



## Full wwPDB EM Validation Report ⓘ

Dec 7, 2022 – 10:42 PM JST

PDB ID : 7W0R  
EMDB ID : EMD-32248  
Title : Active state CI from Q10-NADH dataset, Subclass 1  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-18  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

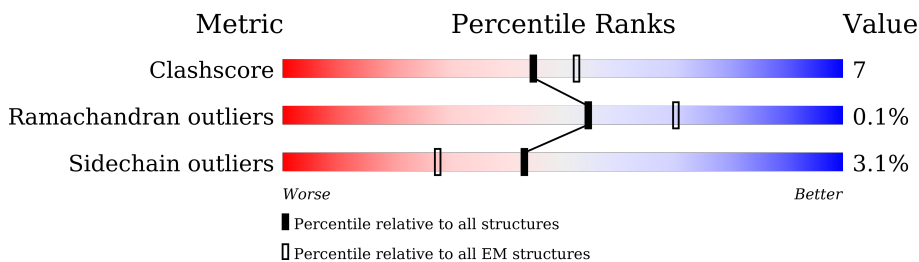
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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.








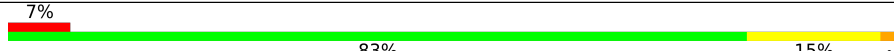
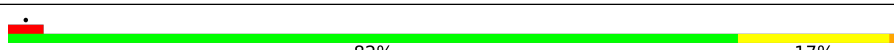

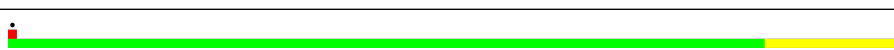

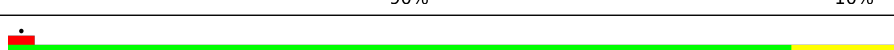
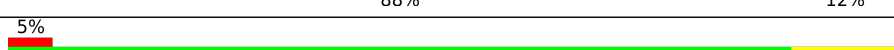

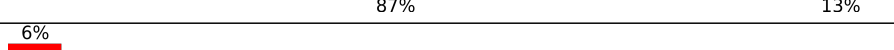
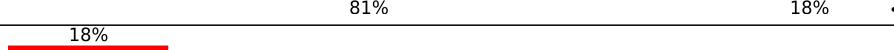
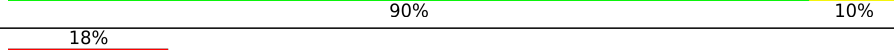

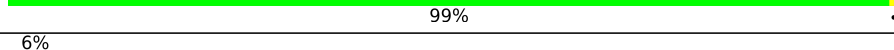

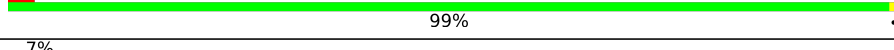
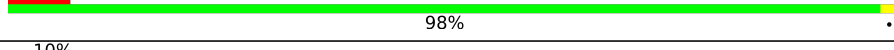
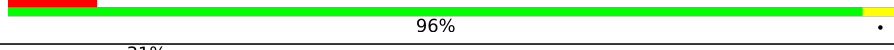
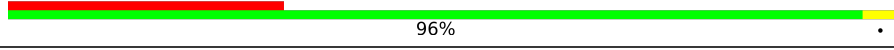
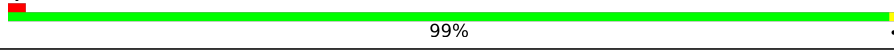
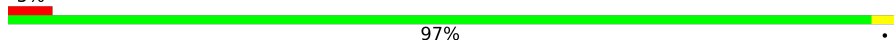
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	

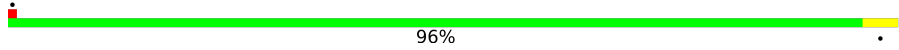
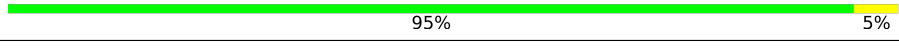
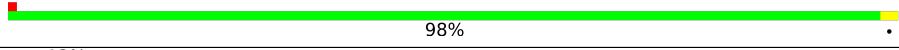
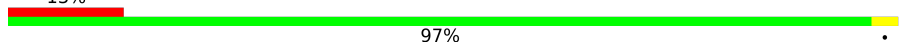

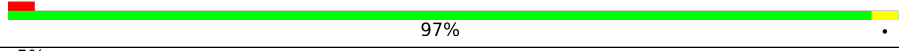
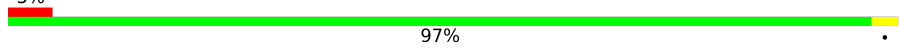
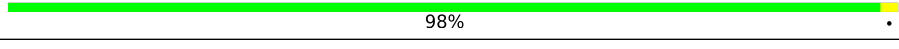
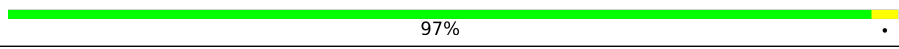
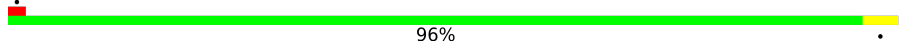
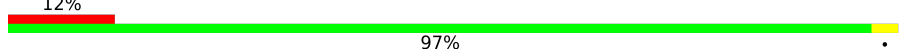
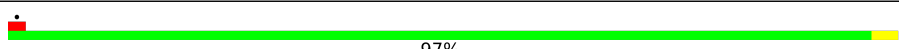
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Mol	Chain	Length	Quality of chain
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	
29	f	49	
30	g	121	
31	h	105	
32	i	347	

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Mol	Chain	Length	Quality of chain
33	j	115	 96% .
34	k	98	 95% 5% .
35	l	606	 98% .
36	m	175	 13% 97% .
37	n	56	 21% 91% 9% .
38	o	128	 97% .
39	p	178	 5% 97% .
40	r	459	 98% .
41	s	318	 97% .
42	u	171	 96% .
43	v	124	 12% 97% .
44	w	320	 97% .

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
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68233 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3330	2103	593	614	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			967	617	179	166	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			687	432	129	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			704	454	104	141	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		



- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4800	3182	744	823	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1295	864	188	230	13		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	980	279	263	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1059	658	202	189	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

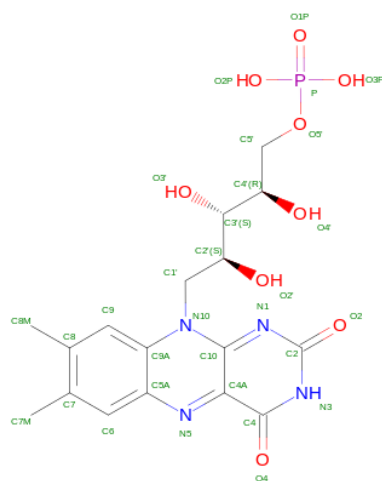
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



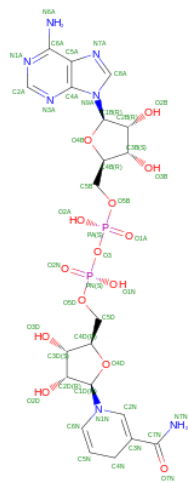
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			16	8	8	
45	B	1	Total	Fe	S	0
			16	8	8	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			16	8	8	
45	M	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).



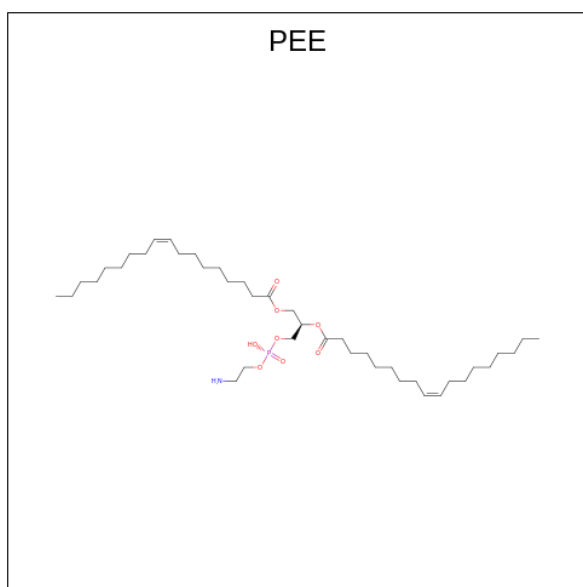
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



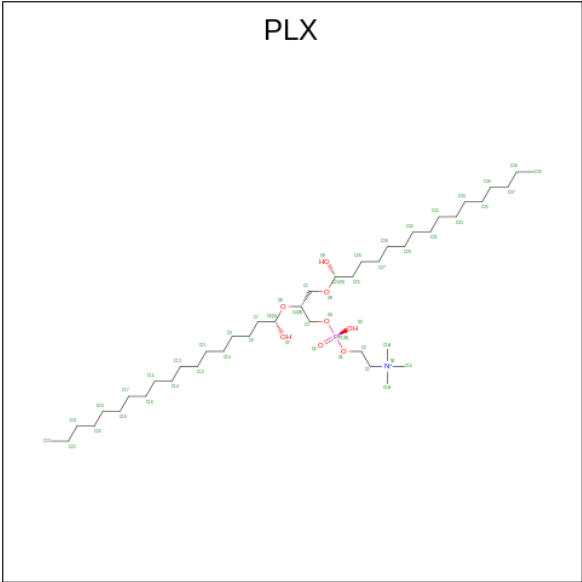
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total 44	C 21	N 7	O 14	P 2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



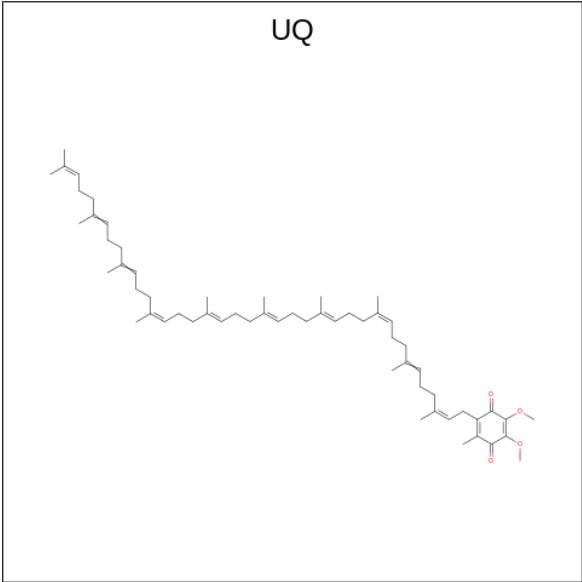
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	j	1	Total	C	N	O	P	0
			92	72	2	16	2	
48	l	1	Total	C	N	O	P	0
			97	77	2	16	2	
48	l	1	Total	C	N	O	P	0
			97	77	2	16	2	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



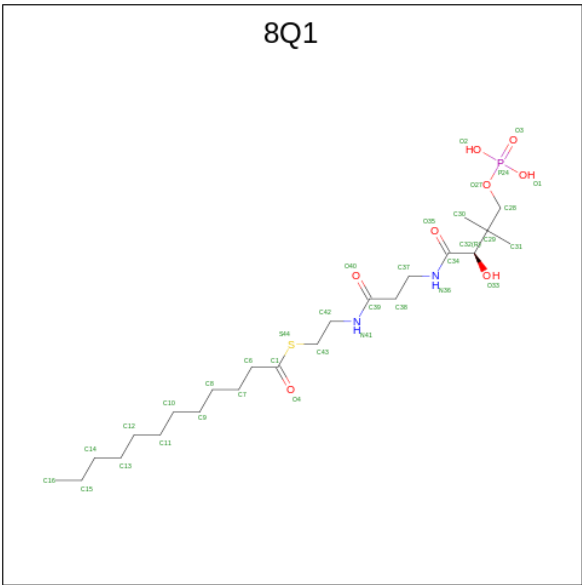
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
49	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 50 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			38	34	4	
50	J	1	Total	C	O	0
			33	29	4	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

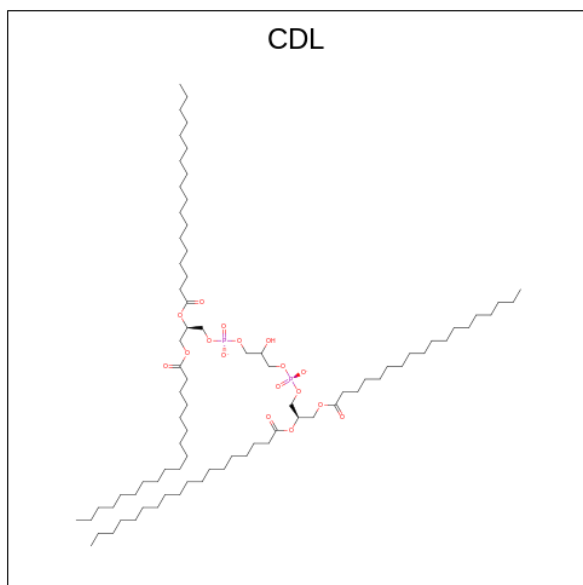
Continued on next page...



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Mol	Chain	Residues	Atoms						AltConf
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

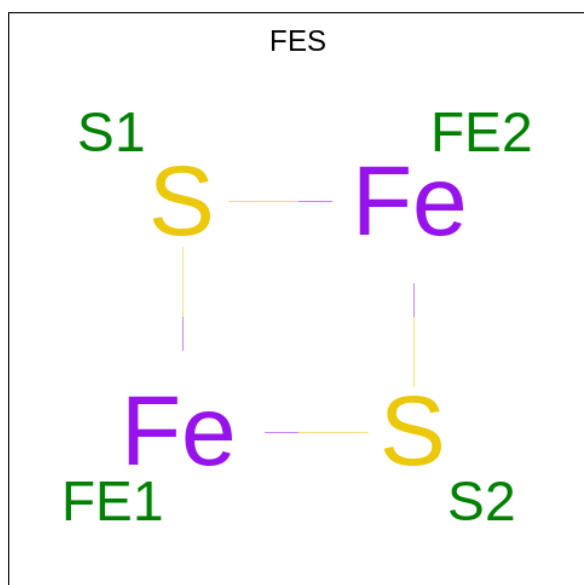
- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	k	1	Total	C	O	P	0
			100	81	17	2	
52	l	1	Total	C	O	P	0
			199	161	34	4	
52	l	1	Total	C	O	P	0
			199	161	34	4	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	r	1	Total	C	O	P	0
			100	81	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	
52	u	1	Total	C	O	P	0
			55	36	17	2	

- # NDP

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total 4	Fe 2	S 2	0
54	O	1	Total 4	Fe 2	S 2	0

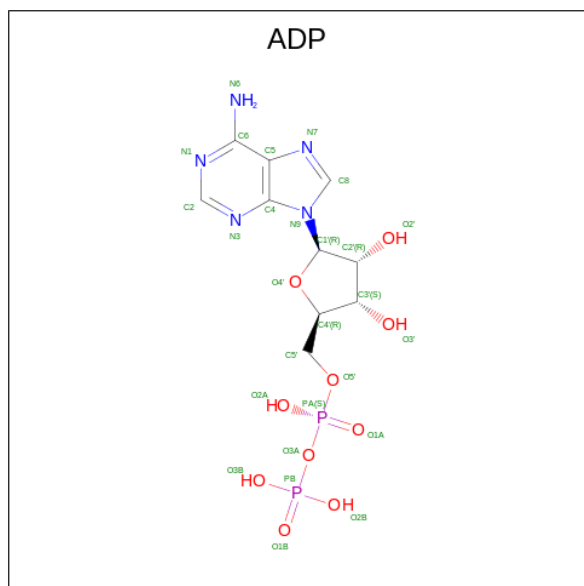
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
55	M	1	Total Mg 1 1	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
56	T	1	Total Zn 1 1	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

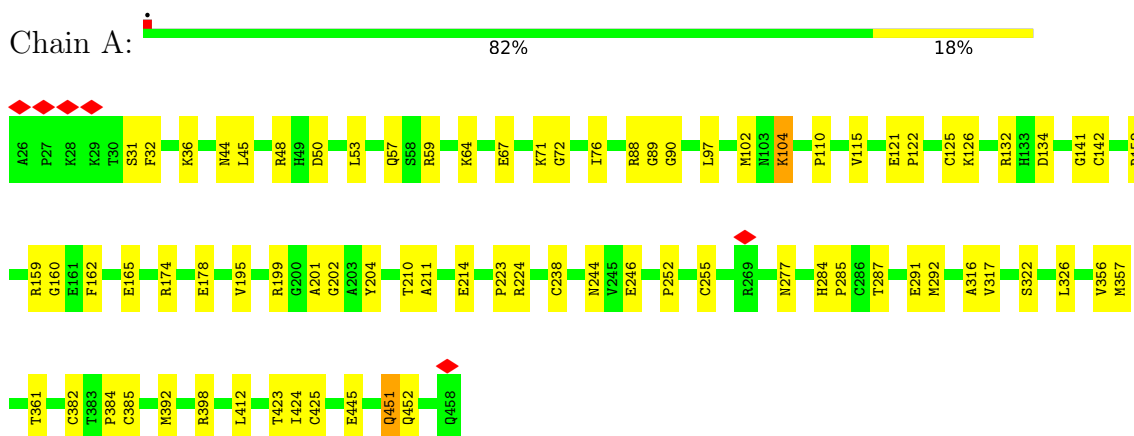


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total 27	C 10	N 5	O 10	P 2	0

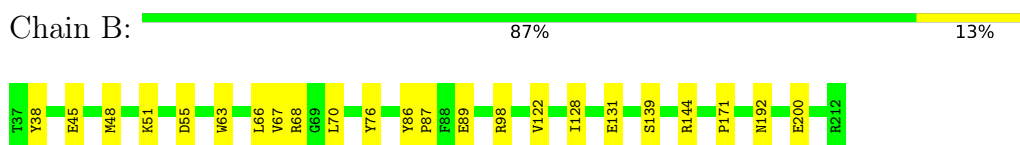
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

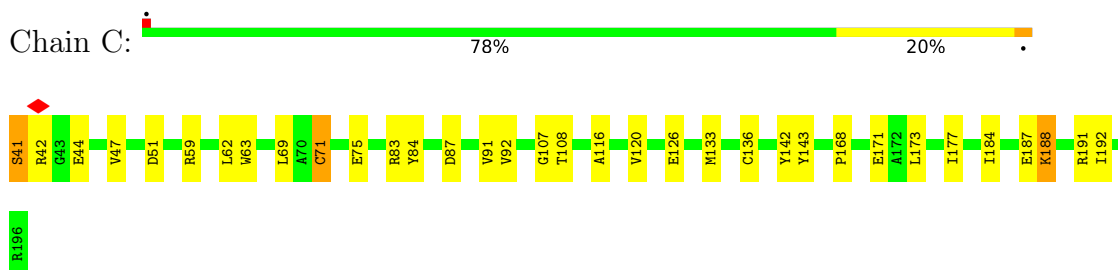
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



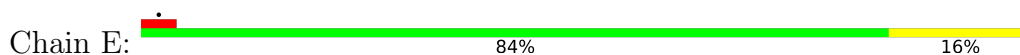
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

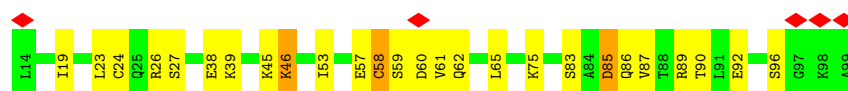


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

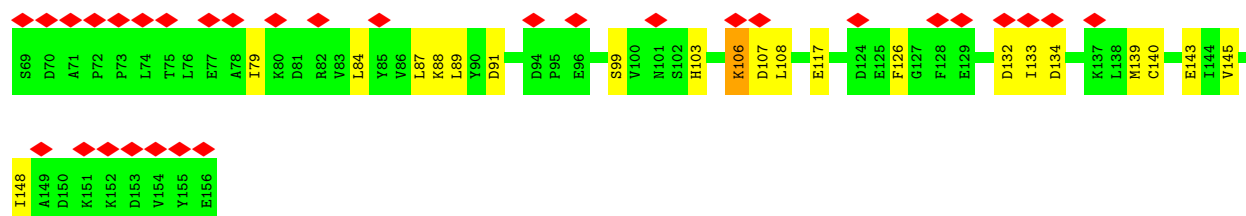
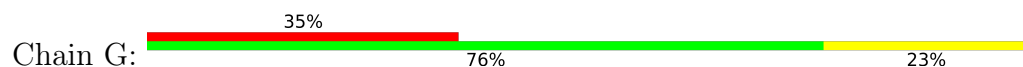




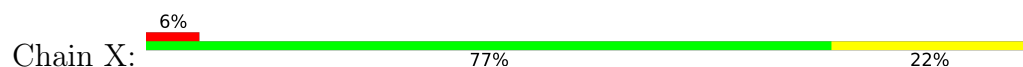
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



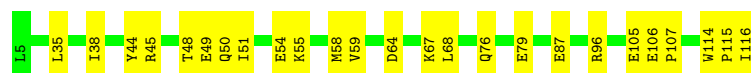
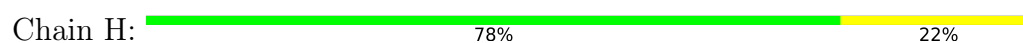
- Molecule 6: Acyl carrier protein



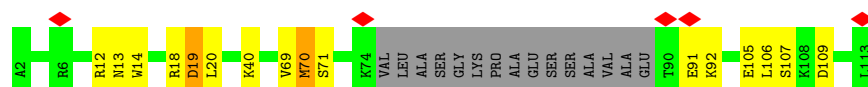
- Molecule 6: Acyl carrier protein



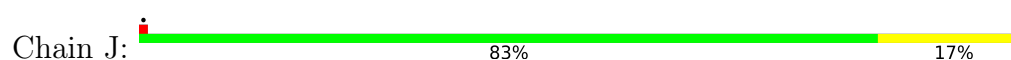
- Molecule 7: Complex I subunit B13

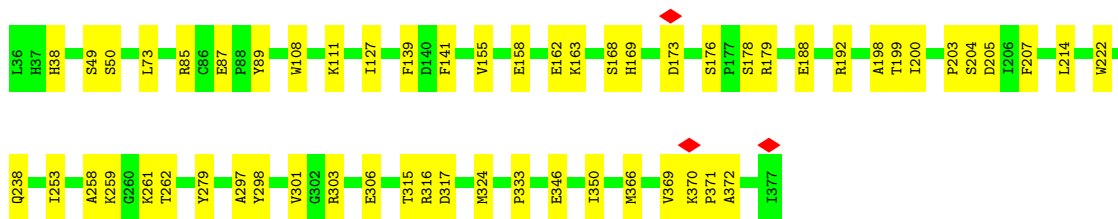


- Molecule 8: Complex I-B14.5a



- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

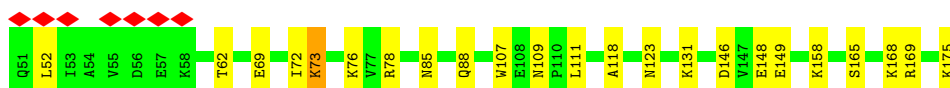
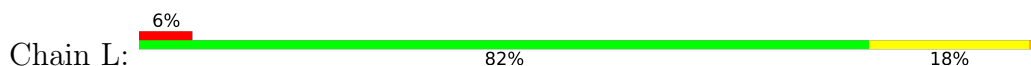




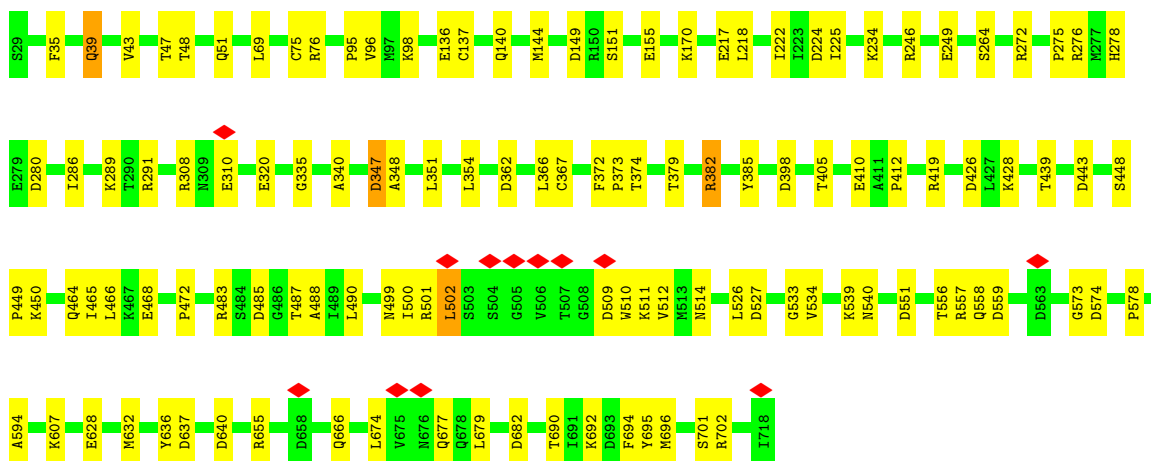
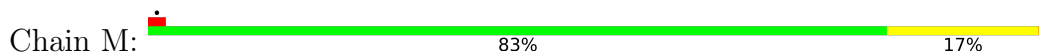
- Molecule 10: Complex I-9kD



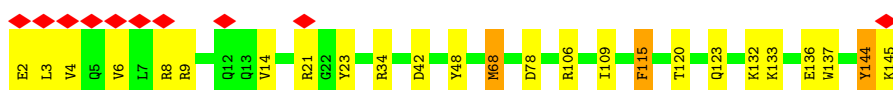
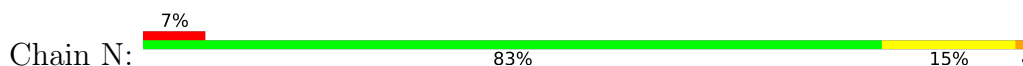
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial




- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

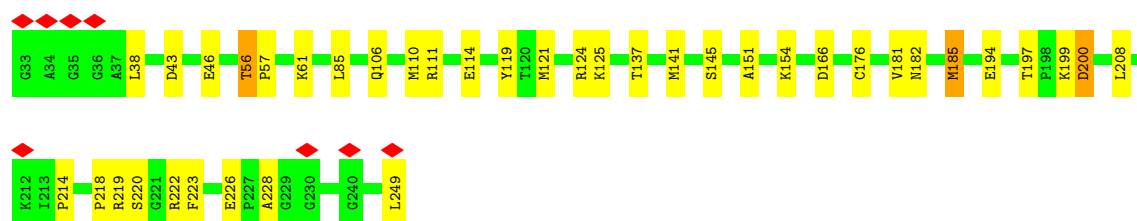


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12




- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:  82% 17%




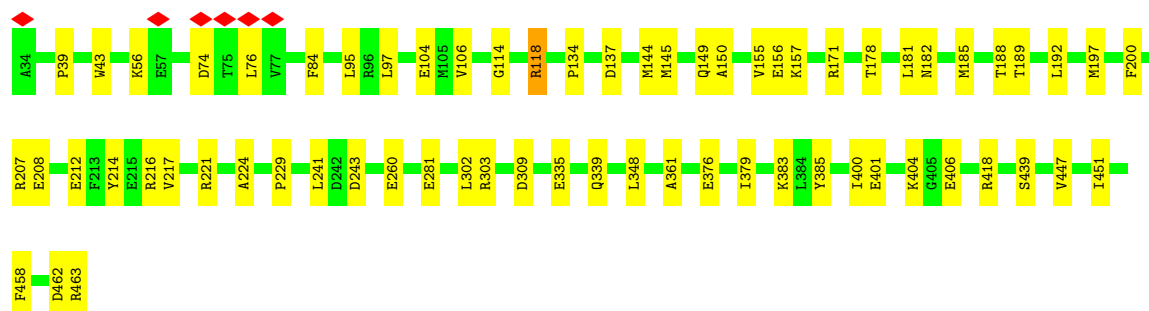
• Molecule 15: Complex I-30kD

Chain P:  86% 14%




• Molecule 16: Complex I-49kD

Chain Q:  85% 15%




• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  90% 10%




• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  88% 12%

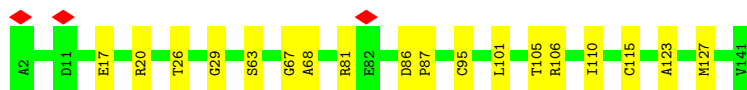
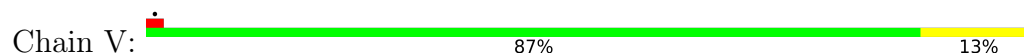


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

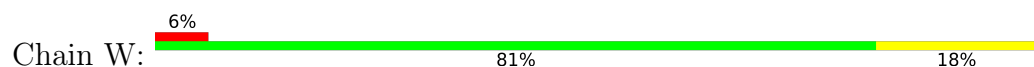
Chain U:  5% 88% 12%



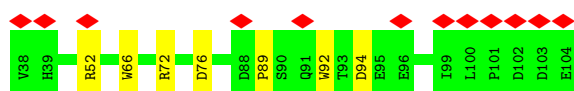
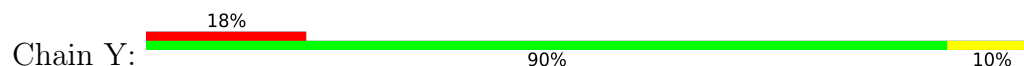
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



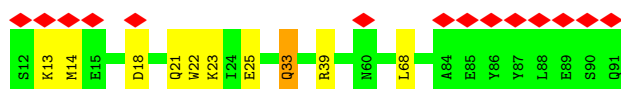
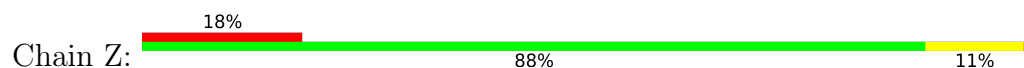
- Molecule 21: Complex I-B16.6



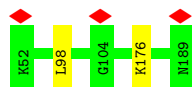
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



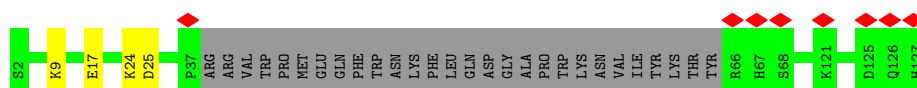
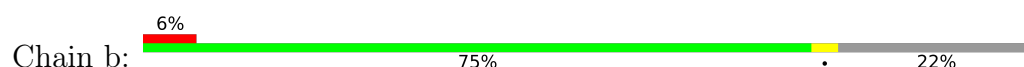
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



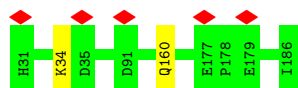
- Molecule 25: Complex I-B17





- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  99%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  98%



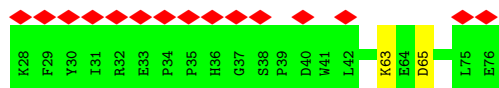
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  96%



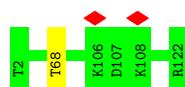
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  96%



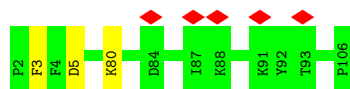
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  99%



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  97%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  98%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  96%



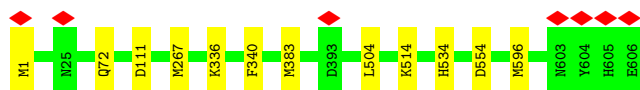
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  95%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  98%






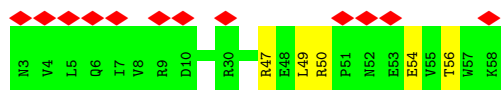
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  13%  97%



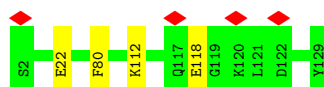
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  21%  91%  9%

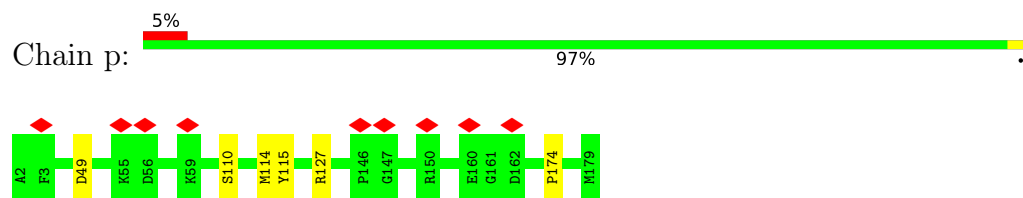


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

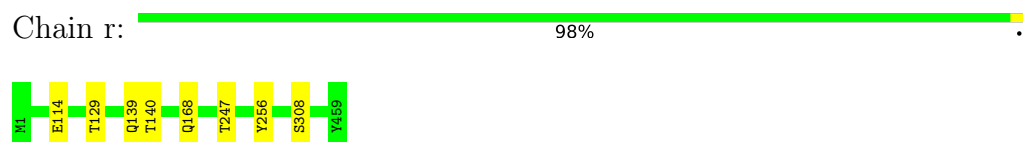
Chain o:  97%



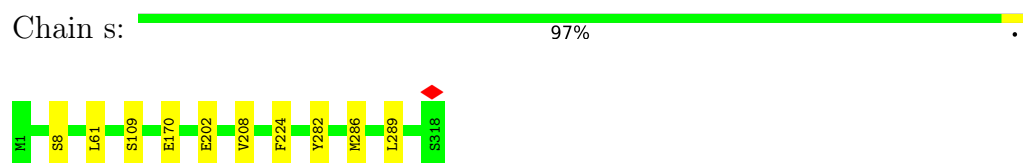
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



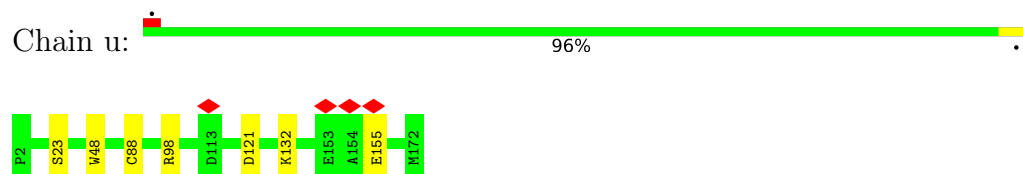
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



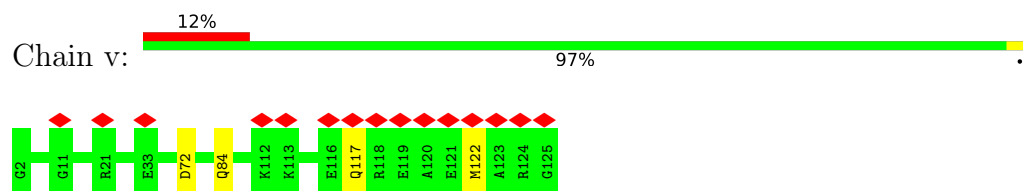
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



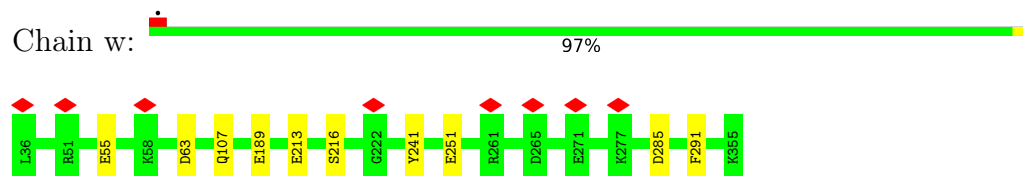
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.202	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0291	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLX, FES, PEE, NAI, ADP, MG, UQ, ZN, NDP, 8Q1, FMN, CDL, SF4, 2MR

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	0.28	0/3406	0.51	0/4603
2	B	0.34	0/1443	0.53	0/1952
3	C	0.34	0/1279	0.52	0/1730
4	E	0.28	0/991	0.51	0/1335
5	F	0.33	0/698	0.62	1/940 (0.1%)
6	G	0.29	0/702	0.51	0/952
6	X	0.28	0/716	0.46	0/968
7	H	0.28	0/929	0.47	0/1258
8	I	0.30	0/798	0.55	0/1079
9	J	0.29	0/2828	0.49	0/3834
10	K	0.28	0/377	0.49	0/509
11	L	0.29	0/1039	0.50	0/1403
12	M	0.29	0/5384	0.52	1/7295 (0.0%)
13	N	0.30	0/1245	0.51	0/1694
14	O	0.28	0/1711	0.48	0/2328
15	P	0.32	0/1789	0.52	0/2436
16	Q	0.32	0/3538	0.51	0/4796
17	S	0.29	0/581	0.53	0/781
18	T	0.31	0/755	0.54	0/1018
19	U	0.27	0/664	0.46	0/912
20	V	0.28	0/1042	0.47	0/1411
21	W	0.29	0/1198	0.50	0/1617
22	Y	0.27	0/610	0.45	0/836
23	Z	0.27	0/660	0.46	0/892
24	a	0.31	0/1184	0.50	0/1603
25	b	0.29	0/844	0.53	0/1149
26	c	0.31	0/1371	0.50	0/1875
27	d	0.28	0/1494	0.51	0/2015
28	e	0.28	0/891	0.50	0/1210
29	f	0.29	0/386	0.47	0/523
30	g	0.31	0/1031	0.48	0/1394
31	h	0.28	0/889	0.51	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.29	0/2773	0.48	0/3768
33	j	0.29	0/938	0.47	0/1281
34	k	0.29	0/759	0.46	0/1029
35	l	0.29	0/4929	0.46	0/6704
36	m	0.30	0/1328	0.45	0/1804
37	n	0.26	0/491	0.52	0/663
38	o	0.29	0/1092	0.50	0/1481
39	p	0.29	0/1586	0.49	0/2150
40	r	0.29	0/3723	0.48	0/5078
41	s	0.30	0/2581	0.47	0/3529
42	u	0.29	0/1436	0.52	0/1938
43	v	0.27	0/1083	0.54	0/1448
44	w	0.28	0/2642	0.48	0/3580
All	All	0.29	0/67834	0.50	2/91991 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	58	CYS	CA-CB-SG	7.09	126.77	114.00
12	M	502	LEU	CA-CB-CG	5.26	127.40	115.30

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	3330	0	3292	54	0
2	B	1412	0	1363	17	0
3	C	1248	0	1254	23	0
4	E	967	0	971	8	0
5	F	687	0	700	16	0
6	G	690	0	669	13	0
6	X	704	0	695	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	910	0	950	15	0
8	I	780	0	808	14	0
9	J	2751	0	2773	31	0
10	K	366	0	338	11	0
11	L	1016	0	1016	15	0
12	M	5296	0	5326	68	0
13	N	1204	0	1162	15	0
14	O	1671	0	1673	26	0
15	P	1738	0	1693	20	0
16	Q	3459	0	3396	38	0
17	S	566	0	561	5	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1021	0	1027	11	0
21	W	1167	0	1155	17	0
22	Y	584	0	529	4	0
23	Z	641	0	620	8	0
24	a	1151	0	1164	0	0
25	b	819	0	835	0	0
26	c	1315	0	1208	0	0
27	d	1461	0	1429	0	0
28	e	867	0	817	0	0
29	f	378	0	356	0	0
30	g	1000	0	994	0	0
31	h	867	0	873	0	0
32	i	2710	0	2874	0	0
33	j	914	0	951	0	0
34	k	748	0	799	0	0
35	l	4800	0	4939	0	0
36	m	1295	0	1263	0	0
37	n	479	0	486	0	0
38	o	1062	0	1072	0	0
39	p	1530	0	1466	0	0
40	r	3631	0	3839	0	0
41	s	2508	0	2607	0	0
42	u	1398	0	1374	0	0
43	v	1059	0	1029	0	0
44	w	2582	0	2531	0	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	A	31	0	19	3	0
47	A	44	0	27	6	0
48	B	51	0	82	4	0
48	C	47	0	71	2	0
48	V	40	0	54	3	0
48	W	41	0	59	1	0
48	i	47	0	71	0	0
48	j	92	0	141	0	0
48	l	97	0	151	0	0
48	r	51	0	82	0	0
49	C	52	0	88	4	0
49	J	52	0	88	2	0
49	a	52	0	88	0	0
49	g	52	0	88	0	0
49	j	52	0	88	0	0
49	r	104	0	176	0	0
50	C	38	0	47	5	0
50	J	33	0	39	6	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	I	51	0	46	1	0
52	V	94	0	138	3	0
52	a	100	0	156	0	0
52	k	100	0	156	0	0
52	l	199	0	307	0	0
52	o	100	0	156	0	0
52	r	100	0	156	0	0
52	s	89	0	125	0	0
52	u	55	0	54	0	0
53	J	48	0	24	1	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	T	1	0	0	0	0
57	w	27	0	11	0	0
All	All	68233	0	69009	419	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 7.

All (419) 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)
20:V:95:CYS:SG	20:V:115:CYS:SG	1.39	1.39
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.22
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.68	1.12
20:V:110:ILE:HD13	48:V:202:PEE:H49	1.51	0.90
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.66	0.77
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.64	0.77
4:E:16:SER:HA	11:L:52:LEU:HD13	1.70	0.74
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.20	0.74
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.20	0.74
11:L:109:ASN:ND2	11:L:111:LEU:O	2.22	0.72
20:V:110:ILE:CD1	48:V:202:PEE:H49	2.19	0.72
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.70	0.71
1:A:50:ASP:O	1:A:59:ARG:NH2	2.23	0.71
8:I:40:LYS:HB3	21:W:7:LYS:H	1.56	0.70
6:G:143:GLU:OE2	6:G:143:GLU:N	2.17	0.69
2:B:45:GLU:OE2	2:B:45:GLU:N	2.20	0.69
9:J:192:ARG:NH1	9:J:198:ALA:O	2.25	0.68
6:G:117:GLU:OE1	6:G:117:GLU:N	4.99	0.68
9:J:222:TRP:HB3	50:J:402:UQ:H152	1.74	0.68
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.75	0.68
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.74	0.67
7:H:54:GLU:O	7:H:58:MET:HG3	1.95	0.67
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.76	0.67
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.27	0.67
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.27	0.66
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.26	0.66
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.76	0.66
11:L:78:ARG:NH2	12:M:249:GLU:OE2	2.22	0.66
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.28	0.66
48:C:302:PEE:H67	49:C:303:PLX:H212	1.77	0.65
9:J:258:ALA:HA	9:J:261:LYS:HD2	1.77	0.65
6:X:140:CYS:HB2	6:X:143:GLU:HG3	1.79	0.65
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.36	0.65
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.30	0.65
8:I:105:GLU:OE2	8:I:105:GLU:HA	1.95	0.65
1:A:357:MET:HB3	1:A:361:THR:HG21	1.80	0.64
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.79	0.64
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.29	0.64
3:C:71:CYS:HB2	45:C:301:SF4:S4	2.39	0.63
12:M:696:MET:HG2	12:M:702:ARG:HA	1.81	0.63
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.78	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.31	0.62
6:G:103:HIS:HB3	6:G:106:LYS:HG3	1.81	0.62
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.81	0.62
21:W:143:TYR:O	48:W:201:PEE:N	2.31	0.62
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.31	0.62
12:M:308:ARG:NH2	12:M:578:PRO:O	2.32	0.62
1:A:48:ARG:NH1	10:K:70:ASN:O	2.32	0.62
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.81	0.62
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.29	0.62
1:A:285:PRO:O	14:O:222:ARG:NH2	2.33	0.61
3:C:75:GLU:OE2	16:Q:221:ARG:NH1	2.33	0.61
14:O:151:ALA:HA	14:O:154:LYS:HE3	1.81	0.61
9:J:163:LYS:HG2	9:J:259:LYS:HE2	1.82	0.61
3:C:133:MET:HG2	3:C:168:PRO:HG2	1.83	0.61
12:M:488:ALA:HB1	12:M:679:LEU:HD12	1.81	0.61
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.83	0.61
8:I:106:LEU:O	8:I:106:LEU:HG	2.02	0.60
13:N:4:VAL:O	13:N:8:ARG:HG3	2.02	0.59
9:J:178:SER:OG	9:J:317:ASP:OD2	2.20	0.59
5:F:57:GLU:O	12:M:655:ARG:NH2	2.35	0.59
12:M:472:PRO:O	12:M:510:TRP:NE1	2.33	0.59
9:J:163:LYS:NZ	9:J:253:ILE:O	2.25	0.59
21:W:56:GLU:OE1	21:W:59:ARG:NH2	2.31	0.59
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.39	0.58
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.36	0.58
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.84	0.58
3:C:59:ARG:NH2	49:C:303:PLX:O3	2.31	0.58
12:M:379:THR:HG21	12:M:526:LEU:HD22	1.84	0.58
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.36	0.58
1:A:89:GLY:O	47:A:503:NAI:H2N	2.03	0.58
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.39	0.58
10:K:69:ASP:OD1	10:K:70:ASN:N	2.36	0.58
16:Q:185:MET:O	16:Q:189:THR:OG1	2.20	0.58
2:B:131:GLU:OE2	2:B:144:ARG:NE	2.36	0.58
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.33	0.57
5:F:23:LEU:HD23	5:F:23:LEU:H	1.69	0.57
9:J:168:SER:O	9:J:203:PRO:HD2	2.04	0.57
7:H:50:GLN:O	7:H:54:GLU:HG3	2.02	0.57
14:O:38:LEU:O	14:O:124:ARG:NH2	2.38	0.57
7:H:44:TYR:O	7:H:48:THR:HG22	2.05	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:140:CYS:HB2	6:G:143:GLU:OE2	2.05	0.56
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.38	0.56
1:A:122:PRO:HG2	1:A:322:SER:HB3	1.88	0.56
1:A:392:MET:HG2	1:A:412:LEU:HD11	1.87	0.56
11:L:131:LYS:NZ	11:L:149:GLU:OE1	2.38	0.56
2:B:38:TYR:O	8:I:107:SER:HB2	2.04	0.56
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.88	0.56
16:Q:447:VAL:O	16:Q:451:ILE:HG13	2.05	0.56
10:K:109:ARG:NH2	14:O:106:GLN:O	2.38	0.56
16:Q:114:GLY:N	16:Q:462:ASP:OD1	2.38	0.55
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.86	0.55
6:X:93:ILE:HG21	6:X:98:LEU:HD13	1.88	0.55
8:I:18:ARG:NH2	16:Q:260:GLU:OE2	2.35	0.55
1:A:64:LYS:HD3	14:O:249:LEU:HD23	1.89	0.55
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.72	0.55
1:A:32:PHE:HB3	1:A:291:GLU:HG2	1.88	0.54
3:C:41:SER:OG	3:C:42:ARG:N	2.40	0.54
1:A:36:LYS:H	1:A:36:LYS:HD2	1.73	0.54
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.47	0.54
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.41	0.54
1:A:445:GLU:OE2	1:A:445:GLU:N	2.39	0.54
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.39	0.54
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.89	0.54
3:C:116:ALA:O	3:C:120:VAL:HG22	2.08	0.54
5:F:89:ARG:HA	5:F:89:ARG:NE	2.22	0.54
6:G:79:ILE:HG22	6:G:145:VAL:HG22	1.88	0.54
48:C:302:PEE:H36	48:C:302:PEE:H71	1.90	0.54
5:F:46:LYS:HE3	12:M:674:LEU:HD21	1.89	0.54
49:J:403:PLX:O4	49:J:403:PLX:O9	2.26	0.54
6:X:103:HIS:CE1	6:X:106:LYS:HE2	2.43	0.54
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.89	0.54
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.90	0.54
18:T:64:GLU:H	18:T:64:GLU:CD	2.11	0.54
8:I:14:TRP:O	21:W:28:ARG:NH2	2.41	0.54
12:M:419:ARG:NH1	12:M:439:THR:O	2.41	0.54
12:M:428:LYS:HE2	12:M:465:ILE:HD13	1.90	0.54
15:P:201:ASP:OD1	15:P:201:ASP:N	2.40	0.54
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.53
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.43	0.53
48:V:202:PEE:H58	48:V:202:PEE:H19	1.90	0.53
4:E:35:LEU:HD13	4:E:87:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.39	0.53
13:N:120:THR:O	13:N:123:GLN:HG2	2.09	0.53
18:T:69:ASP:O	18:T:73:GLU:HG3	2.08	0.53
1:A:88:ARG:HG3	1:A:246:GLU:HG2	1.91	0.53
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.90	0.53
9:J:50:SER:OG	15:P:225:GLU:OE2	2.26	0.52
9:J:199:THR:OG1	9:J:258:ALA:O	2.25	0.52
16:Q:281:GLU:CD	16:Q:281:GLU:H	2.13	0.52
3:C:41:SER:N	3:C:44:GLU:OE2	2.43	0.52
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.43	0.52
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.44	0.52
5:F:86:GLN:O	5:F:90:THR:HG22	2.09	0.52
11:L:78:ARG:NE	11:L:148:GLU:OE2	2.32	0.52
2:B:38:TYR:CE2	8:I:106:LEU:HD13	2.45	0.52
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.91	0.52
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.92	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.91	0.52
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.10	0.51
1:A:44:ASN:HB3	1:A:134:ASP:OD1	2.09	0.51
5:F:61:VAL:HG22	5:F:62:GLN:HB2	1.92	0.51
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.45	0.51
17:S:69:ILE:HG22	17:S:69:ILE:O	2.09	0.51
19:U:27:GLY:O	19:U:31:ILE:HG23	2.10	0.51
12:M:249:GLU:HG2	12:M:276:ARG:HD3	1.93	0.51
7:H:48:THR:HA	7:H:51:ILE:HG12	1.93	0.51
1:A:284:HIS:HB3	14:O:228:ALA:H	1.76	0.51
48:B:303:PEE:H38	19:U:25:ILE:HG12	1.94	0.50
12:M:695:TYR:O	12:M:701:SER:OG	2.29	0.50
11:L:85:ASN:HD21	12:M:136:GLU:HG2	1.76	0.50
6:X:115:GLN:NE2	6:X:138:LEU:O	2.44	0.50
3:C:84:TYR:CE1	3:C:171:GLU:HG3	2.47	0.50
3:C:184:ILE:O	3:C:187:GLU:HG2	2.12	0.50
12:M:264:SER:OG	12:M:272:ARG:HG2	2.12	0.50
13:N:144:TYR:CZ	13:N:145:LYS:HD3	2.47	0.50
19:U:26:GLY:O	19:U:30:ILE:HD12	2.11	0.50
21:W:93:GLU:O	21:W:97:ILE:HG13	2.12	0.50
1:A:174:ARG:O	1:A:178:GLU:HG2	2.12	0.49
3:C:63:TRP:CD1	3:C:92:VAL:HG22	2.47	0.49
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.94	0.49
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.94	0.49
5:F:92:GLU:O	5:F:96:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:428:LYS:NZ	12:M:443:ASP:OD1	2.46	0.49
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.94	0.49
9:J:262:THR:O	9:J:333:PRO:HD2	2.12	0.49
10:K:87:LEU:HD12	14:O:85:LEU:HD13	1.94	0.49
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.51	0.49
9:J:87:GLU:HG3	9:J:89:TYR:H	1.77	0.49
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.93	0.49
14:O:185:MET:HB3	14:O:194:GLU:HA	1.93	0.49
12:M:449:PRO:HB2	12:M:679:LEU:HD23	1.95	0.48
21:W:48:TRP:O	21:W:52:LYS:HG2	2.13	0.48
52:I:201:CDL:H511	52:I:201:CDL:H542	1.67	0.48
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.96	0.48
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.95	0.48
9:J:297:ALA:O	9:J:301:VAL:HG13	2.13	0.48
13:N:136:GLU:OE2	13:N:136:GLU:N	2.44	0.48
20:V:67:GLY:HA2	52:V:201:CDL:H221	1.94	0.48
1:A:160:GLY:O	1:A:199:ARG:NH2	2.47	0.48
5:F:26:ARG:HH11	5:F:26:ARG:HB2	1.78	0.48
1:A:316:ALA:HB1	1:A:326:LEU:HD12	1.96	0.48
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.96	0.48
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.93	0.48
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.96	0.48
15:P:127:GLU:OE1	15:P:144:LYS:HE3	2.13	0.48
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.95	0.48
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.96	0.48
10:K:77:GLN:OE1	10:K:77:GLN:N	2.47	0.48
9:J:204:SER:OG	9:J:238:GLN:O	2.32	0.48
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.29	0.48
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.96	0.47
3:C:87:ASP:OD1	3:C:92:VAL:HG12	2.13	0.47
7:H:59:VAL:HG22	7:H:68:LEU:HD21	1.95	0.47
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.96	0.47
5:F:85:ASP:OD1	5:F:85:ASP:N	2.47	0.47
3:C:173:LEU:O	3:C:177:ILE:HG12	2.15	0.47
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.47	0.47
23:Z:25:GLU:OE2	23:Z:25:GLU:N	2.37	0.47
8:I:69:VAL:O	15:P:76:VAL:HB	2.14	0.47
12:M:335:GLY:HA2	12:M:362:ASP:O	2.13	0.47
14:O:56:THR:HG22	14:O:57:PRO:HD2	1.97	0.47
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.95	0.47
12:M:509:ASP:OD1	12:M:509:ASP:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:47:ASP:O	18:T:52:ARG:NH1	2.48	0.47
12:M:499:ASN:HA	12:M:502:LEU:HG	1.96	0.47
20:V:29:GLY:O	20:V:63:SER:HB3	2.15	0.47
6:X:96:GLU:H	6:X:96:GLU:CD	2.19	0.47
3:C:62:LEU:O	3:C:91:VAL:HA	2.15	0.46
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.96	0.46
50:J:402:UQ:H202	50:J:402:UQ:H172	1.81	0.46
18:T:79:VAL:O	18:T:121:PRO:HD3	2.15	0.46
6:X:114:ASP:O	6:X:118:ILE:HD12	2.15	0.46
13:N:6:VAL:HG12	13:N:9:ARG:HH12	1.79	0.46
14:O:197:THR:OG1	14:O:200:ASP:OD2	2.32	0.46
21:W:90:ASN:ND2	21:W:123:GLU:O	2.48	0.46
1:A:72:GLY:O	1:A:76:ILE:HG13	2.16	0.46
7:H:64:ASP:HB3	7:H:67:LYS:HB2	1.97	0.46
20:V:123:ALA:O	20:V:127:MET:HG3	2.16	0.46
9:J:141:PHE:HB2	9:J:179:ARG:HE	1.81	0.46
14:O:199:LYS:HE2	14:O:199:LYS:HB3	1.80	0.46
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.98	0.46
1:A:104:LYS:HD3	1:A:104:LYS:N	2.30	0.46
1:A:210:THR:HB	1:A:224:ARG:H	1.81	0.46
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.41	0.46
1:A:125:CYS:H	1:A:277:ASN:ND2	2.14	0.46
8:I:70:MET:O	8:I:70:MET:SD	2.74	0.46
12:M:573:GLY:HA3	13:N:137:TRP:CG	2.51	0.46
11:L:168:LYS:HA	11:L:168:LYS:HD3	1.66	0.46
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.98	0.46
14:O:200:ASP:OD2	14:O:200:ASP:N	2.49	0.46
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.98	0.46
6:X:79:ILE:O	6:X:83:VAL:HG23	2.16	0.46
48:B:303:PEE:H58	48:B:303:PEE:H64	1.66	0.45
12:M:464:GLN:O	12:M:468:GLU:HG2	2.15	0.45
14:O:220:SER:O	14:O:220:SER:OG	2.31	0.45
1:A:67:GLU:O	1:A:71:LYS:HG2	2.17	0.45
1:A:122:PRO:HA	14:O:176:CYS:SG	2.56	0.45
1:A:152:ARG:NH2	10:K:99:PRO:O	2.49	0.45
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.98	0.45
19:U:47:ARG:HE	19:U:47:ARG:HA	4.77	0.45
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.98	0.45
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	1.97	0.45
23:Z:18:ASP:O	23:Z:21:GLN:HG2	2.17	0.45
1:A:110:PRO:O	1:A:238:CYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:H	1:A:326:LEU:HD23	1.81	0.45
9:J:303:ARG:HB2	9:J:316:ARG:HD3	1.98	0.45
16:Q:241:LEU:HD22	16:Q:348:LEU:HD23	1.99	0.45
23:Z:33:GLN:CA	23:Z:33:GLN:HE21	2.30	0.45
3:C:44:GLU:HA	3:C:47:VAL:HG22	1.98	0.45
3:C:92:VAL:HG21	50:C:304:UQ:H103	1.97	0.45
13:N:3:LEU:O	13:N:6:VAL:HG22	2.16	0.45
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.97	0.45
12:M:48:THR:HA	12:M:95:PRO:HA	1.99	0.45
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.81	0.45
4:E:120:SER:O	4:E:124:VAL:HG13	2.16	0.45
12:M:170:LYS:HB2	12:M:234:LYS:HG3	1.99	0.45
2:B:128:ILE:O	15:P:231:ARG:NH2	2.50	0.45
21:W:120:MET:O	21:W:120:MET:HG2	2.16	0.45
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.46	0.45
8:I:13:ASN:ND2	8:I:19:ASP:HA	2.32	0.44
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.99	0.44
16:Q:335:GLU:OE2	16:Q:339:GLN:NE2	2.40	0.44
52:V:201:CDL:H512	52:V:201:CDL:H542	1.69	0.44
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.97	0.44
19:U:53:TYR:HB2	21:W:72:MET:SD	2.58	0.44
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.26	0.44
14:O:125:LYS:HE3	14:O:125:LYS:HB2	1.60	0.44
18:T:51:ARG:HG2	18:T:54:ARG:HH21	1.82	0.44
50:J:402:UQ:H103	50:J:402:UQ:H121	1.86	0.44
21:W:105:LYS:HD2	21:W:105:LYS:HA	1.80	0.44
12:M:320:GLU:OE1	12:M:320:GLU:N	2.46	0.44
22:Y:72:ARG:NE	22:Y:76:ASP:OD2	2.41	0.44
50:J:402:UQ:H71	50:J:402:UQ:HM51	1.68	0.44
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.48	0.44
19:U:40:ASN:O	19:U:44:ARG:HG3	2.18	0.44
21:W:99:LYS:HE2	21:W:99:LYS:HB3	1.65	0.44
49:C:303:PLX:H102	49:C:303:PLX:H261	2.00	0.44
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.21	0.44
22:Y:52:ARG:HD2	22:Y:52:ARG:HA	1.81	0.44
1:A:195:VAL:O	10:K:97:ARG:NH1	2.49	0.44
4:E:62:LYS:O	4:E:66:MET:HG2	2.17	0.44
50:J:402:UQ:H201	50:J:402:UQ:H221	1.66	0.44
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.53	0.44
6:G:89:LEU:HD12	6:G:89:LEU:HA	1.76	0.43
11:L:107:TRP:HH2	11:L:118:ALA:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:289:LYS:HE2	12:M:694:PHE:O	2.18	0.43
14:O:46:GLU:OE1	14:O:46:GLU:N	2.51	0.43
13:N:68:MET:HB3	13:N:115:PHE:HE2	1.83	0.43
2:B:63:TRP:O	2:B:67:VAL:HG23	2.18	0.43
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.18	0.43
5:F:59:SER:OG	5:F:60:ASP:N	2.51	0.43
12:M:487:THR:HB	12:M:677:GLN:OE1	2.18	0.43
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.00	0.43
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.35	0.43
12:M:556:THR:OG1	12:M:557:ARG:N	2.52	0.43
21:W:57:ARG:HA	21:W:60:LEU:HD12	2.00	0.43
6:G:87:LEU:HD23	6:G:87:LEU:HA	2.28	0.43
9:J:155:VAL:HA	9:J:158:GLU:HG2	1.98	0.43
16:Q:192:LEU:HD12	16:Q:197:MET:HA	2.00	0.43
20:V:101:LEU:O	20:V:105:THR:HG23	2.18	0.43
12:M:367:CYS:HB3	12:M:533:GLY:O	2.17	0.43
19:U:47:ARG:HA	19:U:47:ARG:NE	4.46	0.43
3:C:84:TYR:HE1	3:C:171:GLU:HG3	1.82	0.43
5:F:83:SER:O	5:F:87:VAL:HG13	2.19	0.43
7:H:96:ARG:HH11	7:H:96:ARG:HB3	1.84	0.43
9:J:204:SER:OG	9:J:204:SER:O	2.37	0.43
23:Z:33:GLN:HE21	23:Z:33:GLN:C	2.22	0.43
2:B:70:LEU:HD11	48:B:303:PEE:H65	2.01	0.43
8:I:109:ASP:OD2	21:W:21:TYR:OH	2.37	0.43
9:J:73:LEU:HD23	9:J:73:LEU:HA	2.07	0.43
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.85	0.43
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.29	0.43
7:H:76:GLN:O	7:H:79:GLU:N	2.41	0.43
9:J:168:SER:OG	9:J:169:HIS:N	2.51	0.43
12:M:382:ARG:NH1	12:M:527:ASP:OD2	2.52	0.43
1:A:45:LEU:HD21	1:A:287:THR:HG22	2.01	0.42
6:G:139:MET:HA	6:G:139:MET:HE3	2.01	0.42
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.48	0.42
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.75	0.42
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.70	0.42
2:B:38:TYR:CZ	8:I:106:LEU:HD13	2.54	0.42
12:M:151:SER:HB2	16:Q:376:GLU:OE1	2.19	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.00	0.42
16:Q:134:PRO:HA	16:Q:137:ASP:HB2	2.00	0.42
16:Q:439:SER:HB2	16:Q:447:VAL:HG22	2.01	0.42
6:X:84:LEU:HD23	6:X:84:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.42
9:J:173:ASP:OD1	9:J:176:SER:HB3	2.19	0.42
12:M:348:ALA:HA	12:M:351:LEU:HD12	2.02	0.42
12:M:556:THR:HG23	12:M:558:GLN:H	1.84	0.42
3:C:143:TYR:CD1	16:Q:118:2MR:HB2	2.54	0.42
12:M:539:LYS:HG2	12:M:540:ASN:CG	2.39	0.42
6:X:141:PRO:O	6:X:145:VAL:HG13	2.20	0.42
14:O:208:LEU:HD13	14:O:214:PRO:HD2	2.00	0.42
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.55	0.42
50:J:402:UQ:H151	50:J:402:UQ:H171	1.82	0.42
12:M:43:VAL:HG21	12:M:96:VAL:HG21	2.02	0.42
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.55	0.42
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.59	0.42
50:C:304:UQ:H262	50:C:304:UQ:H221	1.63	0.42
8:I:12:ARG:HB3	8:I:20:LEU:HD12	2.02	0.42
11:L:73:LYS:HD2	11:L:73:LYS:HA	1.84	0.42
12:M:372:PHE:CZ	12:M:385:TYR:HB3	2.55	0.42
12:M:485:ASP:HA	12:M:677:GLN:HE22	1.85	0.42
13:N:78:ASP:OD1	13:N:78:ASP:N	2.52	0.42
50:C:304:UQ:H72	50:C:304:UQ:HM51	1.70	0.42
49:J:403:PLX:H111	49:J:403:PLX:H82	1.77	0.42
21:W:52:LYS:HB3	21:W:52:LYS:HE2	2.25	0.42
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.86	0.41
12:M:340:ALA:HB3	12:M:366:LEU:HD23	2.02	0.41
12:M:690:THR:HG22	12:M:692:LYS:HG2	2.01	0.41
23:Z:23:LYS:HB3	23:Z:25:GLU:OE2	2.19	0.41
7:H:38:ILE:O	7:H:45:ARG:NH1	2.46	0.41
9:J:111:LYS:HE3	9:J:139:PHE:CE2	2.55	0.41
9:J:207:PHE:HB2	9:J:214:LEU:HG	2.02	0.41
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.53	0.41
1:A:201:ALA:C	14:O:121:MET:HG3	2.40	0.41
1:A:211:ALA:HB2	1:A:223:PRO:HG3	2.01	0.41
1:A:317:VAL:HG22	1:A:356:VAL:HG22	2.02	0.41
5:F:39:LYS:HA	5:F:39:LYS:HD2	1.77	0.41
7:H:35:LEU:HD13	7:H:49:GLU:HG3	2.02	0.41
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.56	0.41
1:A:53:LEU:O	1:A:57:GLN:HG3	2.21	0.41
1:A:382:CYS:HB3	1:A:424:ILE:HD12	2.01	0.41
6:G:103:HIS:O	6:G:108:LEU:HD12	2.20	0.41
10:K:105:ARG:HH22	12:M:426:ASP:CG	2.23	0.41
12:M:35:PHE:HA	12:M:39:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.36	0.41
49:C:303:PLX:H222	49:C:303:PLX:H192	1.84	0.41
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.37	0.41
48:B:303:PEE:H43	48:B:303:PEE:H37	1.79	0.41
15:P:126:PHE:HE2	15:P:149:GLU:HG3	1.86	0.41
20:V:26:THR:HB	20:V:68:ALA:HB2	2.03	0.41
20:V:86:ASP:HA	20:V:87:PRO:HD3	1.94	0.41
3:C:188:LYS:O	3:C:192:ILE:HD12	2.21	0.41
5:F:19:ILE:HD11	5:F:53:ILE:HG12	2.02	0.41
9:J:369:VAL:HG12	9:J:369:VAL:O	2.21	0.41
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.56	0.41
14:O:61:LYS:HA	14:O:61:LYS:HD3	1.76	0.41
1:A:126:LYS:HG2	1:A:277:ASN:HD21	1.84	0.41
1:A:202:GLY:N	14:O:121:MET:HG3	2.36	0.41
1:A:451:GLN:HG3	1:A:452:GLN:N	2.36	0.41
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.02	0.41
12:M:354:LEU:HD12	12:M:354:LEU:HA	1.90	0.41
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.54	0.41
17:S:4:GLU:O	17:S:7:PRO:HD2	2.21	0.41
20:V:106:ARG:HG3	20:V:106:ARG:HH11	1.85	0.41
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.61	0.41
2:B:51:LYS:HE2	2:B:51:LYS:HB2	1.88	0.41
50:C:304:UQ:H202	50:C:304:UQ:H172	1.72	0.41
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.36	0.41
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.03	0.41
6:X:80:LYS:HE2	6:X:80:LYS:HB3	1.78	0.41
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.56	0.41
50:C:304:UQ:H102	50:C:304:UQ:H122	1.81	0.40
3:C:108:THR:HA	3:C:136:CYS:HB3	2.03	0.40
6:G:84:LEU:HD12	6:G:84:LEU:HA	1.82	0.40
12:M:373:PRO:HG2	12:M:490:LEU:HD22	2.03	0.40
1:A:159:ARG:NH2	14:O:176:CYS:O	2.45	0.40
1:A:201:ALA:O	14:O:119:TYR:HB3	2.21	0.40
9:J:350:ILE:HG21	9:J:366:MET:HG3	2.03	0.40
16:Q:157:LYS:HE3	16:Q:157:LYS:HB2	1.88	0.40
52:V:201:CDL:H342	52:V:201:CDL:H371	1.54	0.40
21:W:103:ASP:OD1	21:W:103:ASP:N	2.53	0.40
6:G:84:LEU:O	6:G:88:LYS:HE3	2.22	0.40
7:H:87:GLU:OE1	15:P:104:THR:OG1	2.28	0.40
8:I:91:GLU:CD	8:I:91:GLU:H	2.24	0.40
11:L:158:LYS:NZ	12:M:69:LEU:O	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:512:VAL:O	12:M:514:ASN:ND2	2.54	0.40
12:M:551:ASP:OD2	12:M:574:ASP:HB3	2.22	0.40
13:N:2:GLU:HG2	13:N:3:LEU:H	1.86	0.40
17:S:27:HIS:CE1	17:S:36:LYS:HD3	2.57	0.40
22:Y:66:TRP:CZ2	23:Z:68:LEU:HD23	2.56	0.40
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.70	0.40
11:L:165:SER:OG	11:L:168:LYS:HB2	2.22	0.40
12:M:448:SER:OG	12:M:450:LYS:HG3	2.22	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	431/433 (100%)	420 (97%)	11 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
6	G	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	13	39
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	325 (96%)	14 (4%)	1 (0%)	41	72
10	K	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
17	S	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	143 (93%)	11 (7%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
33	j	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	17	46
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
36	m	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	25	56
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	25	56
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	41	72
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/124 (98%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	w	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
All	All	8174/8312 (98%)	7861 (96%)	307 (4%)	6 (0%)	54	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
9	J	38	HIS
41	s	208	VAL
36	m	25	SER
39	p	174	PRO
33	j	40	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	339 (98%)	7 (2%)	55	84
2	B	151/151 (100%)	146 (97%)	5 (3%)	38	72
3	C	132/132 (100%)	126 (96%)	6 (4%)	27	60
4	E	106/107 (99%)	101 (95%)	5 (5%)	26	59
5	F	75/76 (99%)	69 (92%)	6 (8%)	12	34
6	G	75/81 (93%)	69 (92%)	6 (8%)	12	34
6	X	79/81 (98%)	76 (96%)	3 (4%)	33	67
7	H	99/99 (100%)	98 (99%)	1 (1%)	76	93
8	I	87/97 (90%)	83 (95%)	4 (5%)	27	60
9	J	296/296 (100%)	289 (98%)	7 (2%)	49	81
10	K	42/42 (100%)	40 (95%)	2 (5%)	25	58
11	L	113/113 (100%)	107 (95%)	6 (5%)	22	54
12	M	580/580 (100%)	561 (97%)	19 (3%)	38	72
13	N	130/130 (100%)	125 (96%)	5 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	183/183 (100%)	172 (94%)	11 (6%)	19	48
15	P	190/190 (100%)	187 (98%)	3 (2%)	62	88
16	Q	370/370 (100%)	362 (98%)	8 (2%)	52	83
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	69	91
19	U	69/69 (100%)	68 (99%)	1 (1%)	67	90
20	V	101/101 (100%)	100 (99%)	1 (1%)	76	93
21	W	122/123 (99%)	116 (95%)	6 (5%)	25	57
22	Y	62/62 (100%)	61 (98%)	1 (2%)	62	88
23	Z	62/62 (100%)	59 (95%)	3 (5%)	25	58
24	a	121/121 (100%)	119 (98%)	2 (2%)	60	87
25	b	90/119 (76%)	86 (96%)	4 (4%)	28	61
26	c	141/141 (100%)	139 (99%)	2 (1%)	67	90
27	d	155/155 (100%)	151 (97%)	4 (3%)	46	79
28	e	96/96 (100%)	92 (96%)	4 (4%)	30	63
29	f	36/45 (80%)	34 (94%)	2 (6%)	21	51
30	g	108/108 (100%)	107 (99%)	1 (1%)	78	94
31	h	93/93 (100%)	90 (97%)	3 (3%)	39	73
32	i	311/311 (100%)	304 (98%)	7 (2%)	50	82
33	j	100/100 (100%)	96 (96%)	4 (4%)	31	65
34	k	85/85 (100%)	80 (94%)	5 (6%)	19	49
35	l	537/540 (99%)	525 (98%)	12 (2%)	52	83
36	m	130/141 (92%)	126 (97%)	4 (3%)	40	74
37	n	53/53 (100%)	48 (91%)	5 (9%)	8	26
38	o	113/113 (100%)	109 (96%)	4 (4%)	36	70
39	p	158/159 (99%)	153 (97%)	5 (3%)	39	73
40	r	410/410 (100%)	402 (98%)	8 (2%)	55	84
41	s	275/275 (100%)	266 (97%)	9 (3%)	38	72
42	u	153/153 (100%)	146 (95%)	7 (5%)	27	60
43	v	111/111 (100%)	107 (96%)	4 (4%)	35	69
44	w	281/283 (99%)	271 (96%)	10 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7163/7240 (99%)	6940 (97%)	223 (3%)	43 74

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	97	LEU
1	A	102	MET
1	A	104	LYS
1	A	292	MET
1	A	425	CYS
1	A	451	GLN
2	B	48	MET
2	B	55	ASP
2	B	68	ARG
2	B	76	TYR
2	B	139	SER
3	C	41	SER
3	C	51	ASP
3	C	71	CYS
3	C	142	TYR
3	C	188	LYS
3	C	191	ARG
4	E	18	LYS
4	E	23	ARG
4	E	25	MET
4	E	41	ARG
4	E	89	GLU
5	F	27	SER
5	F	38	GLU
5	F	46	LYS
5	F	65	LEU
5	F	75	LYS
5	F	85	ASP
6	G	91	ASP
6	G	99	SER
6	G	106	LYS
6	G	107	ASP
6	G	132	ASP
6	G	134	ASP
7	H	116	ILE
8	I	19	ASP

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Mol	Chain	Res	Type
8	I	70	MET
8	I	71	SER
8	I	92	LYS
9	J	85	ARG
9	J	108	TRP
9	J	162	GLU
9	J	205	ASP
9	J	298	TYR
9	J	324	MET
9	J	370	LYS
10	K	85	THR
10	K	103	SER
11	L	69	GLU
11	L	73	LYS
11	L	76	LYS
11	L	88	GLN
11	L	146	ASP
11	L	169	ARG
12	M	39	GLN
12	M	75	CYS
12	M	76	ARG
12	M	98	LYS
12	M	310	GLU
12	M	347	ASP
12	M	374	THR
12	M	382	ARG
12	M	398	ASP
12	M	501	ARG
12	M	511	LYS
12	M	534	VAL
12	M	559	ASP
12	M	628	GLU
12	M	632	MET
12	M	636	TYR
12	M	637	ASP
12	M	640	ASP
12	M	666	GLN
13	N	21	ARG
13	N	68	MET
13	N	115	PHE
13	N	133	LYS
13	N	144	TYR

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Mol	Chain	Res	Type
14	O	43	ASP
14	O	56	THR
14	O	110	MET
14	O	137	THR
14	O	141	MET
14	O	145	SER
14	O	166	ASP
14	O	181	VAL
14	O	185	MET
14	O	200	ASP
14	O	219	ARG
15	P	52	ASP
15	P	80	CYS
15	P	172	ASP
16	Q	56	LYS
16	Q	74	ASP
16	Q	76	LEU
16	Q	104	GLU
16	Q	144	MET
16	Q	145	MET
16	Q	217	VAL
16	Q	463	ARG
18	T	122	HIS
19	U	65	ASP
20	V	81	ARG
21	W	34	SER
21	W	49	SER
21	W	64	ASP
21	W	99	LYS
21	W	115	ARG
21	W	135	SER
6	X	96	GLU
6	X	101	ASN
6	X	137	LYS
22	Y	94	ASP
23	Z	14	MET
23	Z	33	GLN
23	Z	39	ARG
24	a	98	LEU
24	a	176	LYS
25	b	9	LYS
25	b	17	GLU

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Mol	Chain	Res	Type
25	b	24	LYS
25	b	25	ASP
26	c	34	LYS
26	c	160	GLN
27	d	55	GLN
27	d	60	ARG
27	d	134	GLN
27	d	144	SER
28	e	63	ASP
28	e	72	ASP
28	e	114	MET
28	e	151	GLU
29	f	63	LYS
29	f	65	ASP
30	g	68	THR
31	h	3	PHE
31	h	5	ASP
31	h	80	LYS
32	i	97	MET
32	i	171	ASN
32	i	223	SER
32	i	244	MET
32	i	321	LYS
32	i	323	MET
32	i	336	VAL
33	j	16	LEU
33	j	31	SER
33	j	86	THR
33	j	87	MET
34	k	6	MET
34	k	10	MET
34	k	53	PHE
34	k	78	LEU
34	k	80	MET
35	l	1	MET
35	l	72	GLN
35	l	111	ASP
35	l	267	MET
35	l	336	LYS
35	l	340	PHE
35	l	383	MET
35	l	504	LEU

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Mol	Chain	Res	Type
35	l	514	LYS
35	l	534	HIS
35	l	554	ASP
35	l	596	MET
36	m	98	MET
36	m	101	PHE
36	m	109	LYS
36	m	135	PHE
37	n	47	ARG
37	n	49	LEU
37	n	50	ARG
37	n	54	GLU
37	n	56	THR
38	o	22	GLU
38	o	80	PHE
38	o	112	LYS
38	o	118	GLU
39	p	49	ASP
39	p	110	SER
39	p	114	MET
39	p	115	TYR
39	p	127	ARG
40	r	114	GLU
40	r	129	THR
40	r	139	GLN
40	r	140	THR
40	r	168	GLN
40	r	247	THR
40	r	256	TYR
40	r	308	SER
41	s	8	SER
41	s	61	LEU
41	s	109	SER
41	s	170	GLU
41	s	202	GLU
41	s	224	PHE
41	s	282	TYR
41	s	286	MET
41	s	289	LEU
42	u	23	SER
42	u	48	TRP
42	u	88	CYS

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Mol	Chain	Res	Type
42	u	98	ARG
42	u	121	ASP
42	u	132	LYS
42	u	155	GLU
43	v	72	ASP
43	v	84	GLN
43	v	117	GLN
43	v	122	MET
44	w	55	GLU
44	w	63	ASP
44	w	107	GLN
44	w	189	GLU
44	w	213	GLU
44	w	216	SER
44	w	241	TYR
44	w	251	GLU
44	w	285	ASP
44	w	291	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
40	r	81	GLN
44	w	235	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
16	2MR	Q	118	16	10,12,13	2.01	2 (20%)	5,13,15	6.30	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.53	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.10	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.93	131.33	119.48
16	Q	118	2MR	CD-NE-CZ	4.65	132.12	123.41
16	Q	118	2MR	CQ2-NH2-CZ	2.87	130.21	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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
51	8Q1	X	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.60	6 (15%)
45	SF4	M	802	12	0,12,12	-	-	-		
51	8Q1	G	201	6	31,34,34	1.67	5 (16%)	40,43,43	1.73	6 (15%)
49	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.64	1 (1%)
48	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.93	2 (4%)
57	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.46	5 (17%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.04	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
54	FES	O	301	14	0,4,4	-	-	-		
52	CDL	u	201	-	54,54,99	1.36	9 (16%)	60,66,111	1.09	4 (6%)
52	CDL	V	201	-	93,93,99	1.10	9 (9%)	99,105,111	0.89	4 (4%)
52	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.90	4 (3%)
48	PEE	V	202	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)
52	CDL	k	101	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.30	9 (18%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.65	1 (1%)
53	NDP	J	401	-	45,52,52	4.55	19 (42%)	53,80,80	1.99	7 (13%)
48	PEE	l	704	-	45,45,50	1.21	6 (13%)	48,50,55	0.99	2 (4%)
49	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.60	1 (1%)
52	CDL	l	702	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
49	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.66	1 (1%)
50	UQ	C	304	-	38,38,63	3.51	11 (28%)	46,49,79	2.93	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	CDL	o	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
45	SF4	C	301	3	0,12,12	-	-	-		
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.57	1 (1%)
48	PEE	j	202	-	40,40,50	1.14	5 (12%)	43,45,55	1.12	3 (6%)
52	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
50	UQ	J	402	-	33,33,63	3.47	10 (30%)	40,43,79	2.69	14 (35%)
54	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)
52	CDL	r	504	-	99,99,99	1.07	8 (8%)	105,111,111	0.90	4 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
49	PLX	r	502	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
52	CDL	s	401	-	88,88,99	1.13	7 (7%)	94,100,111	0.94	4 (4%)
48	PEE	l	703	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
49	PLX	J	403	-	51,51,51	1.13	3 (5%)	55,59,59	0.61	1 (1%)
48	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	1.02	2 (3%)
48	PEE	i	401	-	46,46,50	1.19	6 (13%)	49,51,55	1.02	2 (4%)
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
52	CDL	I	201	-	50,50,99	1.39	8 (16%)	56,62,111	1.11	4 (7%)
47	NAI	A	503	-	42,48,48	4.92	18 (42%)	47,73,73	1.33	7 (14%)

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
51	8Q1	X	201	6	-	16/41/41/41	-
45	SF4	M	802	12	-	-	0/6/5/5
51	8Q1	G	201	6	-	12/41/41/41	-
49	PLX	j	203	-	-	26/55/55/55	-
48	PEE	W	201	-	-	19/44/44/54	-
57	ADP	w	401	-	-	4/12/32/32	0/3/3/3
48	PEE	B	303	-	-	27/54/54/54	-
45	SF4	B	302	2	-	-	0/6/5/5
54	FES	O	301	14	-	-	0/1/1/1
52	CDL	u	201	-	-	36/65/65/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CDL	V	201	-	-	59/104/104/110	-
52	CDL	l	701	-	-	64/109/109/110	-
48	PEE	V	202	-	-	26/43/43/54	-
52	CDL	k	101	-	-	62/110/110/110	-
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	C	303	-	-	31/55/55/55	-
53	NDP	J	401	-	-	11/30/77/77	0/4/5/5
48	PEE	l	704	-	-	29/49/49/54	-
49	PLX	r	503	-	-	30/55/55/55	-
52	CDL	l	702	-	-	58/110/110/110	-
49	PLX	g	201	-	-	32/55/55/55	-
50	UQ	C	304	-	-	13/33/57/87	0/1/1/1
52	CDL	o	201	-	-	65/110/110/110	-
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	a	202	-	-	30/55/55/55	-
48	PEE	j	202	-	-	20/44/44/54	-
52	CDL	a	201	-	-	50/110/110/110	-
50	UQ	J	402	-	-	10/27/51/87	0/1/1/1
54	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	j	201	-	-	26/54/54/54	-
52	CDL	r	504	-	-	64/110/110/110	-
45	SF4	A	501	1	-	-	0/6/5/5
49	PLX	r	502	-	-	32/55/55/55	-
52	CDL	s	401	-	-	49/99/99/110	-
48	PEE	l	703	-	-	31/54/54/54	-
49	PLX	J	403	-	-	34/55/55/55	-
48	PEE	r	501	-	-	32/54/54/54	-
48	PEE	i	401	-	-	20/50/50/54	-
48	PEE	C	302	-	-	28/50/50/54	-
52	CDL	I	201	-	-	30/61/61/110	-
47	NAI	A	503	-	-	8/25/72/72	0/5/5/5

All (240) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4B-C1B	16.17	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.34	1.30	1.53
53	J	401	NDP	C3B-C2B	-12.96	1.24	1.52
53	J	401	NDP	C6N-C5N	12.22	1.55	1.33
53	J	401	NDP	O4D-C4D	10.68	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.28	1.26	1.53
53	J	401	NDP	C3D-C4D	-9.98	1.27	1.53
50	J	402	UQ	C18-C19	9.63	1.56	1.33
50	C	304	UQ	C18-C19	9.50	1.55	1.33
50	J	402	UQ	C13-C14	9.28	1.55	1.33
50	C	304	UQ	C23-C24	9.16	1.54	1.33
50	J	402	UQ	C8-C9	9.11	1.54	1.33
50	C	304	UQ	C13-C14	9.05	1.54	1.33
50	C	304	UQ	C8-C9	8.98	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.30	1.26	1.45
53	J	401	NDP	O4B-C4B	-8.23	1.26	1.45
53	J	401	NDP	O4B-C1B	7.98	1.52	1.41
50	J	402	UQ	C23-C24	7.87	1.55	1.32
47	A	503	NAI	C2D-C1D	-7.66	1.29	1.53
50	C	304	UQ	C28-C29	7.64	1.54	1.32
57	w	401	ADP	O4'-C4'	7.56	1.61	1.45
53	J	401	NDP	C2N-C3N	7.35	1.55	1.34
57	w	401	ADP	O4'-C1'	-6.95	1.31	1.41
47	A	503	NAI	O4D-C4D	6.89	1.60	1.45
47	A	503	NAI	C2D-C3D	5.80	1.69	1.53
47	A	503	NAI	C7N-N7N	5.71	1.48	1.33
53	J	401	NDP	P2B-O2B	5.57	1.69	1.59
51	X	201	8Q1	C34-N36	5.40	1.45	1.33
51	G	201	8Q1	C34-N36	5.37	1.45	1.33
51	X	201	8Q1	C39-N41	5.33	1.45	1.33
47	A	503	NAI	O4D-C1D	5.30	1.54	1.42
53	J	401	NDP	C3B-C4B	5.29	1.66	1.53
51	G	201	8Q1	C39-N41	5.12	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.11	1.39	1.49
53	J	401	NDP	O4D-C1D	-4.94	1.30	1.42
53	J	401	NDP	C6N-N1N	4.77	1.49	1.37
47	A	503	NAI	O2B-C2B	4.47	1.53	1.43
53	J	401	NDP	O2D-C2D	-4.25	1.33	1.43
53	J	401	NDP	C7N-N7N	4.11	1.44	1.33
53	J	401	NDP	C6A-N6A	4.05	1.48	1.34
47	A	503	NAI	C6N-C5N	3.91	1.40	1.33
57	w	401	ADP	C6-N6	3.84	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	703	PEE	C18-C19	3.75	1.53	1.31
48	C	302	PEE	C18-C19	3.74	1.53	1.31
48	V	202	PEE	C18-C19	3.72	1.53	1.31
48	B	303	PEE	C18-C19	3.72	1.53	1.31
48	r	501	PEE	C18-C19	3.72	1.53	1.31
48	j	201	PEE	C18-C19	3.71	1.53	1.31
48	j	202	PEE	C18-C19	3.70	1.53	1.31
48	W	201	PEE	C18-C19	3.70	1.53	1.31
48	l	704	PEE	C18-C19	3.68	1.53	1.31
48	i	401	PEE	C18-C19	3.67	1.53	1.31
48	V	202	PEE	C39-C38	3.65	1.53	1.31
48	l	704	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.64	1.52	1.31
48	r	501	PEE	C39-C38	3.64	1.52	1.31
48	l	703	PEE	C39-C38	3.63	1.52	1.31
46	A	502	FMN	C4A-N5	3.63	1.37	1.30
48	i	401	PEE	C39-C38	3.62	1.52	1.31
48	C	302	PEE	C39-C38	3.62	1.52	1.31
52	l	701	CDL	OA8-CA7	3.61	1.43	1.33
48	j	201	PEE	C39-C38	3.60	1.52	1.31
47	A	503	NAI	C6A-N6A	3.54	1.47	1.34
52	l	702	CDL	OA8-CA7	3.49	1.43	1.33
52	u	201	CDL	OA8-CA7	3.47	1.43	1.33
47	A	503	NAI	C7N-C3N	3.47	1.56	1.48
52	s	401	CDL	OA8-CA7	3.46	1.43	1.33
52	a	201	CDL	OA8-CA7	3.45	1.43	1.33
52	o	201	CDL	OA8-CA7	3.44	1.43	1.33
52	I	201	CDL	OA8-CA7	3.42	1.43	1.33
57	w	401	ADP	O2'-C2'	-3.41	1.34	1.43
52	V	201	CDL	OA8-CA7	3.39	1.43	1.33
52	k	101	CDL	OA8-CA7	3.39	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.35	1.40	1.48
52	r	504	CDL	OA8-CA7	3.34	1.43	1.33
52	V	201	CDL	OA6-CA5	3.16	1.43	1.34
52	k	101	CDL	OA6-CA5	3.12	1.43	1.34
57	w	401	ADP	O3'-C3'	3.11	1.50	1.43
52	a	201	CDL	OB6-CB5	3.07	1.43	1.34
52	u	201	CDL	OB8-CB7	3.03	1.42	1.33
52	l	701	CDL	OB8-CB7	3.03	1.42	1.33
52	o	201	CDL	OB6-CB5	3.01	1.42	1.34
53	J	401	NDP	O3D-C3D	3.01	1.50	1.43
52	l	702	CDL	OB8-CB7	2.98	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	s	401	CDL	OA6-CA5	2.97	1.42	1.34
52	u	201	CDL	OA6-CA5	2.97	1.42	1.34
52	s	401	CDL	OB6-CB5	2.97	1.42	1.34
52	o	201	CDL	OB8-CB7	2.97	1.42	1.33
52	I	201	CDL	OB6-CB5	2.96	1.42	1.34
52	l	702	CDL	OA6-CA5	2.95	1.42	1.34
52	l	701	CDL	OB6-CB5	2.95	1.42	1.34
52	o	201	CDL	OA6-CA5	2.94	1.42	1.34
52	u	201	CDL	OB6-CB5	2.93	1.42	1.34
52	k	101	CDL	OB8-CB7	2.93	1.41	1.33
49	g	201	PLX	O6-C4	-2.93	1.40	1.44
52	I	201	CDL	OB8-CB7	2.92	1.41	1.33
52	l	702	CDL	OB6-CB5	2.92	1.42	1.34
52	r	504	CDL	OB6-CB5	2.92	1.42	1.34
52	I	201	CDL	OA6-CA5	2.92	1.42	1.34
52	r	504	CDL	OB8-CB7	2.91	1.41	1.33
52	a	201	CDL	OB8-CB7	2.91	1.41	1.33
52	a	201	CDL	OA6-CA5	2.90	1.42	1.34
52	r	504	CDL	OA6-CA5	2.90	1.42	1.34
53	J	401	NDP	C7N-C3N	2.90	1.54	1.48
52	V	201	CDL	OB8-CB7	2.89	1.41	1.33
52	k	101	CDL	OB6-CB5	2.88	1.42	1.34
49	a	202	PLX	O6-C4	-2.86	1.40	1.44
52	V	201	CDL	OB6-CB5	2.82	1.42	1.34
52	l	701	CDL	OA6-CA5	2.82	1.42	1.34
52	s	401	CDL	OB8-CB7	2.74	1.41	1.33
49	j	203	PLX	O6-C4	-2.74	1.40	1.44
49	C	303	PLX	O6-C4	-2.68	1.41	1.44
49	r	502	PLX	O6-C4	-2.63	1.41	1.44
49	r	503	PLX	O6-C4	-2.62	1.41	1.44
50	J	402	UQ	C7-C8	2.62	1.54	1.50
50	C	304	UQ	C6-C1	2.61	1.54	1.46
50	J	402	UQ	C6-C1	2.61	1.54	1.46
52	r	504	CDL	OA6-CA4	-2.53	1.40	1.46
47	A	503	NAI	O3B-C3B	-2.53	1.37	1.43
48	j	201	PEE	O2-C2	-2.51	1.40	1.46
52	l	701	CDL	OA6-CA4	-2.49	1.40	1.46
48	C	302	PEE	O2-C2	-2.49	1.40	1.46
48	j	202	PEE	O3-C30	2.48	1.40	1.33
48	V	202	PEE	O3-C30	2.46	1.40	1.33
48	B	303	PEE	O3-C30	2.46	1.40	1.33
48	l	704	PEE	O3-C30	2.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	o	201	CDL	OA6-CA4	-2.44	1.40	1.46
48	B	303	PEE	O2-C2	-2.44	1.40	1.46
52	I	201	CDL	OA6-CA4	-2.44	1.40	1.46
48	C	302	PEE	O3-C30	2.43	1.40	1.33
52	s	401	CDL	OA6-CA4	-2.43	1.40	1.46
48	W	201	PEE	O2-C2	-2.43	1.40	1.46
48	l	703	PEE	O2-C2	-2.43	1.40	1.46
48	i	401	PEE	O2-C2	-2.41	1.40	1.46
48	l	703	PEE	O3-C30	2.41	1.40	1.33
51	X	201	8Q1	C1-S44	2.41	1.82	1.76
49	J	403	PLX	C7-C6	2.40	1.55	1.50
48	W	201	PEE	O3-C30	2.40	1.40	1.33
52	a	201	CDL	OA6-CA4	-2.40	1.40	1.46
48	j	201	PEE	O3-C30	2.39	1.40	1.33
49	r	502	PLX	C7-C6	2.39	1.55	1.50
48	j	202	PEE	O2-C2	-2.39	1.40	1.46
53	J	401	NDP	O2B-C2B	2.38	1.52	1.44
48	r	501	PEE	O2-C2	-2.37	1.40	1.46
49	j	203	PLX	C7-C6	2.37	1.55	1.50
52	u	201	CDL	OA6-CA4	-2.37	1.40	1.46
51	G	201	8Q1	O40-C39	-2.36	1.18	1.23
48	r	501	PEE	O3-C30	2.35	1.40	1.33
48	V	202	PEE	O2-C2	-2.35	1.40	1.46
49	C	303	PLX	C7-C6	2.34	1.55	1.50
52	V	201	CDL	OB6-CB4	-2.34	1.40	1.46
48	l	704	PEE	O2-C2	-2.33	1.40	1.46
48	i	401	PEE	O3-C30	2.33	1.40	1.33
51	G	201	8Q1	C1-S44	2.32	1.81	1.76
52	k	101	CDL	OB6-CB4	-2.32	1.40	1.46
48	W	201	PEE	O2-C10	2.31	1.40	1.34
48	V	202	PEE	O2-C10	2.31	1.40	1.34
51	G	201	8Q1	O35-C34	-2.31	1.18	1.23
47	A	503	NAI	PN-O5D	2.30	1.68	1.59
51	X	201	8Q1	O40-C39	-2.30	1.18	1.23
49	a	202	PLX	C7-C6	2.30	1.55	1.50
49	g	201	PLX	C7-C6	2.29	1.55	1.50
52	l	702	CDL	OA6-CA4	-2.29	1.40	1.46
49	r	503	PLX	C7-C6	2.28	1.55	1.50
52	l	701	CDL	OB6-CB4	-2.28	1.40	1.46
48	l	703	PEE	O2-C10	2.27	1.40	1.34
51	X	201	8Q1	O35-C34	-2.27	1.18	1.23
48	l	704	PEE	O2-C10	2.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	UQ	C7-C8	2.26	1.53	1.50
52	k	101	CDL	OA6-CA4	-2.26	1.41	1.46
46	A	502	FMN	C10-N1	2.25	1.37	1.33
52	l	702	CDL	OB6-CB4	-2.25	1.41	1.46
48	B	303	PEE	O2-C10	2.24	1.40	1.34
52	u	201	CDL	OB6-CB4	-2.23	1.41	1.46
48	W	201	PEE	O3-C3	-2.23	1.40	1.45
53	J	401	NDP	C2D-C3D	2.22	1.59	1.53
48	r	501	PEE	O3-C3	-2.22	1.40	1.45
52	l	702	CDL	PB2-OB2	2.21	1.68	1.59
48	i	401	PEE	O2-C10	2.21	1.40	1.34
52	o	201	CDL	PB2-OB2	2.21	1.68	1.59
52	I	201	CDL	OB6-CB4	-2.20	1.41	1.46
53	J	401	NDP	O7N-C7N	-2.20	1.19	1.24
52	V	201	CDL	PB2-OB2	2.19	1.68	1.59
48	j	201	PEE	O2-C10	2.19	1.40	1.34
48	j	202	PEE	O2-C10	2.19	1.40	1.34
52	o	201	CDL	PB2-OB5	2.18	1.68	1.59
48	r	501	PEE	O2-C10	2.18	1.40	1.34
50	J	402	UQ	O4-C4	-2.18	1.18	1.23
48	l	703	PEE	O3-C3	-2.17	1.40	1.45
48	C	302	PEE	O2-C10	2.16	1.40	1.34
48	i	401	PEE	O3-C3	-2.16	1.40	1.45
50	C	304	UQ	O4-C4	-2.16	1.18	1.23
52	r	504	CDL	PB2-OB5	2.16	1.68	1.59
47	A	503	NAI	C5B-C4B	2.16	1.58	1.51
52	r	504	CDL	OB6-CB4	-2.15	1.41	1.46
52	s	401	CDL	PB2-OB2	2.15	1.68	1.59
52	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
52	u	201	CDL	PB2-OB5	2.15	1.68	1.59
52	a	201	CDL	PB2-OB5	2.14	1.68	1.59
49	a	202	PLX	P1-O4	2.14	1.68	1.59
52	o	201	CDL	OB6-CB4	-2.14	1.41	1.46
50	C	304	UQ	O3-CM3	-2.14	1.40	1.45
48	j	201	PEE	O3-C3	-2.14	1.40	1.45
52	l	701	CDL	PB2-OB5	2.14	1.67	1.59
52	s	401	CDL	OB6-CB4	-2.13	1.41	1.46
52	a	201	CDL	PB2-OB2	2.13	1.67	1.59
52	I	201	CDL	PB2-OB5	2.13	1.67	1.59
52	u	201	CDL	PB2-OB2	2.13	1.67	1.59
52	k	101	CDL	PB2-OB2	2.12	1.67	1.59
52	V	201	CDL	PB2-OB5	2.12	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	O3-C3	-2.12	1.40	1.45
52	V	201	CDL	C11-CA5	2.12	1.56	1.50
52	r	504	CDL	PB2-OB2	2.12	1.67	1.59
52	l	701	CDL	PB2-OB2	2.11	1.67	1.59
49	C	303	PLX	P1-O1	2.11	1.67	1.59
52	l	702	CDL	PB2-OB5	2.11	1.67	1.59
52	k	101	CDL	PB2-OB5	2.10	1.67	1.59
48	B	303	PEE	O3-C3	-2.09	1.40	1.45
48	V	202	PEE	O3-C3	-2.09	1.40	1.45
52	I	201	CDL	PB2-OB2	2.09	1.67	1.59
49	j	203	PLX	P1-O4	2.08	1.67	1.59
49	J	403	PLX	P1-O4	2.08	1.67	1.59
50	J	402	UQ	O1-C1	-2.08	1.18	1.23
49	r	502	PLX	P1-O4	2.07	1.67	1.59
50	C	304	UQ	O1-C1	-2.07	1.18	1.23
49	J	403	PLX	O6-C4	-2.06	1.41	1.44
49	g	201	PLX	P1-O4	2.06	1.67	1.59
51	X	201	8Q1	C6-C1	2.06	1.53	1.50
49	C	303	PLX	P1-O4	2.05	1.67	1.59
48	j	202	PEE	O3-C3	-2.05	1.40	1.45
52	V	201	CDL	OA6-CA4	-2.05	1.41	1.46
50	C	304	UQ	C21-C19	2.04	1.55	1.51
49	j	203	PLX	P1-O1	2.04	1.67	1.59
48	l	704	PEE	O3-C3	-2.03	1.40	1.45
50	J	402	UQ	C21-C19	2.03	1.55	1.51
49	r	503	PLX	P1-O4	2.03	1.67	1.59
52	u	201	CDL	C11-CA5	2.02	1.56	1.50
49	a	202	PLX	P1-O1	2.01	1.67	1.59
50	J	402	UQ	O3-CM3	-2.01	1.40	1.45

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	304	UQ	C7-C8-C9	-8.36	112.88	126.79
50	J	402	UQ	C7-C8-C9	-7.88	113.67	126.79
53	J	401	NDP	C3N-C2N-N1N	-7.79	111.98	123.10
51	G	201	8Q1	C6-C1-S44	7.09	121.72	113.46
53	J	401	NDP	C1D-N1N-C2N	-6.95	109.53	121.11
50	C	304	UQ	C17-C18-C19	-6.37	112.32	127.66
50	C	304	UQ	C12-C13-C14	-6.36	112.35	127.66
50	C	304	UQ	C22-C23-C24	-5.79	113.72	127.66
51	X	201	8Q1	C6-C1-S44	5.79	120.19	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	402	UQ	C17-C18-C19	-5.78	113.75	127.66
50	J	402	UQ	C12-C13-C14	-5.65	114.07	127.66
53	J	401	NDP	C1D-N1N-C6N	-5.60	108.77	120.83
57	w	401	ADP	N3-C2-N1	-4.58	121.52	128.68
48	j	202	PEE	O2-C10-C11	4.56	121.33	111.50
50	C	304	UQ	C10-C9-C8	-4.49	112.17	123.68
50	C	304	UQ	C27-C28-C29	-4.48	112.45	127.75
48	r	501	PEE	O2-C10-C11	4.43	121.06	111.50
47	A	503	NAI	N3A-C2A-N1A	-4.39	121.82	128.68
50	C	304	UQ	C20-C19-C18	-4.31	112.61	123.68
52	V	201	CDL	OA6-CA5-C11	4.30	120.78	111.50
50	J	402	UQ	C22-C23-C24	-4.29	113.08	127.75
52	s	401	CDL	OB6-CB5-C51	4.24	120.63	111.50
50	J	402	UQ	C10-C9-C8	-4.18	112.96	123.68
48	B	303	PEE	O2-C10-C11	4.17	120.48	111.50
53	J	401	NDP	N3A-C2A-N1A	-4.16	122.17	128.68
50	C	304	UQ	C11-C9-C8	-4.15	112.72	121.12
52	l	701	CDL	OB6-CB5-C51	4.13	120.41	111.50
50	J	402	UQ	C21-C19-C18	-4.09	112.84	121.12
52	o	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
50	C	304	UQ	C25-C24-C23	-4.08	113.22	123.68
52	k	101	CDL	OB6-CB5-C51	4.08	120.28	111.50
50	C	304	UQ	C21-C19-C18	-4.07	112.88	121.12
52	s	401	CDL	OA6-CA5-C11	4.06	120.26	111.50
48	V	202	PEE	O2-C10-C11	4.02	120.17	111.50
48	l	704	PEE	O2-C10-C11	4.01	120.15	111.50
51	G	201	8Q1	O4-C1-C6	-4.01	119.25	123.99
52	r	504	CDL	OB6-CB5-C51	4.01	120.15	111.50
52	l	702	CDL	OB6-CB5-C51	4.01	120.13	111.50
52	u	201	CDL	OA6-CA5-C11	3.99	120.11	111.50
50	J	402	UQ	C20-C19-C18	-3.99	113.44	123.68
48	C	302	PEE	O2-C10-C11	3.97	120.06	111.50
52	l	701	CDL	OA6-CA5-C11	3.96	120.04	111.50
50	C	304	UQ	C26-C24-C23	-3.96	113.11	121.12
52	V	201	CDL	OB6-CB5-C51	3.95	120.02	111.50
52	a	201	CDL	OB6-CB5-C51	3.94	119.99	111.50
52	a	201	CDL	OA6-CA5-C11	3.92	119.95	111.50
50	C	304	UQ	C15-C14-C13	-3.91	113.65	123.68
52	u	201	CDL	OB6-CB5-C51	3.91	119.92	111.50
52	l	702	CDL	OA6-CA5-C11	3.90	119.91	111.50
50	J	402	UQ	C16-C14-C13	-3.87	113.29	121.12
48	i	401	PEE	O2-C10-C11	3.85	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	j	201	PEE	O2-C10-C11	3.85	119.80	111.50
52	I	201	CDL	OA6-CA5-C11	3.85	119.80	111.50
52	I	201	CDL	OB6-CB5-C51	3.84	119.78	111.50
52	r	504	CDL	OA6-CA5-C11	3.81	119.72	111.50
50	C	304	UQ	C16-C14-C13	-3.78	113.46	121.12
50	J	402	UQ	C15-C14-C13	-3.77	114.01	123.68
52	o	201	CDL	OA6-CA5-C11	3.71	119.49	111.50
48	W	201	PEE	O2-C10-C11	3.70	119.47	111.50
48	l	703	PEE	O2-C10-C11	3.69	119.46	111.50
50	J	402	UQ	C11-C9-C8	-3.66	113.70	121.12
51	X	201	8Q1	O4-C1-C6	-3.63	119.70	123.99
52	k	101	CDL	OA6-CA5-C11	3.56	119.18	111.50
50	C	304	UQ	C30-C29-C28	-3.42	112.76	122.65
46	A	502	FMN	C4-N3-C2	-3.38	119.40	125.64
50	C	304	UQ	C31-C29-C28	-3.30	113.10	122.65
50	J	402	UQ	C25-C24-C23	-3.29	113.14	122.65
50	J	402	UQ	C26-C24-C23	-3.27	113.19	122.65
51	X	201	8Q1	C37-C38-C39	3.24	117.76	112.36
52	u	201	CDL	OA8-CA7-C31	3.14	119.61	111.38
52	l	701	CDL	OA8-CA7-C31	3.10	121.63	111.91
48	B	303	PEE	O3-C30-C31	3.05	121.49	111.91
47	A	503	NAI	C3B-C2B-C1B	2.86	105.29	100.98
48	l	703	PEE	O3-C30-C31	2.83	120.78	111.91
51	G	201	8Q1	C37-C38-C39	2.82	117.06	112.36
47	A	503	NAI	C3D-C2D-C1D	2.79	106.73	101.43
47	A	503	NAI	C2D-C3D-C4D	2.79	108.06	102.64
51	X	201	8Q1	C43-S44-C1	2.76	110.46	101.87
51	G	201	8Q1	O4-C1-S44	-2.76	119.03	122.61
52	k	101	CDL	OB8-CB7-C71	2.75	120.55	111.91
48	i	401	PEE	O3-C30-C31	2.74	120.52	111.91
52	r	504	CDL	OB8-CB7-C71	2.73	120.48	111.91
52	l	702	CDL	OB8-CB7-C71	2.72	120.45	111.91
46	A	502	FMN	C4A-C4-N3	2.72	120.09	113.19
52	a	201	CDL	OB8-CB7-C71	2.71	120.42	111.91
52	l	702	CDL	OA8-CA7-C31	2.71	120.42	111.91
52	k	101	CDL	OA8-CA7-C31	2.71	120.41	111.91
52	o	201	CDL	OB8-CB7-C71	2.68	120.30	111.91
52	o	201	CDL	OA8-CA7-C31	2.67	120.27	111.91
52	s	401	CDL	OA8-CA7-C31	2.66	120.26	111.91
52	I	201	CDL	OB8-CB7-C71	2.66	120.25	111.91
52	I	201	CDL	OA8-CA7-C31	2.65	120.22	111.91
48	j	202	PEE	O3-C30-C31	2.65	120.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	l	701	CDL	OB8-CB7-C71	2.65	120.21	111.91
47	A	503	NAI	C4A-C5A-N7A	-2.64	106.64	109.40
47	A	503	NAI	C4D-O4D-C1D	-2.64	103.64	109.47
48	r	501	PEE	O3-C30-C31	2.63	120.17	111.91
52	u	201	CDL	OB8-CB7-C71	2.62	120.14	111.91
48	C	302	PEE	O3-C30-C31	2.61	120.10	111.91
49	g	201	PLX	C1A-N1-C1	2.61	120.60	109.92
48	l	704	PEE	O3-C30-C31	2.60	120.08	111.91
53	J	401	NDP	PN-O3-PA	-2.60	123.90	132.83
48	j	202	PEE	C2-O2-C10	-2.58	111.43	117.79
57	w	401	ADP	PA-O3A-PB	-2.58	123.98	132.83
53	J	401	NDP	C2B-C3B-C4B	2.57	107.58	101.99
52	V	201	CDL	OB8-CB7-C71	2.57	119.98	111.91
46	A	502	FMN	O4-C4-C4A	-2.57	119.79	126.60
52	r	504	CDL	OA8-CA7-C31	2.56	119.94	111.91
48	j	201	PEE	O3-C30-C31	2.54	119.89	111.91
48	V	202	PEE	O3-C30-C31	2.53	119.83	111.91
46	A	502	FMN	C4A-C10-N10	2.52	120.17	116.48
52	a	201	CDL	OA8-CA7-C31	2.52	119.81	111.91
50	J	402	UQ	CM5-C5-C6	-2.50	120.31	124.40
52	s	401	CDL	OB8-CB7-C71	2.48	119.69	111.91
49	r	503	PLX	C1A-N1-C1	2.48	120.06	109.92
49	j	203	PLX	C1A-N1-C1	2.48	120.05	109.92
49	r	502	PLX	C1A-N1-C1	2.48	120.05	109.92
46	A	502	FMN	C4A-C10-N1	-2.46	119.02	124.73
51	X	201	8Q1	C38-C39-N41	2.40	120.45	116.42
57	w	401	ADP	O4'-C1'-C2'	-2.39	103.43	106.93
53	J	401	NDP	C4A-C5A-N7A	-2.38	106.92	109.40
51	G	201	8Q1	C38-C39-N41	2.35	120.38	116.42
50	C	304	UQ	CM5-C5-C6	-2.33	120.60	124.40
49	C	303	PLX	C1A-N1-C1	2.29	119.27	109.92
52	V	201	CDL	OA8-CA7-C31	2.28	119.07	111.91
48	W	201	PEE	O3-C30-C31	2.28	119.06	111.91
57	w	401	ADP	C4-C5-N7	-2.28	107.02	109.40
49	J	403	PLX	C1A-N1-C1	2.28	119.23	109.92
49	a	202	PLX	C1A-N1-C1	2.26	119.17	109.92
46	A	502	FMN	C10-C4A-N5	-2.21	120.17	124.86
51	G	201	8Q1	O27-C28-C29	-2.21	107.00	110.55
46	A	502	FMN	C5A-C9A-N10	2.20	120.22	117.95
50	C	304	UQ	C10-C9-C11	-2.19	111.59	115.27
47	A	503	NAI	PN-O3-PA	-2.14	125.48	132.83
51	X	201	8Q1	C32-C34-N36	2.12	120.80	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C9A-C5A-N5	-2.11	120.14	122.43
46	A	502	FMN	C4-C4A-C10	2.05	120.23	116.79
57	w	401	ADP	C2'-C3'-C4'	2.02	106.57	102.64
50	J	402	UQ	C10-C9-C11	-2.01	111.89	115.27

There are no chirality outliers.

All (1088) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	C5B-O5B-PA-O3
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	O4-C10-O2-C2
48	C	302	PEE	C11-C10-O2-C2
48	C	302	PEE	O4-C10-O2-C2
48	C	302	PEE	C1-O3P-P-O1P
48	V	202	PEE	C11-C10-O2-C2
48	V	202	PEE	C1-O3P-P-O2P
48	V	202	PEE	C1-O3P-P-O1P
48	V	202	PEE	C1-O3P-P-O4P
48	V	202	PEE	C4-O4P-P-O3P
48	V	202	PEE	C4-O4P-P-O2P
48	V	202	PEE	C4-O4P-P-O1P
48	V	202	PEE	C39-C40-C41-C42
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	i	401	PEE	C11-C10-O2-C2
48	i	401	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O1P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O1P
48	l	703	PEE	O4-C10-O2-C2
48	l	703	PEE	C4-O4P-P-O3P
48	l	703	PEE	C4-O4P-P-O2P
48	l	703	PEE	C4-O4P-P-O1P
48	l	704	PEE	C1-O3P-P-O2P
48	l	704	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C1-O3P-P-O4P
48	l	704	PEE	C37-C38-C39-C40
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	N1-C1-C2-O1
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-O4-P1-O2
49	J	403	PLX	C2-O1-P1-O2
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	O9-C24-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	O9-C24-C25-C26
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O9-C24-O8-C5
49	j	203	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C25-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	O9-C24-O8-C5
50	C	304	UQ	C7-C8-C9-C11
50	C	304	UQ	C12-C13-C14-C15
50	C	304	UQ	C17-C18-C19-C21
50	C	304	UQ	C22-C23-C24-C26
50	J	402	UQ	C7-C8-C9-C10
50	J	402	UQ	C19-C21-C22-C23
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O3
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	O4-C1-S44-C43
51	X	201	8Q1	C6-C1-S44-C43

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Mol	Chain	Res	Type	Atoms
51	X	201	8Q1	O27-C28-C29-C30
51	X	201	8Q1	O27-C28-C29-C31
51	X	201	8Q1	O27-C28-C29-C32
51	X	201	8Q1	N41-C42-C43-S44
51	X	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
52	I	201	CDL	CB2-C1-CA2-OA2
52	I	201	CDL	CA2-OA2-PA1-OA3
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	OA5-CA3-CA4-OA6
52	I	201	CDL	CB2-OB2-PB2-OB3
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB2-C1-CA2-OA2
52	V	201	CDL	CA2-C1-CB2-OB2
52	V	201	CDL	CA2-OA2-PA1-OA3
52	V	201	CDL	CA2-OA2-PA1-OA4
52	V	201	CDL	CA2-OA2-PA1-OA5
52	V	201	CDL	C11-CA5-OA6-CA4
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-C1-CB2-OB2
52	a	201	CDL	CB2-OB2-PB2-OB3
52	k	101	CDL	CA2-OA2-PA1-OA3
52	k	101	CDL	OA5-CA3-CA4-OA6
52	k	101	CDL	CB2-OB2-PB2-OB3
52	k	101	CDL	CB3-OB5-PB2-OB2
52	k	101	CDL	CB3-OB5-PB2-OB3
52	k	101	CDL	CB3-OB5-PB2-OB4
52	l	701	CDL	O1-C1-CA2-OA2
52	l	701	CDL	CA3-OA5-PA1-OA3
52	l	701	CDL	OA9-CA7-OA8-CA6
52	l	701	CDL	C31-CA7-OA8-CA6
52	l	701	CDL	CB2-OB2-PB2-OB3
52	l	701	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB2-OB2-PB2-OB5
52	l	702	CDL	CB2-C1-CA2-OA2
52	l	702	CDL	CA3-OA5-PA1-OA3
52	l	702	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	CB2-C1-CA2-OA2
52	o	201	CDL	CA3-OA5-PA1-OA3
52	o	201	CDL	CB2-OB2-PB2-OB3
52	r	504	CDL	O1-C1-CA2-OA2
52	r	504	CDL	CB2-C1-CA2-OA2
52	r	504	CDL	CA2-OA2-PA1-OA3
52	r	504	CDL	CB2-OB2-PB2-OB3
52	r	504	CDL	CB2-OB2-PB2-OB4
52	r	504	CDL	CB2-OB2-PB2-OB5
52	r	504	CDL	CB3-OB5-PB2-OB3
52	r	504	CDL	CB3-OB5-PB2-OB4
52	s	401	CDL	O1-C1-CA2-OA2
52	s	401	CDL	CA2-C1-CB2-OB2
52	u	201	CDL	CB2-C1-CA2-OA2
52	u	201	CDL	CB2-OB2-PB2-OB3
52	u	201	CDL	CB2-OB2-PB2-OB4
52	u	201	CDL	CB3-OB5-PB2-OB3
52	u	201	CDL	CB3-OB5-PB2-OB4
53	J	401	NDP	C5B-O5B-PA-O1A
53	J	401	NDP	O4B-C4B-C5B-O5B
53	J	401	NDP	C2N-C3N-C7N-N7N
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
48	i	401	PEE	O5-C30-O3-C3
52	s	401	CDL	OA9-CA7-OA8-CA6
48	i	401	PEE	C31-C30-O3-C3
52	s	401	CDL	C31-CA7-OA8-CA6
48	V	202	PEE	O4-C10-O2-C2
48	i	401	PEE	O4-C10-O2-C2
52	V	201	CDL	OA7-CA5-OA6-CA4
52	a	201	CDL	OB7-CB5-OB6-CB4
48	l	703	PEE	C11-C10-O2-C2
49	g	201	PLX	C9-C10-C11-C12
52	l	702	CDL	C71-CB7-OB8-CB6
48	j	201	PEE	C17-C18-C19-C20
52	r	504	CDL	C74-C75-C76-C77
50	C	304	UQ	C27-C28-C29-C31
50	C	304	UQ	C7-C8-C9-C10
50	J	402	UQ	C7-C8-C9-C11
50	J	402	UQ	C12-C13-C14-C16
52	u	201	CDL	C55-C56-C57-C58
52	s	401	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
52	I	201	CDL	O1-C1-CA2-OA2
52	I	201	CDL	O1-C1-CB2-OB2
52	V	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CA2-OA2
52	k	101	CDL	O1-C1-CB2-OB2
52	l	702	CDL	O1-C1-CA2-OA2
52	o	201	CDL	O1-C1-CA2-OA2
52	u	201	CDL	O1-C1-CA2-OA2
48	j	202	PEE	C31-C30-O3-C3
52	a	201	CDL	C51-CB5-OB6-CB4
52	k	101	CDL	C11-CA5-OA6-CA4
52	o	201	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C30-C31-C32-C33
52	k	101	CDL	C73-C74-C75-C76
52	o	201	CDL	C32-C33-C34-C35
52	u	201	CDL	C74-C75-C76-C77
49	g	201	PLX	C7-C8-C9-C10
52	l	701	CDL	C55-C56-C57-C58
53	J	401	NDP	O4D-C4D-C5D-O5D
52	r	504	CDL	C60-C61-C62-C63
52	l	702	CDL	OB9-CB7-OB8-CB6
52	a	201	CDL	C36-C37-C38-C39
50	J	402	UQ	C22-C23-C24-C26
50	J	402	UQ	C13-C14-C16-C17
50	J	402	UQ	C18-C19-C21-C22
49	C	303	PLX	C27-C28-C29-C30
49	j	203	PLX	C13-C14-C15-C16
48	j	201	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
49	r	502	PLX	C9-C10-C11-C12
48	j	202	PEE	O5-C30-O3-C3
49	J	403	PLX	C11-C10-C9-C8
49	g	201	PLX	C17-C18-C19-C20
52	l	701	CDL	CB2-C1-CA2-OA2
52	l	701	CDL	CA2-C1-CB2-OB2
52	o	201	CDL	CA2-C1-CB2-OB2
52	u	201	CDL	CA2-C1-CB2-OB2
52	k	101	CDL	OA7-CA5-OA6-CA4
48	l	703	PEE	O5-C30-O3-C3
49	g	201	PLX	C2-C1-N1-C1A
52	a	201	CDL	C71-CB7-OB8-CB6
52	s	401	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C35-C36-C37-C38
52	s	401	CDL	C33-C34-C35-C36
48	l	703	PEE	O3P-C1-C2-O2
52	s	401	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	O1-C1-CB2-OB2
49	g	201	PLX	O6-C4-C5-O8
52	l	702	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	OA6-CA4-CA6-OA8
52	s	401	CDL	OB6-CB4-CB6-OB8
52	u	201	CDL	OA6-CA4-CA6-OA8
52	V	201	CDL	C59-C60-C61-C62
52	V	201	CDL	C62-C63-C64-C65
52	k	101	CDL	C60-C61-C62-C63
49	a	202	PLX	C19-C20-C21-C22
52	V	201	CDL	C34-C35-C36-C37
52	l	701	CDL	C58-C59-C60-C61
52	l	702	CDL	C11-C12-C13-C14
48	j	201	PEE	C11-C10-O2-C2
52	r	504	CDL	C51-CB5-OB6-CB4
52	k	101	CDL	CA7-C31-C32-C33
52	k	101	CDL	C40-C41-C42-C43
48	V	202	PEE	C10-C11-C12-C13
52	u	201	CDL	CB5-C51-C52-C53
48	r	501	PEE	C17-C18-C19-C20
48	W	201	PEE	C10-C11-C12-C13
48	r	501	PEE	C10-C11-C12-C13
52	I	201	CDL	CA7-C31-C32-C33
52	a	201	CDL	CB5-C51-C52-C53
52	l	701	CDL	CB5-C51-C52-C53
52	l	702	CDL	CA7-C31-C32-C33
52	o	201	CDL	CB7-C71-C72-C73
53	J	401	NDP	C3D-C4D-C5D-O5D
52	k	101	CDL	C36-C37-C38-C39
52	o	201	CDL	OB7-CB5-OB6-CB4
48	B	303	PEE	C34-C35-C36-C37
48	V	202	PEE	C11-C12-C13-C14
49	g	201	PLX	C2-C1-N1-C1B
48	i	401	PEE	C10-C11-C12-C13
52	l	701	CDL	CB7-C71-C72-C73
52	a	201	CDL	OB9-CB7-OB8-CB6
52	s	401	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
50	C	304	UQ	C9-C11-C12-C13
52	V	201	CDL	O1-C1-CB2-OB2
52	a	201	CDL	O1-C1-CB2-OB2
52	l	701	CDL	O1-C1-CB2-OB2
52	o	201	CDL	O1-C1-CB2-OB2
52	o	201	CDL	C71-CB7-OB8-CB6
48	j	201	PEE	O5-C30-O3-C3
48	r	501	PEE	C15-C16-C17-C18
48	B	303	PEE	C17-C18-C19-C20
48	W	201	PEE	C17-C18-C19-C20
48	l	703	PEE	C37-C38-C39-C40
48	r	501	PEE	C41-C42-C43-C44
49	r	502	PLX	C7-C8-C9-C10
48	l	704	PEE	C11-C10-O2-C2
48	C	302	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O4P
48	r	501	PEE	C1-O3P-P-O4P
49	J	403	PLX	C2-O1-P1-O4
49	a	202	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O4
49	r	502	PLX	C3-O4-P1-O1
49	r	503	PLX	C2-O1-P1-O4
52	I	201	CDL	CA2-OA2-PA1-OA5
52	I	201	CDL	CB2-OB2-PB2-OB5
52	I	201	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB3-OB5-PB2-OB2
52	k	101	CDL	CA3-OA5-PA1-OA2
52	l	702	CDL	CA3-OA5-PA1-OA2
52	o	201	CDL	CA2-OA2-PA1-OA5
52	o	201	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CB3-OB5-PB2-OB2
52	r	504	CDL	CA2-OA2-PA1-OA5
52	r	504	CDL	CB3-OB5-PB2-OB2
52	s	401	CDL	CA2-OA2-PA1-OA5
52	u	201	CDL	CB2-OB2-PB2-OB5
52	u	201	CDL	CB3-OB5-PB2-OB2
53	J	401	NDP	C2D-C1D-N1N-C6N
52	V	201	CDL	C71-CB7-OB8-CB6
52	u	201	CDL	CB7-C71-C72-C73
52	s	401	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	O4-C10-O2-C2
52	r	504	CDL	OB7-CB5-OB6-CB4
52	I	201	CDL	C51-C52-C53-C54
52	l	701	CDL	C71-CB7-OB8-CB6
49	C	303	PLX	O6-C6-C7-C8
49	g	201	PLX	O8-C24-C25-C26
49	r	502	PLX	O6-C6-C7-C8
52	l	702	CDL	CB5-C51-C52-C53
48	C	302	PEE	C32-C33-C34-C35
48	j	201	PEE	C42-C43-C44-C45
52	k	101	CDL	C58-C59-C60-C61
52	s	401	CDL	C36-C37-C38-C39
52	s	401	CDL	C73-C74-C75-C76
48	j	202	PEE	C11-C10-O2-C2
48	W	201	PEE	C21-C22-C23-C24
48	l	703	PEE	C34-C35-C36-C37
52	V	201	CDL	C51-C52-C53-C54
52	a	201	CDL	C37-C38-C39-C40
52	k	101	CDL	C55-C56-C57-C58
52	l	701	CDL	C13-C14-C15-C16
52	l	701	CDL	C59-C60-C61-C62
52	l	701	CDL	C62-C63-C64-C65
52	r	504	CDL	C31-C32-C33-C34
52	s	401	CDL	C71-C72-C73-C74
52	u	201	CDL	C71-C72-C73-C74
48	V	202	PEE	C32-C33-C34-C35
48	l	703	PEE	C31-C32-C33-C34
48	r	501	PEE	C21-C22-C23-C24
49	a	202	PLX	C14-C15-C16-C17
52	a	201	CDL	C60-C61-C62-C63
52	k	101	CDL	C71-C72-C73-C74
52	l	701	CDL	C56-C57-C58-C59
52	l	702	CDL	C15-C16-C17-C18
52	l	702	CDL	C34-C35-C36-C37
52	l	702	CDL	C59-C60-C61-C62
52	u	201	CDL	C73-C74-C75-C76
48	j	202	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
49	a	202	PLX	C13-C14-C15-C16
49	j	203	PLX	C14-C15-C16-C17
49	r	502	PLX	C34-C35-C36-C37
49	r	503	PLX	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	C36-C37-C38-C39
48	B	303	PEE	C14-C15-C16-C17
48	l	704	PEE	C33-C34-C35-C36
49	C	303	PLX	C28-C29-C30-C31
49	J	403	PLX	C9-C10-C11-C12
49	J	403	PLX	C7-C8-C9-C10
49	r	503	PLX	C13-C14-C15-C16
52	V	201	CDL	C58-C59-C60-C61
52	l	701	CDL	C75-C76-C77-C78
49	J	403	PLX	C14-C15-C16-C17
49	g	201	PLX	C28-C29-C30-C31
49	j	203	PLX	C34-C35-C36-C37
52	V	201	CDL	C37-C38-C39-C40
52	l	701	CDL	C71-C72-C73-C74
52	l	701	CDL	C74-C75-C76-C77
52	l	701	CDL	CA7-C31-C32-C33
48	l	704	PEE	C20-C21-C22-C23
49	r	502	PLX	C33-C34-C35-C36
52	V	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C32-C33-C34-C35
52	o	201	CDL	C55-C56-C57-C58
52	o	201	CDL	C59-C60-C61-C62
52	s	401	CDL	C17-C18-C19-C20
49	g	201	PLX	C13-C14-C15-C16
49	r	503	PLX	C28-C29-C30-C31
52	a	201	CDL	C35-C36-C37-C38
52	l	702	CDL	C51-C52-C53-C54
48	r	501	PEE	C11-C12-C13-C14
49	J	403	PLX	C25-C26-C27-C28
49	j	203	PLX	C31-C32-C33-C34
51	X	201	8Q1	C12-C13-C14-C15
52	V	201	CDL	C55-C56-C57-C58
52	a	201	CDL	C22-C23-C24-C25
52	k	101	CDL	C21-C22-C23-C24
52	l	701	CDL	C52-C53-C54-C55
52	o	201	CDL	C60-C61-C62-C63
52	r	504	CDL	C83-C84-C85-C86
52	s	401	CDL	C51-C52-C53-C54
49	J	403	PLX	C33-C34-C35-C36
49	j	203	PLX	C7-C8-C9-C10
49	r	503	PLX	C12-C13-C14-C15
52	l	702	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C74-C75-C76-C77
52	s	401	CDL	C55-C56-C57-C58
52	I	201	CDL	C51-CB5-OB6-CB4
49	C	303	PLX	C13-C14-C15-C16
49	C	303	PLX	C10-C11-C12-C13
49	J	403	PLX	C27-C28-C29-C30
49	a	202	PLX	C16-C17-C18-C19
49	a	202	PLX	C25-C26-C27-C28
49	g	201	PLX	C18-C19-C20-C21
49	g	201	PLX	C32-C33-C34-C35
49	r	503	PLX	C25-C26-C27-C28
52	s	401	CDL	C31-C32-C33-C34
52	s	401	CDL	CB5-C51-C52-C53
48	i	401	PEE	C23-C24-C25-C26
48	l	703	PEE	C21-C22-C23-C24
49	g	201	PLX	C33-C34-C35-C36
49	r	503	PLX	C31-C32-C33-C34
49	r	503	PLX	C32-C33-C34-C35
52	V	201	CDL	C35-C36-C37-C38
52	a	201	CDL	C52-C53-C54-C55
52	k	101	CDL	C32-C33-C34-C35
52	k	101	CDL	C56-C57-C58-C59
52	l	701	CDL	C73-C74-C75-C76
52	o	201	CDL	C34-C35-C36-C37
52	r	504	CDL	C19-C20-C21-C22
52	r	504	CDL	C63-C64-C65-C66
52	s	401	CDL	C11-C12-C13-C14
52	s	401	CDL	C75-C76-C77-C78
52	u	201	CDL	C54-C55-C56-C57
48	B	303	PEE	O3P-C1-C2-C3
50	J	402	UQ	C9-C11-C12-C13
48	B	303	PEE	C31-C32-C33-C34
48	j	202	PEE	C11-C12-C13-C14
49	r	502	PLX	C27-C28-C29-C30
49	r	502	PLX	C28-C29-C30-C31
52	I	201	CDL	C71-C72-C73-C74
52	k	101	CDL	C39-C40-C41-C42
52	l	701	CDL	C42-C43-C44-C45
52	o	201	CDL	C13-C14-C15-C16
52	o	201	CDL	C37-C38-C39-C40
52	r	504	CDL	C32-C33-C34-C35
52	r	504	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
52	r	504	CDL	C71-C72-C73-C74
52	s	401	CDL	C52-C53-C54-C55
48	W	201	PEE	C12-C13-C14-C15
49	g	201	PLX	C10-C11-C12-C13
49	r	502	PLX	C14-C15-C16-C17
52	o	201	CDL	C56-C57-C58-C59
52	s	401	CDL	C59-C60-C61-C62
52	V	201	CDL	CB7-C71-C72-C73
52	s	401	CDL	CB7-C71-C72-C73
52	V	201	CDL	OB9-CB7-OB8-CB6
52	l	701	CDL	OB9-CB7-OB8-CB6
49	j	203	PLX	C33-C34-C35-C36
48	j	202	PEE	C14-C15-C16-C17
48	l	704	PEE	C31-C32-C33-C34
49	r	502	PLX	C30-C31-C32-C33
52	r	504	CDL	C62-C63-C64-C65
49	r	503	PLX	C10-C11-C12-C13
52	V	201	CDL	C71-C72-C73-C74
52	l	702	CDL	CB7-C71-C72-C73
52	o	201	CDL	OB9-CB7-OB8-CB6
49	J	403	PLX	C31-C32-C33-C34
52	l	701	CDL	C19-C20-C21-C22
49	C	303	PLX	C3-C4-C5-O8
52	k	101	CDL	CB3-CB4-CB6-OB8
52	o	201	CDL	C52-C53-C54-C55
48	r	501	PEE	C11-C10-O2-C2
49	a	202	PLX	C10-C11-C12-C13
52	s	401	CDL	C54-C55-C56-C57
49	g	201	PLX	O7-C6-C7-C8
48	C	302	PEE	C13-C14-C15-C16
49	C	303	PLX	C33-C34-C35-C36
49	J	403	PLX	C13-C14-C15-C16
52	o	201	CDL	C33-C34-C35-C36
48	B	303	PEE	C35-C36-C37-C38
48	i	401	PEE	C35-C36-C37-C38
49	C	303	PLX	C19-C20-C21-C22
52	r	504	CDL	C14-C15-C16-C17
48	l	703	PEE	C32-C33-C34-C35
52	a	201	CDL	C73-C74-C75-C76
52	s	401	CDL	C14-C15-C16-C17
48	C	302	PEE	C43-C44-C45-C46
52	I	201	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C79-C80-C81-C82
48	r	501	PEE	O4-C10-O2-C2
52	I	201	CDL	OB7-CB5-OB6-CB4
50	J	402	UQ	C17-C18-C19-C21
52	o	201	CDL	C75-C76-C77-C78
52	r	504	CDL	C43-C44-C45-C46
52	r	504	CDL	C54-C55-C56-C57
48	C	302	PEE	C42-C43-C44-C45
49	J	403	PLX	C29-C30-C31-C32
49	a	202	PLX	C33-C34-C35-C36
49	g	201	PLX	C27-C28-C29-C30
49	j	203	PLX	C29-C30-C31-C32
52	l	702	CDL	C55-C56-C57-C58
52	l	702	CDL	C75-C76-C77-C78
49	g	201	PLX	C2-C1-N1-C1C
52	a	201	CDL	CA5-C11-C12-C13
49	j	203	PLX	C16-C17-C18-C19
52	a	201	CDL	C11-C12-C13-C14
52	a	201	CDL	C74-C75-C76-C77
52	s	401	CDL	C11-CA5-OA6-CA4
52	o	201	CDL	C82-C83-C84-C85
52	r	504	CDL	C41-C42-C43-C44
52	s	401	CDL	C16-C17-C18-C19
52	r	504	CDL	CA7-C31-C32-C33
49	g	201	PLX	C30-C31-C32-C33
49	r	502	PLX	C11-C10-C9-C8
49	a	202	PLX	C9-C10-C11-C12
48	i	401	PEE	C11-C12-C13-C14
49	j	203	PLX	C9-C10-C11-C12
48	V	202	PEE	C35-C36-C37-C38
52	l	702	CDL	OB7-CB5-OB6-CB4
52	k	101	CDL	CB5-C51-C52-C53
48	l	704	PEE	C31-C30-O3-C3
52	k	101	CDL	C71-CB7-OB8-CB6
52	r	504	CDL	C23-C24-C25-C26
52	r	504	CDL	C75-C76-C77-C78
48	B	303	PEE	C12-C13-C14-C15
52	l	702	CDL	C33-C34-C35-C36
52	V	201	CDL	C12-C13-C14-C15
52	a	201	CDL	C39-C40-C41-C42
52	u	201	CDL	C52-C53-C54-C55
49	r	503	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C16-C17-C18-C19
52	l	701	CDL	C82-C83-C84-C85
52	k	101	CDL	C15-C16-C17-C18
52	V	201	CDL	C51-CB5-OB6-CB4
52	l	701	CDL	C11-CA5-OA6-CA4
52	l	701	CDL	C51-CB5-OB6-CB4
52	l	702	CDL	C51-CB5-OB6-CB4
52	o	201	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	C13-C14-C15-C16
49	a	202	PLX	C35-C36-C37-C38
48	j	201	PEE	C13-C14-C15-C16
49	C	303	PLX	C7-C8-C9-C10
49	J	403	PLX	C10-C11-C12-C13
52	V	201	CDL	OB7-CB5-OB6-CB4
52	l	701	CDL	OA7-CA5-OA6-CA4
49	r	503	PLX	C15-C16-C17-C18
52	r	504	CDL	C59-C60-C61-C62
49	C	303	PLX	O6-C4-C5-O8
52	k	101	CDL	OB6-CB4-CB6-OB8
52	l	701	CDL	OA6-CA4-CA6-OA8
49	a	202	PLX	C30-C31-C32-C33
52	o	201	CDL	C51-C52-C53-C54
48	V	202	PEE	C31-C32-C33-C34
49	r	502	PLX	C12-C13-C14-C15
49	r	503	PLX	C7-C8-C9-C10
52	l	701	CDL	C80-C81-C82-C83
52	o	201	CDL	C62-C63-C64-C65
52	s	401	CDL	C35-C36-C37-C38
48	C	302	PEE	C35-C36-C37-C38
48	j	201	PEE	C15-C16-C17-C18
50	C	304	UQ	C18-C19-C21-C22
48	W	201	PEE	C13-C14-C15-C16
49	j	203	PLX	C27-C28-C29-C30
48	V	202	PEE	C17-C18-C19-C20
52	l	702	CDL	C52-C53-C54-C55
52	o	201	CDL	C11-C12-C13-C14
48	V	202	PEE	C31-C30-O3-C3
52	k	101	CDL	OB9-CB7-OB8-CB6
52	l	701	CDL	OB7-CB5-OB6-CB4
52	s	401	CDL	OA7-CA5-OA6-CA4
48	l	704	PEE	C12-C13-C14-C15
48	r	501	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C62-C63-C64-C65
48	j	201	PEE	C38-C39-C40-C41
48	i	401	PEE	C1-O3P-P-O4P
49	r	502	PLX	C2-O1-P1-O4
52	a	201	CDL	CB2-OB2-PB2-OB5
52	o	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CA2-OA2-PA1-OA5
52	u	201	CDL	CA3-OA5-PA1-OA2
48	W	201	PEE	C24-C25-C26-C27
52	k	101	CDL	C37-C38-C39-C40
52	l	701	CDL	C17-C18-C19-C20
48	j	201	PEE	C21-C22-C23-C24
48	l	704	PEE	O5-C30-O3-C3
48	l	703	PEE	O3P-C1-C2-C3
52	a	201	CDL	OA5-CA3-CA4-CA6
52	s	401	CDL	OA5-CA3-CA4-CA6
52	r	504	CDL	C52-C53-C54-C55
52	u	201	CDL	C51-C52-C53-C54
49	r	503	PLX	C14-C15-C16-C17
52	k	101	CDL	C59-C60-C61-C62
52	l	702	CDL	C57-C58-C59-C60
49	r	503	PLX	C16-C17-C18-C19
52	k	101	CDL	C74-C75-C76-C77
52	o	201	CDL	C83-C84-C85-C86
48	W	201	PEE	C11-C12-C13-C14
49	g	201	PLX	C25-C26-C27-C28
48	W	201	PEE	C31-C30-O3-C3
52	I	201	CDL	CA2-C1-CB2-OB2
52	l	702	CDL	C62-C63-C64-C65
52	V	201	CDL	C75-C76-C77-C78
52	l	702	CDL	C38-C39-C40-C41
52	r	504	CDL	C84-C85-C86-C87
48	B	303	PEE	C20-C21-C22-C23
49	C	303	PLX	C31-C32-C33-C34
52	a	201	CDL	C20-C21-C22-C23
52	o	201	CDL	C36-C37-C38-C39
48	C	302	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
49	g	201	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
52	o	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	CB3-CB4-CB6-OB8
52	s	401	CDL	CB3-CB4-CB6-OB8
52	u	201	CDL	CA3-CA4-CA6-OA8
52	a	201	CDL	C75-C76-C77-C78
52	l	702	CDL	C64-C65-C66-C67
49	r	502	PLX	C4-C5-O8-C24
52	u	201	CDL	C75-C76-C77-C78
52	s	401	CDL	C18-C19-C20-C21
49	J	403	PLX	C36-C37-C38-C39
49	j	203	PLX	C11-C12-C13-C14
52	l	702	CDL	C41-C42-C43-C44
48	r	501	PEE	C36-C37-C38-C39
48	C	302	PEE	C34-C35-C36-C37
49	a	202	PLX	C7-C8-C9-C10
48	j	202	PEE	C15-C16-C17-C18
49	j	203	PLX	C25-C26-C27-C28
52	k	101	CDL	C14-C15-C16-C17
52	l	702	CDL	C21-C22-C23-C24
48	j	201	PEE	C34-C35-C36-C37
49	j	203	PLX	C12-C13-C14-C15
52	a	201	CDL	C71-C72-C73-C74
52	u	201	CDL	C57-C58-C59-C60
48	l	703	PEE	C13-C14-C15-C16
52	l	702	CDL	C17-C18-C19-C20
52	k	101	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C11-C10-C9-C8
49	g	201	PLX	C16-C17-C18-C19
48	V	202	PEE	C33-C34-C35-C36
49	j	203	PLX	C18-C19-C20-C21
52	V	201	CDL	C72-C73-C74-C75
52	u	201	CDL	C72-C73-C74-C75
48	B	303	PEE	C31-C30-O3-C3
48	r	501	PEE	C31-C30-O3-C3
48	W	201	PEE	O3P-C1-C2-O2
49	J	403	PLX	O4-C3-C4-O6
49	r	502	PLX	O4-C3-C4-O6
52	k	101	CDL	OB5-CB3-CB4-OB6
52	l	701	CDL	OA5-CA3-CA4-OA6
52	o	201	CDL	C57-C58-C59-C60
48	V	202	PEE	O5-C30-O3-C3
52	a	201	CDL	C54-C55-C56-C57
48	j	202	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C24-C25-C26-C27
52	a	201	CDL	C84-C85-C86-C87
52	l	702	CDL	C32-C33-C34-C35
52	o	201	CDL	OB6-CB4-CB6-OB8
49	C	303	PLX	C11-C12-C13-C14
52	o	201	CDL	OA7-CA5-OA6-CA4
48	j	202	PEE	C12-C13-C14-C15
52	l	701	CDL	C31-C32-C33-C34
52	l	701	CDL	C51-C52-C53-C54
50	C	304	UQ	C17-C18-C19-C20
52	k	101	CDL	C52-C53-C54-C55
48	B	303	PEE	C36-C37-C38-C39
52	r	504	CDL	C72-C71-CB7-OB8
48	W	201	PEE	O5-C30-O3-C3
49	r	502	PLX	C31-C32-C33-C34
49	C	303	PLX	C14-C15-C16-C17
52	k	101	CDL	C33-C34-C35-C36
52	I	201	CDL	C52-C53-C54-C55
52	V	201	CDL	C73-C74-C75-C76
52	l	702	CDL	C77-C78-C79-C80
48	B	303	PEE	C38-C39-C40-C41
48	r	501	PEE	C38-C39-C40-C41
48	C	302	PEE	O3P-C1-C2-C3
52	I	201	CDL	OB5-CB3-CB4-CB6
52	V	201	CDL	OA5-CA3-CA4-CA6
52	k	101	CDL	OA5-CA3-CA4-CA6
52	u	201	CDL	OA5-CA3-CA4-CA6
48	l	703	PEE	C30-C31-C32-C33
52	r	504	CDL	CA5-C11-C12-C13
48	C	302	PEE	O4P-C4-C5-N
48	l	704	PEE	O4P-C4-C5-N
48	C	302	PEE	C12-C13-C14-C15
49	C	303	PLX	C25-C26-C27-C28
52	l	702	CDL	C58-C59-C60-C61
52	r	504	CDL	C77-C78-C79-C80
52	l	702	CDL	C60-C61-C62-C63
48	i	401	PEE	C12-C13-C14-C15
48	j	202	PEE	C33-C34-C35-C36
52	V	201	CDL	C54-C55-C56-C57
52	l	702	CDL	C78-C79-C80-C81
52	k	101	CDL	C64-C65-C66-C67
48	j	201	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C11-C12-C13-C14
52	r	504	CDL	C13-C14-C15-C16
52	l	702	CDL	C14-C15-C16-C17
52	s	401	CDL	C32-C33-C34-C35
52	o	201	CDL	C39-C40-C41-C42
48	j	202	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8
52	l	701	CDL	CA3-CA4-CA6-OA8
52	l	702	CDL	CA3-CA4-CA6-OA8
49	C	303	PLX	C12-C13-C14-C15
52	V	201	CDL	C36-C37-C38-C39
52	k	101	CDL	C13-C14-C15-C16
48	l	704	PEE	C22-C23-C24-C25
52	o	201	CDL	C17-C18-C19-C20
52	o	201	CDL	C84-C85-C86-C87
49	r	503	PLX	C18-C19-C20-C21
48	r	501	PEE	C4-O4P-P-O3P
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C3-O4-P1-O1
49	a	202	PLX	C5-C4-O6-C6
49	r	503	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
52	k	101	CDL	CB2-OB2-PB2-OB5
48	l	703	PEE	C10-C11-C12-C13
48	r	501	PEE	O5-C30-O3-C3
47	A	503	NAI	C2D-C1D-N1N-C2N
49	C	303	PLX	O9-C24-C25-C26
52	l	701	CDL	C12-C13-C14-C15
48	B	303	PEE	O3P-C1-C2-O2
49	r	503	PLX	O4-C3-C4-O6
52	V	201	CDL	OB5-CB3-CB4-OB6
52	l	701	CDL	OB5-CB3-CB4-OB6
52	u	201	CDL	OB5-CB3-CB4-OB6
49	a	202	PLX	C28-C29-C30-C31
52	l	702	CDL	C84-C85-C86-C87
52	s	401	CDL	C77-C78-C79-C80
48	l	703	PEE	C15-C16-C17-C18
48	B	303	PEE	O5-C30-O3-C3
49	r	502	PLX	C10-C11-C12-C13
52	V	201	CDL	C44-C45-C46-C47
52	l	701	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
52	s	401	CDL	O1-C1-CB2-OB2
52	r	504	CDL	C35-C36-C37-C38
52	V	201	CDL	OB6-CB4-CB6-OB8
52	r	504	CDL	OA6-CA4-CA6-OA8
52	V	201	CDL	C64-C65-C66-C67
52	s	401	CDL	C40-C41-C42-C43
52	k	101	CDL	CA2-C1-CB2-OB2
49	r	503	PLX	C27-C28-C29-C30
51	G	201	8Q1	C7-C8-C9-C10
52	l	702	CDL	C82-C83-C84-C85
52	o	201	CDL	C42-C43-C44-C45
49	r	502	PLX	C16-C17-C18-C19
48	V	202	PEE	C2-C1-O3P-P
52	k	101	CDL	CA4-CA3-OA5-PA1
48	r	501	PEE	C40-C41-C42-C43
48	j	201	PEE	C32-C33-C34-C35
49	J	403	PLX	C28-C29-C30-C31
52	o	201	CDL	C12-C13-C14-C15
48	i	401	PEE	C18-C19-C20-C21
51	G	201	8Q1	O4-C1-S44-C43
52	a	201	CDL	C76-C77-C78-C79
52	r	504	CDL	C64-C65-C66-C67
48	r	501	PEE	C33-C34-C35-C36
49	j	203	PLX	C10-C11-C12-C13
52	a	201	CDL	C64-C65-C66-C67
49	g	201	PLX	C12-C13-C14-C15
48	V	202	PEE	C18-C19-C20-C21
49	r	502	PLX	C6-C7-C8-C9
49	g	201	PLX	O6-C6-C7-C8
49	j	203	PLX	O6-C6-C7-C8
48	W	201	PEE	O3P-C1-C2-C3
49	J	403	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
52	I	201	CDL	OA5-CA3-CA4-CA6
52	l	701	CDL	OA5-CA3-CA4-CA6
52	u	201	CDL	OB5-CB3-CB4-CB6
51	X	201	8Q1	C9-C10-C11-C12
52	s	401	CDL	C15-C16-C17-C18
52	r	504	CDL	C55-C56-C57-C58
52	r	504	CDL	C15-C16-C17-C18
52	r	504	CDL	C12-C13-C14-C15
48	B	303	PEE	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	C63-C64-C65-C66
52	a	201	CDL	C82-C83-C84-C85
52	V	201	CDL	C43-C44-C45-C46
51	G	201	8Q1	C6-C1-S44-C43
52	V	201	CDL	CA6-CA4-OA6-CA5
48	r	501	PEE	C14-C15-C16-C17
52	a	201	CDL	C38-C39-C40-C41
48	r	501	PEE	C44-C45-C46-C47
52	V	201	CDL	CA4-CA3-OA5-PA1
52	r	504	CDL	C1-CB2-OB2-PB2
48	C	302	PEE	O3P-C1-C2-O2
48	j	201	PEE	O3P-C1-C2-O2
52	I	201	CDL	OB5-CB3-CB4-OB6
52	l	702	CDL	OA5-CA3-CA4-OA6
48	l	703	PEE	C33-C34-C35-C36
51	G	201	8Q1	C12-C13-C14-C15
49	C	303	PLX	C9-C10-C11-C12
48	l	703	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
52	I	201	CDL	C71-CB7-OB8-CB6
52	k	101	CDL	C20-C21-C22-C23
53	J	401	NDP	C5B-O5B-PA-O3
52	a	201	CDL	C18-C19-C20-C21
48	l	704	PEE	C15-C16-C17-C18
52	l	702	CDL	C54-C55-C56-C57
52	l	701	CDL	C37-C38-C39-C40
53	J	401	NDP	PN-O3-PA-O1A
57	w	401	ADP	PB-O3A-PA-O1A
49	a	202	PLX	C18-C19-C20-C21
52	k	101	CDL	C84-C85-C86-C87
52	k	101	CDL	C62-C63-C64-C65
48	l	704	PEE	C14-C15-C16-C17
52	l	701	CDL	CA2-OA2-PA1-OA5
52	l	701	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CA2-OA2-PA1-OA5
53	J	401	NDP	O4D-C1D-N1N-C6N
48	l	703	PEE	C11-C12-C13-C14
49	J	403	PLX	C16-C17-C18-C19
49	j	203	PLX	C19-C20-C21-C22
52	l	701	CDL	C24-C25-C26-C27
52	V	201	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
52	l	701	CDL	CB4-CB3-OB5-PB2
52	V	201	CDL	C14-C15-C16-C17
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
48	C	302	PEE	C1-O3P-P-O2P
48	W	201	PEE	C4-O4P-P-O2P
48	i	401	PEE	C1-O3P-P-O1P
48	l	704	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C4-O4P-P-O2P
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C2-O1-P1-O3
49	g	201	PLX	C2-O1-P1-O3
49	j	203	PLX	C3-O4-P1-O3
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
52	I	201	CDL	CB3-OB5-PB2-OB4
52	V	201	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CB2-OB2-PB2-OB4
52	k	101	CDL	CA3-OA5-PA1-OA4
52	k	101	CDL	CB2-OB2-PB2-OB4
52	l	701	CDL	CB3-OB5-PB2-OB3
52	l	701	CDL	CB3-OB5-PB2-OB4
52	o	201	CDL	CA2-OA2-PA1-OA4
52	o	201	CDL	CB2-OB2-PB2-OB4
52	o	201	CDL	CB3-OB5-PB2-OB3
52	o	201	CDL	CB3-OB5-PB2-OB4
52	r	504	CDL	CA2-OA2-PA1-OA4
52	s	401	CDL	CA2-OA2-PA1-OA4
57	w	401	ADP	C5'-O5'-PA-O1A
48	V	202	PEE	O3P-C1-C2-C3
48	j	201	PEE	O3P-C1-C2-C3
48	l	704	PEE	O3P-C1-C2-C3
49	r	502	PLX	O4-C3-C4-C5
52	V	201	CDL	OB5-CB3-CB4-CB6
52	l	702	CDL	OA5-CA3-CA4-CA6
48	l	703	PEE	C44-C45-C46-C47
52	l	702	CDL	C39-C40-C41-C42
52	I	201	CDL	OB9-CB7-OB8-CB6
52	V	201	CDL	C33-C34-C35-C36
52	V	201	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C31-C32-C33-C34
49	C	303	PLX	C1-C2-O1-P1
49	a	202	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
52	o	201	CDL	C32-C31-CA7-OA8
48	j	201	PEE	C14-C15-C16-C17
48	j	202	PEE	C24-C25-C26-C27
52	V	201	CDL	C74-C75-C76-C77
48	V	202	PEE	O3P-C1-C2-O2
48	l	704	PEE	O3P-C1-C2-O2
52	l	702	CDL	C32-C31-CA7-OA8
49	g	201	PLX	C11-C12-C13-C14
49	C	303	PLX	C2-C1-N1-C1A
47	A	503	NAI	C2D-C1D-N1N-C6N
48	V	202	PEE	C13-C14-C15-C16
48	j	201	PEE	C44-C45-C46-C47
48	l	704	PEE	C1-C2-C3-O3
49	J	403	PLX	N1-C1-C2-O1
52	l	702	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	O2-C2-C3-O3
48	j	202	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
49	a	202	PLX	O6-C4-C5-O8
52	l	702	CDL	OB6-CB4-CB6-OB8
48	j	202	PEE	C13-C14-C15-C16
52	l	701	CDL	C32-C33-C34-C35
52	o	201	CDL	C54-C55-C56-C57
48	i	401	PEE	C24-C25-C26-C27
52	o	201	CDL	C64-C65-C66-C67
48	i	401	PEE	C14-C15-C16-C17
52	o	201	CDL	C73-C74-C75-C76
48	l	703	PEE	C42-C43-C44-C45
49	j	203	PLX	O8-C24-C25-C26
49	C	303	PLX	C16-C17-C18-C19
52	k	101	CDL	C41-C42-C43-C44
48	r	501	PEE	C18-C19-C20-C21
49	r	503	PLX	C11-C10-C9-C8
52	r	504	CDL	C36-C37-C38-C39
47	A	503	NAI	O4D-C1D-N1N-C2N
48	B	303	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
51	X	201	8Q1	C11-C12-C13-C14
52	a	201	CDL	C14-C15-C16-C17
52	r	504	CDL	C53-C54-C55-C56
52	k	101	CDL	C51-C52-C53-C54
52	l	701	CDL	C39-C40-C41-C42
48	l	703	PEE	C3-C2-O2-C10
52	k	101	CDL	OB5-CB3-CB4-CB6
52	o	201	CDL	OA5-CA3-CA4-CA6
52	o	201	CDL	C21-C22-C23-C24
52	r	504	CDL	CB5-C51-C52-C53
49	a	202	PLX	C36-C37-C38-C39
46	A	502	FMN	C5'-O5'-P-O1P
52	V	201	CDL	OA5-CA3-CA4-OA6
52	a	201	CDL	OA5-CA3-CA4-OA6
52	o	201	CDL	OA5-CA3-CA4-OA6
52	V	201	CDL	C32-C33-C34-C35
52	s	401	CDL	C83-C84-C85-C86
52	r	504	CDL	OB6-CB4-CB6-OB8
48	l	704	PEE	C4-O4P-P-O3P
49	g	201	PLX	C3-O4-P1-O1
52	r	504	CDL	CA3-OA5-PA1-OA2
52	s	401	CDL	CB3-OB5-PB2-OB2
53	J	401	NDP	C3B-C4B-C5B-O5B
48	l	703	PEE	C1-C2-C3-O3
52	r	504	CDL	CA3-CA4-CA6-OA8
49	r	503	PLX	C19-C20-C21-C22
52	l	701	CDL	C23-C24-C25-C26
49	r	502	PLX	C35-C36-C37-C38
49	j	203	PLX	C26-C27-C28-C29
52	l	701	CDL	C16-C17-C18-C19
52	k	101	CDL	C1-CB2-OB2-PB2
52	r	504	CDL	CB4-CB3-OB5-PB2
48	j	201	PEE	C22-C23-C24-C25
52	o	201	CDL	C61-C62-C63-C64
52	V	201	CDL	CA5-C11-C12-C13
48	l	704	PEE	C18-C19-C20-C21
49	C	303	PLX	C34-C35-C36-C37
49	g	201	PLX	C19-C20-C21-C22
52	l	702	CDL	C43-C44-C45-C46
48	B	303	PEE	C32-C33-C34-C35
48	W	201	PEE	C19-C20-C21-C22
48	i	401	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C11-C10-C9-C8
48	l	704	PEE	C23-C24-C25-C26
52	a	201	CDL	C31-C32-C33-C34
49	J	403	PLX	C24-C25-C26-C27
48	V	202	PEE	C30-C31-C32-C33
52	a	201	CDL	C12-C13-C14-C15
48	j	202	PEE	C23-C24-C25-C26
48	l	703	PEE	C40-C41-C42-C43
49	a	202	PLX	C29-C30-C31-C32
52	l	702	CDL	C12-C11-CA5-OA6
52	s	401	CDL	C61-C62-C63-C64
52	k	101	CDL	C1-CA2-OA2-PA1
48	r	501	PEE	C32-C33-C34-C35
51	G	201	8Q1	N41-C42-C43-S44
52	o	201	CDL	C35-C36-C37-C38
49	r	503	PLX	C11-C12-C13-C14
52	k	101	CDL	C44-C45-C46-C47
48	C	302	PEE	C15-C16-C17-C18
52	l	701	CDL	C54-C55-C56-C57
48	B	303	PEE	C23-C24-C25-C26
49	a	202	PLX	C11-C12-C13-C14
51	G	201	8Q1	O27-C28-C29-C30
50	C	304	UQ	C22-C23-C24-C25
48	l	704	PEE	C21-C22-C23-C24
49	j	203	PLX	C30-C31-C32-C33
52	o	201	CDL	C44-C45-C46-C47
48	l	703	PEE	C39-C40-C41-C42
49	r	503	PLX	C24-C25-C26-C27
48	r	501	PEE	C31-C32-C33-C34
52	s	401	CDL	C72-C71-CB7-OB8
48	V	202	PEE	C38-C39-C40-C41
49	C	303	PLX	C5-C4-O6-C6
48	B	303	PEE	C11-C12-C13-C14
52	r	504	CDL	C44-C45-C46-C47
52	V	201	CDL	C52-C51-CB5-OB6
49	j	203	PLX	C36-C37-C38-C39
48	j	201	PEE	C40-C41-C42-C43
52	k	101	CDL	C75-C76-C77-C78
48	W	201	PEE	C34-C35-C36-C37
48	r	501	PEE	C34-C35-C36-C37
52	l	702	CDL	C61-C62-C63-C64
51	X	201	8Q1	C42-C43-S44-C1

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Mol	Chain	Res	Type	Atoms
52	o	201	CDL	C31-CA7-OA8-CA6
47	A	503	NAI	O4D-C1D-N1N-C6N
49	J	403	PLX	C32-C33-C34-C35
52	V	201	CDL	C40-C41-C42-C43
48	C	302	PEE	C37-C38-C39-C40
48	C	302	PEE	C16-C17-C18-C19
52	r	504	CDL	C39-C40-C41-C42
52	k	101	CDL	C78-C79-C80-C81
52	r	504	CDL	C72-C71-CB7-OB9
52	u	201	CDL	OB9-CB7-OB8-CB6
52	o	201	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C18-C19-C20-C21
48	W	201	PEE	C16-C17-C18-C19
48	j	202	PEE	C16-C17-C18-C19
48	l	704	PEE	C38-C39-C40-C41
49	C	303	PLX	O8-C24-C25-C26
52	k	101	CDL	C22-C23-C24-C25
48	B	303	PEE	C22-C23-C24-C25
48	l	704	PEE	C34-C35-C36-C37
52	a	201	CDL	C40-C41-C42-C43
52	o	201	CDL	C76-C77-C78-C79
52	l	701	CDL	OB5-CB3-CB4-CB6
51	X	201	8Q1	O33-C32-C34-O35
52	k	101	CDL	C43-C44-C45-C46
51	X	201	8Q1	C1-C6-C7-C8
48	j	201	PEE	C23-C24-C25-C26
52	l	701	CDL	C44-C45-C46-C47
48	i	401	PEE	C36-C37-C38-C39
48	B	303	PEE	O2-C10-C11-C12
52	a	201	CDL	C32-C31-CA7-OA8
52	r	504	CDL	C52-C51-CB5-OB6
52	o	201	CDL	C19-C20-C21-C22
52	k	101	CDL	CA2-OA2-PA1-OA5
52	l	701	CDL	CA3-OA5-PA1-OA2
49	C	303	PLX	C2-C1-N1-C1C
52	u	201	CDL	C72-C71-CB7-OB8
48	B	303	PEE	C39-C40-C41-C42
48	l	703	PEE	C19-C20-C21-C22
49	J	403	PLX	C35-C36-C37-C38
52	a	201	CDL	C53-C54-C55-C56
49	a	202	PLX	C27-C28-C29-C30
52	l	702	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
48	V	202	PEE	C16-C17-C18-C19
48	r	501	PEE	C16-C17-C18-C19
46	A	502	FMN	O4'-C4'-C5'-O5'
52	k	101	CDL	C52-C51-CB5-OB6
52	s	401	CDL	C12-C11-CA5-OA6
51	G	201	8Q1	C11-C12-C13-C14
49	j	203	PLX	C7-C6-O6-C4
52	V	201	CDL	CB3-CB4-CB6-OB8
49	r	502	PLX	C18-C19-C20-C21
49	a	202	PLX	C32-C33-C34-C35
49	a	202	PLX	C24-C25-C26-C27
52	o	201	CDL	CA7-C31-C32-C33
48	C	302	PEE	C38-C39-C40-C41
52	r	504	CDL	C61-C62-C63-C64
52	l	702	CDL	C44-C45-C46-C47
52	r	504	CDL	C12-C11-CA5-OA6
52	a	201	CDL	OB5-CB3-CB4-CB6
48	C	302	PEE	O3-C30-C31-C32
52	I	201	CDL	C12-C11-CA5-OA6
48	l	704	PEE	C32-C33-C34-C35
48	C	302	PEE	O2-C10-C11-C12
52	I	201	CDL	C72-C71-CB7-OB8
52	u	201	CDL	C52-C51-CB5-OB6
49	J	403	PLX	O9-C24-C25-C26
53	J	401	NDP	C2B-O2B-P2B-O2X
52	u	201	CDL	C71-CB7-OB8-CB6
52	l	701	CDL	C12-C11-CA5-OA7
52	l	701	CDL	C60-C61-C62-C63
52	o	201	CDL	C71-C72-C73-C74
50	C	304	UQ	C23-C24-C26-C27
48	W	201	PEE	C18-C19-C20-C21
52	a	201	CDL	C12-C11-CA5-OA6
52	r	504	CDL	C24-C25-C26-C27
50	C	304	UQ	C14-C16-C17-C18
52	s	401	CDL	C12-C13-C14-C15
52	l	702	CDL	C12-C13-C14-C15
47	A	503	NAI	O4B-C4B-C5B-O5B
48	r	501	PEE	C42-C43-C44-C45
50	C	304	UQ	C1-C2-O2-CM2
52	V	201	CDL	C12-C11-CA5-OA6
52	l	702	CDL	C72-C71-CB7-OB9
49	a	202	PLX	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C52-C51-CB5-OB7
52	r	504	CDL	C52-C51-CB5-OB7
52	l	701	CDL	C72-C71-CB7-OB8
48	i	401	PEE	C16-C17-C18-C19
52	a	201	CDL	C12-C11-CA5-OA7
52	a	201	CDL	C32-C31-CA7-OA9
52	r	504	CDL	C12-C11-CA5-OA7
52	s	401	CDL	C12-C11-CA5-OA7
49	r	502	PLX	C13-C14-C15-C16
49	g	201	PLX	C6-C7-C8-C9
48	B	303	PEE	C21-C22-C23-C24
52	r	504	CDL	OA7-CA5-OA6-CA4
52	I	201	CDL	C12-C11-CA5-OA7
52	u	201	CDL	C72-C71-CB7-OB9
48	i	401	PEE	C4-O4P-P-O2P
49	C	303	PLX	C2-C1-N1-C1B
52	a	201	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	CB3-OB5-PB2-OB3
52	r	504	CDL	CA3-OA5-PA1-OA3
48	j	202	PEE	C10-C11-C12-C13
52	a	201	CDL	C24-C25-C26-C27
48	B	303	PEE	O4-C10-C11-C12
48	C	302	PEE	O5-C30-C31-C32
52	V	201	CDL	C80-C81-C82-C83
48	i	401	PEE	C38-C39-C40-C41
48	l	703	PEE	C14-C15-C16-C17
48	B	303	PEE	C5-C4-O4P-P
48	l	704	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
49	J	403	PLX	C1-C2-O1-P1
52	u	201	CDL	C52-C51-CB5-OB7
52	I	201	CDL	C72-C71-CB7-OB9
48	l	703	PEE	C16-C17-C18-C19
48	C	302	PEE	C41-C42-C43-C44
48	C	302	PEE	O4-C10-C11-C12
51	G	201	8Q1	C28-C29-C32-C34
52	a	201	CDL	OB5-CB3-CB4-OB6
52	s	401	CDL	C13-C14-C15-C16
52	r	504	CDL	OB9-CB7-OB8-CB6
52	r	504	CDL	C42-C43-C44-C45
48	C	302	PEE	C44-C45-C46-C47
51	X	201	8Q1	C11-C10-C9-C8

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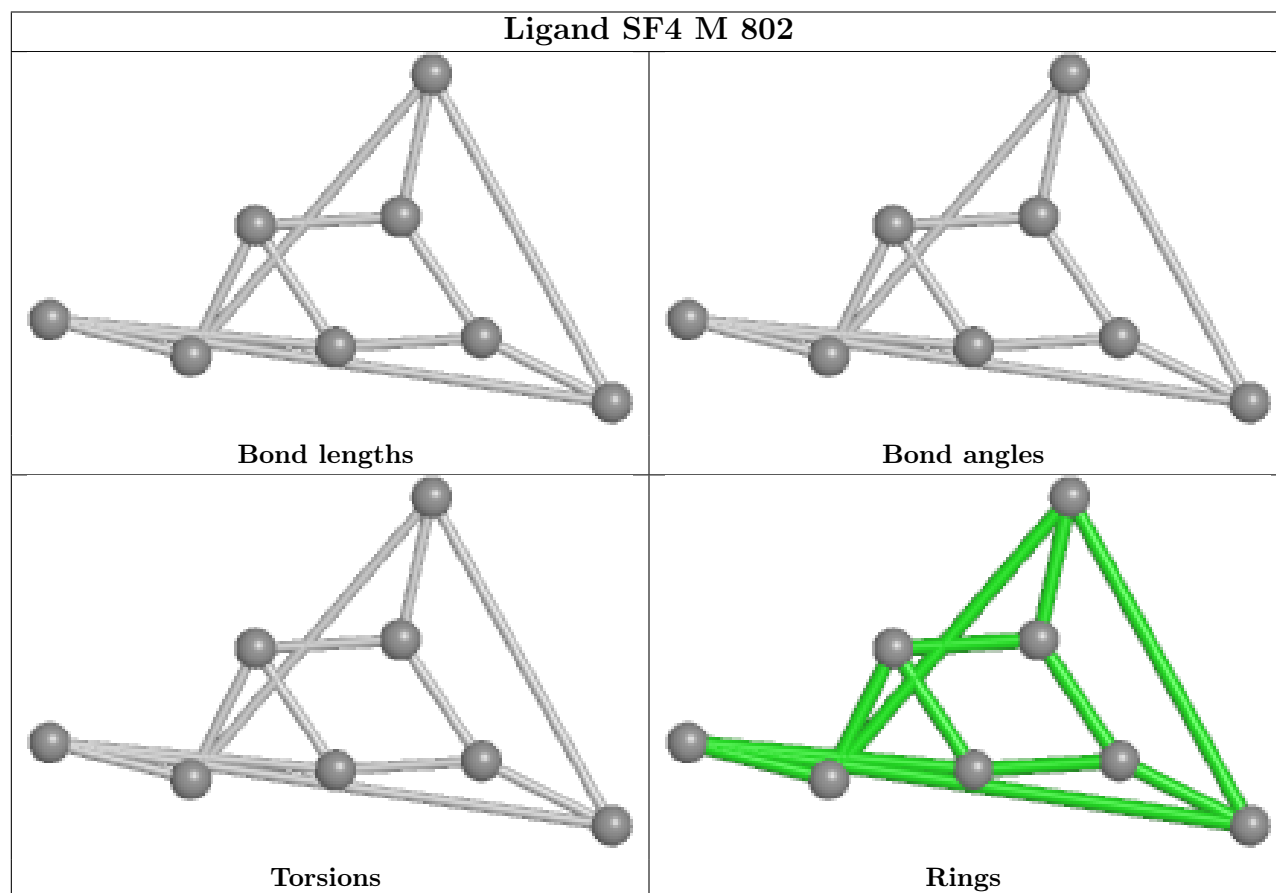
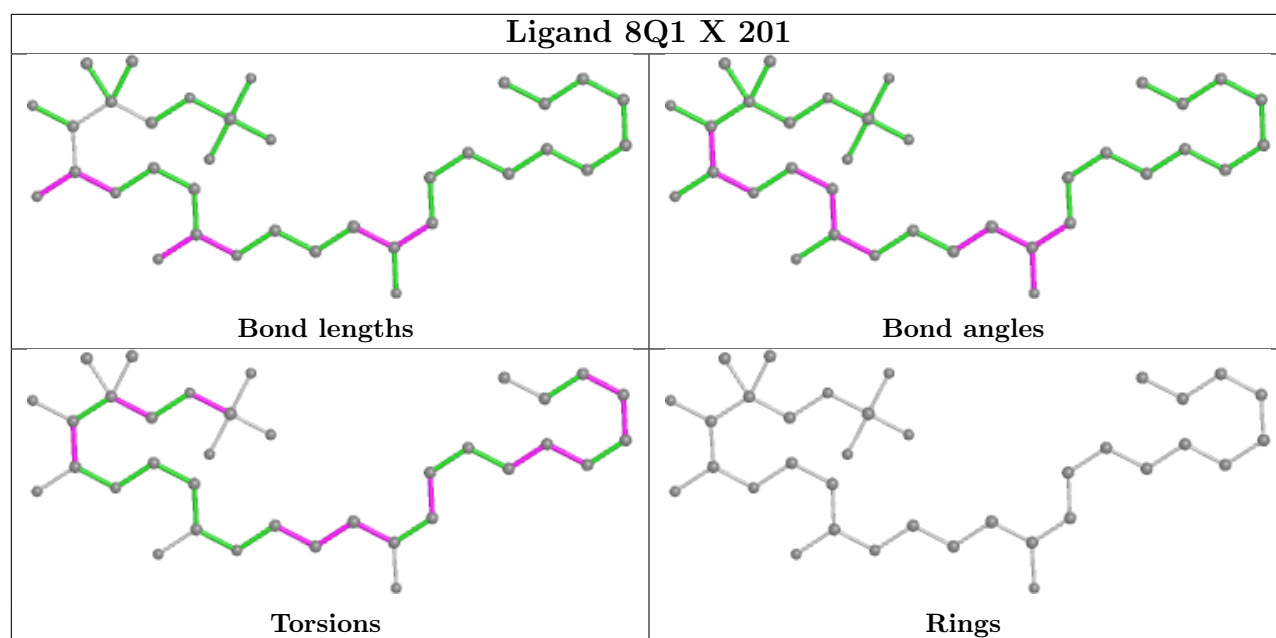
Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C12-C13-C14-C15
52	V	201	CDL	C12-C11-CA5-OA7
52	l	701	CDL	C72-C71-CB7-OB9
52	s	401	CDL	C57-C58-C59-C60
50	J	402	UQ	C20-C19-C21-C22

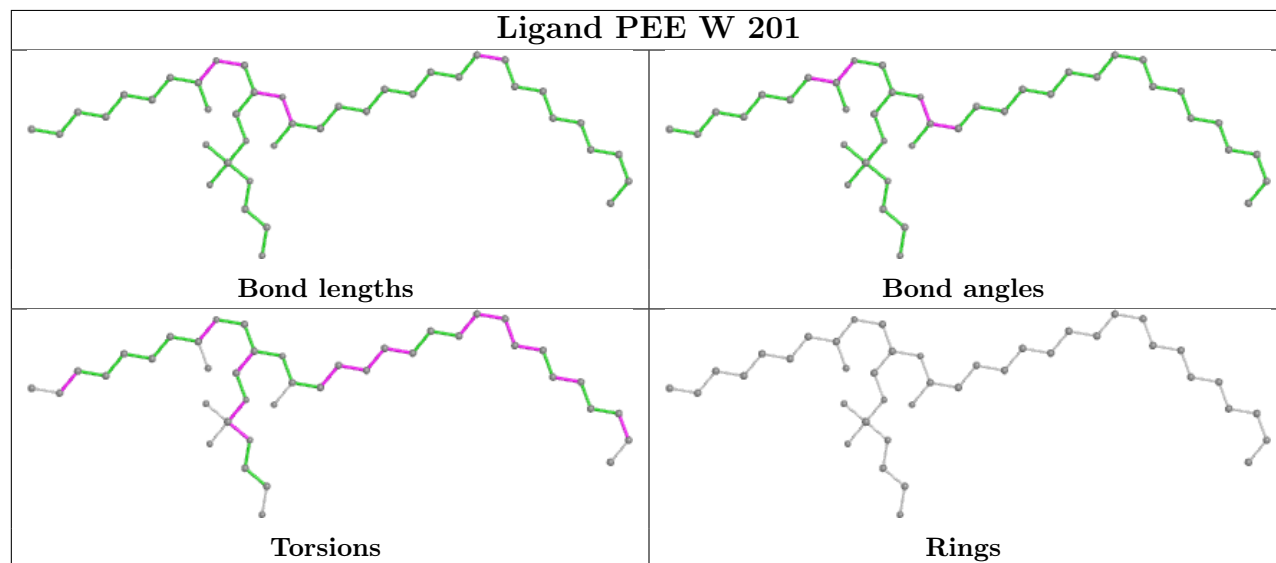
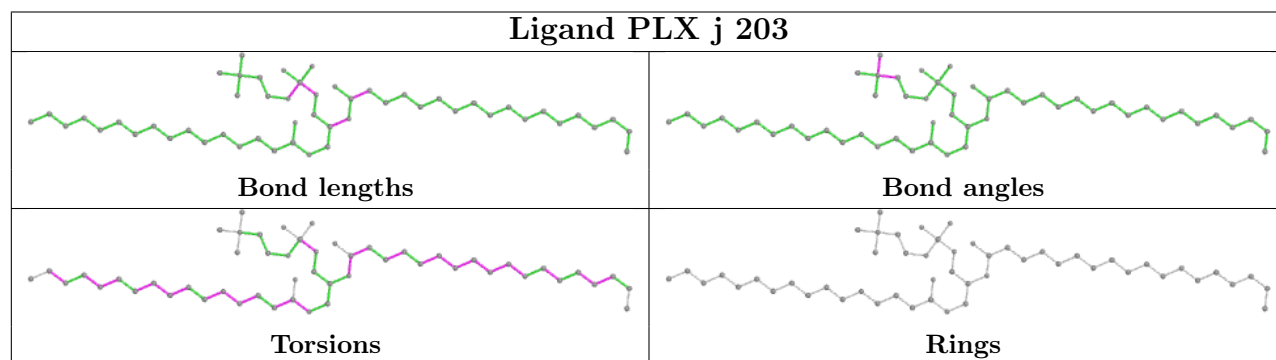
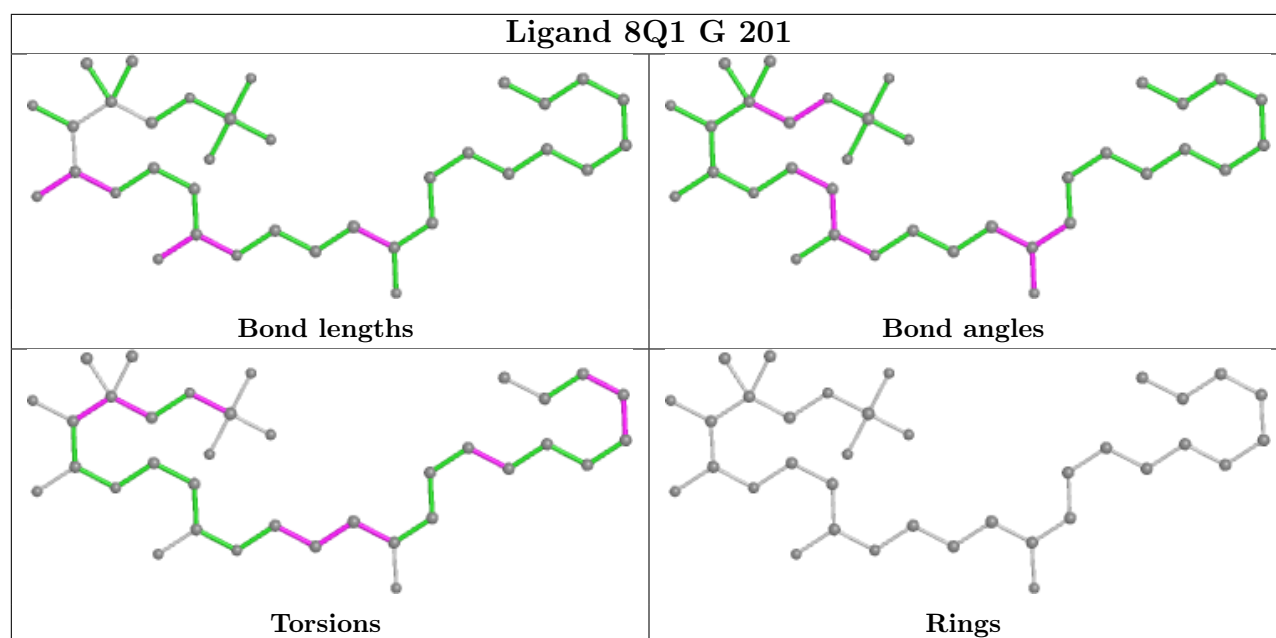
There are no ring outliers.

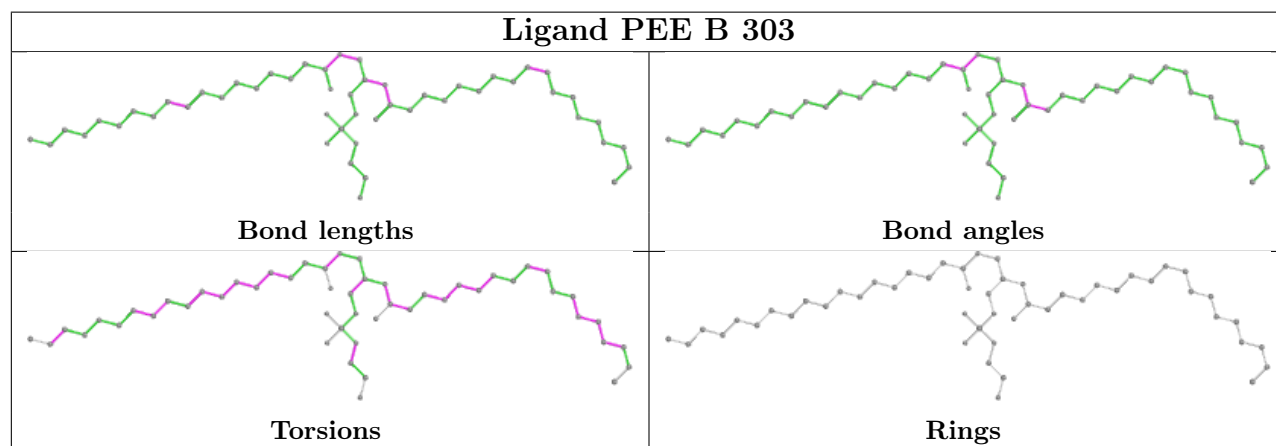
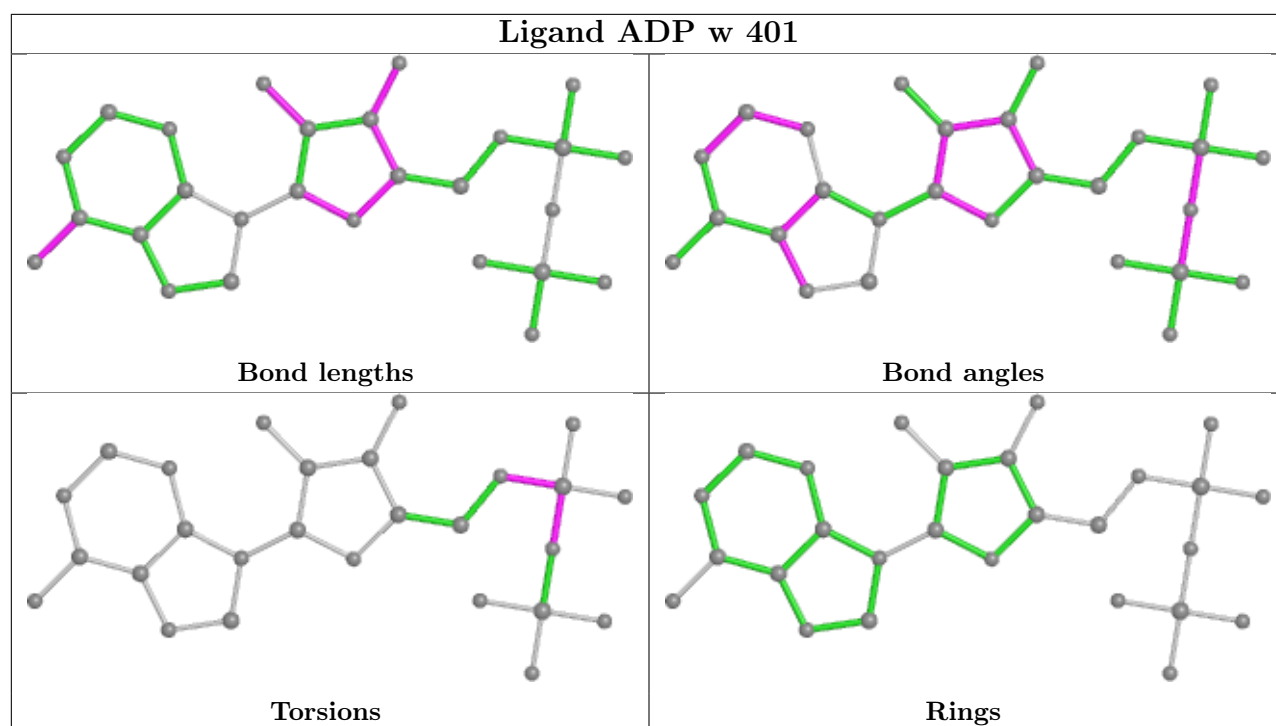
15 monomers are involved in 44 short contacts:

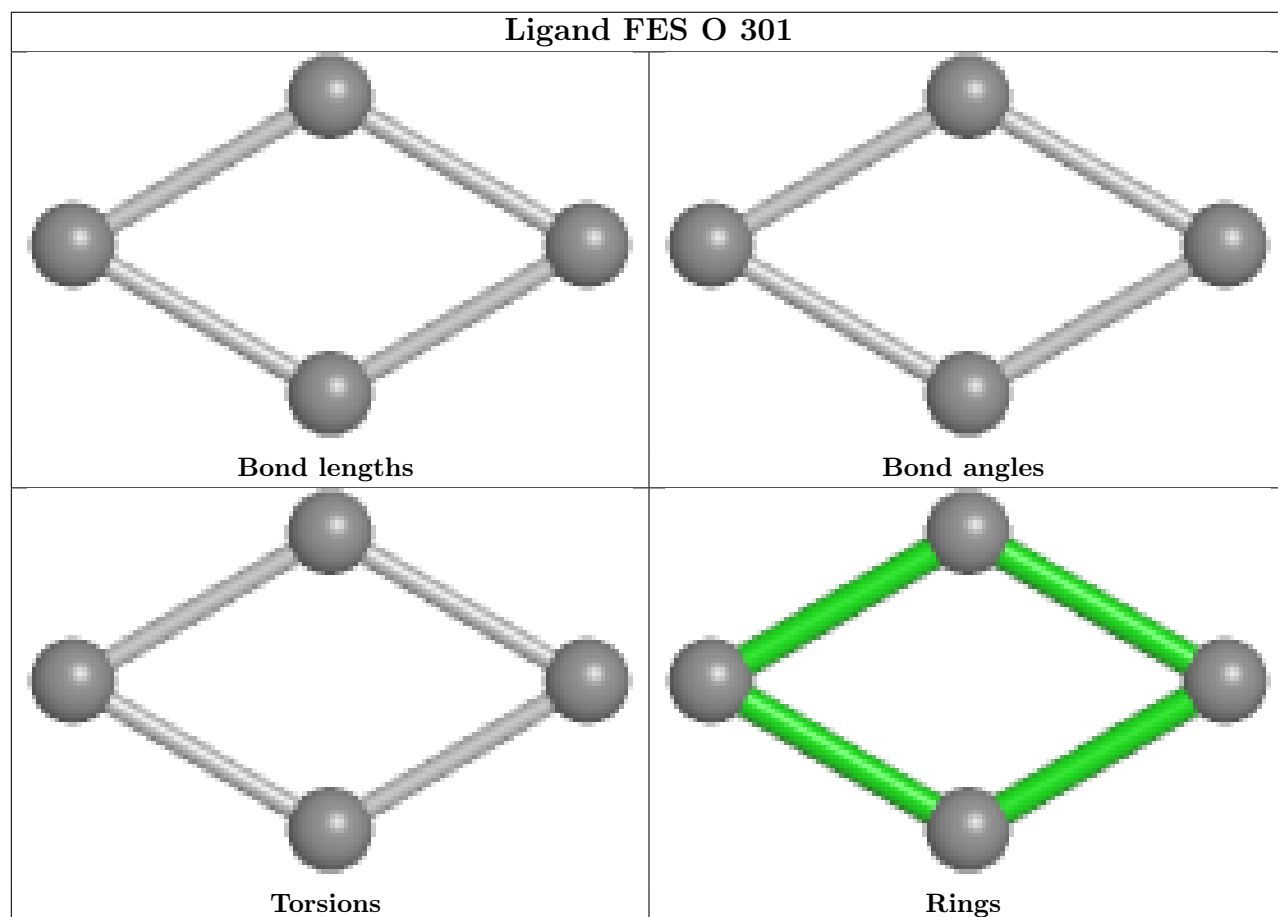
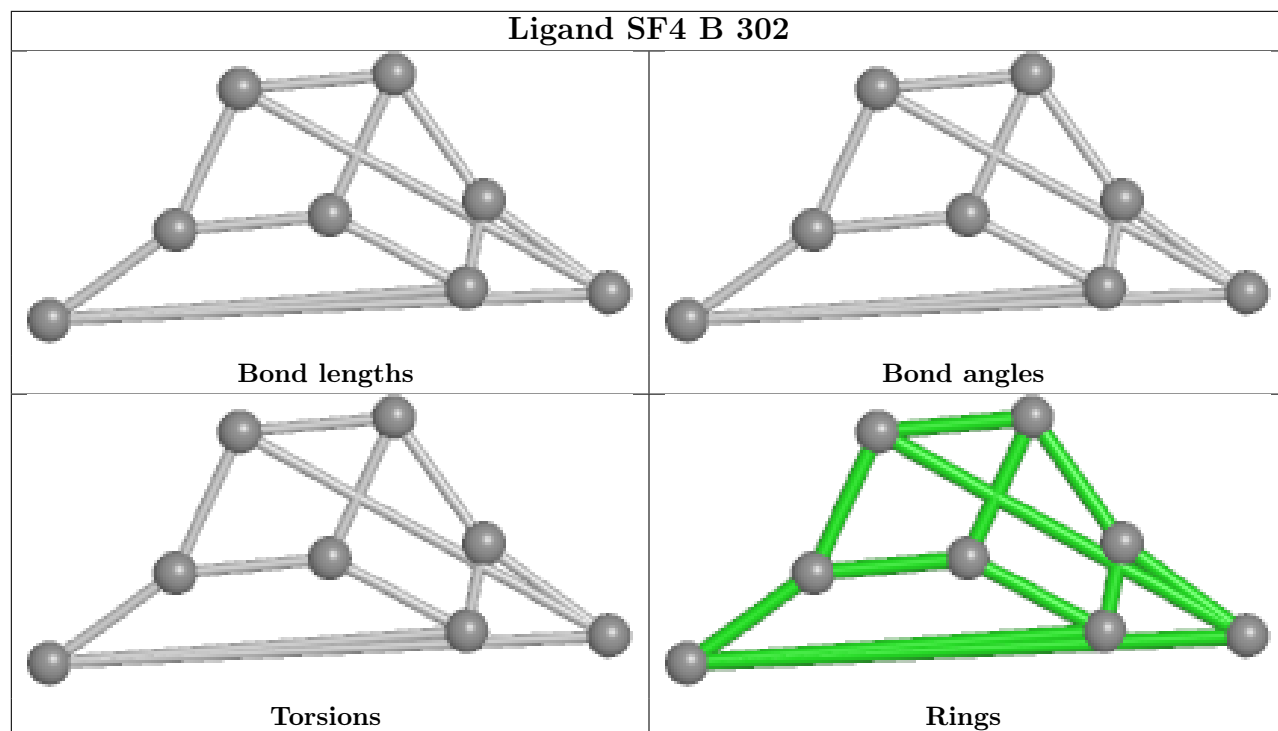
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	W	201	PEE	1	0
48	B	303	PEE	4	0
52	V	201	CDL	3	0
48	V	202	PEE	3	0
46	A	502	FMN	3	0
49	C	303	PLX	4	0
53	J	401	NDP	1	0
50	C	304	UQ	5	0
45	C	301	SF4	2	0
50	J	402	UQ	6	0
45	A	501	SF4	2	0
49	J	403	PLX	2	0
48	C	302	PEE	2	0
52	I	201	CDL	1	0
47	A	503	NAI	6	0

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.

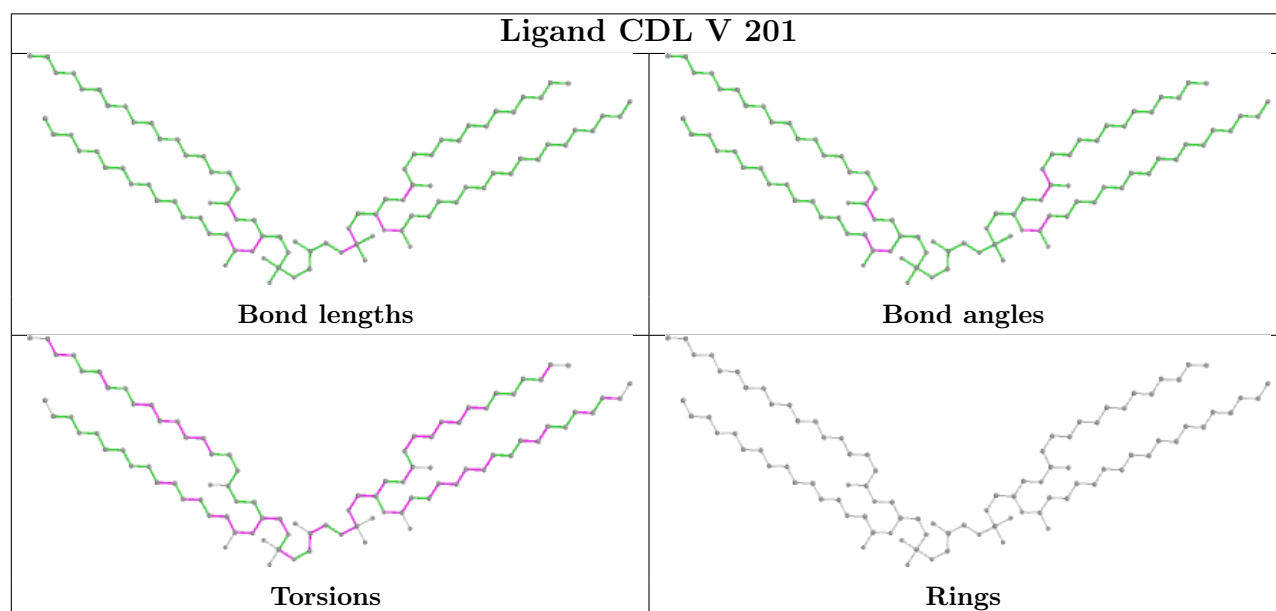
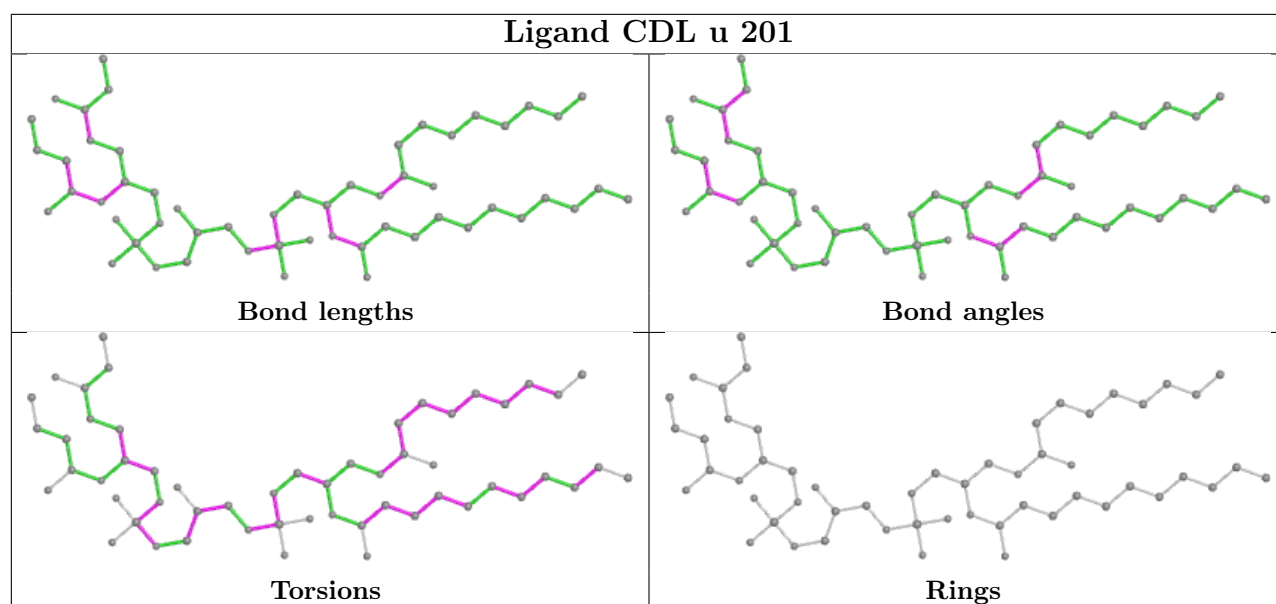


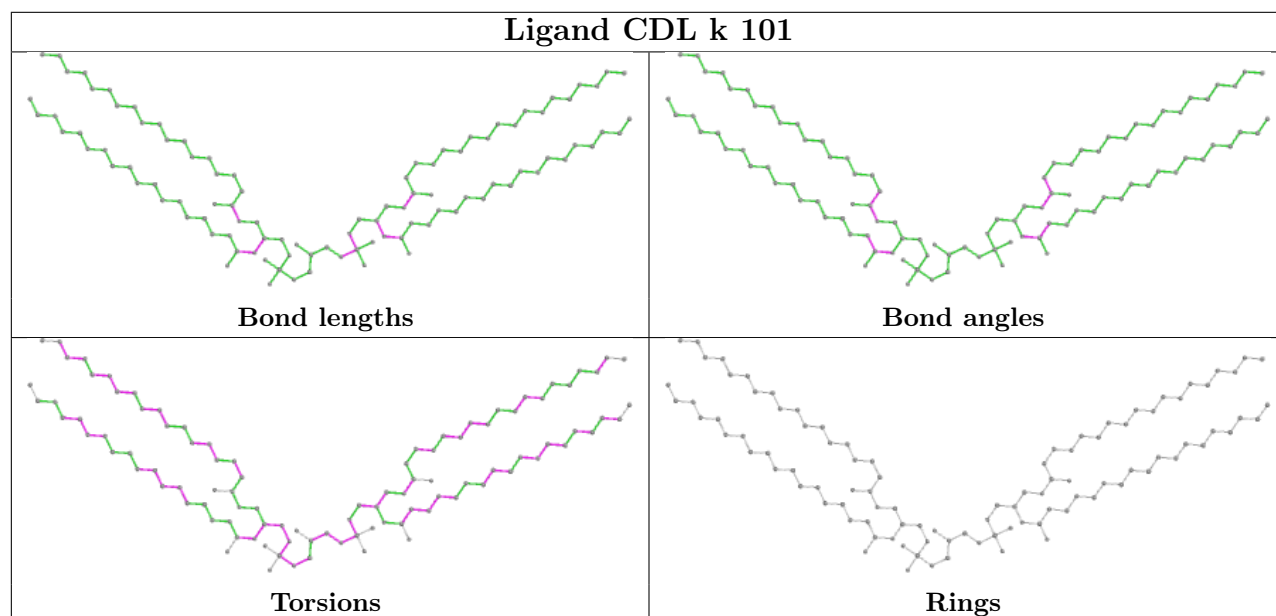
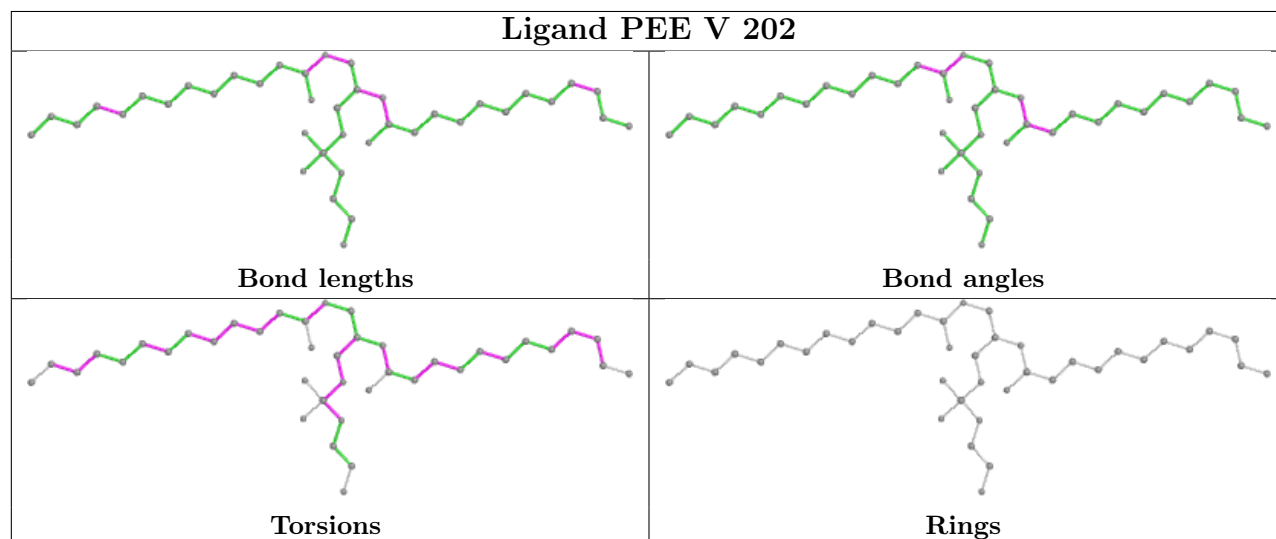
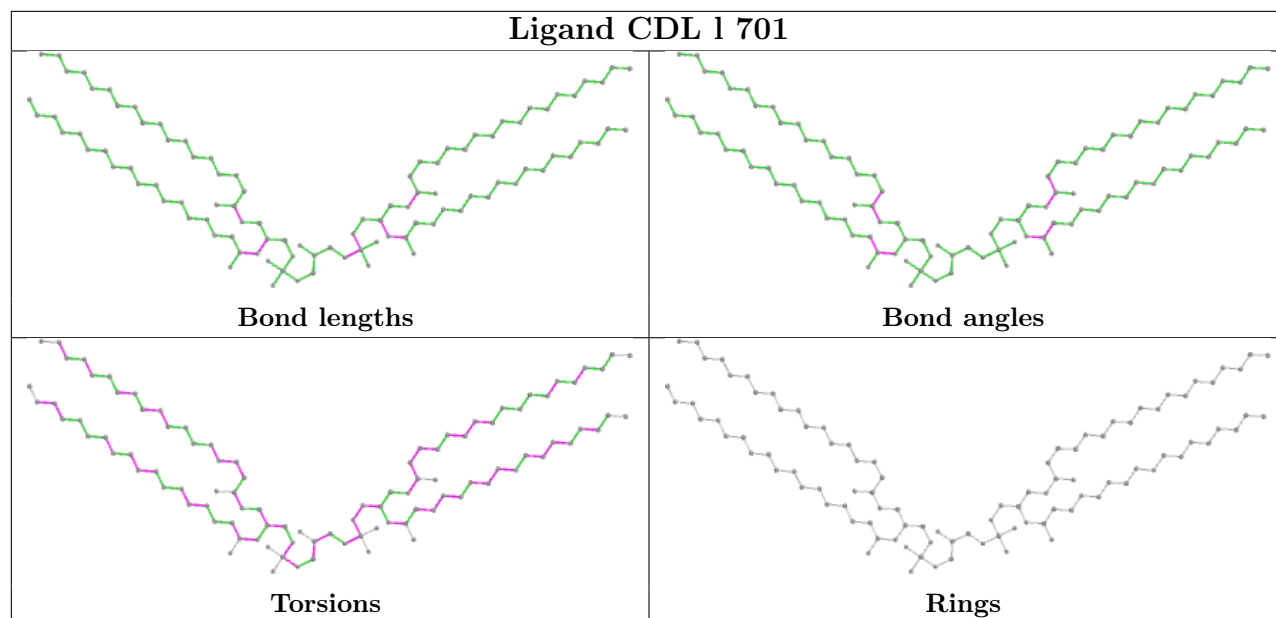


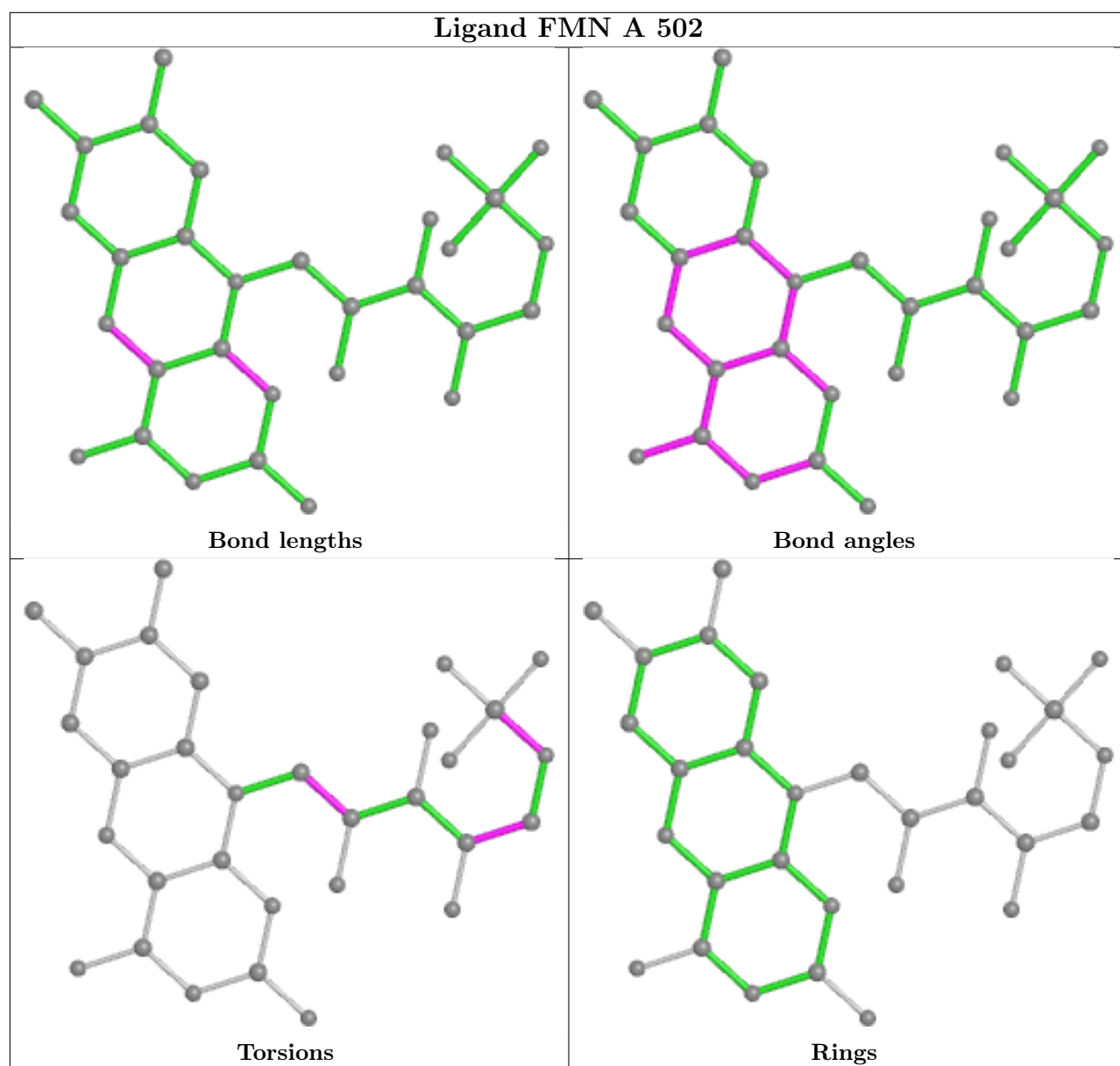


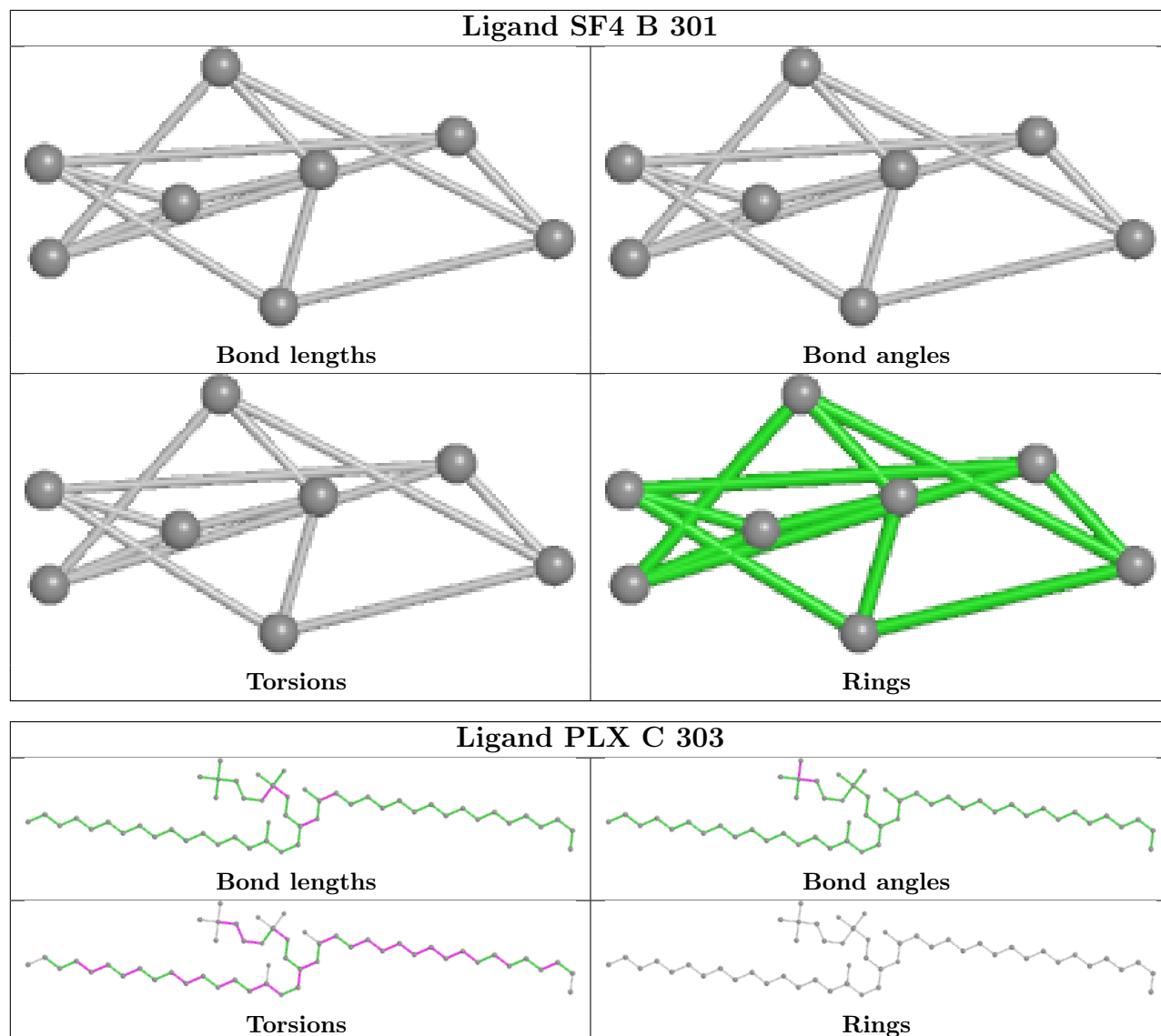


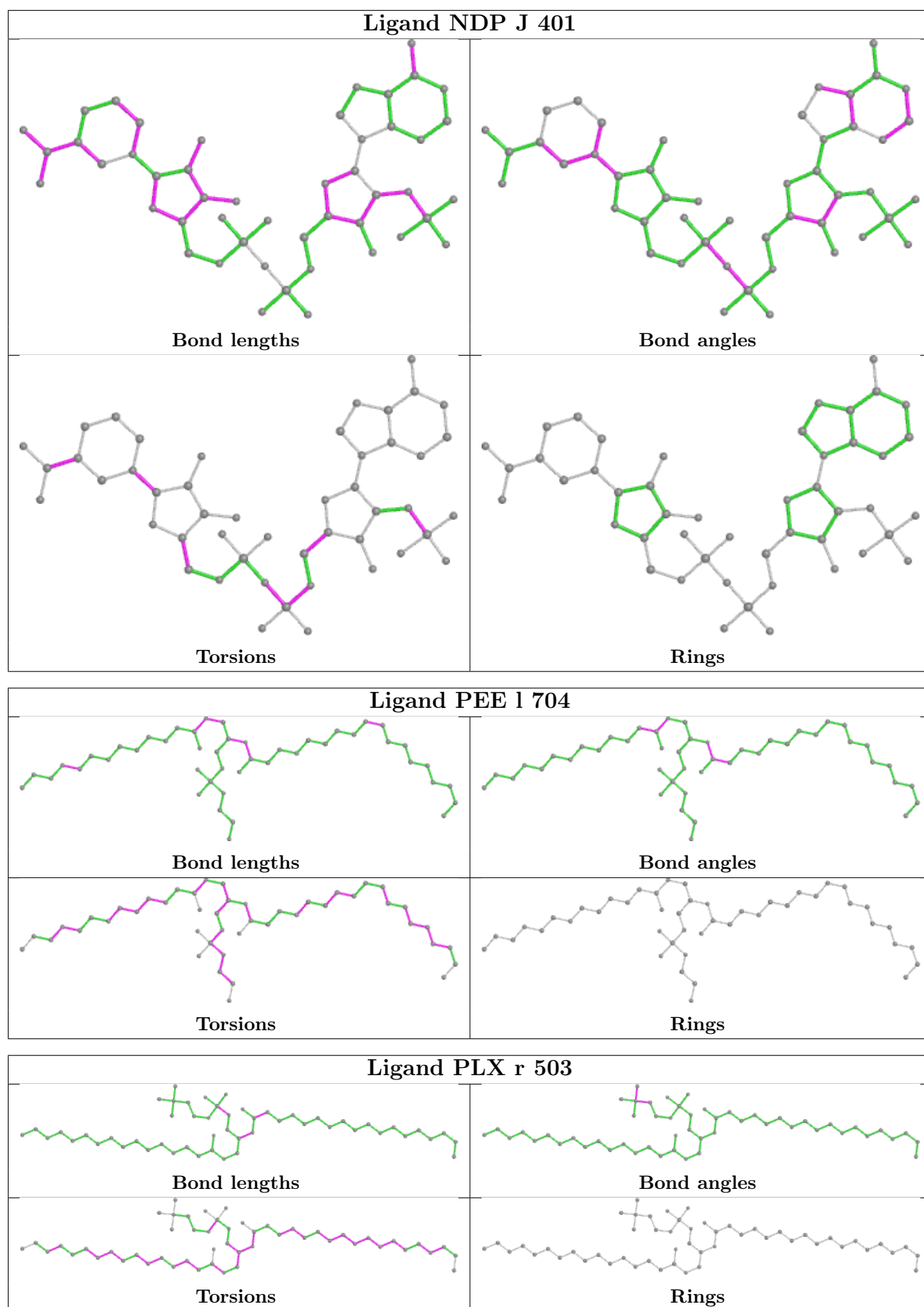


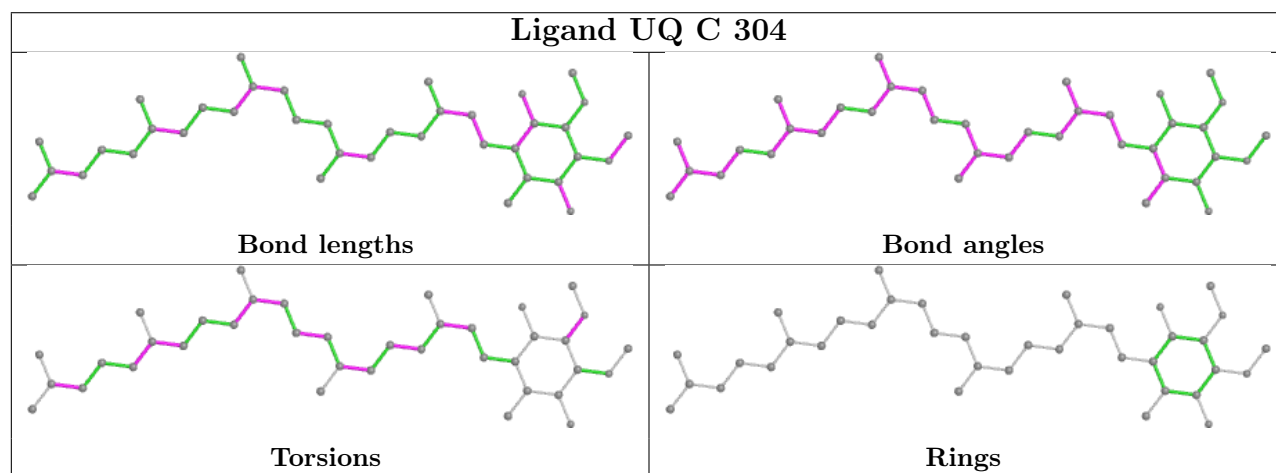
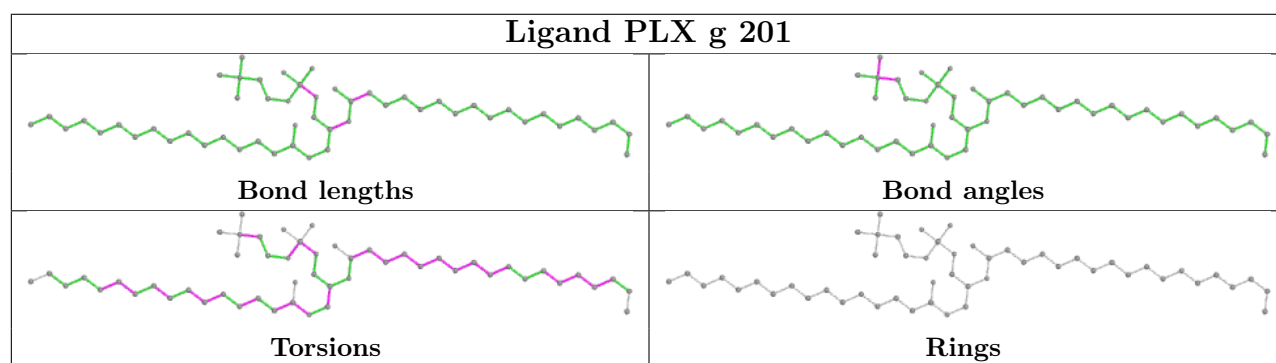
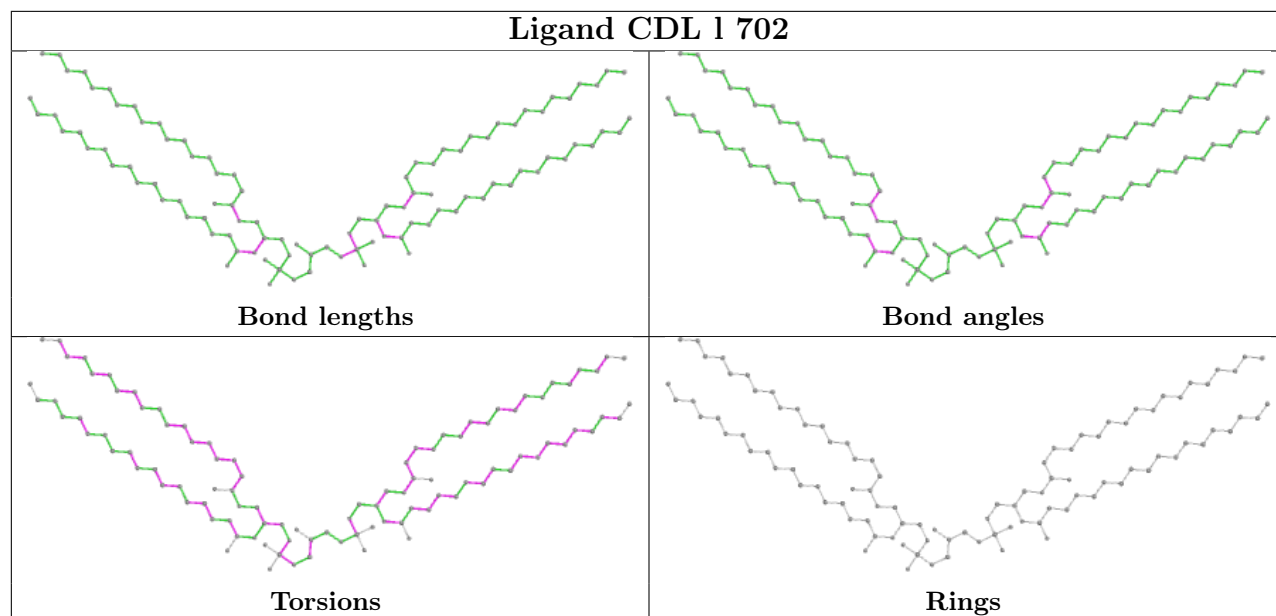


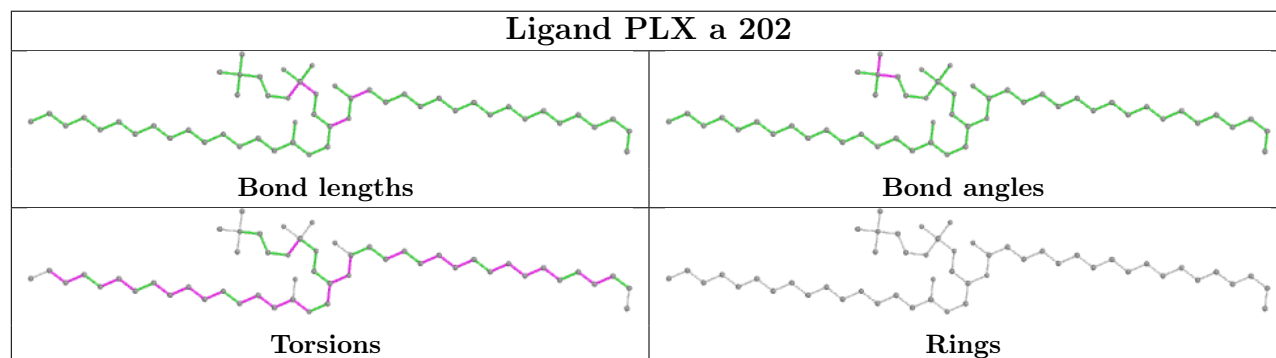
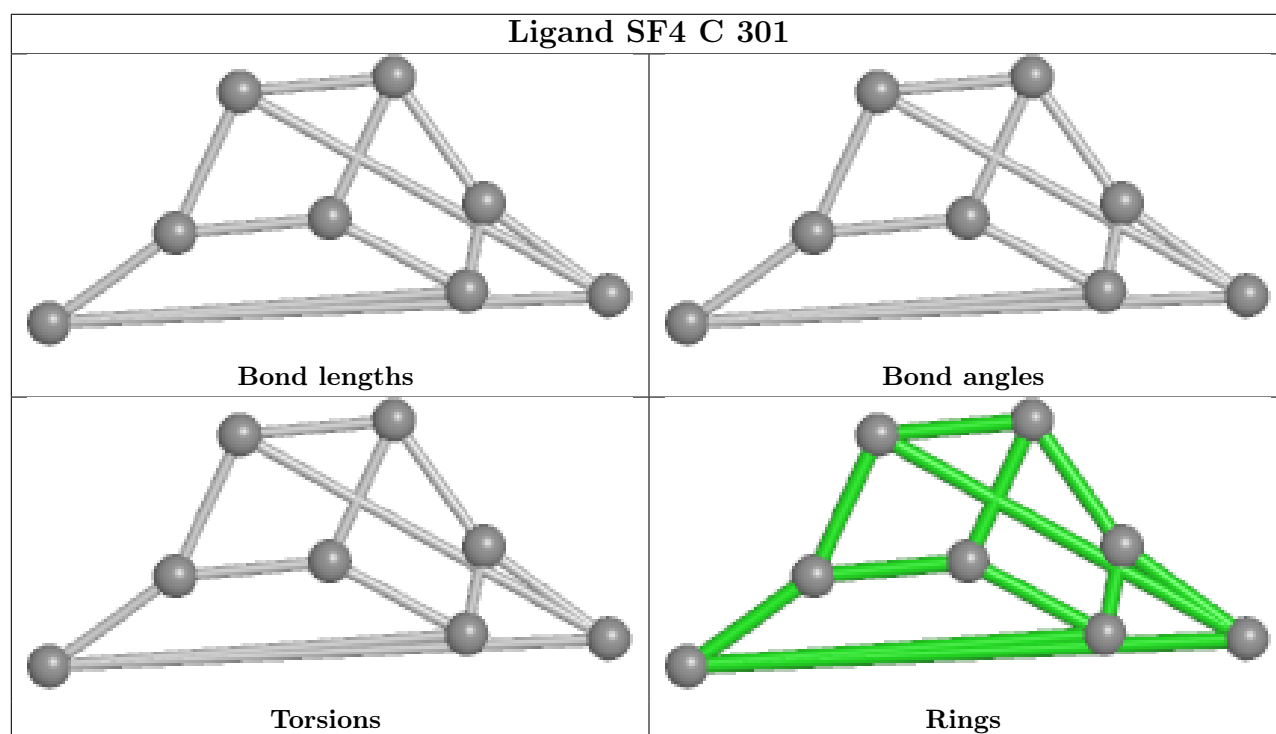
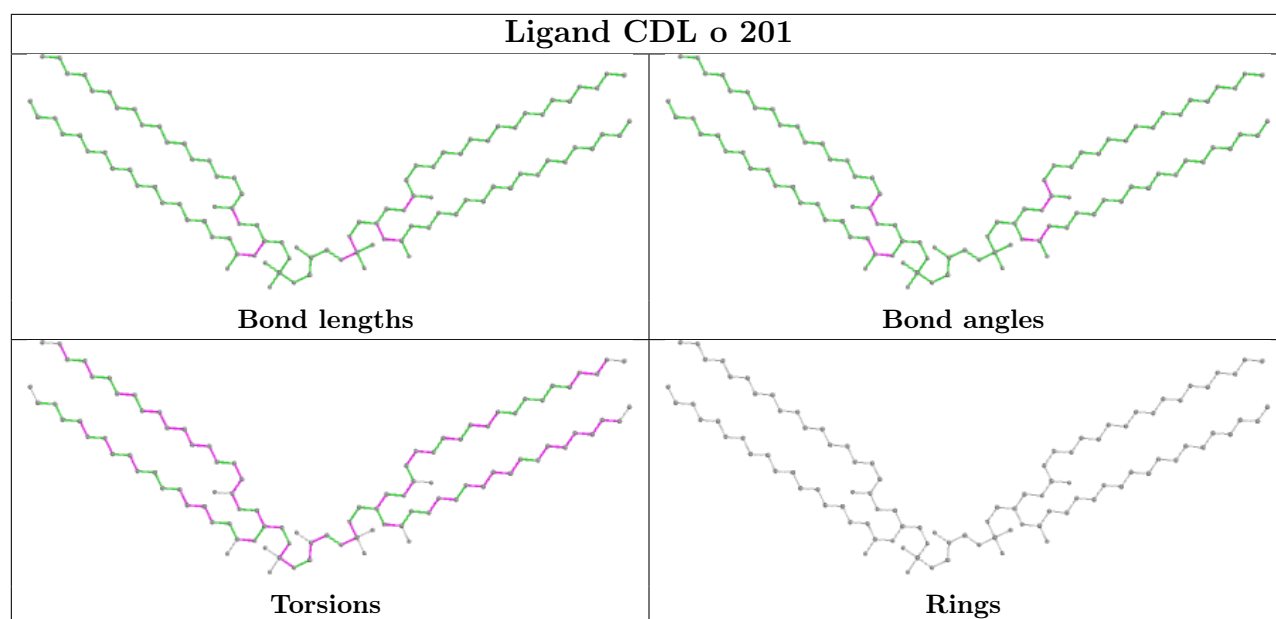


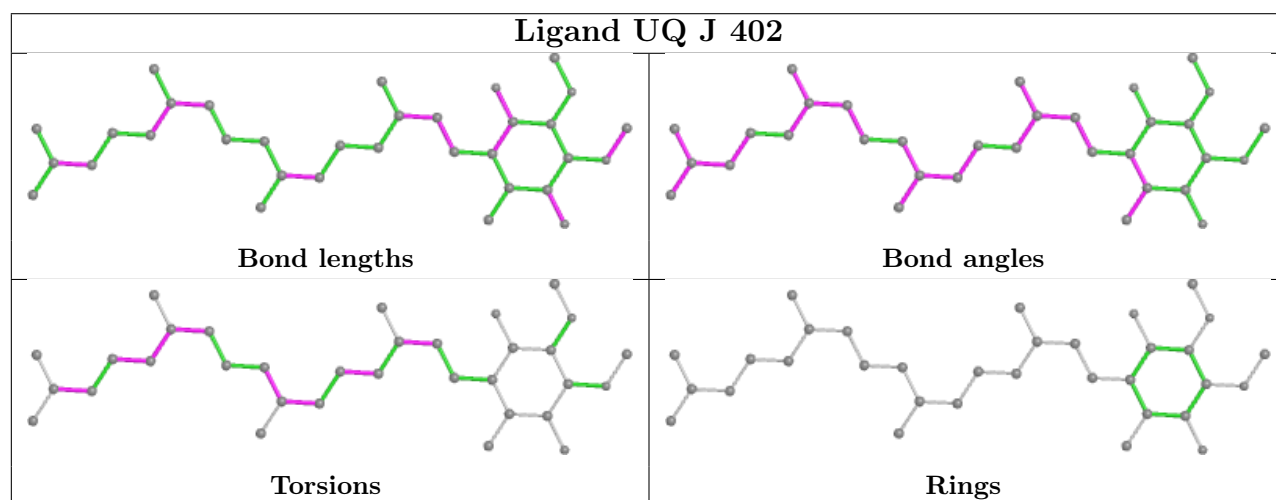
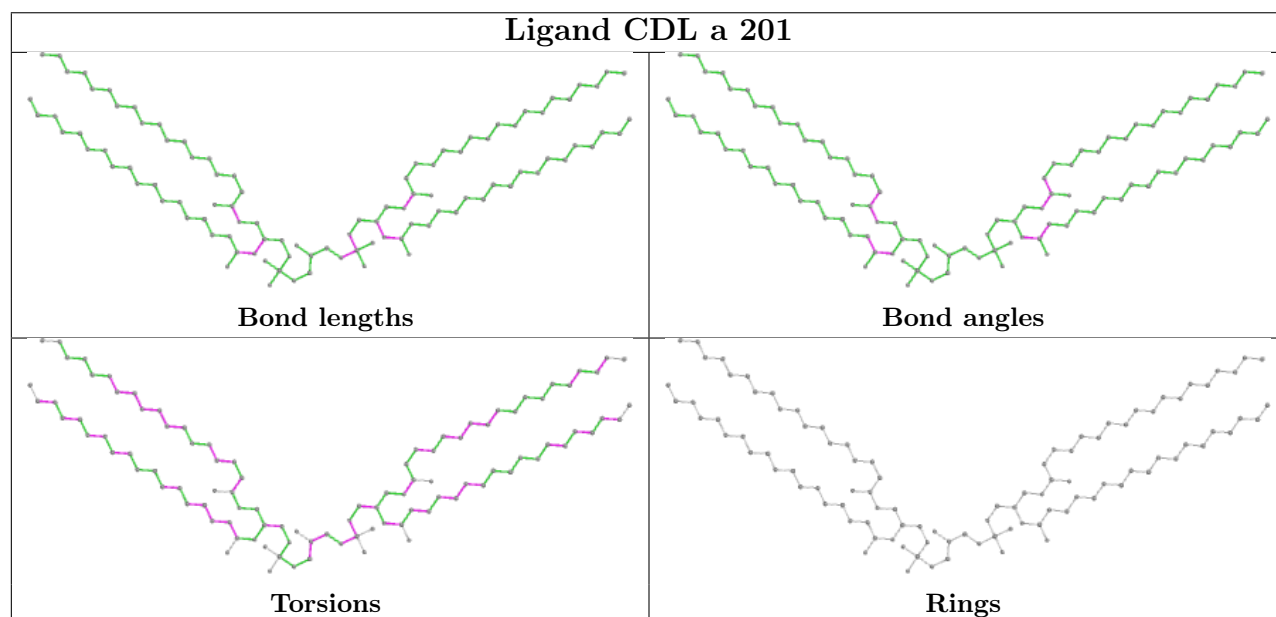
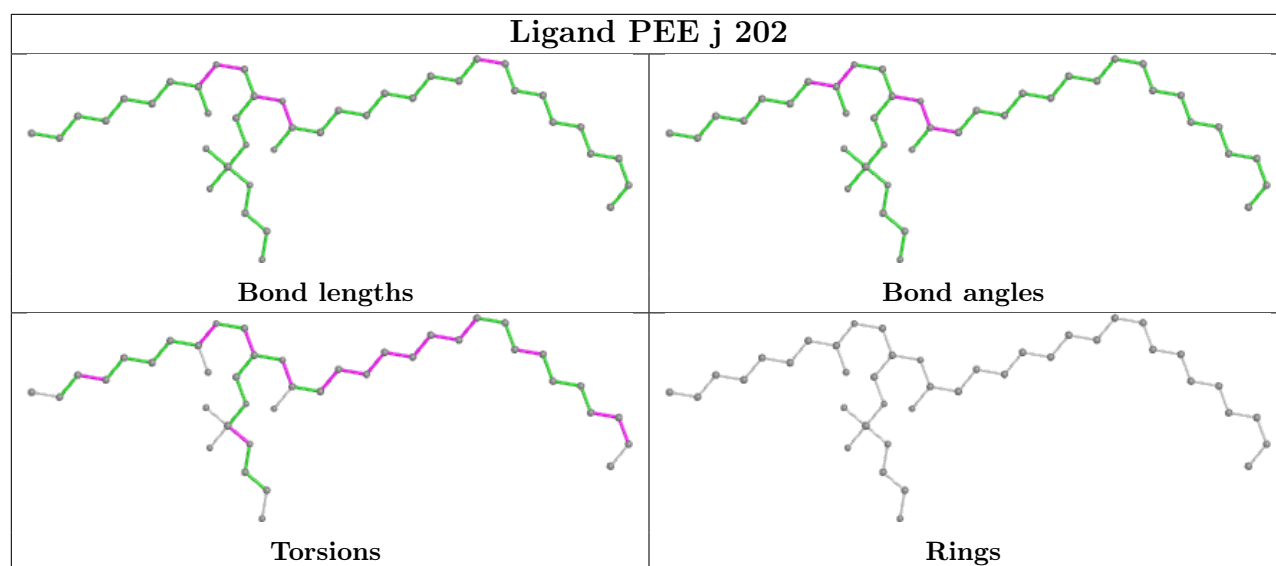




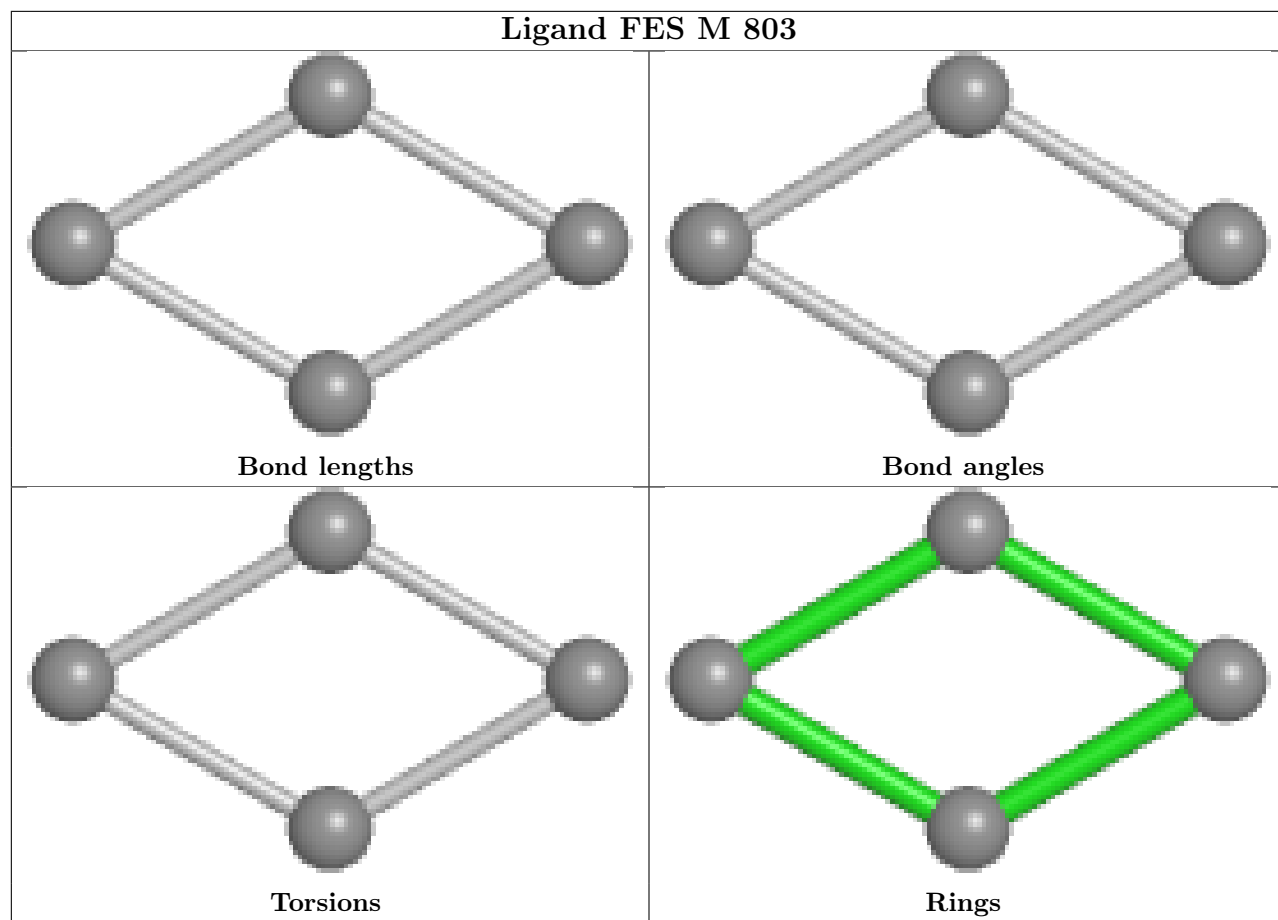


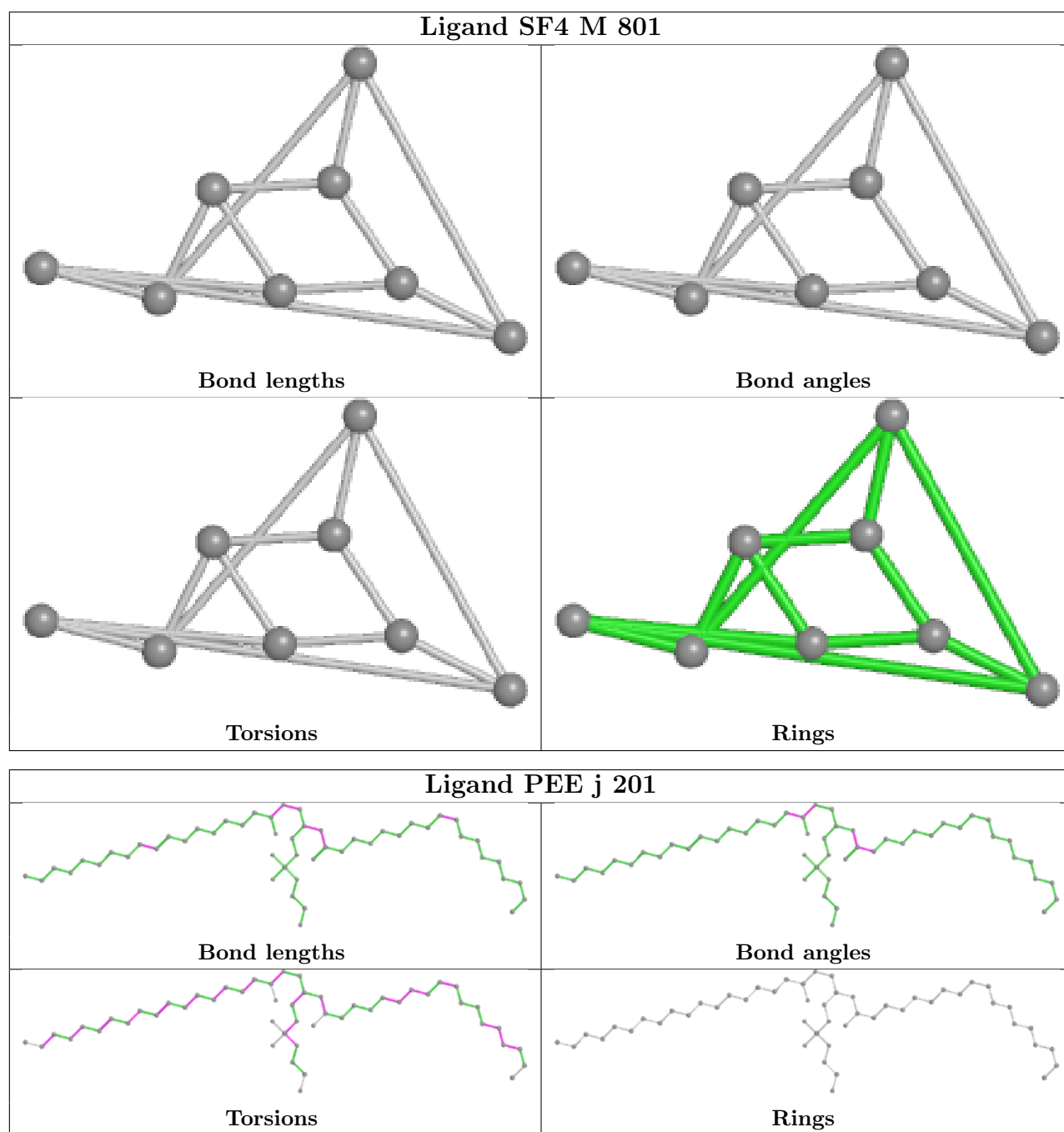


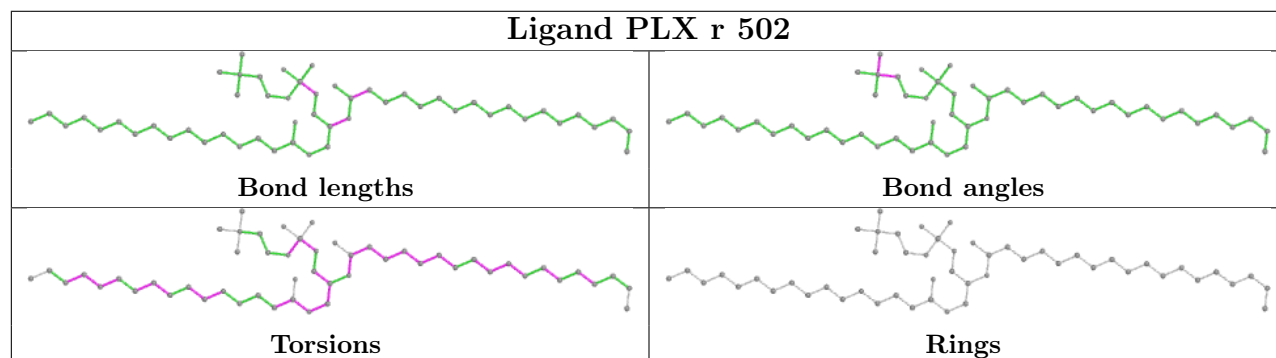
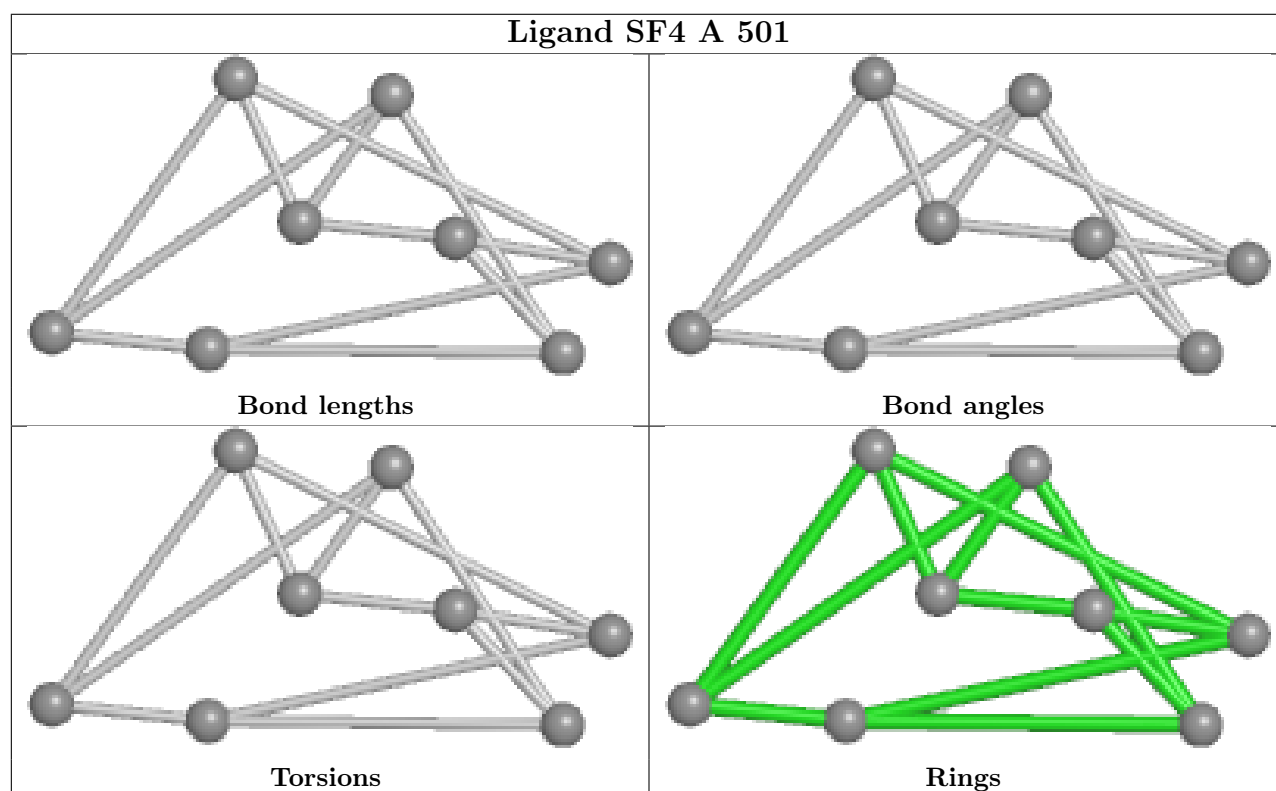
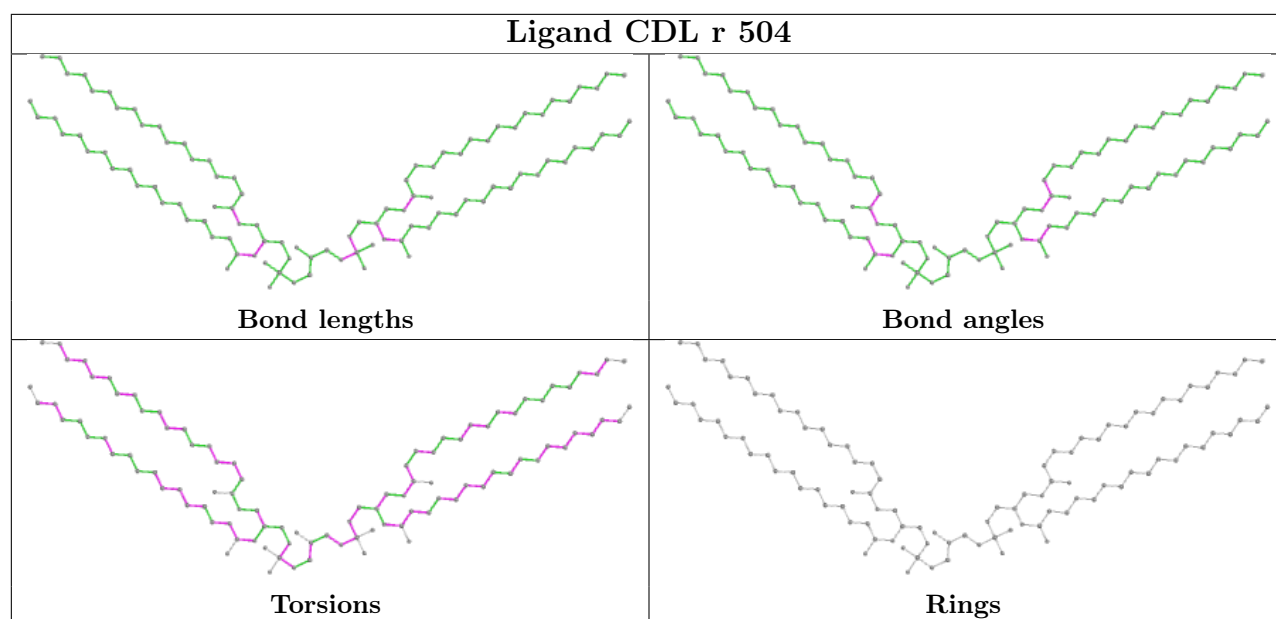


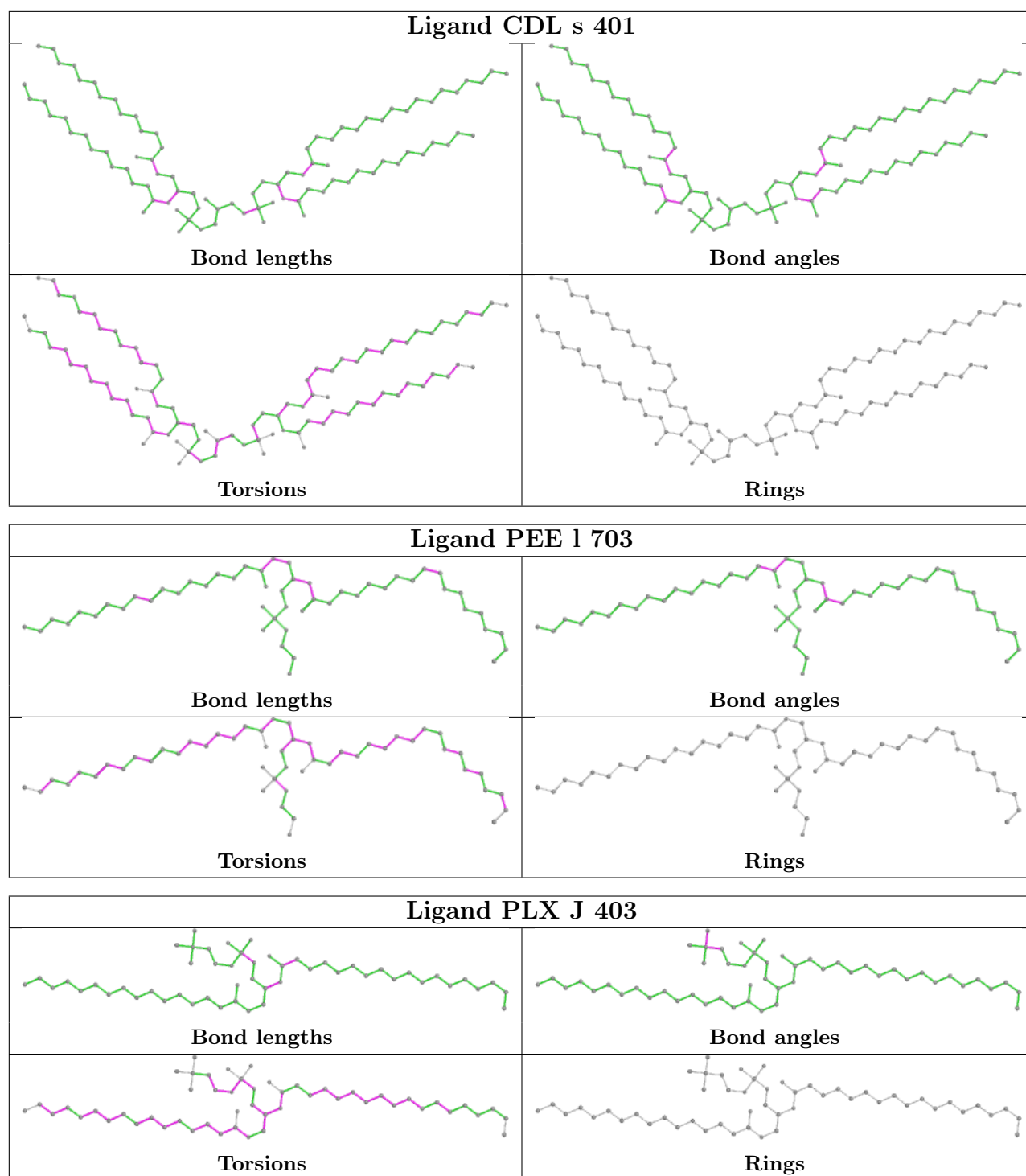


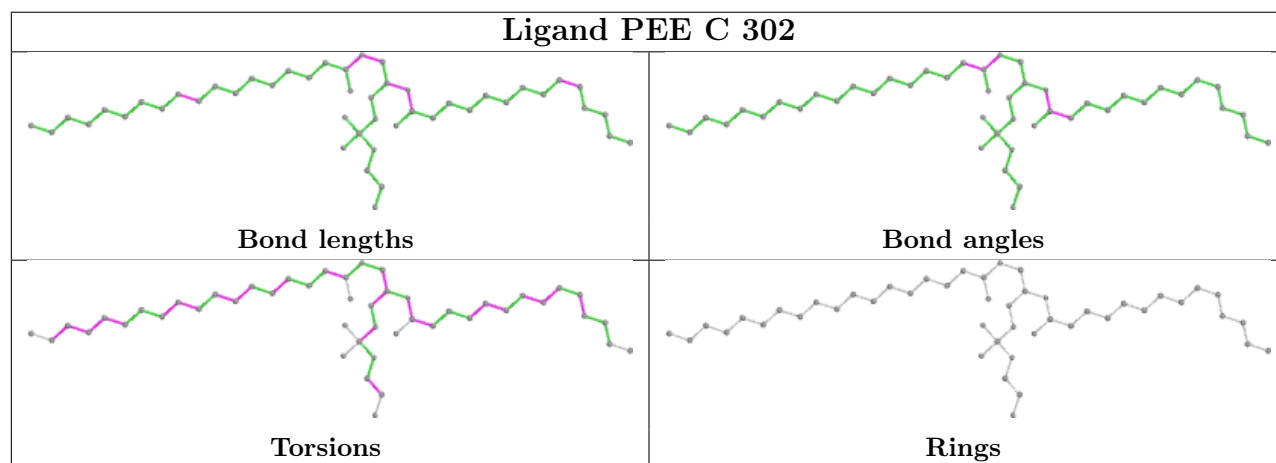
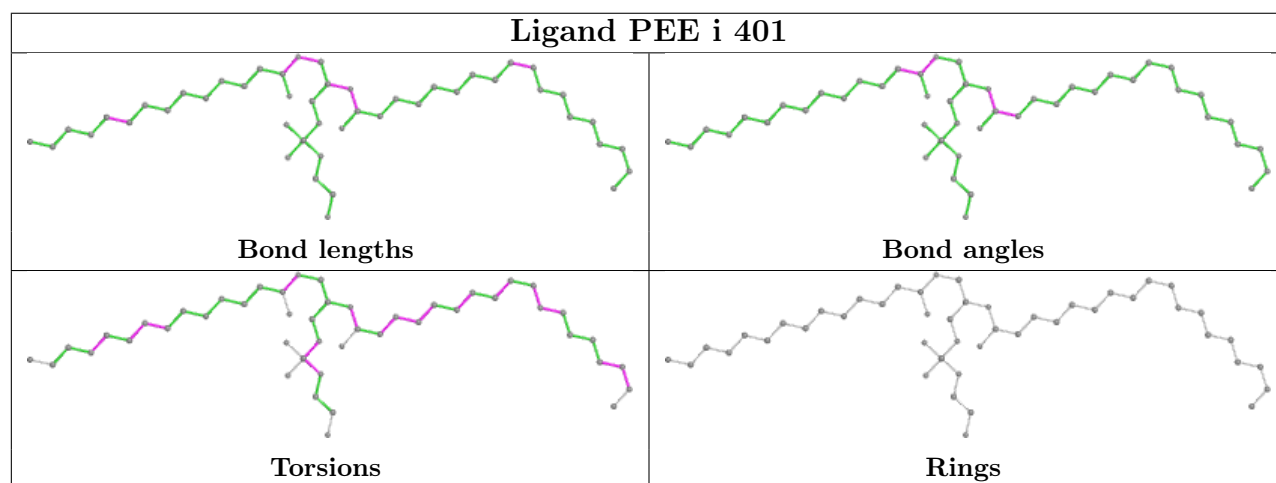
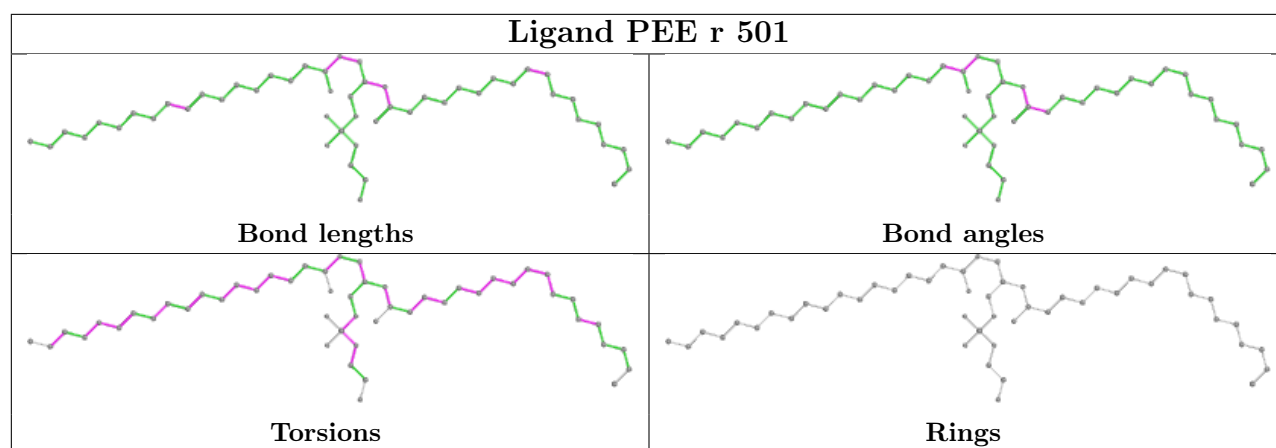




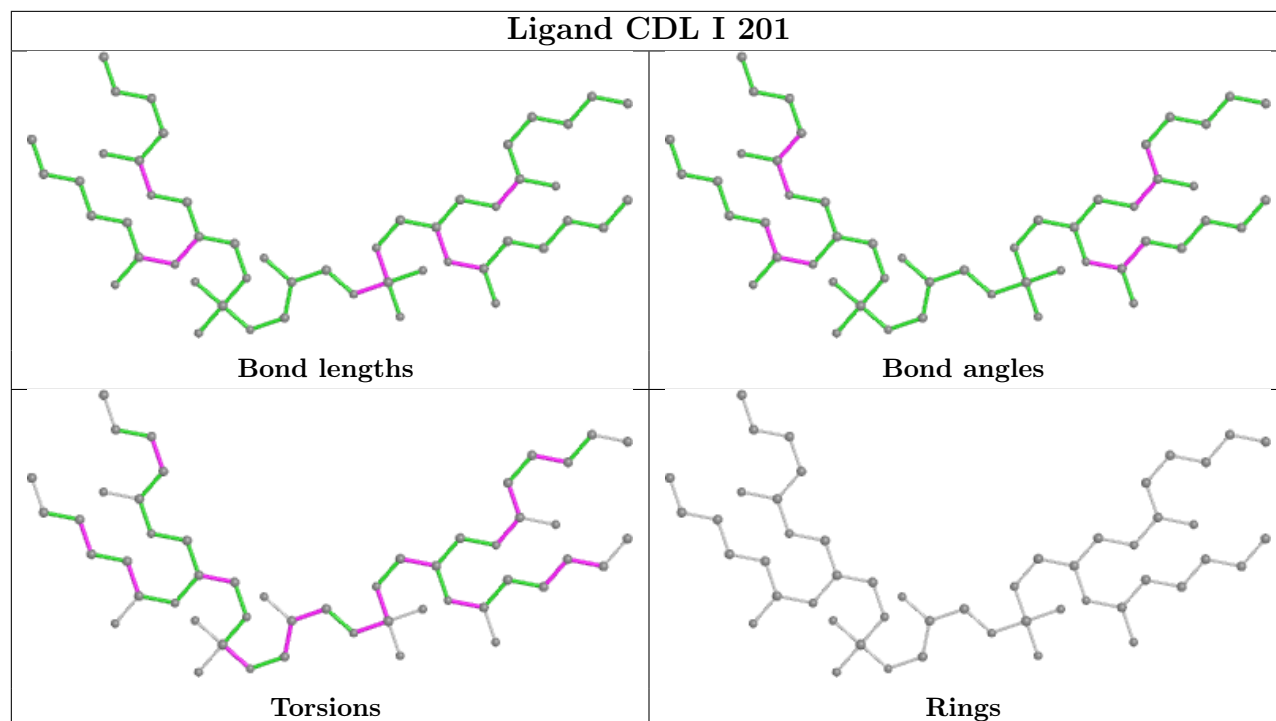




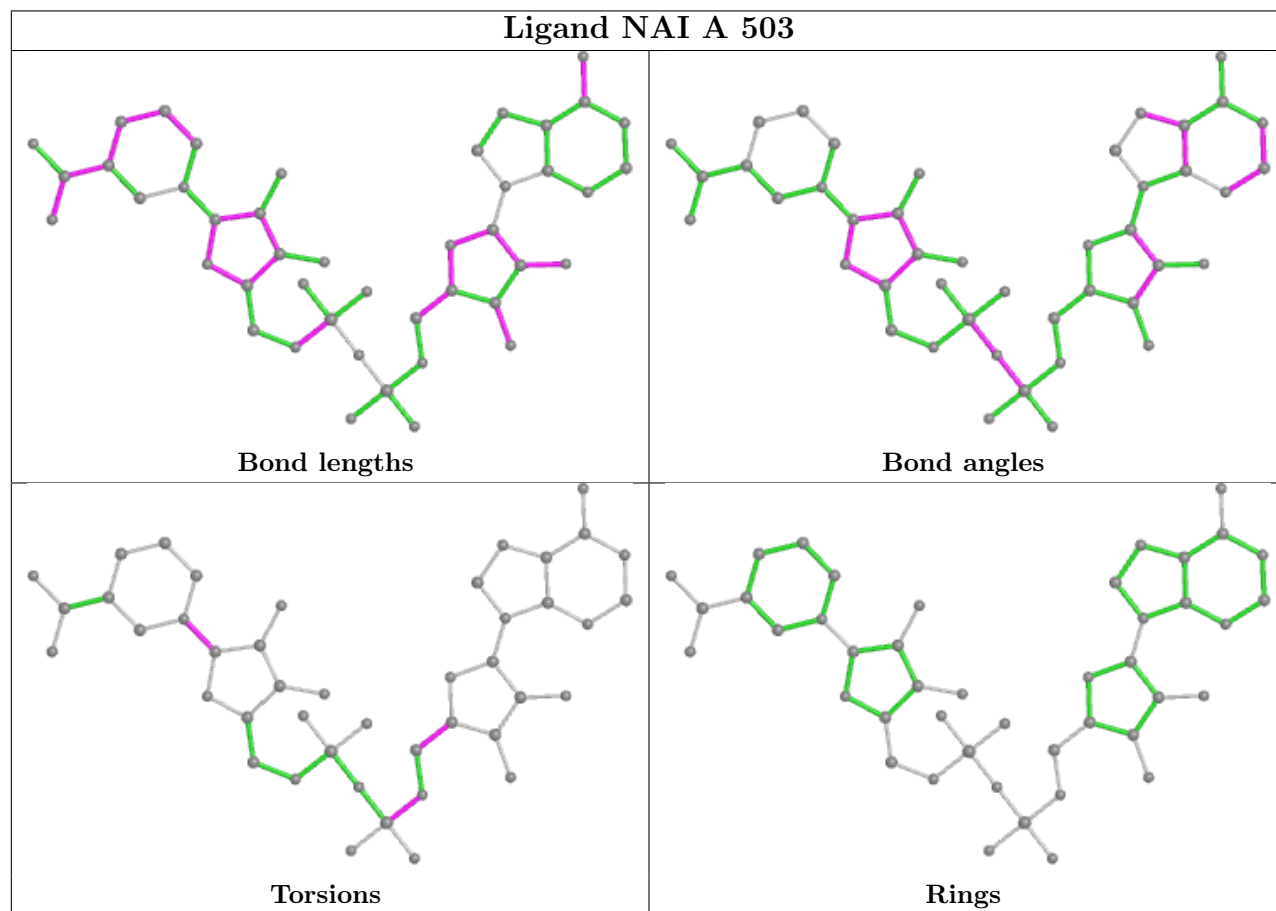




## Ligand CDL I 201



## Ligand NAI A 503



## 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.

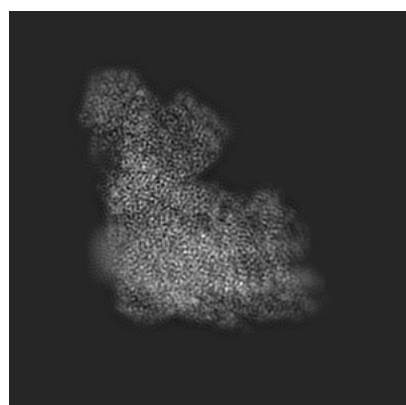
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32248. These allow visual inspection of the internal detail of the map and identification of artifacts.

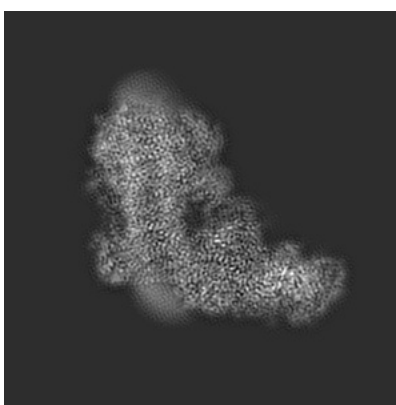
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

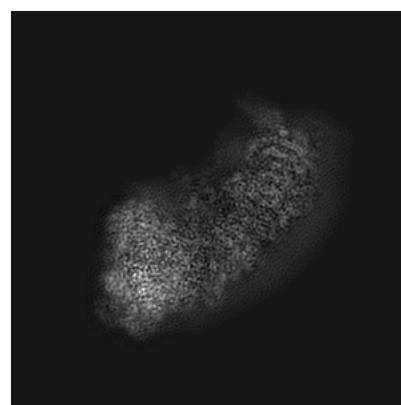
#### 6.1.1 Primary map



X



Y

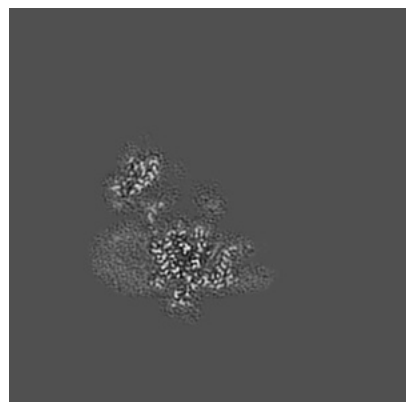


Z

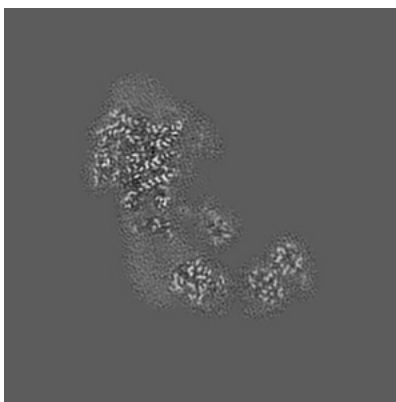
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

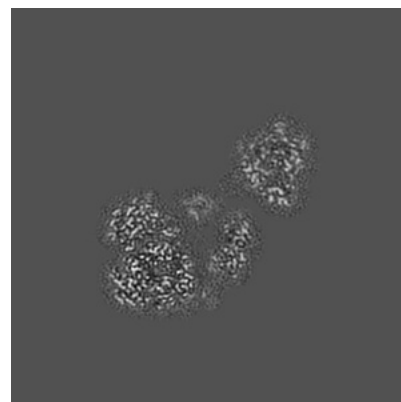
#### 6.2.1 Primary map



X Index: 155



Y Index: 155



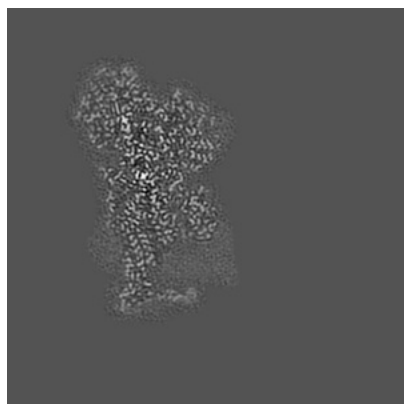
Z Index: 155



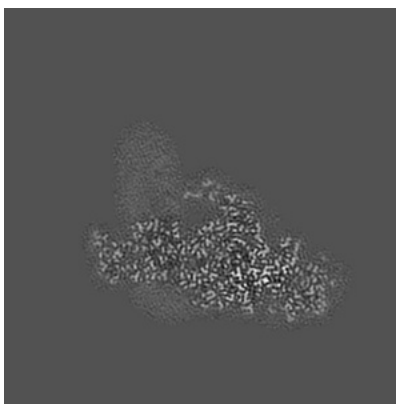
The images above show central slices of the map in three orthogonal directions.

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

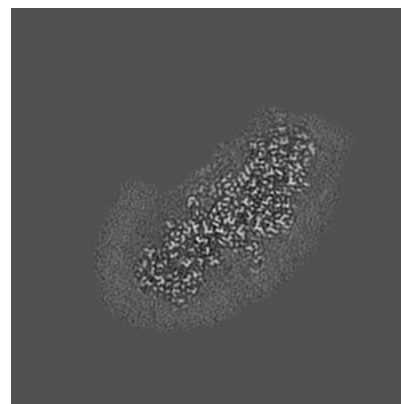
### 6.3.1 Primary map



X Index: 102



Y Index: 101

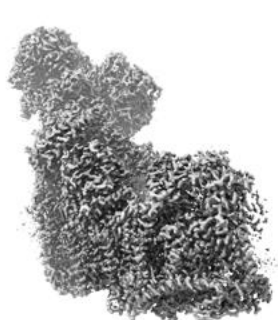


Z Index: 122

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

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

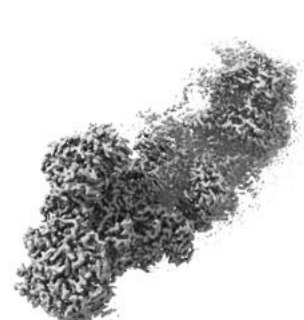
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0291. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

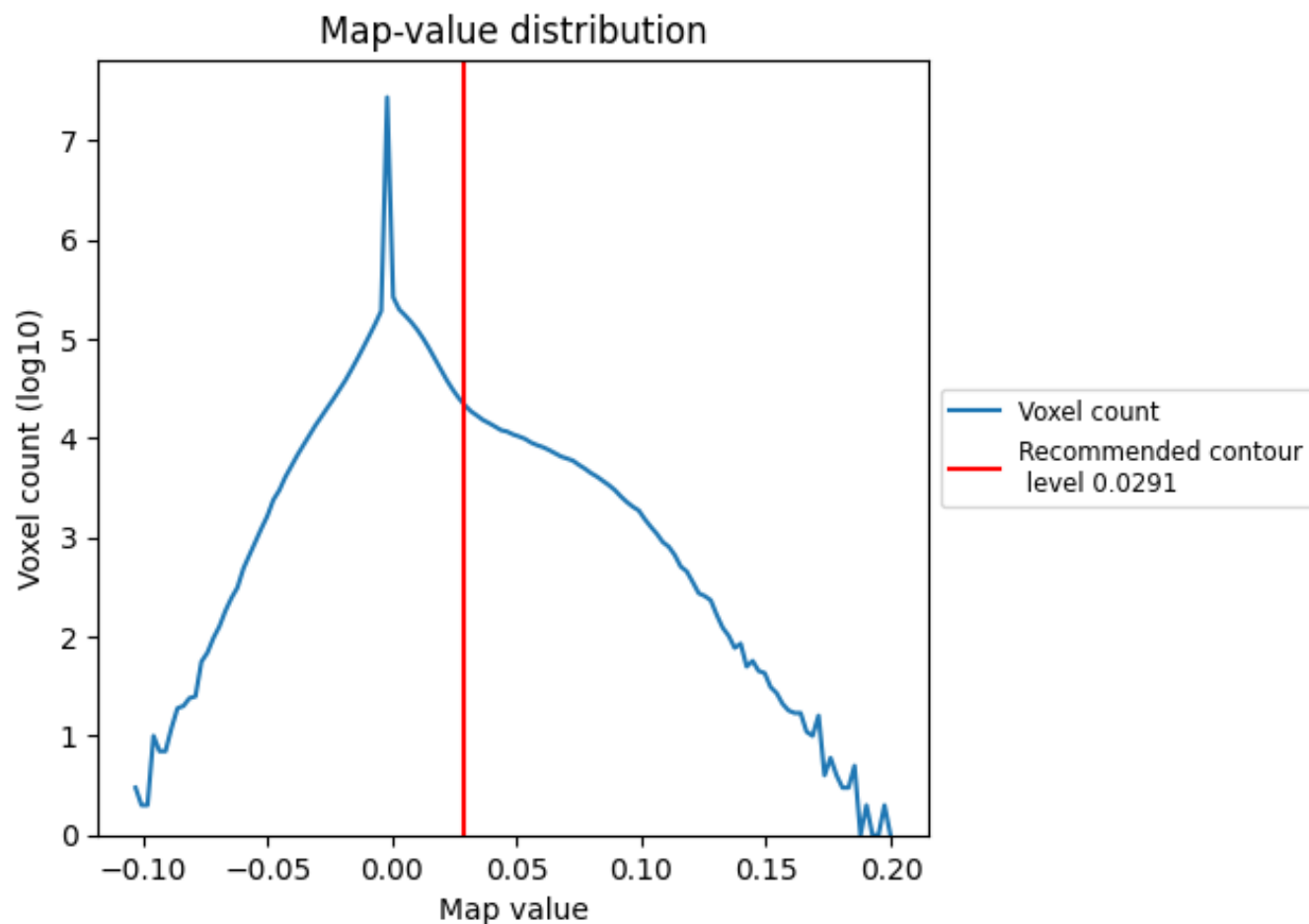
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

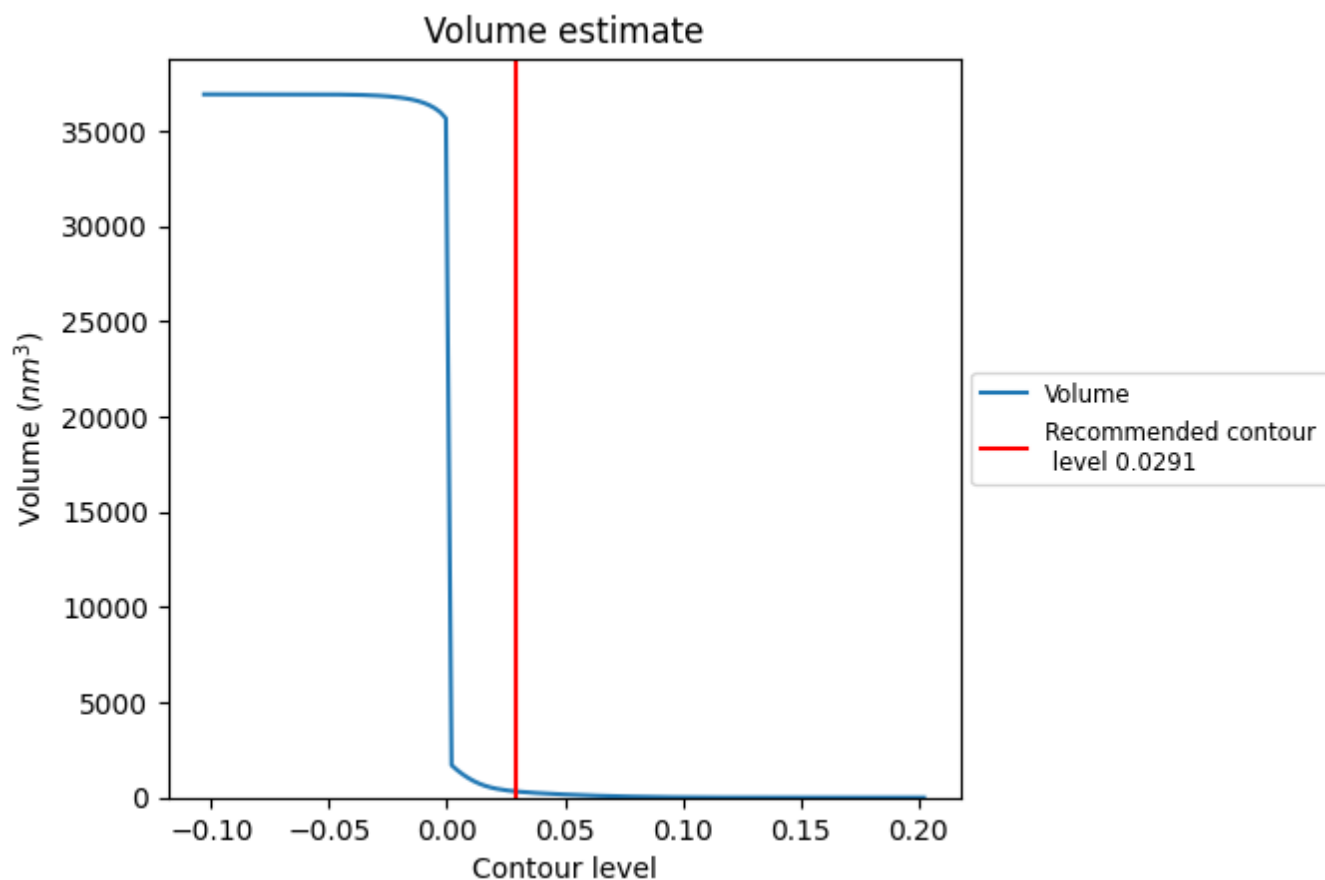
This section contains the results of statistical analysis of the map.

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



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

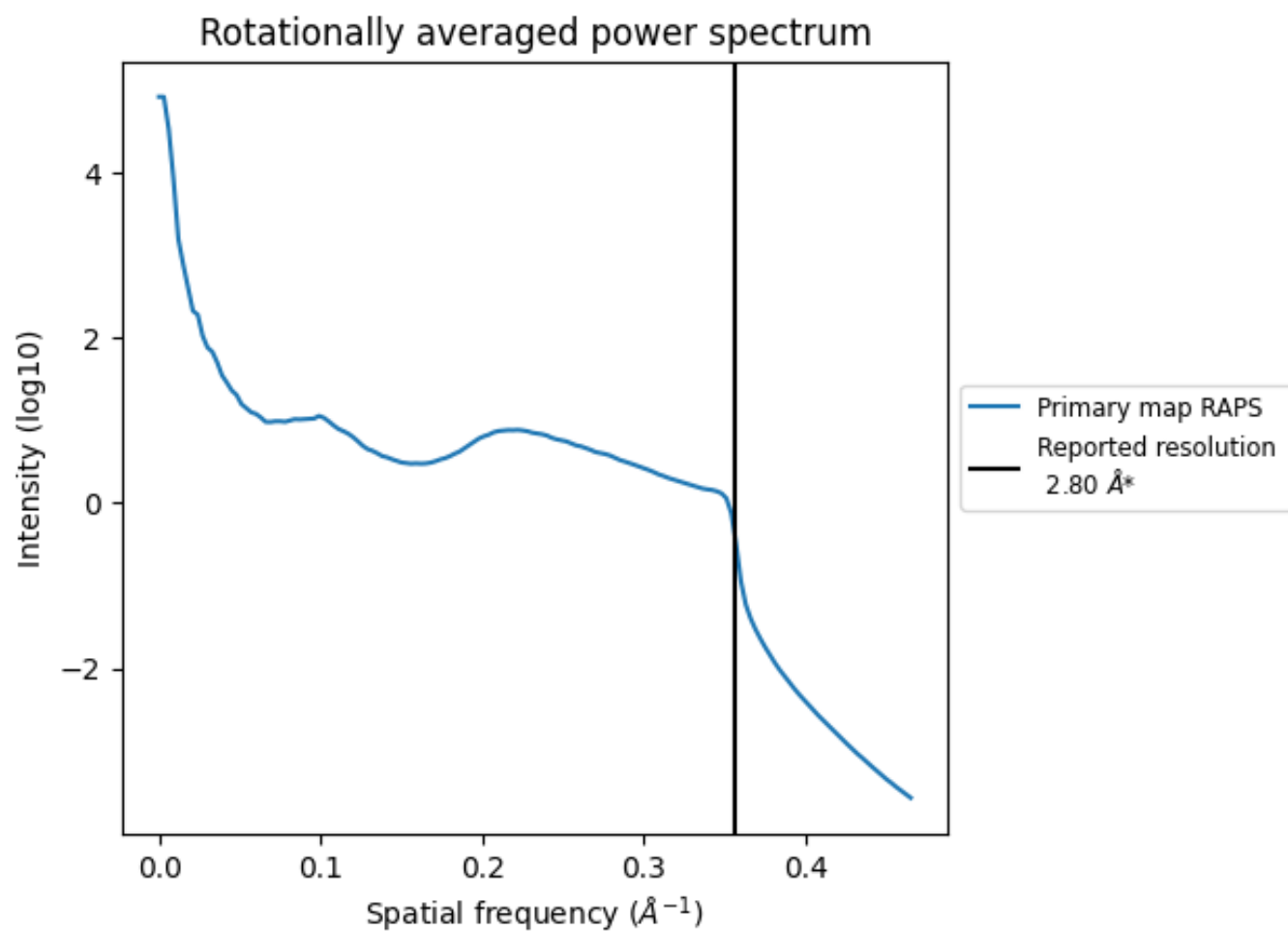
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm<sup>3</sup>; this corresponds to an approximate mass of 294 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 0.357 Å<sup>-1</sup>

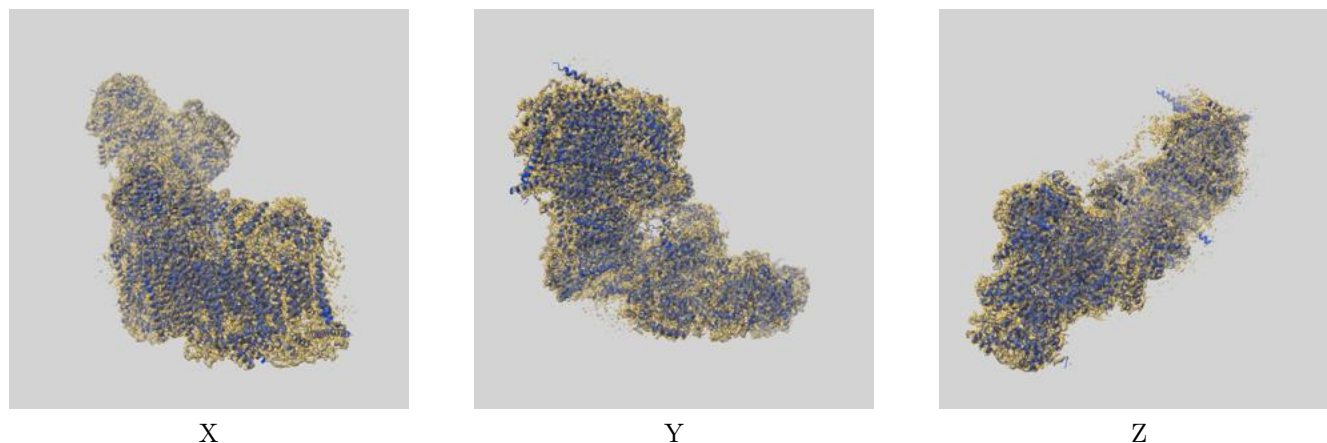
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

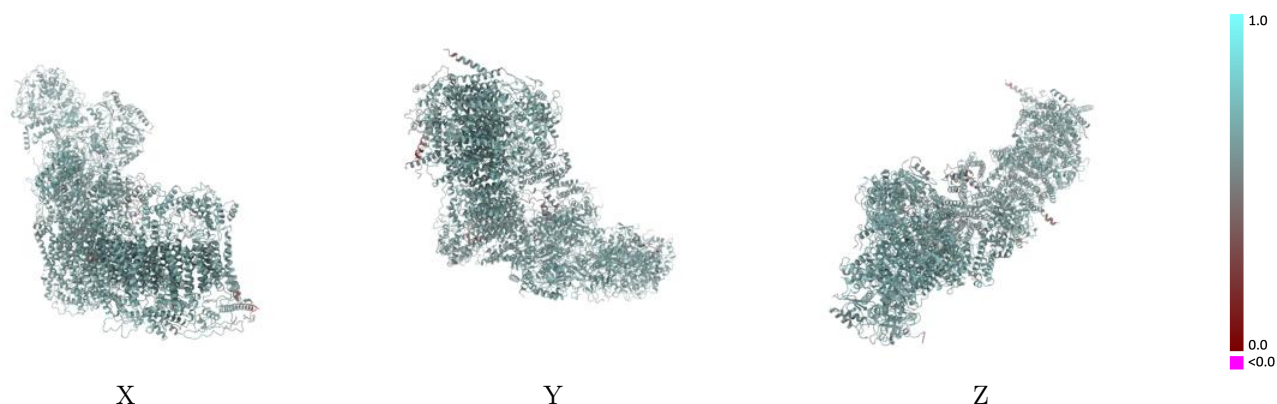
This section contains information regarding the fit between EMDB map EMD-32248 and PDB model 7W0R. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



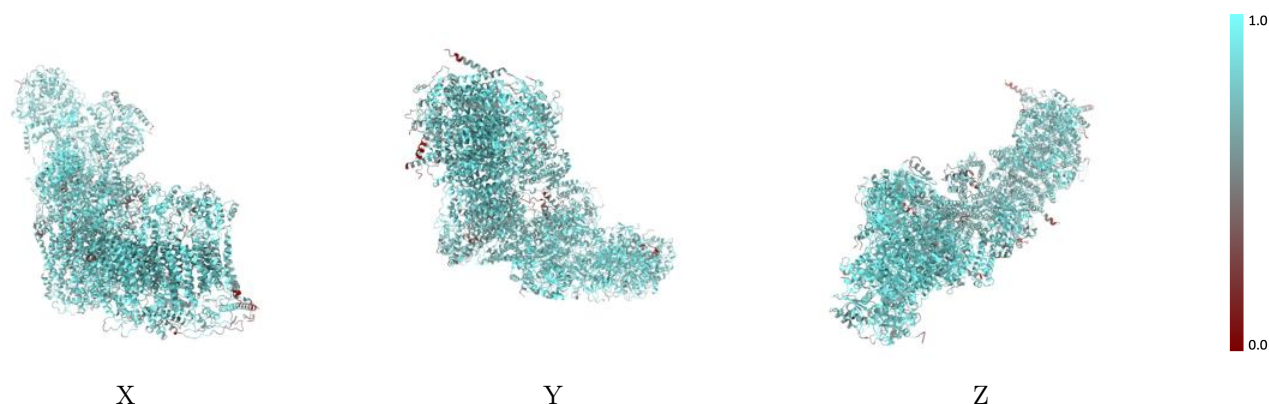
The images above show the 3D surface view of the map at the recommended contour level 0.0291 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

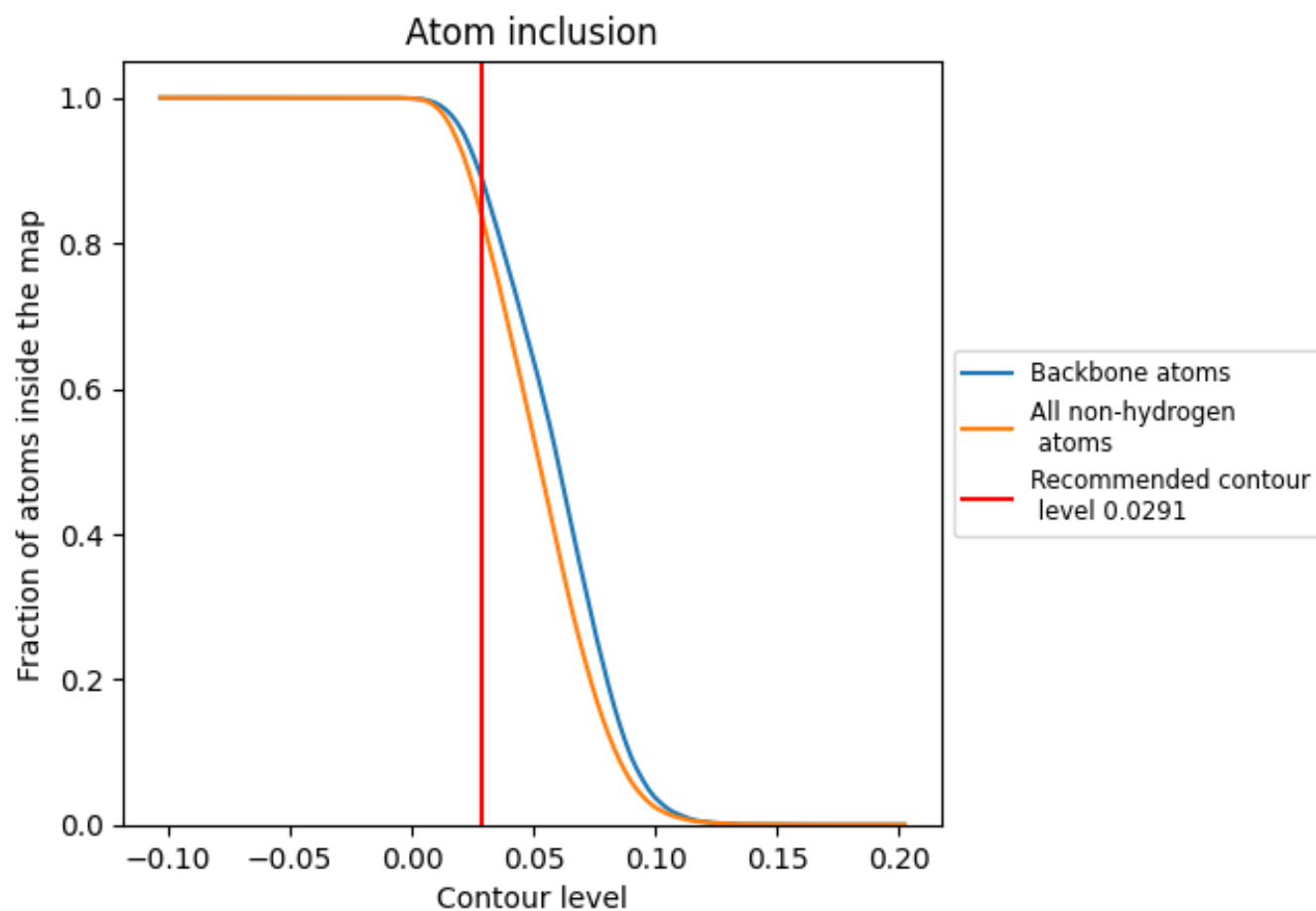
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0291).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.0291) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8341	 0.6160
A	 0.8326	 0.6120
B	 0.9354	 0.6480
C	 0.8959	 0.6430
E	 0.8529	 0.6290
F	 0.7186	 0.5620
G	 0.5243	 0.4870
H	 0.8525	 0.6120
I	 0.7844	 0.6130
J	 0.8610	 0.6230
K	 0.7718	 0.6080
L	 0.8702	 0.6390
M	 0.8794	 0.6280
N	 0.8343	 0.6230
O	 0.8048	 0.5940
P	 0.9415	 0.6530
Q	 0.9245	 0.6480
S	 0.8859	 0.6250
T	 0.8615	 0.6310
U	 0.7822	 0.5940
V	 0.7410	 0.5980
W	 0.8174	 0.6070
X	 0.7381	 0.5930
Y	 0.6977	 0.5540
Z	 0.6416	 0.5440
a	 0.8165	 0.6220
b	 0.7708	 0.5910
c	 0.8139	 0.6110
d	 0.7703	 0.5950
e	 0.7766	 0.6000
f	 0.6351	 0.5580
g	 0.8443	 0.6200
h	 0.8180	 0.5990
i	 0.9143	 0.6380
j	 0.8103	 0.6240



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*Continued from previous page...*

Chain	Atom inclusion	Q-score
k	 0.8171	 0.6210
l	 0.8336	 0.6190
m	 0.7733	 0.5880
n	 0.6832	 0.5730
o	 0.7617	 0.6050
p	 0.8052	 0.6060
r	 0.8759	 0.6310
s	 0.9012	 0.6380
u	 0.8058	 0.6010
v	 0.6843	 0.5550
w	 0.8201	 0.6070