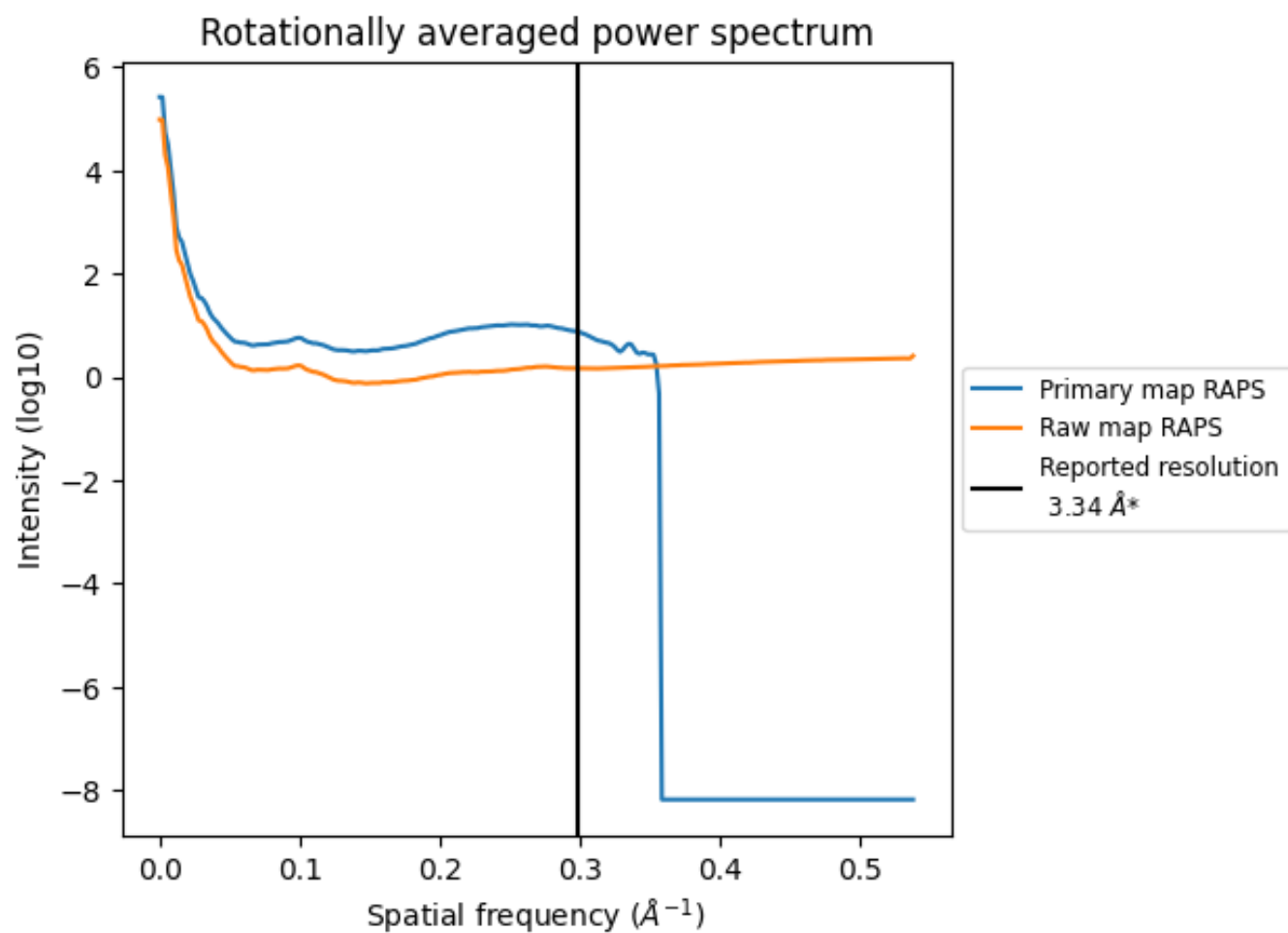
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323 nm³; this corresponds to an approximate mass of 292 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 ⓘ

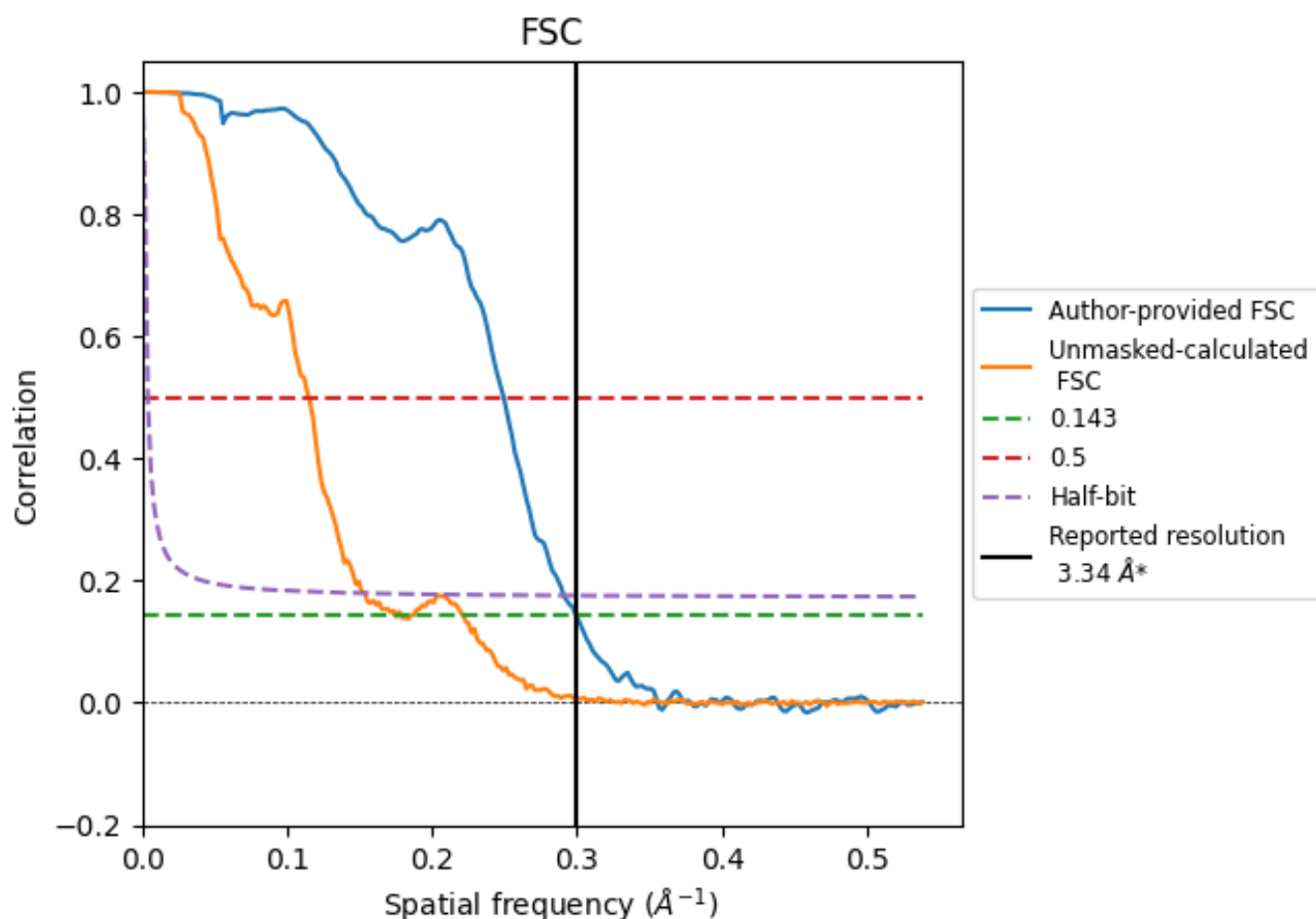


*Reported resolution corresponds to spatial frequency of 0.299 \AA^{-1}

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 0.299 \AA^{-1}

8.2 Resolution estimates [i](#)

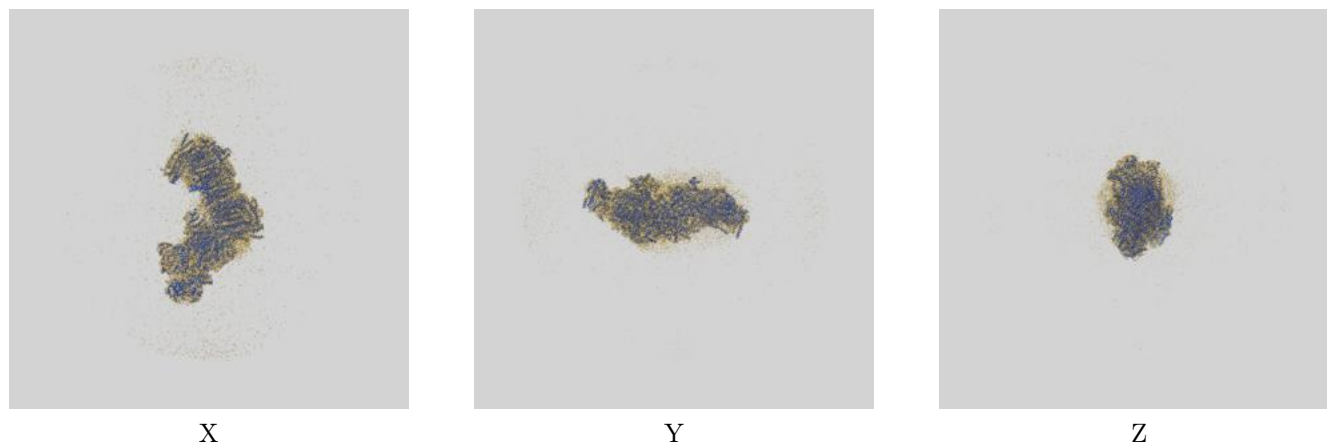
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	4.01	3.44
Unmasked-calculated*	5.71	8.70	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.71 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

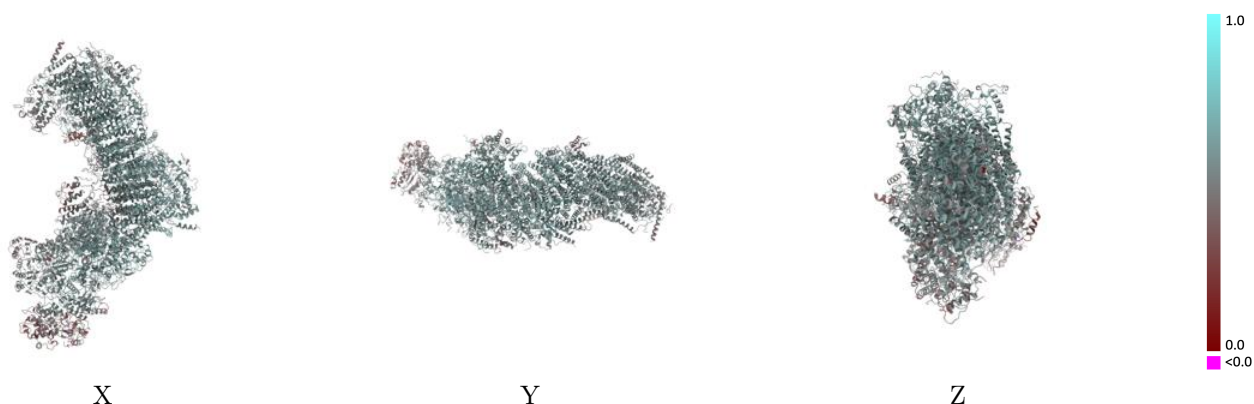
This section contains information regarding the fit between EMDB map EMD-52876 and PDB model 9IHP. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



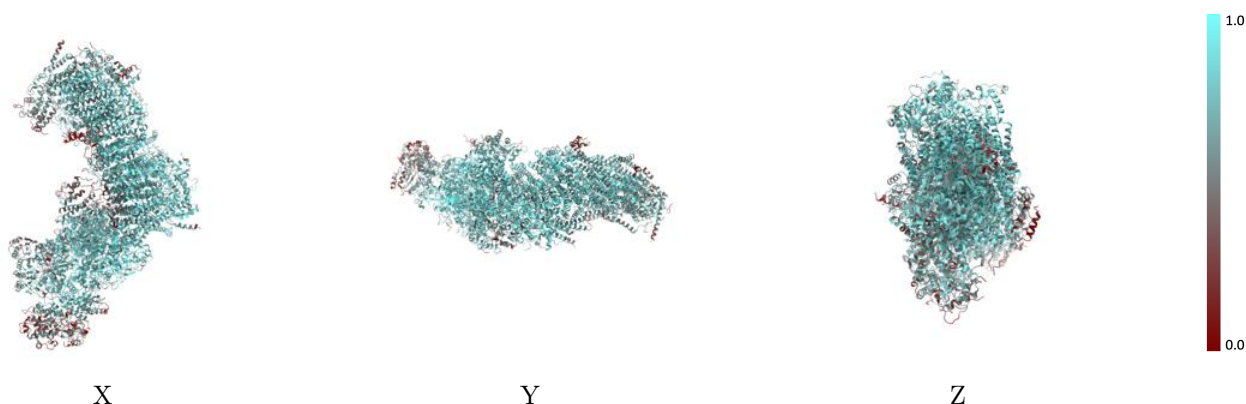
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



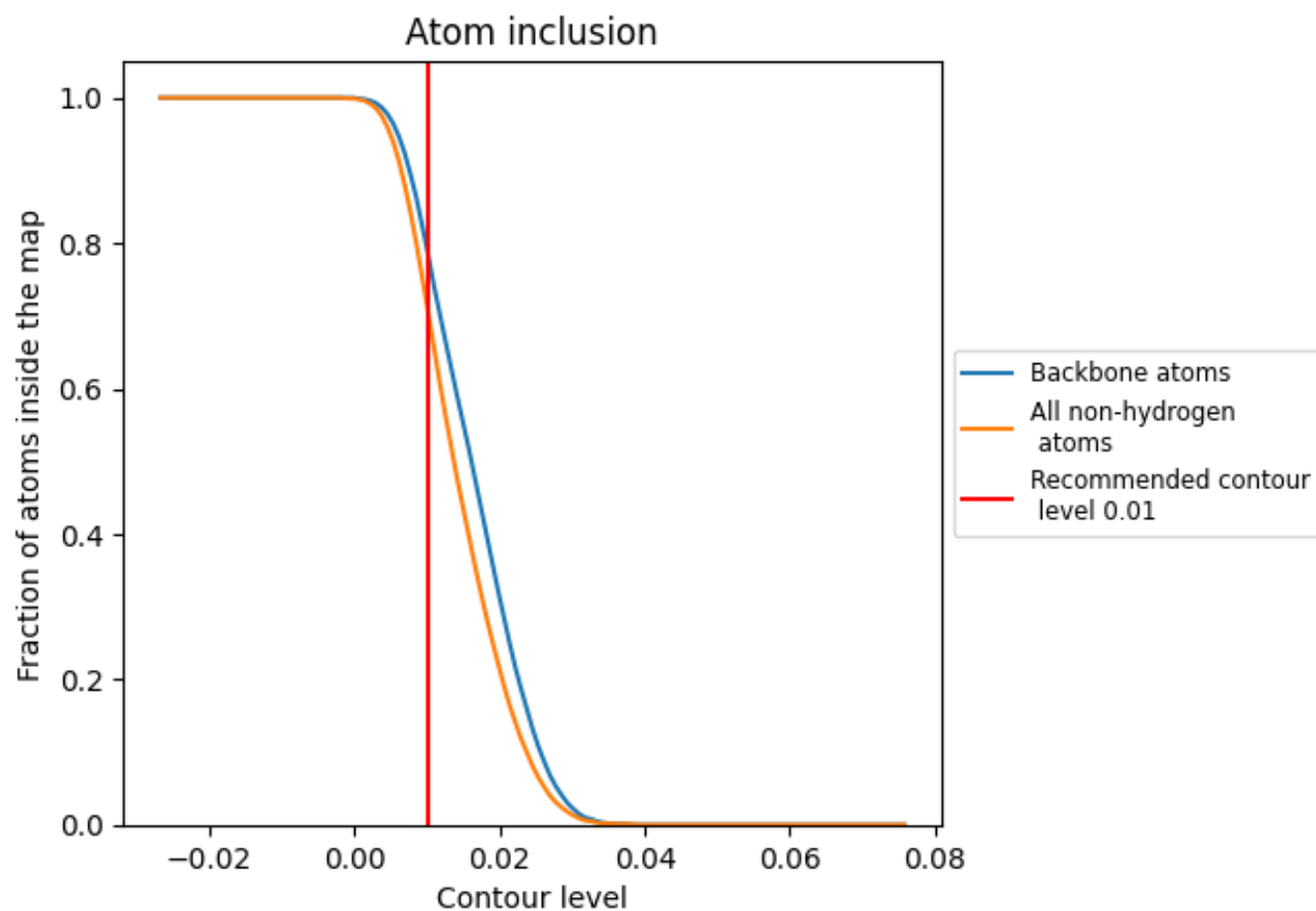
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 72% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.5420
A	 0.6360	 0.5310
B	 0.8120	 0.5760
C	 0.8100	 0.5680
D	 0.8030	 0.5820
E	 0.5510	 0.4500
F	 0.4810	 0.4390
G	 0.7510	 0.5410
H	 0.7560	 0.5700
I	 0.8640	 0.5930
J	 0.7180	 0.5630
K	 0.7410	 0.5540
L	 0.7280	 0.5500
M	 0.7830	 0.5770
N	 0.8090	 0.5830
O	 0.7870	 0.5710
P	 0.6850	 0.5200
Q	 0.7040	 0.5400
R	 0.7730	 0.5530
S	 0.4770	 0.4410
T	 0.3640	 0.4220
U	 0.4460	 0.4580
V	 0.6970	 0.5260
W	 0.6710	 0.4880
X	 0.7950	 0.5700
Y	 0.7260	 0.5520
Z	 0.8060	 0.5760
a	 0.7830	 0.5760
b	 0.7950	 0.5920
c	 0.7090	 0.5340
d	 0.8020	 0.5760
e	 0.8170	 0.5760
f	 0.6960	 0.5360
g	 0.4420	 0.4750
h	 0.7210	 0.5510



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.6670	 0.5280
j	 0.5390	 0.4900
k	 0.5300	 0.4670
l	 0.6250	 0.5310
m	 0.6390	 0.5470
n	 0.5570	 0.4810
o	 0.6030	 0.4990
p	 0.7850	 0.5580
q	 0.8190	 0.5710