



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:54 AM JST

PDB ID : 7W0R / pdb_00007w0r
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

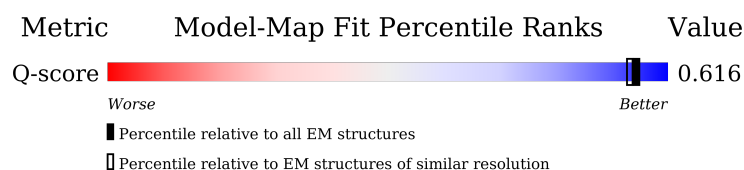
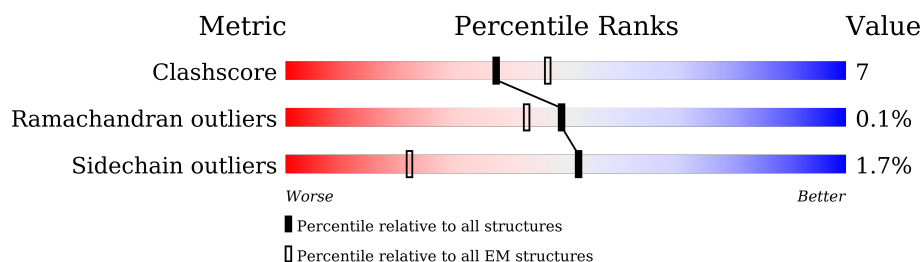
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	

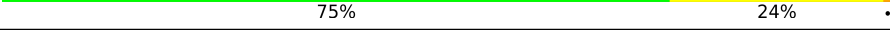
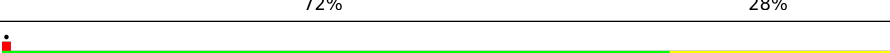
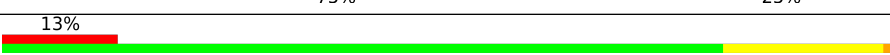
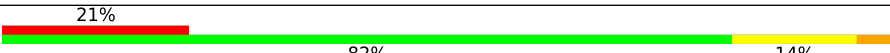
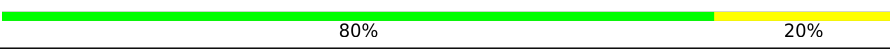
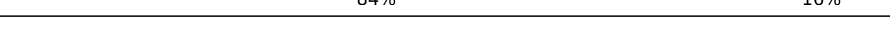
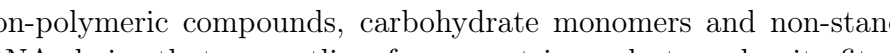
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	124	
44	w	320	

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		

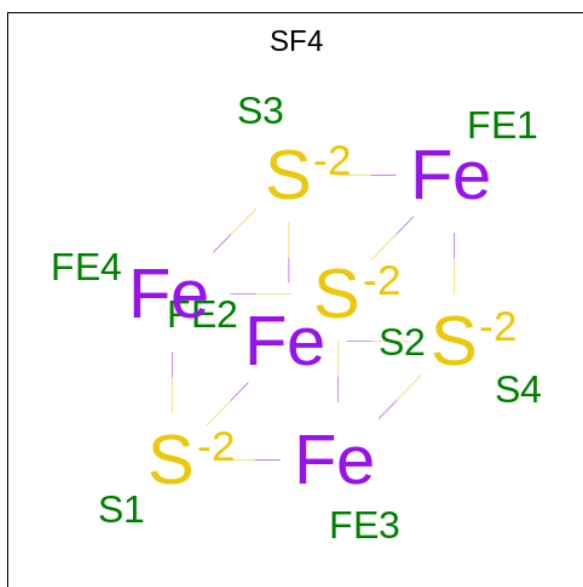
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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.

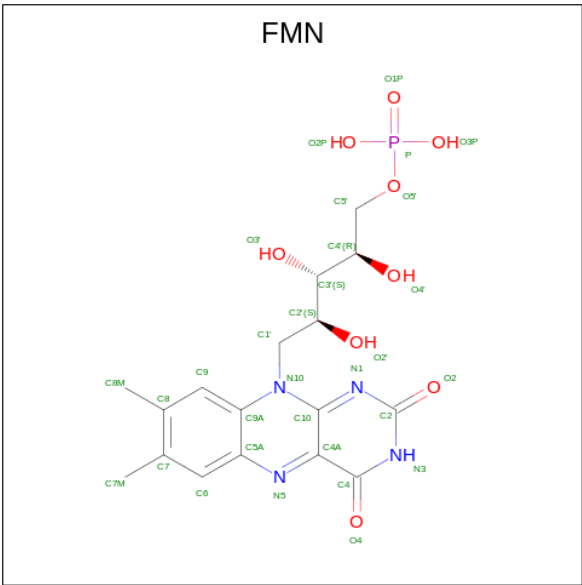
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

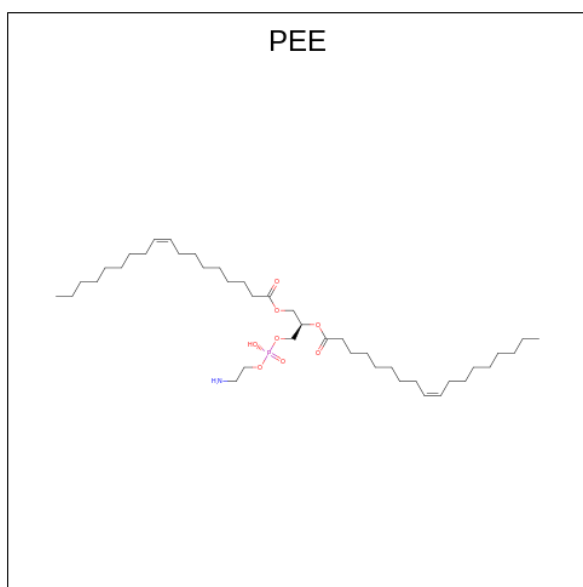
- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

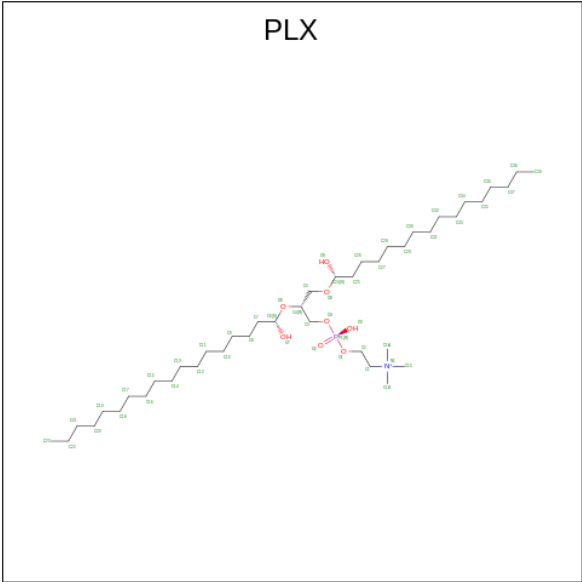
- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).





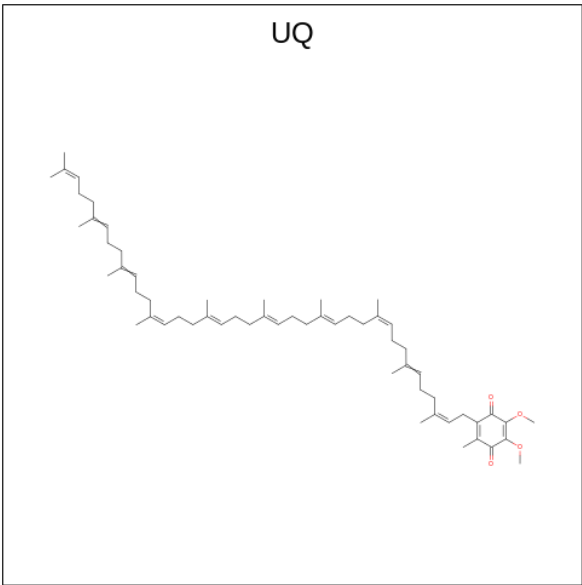
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
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 (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



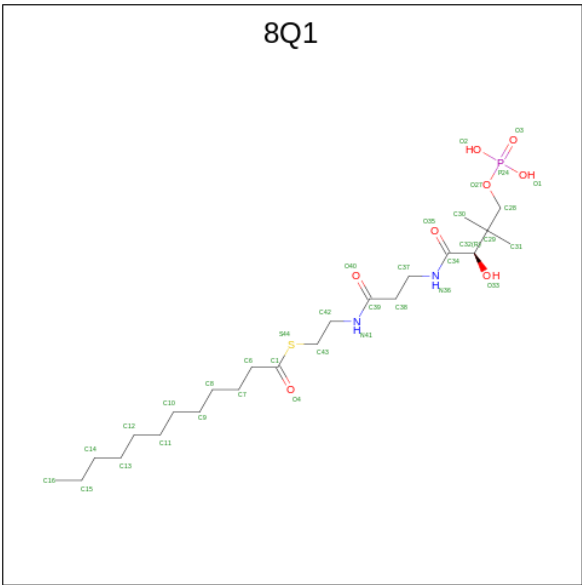
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (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 (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



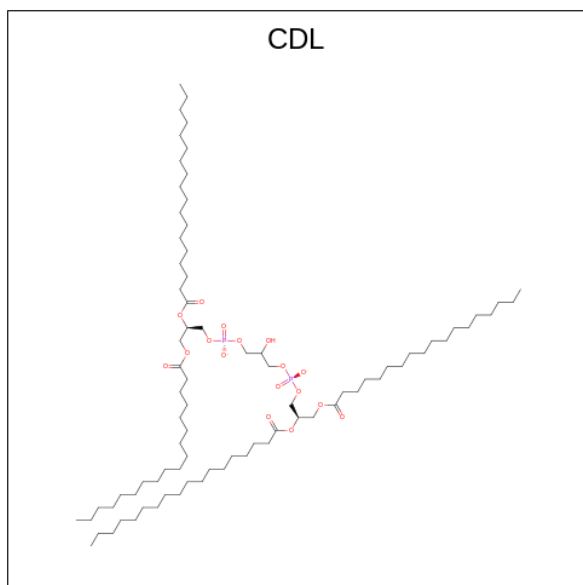
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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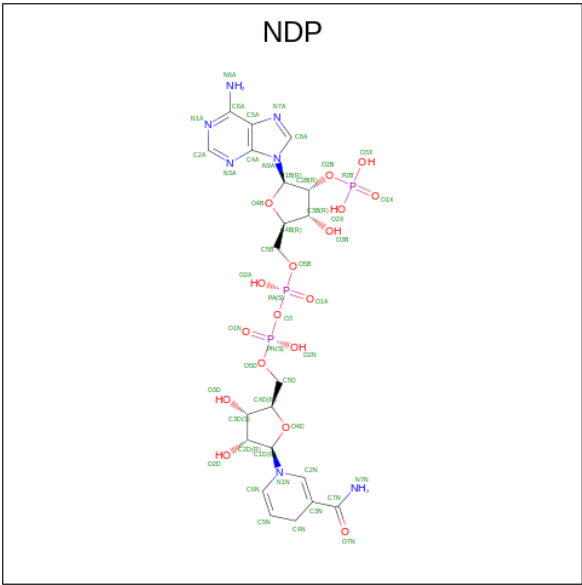
Mol	Chain	Residues	Atoms						AltConf
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



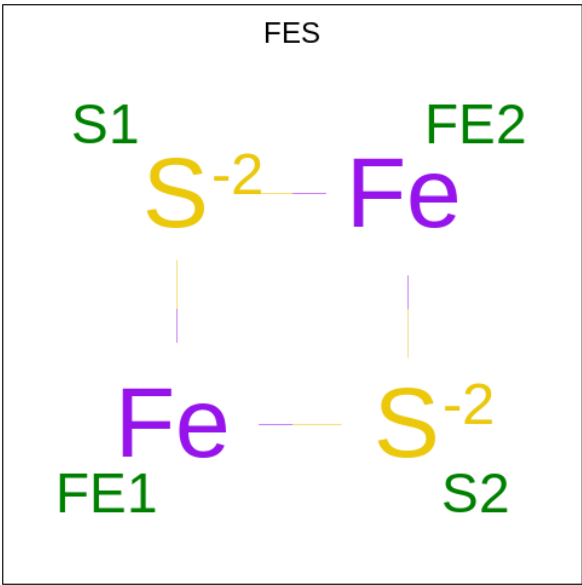
Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	k	1	Total	C	O	P	0
			100	81	17	2	
52	l	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			100	81	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	r	1	Total	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	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	J	1	48	21	7	17	3	0

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

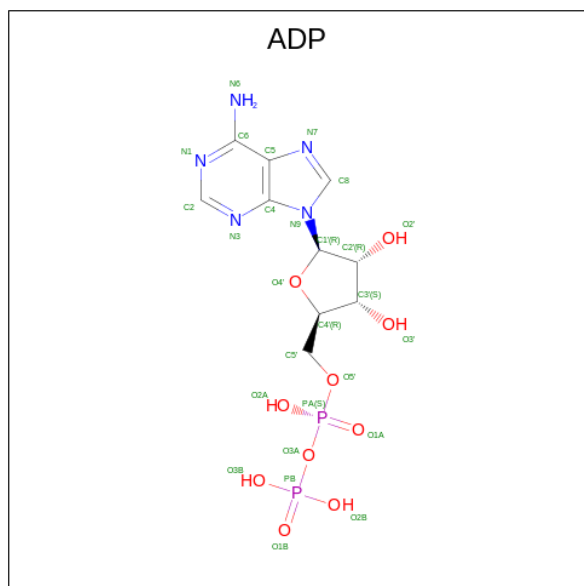
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

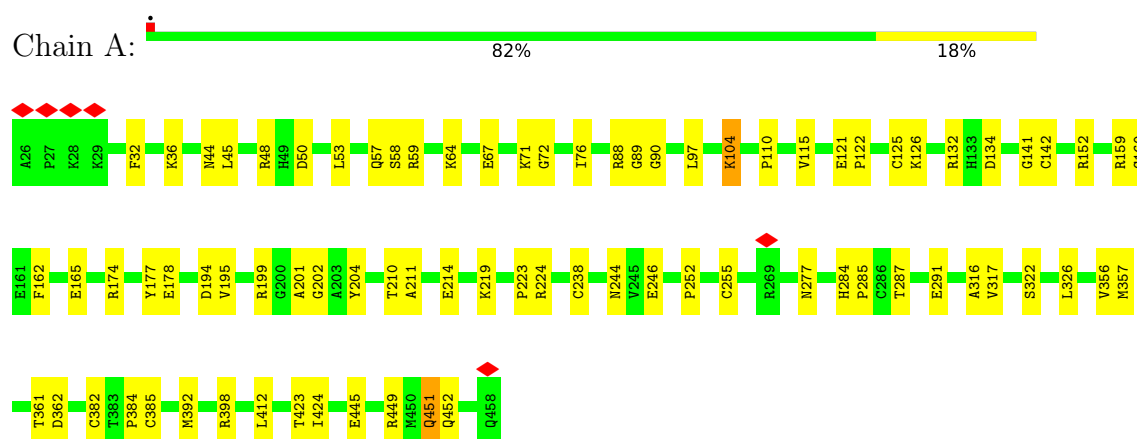


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

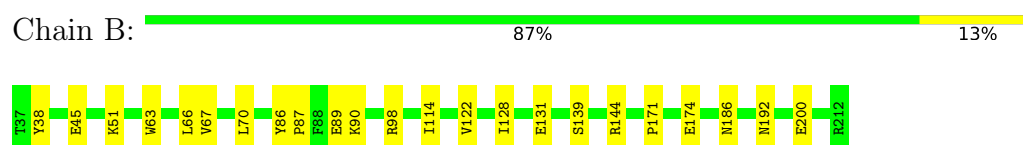
3 Residue-property plots

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.

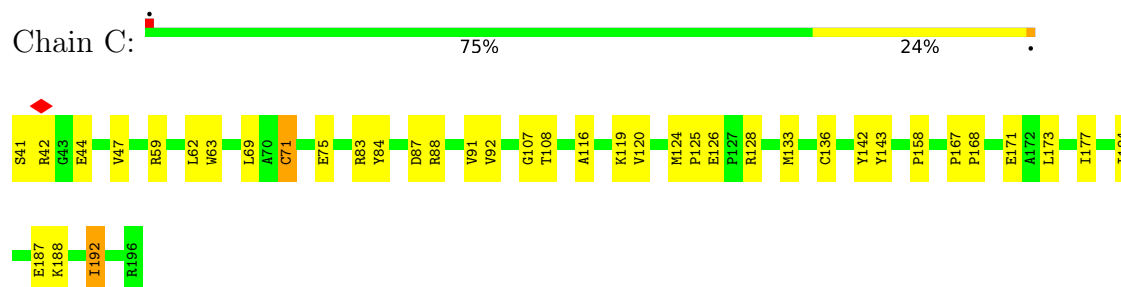
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



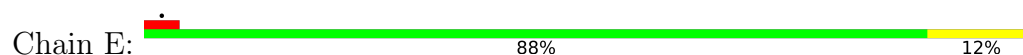
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

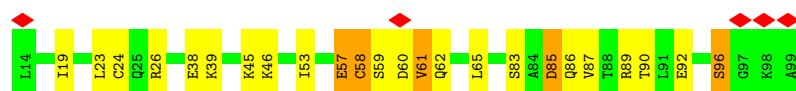


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

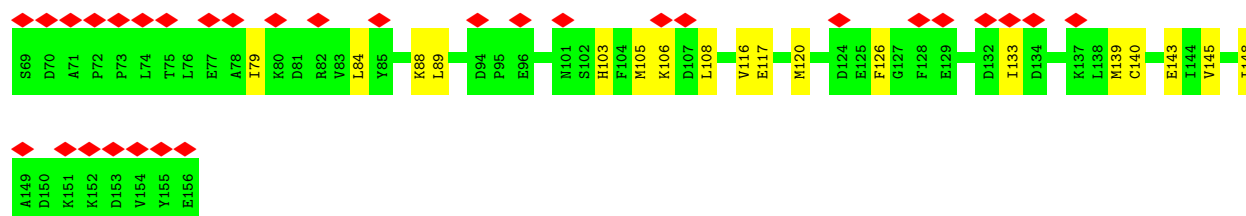
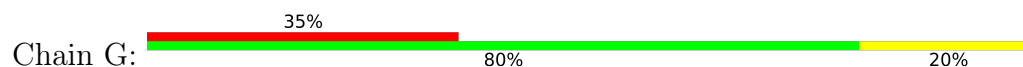




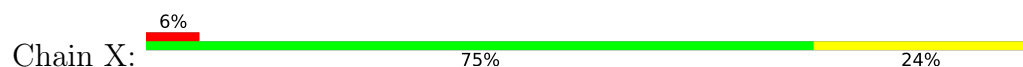
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



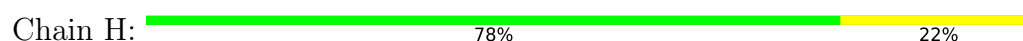
- Molecule 6: Acyl carrier protein



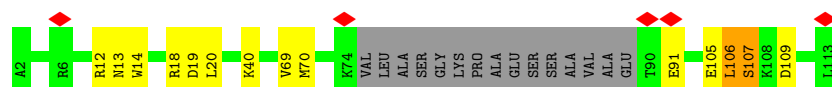
- Molecule 6: Acyl carrier protein



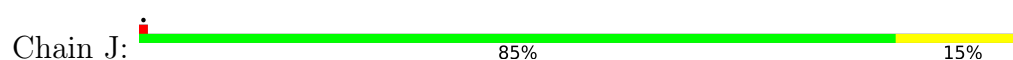
- Molecule 7: Complex I subunit B13

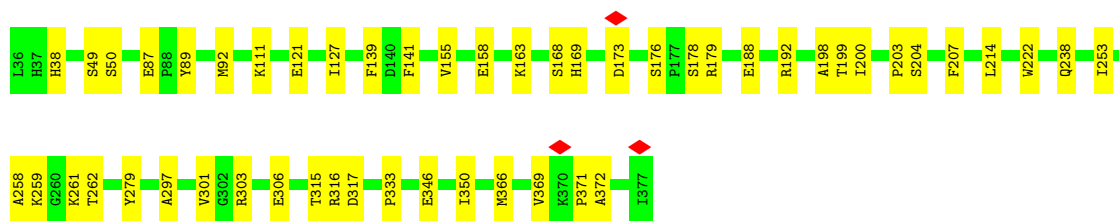


- Molecule 8: Complex I-B14.5a

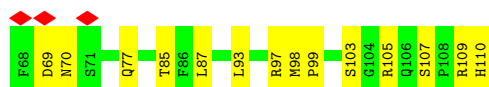


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

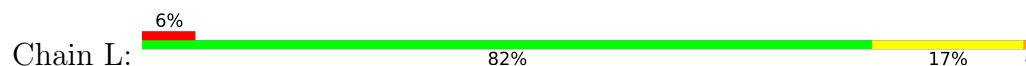




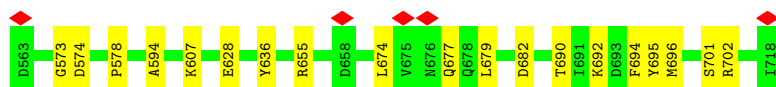
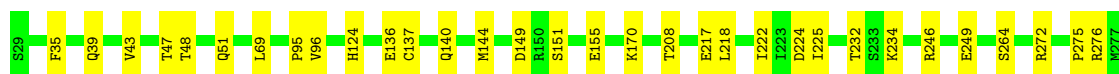
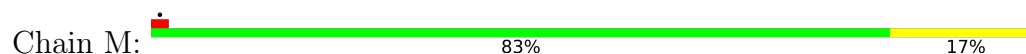
• Molecule 10: Complex I-9kD



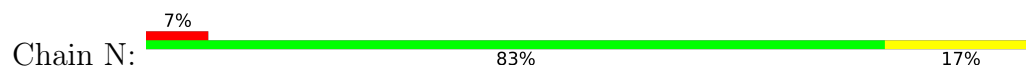
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

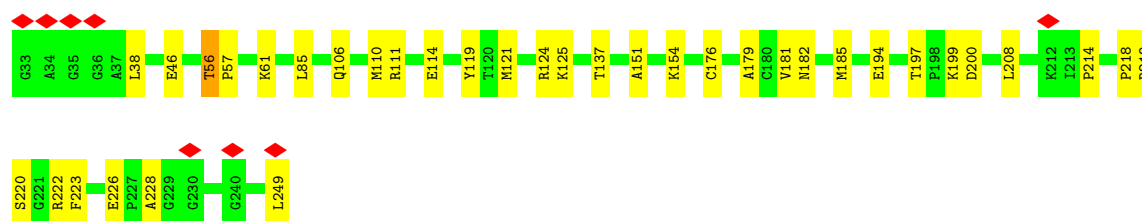


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

Chain O:  83% 16%



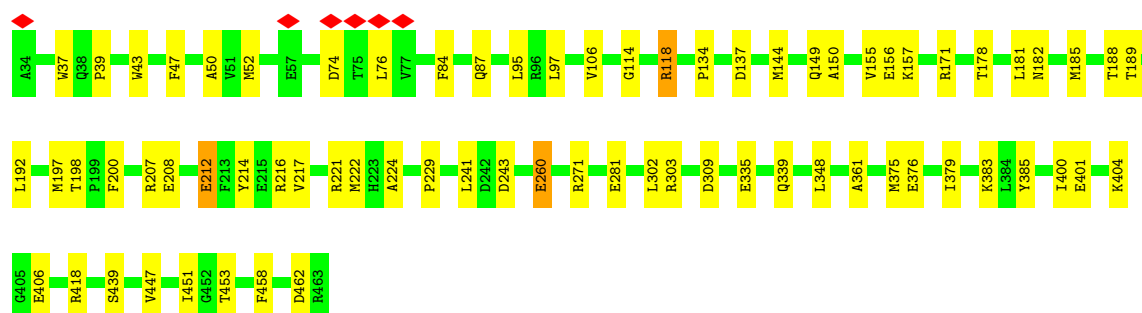
• Molecule 15: Complex I-30kD

Chain P:  85% 15%



• Molecule 16: Complex I-49kD

Chain Q:  83% 16%



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

Chain S:  81% 16%



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

Chain T:  89% 11%

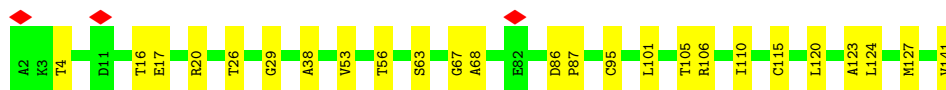
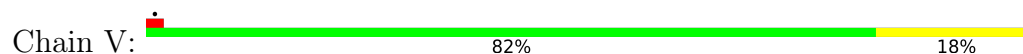


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

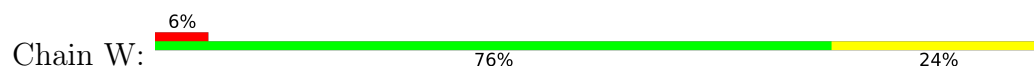
Chain U:  5% 88% 12%



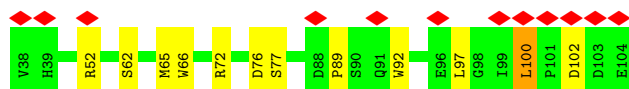
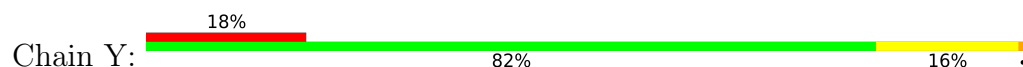
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



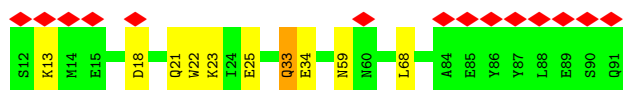
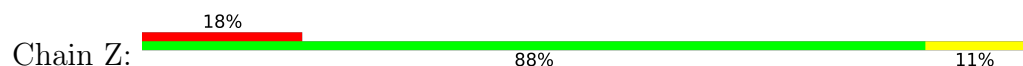
- Molecule 21: Complex I-B16.6



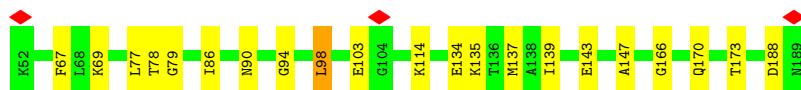
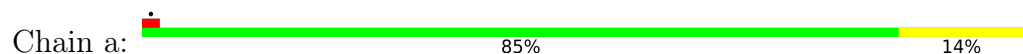
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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

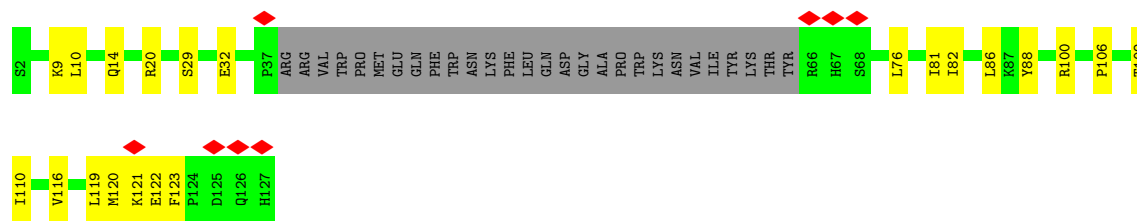


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 25: Complex I-B17





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

Chain c: 86% 13%



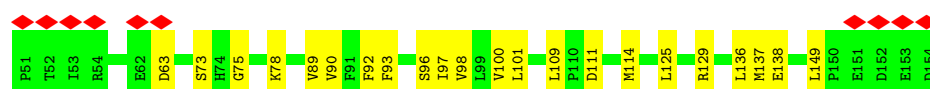
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 7% 80% 19%



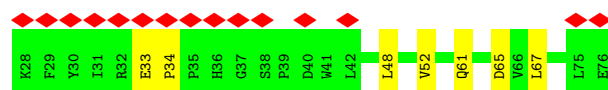
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 10% 79% 21%



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

Chain f: 31% 86% 14%

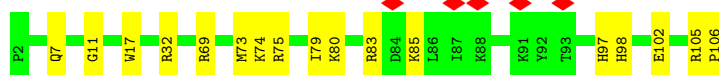
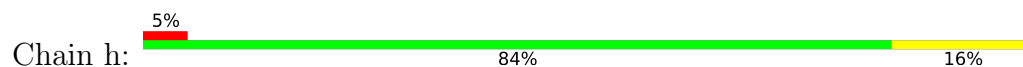


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

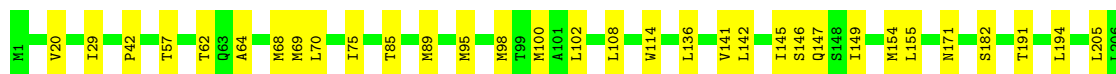
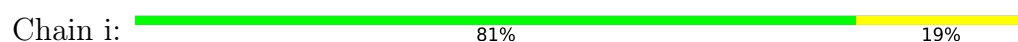
Chain g: 89% 11%



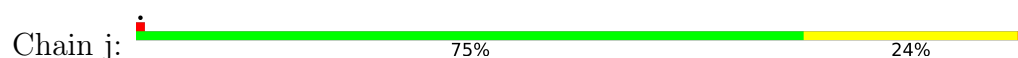
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



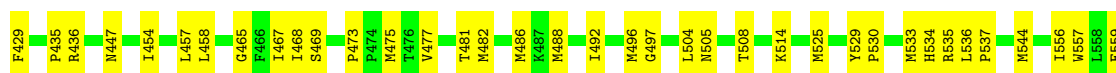
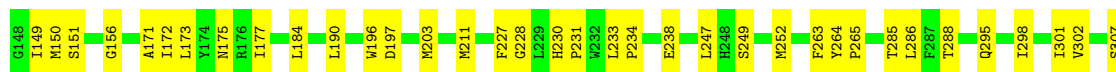
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

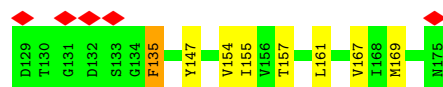
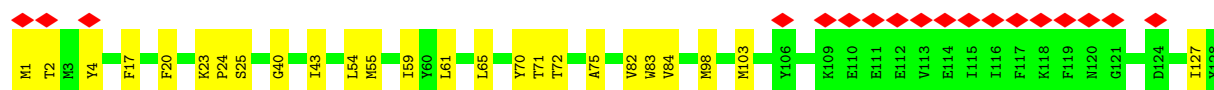
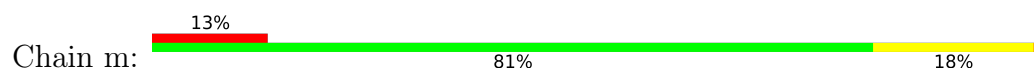


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

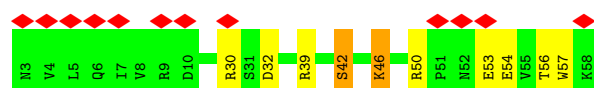
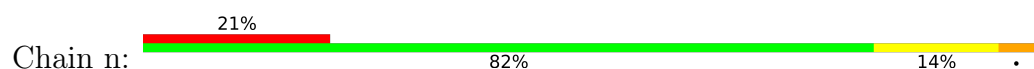




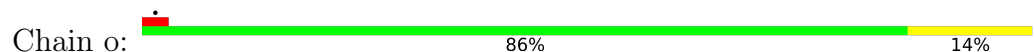
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



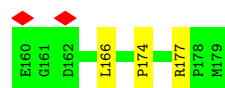
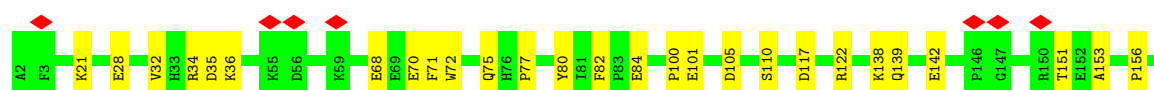
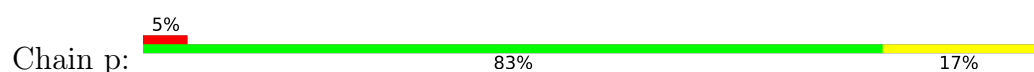
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



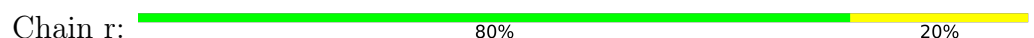
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

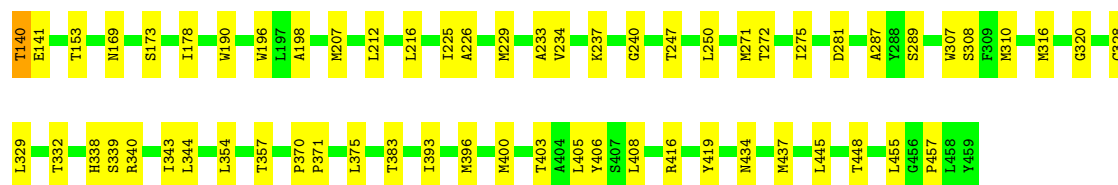


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

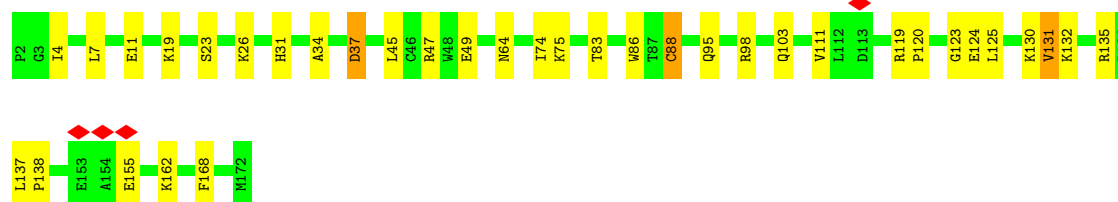
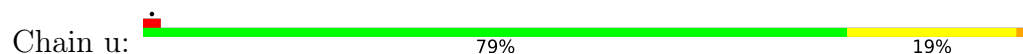




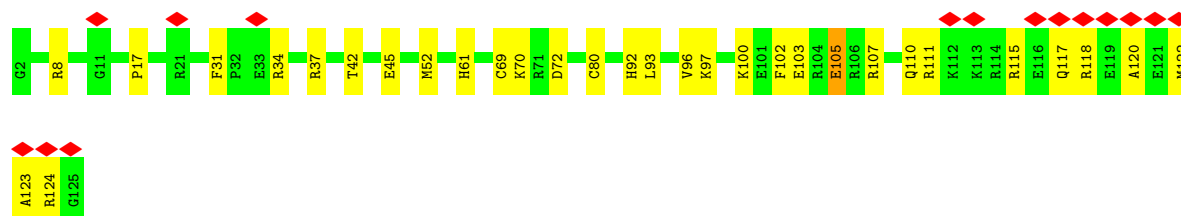
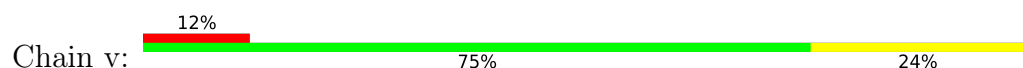
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



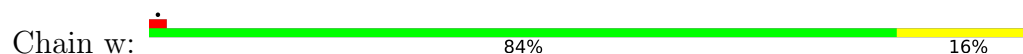
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- 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: NDP, MG, SF4, PEE, CDL, 2MR, ZN, UQ, ADP, FES, FMN, NAI, 8Q1, PLX

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	0.17	0/3406	0.32	0/4603
2	B	0.22	0/1443	0.34	0/1952
3	C	0.22	0/1279	0.32	0/1730
4	E	0.17	0/991	0.30	0/1335
5	F	0.20	0/698	0.49	3/940 (0.3%)
6	G	0.19	0/702	0.45	0/952
6	X	0.16	0/716	0.34	0/968
7	H	0.19	0/929	0.35	0/1258
8	I	0.20	0/798	0.54	2/1079 (0.2%)
9	J	0.18	0/2828	0.31	0/3834
10	K	0.14	0/377	0.24	0/509
11	L	0.20	0/1039	0.31	0/1403
12	M	0.19	0/5384	0.35	0/7295
13	N	0.20	0/1245	0.40	0/1694
14	O	0.16	0/1711	0.33	0/2328
15	P	0.21	0/1789	0.33	0/2436
16	Q	0.22	0/3538	0.36	0/4796
17	S	0.21	0/581	0.41	0/781
18	T	0.17	0/755	0.30	0/1018
19	U	0.15	0/664	0.31	0/912
20	V	0.24	0/1042	0.41	0/1411
21	W	0.19	0/1198	0.32	0/1617
22	Y	0.15	0/610	0.29	0/836
23	Z	0.14	0/660	0.29	0/892
24	a	0.19	0/1184	0.31	0/1603
25	b	0.17	0/844	0.33	0/1149
26	c	0.18	0/1371	0.36	0/1875
27	d	0.20	0/1494	0.51	6/2015 (0.3%)
28	e	0.17	0/891	0.33	0/1210
29	f	0.18	0/386	0.35	0/523
30	g	0.17	0/1031	0.31	0/1394
31	h	0.17	0/889	0.32	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.21	0/2773	0.38	0/3768
33	j	0.23	0/938	0.41	0/1281
34	k	0.22	0/759	0.37	0/1029
35	l	0.18	0/4929	0.35	0/6704
36	m	0.20	0/1328	0.36	0/1804
37	n	0.14	0/491	0.28	0/663
38	o	0.16	0/1092	0.30	0/1481
39	p	0.17	0/1586	0.31	0/2150
40	r	0.21	0/3723	0.36	0/5078
41	s	0.22	0/2581	0.39	0/3529
42	u	0.17	0/1436	0.36	0/1938
43	v	0.15	0/1083	0.31	0/1448
44	w	0.16	0/2642	0.31	0/3580
All	All	0.19	0/67834	0.35	11/91991 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	106	LEU	N-CA-C	7.86	121.41	109.62
8	I	107	SER	N-CA-C	7.71	120.66	111.02
27	d	13	PRO	CA-C-N	7.69	127.40	119.56
27	d	13	PRO	C-N-CA	7.69	127.40	119.56
27	d	12	GLU	CA-C-N	6.57	127.14	120.38
27	d	12	GLU	C-N-CA	6.57	127.14	120.38
27	d	10	TYR	CA-C-N	5.85	125.61	119.76
27	d	10	TYR	C-N-CA	5.85	125.61	119.76
5	F	58	CYS	CA-CB-SG	5.38	126.77	114.40
5	F	57	GLU	CA-C-N	5.37	130.74	120.97
5	F	57	GLU	C-N-CA	5.37	130.74	120.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	57	0
2	B	1412	0	1363	19	0
3	C	1248	0	1254	29	0
4	E	967	0	971	9	0
5	F	687	0	700	16	0
6	G	690	0	669	13	0
6	X	704	0	695	14	0
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	12	0
11	L	1016	0	1016	17	0
12	M	5296	0	5326	72	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	29	0
15	P	1738	0	1693	21	0
16	Q	3459	0	3396	49	0
17	S	566	0	561	13	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1021	0	1027	16	0
21	W	1167	0	1155	32	0
22	Y	584	0	529	11	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	17	0
25	b	819	0	835	18	0
26	c	1315	0	1208	19	0
27	d	1461	0	1429	26	0
28	e	867	0	817	20	0
29	f	378	0	356	3	0
30	g	1000	0	994	10	0
31	h	867	0	873	15	0
32	i	2710	0	2874	52	0
33	j	914	0	951	26	0
34	k	748	0	799	24	0
35	l	4800	0	4939	111	0
36	m	1295	0	1263	31	0
37	n	479	0	486	8	0
38	o	1062	0	1072	12	0
39	p	1530	0	1466	22	0
40	r	3631	0	3839	68	0
41	s	2508	0	2607	54	0
42	u	1398	0	1374	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1059	0	1029	25	0
44	w	2582	0	2531	29	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
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	4	0
48	j	92	0	141	5	0
48	l	97	0	151	11	0
48	r	51	0	82	4	0
49	C	52	0	88	4	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	4	0
49	j	52	0	88	2	0
49	r	104	0	176	10	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	2	0
52	I	51	0	46	1	0
52	V	94	0	138	5	0
52	a	100	0	156	8	0
52	k	100	0	156	11	0
52	l	199	0	307	15	0
52	o	100	0	156	5	0
52	r	100	0	156	10	0
52	s	89	0	125	5	0
52	u	55	0	54	3	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	2	0
All	All	68233	0	69009	1024	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 (1024) 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
32:i:68:MET:HE1	34:k:37:MET:HE2	1.58	0.84
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.45	0.82
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.63	0.79
35:l:387:THR:HG22	35:l:465:GLY:H	1.48	0.79
32:i:146:SER:HA	32:i:149:ILE:HG12	1.66	0.77
36:m:82:VAL:HG21	52:s:401:CDL:HB31	1.64	0.77
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
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.66	0.76
4:E:16:SER:HA	11:L:52:LEU:HD13	1.70	0.74
34:k:6:MET:HG2	36:m:103:MET:HE3	1.70	0.74
16:Q:52:MET:O	32:i:171:ASN:ND2	2.20	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
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.21	0.73
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
32:i:89:MET:HE1	32:i:98:MET:HE3	1.71	0.72
21:W:94:GLU:HG3	31:h:79:ILE:HD13	1.70	0.72
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.70	0.71
41:s:307:LEU:O	41:s:311:THR:HB	1.90	0.71
32:i:278:MET:O	32:i:282:MET:HG3	1.90	0.71
1:A:50:ASP:O	1:A:59:ARG:NH2	2.23	0.71
35:l:228:GLY:HA3	48:l:703:PEE:H38	1.71	0.71
27:d:38:ASP:OD1	27:d:39:LEU:N	2.24	0.71
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.71	0.70
8:I:40:LYS:HB3	21:W:7:LYS:H	1.56	0.70
51:X:201:8Q1:C11	39:p:70:GLU:OE1	2.40	0.69
6:G:143:GLU:OE2	6:G:143:GLU:N	2.17	0.69
16:Q:87:GLN:HB3	33:j:39:CYS:O	1.92	0.69
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.26	0.69
2:B:45:GLU:OE2	2:B:45:GLU:N	2.20	0.69
44:w:125:ASP:O	44:w:130:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:97:THR:O	35:l:101:MET:HG3	1.93	0.69
41:s:13:ILE:O	41:s:17:VAL:HG23	1.92	0.69
40:r:307:TRP:HA	40:r:310:MET:HE2	1.74	0.69
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.75	0.69
9:J:192:ARG:NH1	9:J:198:ALA:O	2.25	0.68
48:i:401:PEE:H37	48:i:401:PEE:H60	1.75	0.68
30:g:117:GLU:OE1	30:g:117:GLU:N	2.19	0.68
41:s:28:LEU:HD22	41:s:275:ALA:HB2	1.75	0.68
52:a:201:CDL:H772	52:a:201:CDL:H212	1.75	0.68
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.74	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
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.76	0.68
42:u:103:GLN:N	42:u:103:GLN:OE1	2.23	0.67
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
41:s:156:MET:HA	41:s:156:MET:HE2	1.76	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
21:W:85:GLN:OE1	31:h:105:ARG:NH1	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
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.60	0.66
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.29	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
52:o:201:CDL:H512	52:o:201:CDL:H712	1.77	0.66
29:f:48:LEU:O	29:f:52:VAL:HG23	1.96	0.65
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
41:s:253:GLU:OE2	41:s:253:GLU:N	2.24	0.65
35:l:150:MET:HE3	35:l:150:MET:HA	1.77	0.65
6:X:140:CYS:HB2	6:X:143:GLU:HG3	1.79	0.65
32:i:20:VAL:HG13	32:i:29:ILE:HG23	1.77	0.65
33:j:38:GLU:HB2	33:j:41:PHE:O	1.97	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
32:i:243:LEU:HD23	52:r:504:CDL:H361	1.79	0.65
28:e:63:ASP:OD2	40:r:338:HIS:NE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:106:TRP:CD1	35:l:447:ASN:HD22	2.15	0.64
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
35:l:227:PHE:O	35:l:230:HIS:ND1	2.31	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
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.80	0.63
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.62
41:s:221:ALA:O	41:s:225:MET:HG3	1.99	0.62
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
31:h:32:ARG:HH11	31:h:32:ARG:HG2	1.63	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
52:l:701:CDL:H432	52:l:701:CDL:H621	1.80	0.62
40:r:31:SER:HB3	40:r:74:PRO:HG3	1.81	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
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.81	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
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.80	0.61
14:O:151:ALA:HA	14:O:154:LYS:HE3	1.81	0.61
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.82	0.61
35:l:375:ILE:HD12	35:l:458:LEU:HD21	1.82	0.61
43:v:93:LEU:O	43:v:97:LYS:HG3	2.00	0.61
9:J:163:LYS:HG2	9:J:259:LYS:HE2	1.82	0.61
24:a:188:ASP:OD1	42:u:47:ARG:NH2	2.33	0.61
3:C:133:MET:HG2	3:C:168:PRO:HG2	1.83	0.61
26:c:46:GLU:OE2	26:c:46:GLU:N	2.27	0.61
12:M:488:ALA:HB1	12:M:679:LEU:HD12	1.81	0.61
3:C:124:MET:HE3	3:C:128:ARG:HB2	1.83	0.61
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.83	0.61
39:p:151:THR:HG23	39:p:153:ALA:H	1.66	0.61
52:l:701:CDL:H242	48:l:704:PEE:H34	1.82	0.61
39:p:84:GLU:OE2	39:p:177:ARG:NH2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ARG:HA	41:s:37:PRO:HA	1.81	0.60
52:s:401:CDL:H332	52:s:401:CDL:H182	1.81	0.60
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.82	0.60
25:b:110:ILE:HG12	27:d:16:ARG:HB3	1.83	0.60
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.83	0.60
27:d:23:GLN:HG2	43:v:72:ASP:HB3	1.84	0.60
26:c:185:GLU:OE1	43:v:97:LYS:NZ	2.35	0.60
40:r:271:MET:HE2	40:r:271:MET:HA	1.84	0.60
8:I:106:LEU:O	8:I:106:LEU:HG	2.02	0.60
20:V:124:LEU:HD11	48:r:501:PEE:H64	1.83	0.59
13:N:4:VAL:O	13:N:8:ARG:HG3	2.02	0.59
35:l:473:PRO:O	35:l:475:MET:HE2	2.03	0.59
36:m:61:LEU:O	41:s:114:TYR:OH	2.20	0.59
52:l:701:CDL:H452	40:r:445:LEU:HB3	1.84	0.59
9:J:178:SER:OG	9:J:317:ASP:OD2	2.20	0.59
27:d:6:ASP:HB3	27:d:9:VAL:HG22	1.85	0.59
44:w:49:THR:HG21	44:w:291:PHE:HB3	1.84	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
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.85	0.59
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.84	0.59
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.36	0.59
9:J:163:LYS:NZ	9:J:253:ILE:O	2.25	0.59
39:p:68:GLU:OE1	39:p:68:GLU:HA	2.03	0.59
52:a:201:CDL:H512	48:l:704:PEE:H52	1.85	0.59
21:W:56:GLU:OE1	21:W:59:ARG:NH2	2.31	0.59
31:h:69:ARG:O	31:h:73:MET:HG3	2.03	0.59
42:u:88:CYS:SG	42:u:103:GLN:NE2	2.76	0.59
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.31	0.58
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
49:J:403:PLX:H222	33:j:16:LEU:HB3	1.85	0.58
52:l:701:CDL:H391	40:r:371:PRO:HD2	1.84	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
32:i:155:LEU:HD22	32:i:278:MET:HE2	1.86	0.58
40:r:226:ALA:HA	40:r:229:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:64:GLU:H	18:T:64:GLU:CD	2.11	0.58
24:a:166:GLY:O	24:a:170:GLN:NE2	2.36	0.58
33:j:18:VAL:HG12	48:j:202:PEE:H16	1.85	0.58
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.85	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:186:ASN:HB3	11:L:112:MET:HE1	1.85	0.58
2:B:131:GLU:OE2	2:B:144:ARG:NE	2.36	0.58
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.86	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
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.57
16:Q:281:GLU:CD	16:Q:281:GLU:H	2.13	0.57
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.37	0.57
41:s:307:LEU:HA	41:s:310:MET:HE2	1.87	0.57
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.86	0.57
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.87	0.57
41:s:101:GLY:O	41:s:105:MET:HG2	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
41:s:218:GLY:O	41:s:222:MET:HG3	2.05	0.57
7:H:44:TYR:O	7:H:48:THR:HG22	2.05	0.57
32:i:68:MET:HE2	32:i:68:MET:HA	1.86	0.57
43:v:92:HIS:O	43:v:96:VAL:HG23	2.04	0.57
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.87	0.56
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.85	0.56
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.86	0.56
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
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.87	0.56
35:l:151:SER:HB2	35:l:252:MET:HE1	1.87	0.56
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.05	0.56
40:r:126:LEU:HD11	40:r:153:THR:HG21	1.88	0.56
40:r:328:CYS:HB3	40:r:437:MET:HE1	1.87	0.56
43:v:103:GLU:O	43:v:107:ARG:HG2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:447:VAL:O	16:Q:451:ILE:HG13	2.05	0.56
33:j:113:TRP:HZ2	41:s:286:MET:HE3	1.70	0.56
38:o:118:GLU:OE1	38:o:120:LYS:HG2	2.05	0.56
24:a:135:LYS:HD2	37:n:32:ASP:HB2	1.88	0.56
33:j:103:ALA:HB2	48:j:201:PEE:H22	1.88	0.56
52:r:504:CDL:H782	52:r:504:CDL:H241	1.88	0.56
32:i:246:VAL:HG11	52:r:504:CDL:H392	1.87	0.56
40:r:207:MET:HE3	40:r:240:GLY:N	2.20	0.56
33:j:57:LEU:HD21	36:m:169:MET:HE3	1.87	0.56
10:K:109:ARG:NH2	14:O:106:GLN:O	2.38	0.56
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.87	0.55
48:l:703:PEE:H55	40:r:405:LEU:HD13	1.88	0.55
37:n:54:GLU:N	37:n:54:GLU:OE1	2.39	0.55
22:Y:72:ARG:HB3	35:l:385:TYR:CD2	2.41	0.55
35:l:106:TRP:HD1	35:l:447:ASN:HD22	1.52	0.55
16:Q:114:GLY:N	16:Q:462:ASP:OD1	2.38	0.55
52:V:201:CDL:H532	35:l:577:VAL:HG22	1.87	0.55
41:s:313:SER:O	41:s:313:SER:OG	2.22	0.55
32:i:238:PRO:HB2	52:r:504:CDL:HA31	1.87	0.55
35:l:128:MET:HE2	35:l:147:VAL:HG11	1.88	0.55
39:p:105:ASP:OD2	39:p:122:ARG:NH1	2.28	0.55
6:X:93:ILE:HG21	6:X:98:LEU:HD13	1.88	0.55
27:d:69:ARG:NH2	37:n:46:LYS:O	2.39	0.55
17:S:70:ASP:O	42:u:75:LYS:NZ	2.37	0.55
8:I:18:ARG:NH2	16:Q:260:GLU:OE2	2.35	0.55
49:J:403:PLX:H101	33:j:24:LEU:HD13	1.88	0.55
28:e:111:ASP:OD2	28:e:114:MET:N	2.39	0.55
40:r:11:LEU:HD23	40:r:14:MET:HE1	1.88	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
21:W:134:LEU:HD21	36:m:2:THR:HB	1.88	0.55
1:A:32:PHE:HB3	1:A:291:GLU:HG2	1.88	0.54
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.38	0.54
41:s:156:MET:HE3	41:s:308:PRO:HG3	1.89	0.54
1:A:36:LYS:H	1:A:36:LYS:HD2	1.73	0.54
3:C:41:SER:OG	3:C:42:ARG:N	2.40	0.54
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.47	0.54
34:k:55:LEU:O	34:k:58:MET:HE3	2.07	0.54
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.41	0.54
40:r:237:LYS:HD2	40:r:316:MET:HG2	1.89	0.54
40:r:272:THR:HA	40:r:275:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:OE2	1:A:445:GLU:N	2.39	0.54
34:k:17:ALA:HB2	52:k:101:CDL:H812	1.88	0.54
48:l:704:PEE:H3	49:r:503:PLX:H1C3	1.90	0.54
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.22	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
17:S:54:ILE:HD11	31:h:106:PRO:HB3	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
40:r:105:PHE:O	40:r:109:THR:OG1	2.25	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
13:N:68:MET:HG3	13:N:81:MET:HE3	1.89	0.54
16:Q:52:MET:HE3	32:i:295:ARG:HD3	1.88	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
25:b:122:GLU:O	25:b:122:GLU:HG3	2.08	0.54
44:w:171:GLU:O	44:w:175:ARG:HG2	2.08	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
33:j:38:GLU:OE1	33:j:38:GLU:HA	2.08	0.54
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.53
16:Q:198:THR:OG1	41:s:275:ALA:O	2.22	0.53
40:r:403:THR:HA	40:r:406:TYR:CE2	2.43	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
35:l:331:MET:HG3	35:l:387:THR:HB	1.90	0.53
52:l:701:CDL:H331	52:l:701:CDL:H591	1.91	0.53
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.29	0.53
4:E:35:LEU:HD13	4:E:87:LYS:HG3	1.91	0.53
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.39	0.53
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.91	0.53
21:W:88:ARG:NH2	42:u:7:LEU:O	2.42	0.53
24:a:134:GLU:OE1	37:m:57:TRP:NE1	2.24	0.53
34:k:2:PRO:HG3	36:m:127:ILE:HD13	1.89	0.53
35:l:492:ILE:O	35:l:496:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:106:PRO:HG2	25:b:120:MET:HE2	1.90	0.53
32:i:147:GLN:CD	32:i:147:GLN:H	2.17	0.53
24:a:78:THR:HG21	28:e:96:SER:HA	1.91	0.53
25:b:121:LYS:O	25:b:121:LYS:HG3	2.08	0.53
21:W:66:GLU:OE2	42:u:123:GLY:N	2.37	0.53
51:X:201:8Q1:C11	39:p:70:GLU:CD	2.82	0.53
33:j:16:LEU:O	33:j:20:ILE:HG12	2.09	0.53
38:o:113:GLU:O	38:o:117:GLN:HG2	2.09	0.53
40:r:91:ARG:NH2	44:w:325:ASP:OD2	2.42	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
52:l:702:CDL:H762	52:l:702:CDL:H592	1.91	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:199:THR:OG1	9:J:258:ALA:O	2.25	0.52
6:X:155:TYR:HA	25:b:20:ARG:HG2	1.90	0.52
49:g:201:PLX:H233	32:i:207:ILE:HD13	1.91	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
40:r:67:VAL:HG12	49:r:503:PLX:H362	1.90	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
32:i:213:LEU:HD13	32:i:329:MET:HE3	1.91	0.52
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.44	0.52
2:B:38:TYR:CE2	8:I:106:LEU:HD13	2.45	0.52
52:a:201:CDL:H401	27:d:44:PRO:HB3	1.91	0.52
28:e:97:ILE:O	28:e:101:LEU:HB2	2.10	0.52
40:r:73:LEU:HA	40:r:76:MET:HE2	1.92	0.52
25:b:10:LEU:HG	25:b:14:GLN:HE21	1.74	0.52
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.90	0.52
35:l:544:MET:HE2	35:l:544:MET:HA	1.92	0.52
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.91	0.52
24:a:103:GLU:OE1	24:a:103:GLU:HA	2.10	0.52
30:g:3:MET:HG2	30:g:4:MET:HG2	1.92	0.52
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.92	0.52
32:i:280:THR:O	32:i:284:MET:HG2	2.09	0.52
40:r:98:MET:HE1	52:r:504:CDL:H212	1.90	0.52
44:w:93:TYR:O	44:w:96:SER:OG	2.28	0.52
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.92	0.52
31:h:32:ARG:HG2	31:h:32:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:31:LYS:O	38:o:35:GLU:HG2	2.10	0.52
40:r:212:LEU:HD21	49:r:502:PLX:H212	1.92	0.52
41:s:222:MET:HA	41:s:225:MET:HE2	1.91	0.52
44:w:258:TYR:CZ	44:w:269:VAL:HG13	2.45	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.91	0.52
40:r:354:LEU:O	40:r:357:THR:HG22	2.10	0.52
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.10	0.51
35:l:429:PHE:HE1	39:p:32:VAL:HG21	1.74	0.51
39:p:28:GLU:OE1	39:p:34:ARG:NH1	2.41	0.51
21:W:97:ILE:HD13	31:h:83:ARG:HG3	1.91	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
6:X:96:GLU:H	6:X:96:GLU:CD	2.19	0.51
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.93	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
35:l:137:LEU:HD21	35:l:263:PHE:HZ	1.76	0.51
12:M:249:GLU:HG2	12:M:276:ARG:HD3	1.93	0.51
20:V:38:ALA:HB2	52:k:101:CDL:H251	1.91	0.51
35:l:298:ILE:O	35:l:302:VAL:HG23	2.11	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
33:j:71:LEU:O	36:m:147:TYR:OH	2.29	0.51
34:k:51:THR:O	34:k:53:PHE:N	2.41	0.51
21:W:105:LYS:HE3	42:u:4:ILE:HD11	1.92	0.51
35:l:129:MET:O	35:l:133:THR:OG1	2.28	0.51
35:l:341:MET:HE2	35:l:454:ILE:HG12	1.92	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
41:s:228:TYR:HA	41:s:231:ILE:HD12	1.93	0.50
6:X:115:GLN:NE2	6:X:138:LEU:O	2.44	0.50
35:l:359:MET:O	35:l:436:ARG:NH2	2.45	0.50
35:l:387:THR:HG22	35:l:465:GLY:N	2.24	0.50
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.93	0.50
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.92	0.50
3:C:84:TYR:CE1	3:C:171:GLU:HG3	2.47	0.50
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.94	0.50
35:l:286:LEU:HD13	35:l:411:MET:SD	2.51	0.50
3:C:184:ILE:O	3:C:187:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.47	0.50
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.94	0.50
9:J:50:SER:OG	15:P:225:GLU:OE2	2.26	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
35:l:346:ILE:HA	35:l:366:MET:HE1	1.94	0.50
40:r:1:MET:SD	40:r:111:THR:HG21	2.52	0.50
21:W:93:GLU:O	21:W:97:ILE:HG13	2.12	0.50
27:d:9:VAL:HG23	27:d:10:TYR:CD2	2.47	0.50
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.94	0.50
35:l:36:VAL:HG13	35:l:122:LEU:HD22	1.94	0.50
24:a:94:GLY:O	27:d:61:TYR:OH	2.27	0.49
1:A:174:ARG:O	1:A:178:GLU:HG2	2.12	0.49
49:J:403:PLX:H201	33:j:16:LEU:HD12	1.94	0.49
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.93	0.49
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.94	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
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.46	0.49
40:r:140:THR:HG23	40:r:141:GLU:OE1	2.12	0.49
40:r:339:SER:HB3	40:r:344:LEU:HD22	1.93	0.49
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.45	0.49
5:F:92:GLU:O	5:F:96:SER:OG	2.30	0.49
12:M:428:LYS:NZ	12:M:443:ASP:OD1	2.46	0.49
25:b:81:ILE:HG23	48:l:704:PEE:H58	1.93	0.49
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.94	0.49
19:U:66:VAL:O	42:u:130:LYS:HE3	2.12	0.49
28:e:92:PHE:O	28:e:96:SER:HB2	2.12	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
22:Y:102:ASP:HA	43:v:115:ARG:HH22	1.77	0.49
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.51	0.49
6:G:105:MET:HE2	6:G:139:MET:HE1	1.95	0.49
9:J:87:GLU:HG3	9:J:89:TYR:H	1.77	0.49
24:a:137:MET:HE1	37:n:42:SER:HA	1.95	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
52:V:201:CDL:H661	35:l:594:THR:HG23	1.94	0.49
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:38:PRO:HG2	38:o:70:TYR:HD1	1.78	0.49
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.40	0.49
37:n:30:ARG:NH1	52:u:201:CDL:OA4	2.46	0.49
42:u:26:LYS:NZ	42:u:95:GLN:O	2.33	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
27:d:127:LYS:O	27:d:130:GLU:HG3	2.12	0.48
35:l:514:LYS:HB2	35:l:514:LYS:HE2	1.67	0.48
40:r:79:ALA:HB3	40:r:229:MET:HE1	1.95	0.48
52:I:201:CDL:H511	52:I:201:CDL:H542	1.67	0.48
26:c:70:MET:HE3	26:c:70:MET:HA	1.95	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
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.95	0.48
6:X:120:MET:SD	39:p:21:LYS:HG3	2.54	0.48
39:p:71:PHE:CD1	39:p:71:PHE:C	2.90	0.48
49:r:502:PLX:H251	49:r:502:PLX:H51	1.44	0.48
43:v:42:THR:OG1	43:v:45:GLU:HG3	2.13	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
32:i:270:MET:HE1	32:i:282:MET:SD	2.54	0.48
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.95	0.48
35:l:401:MET:HE2	35:l:482:MET:HB3	1.96	0.48
1:A:160:GLY:O	1:A:199:ARG:NH2	2.47	0.48
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.96	0.48
5:F:26:ARG:HH11	5:F:26:ARG:HB2	1.78	0.48
11:L:99:MET:HE2	11:L:126:LEU:HD12	1.96	0.48
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.95	0.48
1:A:214:GLU:OE2	1:A:219:LYS:NZ	2.39	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
25:b:109:THR:HG22	25:b:116:VAL:HG22	1.95	0.48
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.48	0.48
40:r:445:LEU:O	40:r:448:THR:HG22	2.12	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
28:e:125:LEU:O	28:e:129:ARG:HG3	2.13	0.48
32:i:70:LEU:HD12	32:i:98:MET:SD	2.54	0.48
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.96	0.48
40:r:106:LEU:HD13	40:r:234:VAL:HG11	1.94	0.48
10:K:77:GLN:OE1	10:K:77:GLN:N	2.47	0.48
24:a:98:LEU:HD23	27:d:63:TYR:CE2	2.48	0.48
52:a:201:CDL:H541	48:l:704:PEE:H16	1.95	0.48
27:d:159:GLN:HG2	27:d:163:MET:HE2	1.94	0.48
38:o:3:PHE:CZ	39:p:70:GLU:HG3	2.48	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
23:Z:59:ASN:O	35:l:364:LYS:NZ	2.37	0.48
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.96	0.48
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.96	0.48
35:l:171:ALA:O	35:l:175:ASN:ND2	2.47	0.48
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.14	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
23:Z:33:GLN:HE21	23:Z:33:GLN:C	2.22	0.47
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.96	0.47
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.96	0.47
5:F:85:ASP:OD1	5:F:85:ASP:N	2.47	0.47
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.47
35:l:145:GLU:HG3	40:r:370:PRO:HG2	1.95	0.47
44:w:256:LEU:HD11	44:w:276:LEU:HD11	1.95	0.47
52:k:101:CDL:H611	52:k:101:CDL:H581	1.63	0.47
52:l:702:CDL:H521	52:l:702:CDL:HB61	1.96	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
12:M:389:THR:O	12:M:390:THR:OG1	2.27	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
21:W:120:MET:HE1	31:h:73:MET:HG2	1.96	0.47
52:k:101:CDL:H161	52:k:101:CDL:H191	1.70	0.47
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.97	0.47
36:m:71:THR:HA	36:m:75:ALA:HB3	1.96	0.47
12:M:509:ASP:OD1	12:M:509:ASP:N	2.42	0.47
18:T:47:ASP:O	18:T:52:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:54:THR:O	44:w:54:THR:OG1	2.32	0.47
12:M:499:ASN:HA	12:M:502:LEU:HG	1.96	0.47
32:i:89:MET:HE1	32:i:98:MET:CE	2.41	0.47
32:i:247:THR:O	32:i:251:MET:HG3	2.14	0.47
52:s:401:CDL:H141	52:s:401:CDL:H171	1.64	0.47
44:w:320:GLY:O	44:w:324:SER:OG	2.20	0.47
12:M:539:LYS:HG2	12:M:540:ASN:CG	2.39	0.47
26:c:34:LYS:HA	26:c:34:LYS:HE2	1.96	0.47
26:c:164:ASN:ND2	26:c:180:PRO:HA	2.30	0.47
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.50	0.47
28:e:129:ARG:HB2	28:e:136:LEU:HD12	1.97	0.47
49:g:201:PLX:H102	49:g:201:PLX:H71	1.65	0.47
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.96	0.47
35:l:51:LEU:HD22	35:l:91:PRO:HG3	1.97	0.47
35:l:184:LEU:HD13	40:r:393:ILE:HG21	1.97	0.47
20:V:29:GLY:O	20:V:63:SER:HB3	2.15	0.47
27:d:164:LEU:HD23	28:e:149:LEU:HD13	1.96	0.47
49:j:203:PLX:H352	36:m:155:ILE:HG23	1.95	0.47
35:l:134:ALA:HB1	35:l:139:GLN:HB3	1.97	0.47
41:s:207:LEU:O	41:s:209:SER:N	2.48	0.47
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.54	0.47
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.97	0.47
49:j:203:PLX:H132	49:j:203:PLX:H161	1.50	0.47
43:v:107:ARG:HA	43:v:110:GLN:HB2	1.97	0.47
3:C:62:LEU:O	3:C:91:VAL:HA	2.15	0.46
3:C:119:LYS:NZ	33:j:32:GLU:OE2	2.47	0.46
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.96	0.46
52:a:201:CDL:H111	48:l:704:PEE:H60	1.97	0.46
28:e:78:LYS:HB2	28:e:78:LYS:NZ	2.29	0.46
1:A:201:ALA:C	14:O:121:MET:HG3	2.40	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
24:a:139:ILE:O	24:a:143:GLU:HG2	2.15	0.46
48:j:202:PEE:H27	52:s:401:CDL:H192	1.98	0.46
34:k:10:MET:HE2	36:m:103:MET:SD	2.55	0.46
35:l:530:PRO:O	35:l:534:HIS:HB2	2.15	0.46
52:l:701:CDL:H801	49:r:503:PLX:H181	1.97	0.46
38:o:116:ILE:HG13	38:o:121:LEU:HD22	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:271:ARG:NH1	41:s:279:ARG:O	2.42	0.46
21:W:90:ASN:ND2	21:W:123:GLU:O	2.48	0.46
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.80	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
32:i:335:LEU:HD21	52:r:504:CDL:H391	1.97	0.46
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.51	0.46
52:o:201:CDL:H792	52:o:201:CDL:H761	1.75	0.46
16:Q:50:ALA:HB1	34:k:98:CYS:SG	2.55	0.46
27:d:36:ILE:HG23	27:d:40:LEU:HD12	1.97	0.46
32:i:270:MET:O	32:i:275:SER:HB3	2.15	0.46
33:j:56:PHE:HB2	36:m:70:TYR:OH	2.16	0.46
38:o:25:ILE:HG21	38:o:30:ARG:CZ	2.46	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
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.98	0.46
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.98	0.46
40:r:8:THR:HG22	40:r:100:ILE:HG23	1.97	0.46
40:r:71:TRP:CG	49:r:503:PLX:H341	2.51	0.46
41:s:149:ILE:HG21	41:s:185:TRP:HB2	1.96	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
10:K:105:ARG:HH22	12:M:426:ASP:CG	2.23	0.46
28:e:125:LEU:HD23	28:e:125:LEU:HA	1.80	0.46
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.81	0.46
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.41	0.46
35:l:313:MET:HE2	35:l:329:ILE:HA	1.97	0.46
52:l:701:CDL:H312	52:l:701:CDL:HA61	1.64	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
31:h:75:ARG:O	31:h:79:ILE:HG13	2.16	0.46
52:s:401:CDL:H401	52:s:401:CDL:H372	1.65	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
52:k:101:CDL:H402	52:k:101:CDL:H432	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:310:LEU:HD23	35:l:313:MET:SD	2.56	0.46
40:r:310:MET:HB3	40:r:455:LEU:HD22	1.98	0.46
41:s:2:PHE:O	41:s:6:ILE:HG13	2.16	0.46
48:B:303:PEE:H58	48:B:303:PEE:H64	1.66	0.45
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.26	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
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.51	0.45
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.51	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
27:d:138:ALA:CB	28:e:137:MET:HG2	2.46	0.45
52:k:101:CDL:H392	52:k:101:CDL:H362	1.75	0.45
52:l:701:CDL:H272	52:l:701:CDL:H241	1.83	0.45
40:r:396:MET:O	40:r:400:MET:HG3	2.15	0.45
52:r:504:CDL:H401	52:r:504:CDL:H221	1.98	0.45
42:u:47:ARG:HE	42:u:47:ARG:HA	1.81	0.45
52:u:201:CDL:H742	52:u:201:CDL:H772	1.44	0.45
10:K:98:MET:HE3	10:K:98:MET:HB3	1.84	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
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.99	0.45
1:A:110:PRO:O	1:A:238:CYS:HB3	2.16	0.45
1:A:326:LEU:H	1:A:326:LEU:HD23	1.81	0.45
50:C:304:UQ:HM53	50:C:304:UQ:H72	1.79	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:HE21	23:Z:33:GLN:CA	2.30	0.45
24:a:86:ILE:O	24:a:90:ASN:ND2	2.47	0.45
35:l:70:THR:HG23	35:l:75:GLU:HG2	1.98	0.45
35:l:156:GLY:HA3	40:r:416:ARG:HH12	1.81	0.45
39:p:72:TRP:O	39:p:75:GLN:HG2	2.16	0.45
39:p:139:GLN:NE2	39:p:156:PRO:O	2.46	0.45
41:s:293:PHE:O	41:s:297:THR:OG1	2.31	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
21:W:68:ARG:CZ	21:W:72:MET:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.97	0.45
32:i:271:THR:HG22	40:r:169:ASN:OD1	2.17	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
12:M:208:THR:HA	14:O:110:MET:HE2	1.98	0.45
34:k:4:VAL:O	34:k:8:ILE:HG12	2.17	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
17:S:1:MET:HE3	17:S:1:MET:HB3	1.73	0.45
35:l:136:ASN:HA	35:l:197:ASP:HA	1.97	0.45
35:l:533:MET:HA	35:l:533:MET:HE2	1.98	0.45
41:s:20:LEU:HD12	41:s:20:LEU:O	2.17	0.45
44:w:65:ASN:OD1	44:w:66:ILE:N	2.41	0.45
8:I:91:GLU:CD	8:I:91:GLU:H	2.24	0.45
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.97	0.45
48:i:401:PEE:H28	48:i:401:PEE:H33	1.85	0.45
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.98	0.45
35:l:249:SER:OG	35:l:336:LYS:HG3	2.16	0.45
35:l:356:ILE:HA	35:l:359:MET:HG3	1.97	0.45
43:v:115:ARG:HG3	43:v:118:ARG:HH21	1.81	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
25:b:100:ARG:HD2	27:d:118:GLY:HA2	1.97	0.45
26:c:40:PRO:HA	38:o:79:ASN:OD1	2.17	0.45
35:l:288:THR:HG21	35:l:307:SER:HB3	1.98	0.45
35:l:559:GLU:O	35:l:563:PRO:HD2	2.16	0.45
41:s:175:ILE:O	41:s:179:TRP:HB3	2.17	0.45
42:u:162:LYS:HA	42:u:162:LYS:HD2	1.71	0.45
44:w:256:LEU:HD21	44:w:276:LEU:HD21	1.99	0.45
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.46	0.45
20:V:53:VAL:HG12	52:k:101:CDL:H341	1.98	0.45
43:v:120:ALA:O	43:v:124:ARG:HG2	2.17	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
24:a:69:LYS:HB3	24:a:69:LYS:HE3	1.57	0.44
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.82	0.44
32:i:136:LEU:HD23	32:i:205:LEU:HD21	1.98	0.44
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:557:TRP:O	35:l:561:ILE:HG12	2.17	0.44
52:u:201:CDL:H581	52:u:201:CDL:H552	1.67	0.44
17:S:12:MET:HE2	17:S:12:MET:HB3	1.69	0.44
30:g:32:ARG:HB3	32:i:339:MET:HE1	1.99	0.44
32:i:68:MET:HE1	34:k:37:MET:CE	2.38	0.44
36:m:2:THR:C	36:m:4:TYR:H	2.25	0.44
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.97	0.44
11:L:158:LYS:NZ	12:M:69:LEU:O	2.35	0.44
19:U:53:TYR:HB2	21:W:72:MET:SD	2.58	0.44
48:j:201:PEE:H59	48:j:201:PEE:H64	1.80	0.44
35:l:56:HIS:CD2	35:l:57:THR:HG23	2.52	0.44
35:l:367:PRO:O	35:l:370:THR:HG22	2.18	0.44
52:o:201:CDL:H321	52:o:201:CDL:H352	1.84	0.44
39:p:35:ASP:OD1	39:p:36:LYS:N	2.49	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
20:V:56:THR:HG21	52:k:101:CDL:H361	2.00	0.44
22:Y:97:LEU:HD12	43:v:107:ARG:HD2	2.00	0.44
31:h:17:TRP:HE3	34:k:55:LEU:HD13	1.83	0.44
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.83	0.44
34:k:37:MET:HE3	34:k:67:ALA:HA	1.99	0.44
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.32	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
52:k:101:CDL:H192	35:l:593:ILE:HD11	2.00	0.44
35:l:378:LEU:HD13	35:l:383:MET:HE2	2.00	0.44
42:u:37:ASP:OD2	42:u:37:ASP:C	2.61	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
44:w:61:THR:HG22	44:w:159:LEU:HD12	1.98	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
24:a:170:GLN:HB2	30:g:6:GLY:O	2.17	0.44
25:b:110:ILE:CG1	27:d:16:ARG:HB3	2.47	0.44
52:l:701:CDL:H551	52:l:701:CDL:H582	1.80	0.44
40:r:1:MET:O	40:r:1:MET:HG3	2.17	0.44
42:u:83:THR:HA	42:u:86:TRP:CD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:67:LEU:HD22	36:m:59:ILE:HD12	2.00	0.44
35:l:8:THR:HB	35:l:82:MET:HE3	2.00	0.44
36:m:1:MET:HA	36:m:4:TYR:CE1	2.53	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
26:c:160:GLN:HB3	26:c:183:HIS:CD2	2.53	0.44
30:g:36:MET:SD	32:i:339:MET:HE2	2.58	0.44
40:r:116:ILE:HG13	42:u:168: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
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
17:S:12:MET:SD	41:s:20:LEU:HA	2.58	0.43
32:i:95:MET:HE2	32:i:149:ILE:HD13	2.00	0.43
39:p:138:LYS:O	39:p:142:GLU:HG2	2.17	0.43
40:r:14:MET:O	40:r:18:SER:OG	2.27	0.43
13:N:68:MET:HB3	13:N:115:PHE:HE2	1.83	0.43
24:a:114:LYS:HB2	24:a:114:LYS:HE3	1.84	0.43
25:b:123:PHE:CZ	43:v:61:HIS:HB2	2.54	0.43
32:i:57:THR:HA	34:k:77:LEU:HD13	2.00	0.43
32:i:244:MET:HB2	32:i:244:MET:HE2	1.74	0.43
34:k:5:TYR:O	34:k:9:ILE:HG13	2.17	0.43
34:k:16:LEU:HA	34:k:36:MET:HE2	1.99	0.43
42:u:137:LEU:HD12	42:u:138:PRO:HD2	2.00	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
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.00	0.43
35:l:336:LYS:HA	35:l:336:LYS:HD3	1.77	0.43
35:l:535:ARG:NH1	38:o:11:LEU:O	2.49	0.43
52:o:201:CDL:H872	52:o:201:CDL:H841	1.77	0.43
44:w:295:ARG:HA	44:w:298:VAL:HG22	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
35:l:475:MET:HB3	43:v:52:MET:HE1	2.01	0.43
35:l:557:TRP:HB3	52:o:201:CDL:H822	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.99	0.43
9:J:155:VAL:HA	9:J:158:GLU:HG2	1.98	0.43
14:O:179:ALA:HB3	14:O:185:MET:HE3	2.00	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
28:e:137:MET:HE3	28:e:137:MET:HB2	1.78	0.43
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.86	0.43
32:i:69:MET:HE1	32:i:100:MET:HE3	1.99	0.43
34:k:64:LEU:O	34:k:67:ALA:HB3	2.18	0.43
36:m:40:GLY:HA2	36:m:43:ILE:HD12	2.00	0.43
12:M:367:CYS:HB3	12:M:533:GLY:O	2.17	0.43
16:Q:37:TRP:CD2	40:r:140:THR:HB	2.53	0.43
48:j:201:PEE:H21	48:j:201:PEE:H27	1.46	0.43
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.53	0.43
35:l:556:ILE:O	35:l:560:THR:OG1	2.35	0.43
42:u:47:ARG:HA	42:u:47:ARG:NE	2.34	0.43
44:w:254:GLU:HG3	44:w:276:LEU:HD22	2.01	0.43
3:C:84:TYR:HE1	3:C:171:GLU:HG3	1.82	0.43
26:c:110:ASP:HA	26:c:113:ILE:HG23	2.00	0.43
31:h:97:HIS:HA	31:h:102:GLU:HB3	2.00	0.43
36:m:65:LEU:N	41:s:114:TYR:OH	2.51	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
49:g:201:PLX:H122	49:g:201:PLX:H91	1.60	0.43
33:j:84:LEU:HD13	41:s:309:ILE:HG23	2.00	0.43
34:k:50:ASN:ND2	36:m:127:ILE:HD12	2.34	0.43
42:u:45:LEU:HD22	42:u:131:VAL:HG13	2.00	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
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.85	0.43
22:Y:62:SER:OG	35:l:371:THR:OG1	2.26	0.43
33:j:17:LEU:HD23	33:j:17:LEU:HA	1.85	0.43
33:j:73:LEU:HD23	33:j:73:LEU:HA	1.82	0.43
35:l:238:GLU:H	35:l:238:GLU:HG2	1.68	0.43
49:r:503:PLX:H1C3	49:r:503:PLX:H22	1.77	0.43
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.35	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
35:l:177:ILE:HG23	48:l:703:PEE:H81	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD21	1:A:287:THR:HG22	2.01	0.42
2:B:90:LYS:NZ	2:B:174:GLU:OE2	2.51	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
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.51	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
14:O:121:MET:HE3	14:O:121:MET:HB3	1.81	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
26:c:113:ILE:HD11	26:c:116:ARG:HD2	2.01	0.42
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.84	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
6:X:129:GLU:HB2	39:p:82:PHE:CD2	2.54	0.42
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.54	0.42
52:a:201:CDL:H392	52:a:201:CDL:H361	1.43	0.42
34:k:16:LEU:HD23	52:k:101:CDL:H841	2.00	0.42
35:l:338:MET:HB2	35:l:457:LEU:HB3	2.01	0.42
40:r:329:LEU:O	40:r:332:THR:OG1	2.33	0.42
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.42
20:V:141:VAL:HG11	32:i:272:LYS:HB3	2.02	0.42
21:W:105:LYS:HG3	42:u:4:ILE:HD11	2.00	0.42
25:b:10:LEU:O	25:b:14:GLN:HG3	2.18	0.42
28:e:73:SER:C	28:e:75:GLY:H	2.28	0.42
28:e:109:LEU:HD22	40:r:43:ASN:HB2	2.02	0.42
33:j:73:LEU:HD12	36:m:55:MET:SD	2.59	0.42
33:j:94:LEU:HD13	36:m:154:VAL:HG13	2.02	0.42
34:k:60:PRO:O	34:k:63:LEU:HB3	2.19	0.42
35:l:393:ASP:OD1	35:l:394:LEU:N	2.53	0.42
40:r:61:LEU:HB2	40:r:457:PRO:HD3	2.00	0.42
40:r:114:GLU:OE2	40:r:116:ILE:HB	2.19	0.42
41:s:54:LYS:HB3	41:s:54:LYS:HE3	1.68	0.42
41:s:55:LEU:HD23	41:s:55:LEU:HA	1.85	0.42
41:s:85:MET:SD	41:s:108:MET:HB2	2.60	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
28:e:90:VAL:HG22	40:r:28:THR:HG21	2.01	0.42
34:k:27:MET:HE2	34:k:27:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:r:504:CDL:H712	52:r:504:CDL:H321	2.01	0.42
3:C:143:TYR:CD1	16:Q:118:2MR:HB2	2.54	0.42
6:X:141:PRO:O	6:X:145:VAL:HG13	2.20	0.42
25:b:29:SER:OG	25:b:32:GLU:HG2	2.19	0.42
35:l:37:LYS:HE3	35:l:37:LYS:HB3	1.79	0.42
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.01	0.42
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.02	0.42
52:r:504:CDL:H742	52:r:504:CDL:H772	1.85	0.42
41:s:84:THR:O	41:s:87:VAL:HG22	2.19	0.42
14:O:208:LEU:HD13	14:O:214:PRO:HD2	2.00	0.42
35:l:230:HIS:N	35:l:231:PRO:HD3	2.35	0.42
49:r:502:PLX:H1C3	49:r:502:PLX:H22	1.76	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
22:Y:92:TRP:CH2	43:v:100:LYS:HG2	2.55	0.42
26:c:78:LEU:HB2	26:c:106:HIS:CD2	2.54	0.42
35:l:125:LEU:O	35:l:129:MET:HG2	2.20	0.42
35:l:488:MET:HB3	35:l:492:ILE:HD13	2.01	0.42
35:l:599:MET:O	35:l:603:ASN:HB3	2.19	0.42
36:m:82:VAL:HG13	36:m:84:VAL:H	1.84	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:124:HIS:HD2	16:Q:375:MET:HE2	1.85	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:68:MET:CG	13:N:81:MET:HE3	2.48	0.42
13:N:78:ASP:OD1	13:N:78:ASP:N	2.52	0.42
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.91	0.42
19:U:70:PRO:HB3	42:u:124:GLU:O	2.20	0.42
33:j:33:LYS:HG2	41:s:61:LEU:HD11	2.02	0.42
40:r:22:MET:HE3	40:r:22:MET:HB3	1.91	0.42
40:r:190:TRP:HZ3	49:r:502:PLX:H102	1.85	0.42
48:r:501:PEE:H68	48:r:501:PEE:H62	1.83	0.42
41:s:49:ILE:H	41:s:49:ILE:HG12	1.65	0.42
41:s:105:MET:HE3	41:s:105:MET:HB3	1.98	0.42
43:v:122:MET:HE3	43:v:123:ALA:N	2.35	0.42
49:J:403:PLX:H111	49:J:403:PLX:H82	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:66:TRP:CD1	48:l:704:PEE:H18	2.55	0.42
35:l:419:THR:HA	35:l:422:TYR:CE2	2.55	0.42
44:w:52:LYS:HB3	44:w:52:LYS:HE2	1.79	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
15:P:68:ILE:C	15:P:70:PRO:HD3	2.44	0.41
23:Z:23:LYS:HB3	23:Z:25:GLU:OE2	2.19	0.41
44:w:132:GLN:HE22	57:w:401:ADP:HN62	1.68	0.41
44:w:173:MET:HB3	44:w:178:PHE:HB2	2.01	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
13:N:85:GLU:H	13:N:85:GLU:CD	2.28	0.41
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.53	0.41
35:l:505:ASN:O	35:l:508:THR:OG1	2.32	0.41
35:l:529:TYR:CZ	35:l:533:MET:HG3	2.55	0.41
43:v:70:LYS:HD3	43:v:80:CYS:SG	2.60	0.41
43:v:117:GLN:HG3	43:v:118:ARG:N	2.34	0.41
1:A:362:ASP:CG	1:A:449:ARG:HH12	2.26	0.41
52:a:201:CDL:H782	28:e:100:VAL:HG22	2.02	0.41
27:d:142:ARG:NE	28:e:138:GLU:O	2.45	0.41
30:g:48:ASN:ND2	30:g:63:GLN:OE1	2.53	0.41
35:l:400:ASN:OD1	35:l:409:LEU:HD11	2.21	0.41
35:l:467:ILE:HG22	35:l:468:ILE:HD12	2.02	0.41
40:r:178:ILE:HD13	40:r:178:ILE:HA	1.85	0.41
49:r:502:PLX:H72	49:r:502:PLX:H101	1.83	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
21:W:97:ILE:CD1	31:h:83:ARG:HG3	2.49	0.41
26:c:141:LEU:HD23	26:c:141:LEU:HA	1.91	0.41
32:i:287:LEU:HB3	48:i:401:PEE:H58	2.00	0.41
52:k:101:CDL:H632	52:k:101:CDL:H602	1.83	0.41
38:o:65:LEU:HD11	40:r:343:ILE:HD11	2.01	0.41
41:s:90:PRO:HD2	41:s:240:ILE:HD13	2.01	0.41
44:w:250:SER:O	44:w:280:LYS:NZ	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:103:HIS:O	6:G:108:LEU:HD12	2.20	0.41
12:M:35:PHE:HA	12:M:39:GLN:O	2.20	0.41
12:M:483:ARG:NH2	12:M:682:ASP:HB3	2.36	0.41
27:d:82:ILE:HD12	27:d:82:ILE:HA	1.90	0.41
30:g:33:LEU:HA	30:g:33:LEU:HD23	1.87	0.41
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.03	0.41
41:s:81:LEU:HD23	41:s:81:LEU:HA	1.88	0.41
44:w:165:SER:O	44:w:168:VAL:HG22	2.20	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
26:c:168:LEU:HD23	26:c:168:LEU:HA	1.88	0.41
27:d:15:ARG:O	27:d:15:ARG:HG3	2.21	0.41
29:f:61:GLN:O	29:f:65:ASP:OD2	2.38	0.41
30:g:85:TYR:CZ	32:i:344:SER:HB2	2.55	0.41
33:j:68:GLU:HG2	36:m:161:LEU:HD13	2.02	0.41
35:l:190:LEU:HD12	40:r:383:THR:HG21	2.02	0.41
35:l:571:MET:HB3	35:l:571:MET:HE2	1.83	0.41
52:l:701:CDL:CA7	52:l:701:CDL:H121	2.51	0.41
44:w:102:LYS:HB2	44:w:102:LYS:HE3	1.93	0.41
44:w:223:ASN:O	44:w:227:MET:HE3	2.19	0.41
48:B:303:PEE:H43	48:B:303:PEE:H37	1.79	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.28	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
24:a:79:GLY:HA3	52:a:201:CDL:H222	2.03	0.41
25:b:10:LEU:HD12	25:b:10:LEU:HA	1.92	0.41
32:i:141:VAL:O	32:i:145:ILE:HG12	2.21	0.41
33:j:53:MET:HE3	33:j:56:PHE:HB3	2.02	0.41
35:l:481:THR:OG1	43:v:92:HIS:ND1	2.30	0.41
39:p:101:GLU:H	39:p:101:GLU:HG3	1.74	0.41
52:r:504:CDL:H841	52:r:504:CDL:H872	1.77	0.41
43:v:31:PHE:CG	43:v:34:ARG:HD3	2.56	0.41
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.38	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
26:c:57:MET:HE1	26:c:76:PRO:HB3	2.03	0.41
27:d:15:ARG:O	27:d:15:ARG:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:182:SER:HB2	32:i:293:TYR:OH	2.21	0.41
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.03	0.41
35:l:247:LEU:HB3	35:l:252:MET:HE3	2.02	0.41
41:s:209:SER:HB3	41:s:213:VAL:HA	2.02	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
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.02	0.41
50:J:402:UQ:HM53	50:J:402:UQ:H71	1.89	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
17:S:54:ILE:HD12	42:u:19:LYS:HG2	2.02	0.41
17:S:66:LEU:HD21	42:u:74:ILE:HG22	2.03	0.41
20:V:106:ARG:HG3	20:V:106:ARG:HH11	1.85	0.41
25:b:76:LEU:HD12	25:b:76:LEU:HA	1.86	0.41
31:h:17:TRP:CD1	31:h:17:TRP:H	2.39	0.41
32:i:64:ALA:O	32:i:68:MET:HG2	2.20	0.41
34:k:1:MET:HE2	34:k:1:MET:HB3	1.88	0.41
35:l:497:GLY:HA2	52:l:702:CDL:H562	2.03	0.41
36:m:98:MET:HE3	36:m:98:MET:HB3	1.73	0.41
40:r:371:PRO:O	40:r:448:THR:OG1	2.29	0.41
41:s:61:LEU:HA	41:s:61:LEU:HD22	1.89	0.41
42:u:31:HIS:NE2	42:u:111:VAL:HG21	2.36	0.41
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.54	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
36:m:54:LEU:HD13	41:s:103:LEU:HB3	2.03	0.41
41:s:87:VAL:HG12	41:s:95:LEU:HD23	2.03	0.41
41:s:142:TYR:CZ	41:s:192:GLU:HG2	2.56	0.41
1:A:451:GLN:HG3	1:A:452:GLN:N	2.36	0.40
50:C:304:UQ:H102	50:C:304:UQ:H122	1.81	0.40
25:b:119:LEU:HD13	25:b:119:LEU:HA	1.92	0.40
35:l:211:MET:HE3	35:l:211:MET:HB2	1.94	0.40
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.56	0.40
52:l:702:CDL:H641	52:l:702:CDL:H612	1.81	0.40
40:r:80:SER:OG	40:r:226:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:370:PRO:CB	40:r:375:LEU:HD22	2.51	0.40
41:s:286:MET:HE2	41:s:286:MET:HB2	1.96	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
21:W:93:GLU:HG2	31:h:98:HIS:CD2	2.56	0.40
27:d:74:ILE:HG23	27:d:156:LEU:HD22	2.02	0.40
32:i:323:MET:H	32:i:323:MET:HG2	1.58	0.40
35:l:9:LEU:HD23	35:l:9:LEU:HA	1.92	0.40
35:l:429:PHE:O	35:l:436:ARG:NH2	2.52	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
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.56	0.40
32:i:147:GLN:H	32:i:147:GLN:NE2	2.18	0.40
48:i:401:PEE:H7	35:l:567:SER:HB3	2.03	0.40
52:l:701:CDL:H561	52:l:701:CDL:H142	2.03	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
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
49:a:202:PLX:H382	28:e:93:PHE:HZ	1.86	0.40
29:f:33:GLU:O	29:f:34:PRO:C	2.64	0.40
35:l:465:GLY:O	35:l:469:SER:OG	2.24	0.40
42:u:11:GLU:CD	42:u:11:GLU:H	2.27	0.40
43:v:17:PRO:HG2	43:v:102:PHE:CZ	2.56	0.40
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.57	0.40
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.70	0.40
6:G:139:MET:HE3	6:G:139:MET:HA	2.03	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
31:h:7:GLN:O	31:h:11:GLY:N	2.54	0.40
35:l:51:LEU:HG	35:l:55:MET:HE3	2.03	0.40
35:l:285:THR:HA	35:l:308:SER:HA	2.03	0.40
35:l:378:LEU:HD23	35:l:378:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:100:PRO:HD3	40:r:419:TYR:CE2	2.57	0.40
41:s:170:GLU:CD	42:u:98:ARG:HH22	2.29	0.40
43:v:69:CYS:SG	43:v:80:CYS:HB3	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	10	34
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%)	36	66
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	14	41
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%)	21	51
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%)	21	51
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	36	66
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
All	All	8174/8312 (98%)	7861 (96%)	307 (4%)	6 (0%)	49	77

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%)	342 (99%)	4 (1%)	63	87
2	B	151/151 (100%)	149 (99%)	2 (1%)	61	86
3	C	132/132 (100%)	129 (98%)	3 (2%)	44	78
4	E	106/107 (99%)	106 (100%)	0	100	100
5	F	75/76 (99%)	70 (93%)	5 (7%)	15	42
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	79/81 (98%)	77 (98%)	2 (2%)	42	76
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	88
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	95
10	K	42/42 (100%)	40 (95%)	2 (5%)	23	56
11	L	113/113 (100%)	111 (98%)	2 (2%)	51	82
12	M	580/580 (100%)	572 (99%)	8 (1%)	59	85
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	90
14	O	183/183 (100%)	179 (98%)	4 (2%)	45	78
15	P	190/190 (100%)	186 (98%)	4 (2%)	47	79
16	Q	370/370 (100%)	364 (98%)	6 (2%)	55	83
17	S	57/58 (98%)	55 (96%)	2 (4%)	32	67
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	72
21	W	122/123 (99%)	118 (97%)	4 (3%)	33	69
22	Y	62/62 (100%)	60 (97%)	2 (3%)	34	70
23	Z	62/62 (100%)	60 (97%)	2 (3%)	34	70
24	a	121/121 (100%)	118 (98%)	3 (2%)	42	76
25	b	90/119 (76%)	88 (98%)	2 (2%)	45	78
26	c	141/141 (100%)	139 (99%)	2 (1%)	59	85
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	81
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	35 (97%)	1 (3%)	38	73
30	g	108/108 (100%)	107 (99%)	1 (1%)	70	89
31	h	93/93 (100%)	90 (97%)	3 (3%)	34	70
32	i	311/311 (100%)	306 (98%)	5 (2%)	55	83
33	j	100/100 (100%)	95 (95%)	5 (5%)	22	54
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/540 (99%)	532 (99%)	5 (1%)	70	89
36	m	130/141 (92%)	129 (99%)	1 (1%)	73	90
37	n	53/53 (100%)	50 (94%)	3 (6%)	18	49
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	89
39	p	158/159 (99%)	156 (99%)	2 (1%)	61	86
40	r	410/410 (100%)	402 (98%)	8 (2%)	48	80
41	s	275/275 (100%)	268 (98%)	7 (2%)	42	76
42	u	153/153 (100%)	147 (96%)	6 (4%)	28	64
43	v	111/111 (100%)	110 (99%)	1 (1%)	70	89
44	w	281/283 (99%)	277 (99%)	4 (1%)	59	85
All	All	7163/7240 (99%)	7042 (98%)	121 (2%)	52	83

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	97	LEU
1	A	104	LYS

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Mol	Chain	Res	Type
1	A	451	GLN
2	B	114	ILE
2	B	139	SER
3	C	71	CYS
3	C	142	TYR
3	C	192	ILE
5	F	38	GLU
5	F	61	VAL
5	F	65	LEU
5	F	85	ASP
5	F	96	SER
7	H	116	ILE
9	J	121	GLU
10	K	85	THR
10	K	103	SER
11	L	88	GLN
11	L	112	MET
12	M	232	THR
12	M	347	ASP
12	M	374	THR
12	M	398	ASP
12	M	534	VAL
12	M	559	ASP
12	M	628	GLU
12	M	636	TYR
13	N	6	VAL
14	O	56	THR
14	O	137	THR
14	O	181	VAL
14	O	219	ARG
15	P	52	ASP
15	P	56	LYS
15	P	80	CYS
15	P	222	GLU
16	Q	74	ASP
16	Q	76	LEU
16	Q	212	GLU
16	Q	217	VAL
16	Q	260	GLU
16	Q	453	THR
17	S	54	ILE
17	S	66	LEU

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Mol	Chain	Res	Type
20	V	4	THR
20	V	16	THR
20	V	120	LEU
21	W	6	VAL
21	W	34	SER
21	W	49	SER
21	W	96	ILE
6	X	74	LEU
6	X	118	ILE
22	Y	77	SER
22	Y	100	LEU
23	Z	33	GLN
23	Z	34	GLU
24	a	77	LEU
24	a	98	LEU
24	a	173	THR
25	b	9	LYS
25	b	82	ILE
26	c	63	GLU
26	c	160	GLN
27	d	55	GLN
27	d	144	SER
27	d	151	SER
29	f	67	LEU
30	g	68	THR
31	h	74	LYS
31	h	80	LYS
31	h	85	LYS
32	i	85	THR
32	i	154	MET
32	i	223	SER
32	i	323	MET
32	i	336	VAL
33	j	16	LEU
33	j	31	SER
33	j	61	THR
33	j	86	THR
33	j	87	MET
35	l	71	LEU
35	l	133	THR
35	l	405	ASN
35	l	477	VAL

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Mol	Chain	Res	Type
35	l	504	LEU
36	m	135	PHE
37	n	42	SER
37	n	46	LYS
37	n	56	THR
38	o	88	LEU
39	p	110	SER
39	p	117	ASP
40	r	1	MET
40	r	103	GLN
40	r	129	THR
40	r	139	GLN
40	r	140	THR
40	r	247	THR
40	r	289	SER
40	r	308	SER
41	s	8	SER
41	s	61	LEU
41	s	81	LEU
41	s	109	SER
41	s	146	LEU
41	s	289	LEU
41	s	296	LEU
42	u	23	SER
42	u	37	ASP
42	u	88	CYS
42	u	131	VAL
42	u	132	LYS
42	u	155	GLU
43	v	105	GLU
44	w	72	ARG
44	w	107	GLN
44	w	216	SER
44	w	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	376	HIS
1	A	393	ASN
4	E	70	ASN

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Mol	Chain	Res	Type
4	E	95	ASN
5	F	48	ASN
5	F	81	ASN
7	H	76	GLN
7	H	83	GLN
8	I	47	HIS
9	J	128	ASN
9	J	150	HIS
10	K	75	ASN
11	L	51	GLN
11	L	71	HIS
12	M	652	ASN
13	N	135	GLN
14	O	74	HIS
14	O	87	GLN
15	P	75	GLN
15	P	77	GLN
15	P	196	HIS
15	P	247	GLN
16	Q	92	HIS
16	Q	162	GLN
16	Q	233	HIS
16	Q	264	ASN
16	Q	454	GLN
21	W	76	GLN
21	W	90	ASN
23	Z	21	GLN
24	a	132	ASN
25	b	89	HIS
26	c	84	GLN
27	d	59	ASN
27	d	107	GLN
27	d	124	ASN
27	d	140	GLN
28	e	65	ASN
28	e	86	ASN
29	f	61	GLN
29	f	62	HIS
29	f	73	ASN
30	g	90	HIS
31	h	98	HIS
32	i	47	ASN

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Mol	Chain	Res	Type
32	i	77	ASN
32	i	120	GLN
32	i	172	GLN
32	i	232	HIS
34	k	52	HIS
35	l	56	HIS
35	l	72	GLN
35	l	135	ASN
35	l	194	ASN
35	l	199	GLN
39	p	33	HIS
39	p	51	HIS
39	p	78	GLN
39	p	141	GLN
40	r	43	ASN
40	r	175	ASN
40	r	279	GLN
41	s	47	GLN
41	s	235	ASN
42	u	65	GLN
42	u	73	GLN
43	v	47	ASN
44	w	85	HIS
44	w	323	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 oligosaccharides 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
54	FES	O	301	14	0,4,4	-	-	-		
49	PLX	j	203	-	51,51,51	1.14	4 (7%)	55,59,59	0.64	1 (1%)
54	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
52	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.85	4 (3%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.57	1 (1%)
50	UQ	C	304	-	38,38,63	3.51	11 (28%)	46,49,79	2.93	17 (36%)
49	PLX	C	303	-	51,51,51	1.14	4 (7%)	55,59,59	0.65	1 (1%)
50	UQ	J	402	-	33,33,63	3.47	10 (30%)	40,43,79	2.69	14 (35%)
52	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.90	4 (3%)
48	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.93	2 (4%)
52	CDL	o	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
48	PEE	l	703	-	50,50,50	1.16	6 (12%)	53,55,55	0.94	2 (3%)
52	CDL	l	702	-	99,99,99	1.08	8 (8%)	105,111,111	0.87	4 (3%)
52	CDL	k	101	-	99,99,99	1.08	8 (8%)	105,111,111	0.86	4 (3%)
48	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	2 (3%)
48	PEE	B	303	-	50,50,50	1.16	6 (12%)	53,55,55	1.04	2 (3%)
52	CDL	I	201	-	50,50,99	1.39	8 (16%)	56,62,111	1.11	4 (7%)
52	CDL	r	504	-	99,99,99	1.07	8 (8%)	105,111,111	0.90	4 (3%)
49	PLX	r	502	-	51,51,51	1.14	3 (5%)	55,59,59	0.63	1 (1%)
57	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.02	11 (26%)
46	FMN	A	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.30	9 (18%)
48	PEE	j	202	-	40,40,50	1.14	5 (12%)	43,45,55	1.12	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	NAI	A	503	-	45,48,48	3.89	19 (42%)	60,73,73	1.79	13 (21%)
49	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.66	1 (1%)
49	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.60	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
48	PEE	l	704	-	45,45,50	1.21	6 (13%)	48,50,55	0.99	2 (4%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	1.00	2 (4%)
48	PEE	i	401	-	46,46,50	1.19	6 (13%)	49,51,55	1.02	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
45	SF4	B	301	2	0,12,12	-	-	-	-	-
51	8Q1	X	201	6	31,34,34	1.69	6 (19%)	40,43,43	1.60	6 (15%)
53	NDP	J	401	-	49,52,52	4.39	22 (44%)	66,80,80	2.19	13 (19%)
49	PLX	J	403	-	51,51,51	1.13	3 (5%)	55,59,59	0.61	1 (1%)
52	CDL	u	201	-	54,54,99	1.36	9 (16%)	60,66,111	1.09	4 (6%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PEE	V	202	-	39,39,50	1.31	6 (15%)	41,44,55	1.04	2 (4%)
51	8Q1	G	201	6	31,34,34	1.67	5 (16%)	40,43,43	1.73	6 (15%)
52	CDL	V	201	-	93,93,99	1.10	9 (9%)	99,105,111	0.89	4 (4%)
48	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	1.02	2 (3%)
52	CDL	s	401	-	88,88,99	1.13	7 (7%)	94,100,111	0.94	4 (4%)

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
54	FES	O	301	14	-	-	0/1/1/1
49	PLX	j	203	-	-	26/55/55/55	-
54	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
52	CDL	a	201	-	-	50/110/110/110	-
49	PLX	a	202	-	-	30/55/55/55	-
50	UQ	C	304	-	-	13/33/57/87	0/1/1/1
49	PLX	C	303	-	-	31/55/55/55	-
50	UQ	J	402	-	-	10/27/51/87	0/1/1/1
52	CDL	l	701	-	-	64/109/109/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	W	201	-	-	19/44/44/54	-
52	CDL	o	201	-	-	65/110/110/110	-
48	PEE	l	703	-	-	31/54/54/54	-
52	CDL	l	702	-	-	58/110/110/110	-
52	CDL	k	101	-	-	62/110/110/110	-
48	PEE	j	201	-	-	26/54/54/54	-
48	PEE	B	303	-	-	27/54/54/54	-
52	CDL	I	201	-	-	30/61/61/110	-
52	CDL	r	504	-	-	64/110/110/110	-
49	PLX	r	502	-	-	32/55/55/55	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
48	PEE	j	202	-	-	20/44/44/54	-
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
49	PLX	g	201	-	-	32/55/55/55	-
49	PLX	r	503	-	-	30/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	l	704	-	-	29/49/49/54	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	C	302	-	-	28/50/50/54	-
48	PEE	i	401	-	-	20/50/50/54	-
51	8Q1	X	201	6	-	16/41/41/41	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	C	301	3	-	-	0/6/5/5
53	NDP	J	401	-	-	11/34/77/77	0/4/5/5
49	PLX	J	403	-	-	34/55/55/55	-
52	CDL	u	201	-	-	36/65/65/110	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	V	202	-	-	26/43/43/54	-
51	8Q1	G	201	6	-	12/41/41/41	-
52	CDL	V	201	-	-	59/104/104/110	-
48	PEE	r	501	-	-	32/54/54/54	-
52	CDL	s	401	-	-	49/99/99/110	-

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
47	A	503	NAI	O4B-C1B	9.13	1.63	1.42
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
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
47	A	503	NAI	C2B-C1B	-7.19	1.30	1.53
47	A	503	NAI	O4D-C4D	6.89	1.60	1.45
53	J	401	NDP	C6A-N6A	5.86	1.48	1.34
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
57	w	401	ADP	C6-N6	5.55	1.48	1.34
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	C6A-N6A	5.12	1.47	1.34
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
53	J	401	NDP	C1B-N9A	-4.49	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.49	1.31	1.42
47	A	503	NAI	O2B-C2B	4.47	1.53	1.43
53	J	401	NDP	O4B-C1B	4.31	1.52	1.42
53	J	401	NDP	O2D-C2D	-4.25	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C7N-N7N	4.11	1.44	1.33
47	A	503	NAI	C6N-C5N	3.91	1.40	1.33
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
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
53	J	401	NDP	C8A-N9A	-3.18	1.31	1.37
52	V	201	CDL	OA6-CA5	3.16	1.43	1.34
57	w	401	ADP	C8-N9	-3.14	1.31	1.37
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
53	J	401	NDP	C5A-N7A	-3.07	1.33	1.39
52	u	201	CDL	OB8-CB7	3.03	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
47	A	503	NAI	C8A-N9A	-2.64	1.32	1.37
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
57	w	401	ADP	C5-N7	-2.29	1.34	1.39
49	g	201	PLX	C7-C6	2.29	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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 (157) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
47	A	503	NAI	C5A-C4A-N3A	-5.96	118.97	126.75
53	J	401	NDP	C5A-C4A-N3A	-5.83	119.14	126.75
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
50	J	402	UQ	C17-C18-C19	-5.78	113.75	127.66
57	w	401	ADP	C5-C4-N3	-5.69	119.32	126.75
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
48	j	202	PEE	O2-C10-C11	4.56	121.33	111.50
57	w	401	ADP	N3-C2-N1	-4.53	121.52	128.60
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	-4.34	121.82	128.60
50	C	304	UQ	C20-C19-C18	-4.31	112.61	123.68
57	w	401	ADP	N3-C4-N9	4.31	134.19	127.08
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
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
47	A	503	NAI	N3A-C4A-N9A	4.13	133.89	127.08
53	J	401	NDP	N3A-C2A-N1A	-4.11	122.17	128.60
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
53	J	401	NDP	N3A-C4A-N9A	4.08	133.81	127.08
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
47	A	503	NAI	C2A-N3A-C4A	3.94	121.07	111.75
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
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
57	w	401	ADP	N9-C8-N7	-3.78	108.74	113.91
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
53	J	401	NDP	C2A-N3A-C4A	3.77	120.65	111.75
57	w	401	ADP	C2-N3-C4	3.77	120.65	111.75
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
47	A	503	NAI	C5A-N7A-C8A	3.69	108.76	103.51
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
57	w	401	ADP	C5-N7-C8	3.59	108.61	103.51
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
47	A	503	NAI	N9A-C8A-N7A	-3.38	109.28	113.91
46	A	502	FMN	C4-N3-C2	-3.38	119.40	125.64
53	J	401	NDP	C5A-N7A-C8A	3.33	108.25	103.51
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
47	A	503	NAI	C4A-C5A-N7A	-3.26	106.64	110.62
53	J	401	NDP	N9A-C8A-N7A	-3.26	109.45	113.91
51	X	201	8Q1	C37-C38-C39	3.24	117.76	112.36
57	w	401	ADP	C4-N9-C8	3.14	109.14	105.73
52	u	201	CDL	OA8-CA7-C31	3.14	119.61	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
53	J	401	NDP	C4A-C5A-N7A	-3.04	106.92	110.62
57	w	401	ADP	C4-C5-N7	-2.95	107.02	110.62
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
52	l	701	CDL	OB8-CB7-C71	2.65	120.21	111.91
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
53	J	401	NDP	C4A-N9A-C8A	2.41	108.33	105.73
51	X	201	8Q1	C38-C39-N41	2.40	120.45	116.42
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
49	J	403	PLX	C1A-N1-C1	2.28	119.23	109.92
47	A	503	NAI	C4A-N9A-C8A	2.26	108.18	105.73
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
46	A	502	FMN	C9A-C5A-N5	-2.11	120.14	122.43
57	w	401	ADP	C4'-O4'-C1'	-2.09	104.86	109.47
46	A	502	FMN	C4-C4A-C10	2.05	120.23	116.79
47	A	503	NAI	C3B-C2B-C1B	2.03	105.29	101.43
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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.

36 monomers are involved in 144 short contacts:

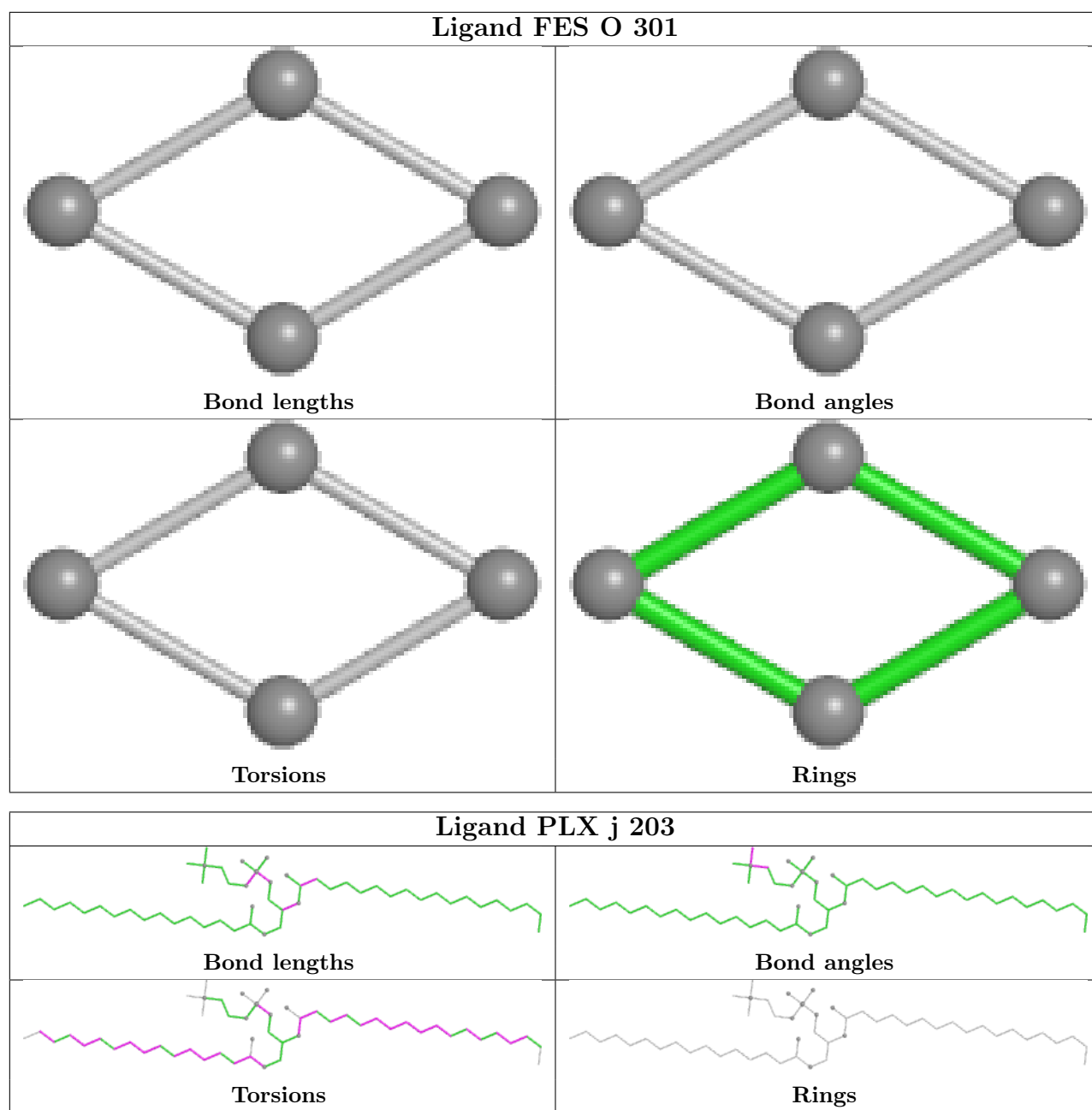
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	j	203	PLX	2	0
52	a	201	CDL	8	0
49	a	202	PLX	1	0
50	C	304	UQ	5	0
49	C	303	PLX	4	0
50	J	402	UQ	6	0
52	l	701	CDL	11	0
48	W	201	PEE	1	0

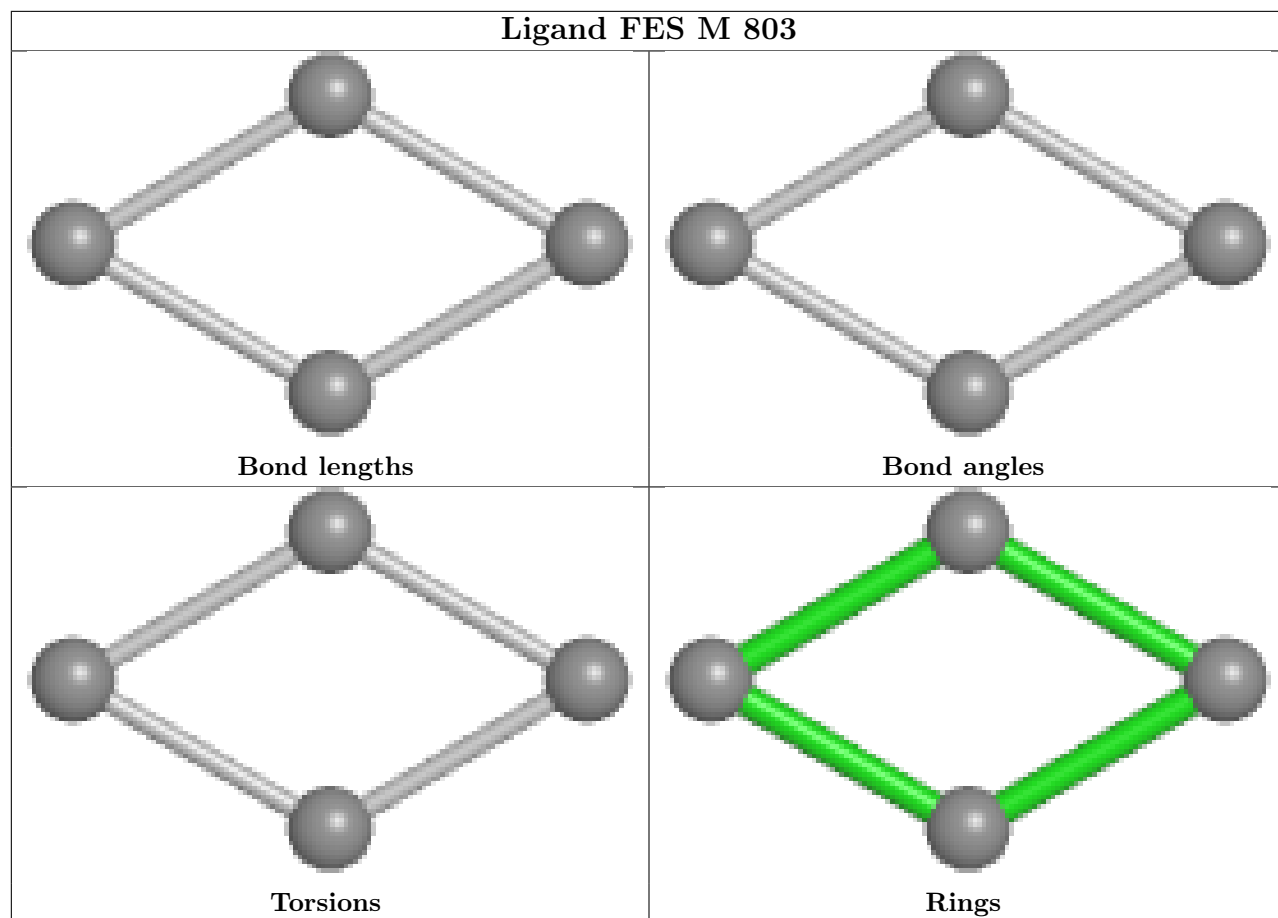
Continued on next page...

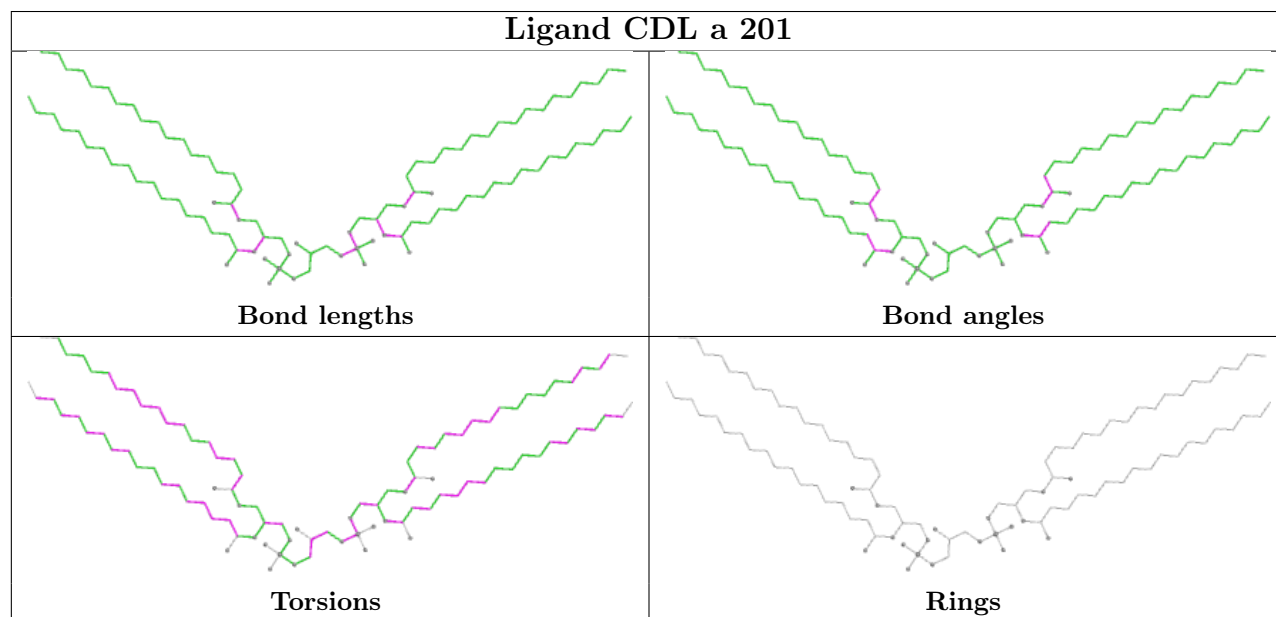
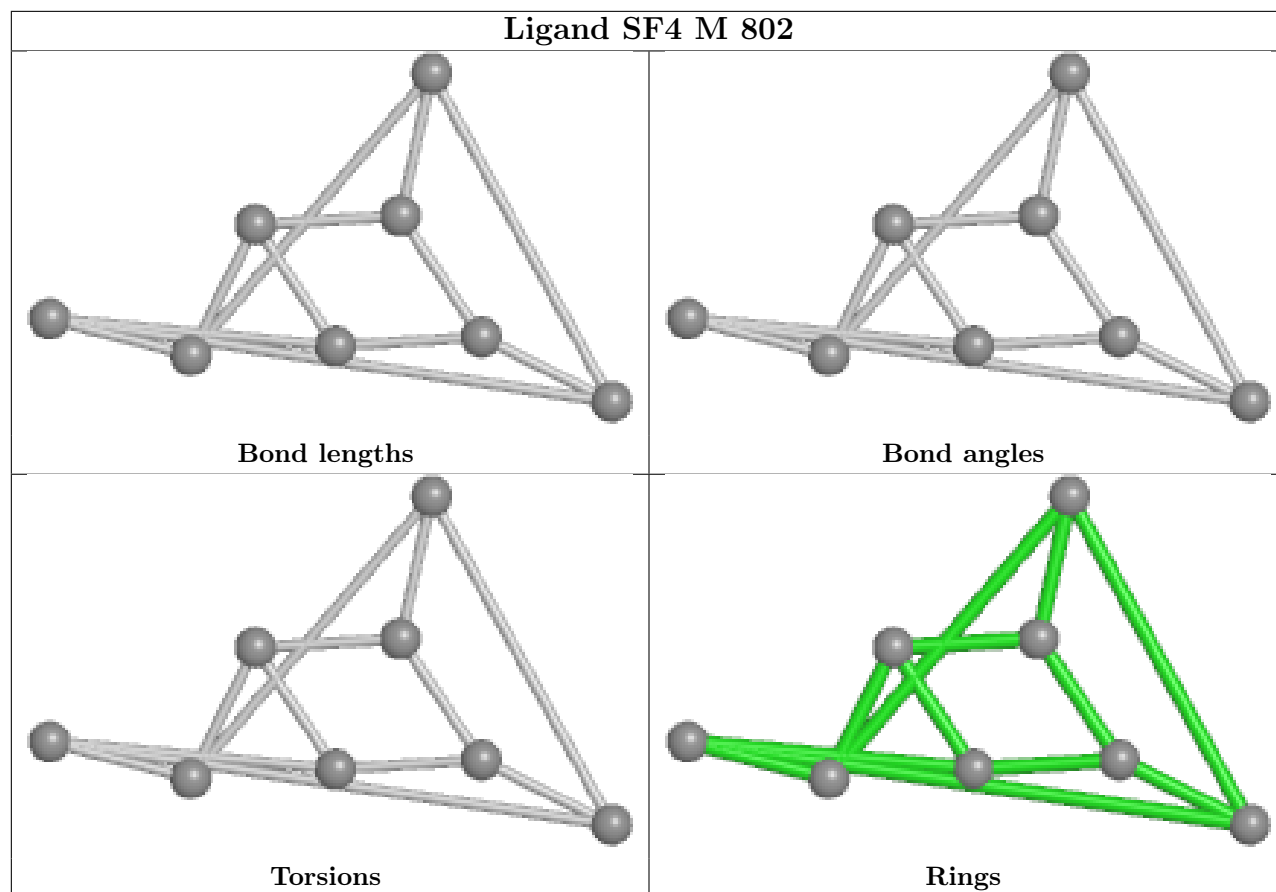
Continued from previous page...

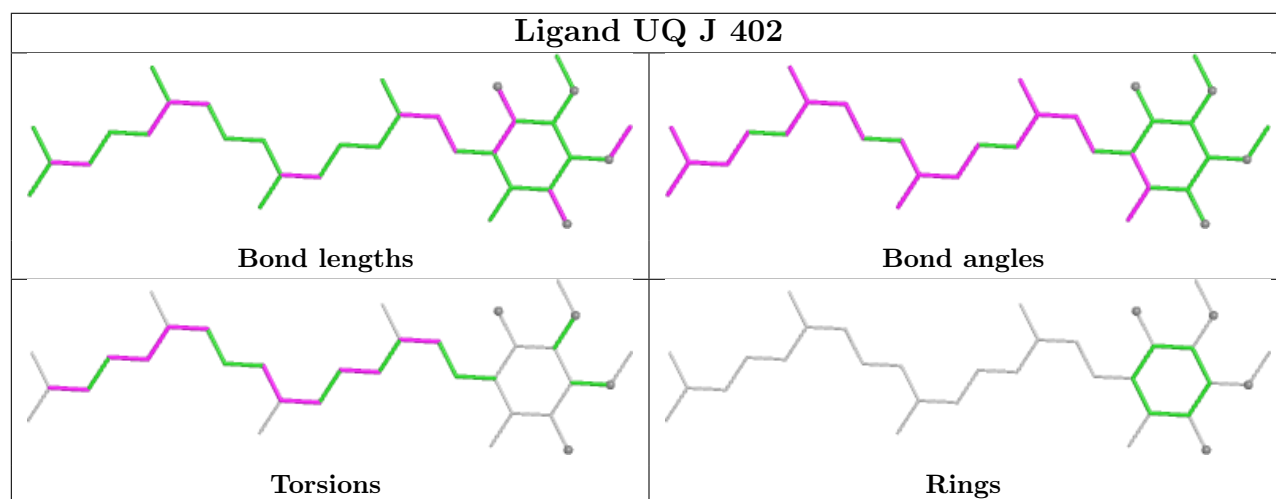
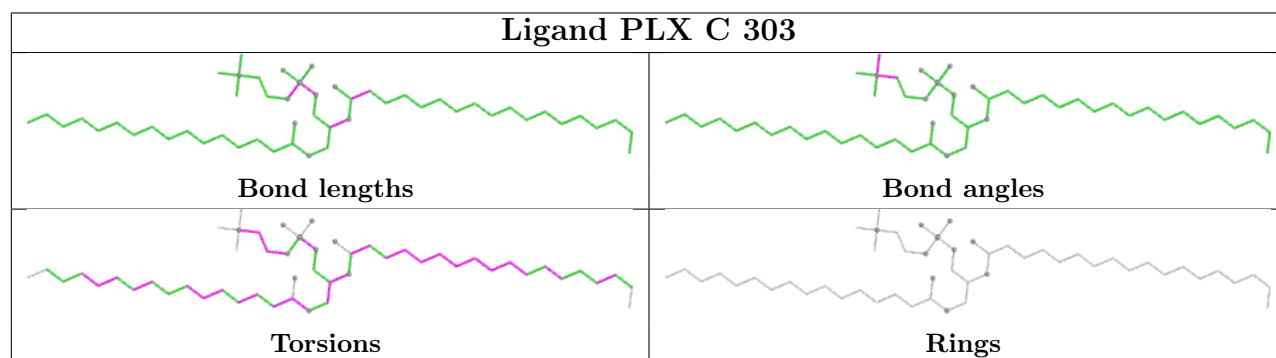
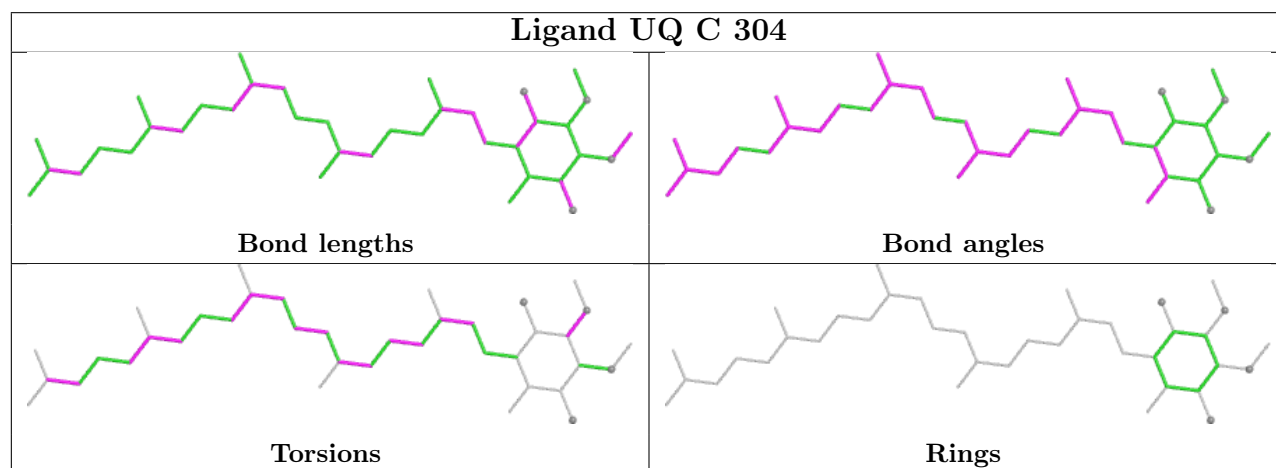
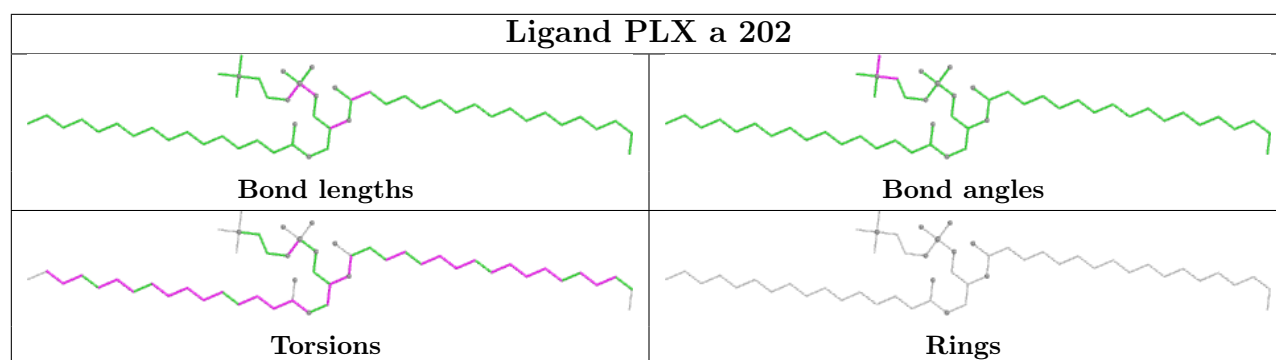
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	o	201	CDL	5	0
48	l	703	PEE	4	0
52	l	702	CDL	4	0
52	k	101	CDL	11	0
48	j	201	PEE	3	0
48	B	303	PEE	4	0
52	I	201	CDL	1	0
52	r	504	CDL	10	0
49	r	502	PLX	5	0
57	w	401	ADP	2	0
46	A	502	FMN	3	0
48	j	202	PEE	2	0
47	A	503	NAI	6	0
49	g	201	PLX	4	0
49	r	503	PLX	5	0
48	l	704	PEE	7	0
48	C	302	PEE	2	0
48	i	401	PEE	4	0
45	C	301	SF4	2	0
51	X	201	8Q1	2	0
53	J	401	NDP	1	0
49	J	403	PLX	5	0
52	u	201	CDL	3	0
45	A	501	SF4	2	0
48	V	202	PEE	3	0
52	V	201	CDL	5	0
48	r	501	PEE	4	0
52	s	401	CDL	5	0

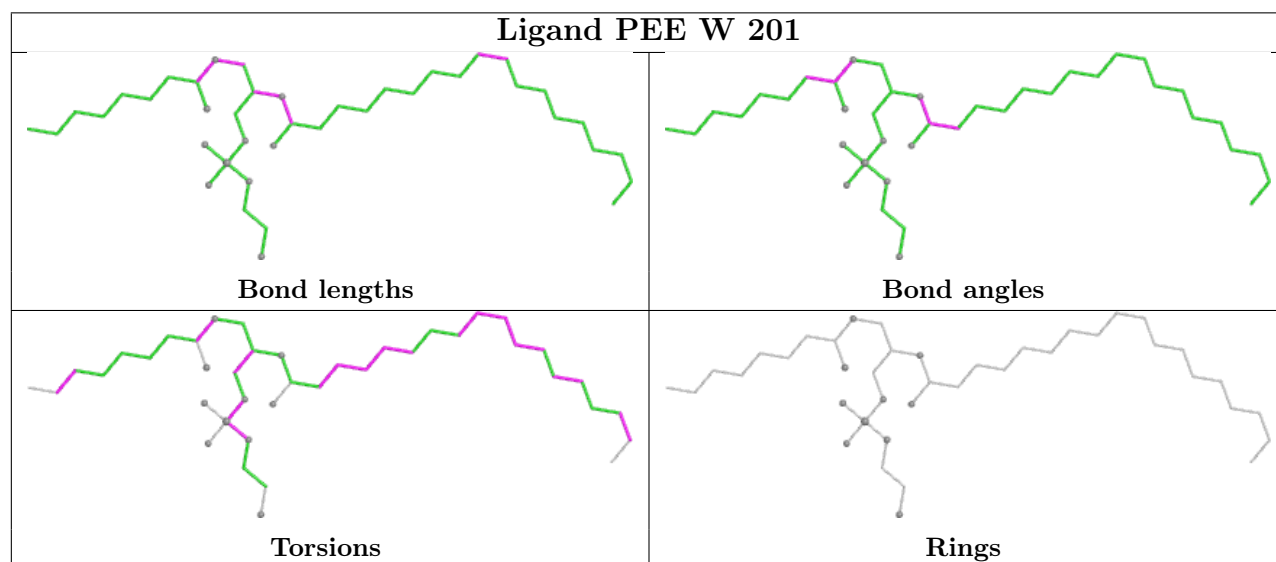
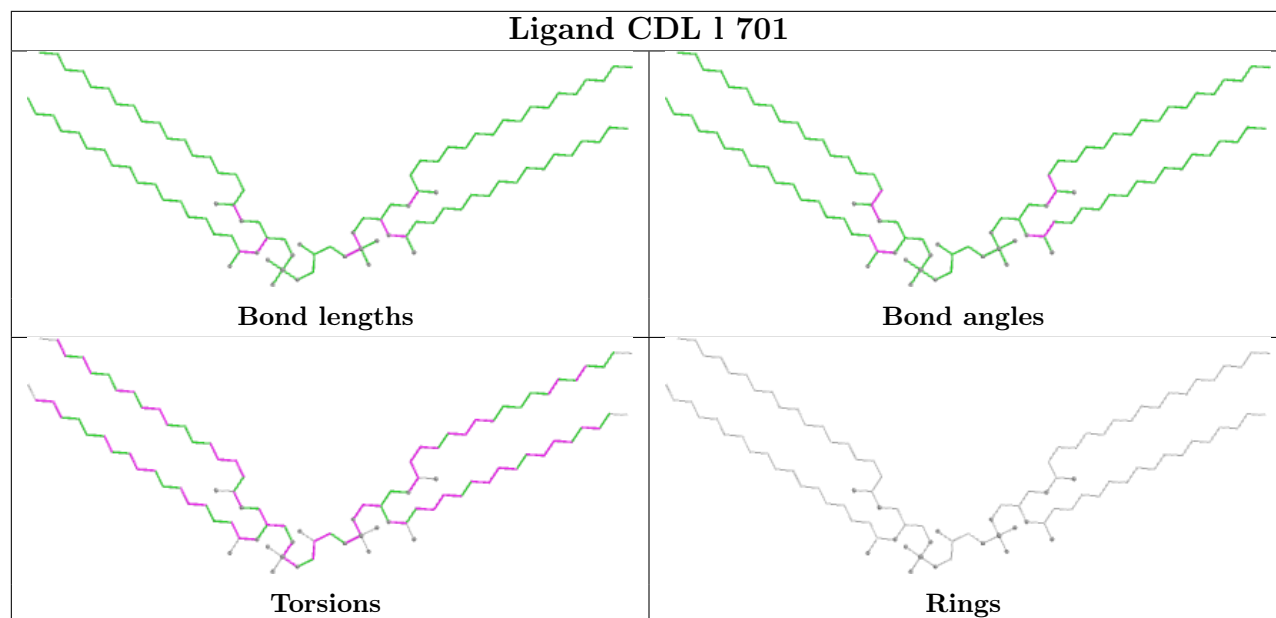
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

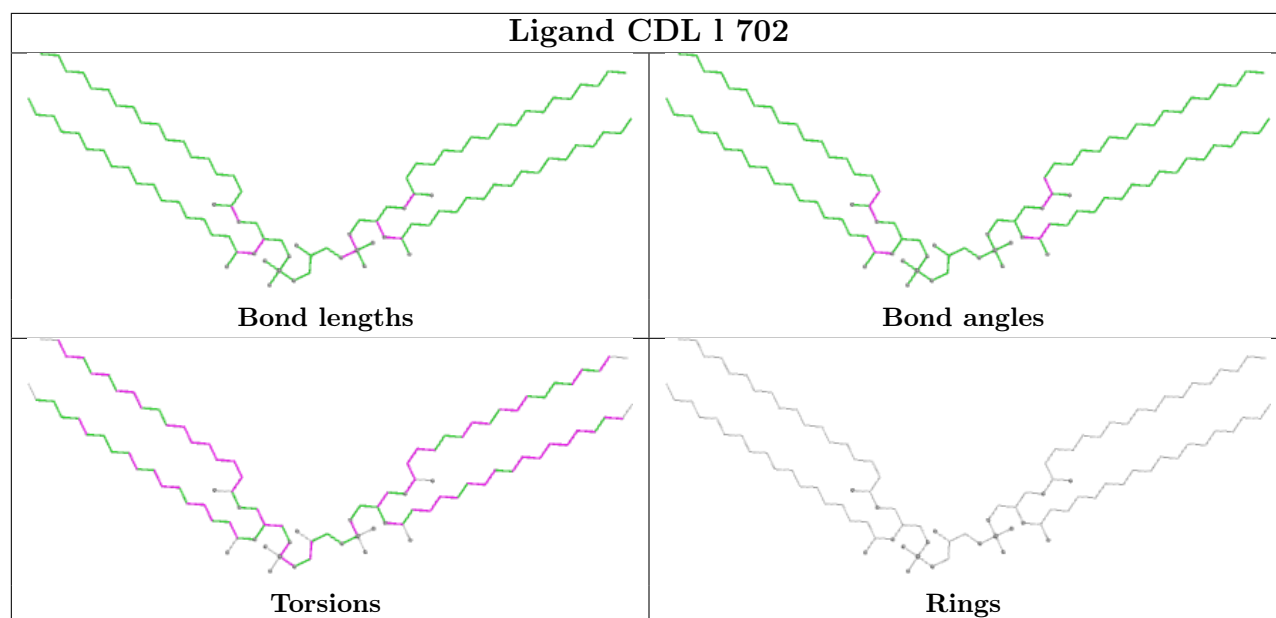
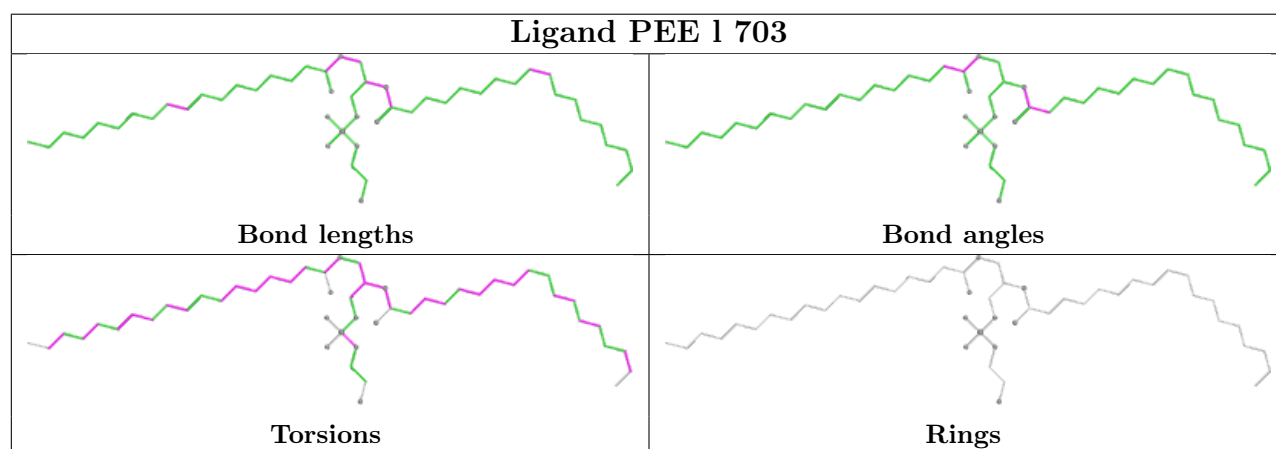
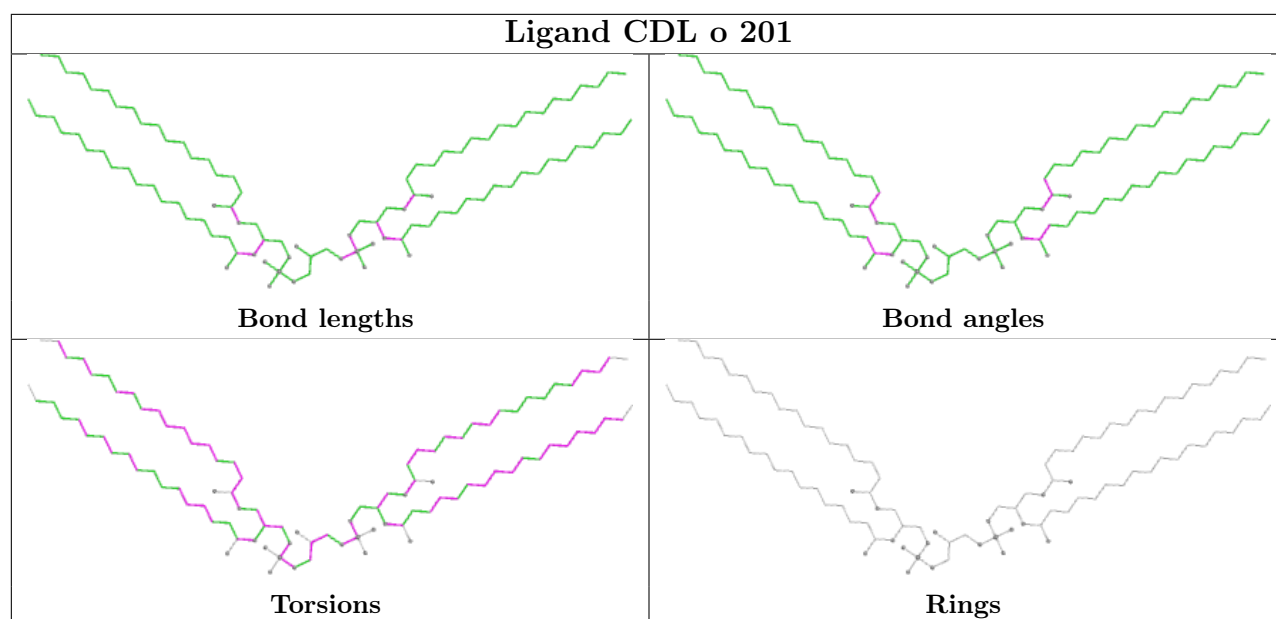


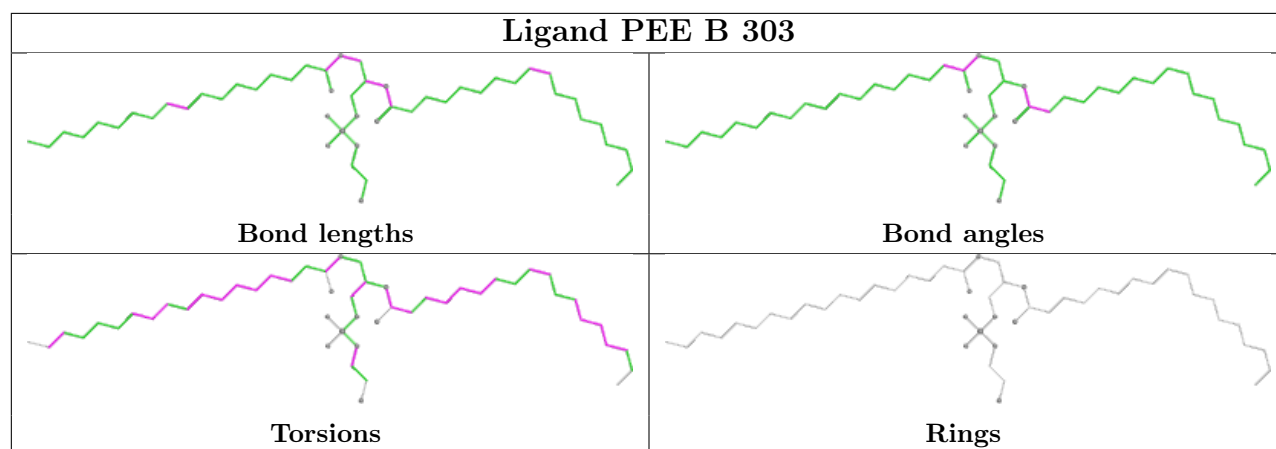
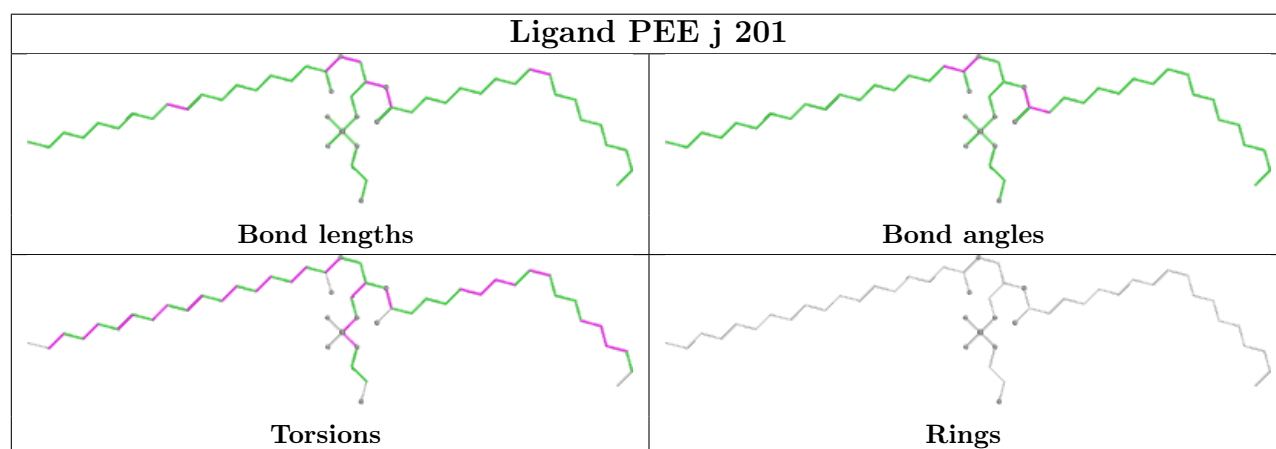
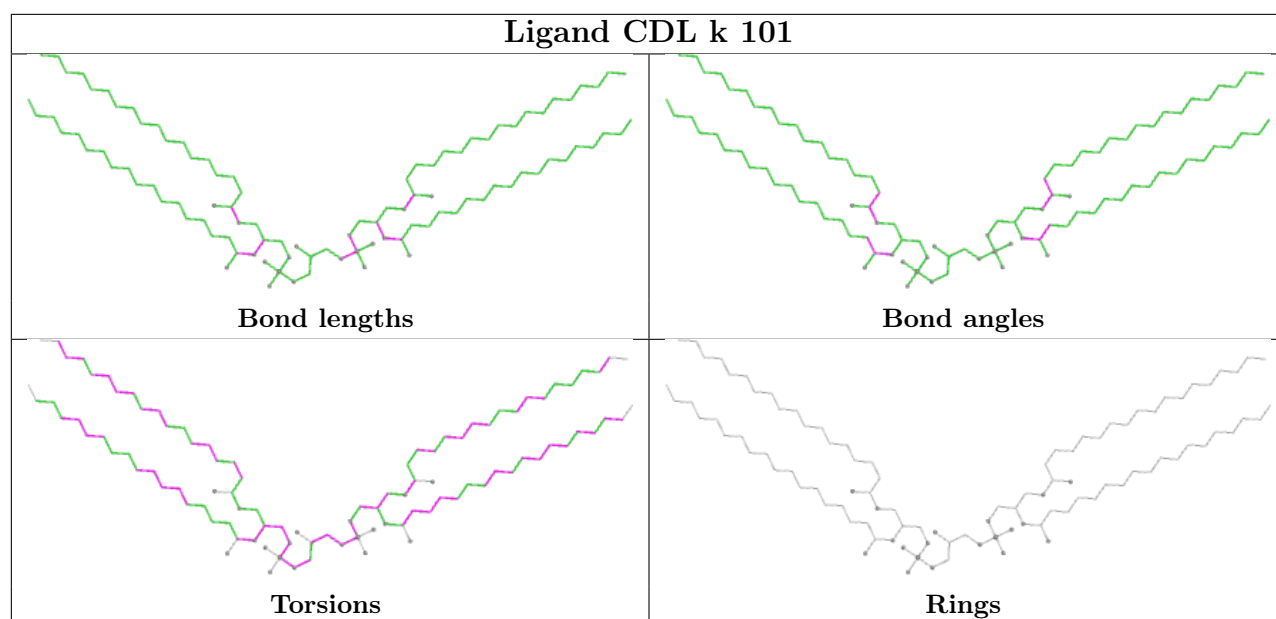


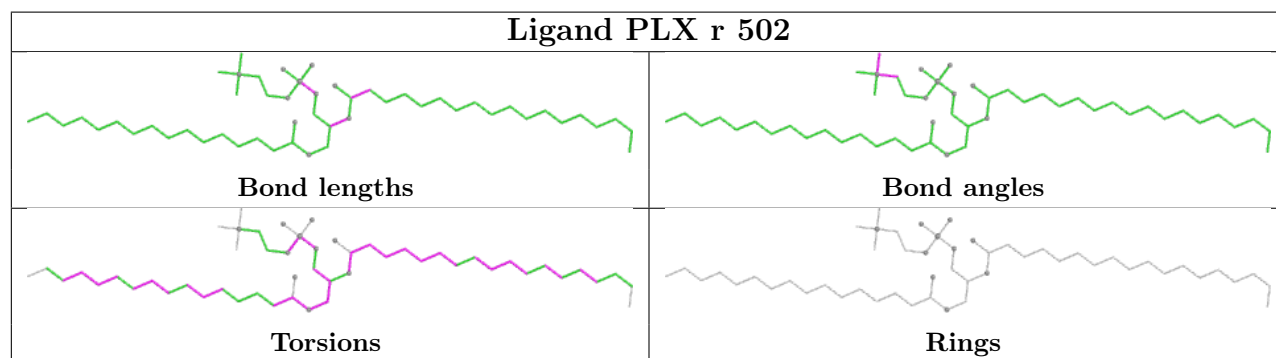
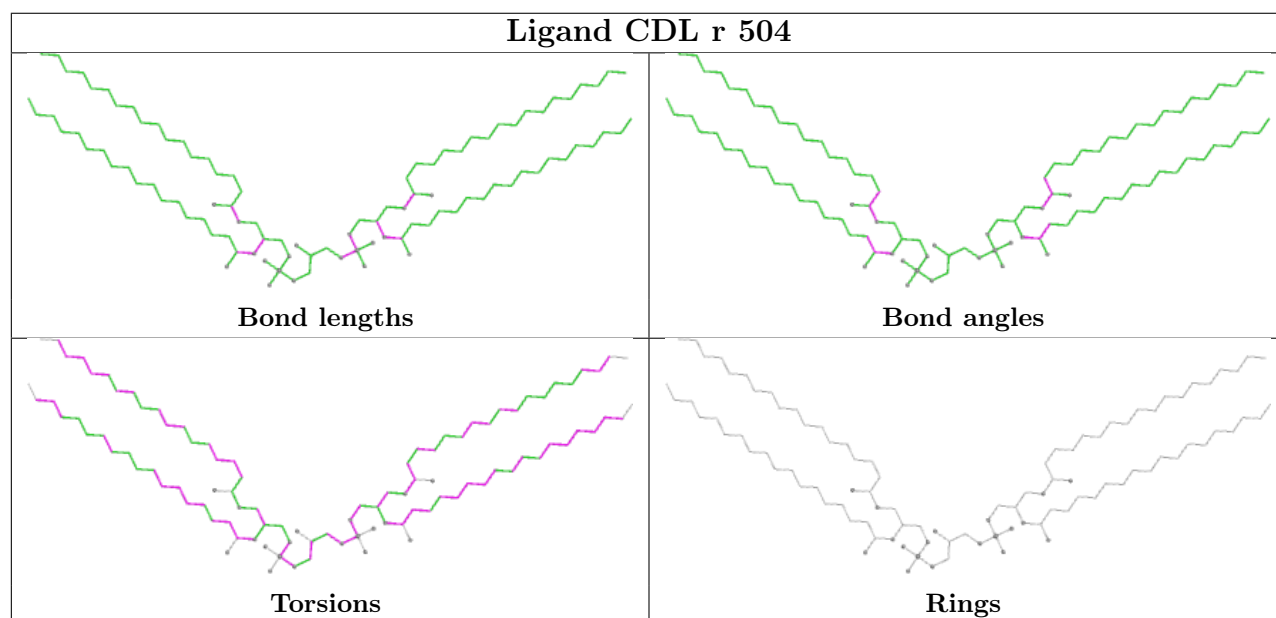
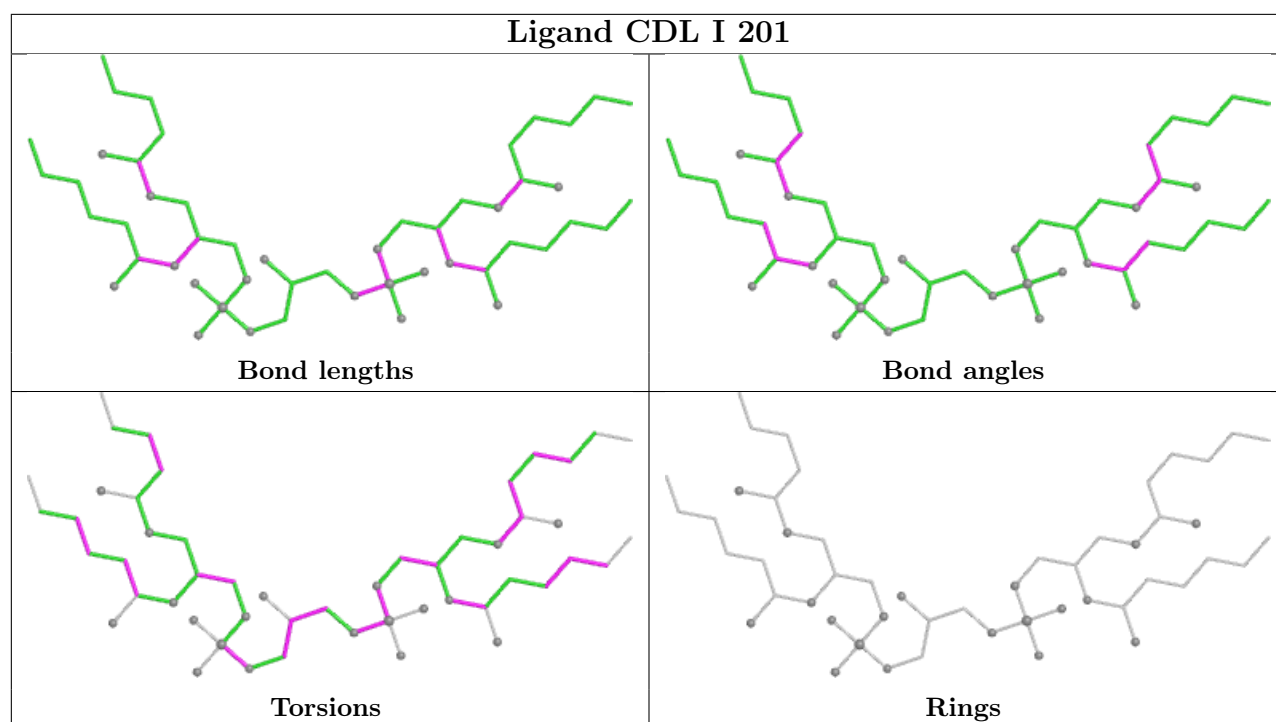


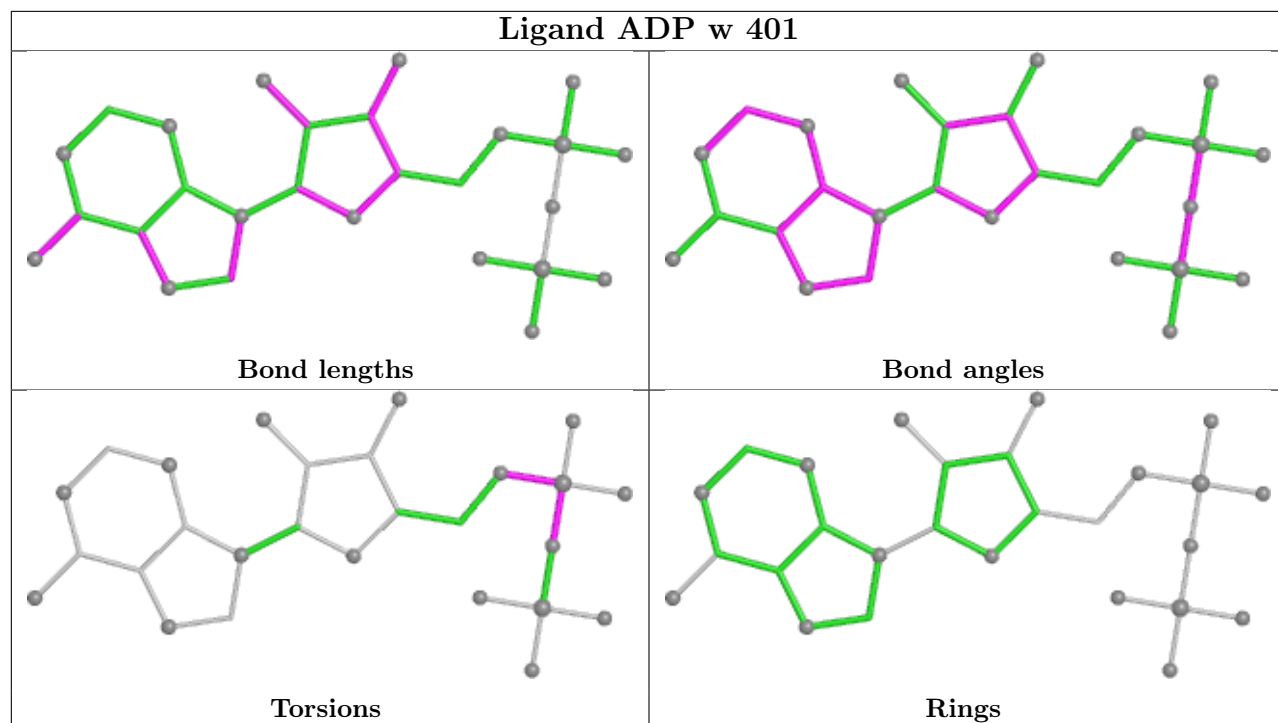


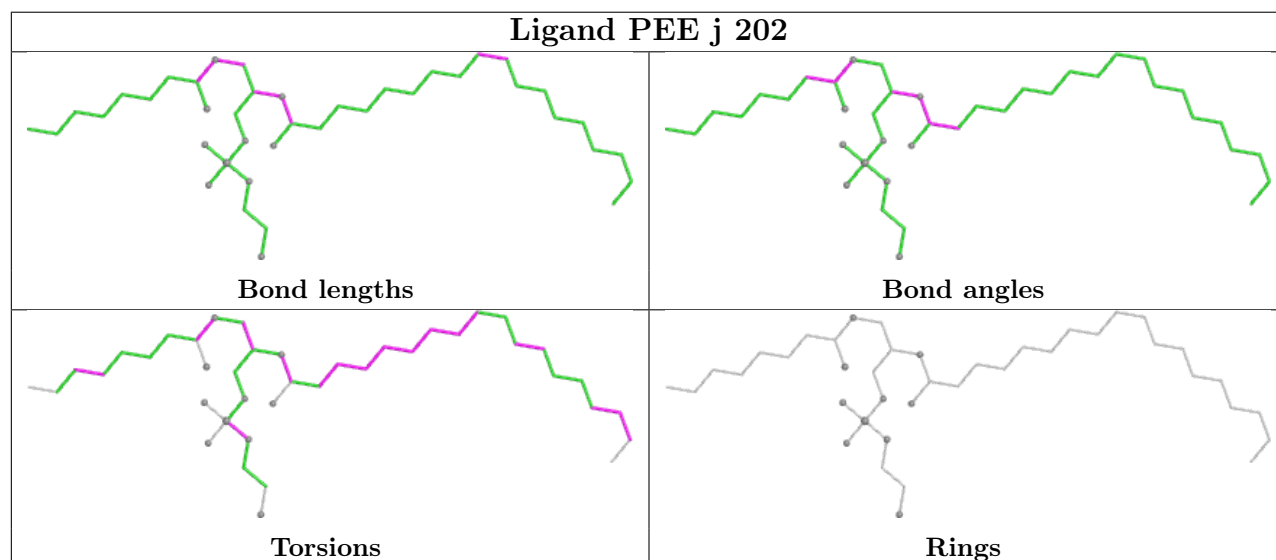
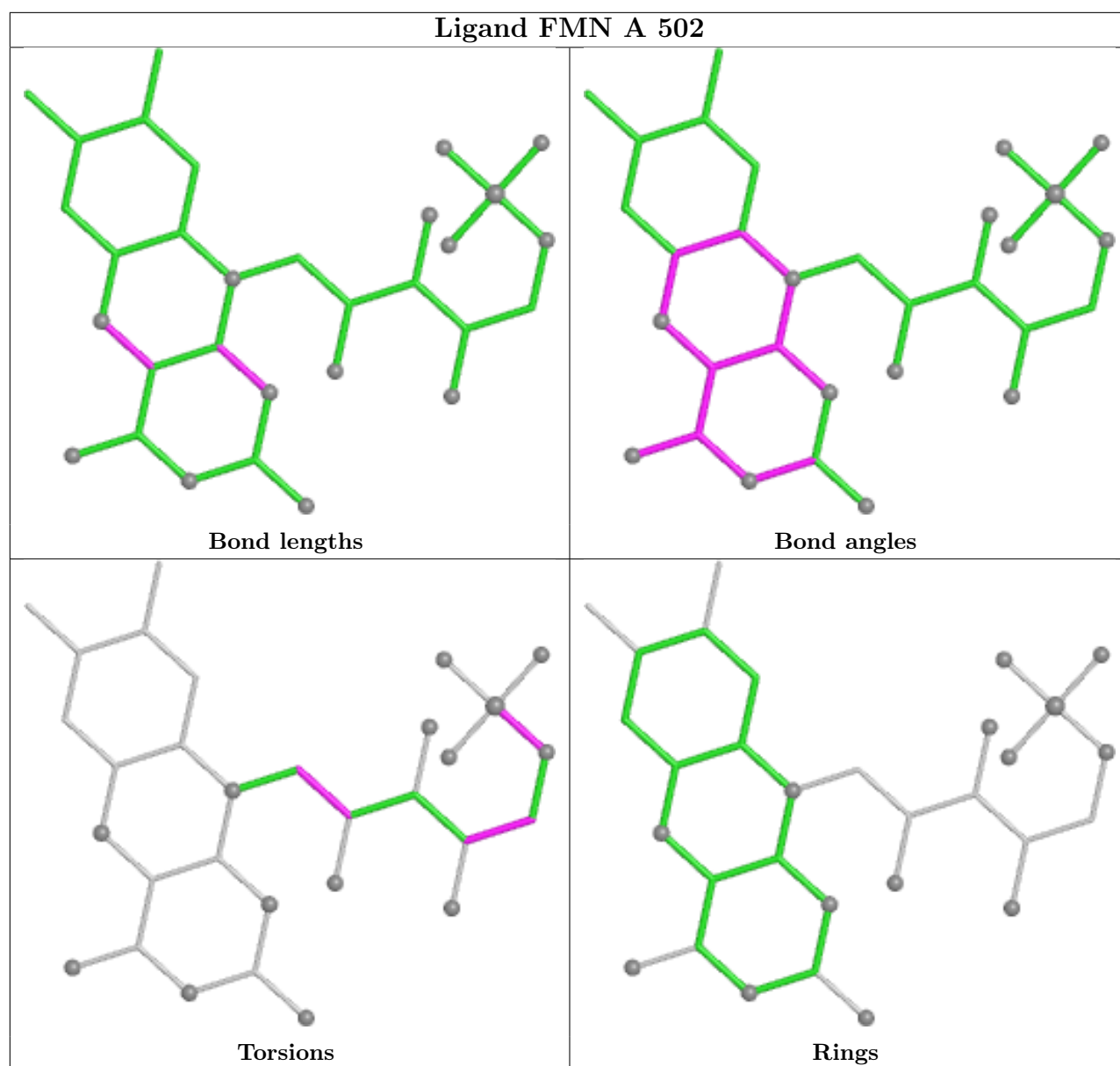


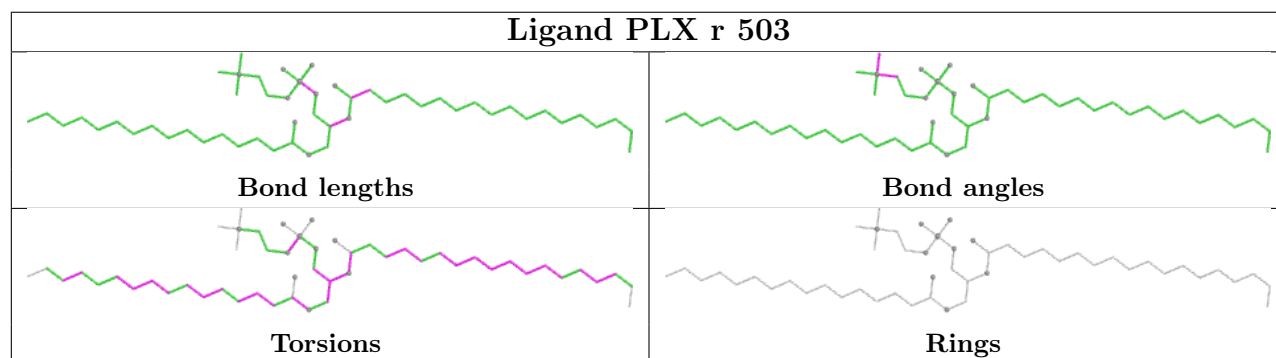
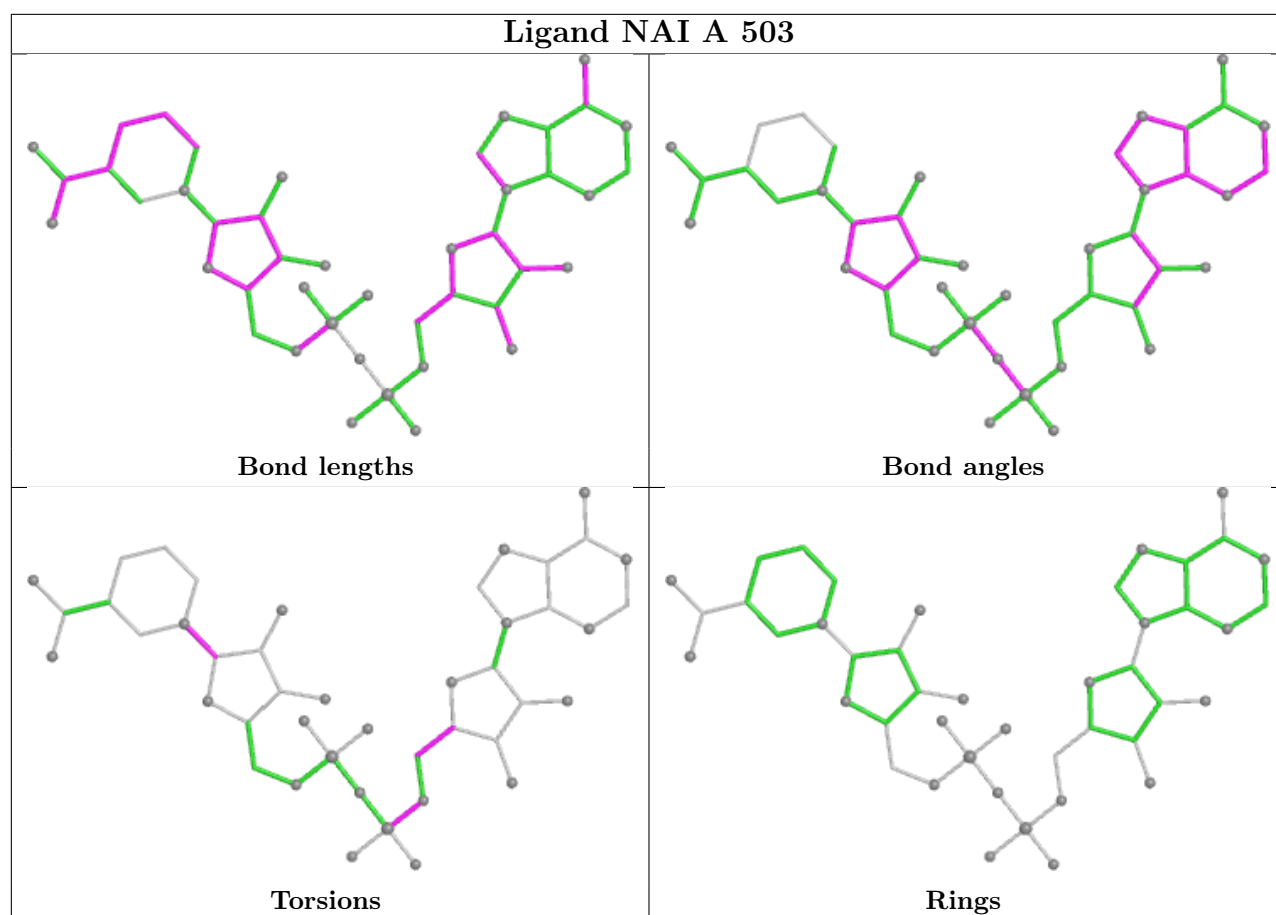


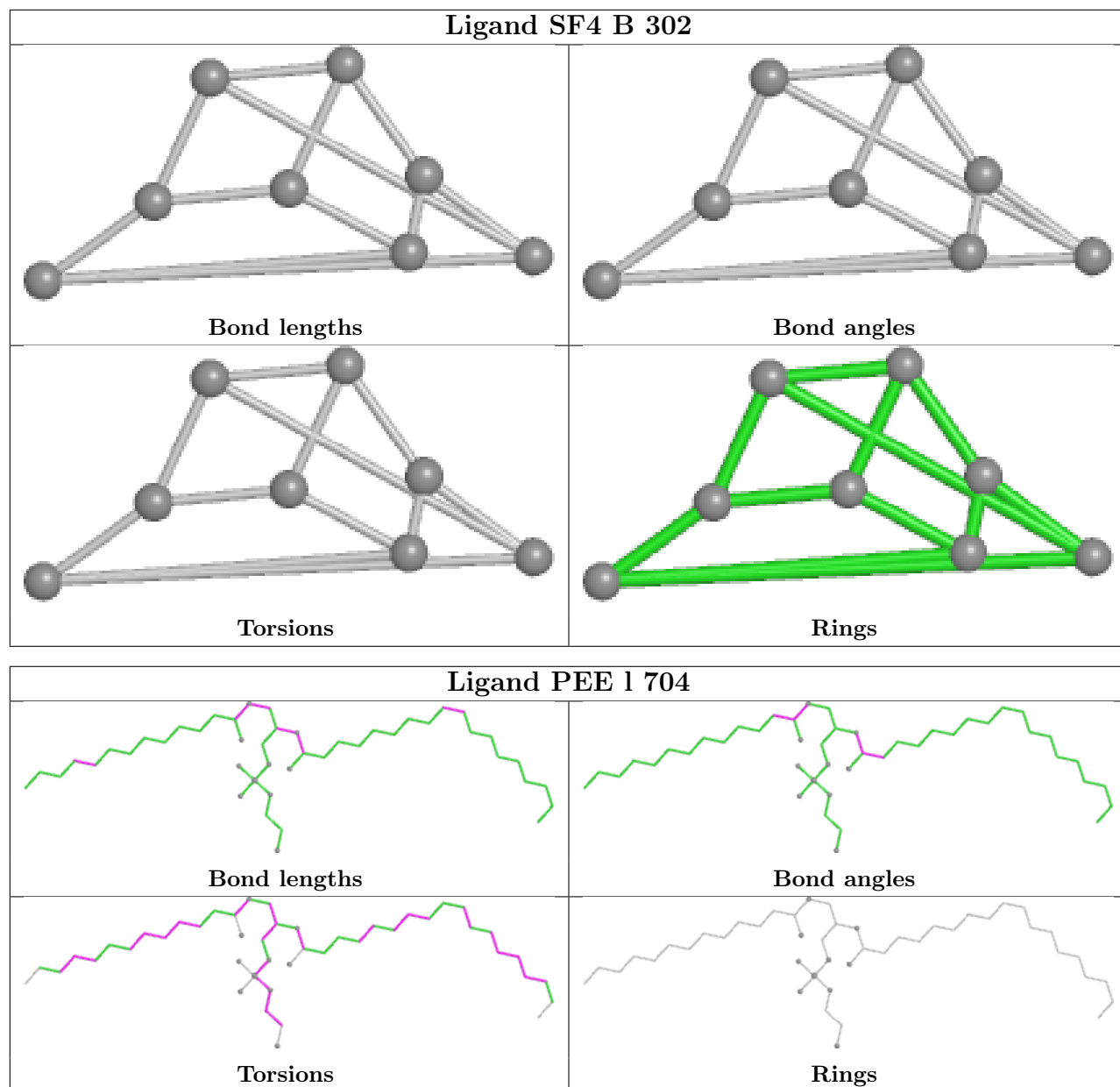


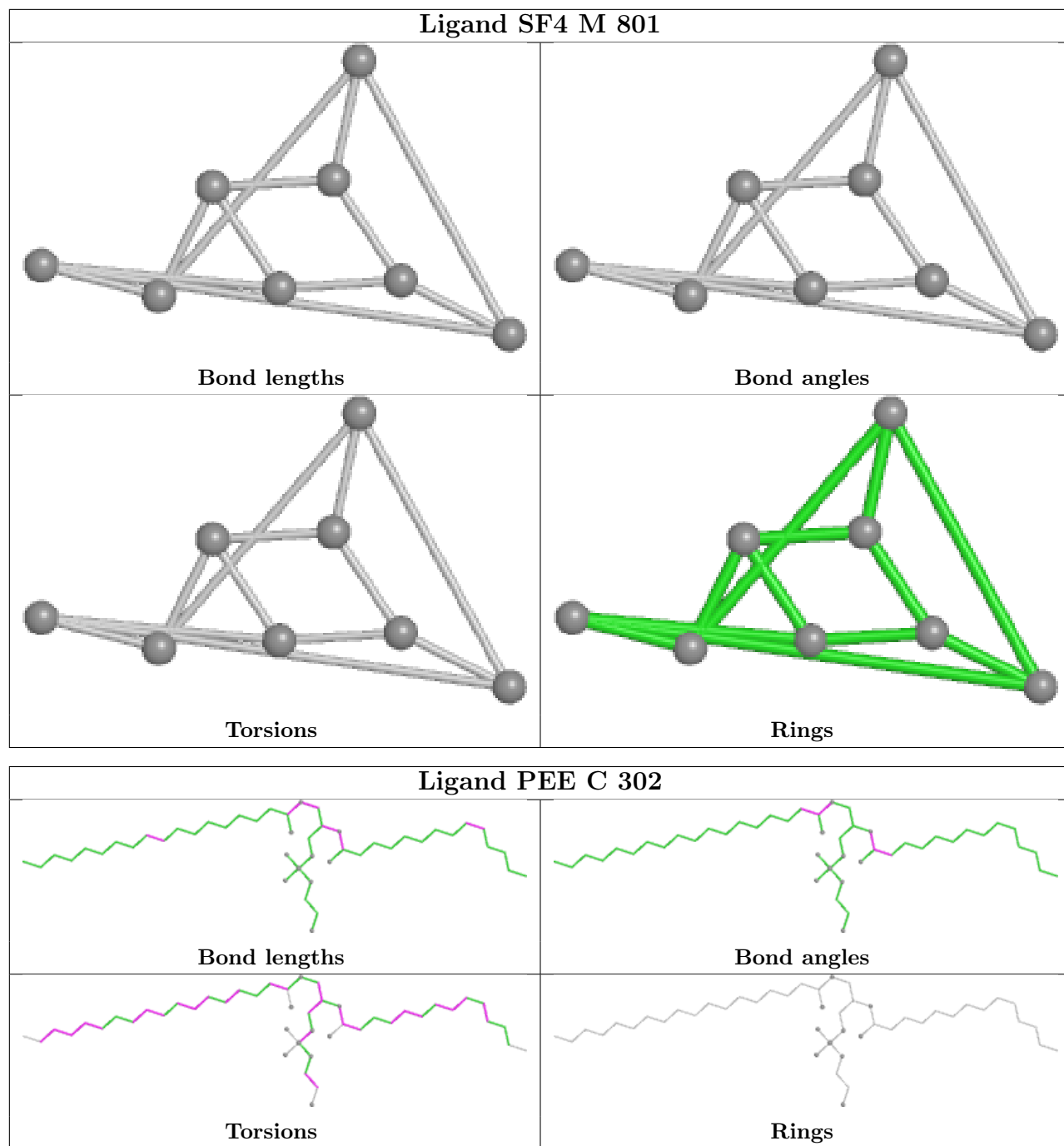


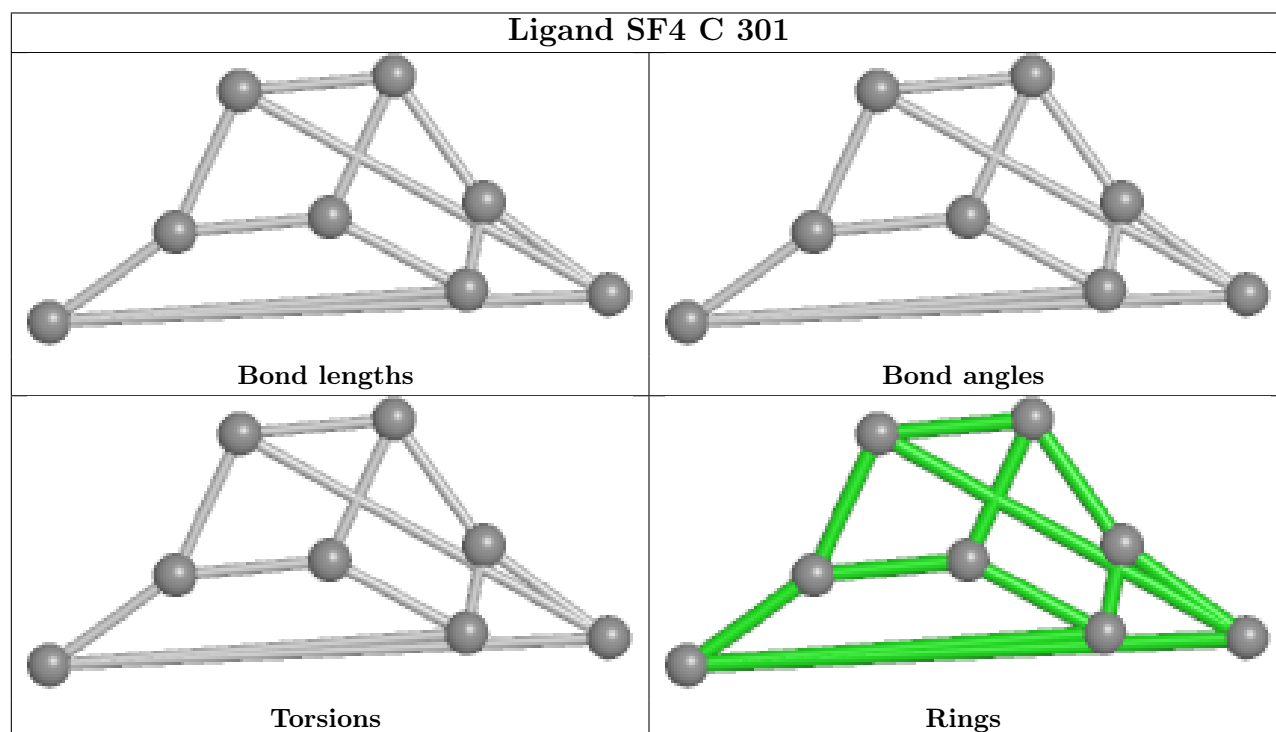
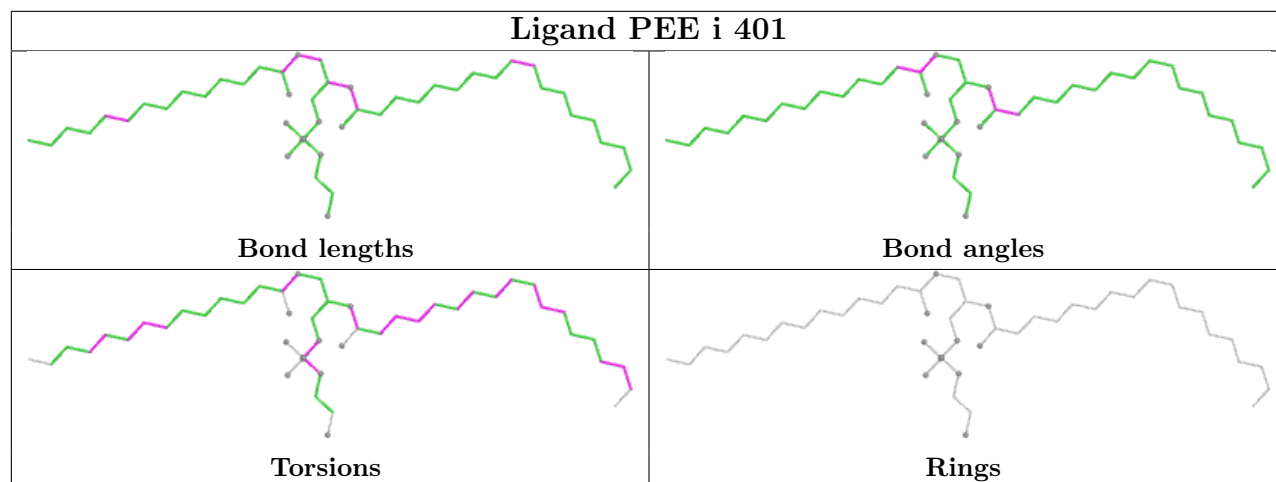


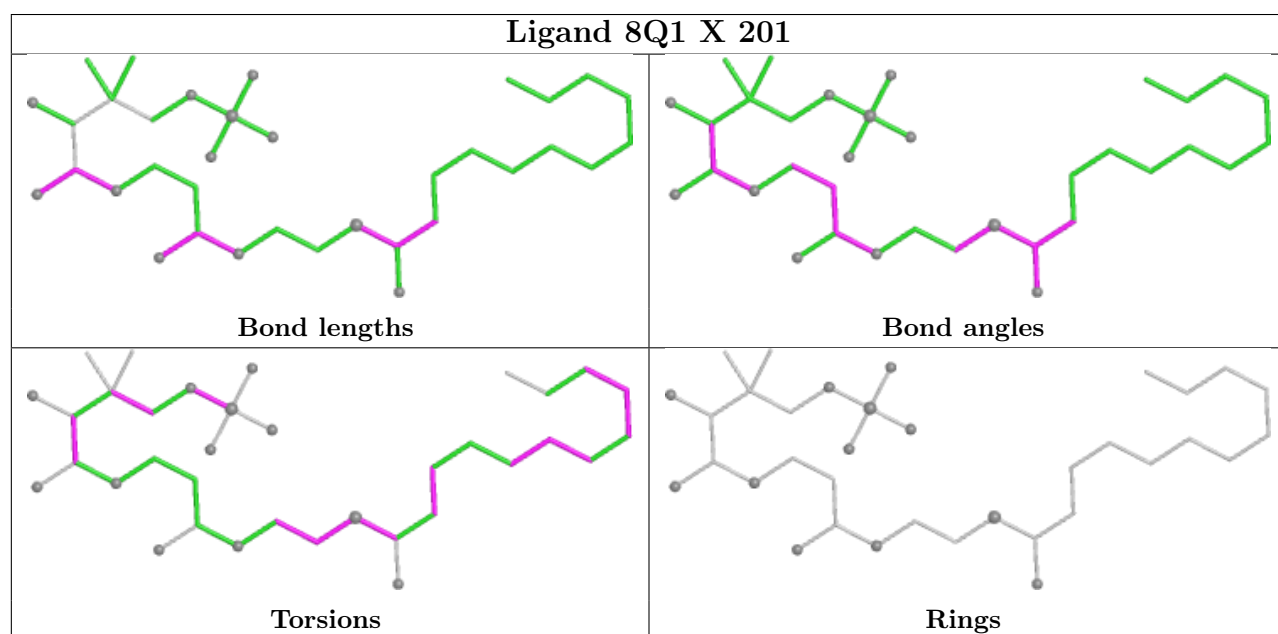
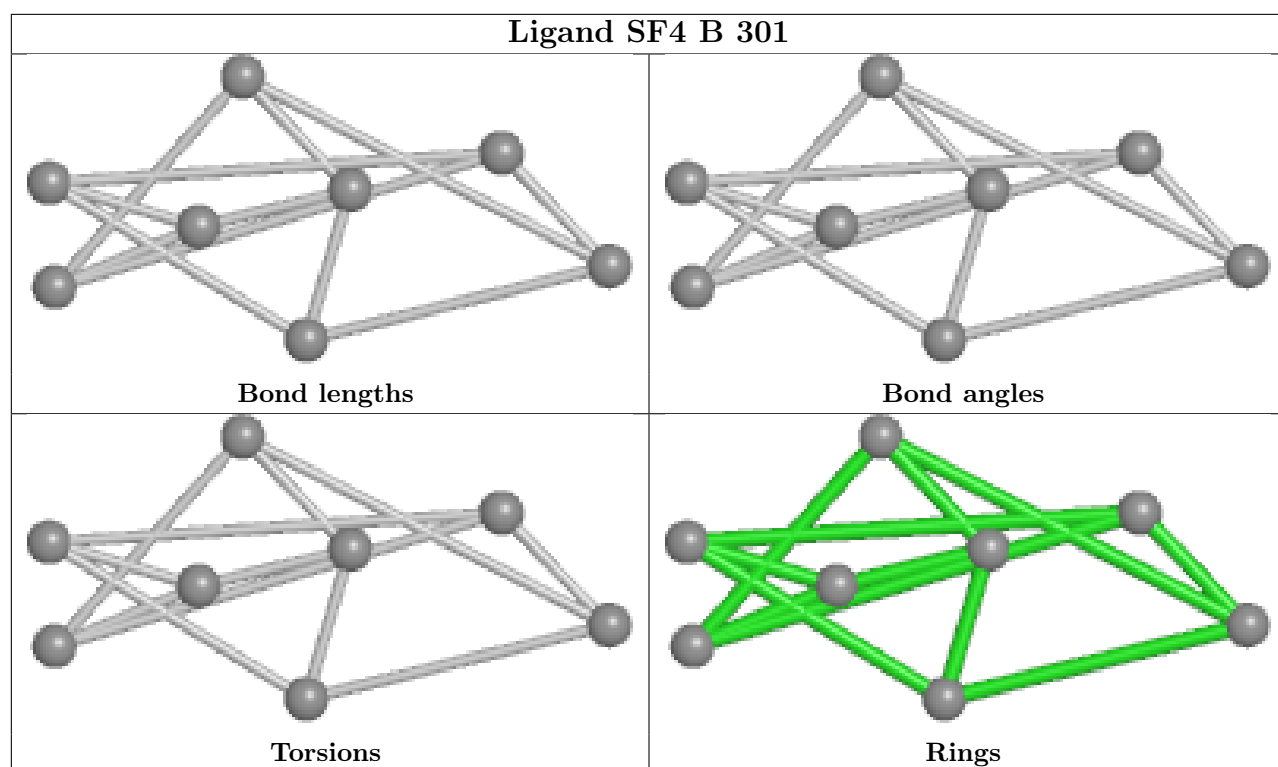


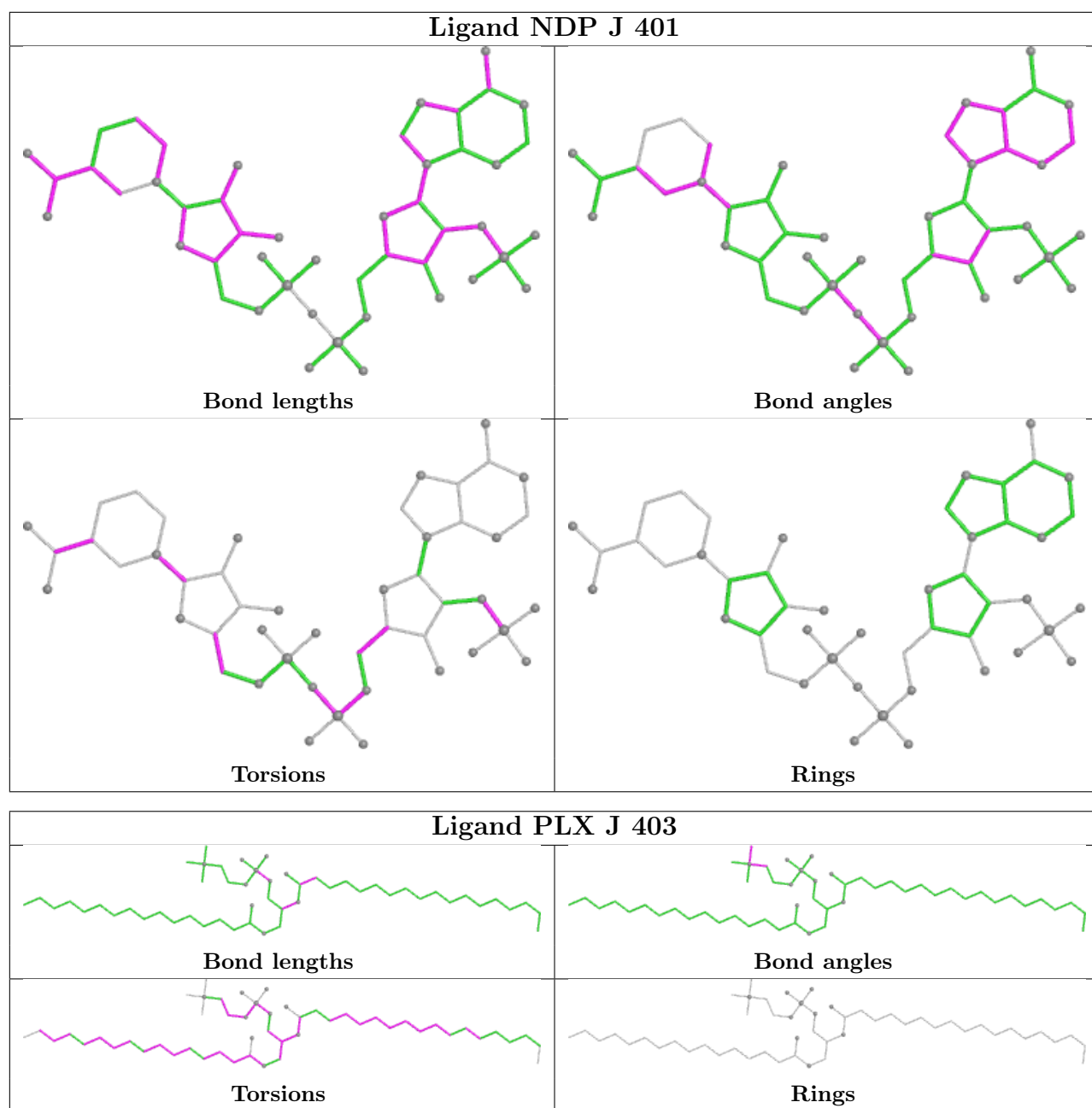




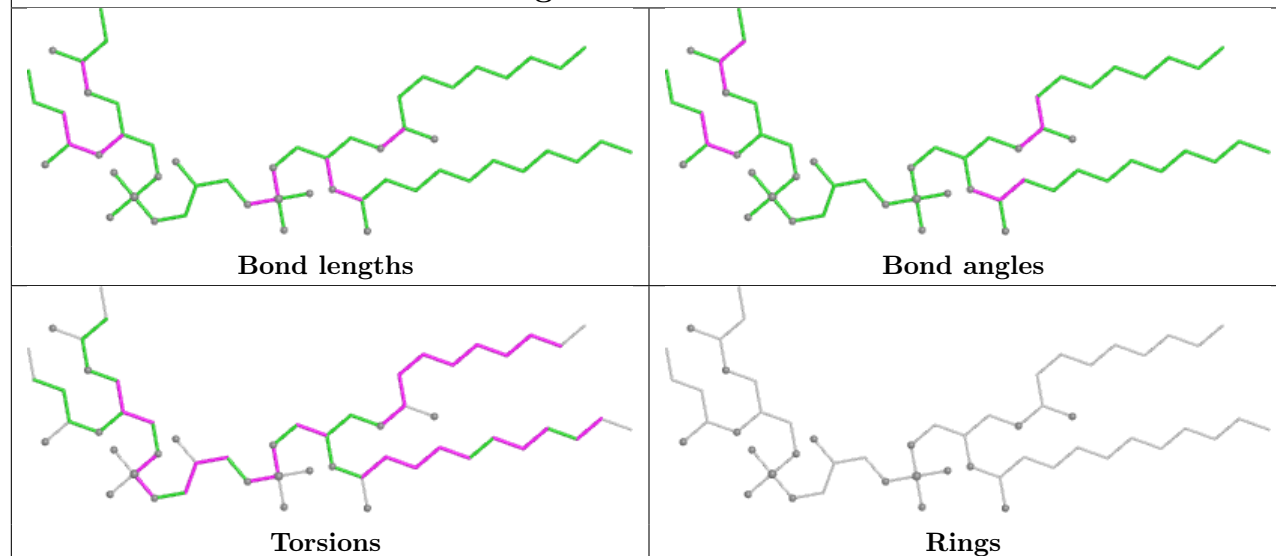




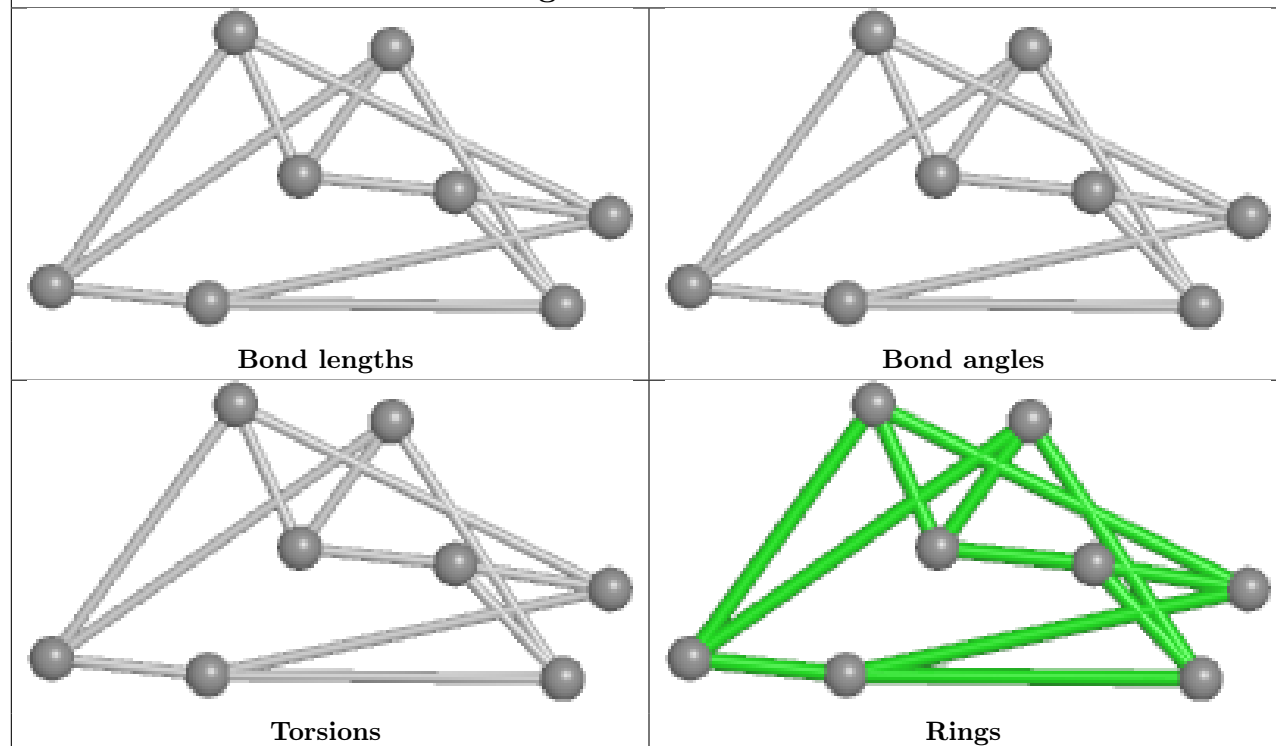


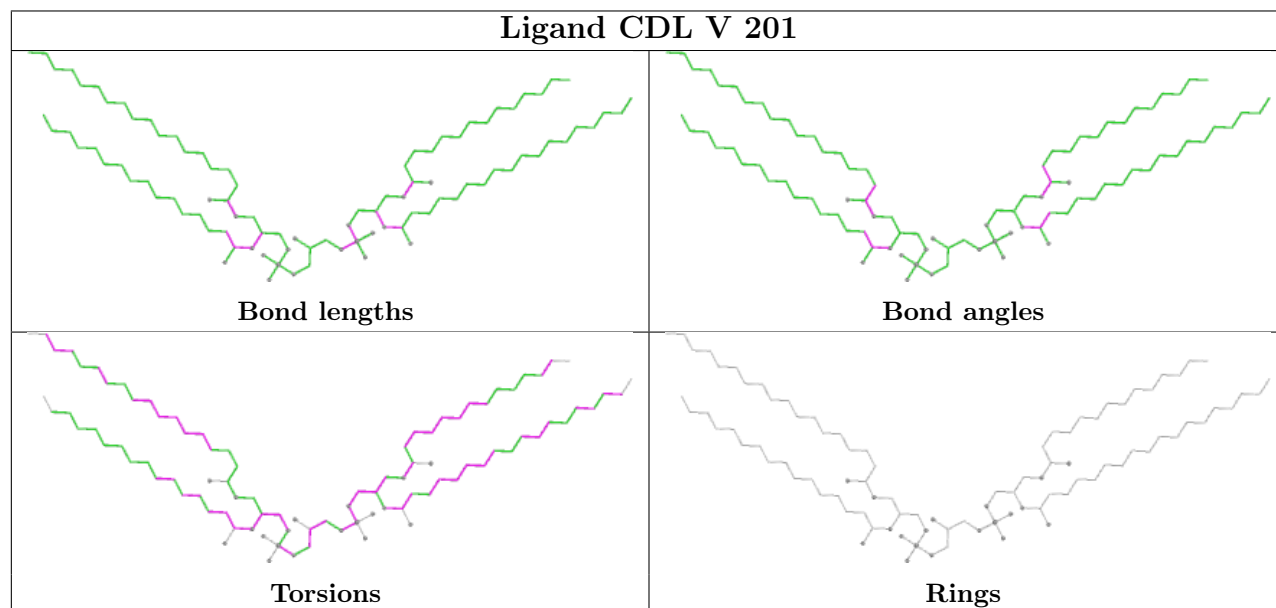
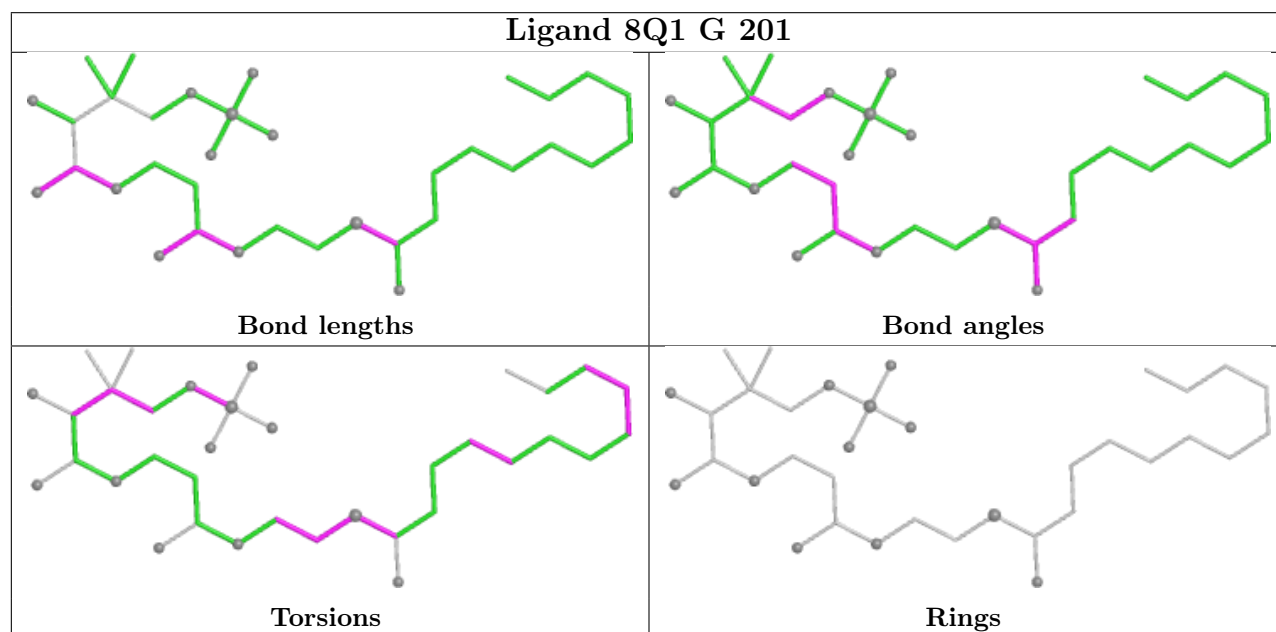
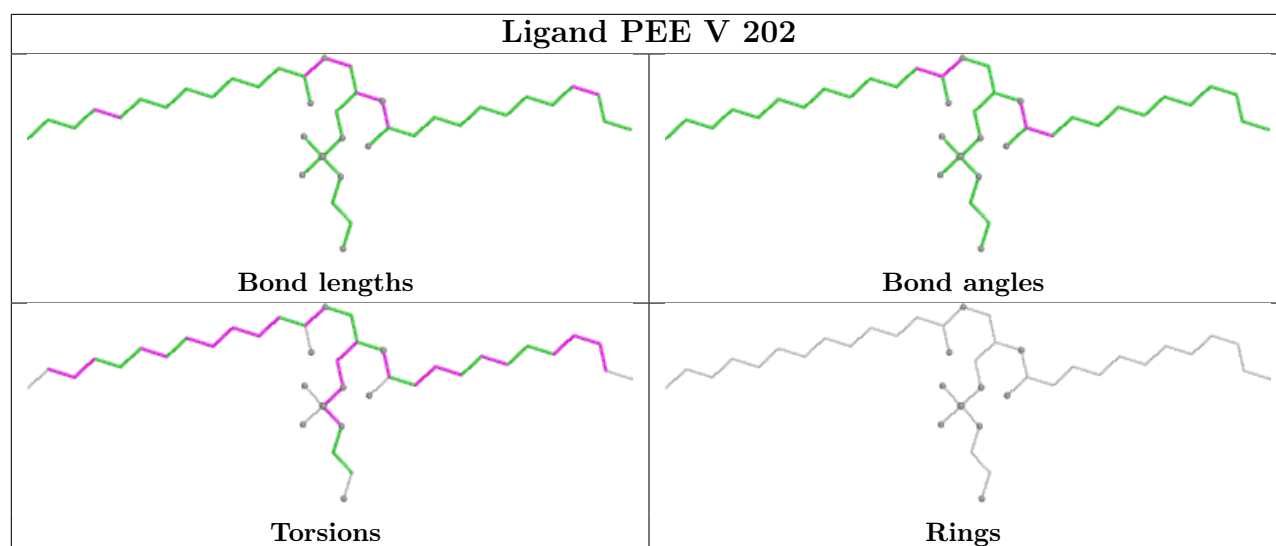


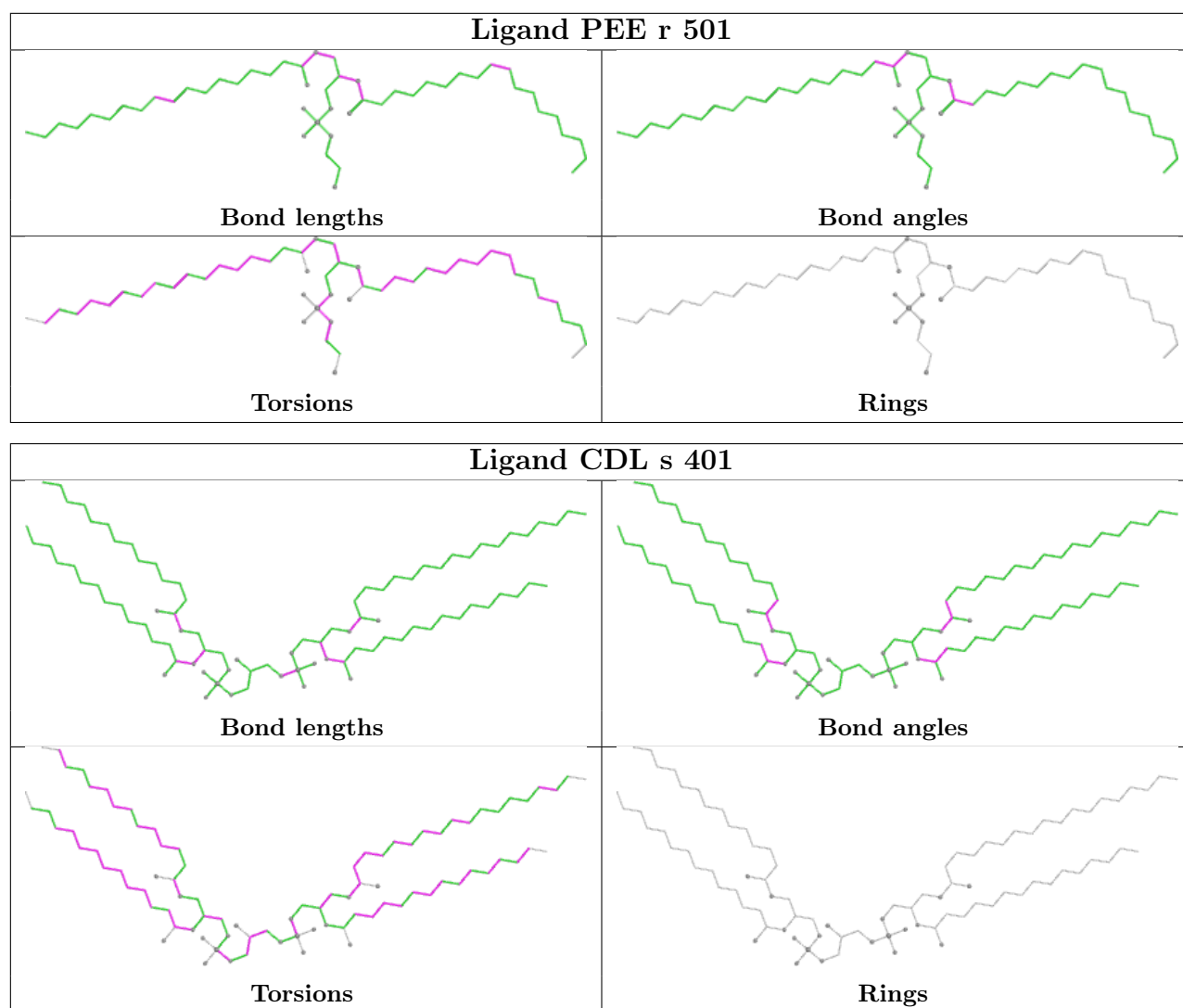
Ligand CDL u 201



Ligand SF4 A 501







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.

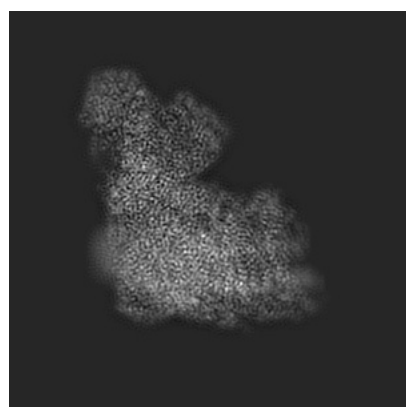
6 Map visualisation [i](#)

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.

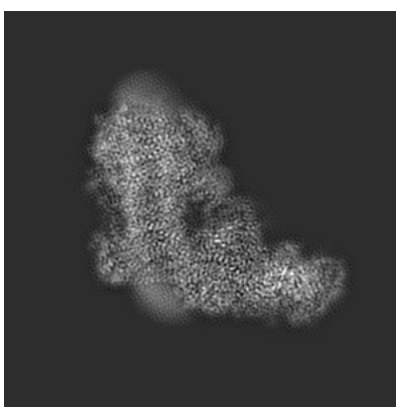
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

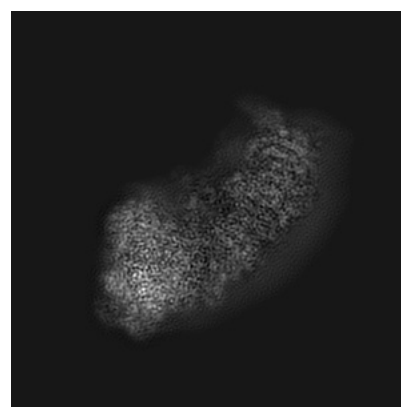
6.1.1 Primary map



X



Y

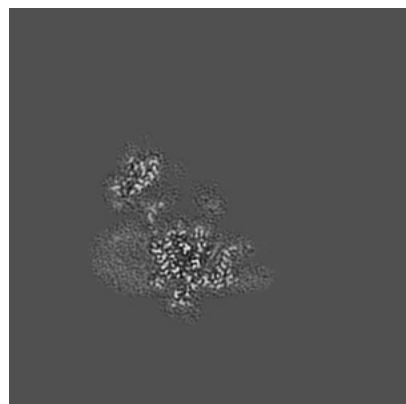


Z

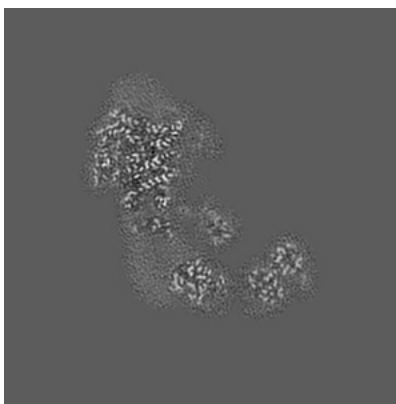
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

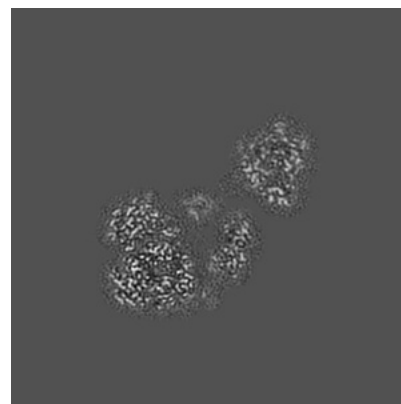
6.2.1 Primary map



X Index: 155



Y Index: 155

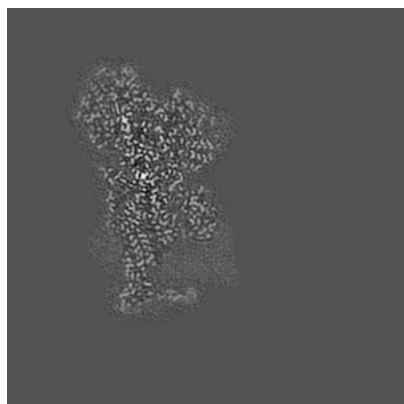


Z Index: 155

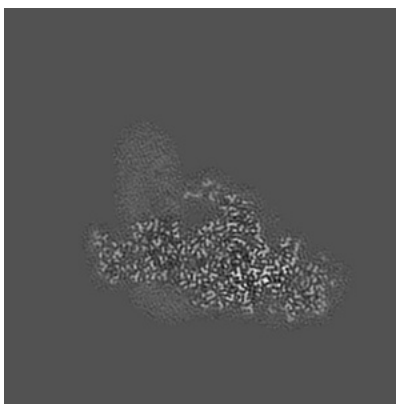
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

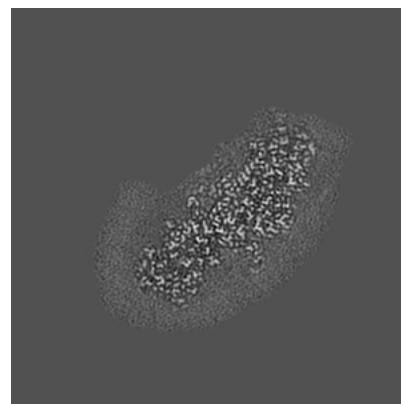
6.3.1 Primary map



X Index: 102



Y Index: 101

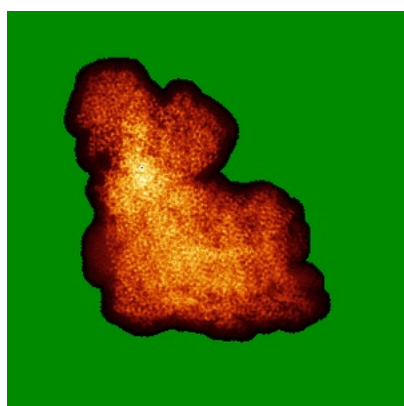


Z Index: 122

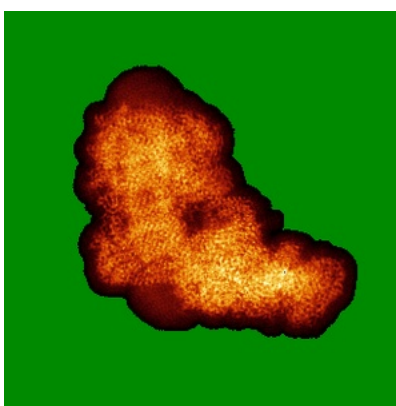
The images above show the largest variance slices of the map in three orthogonal directions.

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

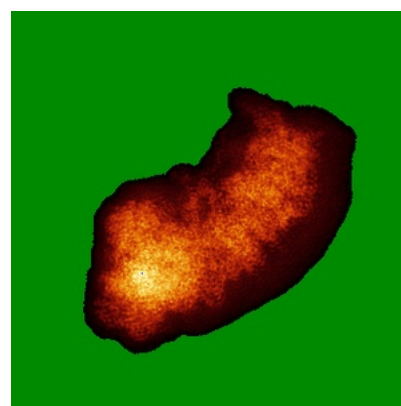
6.4.1 Primary map



X



Y

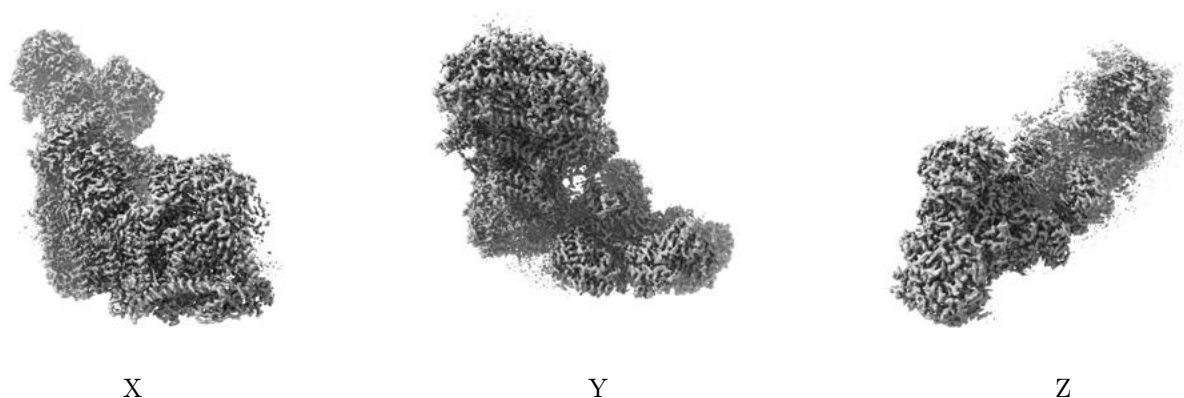


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

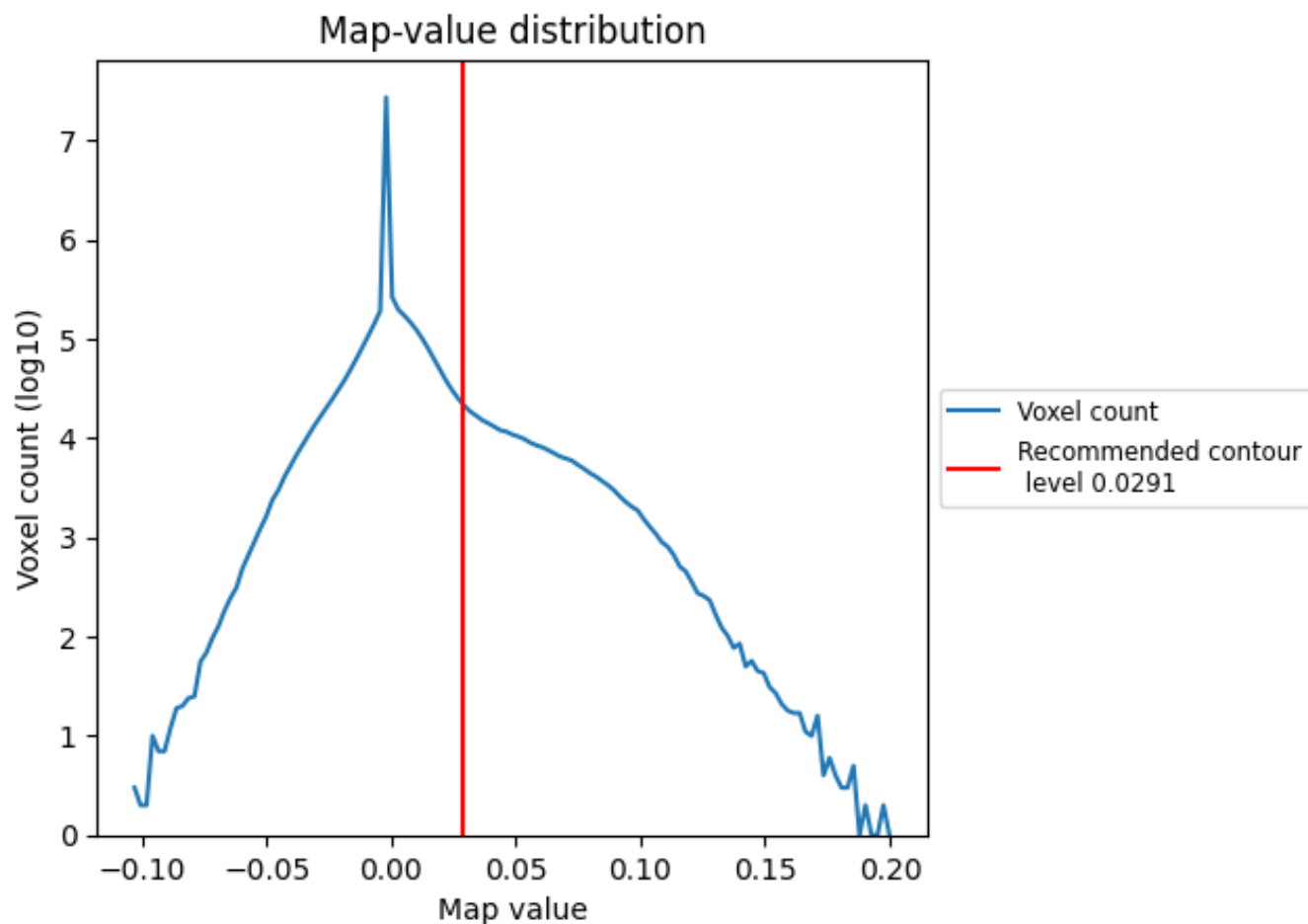
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

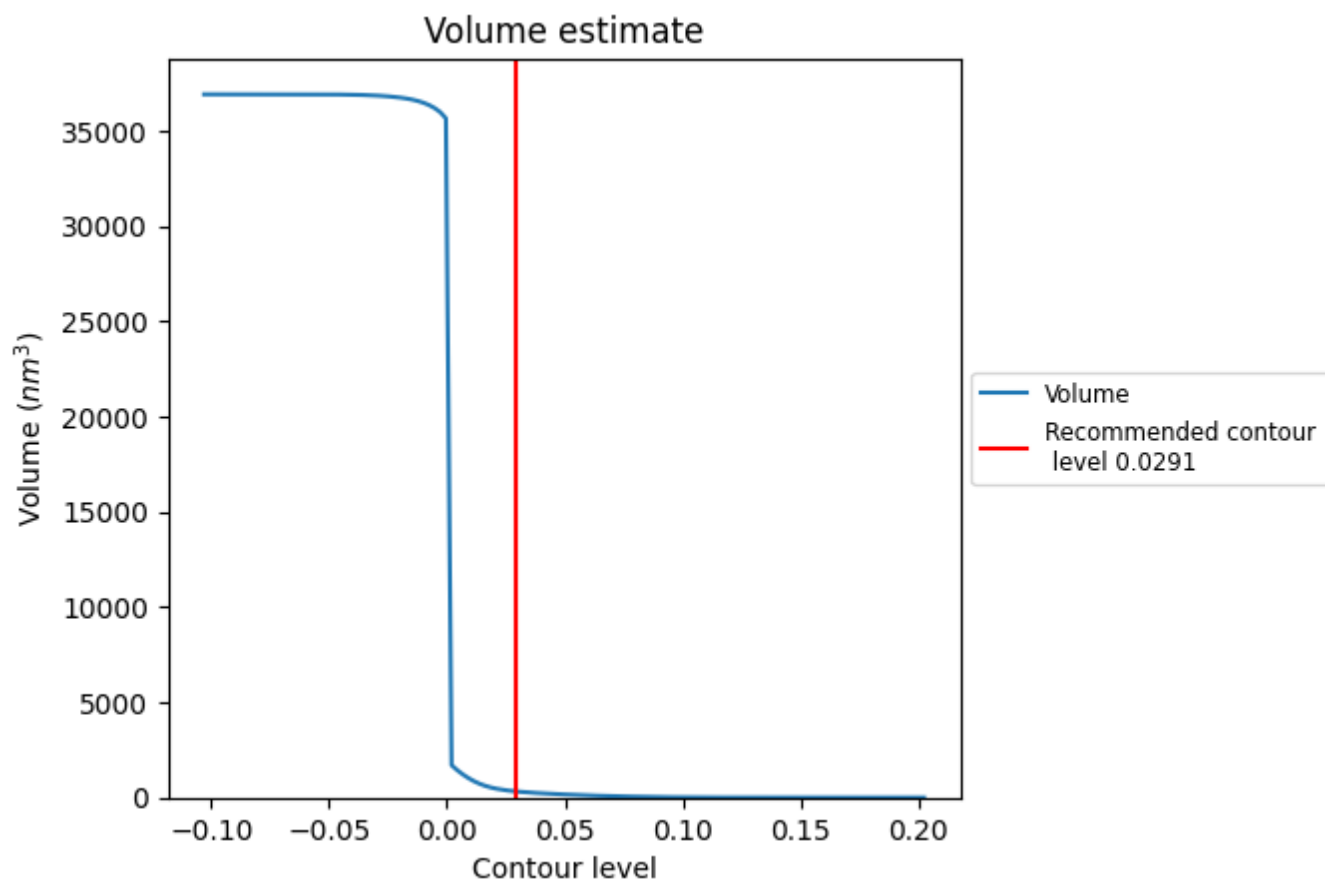
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

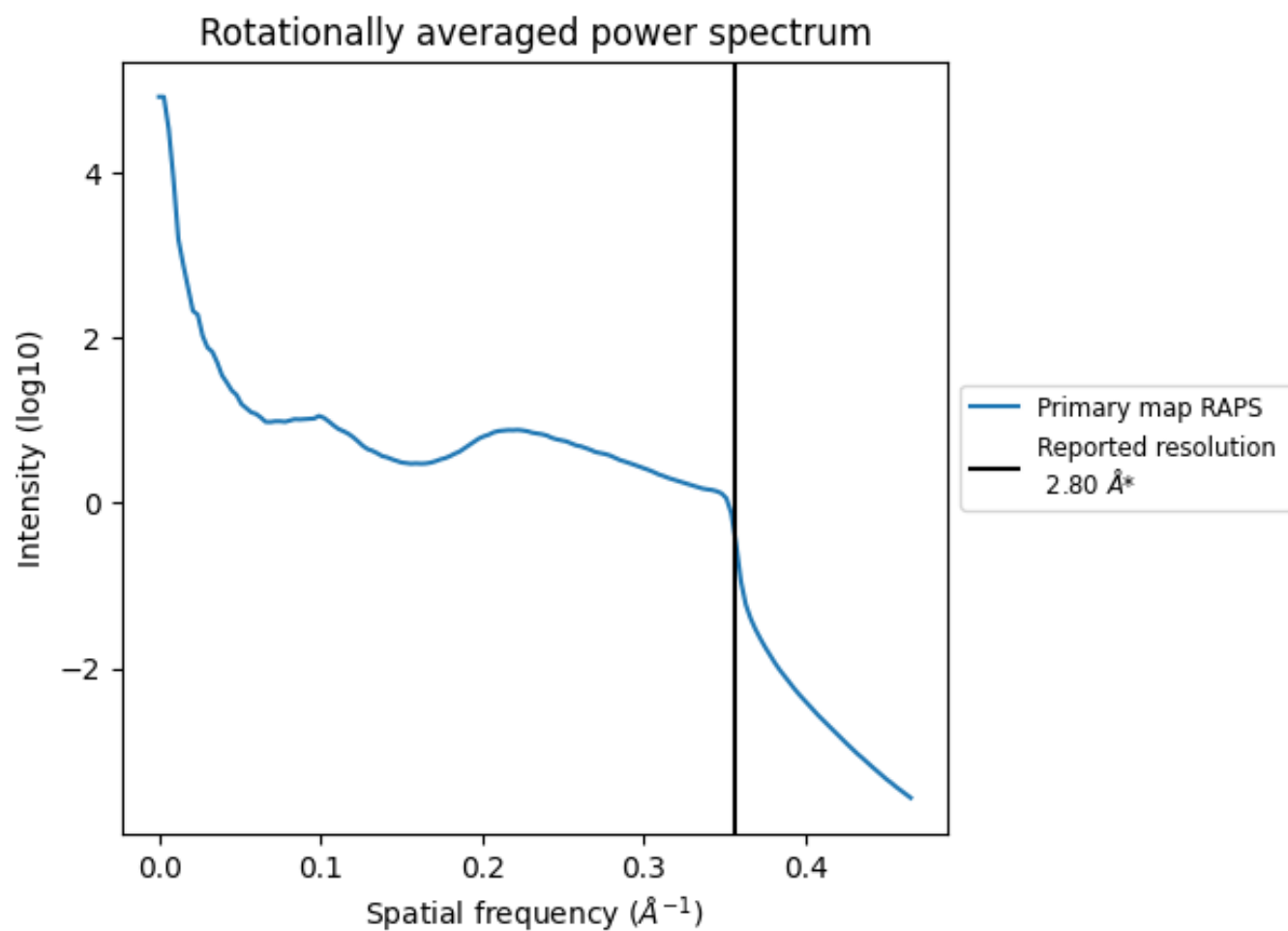
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326 nm³; 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⁻¹

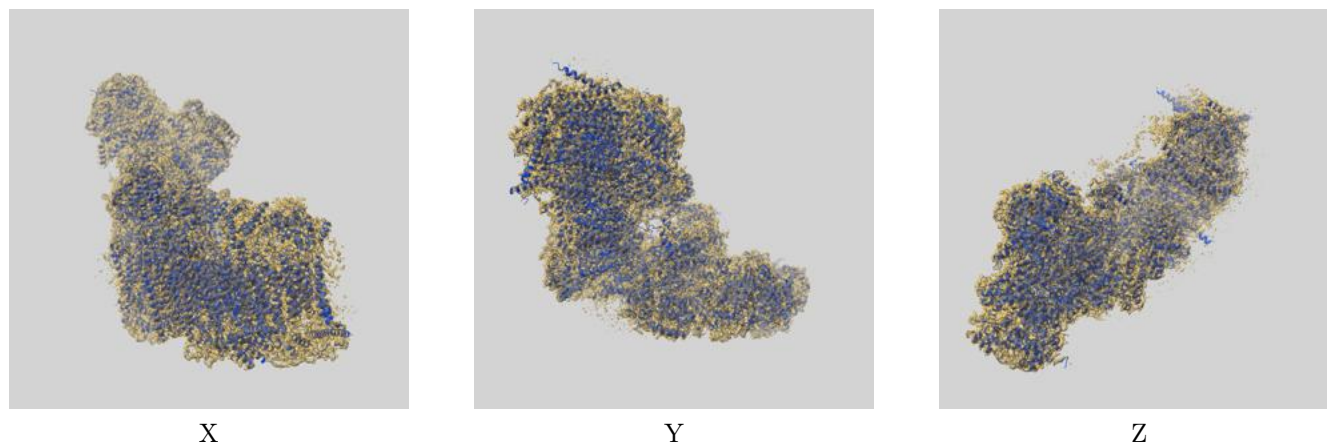
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

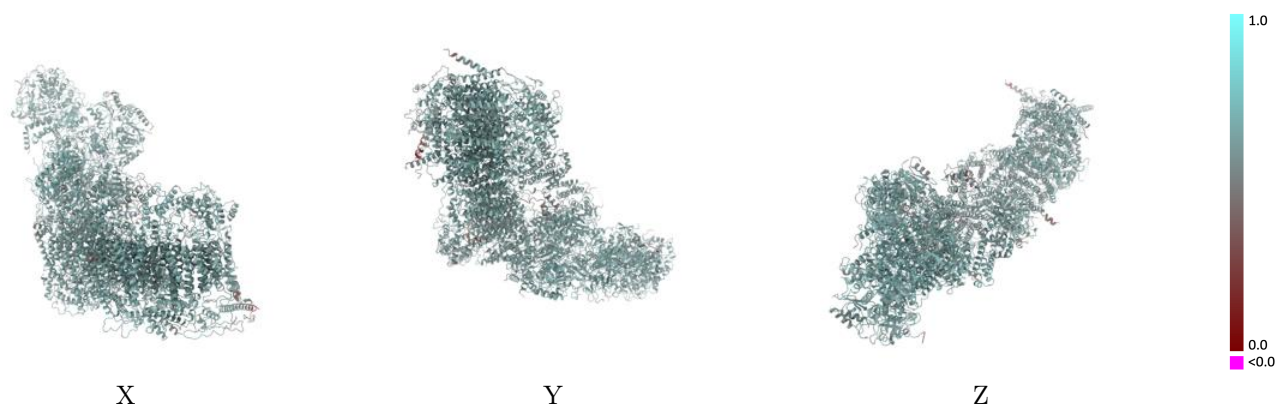
This section contains information regarding the fit between EMDB map EMD-32248 and PDB model 7W0R. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



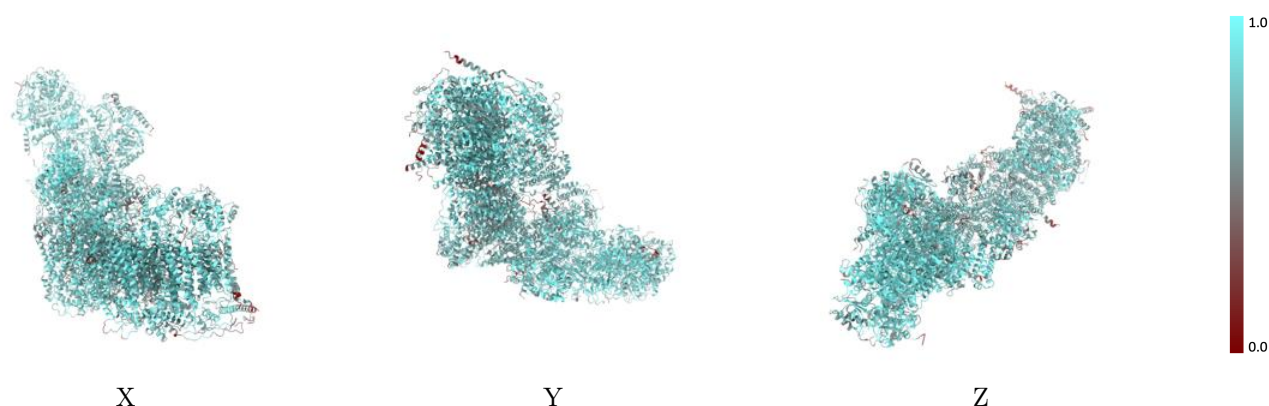
The images above show the 3D surface view of the map at the recommended contour level 0.0291 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



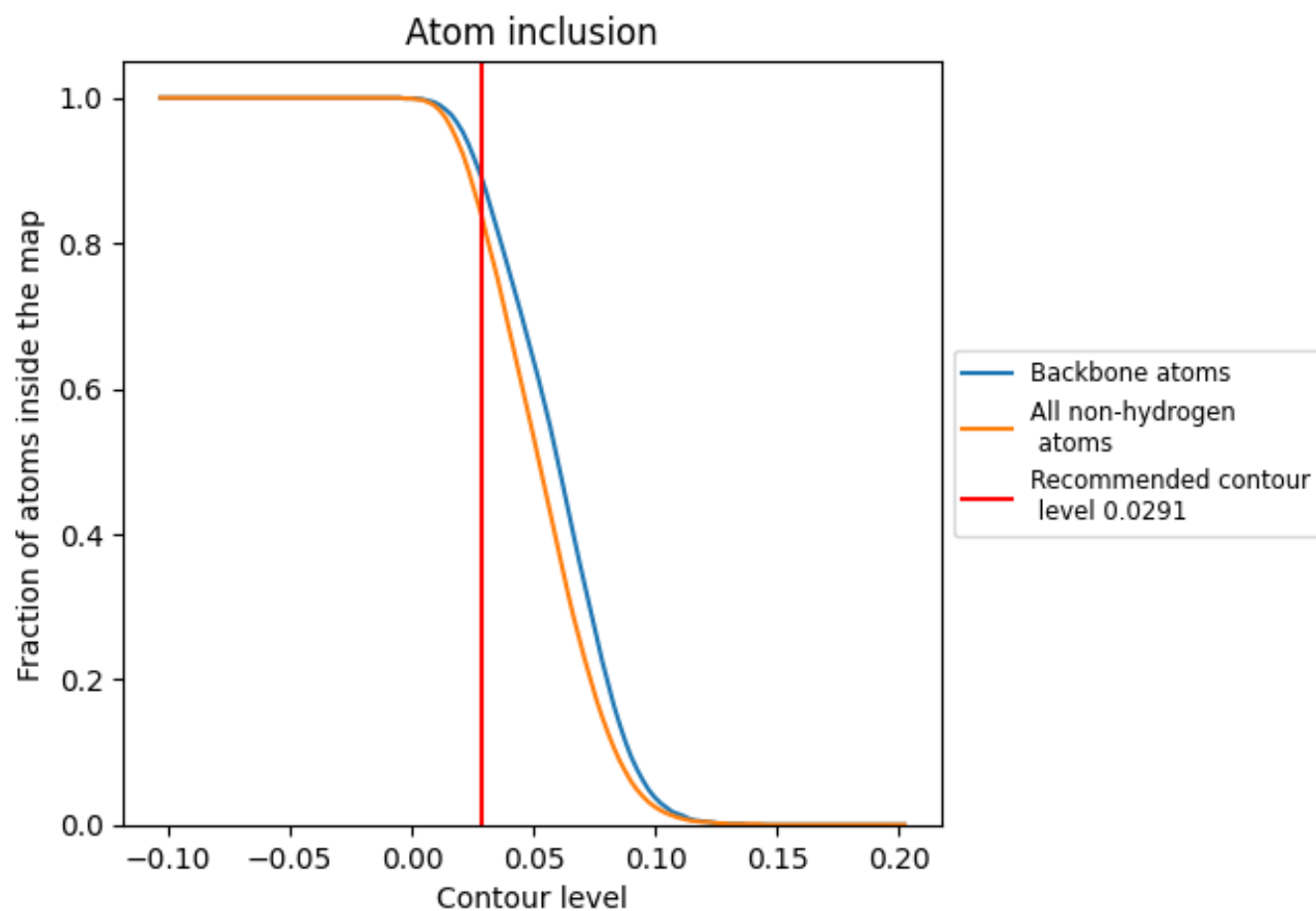
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8340	 0.6160
A	 0.8330	 0.6120
B	 0.9350	 0.6480
C	 0.8960	 0.6430
E	 0.8530	 0.6290
F	 0.7190	 0.5620
G	 0.5240	 0.4870
H	 0.8530	 0.6120
I	 0.7840	 0.6130
J	 0.8610	 0.6230
K	 0.7720	 0.6080
L	 0.8700	 0.6390
M	 0.8790	 0.6280
N	 0.8340	 0.6230
O	 0.8050	 0.5940
P	 0.9420	 0.6530
Q	 0.9240	 0.6480
S	 0.8860	 0.6250
T	 0.8620	 0.6310
U	 0.7820	 0.5940
V	 0.7410	 0.5980
W	 0.8170	 0.6070
X	 0.7380	 0.5930
Y	 0.6980	 0.5540
Z	 0.6420	 0.5440
a	 0.8170	 0.6220
b	 0.7710	 0.5910
c	 0.8140	 0.6110
d	 0.7700	 0.5950
e	 0.7770	 0.6000
f	 0.6350	 0.5580
g	 0.8440	 0.6200
h	 0.8180	 0.5990
i	 0.9140	 0.6380
j	 0.8100	 0.6240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.8170	 0.6210
l	 0.8340	 0.6190
m	 0.7730	 0.5880
n	 0.6830	 0.5730
o	 0.7620	 0.6050
p	 0.8050	 0.6060
r	 0.8760	 0.6310
s	 0.9010	 0.6380
u	 0.8060	 0.6010
v	 0.6840	 0.5550
w	 0.8200	 0.6070