



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:40 PM UTC

PDB ID : 7W2Y / pdb_00007w2y
EMDB ID : EMD-32267
Title : Active state CI from DQ-NADH dataset, Subclass 3
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-24
Resolution : 2.70 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

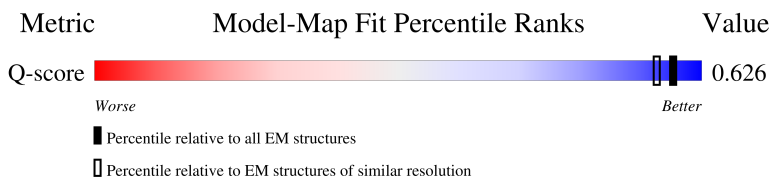
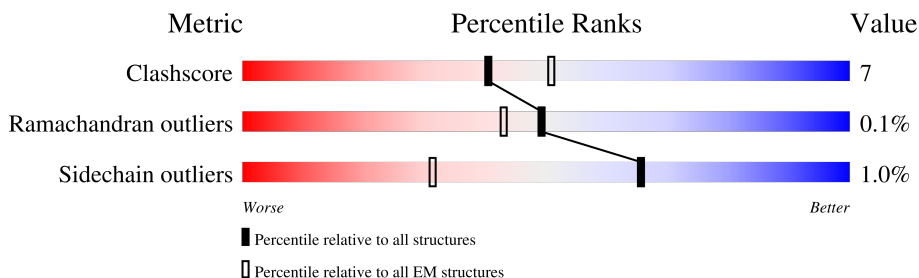
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	 81% 18%
2	B	176	 84% 16%
3	C	156	 81% 19%
4	E	115	 87% 13%

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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	122	
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	125	
44	w	320	

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68232 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
			971	619	179	168	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
			693	447	103	138	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
			2748	1782	481	476	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
			1161	749	197	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	122	Total	C	N	O	S	0	0
			1005	653	174	172	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
			1277	852	187	225	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
			1534	982	279	265	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
			1028	642	195	182	9		

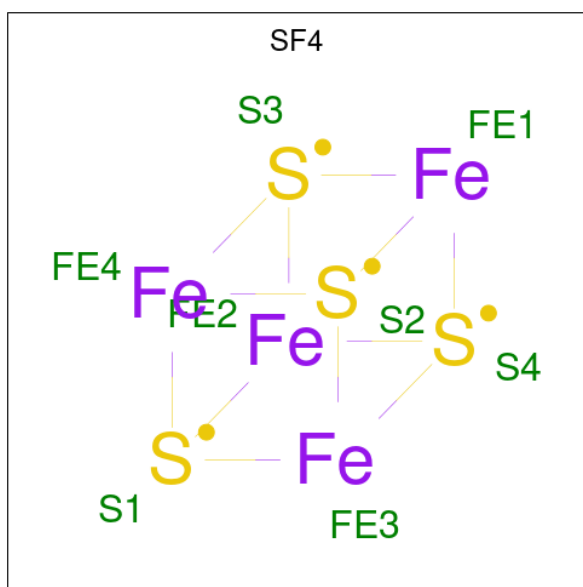
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

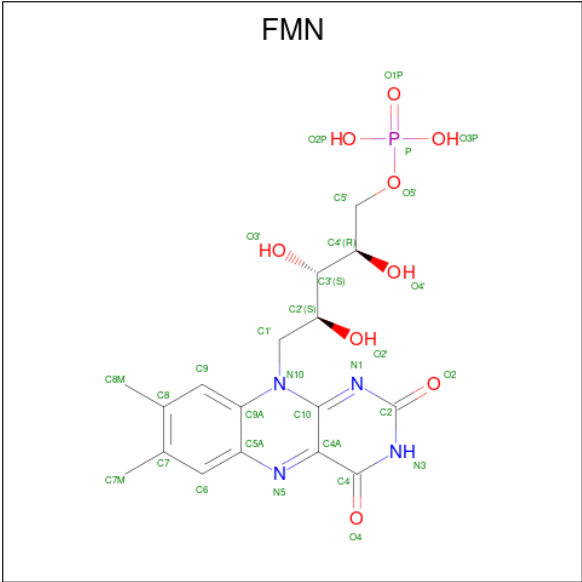
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

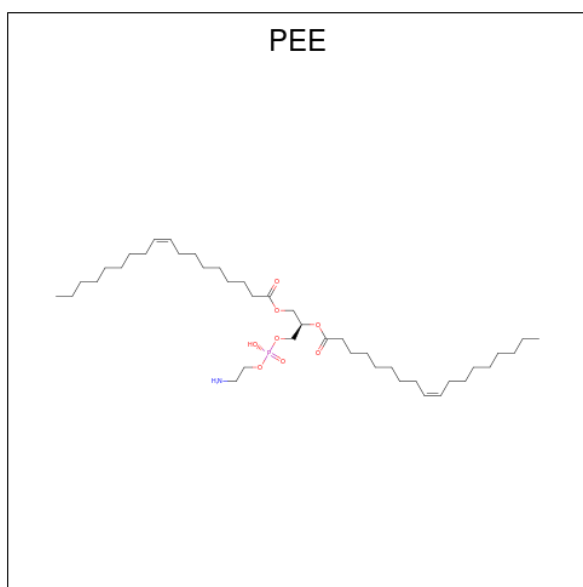
- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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	

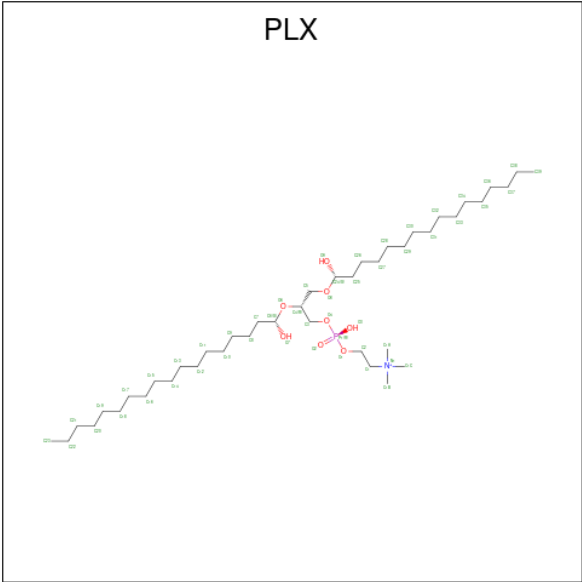
- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).





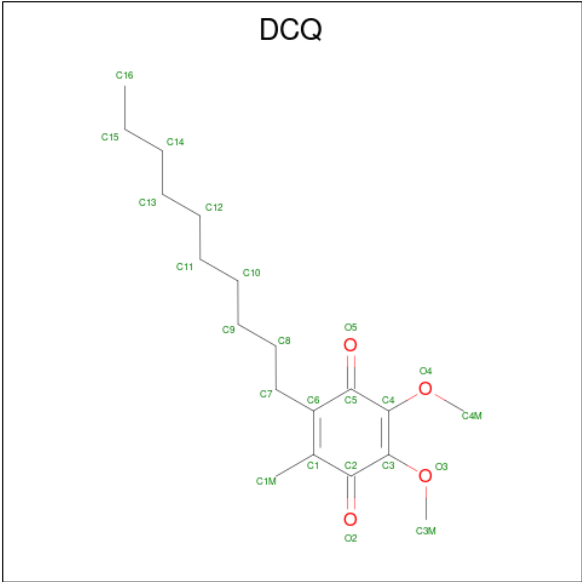
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41	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).



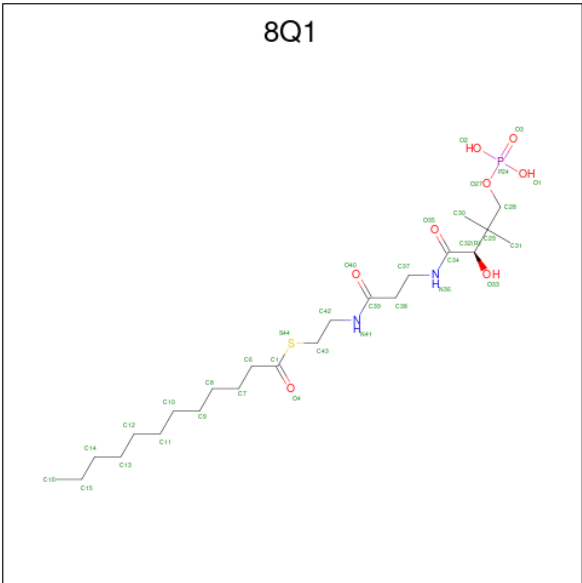
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄) (labeled as "Ligand of Interest" by depositor).



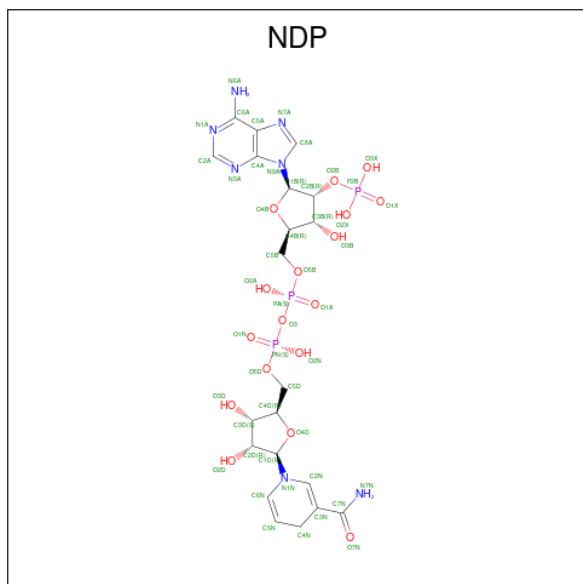
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			23	19	4	

- 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).



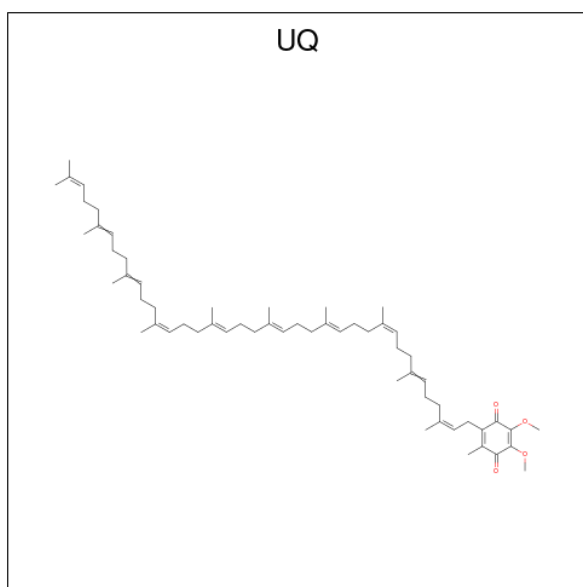
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 52 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).



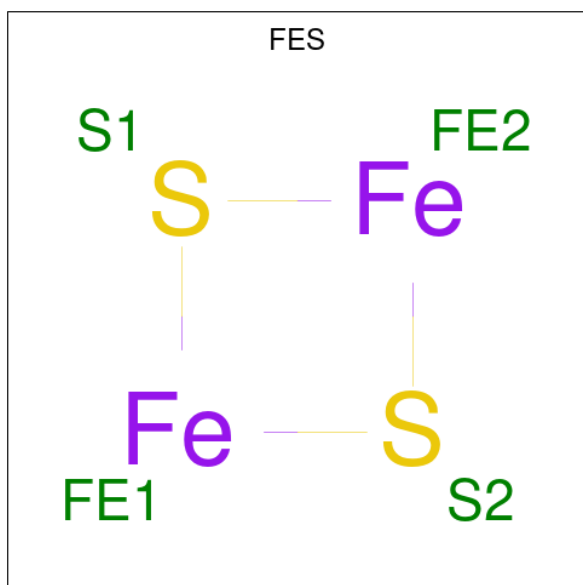
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

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

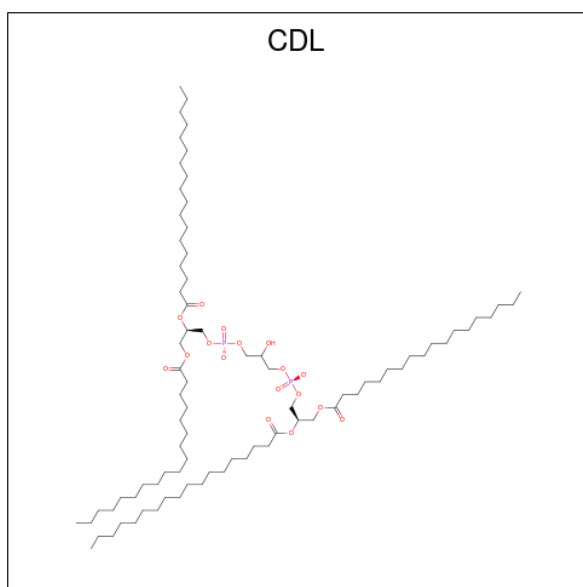


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

- 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 CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

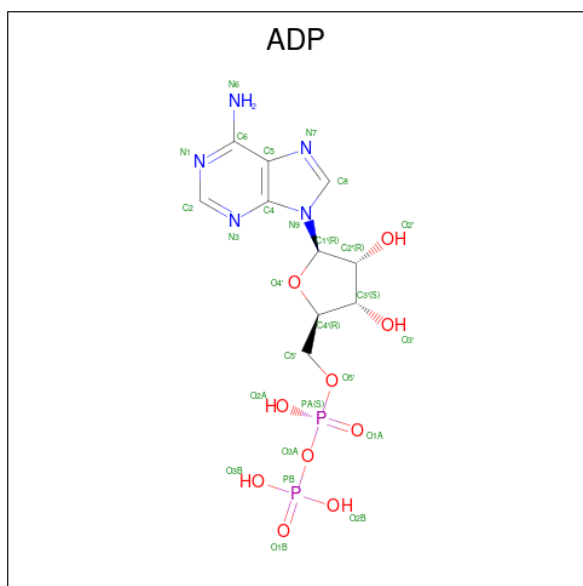


Mol	Chain	Residues	Atoms				AltConf
56	N	1	Total	C	O	P	0
			51	32	17	2	
56	V	1	Total	C	O	P	0
			94	75	17	2	
56	V	1	Total	C	O	P	0
			100	81	17	2	
56	V	1	Total	C	O	P	0
			100	81	17	2	
56	a	1	Total	C	O	P	0
			100	81	17	2	
56	i	1	Total	C	O	P	0
			87	68	17	2	
56	l	1	Total	C	O	P	0
			99	80	17	2	
56	l	1	Total	C	O	P	0
			92	73	17	2	
56	n	1	Total	C	O	P	0
			55	36	17	2	
56	r	1	Total	C	O	P	0
			100	81	17	2	
56	s	1	Total	C	O	P	0
			89	70	17	2	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

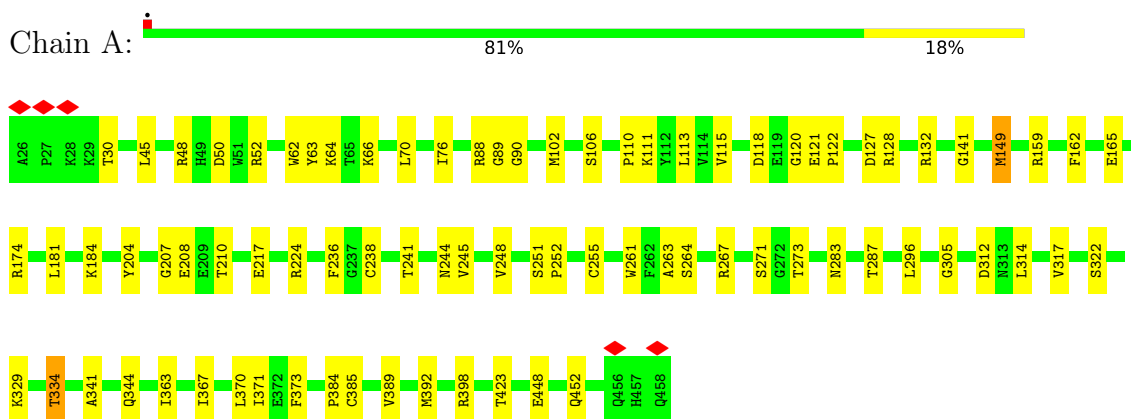


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

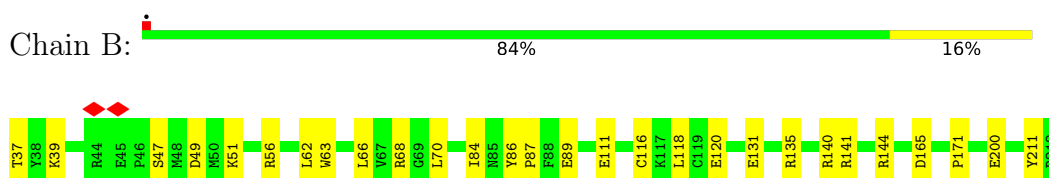
3 Residue-property plots

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.

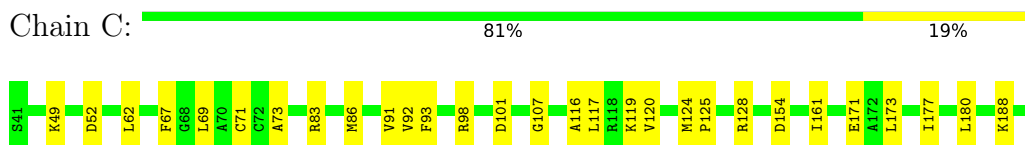
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



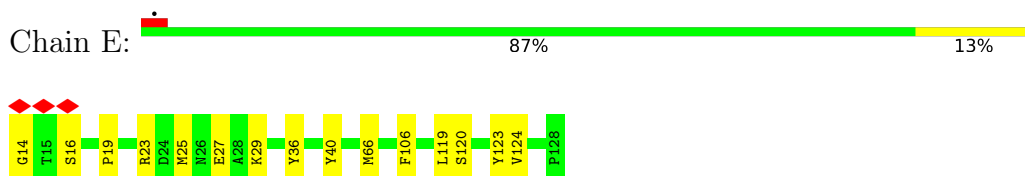
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



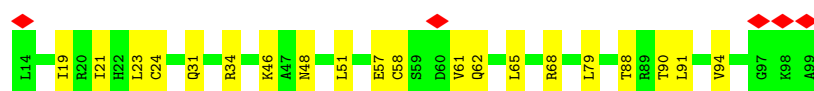
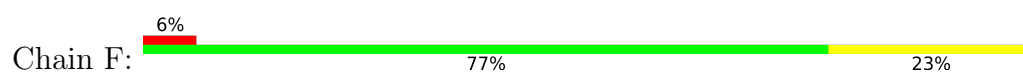
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



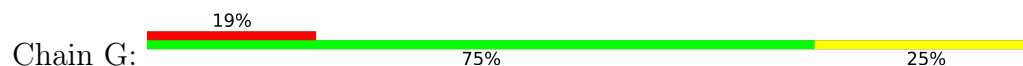
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



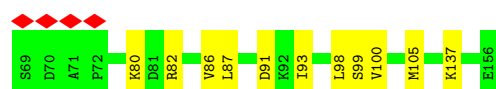
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



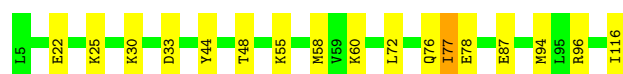
- Molecule 6: Acyl carrier protein



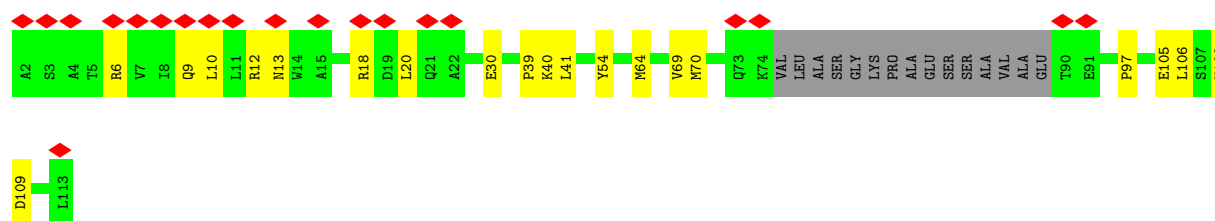
- Molecule 6: Acyl carrier protein



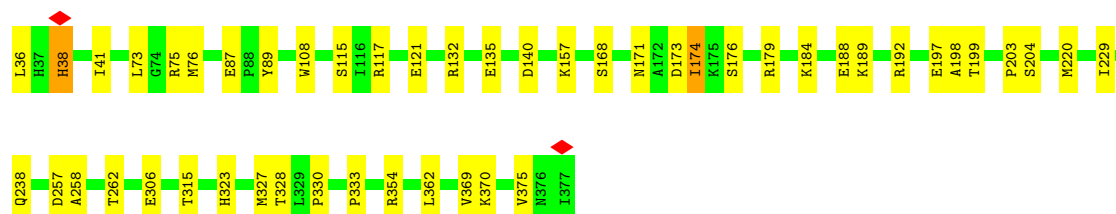
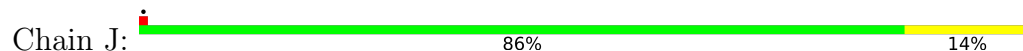
- Molecule 7: Complex I subunit B13



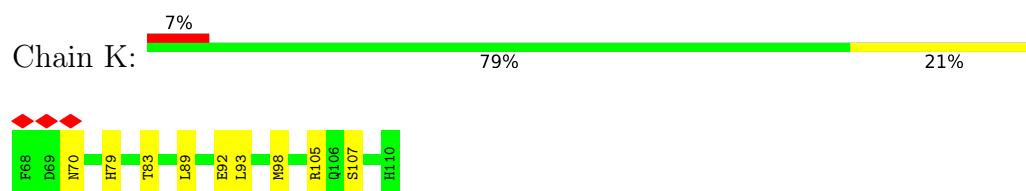
- Molecule 8: Complex I-B14.5a



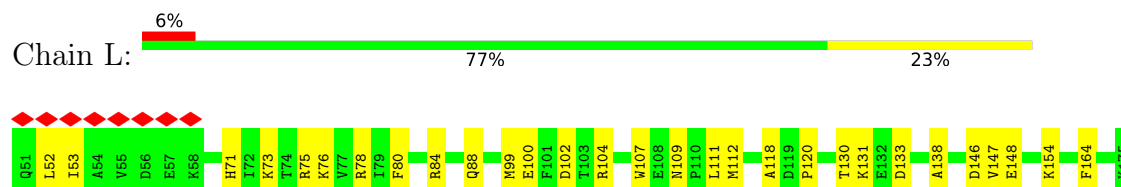
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



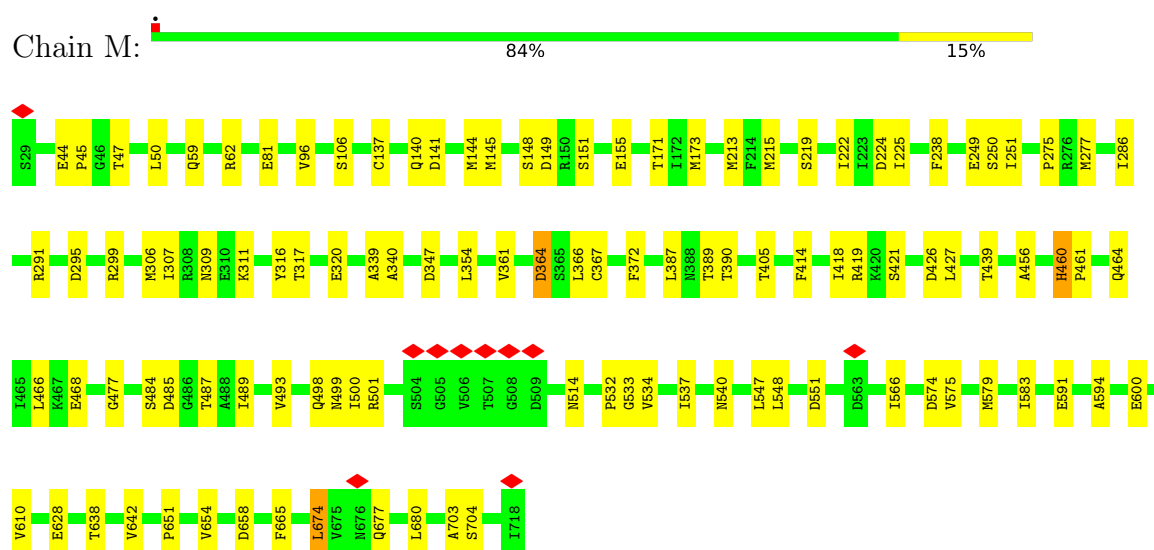
- Molecule 10: Complex I-9kD



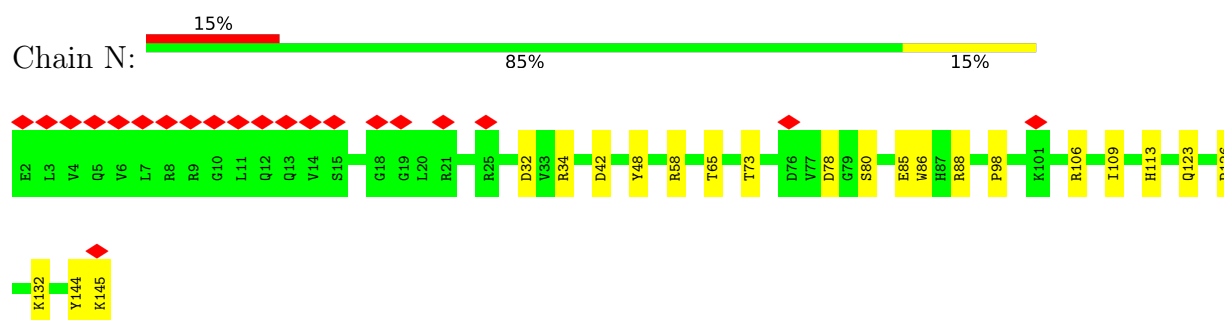
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



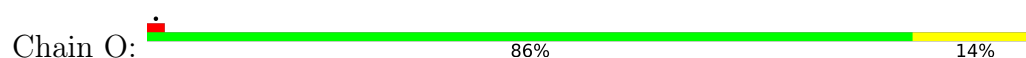
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



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





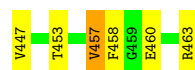
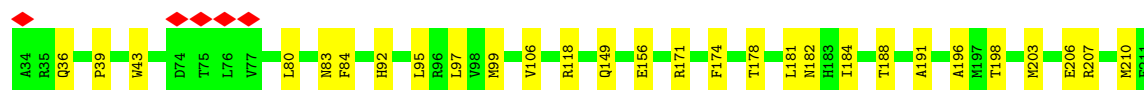
• Molecule 15: Complex I-30kD

Chain P: 84% 16%



• Molecule 16: Complex I-49kD

Chain Q: 84% 15%



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

Chain S: 84% 16%



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

Chain T: 8% 89% 10%



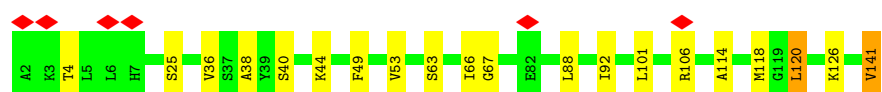
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 5% 90% 10%



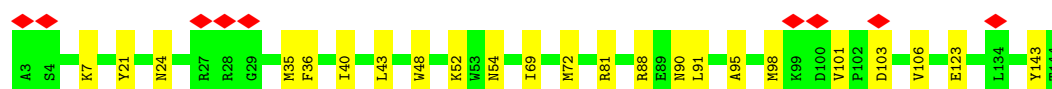
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  86% 13%



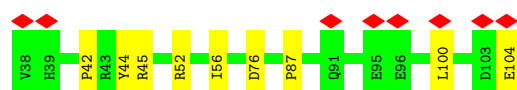
- Molecule 21: Complex I-B16.6

Chain W:  6% 84% 16%



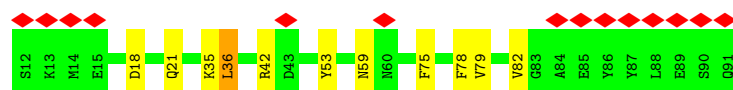
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  12% 87% 13%



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

Chain Z:  18% 86% 12%



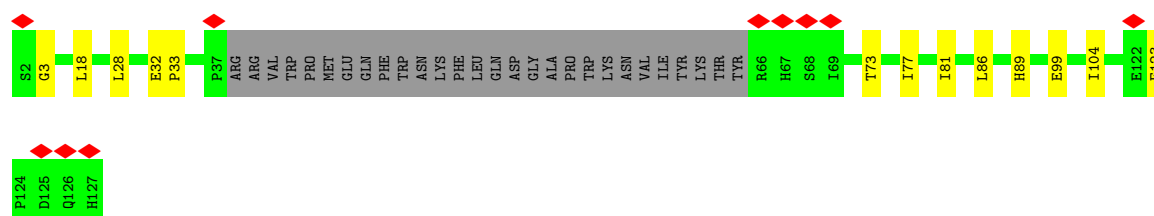
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  89% 11%

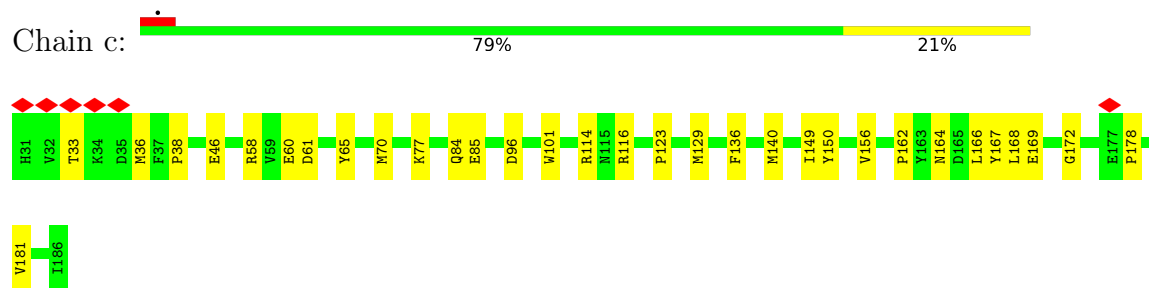


- Molecule 25: Complex I-B17

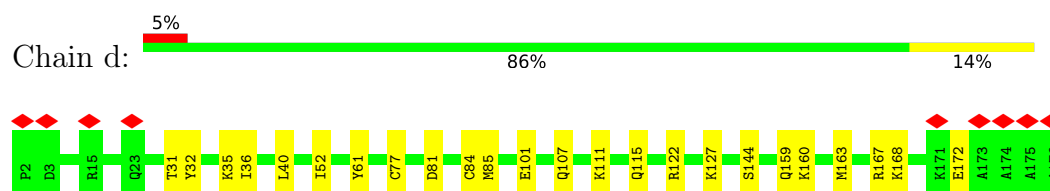
Chain b:  8% 67% 10% 22%



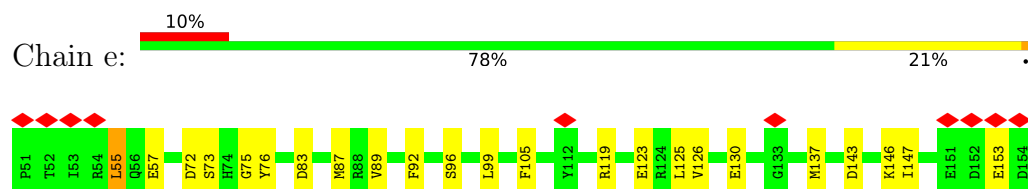
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



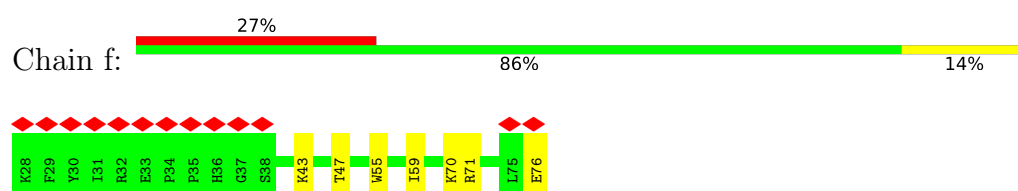
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



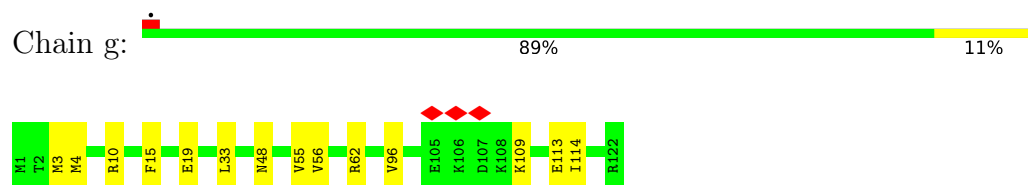
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



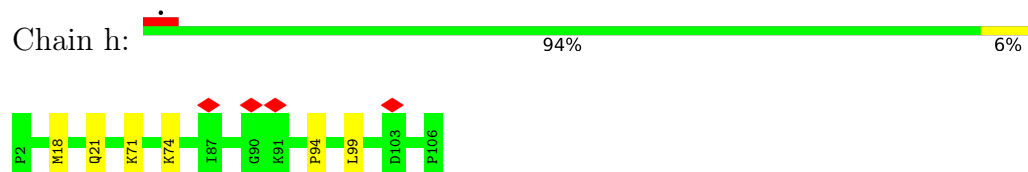
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



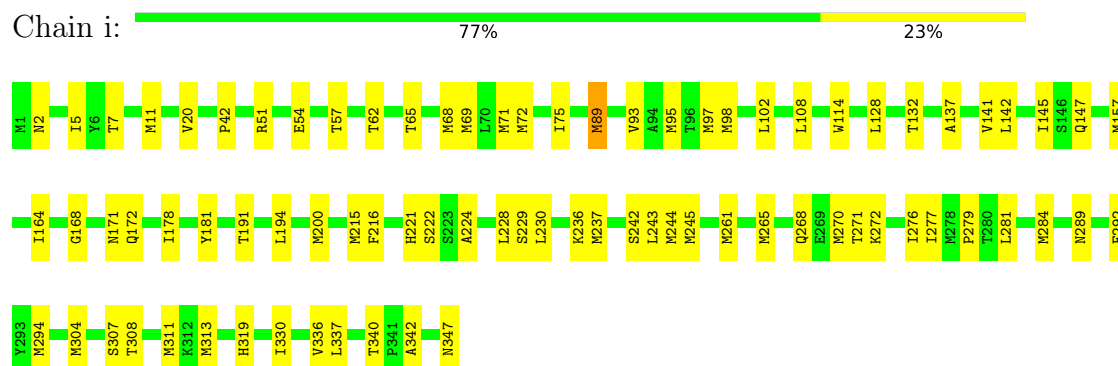
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



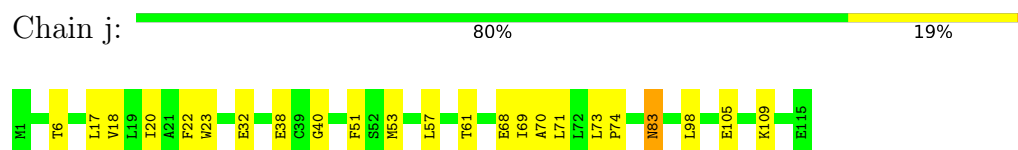
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



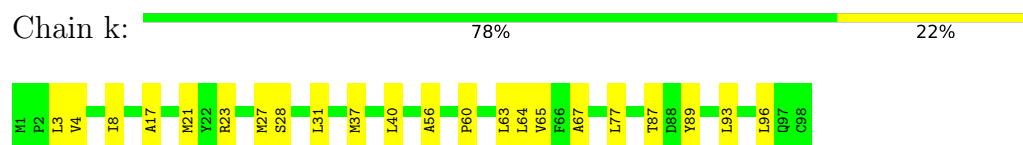
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



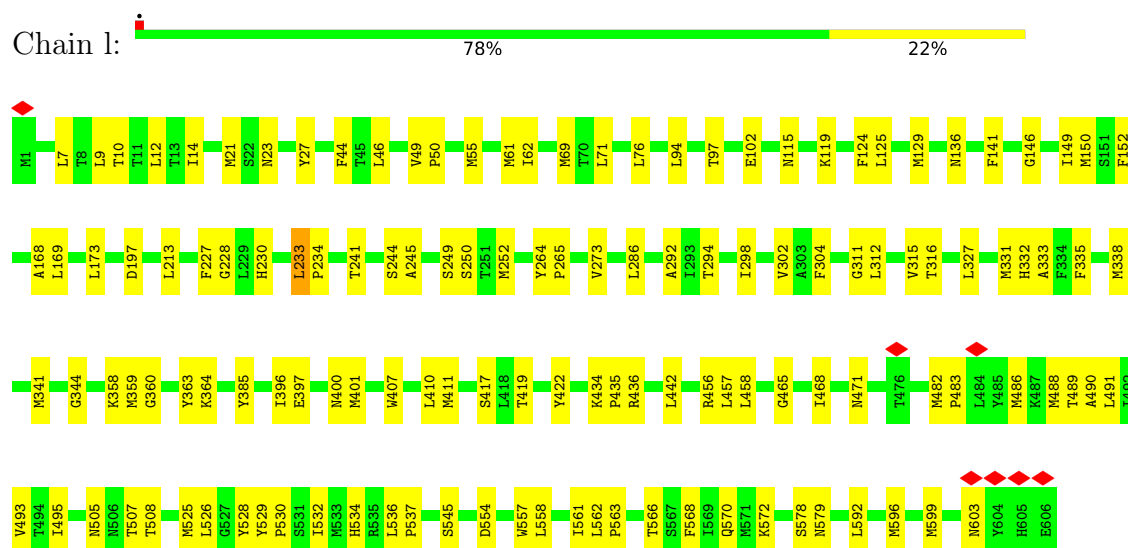
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



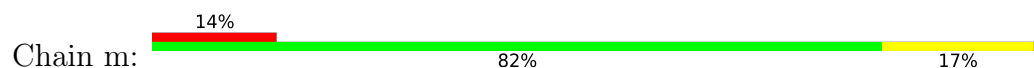
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

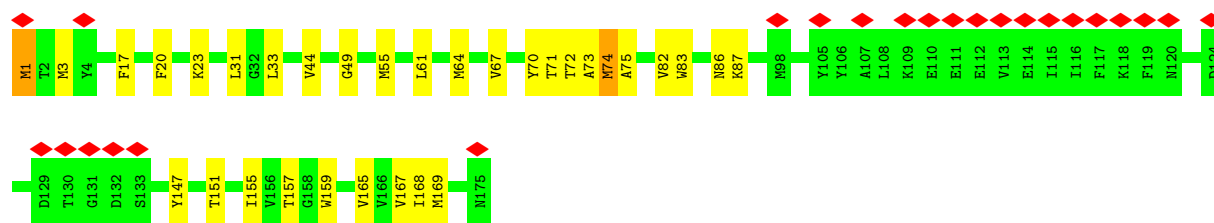


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

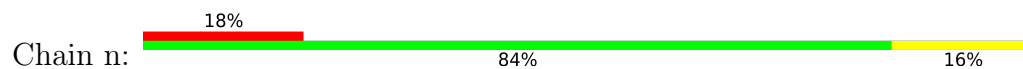


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

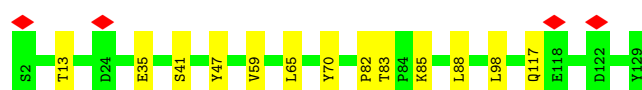




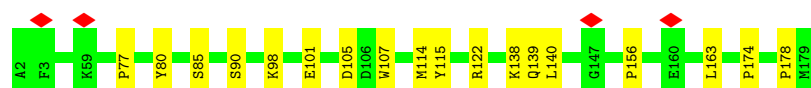
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



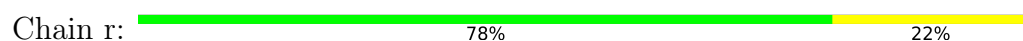
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



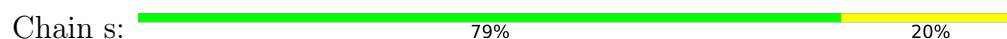
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

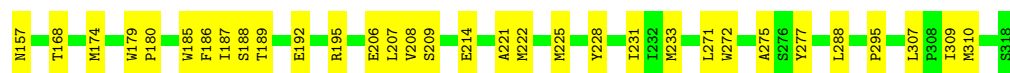


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

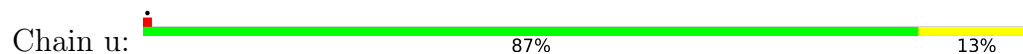


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

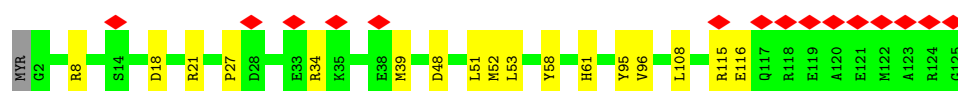
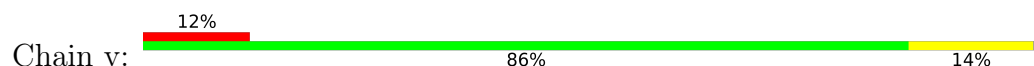




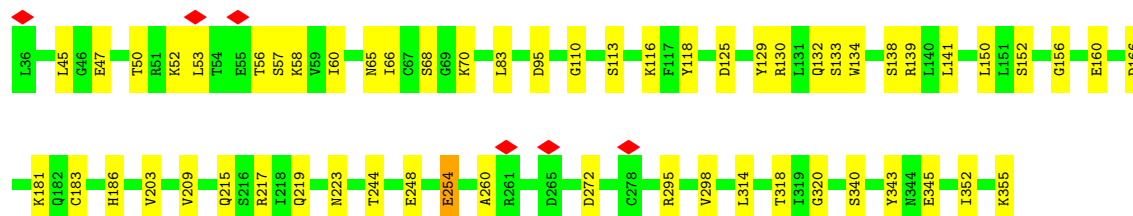
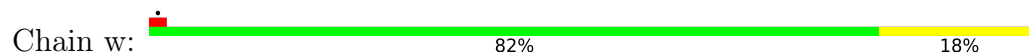
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- 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	184754	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	0.191	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0254	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: UQ, MG, PLX, FES, ZN, SF4, 2MR, DCQ, NAI, PEE, CDL, NDP, FMN, 8Q1, ADP

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	0.12	0/3406	0.31	0/4603
2	B	0.13	0/1443	0.31	0/1952
3	C	0.17	0/1279	0.37	0/1730
4	E	0.12	0/995	0.30	0/1340
5	F	0.14	0/698	0.37	0/940
6	G	0.13	0/702	0.34	0/952
6	X	0.11	0/704	0.29	0/953
7	H	0.13	0/929	0.36	0/1258
8	I	0.14	0/798	0.36	0/1079
9	J	0.13	0/2825	0.32	0/3830
10	K	0.09	0/377	0.25	0/509
11	L	0.16	0/1039	0.42	1/1403 (0.1%)
12	M	0.14	0/5384	0.35	2/7295 (0.0%)
13	N	0.13	0/1245	0.31	0/1694
14	O	0.13	0/1711	0.35	0/2328
15	P	0.14	0/1789	0.40	2/2436 (0.1%)
16	Q	0.14	0/3538	0.32	0/4796
17	S	0.15	0/581	0.40	0/781
18	T	0.10	0/755	0.28	0/1018
19	U	0.11	0/664	0.26	0/912
20	V	0.11	0/1042	0.25	0/1411
21	W	0.13	0/1192	0.29	0/1610
22	Y	0.12	0/610	0.31	0/836
23	Z	0.10	0/660	0.29	0/892
24	a	0.13	0/1184	0.31	0/1603
25	b	0.15	0/844	0.37	0/1149
26	c	0.12	0/1371	0.34	0/1875
27	d	0.12	0/1494	0.30	0/2015
28	e	0.13	0/891	0.33	0/1210
29	f	0.11	0/386	0.28	0/523
30	g	0.12	0/1036	0.29	0/1401
31	h	0.13	0/889	0.32	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.16	0/2773	0.35	0/3768
33	j	0.14	0/938	0.34	0/1281
34	k	0.16	0/759	0.32	0/1029
35	l	0.14	0/4929	0.34	0/6704
36	m	0.15	0/1309	0.35	0/1780
37	n	0.12	0/491	0.30	0/663
38	o	0.13	0/1092	0.32	0/1481
39	p	0.12	0/1590	0.28	0/2155
40	r	0.16	0/3723	0.35	0/5078
41	s	0.17	0/2581	0.38	0/3529
42	u	0.11	0/1436	0.31	0/1938
43	v	0.13	0/1052	0.32	0/1411
44	w	0.12	0/2642	0.31	0/3580
All	All	0.14	0/67776	0.33	5/91921 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	73	LYS	N-CA-C	6.55	118.21	111.14
15	P	44	ARG	CA-C-N	5.85	125.55	119.05
15	P	44	ARG	C-N-CA	5.85	125.55	119.05
12	M	460	HIS	CA-C-N	5.59	125.25	119.05
12	M	460	HIS	C-N-CA	5.59	125.25	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	56	0
2	B	1412	0	1363	23	0
3	C	1248	0	1254	24	0
4	E	971	0	975	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	687	0	700	12	0
6	G	690	0	669	13	0
6	X	693	0	671	9	0
7	H	910	0	950	13	0
8	I	780	0	808	17	0
9	J	2748	0	2771	30	0
10	K	366	0	338	7	0
11	L	1016	0	1016	25	0
12	M	5296	0	5326	64	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	20	0
15	P	1738	0	1693	31	0
16	Q	3459	0	3396	43	0
17	S	566	0	561	8	0
18	T	741	0	701	7	0
19	U	643	0	642	6	0
20	V	1021	0	1025	16	0
21	W	1161	0	1144	20	0
22	Y	584	0	529	6	0
23	Z	641	0	620	8	0
24	a	1151	0	1164	14	0
25	b	819	0	835	12	0
26	c	1315	0	1208	25	0
27	d	1461	0	1429	16	0
28	e	867	0	817	24	0
29	f	378	0	356	5	0
30	g	1005	0	999	12	0
31	h	867	0	871	3	0
32	i	2710	0	2874	62	0
33	j	914	0	951	22	0
34	k	748	0	799	21	0
35	l	4800	0	4939	101	0
36	m	1277	0	1239	31	0
37	n	479	0	486	5	0
38	o	1062	0	1072	12	0
39	p	1534	0	1470	12	0
40	r	3631	0	3839	73	0
41	s	2508	0	2607	52	0
42	u	1398	0	1374	18	0
43	v	1028	0	982	15	0
44	w	2582	0	2531	34	0
45	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	5	0
47	A	44	0	27	7	0
48	B	51	0	82	5	0
48	C	47	0	71	3	0
48	V	40	0	54	2	0
48	W	41	0	59	0	0
48	j	92	0	141	8	0
48	l	97	0	151	6	0
48	r	51	0	82	8	0
49	C	52	0	88	4	0
49	J	52	0	88	8	0
49	a	52	0	88	2	0
49	e	52	0	88	5	0
49	g	52	0	88	3	0
49	j	52	0	88	5	0
49	r	52	0	88	6	0
50	C	23	0	30	2	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	J	48	0	25	2	0
53	J	33	0	39	1	0
53	s	38	0	47	2	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	N	51	0	46	0	0
56	V	294	0	450	25	0
56	a	100	0	156	7	0
56	i	87	0	124	4	0
56	l	191	0	288	19	0
56	n	55	0	54	1	0
56	r	100	0	156	10	0
56	s	89	0	125	5	0
57	T	1	0	0	0	0
58	w	27	0	11	2	0
All	All	68232	0	68974	955	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 (955) 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)
15:P:44:ARG:CB	15:P:45:PRO:HD3	1.58	1.33
15:P:44:ARG:HB3	15:P:45:PRO:CD	1.57	1.31
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.23
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.68	1.11
41:s:24:GLU:OE1	41:s:271:LEU:HD22	1.77	0.85
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.60	0.83
1:A:121:GLU:HG2	47:A:503:NAI:H42N	1.61	0.82
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.62	0.81
41:s:222:MET:HA	41:s:225:MET:HE2	1.63	0.80
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.63	0.79
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.64	0.78
36:m:82:VAL:HG21	56:s:401:CDL:HB31	1.65	0.77
15:P:44:ARG:HB3	15:P:45:PRO:HD3	0.79	0.76
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.68	0.76
8:I:40:LYS:HB3	21:W:7:LYS:H	1.51	0.76
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.75
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.67	0.75
3:C:98:ARG:HD2	41:s:61:LEU:HD21	1.71	0.73
33:j:70:ALA:HA	36:m:55:MET:HE2	1.69	0.73
15:P:44:ARG:CG	15:P:45:PRO:HD3	2.19	0.73
40:r:17:MET:HE3	56:r:503:CDL:H581	1.71	0.73
37:n:47:ARG:NH1	37:n:53:GLU:OE2	2.21	0.73
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.22	0.72
44:w:125:ASP:O	44:w:130:ARG:NH2	2.22	0.72
1:A:149:MET:HE3	1:A:241:THR:HB	1.71	0.72
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.23	0.71
35:l:483:PRO:HD2	35:l:486:MET:HE3	1.72	0.71
35:l:69:MET:HE3	35:l:71:LEU:HD21	1.73	0.70
11:L:109:ASN:ND2	11:L:111:LEU:O	2.25	0.70
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.25	0.70
27:d:31:THR:HG22	27:d:35:LYS:HE2	1.74	0.70
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.73	0.69
12:M:213:MET:HB3	12:M:215:MET:HG2	1.74	0.69
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.73	0.69
40:r:191:SER:HB3	48:r:501:PEE:H2	1.76	0.68
9:J:132:ARG:HH21	52:J:401:NDP:H51A	1.59	0.68
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.76	0.68
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.27	0.67
32:i:270:MET:HE3	32:i:279:PRO:HG3	1.77	0.67
12:M:456:ALA:O	12:M:499:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:r:503:CDL:H401	56:r:503:CDL:H221	1.74	0.67
2:B:47:SER:O	2:B:56:ARG:NH2	2.27	0.67
33:j:57:LEU:HD21	36:m:169:MET:HE3	1.77	0.67
44:w:47:GLU:OE2	44:w:52:LYS:NZ	2.27	0.67
12:M:501:ARG:HH21	12:M:665:PHE:HD2	1.42	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.66
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.77	0.66
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.78	0.66
14:O:182:ASN:HB3	14:O:194:GLU:HB2	1.77	0.66
28:e:119:ARG:O	28:e:123:GLU:HG3	1.96	0.65
9:J:192:ARG:NH1	9:J:198:ALA:O	2.30	0.65
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.28	0.64
3:C:119:LYS:NZ	33:j:32:GLU:OE1	2.28	0.64
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.80	0.64
11:L:75:ARG:HD2	11:L:104:ARG:NH2	2.13	0.64
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.78	0.64
1:A:102:MET:O	1:A:111:LYS:NZ	2.31	0.64
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.28	0.64
24:a:78:THR:HG21	28:e:96:SER:HA	1.78	0.64
26:c:36:MET:HA	26:c:36:MET:HE2	1.80	0.64
40:r:72:LEU:HD11	40:r:233:ALA:HB3	1.80	0.64
26:c:168:LEU:HA	26:c:172:GLY:HA2	1.80	0.64
41:s:221:ALA:O	41:s:225:MET:HG3	1.98	0.63
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.39	0.63
29:f:55:TRP:O	29:f:59:ILE:HG12	1.98	0.63
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.79	0.63
12:M:224:ASP:OD1	12:M:291:ARG:NH1	2.32	0.63
30:g:10:ARG:NH2	32:i:347:ASN:O	2.32	0.63
56:l:701:CDL:H432	56:l:701:CDL:H621	1.80	0.63
56:l:702:CDL:H322	56:l:702:CDL:H121	1.80	0.63
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.81	0.63
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.33	0.62
32:i:171:ASN:ND2	35:l:578:SER:OG	2.25	0.62
23:Z:75:PHE:O	23:Z:79:VAL:HG23	1.99	0.62
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.80	0.62
35:l:227:PHE:O	35:l:230:HIS:ND1	2.33	0.62
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.82	0.62
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.82	0.62
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.82	0.62
1:A:448:GLU:O	1:A:452:GLN:HG2	2.00	0.62
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.33	0.61
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.80	0.61
12:M:460:HIS:ND1	12:M:461:PRO:HD2	2.15	0.61
8:I:6:ARG:HH21	8:I:10:LEU:HD11	1.65	0.61
32:i:265:MET:O	32:i:268:GLN:HG3	1.99	0.61
39:p:105:ASP:OD1	39:p:122:ARG:NH1	2.22	0.61
3:C:73:ALA:HB3	50:C:304:DCQ:H4MB	1.83	0.61
30:g:62:ARG:NH2	44:w:355:LYS:O	2.34	0.61
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.81	0.61
9:J:117:ARG:O	9:J:121:GLU:HG3	2.00	0.61
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.83	0.60
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.83	0.60
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.83	0.60
3:C:52:ASP:HB3	49:C:303:PLX:H251	1.83	0.60
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.49	0.60
3:C:92:VAL:HG11	53:s:402:UQ:H103	1.83	0.60
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.83	0.60
1:A:48:ARG:NH1	10:K:70:ASN:O	2.32	0.60
6:G:79:ILE:HG22	6:G:145:VAL:HG12	1.83	0.60
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.84	0.60
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.83	0.60
1:A:121:GLU:HG2	47:A:503:NAI:C4N	2.31	0.59
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.84	0.59
56:s:401:CDL:HA61	56:s:401:CDL:H132	1.84	0.59
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.83	0.59
9:J:174:ILE:HD11	9:J:189:LYS:HE2	1.84	0.59
11:L:84:ARG:NH1	11:L:88:GLN:O	2.35	0.59
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.50	0.59
12:M:306:MET:HB2	12:M:583:ILE:HB	1.84	0.59
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.35	0.59
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.84	0.59
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.34	0.59
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.32	0.59
32:i:71:MET:HE3	34:k:63:LEU:HD21	1.83	0.59
32:i:93:VAL:HG22	35:l:603:ASN:HD21	1.66	0.59
35:l:491:LEU:O	35:l:495:ILE:HD12	2.02	0.59
48:r:501:PEE:H79	48:r:501:PEE:H37	1.85	0.59
14:O:207:GLU:HG2	14:O:212:LYS:HB2	1.83	0.59
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.59
35:l:410:LEU:HD23	35:l:411:MET:HE2	1.85	0.59
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:201:MET:HG3	48:r:501:PEE:H34	1.84	0.59
41:s:109:SER:OG	41:s:192:GLU:OE2	2.20	0.59
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.83	0.59
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.84	0.59
56:V:204:CDL:H812	34:k:17:ALA:HB2	1.85	0.59
49:e:201:PLX:H202	56:l:701:CDL:H801	1.84	0.59
8:I:9:GLN:O	8:I:13:ASN:ND2	2.36	0.59
40:r:1:MET:HE3	40:r:111:THR:HG21	1.84	0.59
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.21	0.59
56:V:204:CDL:H332	56:V:204:CDL:H222	1.84	0.58
40:r:310:MET:HB3	40:r:455:LEU:HD22	1.86	0.58
16:Q:184:ILE:O	16:Q:188:THR:OG1	2.20	0.58
6:G:94:ASP:OD1	6:G:97:LYS:N	2.36	0.58
20:V:88:LEU:O	20:V:92:ILE:HG13	2.03	0.58
32:i:7:THR:HG23	56:i:401:CDL:H522	1.85	0.58
2:B:62:LEU:HD12	21:W:35:MET:HE3	1.86	0.58
41:s:307:LEU:HA	41:s:310:MET:HE2	1.85	0.58
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.86	0.58
35:l:545:SER:OG	40:r:274:SER:O	2.20	0.58
22:Y:52:ARG:O	22:Y:56:ILE:HG13	2.04	0.58
41:s:62:ARG:HG2	41:s:68:ILE:HD13	1.86	0.57
31:h:18:MET:HE3	34:k:56:ALA:HA	1.85	0.57
35:l:359:MET:O	35:l:436:ARG:NH2	2.36	0.57
1:A:263:ALA:HA	1:A:271:SER:HB3	1.85	0.57
3:C:154:ASP:OD1	3:C:154:ASP:N	2.35	0.57
26:c:46:GLU:OE1	26:c:46:GLU:N	2.36	0.57
35:l:419:THR:HA	35:l:422:TYR:CE2	2.40	0.57
40:r:201:MET:HA	40:r:201:MET:HE2	1.86	0.57
35:l:417:SER:OG	35:l:493:VAL:HG13	2.05	0.56
33:j:22:PHE:HB3	48:j:202:PEE:H2	1.87	0.56
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.87	0.56
41:s:7:LEU:HD23	41:s:10:ILE:HD11	1.87	0.56
30:g:109:LYS:HE2	30:g:113:GLU:HG3	1.88	0.56
28:e:126:VAL:O	28:e:130:GLU:HG2	2.06	0.56
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.86	0.56
56:l:701:CDL:H601	56:l:701:CDL:H772	1.86	0.56
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.87	0.56
4:E:40:TYR:HB3	6:G:120:MET:HE1	1.87	0.56
13:N:65:THR:O	13:N:73:THR:OG1	2.23	0.56
48:j:201:PEE:H26	41:s:295:PRO:HB3	1.87	0.56
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CD1	1:A:64:LYS:HG2	2.40	0.56
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.41	0.56
5:F:90:THR:O	5:F:94:VAL:HG23	2.06	0.56
35:l:294:THR:HG22	56:l:702:CDL:HB61	1.88	0.56
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.41	0.56
12:M:464:GLN:NE2	12:M:468:GLU:OE1	2.39	0.56
41:s:101:GLY:O	41:s:105:MET:HG3	2.07	0.55
44:w:132:GLN:NE2	44:w:166:ASP:OD2	2.38	0.55
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.88	0.55
4:E:25:MET:O	4:E:29:LYS:HG3	2.07	0.55
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.36	0.55
15:P:43:THR:HA	15:P:47:ILE:HD12	1.87	0.55
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.87	0.55
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.46	0.55
56:V:202:CDL:H561	56:V:202:CDL:H731	1.88	0.55
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.89	0.55
9:J:73:LEU:HA	9:J:76:MET:HE2	1.89	0.55
32:i:11:MET:HG2	56:i:401:CDL:H581	1.87	0.55
41:s:146:LEU:HD12	41:s:188:SER:HB3	1.88	0.55
24:a:166:GLY:O	24:a:170:GLN:NE2	2.36	0.55
49:g:201:PLX:H332	32:i:342:ALA:HB3	1.87	0.55
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.41	0.55
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.25	0.55
17:S:34:LYS:NZ	17:S:61:HIS:O	2.33	0.55
12:M:485:ASP:HB3	12:M:680:LEU:HD13	1.90	0.54
28:e:55:LEU:HD12	44:w:318:THR:HG22	1.89	0.54
29:f:43:LYS:O	29:f:47:THR:HG23	2.07	0.54
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.22	0.54
6:G:82:ARG:NE	6:G:125:GLU:OE2	2.41	0.54
56:l:701:CDL:H242	48:l:704:PEE:H34	1.88	0.54
36:m:61:LEU:O	41:s:114:TYR:OH	2.24	0.54
11:L:99:MET:HE2	11:L:138:ALA:HB2	1.88	0.54
49:e:201:PLX:H162	56:l:701:CDL:H822	1.89	0.54
40:r:339:SER:HB3	40:r:344:LEU:HD22	1.89	0.54
56:r:503:CDL:H271	56:r:503:CDL:H721	1.89	0.54
49:J:403:PLX:H201	33:j:20:ILE:HD11	1.89	0.54
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.88	0.54
1:A:45:LEU:HD21	1:A:287:THR:HG22	1.87	0.54
26:c:70:MET:HE2	38:o:85:LYS:HE3	1.89	0.54
5:F:46:LYS:HG3	12:M:674:LEU:HD21	1.89	0.54
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:143:ASP:HB3	28:e:146:LYS:HG3	1.89	0.54
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.90	0.54
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.39	0.54
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.90	0.54
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.90	0.54
18:T:49:ASP:OD2	18:T:51:ARG:NH2	2.40	0.54
20:V:120:LEU:HD21	49:r:502:PLX:H341	1.90	0.54
30:g:3:MET:HG2	30:g:4:MET:HG3	1.90	0.53
21:W:88:ARG:HH21	42:u:9:THR:HG22	1.72	0.53
32:i:200:MET:SD	32:i:265:MET:HB3	2.49	0.53
42:u:83:THR:HA	42:u:86:TRP:CD1	2.43	0.53
9:J:75:ARG:NH2	15:P:215:GLU:OE2	2.41	0.53
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.44	0.53
35:l:298:ILE:O	35:l:302:VAL:HG23	2.09	0.53
40:r:325:MET:HE2	40:r:362:ALA:HB2	1.91	0.53
31:h:71:LYS:HA	31:h:74:LYS:HG2	1.90	0.53
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.89	0.53
35:l:228:GLY:HA3	48:l:703:PEE:H38	1.91	0.53
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.44	0.53
1:A:89:GLY:O	47:A:503:NAI:H2N	2.09	0.53
7:H:76:GLN:O	7:H:78:GLU:N	2.41	0.53
21:W:98:MET:HE3	21:W:101:VAL:HG21	1.91	0.53
6:X:82:ARG:O	6:X:86:VAL:HG23	2.09	0.53
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.91	0.53
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.89	0.53
12:M:566:ILE:HD13	12:M:579:MET:HE3	1.91	0.53
26:c:136:PHE:O	26:c:140:MET:HG2	2.09	0.53
5:F:19:ILE:HD12	5:F:51:LEU:HD21	1.91	0.53
2:B:68:ARG:NH2	16:Q:260:GLU:OE2	2.40	0.52
56:V:202:CDL:H871	35:l:558:LEU:HD21	1.90	0.52
56:a:201:CDL:H321	48:l:704:PEE:H58	1.91	0.52
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.90	0.52
6:X:87:LEU:HB3	6:X:98:LEU:HD21	1.92	0.52
49:j:203:PLX:H352	36:m:155:ILE:HG23	1.90	0.52
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.91	0.52
31:h:94:PRO:HG2	31:h:99:LEU:HD11	1.92	0.52
27:d:160:LYS:NZ	30:g:114:ILE:O	2.41	0.52
40:r:114:GLU:OE2	40:r:116:ILE:HB	2.09	0.52
40:r:403:THR:HA	40:r:406:TYR:CE2	2.44	0.52
1:A:261:TRP:O	1:A:264:SER:OG	2.28	0.52
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:55:VAL:HG21	56:r:503:CDL:HB61	1.91	0.52
42:u:80:GLU:CD	42:u:80:GLU:H	2.18	0.52
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.91	0.52
2:B:111:GLU:O	2:B:141:ARG:NH1	2.43	0.52
27:d:163:MET:HE1	28:e:147:ILE:HD12	1.92	0.52
1:A:50:ASP:OD1	1:A:52:ARG:NH1	2.42	0.52
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.45	0.52
30:g:19:GLU:HG2	42:u:158:LEU:HD22	1.91	0.52
40:r:243:MET:HB3	40:r:301:ILE:HG21	1.92	0.52
8:I:109:ASP:OD2	21:W:21:TYR:OH	2.28	0.52
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.90	0.52
43:v:21:ARG:O	43:v:21:ARG:HG2	2.09	0.52
56:V:204:CDL:H592	56:V:204:CDL:H782	1.92	0.52
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.90	0.52
12:M:372:PHE:H	12:M:532:PRO:HB2	1.74	0.52
56:l:701:CDL:H791	56:l:701:CDL:H582	1.92	0.52
7:H:58:MET:HE3	7:H:72:LEU:HD23	1.92	0.51
12:M:250:SER:OG	12:M:251:ILE:N	2.42	0.51
48:r:501:PEE:H29	48:r:501:PEE:H71	1.92	0.51
27:d:81:ASP:O	27:d:85:MET:HG3	2.11	0.51
56:l:702:CDL:H201	56:l:702:CDL:H861	1.91	0.51
32:i:72:MET:HB2	34:k:40:LEU:HD21	1.91	0.51
32:i:265:MET:HE3	32:i:340:THR:HG21	1.91	0.51
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.92	0.51
42:u:79:ALA:O	42:u:83:THR:OG1	2.27	0.51
37:n:17:VAL:HG13	40:r:7:PRO:HB3	1.92	0.51
13:N:78:ASP:OD2	13:N:80:SER:OG	2.27	0.51
33:j:53:MET:HE1	36:m:70:TYR:CD1	2.46	0.51
40:r:122:PHE:CZ	40:r:206:LYS:HD2	2.46	0.51
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.92	0.51
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.46	0.51
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.92	0.51
12:M:299:ARG:NH1	12:M:703:ALA:O	2.42	0.51
34:k:27:MET:HE1	36:m:70:TYR:HB3	1.92	0.51
40:r:282:LEU:HD13	40:r:342:MET:HG3	1.91	0.51
4:E:120:SER:O	4:E:124:VAL:HG22	2.11	0.51
20:V:25:SER:OG	20:V:67:GLY:O	2.22	0.51
56:V:204:CDL:H222	56:V:204:CDL:H351	1.92	0.51
1:A:88:ARG:NH2	1:A:273:THR:O	2.44	0.51
6:G:138:LEU:HD13	6:G:144:ILE:HA	1.91	0.51
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.41	0.51
56:V:202:CDL:H361	38:o:88:LEU:HD21	1.93	0.51
27:d:168:LYS:O	27:d:172:GLU:HG2	2.11	0.51
32:i:128:LEU:O	32:i:132:THR:OG1	2.25	0.51
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.93	0.51
21:W:54:ASN:HD22	41:s:156:MET:HE3	1.76	0.50
26:c:96:ASP:N	26:c:96:ASP:OD1	2.43	0.50
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.93	0.50
40:r:266:MET:O	40:r:269:MET:HG2	2.10	0.50
4:E:119:LEU:HD22	4:E:123:TYR:CZ	2.46	0.50
11:L:102:ASP:OD1	11:L:102:ASP:N	2.44	0.50
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.76	0.50
26:c:149:ILE:HG22	26:c:150:TYR:CD1	2.46	0.50
33:j:68:GLU:HG3	33:j:98:LEU:HD13	1.93	0.50
35:l:250:SER:HB2	35:l:333:ALA:HA	1.92	0.50
1:A:122:PRO:HA	14:O:176:CYS:SG	2.50	0.50
5:F:23:LEU:O	5:F:57:GLU:HA	2.11	0.50
56:V:202:CDL:H861	38:o:98:LEU:HD11	1.94	0.50
9:J:87:GLU:HG3	9:J:89:TYR:H	1.77	0.50
20:V:67:GLY:HA2	56:V:201:CDL:H221	1.93	0.50
48:V:203:PEE:H7	35:l:568:PHE:HE2	1.76	0.50
56:l:701:CDL:H311	56:l:701:CDL:H561	1.93	0.50
40:r:118:PHE:O	40:r:122:PHE:HB3	2.12	0.50
40:r:266:MET:HB3	40:r:395:LEU:HD13	1.93	0.50
9:J:135:GLU:HG2	9:J:140:ASP:HA	1.93	0.50
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.41	0.50
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.94	0.50
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.92	0.50
34:k:87:THR:HG22	34:k:89:TYR:H	1.75	0.50
49:j:203:PLX:H251	36:m:151:THR:HG21	1.93	0.50
26:c:60:GLU:OE1	26:c:60:GLU:N	2.44	0.50
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.94	0.50
32:i:284:MET:HE1	40:r:155:ALA:HA	1.93	0.50
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.93	0.50
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.94	0.50
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.93	0.50
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.76	0.50
14:O:213:ILE:HD12	14:O:214:PRO:HD2	1.94	0.50
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.94	0.50
35:l:245:ALA:O	35:l:249:SER:OG	2.24	0.50
39:p:139:GLN:NE2	39:p:156:PRO:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:203:PHE:O	40:r:207:MET:HG2	2.11	0.50
56:V:202:CDL:HB4	38:o:82:PRO:HB2	1.94	0.49
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.92	0.49
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.76	0.49
38:o:83:THR:HG22	38:o:85:LYS:H	1.77	0.49
1:A:210:THR:HB	1:A:224:ARG:H	1.77	0.49
12:M:44:GLU:HG3	12:M:45:PRO:HD2	1.93	0.49
18:T:34:THR:HG21	18:T:52:ARG:NH1	2.27	0.49
20:V:106:ARG:HE	20:V:106:ARG:HA	1.77	0.49
25:b:81:ILE:HD13	48:l:704:PEE:H64	1.94	0.49
49:j:203:PLX:H341	49:j:203:PLX:H151	1.94	0.49
1:A:210:THR:HB	1:A:224:ARG:HG3	1.94	0.49
13:N:85:GLU:HG2	13:N:86:TRP:H	1.77	0.49
35:l:396:ILE:HG21	35:l:490:ALA:HB2	1.95	0.49
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.94	0.49
12:M:340:ALA:HB3	12:M:366:LEU:HD13	1.94	0.49
16:Q:210:MET:HE2	16:Q:247:PHE:HZ	1.77	0.49
44:w:58:LYS:O	44:w:60:ILE:HG13	2.12	0.49
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.94	0.49
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.94	0.49
6:G:93:ILE:HG21	6:G:98:LEU:HD13	1.94	0.49
6:G:93:ILE:HD11	6:G:110:LEU:HD11	1.94	0.49
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.94	0.49
28:e:92:PHE:O	28:e:96:SER:HB2	2.13	0.49
30:g:48:ASN:HB3	30:g:55:VAL:HA	1.94	0.49
40:r:105:PHE:O	40:r:109:THR:OG1	2.24	0.49
49:r:502:PLX:H6	49:r:502:PLX:H261	1.95	0.49
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.94	0.49
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.47	0.49
38:o:65:LEU:HD11	40:r:343:ILE:HD11	1.94	0.49
40:r:370:PRO:HG3	40:r:375:LEU:HD13	1.94	0.49
4:E:23:ARG:HB2	4:E:27:GLU:OE2	2.13	0.49
11:L:112:MET:SD	13:N:126:PRO:HB2	2.52	0.49
21:W:69:ILE:HA	21:W:72:MET:HE3	1.95	0.49
22:Y:76:ASP:O	35:l:385:TYR:OH	2.23	0.49
35:l:561:ILE:HG13	35:l:562:LEU:H	1.77	0.49
1:A:128:ARG:O	1:A:132:ARG:HG2	2.12	0.48
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.95	0.48
44:w:50:THR:HA	44:w:53:LEU:HD23	1.93	0.48
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.48	0.48
16:Q:80:LEU:HD11	41:s:126:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:54:ARG:O	18:T:58:ARG:NH2	2.45	0.48
20:V:38:ALA:HB2	56:V:204:CDL:H251	1.95	0.48
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.94	0.48
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.49	0.48
9:J:179:ARG:HG2	9:J:179:ARG:HH11	1.78	0.48
12:M:390:THR:HA	12:M:600:GLU:HG2	1.95	0.48
13:N:144:TYR:CZ	13:N:145:LYS:HD2	2.48	0.48
23:Z:18:ASP:O	23:Z:21:GLN:NE2	2.30	0.48
48:j:202:PEE:H31	56:s:401:CDL:H222	1.94	0.48
24:a:134:GLU:HG2	37:n:38:PHE:O	2.13	0.48
26:c:58:ARG:NH1	26:c:61:ASP:OD1	2.46	0.48
26:c:166:LEU:HB3	26:c:169:GLU:HB2	1.96	0.48
32:i:11:MET:HE1	56:i:401:CDL:H771	1.95	0.48
32:i:277:ILE:O	32:i:281:LEU:HG	2.14	0.48
2:B:120:GLU:OE2	15:P:231:ARG:NH1	2.47	0.48
11:L:107:TRP:HH2	11:L:118:ALA:HB2	1.79	0.48
12:M:591:GLU:HG2	12:M:610:VAL:HG23	1.93	0.48
19:U:66:VAL:O	42:u:130:LYS:HE3	2.13	0.48
35:l:27:TYR:O	35:l:115:ASN:ND2	2.42	0.48
48:C:302:PEE:H70	48:C:302:PEE:H36	1.96	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.78	0.48
56:l:701:CDL:H331	56:l:701:CDL:H142	1.95	0.48
12:M:295:ASP:OD1	12:M:704:SER:OG	2.29	0.48
23:Z:59:ASN:O	35:l:364:LYS:NZ	2.47	0.48
23:Z:78:PHE:O	23:Z:82:VAL:HG23	2.13	0.48
29:f:70:LYS:HE3	29:f:76:GLU:HB2	1.95	0.48
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.96	0.48
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.95	0.48
9:J:354:ARG:NH1	9:J:362:LEU:O	2.46	0.48
41:s:157:ASN:OD1	41:s:168:THR:OG1	2.28	0.48
48:C:302:PEE:H35	49:C:303:PLX:H392	1.96	0.48
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.47	0.48
9:J:38:HIS:CE1	13:N:132:LYS:HE3	2.49	0.48
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.48
43:v:8:ARG:NH2	43:v:18:ASP:OD1	2.46	0.48
14:O:134:VAL:HG22	14:O:186:VAL:HG22	1.94	0.48
35:l:505:ASN:O	35:l:508:THR:HG22	2.14	0.48
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.39	0.47
9:J:199:THR:OG1	9:J:258:ALA:O	2.29	0.47
14:O:177:LEU:HD13	14:O:187:GLN:HB2	1.96	0.47
32:i:244:MET:HE3	32:i:244:MET:HB2	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:MET:HE2	3:C:128:ARG:HB2	1.97	0.47
7:H:96:ARG:HG2	7:H:96:ARG:HH11	1.78	0.47
16:Q:84:PHE:HB2	16:Q:99:MET:HE2	1.97	0.47
21:W:91:LEU:HD22	42:u:7:LEU:HD12	1.96	0.47
36:m:3:MET:HE2	36:m:3:MET:HA	1.96	0.47
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.49	0.47
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.97	0.47
49:r:502:PLX:H101	49:r:502:PLX:H72	1.57	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.95	0.47
12:M:651:PRO:O	12:M:654:VAL:HG22	2.14	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.97	0.47
25:b:73:THR:HA	25:b:77:ILE:HD12	1.96	0.47
3:C:49:LYS:HA	3:C:49:LYS:HD3	1.70	0.47
9:J:168:SER:O	9:J:203:PRO:HD2	2.14	0.47
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.96	0.47
35:l:401:MET:HE3	35:l:401:MET:HB3	1.74	0.47
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.97	0.47
49:J:403:PLX:H32	33:j:23:TRP:HZ3	1.79	0.47
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.50	0.47
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.97	0.47
21:W:95:ALA:HA	21:W:106:VAL:HG21	1.96	0.47
56:a:201:CDL:H171	56:a:201:CDL:H712	1.96	0.47
26:c:85:GLU:OE2	38:o:13:THR:OG1	2.28	0.47
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.50	0.47
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.95	0.47
49:j:203:PLX:H132	49:j:203:PLX:H161	1.44	0.47
35:l:136:ASN:HA	35:l:197:ASP:HA	1.96	0.47
39:p:101:GLU:OE1	39:p:122:ARG:NH2	2.41	0.47
40:r:357:THR:O	40:r:361:VAL:HG23	2.14	0.47
43:v:39:MET:SD	43:v:58:TYR:HA	2.55	0.47
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.95	0.47
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.97	0.47
48:V:203:PEE:H7	35:l:568:PHE:CE2	2.50	0.47
28:e:137:MET:HE3	28:e:137:MET:HB2	1.82	0.47
35:l:327:LEU:O	35:l:331:MET:HG2	2.15	0.47
49:J:403:PLX:H251	49:J:403:PLX:H282	1.58	0.47
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.97	0.47
20:V:49:PHE:O	20:V:53:VAL:HG23	2.15	0.47
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.97	0.47
35:l:10:THR:O	35:l:14:ILE:HG23	2.14	0.47
40:r:72:LEU:HD12	40:r:234:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD2	1:A:245:VAL:HB	2.15	0.47
12:M:638:THR:O	12:M:642:VAL:HG23	2.14	0.47
20:V:66:ILE:HD11	20:V:101:LEU:HB2	1.95	0.47
21:W:48:TRP:CZ2	21:W:52:LYS:HE2	2.50	0.47
49:e:201:PLX:H222	35:l:23:ASN:HB2	1.97	0.47
40:r:104:LEU:O	40:r:108:MET:HG3	2.15	0.47
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.95	0.46
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.96	0.46
24:a:95:GLU:OE1	56:a:201:CDL:O1	2.22	0.46
35:l:119:LYS:NZ	56:l:701:CDL:OA3	2.48	0.46
9:J:369:VAL:HG12	9:J:369:VAL:O	2.16	0.46
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.50	0.46
34:k:37:MET:HE1	34:k:63:LEU:HD22	1.96	0.46
35:l:312:LEU:O	35:l:315:VAL:HG22	2.14	0.46
1:A:110:PRO:O	1:A:238:CYS:HB3	2.16	0.46
1:A:248:VAL:O	1:A:251:SER:OG	2.27	0.46
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.50	0.46
12:M:309:ASN:OD1	12:M:311:LYS:N	2.42	0.46
12:M:460:HIS:CG	12:M:461:PRO:HD2	2.50	0.46
24:a:60:SER:HB2	39:p:107:TRP:HA	1.97	0.46
26:c:129:MET:HB3	35:l:528:TYR:CG	2.50	0.46
35:l:557:TRP:O	35:l:561:ILE:HG12	2.16	0.46
40:r:94:LEU:HD21	56:r:503:CDL:H312	1.97	0.46
44:w:95:ASP:OD1	44:w:95:ASP:N	2.47	0.46
1:A:66:LYS:O	1:A:70:LEU:HG	2.15	0.46
2:B:116:CYS:SG	2:B:118:LEU:HG	2.55	0.46
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.98	0.46
20:V:38:ALA:HA	56:V:204:CDL:H201	1.97	0.46
27:d:127:LYS:HA	27:d:127:LYS:HD3	1.76	0.46
32:i:65:THR:O	32:i:69:MET:HG3	2.16	0.46
32:i:311:MET:HE2	32:i:311:MET:HB2	1.78	0.46
35:l:562:LEU:HD21	48:r:501:PEE:H45	1.98	0.46
39:p:138:LYS:HD3	39:p:138:LYS:HA	1.65	0.46
12:M:485:ASP:HA	12:M:677:GLN:OE1	2.16	0.46
12:M:489:ILE:O	12:M:493:VAL:HG23	2.15	0.46
15:P:44:ARG:CB	15:P:45:PRO:CD	2.36	0.46
1:A:118:ASP:O	1:A:159:ARG:HD2	2.16	0.46
21:W:54:ASN:ND2	41:s:156:MET:HE3	2.30	0.46
26:c:129:MET:HB2	35:l:532:ILE:HD11	1.98	0.46
28:e:55:LEU:HD11	44:w:320:GLY:HA2	1.98	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:10:MET:HE1	56:r:503:CDL:H632	1.97	0.46
5:F:61:VAL:HG23	5:F:62:GLN:H	1.81	0.46
7:H:25:LYS:HE2	7:H:60:LYS:HG2	1.97	0.46
12:M:547:LEU:HD11	12:M:579:MET:HE2	1.98	0.46
23:Z:35:LYS:HB3	23:Z:35:LYS:HE2	1.72	0.46
27:d:32:TYR:CE2	27:d:36:ILE:HD11	2.50	0.46
34:k:17:ALA:O	34:k:21:MET:HG3	2.15	0.46
56:l:701:CDL:H202	56:l:701:CDL:H231	1.81	0.46
40:r:342:MET:HE3	40:r:413:THR:HG21	1.98	0.46
41:s:207:LEU:O	41:s:209:SER:N	2.48	0.46
44:w:244:THR:O	44:w:248:GLU:HB2	2.15	0.46
22:Y:44:TYR:O	22:Y:45:ARG:HB2	2.16	0.46
32:i:98:MET:HE2	32:i:98:MET:HB2	1.86	0.46
32:i:268:GLN:O	32:i:271:THR:OG1	2.33	0.46
32:i:313:MET:HE3	44:w:141:LEU:HD22	1.97	0.46
42:u:77:HIS:CE1	42:u:115:LEU:HD21	2.50	0.46
1:A:334:THR:O	1:A:334:THR:OG1	2.30	0.46
7:H:22:GLU:OE1	7:H:22:GLU:N	2.33	0.46
12:M:339:ALA:HB1	12:M:537:ILE:HD12	1.98	0.46
28:e:55:LEU:CD2	28:e:57:GLU:HB2	2.46	0.46
28:e:72:ASP:OD1	28:e:72:ASP:N	2.48	0.46
28:e:99:LEU:HD12	28:e:99:LEU:HA	1.84	0.46
32:i:54:GLU:HG3	34:k:93:LEU:HB3	1.97	0.46
35:l:558:LEU:HD23	35:l:561:ILE:HD11	1.97	0.46
36:m:31:LEU:HD21	56:s:401:CDL:H542	1.96	0.46
41:s:20:LEU:HD12	41:s:20:LEU:O	2.15	0.46
2:B:89:GLU:OE1	13:N:58:ARG:HD2	2.16	0.46
9:J:370:LYS:HD2	9:J:370:LYS:O	2.16	0.46
12:M:421:SER:OG	12:M:427:LEU:HD22	2.16	0.46
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.97	0.46
56:a:201:CDL:H572	48:l:704:PEE:H20	1.97	0.46
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.16	0.46
33:j:109:LYS:HA	33:j:109:LYS:HD3	1.66	0.46
35:l:592:LEU:O	35:l:596:MET:HG3	2.16	0.46
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.98	0.46
44:w:68:SER:HA	44:w:217:ARG:HH21	1.81	0.46
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.59	0.45
26:c:84:GLN:HG2	26:c:114:ARG:HB2	1.96	0.45
41:s:20:LEU:HG	41:s:228:TYR:CD2	2.51	0.45
7:H:30:LYS:NZ	44:w:272:ASP:OD1	2.41	0.45
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:40:SER:HA	56:V:201:CDL:HB62	1.96	0.45
56:a:201:CDL:H361	56:a:201:CDL:H392	1.59	0.45
34:k:4:VAL:O	34:k:8:ILE:HG12	2.16	0.45
3:C:188:LYS:HB2	3:C:188:LYS:HE3	1.59	0.45
12:M:405:THR:HB	12:M:477:GLY:HA3	1.98	0.45
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.98	0.45
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.17	0.45
40:r:406:TYR:O	40:r:409:TYR:HB3	2.16	0.45
42:u:19:LYS:HE3	42:u:19:LYS:HB3	1.83	0.45
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.51	0.45
35:l:363:TYR:HD1	35:l:364:LYS:HG2	1.82	0.45
41:s:186:PHE:O	41:s:189:THR:OG1	2.27	0.45
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.51	0.45
8:I:30:GLU:CD	8:I:30:GLU:H	2.25	0.45
13:N:85:GLU:HG2	13:N:86:TRP:N	2.32	0.45
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.98	0.45
1:A:283:ASN:ND2	1:A:305:GLY:O	2.49	0.45
49:J:403:PLX:H92	49:J:403:PLX:H122	1.66	0.45
17:S:63:THR:HG23	42:u:21:SER:HB2	1.98	0.45
56:V:202:CDL:H782	35:l:557:TRP:CD2	2.51	0.45
26:c:46:GLU:H	26:c:46:GLU:CD	2.23	0.45
35:l:338:MET:HA	35:l:341:MET:HE2	1.99	0.45
56:l:701:CDL:H391	40:r:371:PRO:HD2	1.99	0.45
43:v:27:PRO:O	43:v:34:ARG:NH1	2.50	0.45
3:C:101:ASP:OD2	41:s:54:LYS:NZ	2.33	0.45
53:J:402:UQ:HM53	53:J:402:UQ:H71	1.79	0.45
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.52	0.45
12:M:389:THR:O	12:M:390:THR:OG1	2.28	0.45
56:V:204:CDL:H362	56:V:204:CDL:H392	1.66	0.45
49:a:202:PLX:H141	28:e:105:PHE:HB2	1.99	0.45
27:d:101:GLU:OE1	28:e:119:ARG:NE	2.44	0.45
48:j:201:PEE:H59	48:j:201:PEE:H64	1.70	0.45
35:l:311:GLY:O	35:l:315:VAL:HG13	2.17	0.45
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.51	0.45
9:J:184:LYS:O	9:J:188:GLU:HG2	2.16	0.45
32:i:51:ARG:HG2	34:k:96:LEU:HD21	1.98	0.45
5:F:68:ARG:NH2	12:M:364:ASP:OD2	2.50	0.45
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.52	0.45
9:J:370:LYS:HB3	9:J:370:LYS:HE3	1.74	0.45
38:o:117:GLN:OE1	38:o:117:GLN:HA	2.16	0.45
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:103:ASP:OD1	21:W:103:ASP:N	2.50	0.45
33:j:61:THR:OG1	33:j:105:GLU:OE2	2.27	0.45
33:j:73:LEU:HD12	36:m:55:MET:HE1	1.98	0.45
37:n:34:LYS:HE2	37:n:34:LYS:HB2	1.68	0.45
41:s:149:ILE:HG21	41:s:185:TRP:HB2	1.99	0.45
44:w:181:LYS:HE3	44:w:181:LYS:HB3	1.64	0.45
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.99	0.45
1:A:217:GLU:OE2	1:A:236:PHE:N	2.43	0.44
7:H:94:MET:HE1	15:P:69:LEU:HD21	1.99	0.44
9:J:36:LEU:HD23	9:J:41:ILE:HG12	1.99	0.44
10:K:89:LEU:O	10:K:93:LEU:HG	2.18	0.44
11:L:76:LYS:HE3	11:L:146:ASP:OD1	2.16	0.44
12:M:151:SER:HB3	16:Q:374:SER:HB3	1.98	0.44
6:X:105:MET:H	6:X:105:MET:HG2	1.61	0.44
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.81	0.44
26:c:162:PRO:HB3	43:v:39:MET:HG3	1.98	0.44
32:i:245:MET:HE3	32:i:245:MET:HB3	1.92	0.44
32:i:261:MET:HB2	32:i:337:LEU:HD12	1.98	0.44
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.80	0.44
35:l:146:GLY:O	35:l:150:MET:HG2	2.17	0.44
56:l:702:CDL:H542	56:l:702:CDL:H511	1.57	0.44
1:A:367:ILE:O	1:A:371:ILE:HG12	2.17	0.44
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.66	0.44
49:C:303:PLX:H1C3	49:C:303:PLX:H21	1.77	0.44
4:E:16:SER:HA	11:L:52:LEU:HD13	2.00	0.44
12:M:47:THR:O	12:M:96:VAL:HG12	2.17	0.44
32:i:89:MET:HE3	32:i:98:MET:HE3	1.99	0.44
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.52	0.44
35:l:400:ASN:HB3	35:l:486:MET:SD	2.57	0.44
35:l:530:PRO:O	35:l:534:HIS:HB2	2.17	0.44
8:I:64:MET:HE2	15:P:80:CYS:SG	2.57	0.44
19:U:59:ASP:OD2	42:u:130:LYS:HD3	2.17	0.44
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.00	0.44
35:l:572:LYS:HA	35:l:572:LYS:HD3	1.82	0.44
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.52	0.44
49:J:403:PLX:H371	49:J:403:PLX:H322	1.99	0.44
12:M:219:SER:O	12:M:222:ILE:HG12	2.17	0.44
56:V:202:CDL:H401	56:V:202:CDL:H371	1.57	0.44
35:l:12:LEU:HD22	35:l:129:MET:HB3	1.99	0.44
56:l:701:CDL:H342	56:l:701:CDL:H372	1.82	0.44
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B:303:PEE:H14	48:B:303:PEE:H20	1.57	0.44
4:E:23:ARG:HD2	11:L:53:ILE:HG22	1.99	0.44
13:N:123:GLN:O	18:T:59:GLN:NE2	2.48	0.44
56:V:204:CDL:H811	56:V:204:CDL:H632	2.00	0.44
26:c:58:ARG:NE	38:o:35:GLU:OE1	2.46	0.44
34:k:64:LEU:O	34:k:67:ALA:HB3	2.17	0.44
49:r:502:PLX:H92	49:r:502:PLX:H121	1.63	0.44
41:s:7:LEU:HA	41:s:10:ILE:HG12	1.99	0.44
3:C:173:LEU:O	3:C:177:ILE:HG12	2.18	0.44
12:M:81:GLU:OE1	12:M:106:SER:OG	2.32	0.44
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.35	0.44
33:j:83:ASN:OD1	33:j:83:ASN:N	2.37	0.44
35:l:554:ASP:OD2	40:r:288:TYR:OH	2.21	0.44
9:J:257:ASP:OD1	9:J:257:ASP:C	2.60	0.44
16:Q:206:GLU:O	16:Q:210:MET:HG3	2.17	0.44
19:U:27:GLY:O	19:U:31:ILE:HG23	2.18	0.44
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.83	0.44
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.53	0.44
35:l:526:LEU:HD12	35:l:530:PRO:HG2	2.00	0.44
40:r:373:ILE:HD11	40:r:444:LEU:HD23	2.00	0.44
44:w:345:GLU:HB3	44:w:352:ILE:HD12	2.00	0.44
3:C:116:ALA:O	3:C:120:VAL:HG22	2.17	0.44
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.34	0.44
17:S:66:LEU:O	17:S:69:ILE:HG12	2.17	0.44
56:a:201:CDL:OA4	25:b:89:HIS:NE2	2.36	0.44
32:i:172:GLN:HB2	32:i:178:ILE:HG13	1.98	0.44
48:j:202:PEE:P	41:s:62:ARG:HH12	2.40	0.44
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.52	0.44
40:r:189:SER:HA	49:r:502:PLX:H1B3	2.00	0.44
53:s:402:UQ:H221	53:s:402:UQ:H262	1.67	0.44
9:J:171:ASN:HA	9:J:327:MET:HE3	2.00	0.44
12:M:367:CYS:HB3	12:M:533:GLY:O	2.18	0.44
14:O:158:ILE:HB	14:O:162:GLU:HB2	2.00	0.44
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.32	0.44
20:V:63:SER:HB3	56:V:201:CDL:H172	2.00	0.44
56:a:201:CDL:H342	56:a:201:CDL:H372	1.92	0.44
32:i:243:LEU:HD22	32:i:330:ILE:HG21	2.00	0.44
35:l:97:THR:HG21	35:l:125:LEU:HD22	2.00	0.44
8:I:70:MET:O	8:I:70:MET:SD	2.76	0.43
40:r:57:PHE:CD1	40:r:113:THR:HG22	2.53	0.43
49:r:502:PLX:H6	49:r:502:PLX:H51	1.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:45:LEU:O	44:w:45:LEU:HD12	2.17	0.43
44:w:215:GLN:O	44:w:219:GLN:NE2	2.51	0.43
2:B:135:ARG:HD3	2:B:141:ARG:HG3	2.00	0.43
5:F:46:LYS:HE3	5:F:46:LYS:HB2	1.79	0.43
16:Q:198:THR:OG1	41:s:275:ALA:O	2.30	0.43
26:c:164:ASN:HA	26:c:181:VAL:HB	1.99	0.43
36:m:33:LEU:HD23	36:m:64:MET:HE3	2.00	0.43
40:r:193:ILE:HD11	40:r:256:TYR:OH	2.18	0.43
41:s:20:LEU:HG	41:s:228:TYR:HD2	1.83	0.43
1:A:90:GLY:HA3	47:A:503:NAI:H1D	2.00	0.43
19:U:39:THR:HG23	41:s:309:ILE:HG22	1.99	0.43
25:b:123:PHE:CZ	43:v:61:HIS:HB2	2.52	0.43
49:e:201:PLX:H352	40:r:443:PRO:HB3	1.99	0.43
32:i:221:HIS:O	32:i:319:HIS:HE1	2.01	0.43
56:r:503:CDL:H761	56:r:503:CDL:H791	1.46	0.43
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.99	0.43
19:U:26:GLY:HA3	48:j:201:PEE:H37	2.00	0.43
21:W:90:ASN:ND2	21:W:123:GLU:O	2.51	0.43
6:X:93:ILE:HG21	6:X:98:LEU:HD22	2.01	0.43
32:i:313:MET:HE1	44:w:138:SER:HA	2.00	0.43
34:k:60:PRO:O	34:k:63:LEU:HB2	2.18	0.43
36:m:82:VAL:HG22	36:m:83:TRP:H	1.83	0.43
36:m:86:ASN:OD1	36:m:87:LYS:N	2.51	0.43
40:r:202:ALA:O	40:r:205:VAL:HG12	2.18	0.43
41:s:68:ILE:HG13	56:s:401:CDL:H121	2.01	0.43
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.59	0.43
49:J:403:PLX:H1C3	49:J:403:PLX:H21	1.76	0.43
14:O:193:TYR:OH	14:O:214:PRO:HG2	2.18	0.43
15:P:156:SER:O	15:P:156:SER:OG	2.34	0.43
33:j:73:LEU:N	33:j:74:PRO:HD2	2.34	0.43
6:G:83:VAL:O	6:G:87:LEU:HG	2.18	0.43
15:P:122:ARG:NH1	15:P:127:GLU:OE1	2.49	0.43
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.00	0.43
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.40	0.43
18:T:104:LYS:HE2	18:T:104:LYS:HB2	1.83	0.43
42:u:83:THR:HA	42:u:86:TRP:NE1	2.34	0.43
1:A:322:SER:HB2	1:A:370:LEU:HD22	2.01	0.43
5:F:31:GLN:HG2	5:F:34:ARG:NH2	2.33	0.43
20:V:114:ALA:O	20:V:118:MET:HG3	2.19	0.43
27:d:77:CYS:SG	27:d:84:CYS:HB3	2.58	0.43
27:d:159:GLN:HE21	27:d:163:MET:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:307:SER:OG	32:i:308:THR:N	2.52	0.43
35:l:241:THR:HG21	35:l:344:GLY:HA3	2.00	0.43
56:l:702:CDL:H671	56:l:702:CDL:H642	1.87	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.53	0.43
41:s:233:MET:HB3	41:s:233:MET:HE3	1.79	0.43
42:u:47:ARG:HA	42:u:47:ARG:HD2	1.79	0.43
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.59	0.43
6:G:119:ILE:HD13	6:G:119:ILE:HA	1.87	0.43
56:V:202:CDL:H242	56:V:202:CDL:H451	2.01	0.43
32:i:230:LEU:HD21	32:i:244:MET:SD	2.58	0.43
35:l:488:MET:HE2	35:l:488:MET:HA	2.00	0.43
1:A:363:ILE:O	1:A:367:ILE:HG12	2.19	0.43
8:I:69:VAL:O	15:P:76:VAL:HB	2.18	0.43
9:J:375:VAL:HG23	9:J:375:VAL:O	2.18	0.43
12:M:460:HIS:HA	12:M:461:PRO:HD3	1.88	0.43
49:e:201:PLX:H341	40:r:71:TRP:CD2	2.54	0.43
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.00	0.43
48:r:501:PEE:H52	48:r:501:PEE:H59	1.76	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.74	0.43
4:E:119:LEU:HD12	12:M:628:GLU:OE1	2.19	0.43
5:F:65:LEU:HD11	5:F:91:LEU:HD13	2.00	0.43
17:S:66:LEU:HD22	17:S:69:ILE:HD13	2.01	0.43
6:X:137:LYS:HA	25:b:3:GLY:HA2	2.00	0.43
27:d:107:GLN:HB3	27:d:111:LYS:NZ	2.33	0.43
32:i:57:THR:HA	34:k:77:LEU:HD13	2.00	0.43
36:m:1:MET:SD	36:m:1:MET:N	2.91	0.43
40:r:287:ALA:O	40:r:291:VAL:HG23	2.19	0.43
43:v:18:ASP:OD2	43:v:21:ARG:NH1	2.42	0.43
44:w:340:SER:HB2	44:w:343:TYR:HD2	1.84	0.43
1:A:115:VAL:HG22	1:A:248:VAL:HG21	2.01	0.42
1:A:267:ARG:NH1	1:A:341:ALA:HB2	2.33	0.42
48:B:303:PEE:H61	48:B:303:PEE:H55	1.70	0.42
12:M:414:PHE:CE2	12:M:418:ILE:HD11	2.54	0.42
13:N:32:ASP:OD1	13:N:34:ARG:HD3	2.19	0.42
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.46	0.42
16:Q:174:PHE:O	16:Q:178:THR:OG1	2.33	0.42
35:l:331:MET:SD	35:l:465:GLY:HA2	2.58	0.42
3:C:86:MET:HE1	3:C:93:PHE:CE2	2.54	0.42
56:V:201:CDL:H352	56:V:201:CDL:H322	1.77	0.42
28:e:125:LEU:HD23	28:e:125:LEU:HA	1.88	0.42
32:i:68:MET:HE2	32:i:68:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:97:MET:HG2	35:l:599:MET:HE1	2.00	0.42
48:j:201:PEE:H22	48:j:201:PEE:H27	1.87	0.42
36:m:74:MET:HE2	36:m:74:MET:HB2	1.86	0.42
56:V:202:CDL:H361	56:V:202:CDL:H331	1.75	0.42
56:V:204:CDL:H581	56:V:204:CDL:H611	1.45	0.42
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.01	0.42
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.01	0.42
39:p:114:MET:H	39:p:114:MET:HG3	1.67	0.42
50:C:304:DCQ:H3MB	16:Q:92:HIS:ND1	2.34	0.42
7:H:33:ASP:OD1	7:H:33:ASP:C	2.62	0.42
11:L:71:HIS:CE1	11:L:120:PRO:HD2	2.54	0.42
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.35	0.42
20:V:36:VAL:HG22	56:V:201:CDL:H742	2.02	0.42
56:V:204:CDL:H131	56:V:204:CDL:H161	1.71	0.42
6:X:98:LEU:HD12	6:X:99:SER:H	1.84	0.42
6:X:98:LEU:HD12	6:X:99:SER:N	2.33	0.42
32:i:68:MET:HE1	34:k:37:MET:SD	2.59	0.42
35:l:21:MET:HE2	35:l:21:MET:HB3	1.96	0.42
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.01	0.42
44:w:57:SER:HB3	44:w:150:LEU:HD11	2.01	0.42
2:B:86:TYR:CE1	3:C:171:GLU:HG2	2.55	0.42
12:M:148:SER:OG	12:M:149:ASP:N	2.53	0.42
14:O:93:LEU:HD12	14:O:122:TYR:HB3	2.01	0.42
26:c:101:TRP:CE3	38:o:47:TYR:HB2	2.55	0.42
35:l:566:THR:O	35:l:570:GLN:HG2	2.20	0.42
36:m:73:ALA:C	36:m:74:MET:HG3	2.44	0.42
36:m:165:VAL:O	36:m:168:ILE:HG12	2.19	0.42
40:r:122:PHE:CE1	40:r:206:LYS:HD2	2.54	0.42
42:u:101:ARG:NH1	42:u:104:GLN:OE1	2.47	0.42
7:H:87:GLU:OE1	15:P:104:THR:OG1	2.36	0.42
49:g:201:PLX:H102	49:g:201:PLX:H71	1.47	0.42
35:l:244:SER:O	35:l:249:SER:HB3	2.20	0.42
35:l:252:MET:HE2	35:l:252:MET:HB3	1.84	0.42
40:r:6:ILE:O	40:r:10:MET:HG2	2.18	0.42
40:r:346:ARG:O	40:r:419:TYR:HA	2.19	0.42
1:A:267:ARG:HH12	1:A:341:ALA:HB2	1.85	0.42
7:H:55:LYS:HE3	15:P:104:THR:HG21	2.00	0.42
7:H:77:ILE:HD12	7:H:78:GLU:N	2.35	0.42
17:S:1:MET:HB2	17:S:3:PHE:CZ	2.54	0.42
17:S:48:MET:HE1	21:W:143:TYR:CE1	2.55	0.42
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:304:MET:HE3	40:r:135:ARG:HH22	1.84	0.42
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.85	0.42
40:r:247:THR:HB	40:r:304:GLN:NE2	2.34	0.42
13:N:80:SER:O	13:N:113:HIS:HE1	2.03	0.42
56:V:202:CDL:H792	56:V:202:CDL:H761	1.55	0.42
23:Z:36:LEU:HD12	23:Z:36:LEU:HA	1.90	0.42
32:i:141:VAL:O	32:i:145:ILE:HG12	2.20	0.42
32:i:222:SER:O	32:i:224:ALA:N	2.53	0.42
1:A:314:LEU:HD11	1:A:317:VAL:HG23	2.01	0.42
3:C:67:PHE:CZ	3:C:117:LEU:HD12	2.55	0.42
16:Q:434:GLY:O	16:Q:438:MET:HG3	2.19	0.42
32:i:2:ASN:HB3	32:i:5:ILE:HG12	2.01	0.42
32:i:128:LEU:HD12	32:i:216:PHE:HB3	2.02	0.42
32:i:168:GLY:HA3	32:i:181:TYR:CE1	2.55	0.42
33:j:51:PHE:O	36:m:73:ALA:HA	2.20	0.42
56:l:701:CDL:H611	56:l:701:CDL:H581	1.68	0.42
36:m:71:THR:HA	36:m:75:ALA:HB3	2.01	0.42
41:s:81:LEU:HD11	41:s:111:LEU:HG	2.01	0.42
3:C:86:MET:HE3	3:C:91:VAL:HG12	2.02	0.42
10:K:79:HIS:ND1	14:O:216:PRO:HD2	2.34	0.42
12:M:277:MET:HE3	12:M:277:MET:HB3	1.98	0.42
13:N:34:ARG:NH2	13:N:58:ARG:O	2.53	0.42
15:P:147:THR:HB	15:P:153:ILE:HD11	2.02	0.42
34:k:37:MET:CE	34:k:63:LEU:HD22	2.50	0.42
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.02	0.42
43:v:39:MET:HE3	43:v:39:MET:HB3	1.99	0.42
7:H:116:ILE:HG12	15:P:121:THR:HG21	2.01	0.41
18:T:39:THR:HG22	18:T:62:VAL:HG22	2.01	0.41
20:V:126:LYS:HA	20:V:126:LYS:HD2	1.91	0.41
24:a:184:LYS:O	24:a:185:THR:OG1	2.36	0.41
32:i:242:SER:HB3	56:r:503:CDL:H331	2.01	0.41
56:l:701:CDL:H722	56:l:701:CDL:HA62	2.02	0.41
40:r:328:CYS:HB2	40:r:437:MET:HE1	2.02	0.41
56:r:503:CDL:H351	56:r:503:CDL:H201	2.02	0.41
1:A:373:PHE:HD1	14:O:175:GLU:HB3	1.84	0.41
2:B:70:LEU:HB3	41:s:272:TRP:CZ2	2.55	0.41
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.02	0.41
8:I:106:LEU:O	8:I:108:LYS:NZ	2.53	0.41
11:L:78:ARG:NE	11:L:148:GLU:OE1	2.50	0.41
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.67	0.41
21:W:36:PHE:O	21:W:40:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:69:LYS:HB2	24:a:69:LYS:HE2	1.85	0.41
24:a:94:GLY:O	27:d:61:TYR:OH	2.28	0.41
24:a:127:ASP:OD1	49:a:202:PLX:H12	2.20	0.41
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.53	0.41
2:B:144:ARG:NH1	11:L:112:MET:O	2.43	0.41
8:I:18:ARG:NH2	21:W:24:ASN:O	2.45	0.41
29:f:71:ARG:HG2	29:f:71:ARG:NH1	2.34	0.41
35:l:341:MET:CE	35:l:457:LEU:HD12	2.50	0.41
35:l:407:TRP:CZ2	35:l:411:MET:HE3	2.55	0.41
40:r:267:TRP:O	40:r:271:MET:HG2	2.21	0.41
5:F:24:CYS:N	5:F:58:CYS:SG	2.93	0.41
10:K:83:THR:HG22	14:O:88:ARG:HE	1.85	0.41
12:M:419:ARG:NH1	12:M:439:THR:O	2.52	0.41
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	2.02	0.41
33:j:69:ILE:HD11	41:s:144:VAL:HA	2.02	0.41
35:l:304:PHE:CZ	35:l:526:LEU:HD22	2.55	0.41
40:r:405:LEU:HD23	40:r:405:LEU:HA	1.90	0.41
40:r:437:MET:HA	40:r:437:MET:HE3	2.01	0.41
41:s:54:LYS:HD2	41:s:54:LYS:C	2.45	0.41
44:w:183:CYS:HA	44:w:314:LEU:HD21	2.02	0.41
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.03	0.41
6:G:84:LEU:O	6:G:88:LYS:HG3	2.20	0.41
9:J:108:TRP:HA	9:J:115:SER:HB3	2.03	0.41
12:M:171:THR:HG23	12:M:173:MET:SD	2.60	0.41
12:M:466:LEU:HD13	12:M:500:ILE:HD11	2.02	0.41
14:O:185:MET:HB2	14:O:185:MET:HE2	1.83	0.41
6:X:91:ASP:OD2	23:Z:42:ARG:NH2	2.49	0.41
22:Y:42:PRO:HG3	35:l:442:LEU:HD13	2.02	0.41
27:d:122:ARG:HA	27:d:122:ARG:HD3	1.90	0.41
28:e:89:VAL:HG21	40:r:25:ILE:HG23	2.02	0.41
32:i:93:VAL:HG22	35:l:603:ASN:ND2	2.34	0.41
35:l:312:LEU:O	35:l:316:THR:HG22	2.21	0.41
39:p:140:LEU:HD23	39:p:140:LEU:HA	1.88	0.41
44:w:65:ASN:OD1	44:w:66:ILE:N	2.42	0.41
2:B:37:THR:HA	8:I:105:GLU:O	2.20	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.21	0.41
12:M:487:THR:HB	12:M:677:GLN:HE22	1.85	0.41
13:N:42:ASP:OD2	13:N:48:TYR:OH	2.25	0.41
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.91	0.41
32:i:215:MET:HE1	32:i:244:MET:HG3	2.02	0.41
33:j:69:ILE:HD13	41:s:147:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:51:LEU:O	43:v:52:MET:HG3	2.20	0.41
1:A:224:ARG:HD2	11:L:164:PHE:CE1	2.56	0.41
9:J:229:ILE:HB	9:J:323:HIS:CD2	2.55	0.41
12:M:50:LEU:HD11	12:M:62:ARG:HE	1.85	0.41
12:M:141:ASP:O	12:M:145:MET:HG2	2.21	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.41
14:O:185:MET:HB3	14:O:194:GLU:HB3	2.02	0.41
16:Q:457:VAL:HG12	16:Q:460:GLU:HG2	2.03	0.41
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.32	0.41
1:A:224:ARG:HD2	11:L:164:PHE:CZ	2.55	0.41
1:A:389:VAL:HA	1:A:392:MET:HE2	2.03	0.41
3:C:62:LEU:HD23	3:C:62:LEU:HA	1.92	0.41
48:C:302:PEE:H15	49:J:403:PLX:H1B1	2.03	0.41
9:J:306:GLU:HG2	9:J:315:THR:HG22	2.02	0.41
15:P:43:THR:HG22	15:P:47:ILE:HD12	2.03	0.41
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.55	0.41
29:f:59:ILE:HG12	29:f:59:ILE:H	1.74	0.41
32:i:228:LEU:HD23	32:i:228:LEU:HA	1.90	0.41
32:i:261:MET:HE2	32:i:340:THR:HA	2.02	0.41
43:v:115:ARG:HD3	43:v:116:GLU:N	2.35	0.41
44:w:254:GLU:H	44:w:254:GLU:HG2	1.65	0.41
1:A:118:ASP:HB3	46:A:502:FMN:O4	2.21	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.03	0.41
1:A:174:ARG:NH1	10:K:92:GLU:OE2	2.54	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
4:E:36:TYR:CE1	6:G:113:LEU:HD13	2.56	0.41
4:E:66:MET:HE3	4:E:106:PHE:HD1	1.85	0.41
11:L:76:LYS:HE3	11:L:146:ASP:CG	2.46	0.41
11:L:78:ARG:HH22	12:M:249:GLU:CD	2.28	0.41
12:M:307:ILE:HG23	12:M:317:THR:HG21	2.02	0.41
14:O:138:THR:HB	14:O:139:PRO:HD3	2.02	0.41
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.32	0.41
26:c:123:PRO:HB2	35:l:525:MET:HE1	2.02	0.41
30:g:33:LEU:HD23	30:g:33:LEU:HA	1.96	0.41
56:i:401:CDL:H811	36:m:159:TRP:CH2	2.56	0.41
33:j:17:LEU:HD23	33:j:17:LEU:HA	1.92	0.41
33:j:71:LEU:O	36:m:147:TYR:OH	2.33	0.41
35:l:486:MET:HA	35:l:489:THR:OG1	2.21	0.41
35:l:561:ILE:HG13	35:l:562:LEU:N	2.36	0.41
36:m:44:VAL:HG12	36:m:49:GLY:O	2.20	0.41
43:v:53:LEU:HD23	43:v:53:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:551:ASP:OD1	12:M:574:ASP:HB3	2.21	0.41
20:V:141:VAL:HG11	32:i:272:LYS:HB3	2.03	0.41
22:Y:100:LEU:HB3	22:Y:104:GLU:OE1	2.20	0.41
28:e:73:SER:O	28:e:75:GLY:N	2.55	0.41
32:i:294:MET:HE2	40:r:130:LEU:HD21	2.03	0.41
35:l:69:MET:HE2	35:l:76:LEU:HD12	2.03	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.56	0.41
35:l:286:LEU:HD22	35:l:411:MET:SD	2.61	0.41
56:n:101:CDL:H531	56:n:101:CDL:H741	2.03	0.41
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.90	0.41
41:s:123:SER:HB3	41:s:214:GLU:HG3	2.03	0.41
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.56	0.41
1:A:63:TYR:CD2	14:O:241:PRO:HB2	2.56	0.40
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.85	0.40
2:B:49:ASP:OD2	2:B:51:LYS:HB2	2.21	0.40
48:B:303:PEE:H56	41:s:187:ILE:HD12	2.02	0.40
8:I:108:LYS:HA	8:I:108:LYS:HD3	1.69	0.40
9:J:204:SER:OG	9:J:238:GLN:O	2.39	0.40
11:L:111:LEU:HG	11:L:112:MET:HG2	2.03	0.40
15:P:197:PRO:HA	15:P:202:PHE:CD2	2.56	0.40
25:b:28:LEU:HD22	25:b:32:GLU:HG3	2.02	0.40
40:r:321:LEU:HD13	40:r:444:LEU:HG	2.01	0.40
1:A:207:GLY:HA3	46:A:502:FMN:N5	2.36	0.40
49:J:403:PLX:H32	33:j:23:TRP:CZ3	2.57	0.40
14:O:143:ARG:HG3	14:O:183:ALA:HB3	2.03	0.40
21:W:88:ARG:HH11	21:W:91:LEU:HD23	1.86	0.40
28:e:87:MET:HE3	28:e:87:MET:HB3	1.88	0.40
48:j:201:PEE:H60	48:j:201:PEE:H55	1.82	0.40
35:l:169:LEU:HD12	35:l:169:LEU:HA	1.93	0.40
35:l:397:GLU:HG2	35:l:482:MET:HE1	2.03	0.40
37:n:50:ARG:HB3	37:n:51:PRO:HD2	2.03	0.40
4:E:19:PRO:HB3	11:L:53:ILE:HG21	2.02	0.40
9:J:262:THR:O	9:J:333:PRO:HD2	2.22	0.40
16:Q:271:ARG:NH2	16:Q:445:ALA:HB1	2.36	0.40
20:V:44:LYS:NZ	35:l:579:ASN:O	2.46	0.40
26:c:65:TYR:CE2	26:c:77:LYS:HG3	2.56	0.40
42:u:18:VAL:HG23	42:u:64:ASN:HD22	1.86	0.40
43:v:108:LEU:HD12	43:v:108:LEU:HA	1.84	0.40
48:B:303:PEE:H7	41:s:288:LEU:HD11	2.03	0.40
3:C:52:ASP:HB3	49:C:303:PLX:H282	2.02	0.40
16:Q:244:ILE:O	16:Q:248:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.87	0.40
49:j:203:PLX:H311	49:j:203:PLX:H282	1.55	0.40
35:l:338:MET:SD	35:l:458:LEU:HD12	2.61	0.40
40:r:104:LEU:HD21	56:r:503:CDL:H861	2.03	0.40
41:s:134:ARG:NH1	41:s:206:GLU:OE1	2.37	0.40
44:w:70:LYS:NZ	44:w:160:GLU:OE1	2.54	0.40
1:A:184:LYS:HB2	10:K:98:MET:CE	2.52	0.40
2:B:171:PRO:HG3	2:B:200:GLU:HG2	2.03	0.40
11:L:80:PHE:CE1	11:L:100:GLU:HG2	2.55	0.40
12:M:144:MET:O	16:Q:362:LYS:HE3	2.22	0.40
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.56	0.40
28:e:55:LEU:HD23	28:e:57:GLU:HB2	2.03	0.40
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.56	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%)	421 (98%)	10 (2%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
5	F	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
6	G	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	14	35
8	I	93/112 (83%)	86 (92%)	7 (8%)	0	100	100
9	J	340/342 (99%)	327 (96%)	12 (4%)	1 (0%)	36	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	676 (98%)	12 (2%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	198 (92%)	17 (8%)	0	100	100
15	P	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	24	48
16	Q	427/430 (99%)	415 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
22	Y	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
23	Z	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
33	j	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	14	35
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	591 (98%)	13 (2%)	0	100	100
36	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	44
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	s	316/318 (99%)	305 (96%)	10 (3%)	1 (0%)	36	60
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
All	All	8175/8314 (98%)	7912 (97%)	257 (3%)	6 (0%)	49	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	44	ARG
7	H	77	ILE
9	J	38	HIS
33	j	40	GLY
39	p	174	PRO
41	s	208	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	341 (99%)	5 (1%)	59	82
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	88
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	73 (97%)	2 (3%)	39	69
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	75/81 (93%)	74 (99%)	1 (1%)	61	83
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	86
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	85
9	J	295/296 (100%)	293 (99%)	2 (1%)	76	90
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	87
12	M	580/580 (100%)	571 (98%)	9 (2%)	55	80
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	370/370 (100%)	364 (98%)	6 (2%)	55	80
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	83
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	66
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	61 (98%)	1 (2%)	55	80
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	140 (99%)	1 (1%)	76	90
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	77
28	e	96/96 (100%)	95 (99%)	1 (1%)	68	86
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	85
32	i	311/311 (100%)	304 (98%)	7 (2%)	44	73
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	86
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	84
35	l	537/540 (99%)	535 (100%)	2 (0%)	84	93
36	m	126/141 (89%)	124 (98%)	2 (2%)	55	80
37	n	53/53 (100%)	51 (96%)	2 (4%)	29	58
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	87
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	83
40	r	410/410 (100%)	404 (98%)	6 (2%)	57	81
41	s	275/275 (100%)	272 (99%)	3 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	u	153/153 (100%)	152 (99%)	1 (1%)	76	90
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	276 (98%)	5 (2%)	51	78
All	All	7148/7241 (99%)	7074 (99%)	74 (1%)	65	86

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	106	SER
1	A	149	MET
1	A	334	THR
1	A	344	GLN
3	C	71	CYS
5	F	48	ASN
5	F	88	THR
7	H	48	THR
8	I	41	LEU
9	J	174	ILE
9	J	220	MET
10	K	107	SER
11	L	154	LYS
12	M	361	VAL
12	M	364	ASP
12	M	484	SER
12	M	498	GLN
12	M	534	VAL
12	M	540	ASN
12	M	575	VAL
12	M	658	ASP
12	M	674	LEU
16	Q	182	ASN
16	Q	217	VAL
16	Q	248	SER
16	Q	258	LEU
16	Q	453	THR
16	Q	457	VAL
18	T	104	LYS
20	V	4	THR
20	V	120	LEU
20	V	141	VAL

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Mol	Chain	Res	Type
6	X	100	VAL
23	Z	36	LEU
26	c	33	THR
27	d	40	LEU
27	d	52	ILE
27	d	144	SER
28	e	55	LEU
31	h	21	GLN
32	i	89	MET
32	i	147	GLN
32	i	157	MET
32	i	164	ILE
32	i	194	LEU
32	i	229	SER
32	i	336	VAL
33	j	83	ASN
34	k	3	LEU
35	l	233	LEU
35	l	507	THR
36	m	1	MET
36	m	74	MET
37	n	19	VAL
37	n	52	ASN
38	o	41	SER
39	p	85	SER
39	p	90	SER
40	r	58	SER
40	r	138	ASN
40	r	179	ILE
40	r	187	SER
40	r	343	ILE
40	r	375	LEU
41	s	24	GLU
41	s	110	SER
41	s	174	MET
42	u	37	ASP
44	w	56	THR
44	w	133	SER
44	w	152	SER
44	w	223	ASN
44	w	254	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	164	ASN
1	A	281	HIS
1	A	284	HIS
3	C	111	ASN
4	E	48	HIS
8	I	29	GLN
9	J	122	HIS
9	J	128	ASN
9	J	138	ASN
9	J	295	HIS
10	K	70	ASN
10	K	106	GLN
11	L	71	HIS
12	M	498	GLN
13	N	113	HIS
14	O	90	ASN
14	O	182	ASN
15	P	82	ASN
15	P	124	ASN
15	P	196	HIS
16	Q	233	HIS
16	Q	285	ASN
18	T	120	GLN
21	W	90	ASN
22	Y	75	HIS
24	a	189	ASN
27	d	55	GLN
28	e	65	ASN
32	i	63	GLN
32	i	120	GLN
35	l	59	GLN
35	l	470	ASN
40	r	30	HIS
40	r	251	ASN
43	v	84	GLN
44	w	37	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	1.99	1 (10%)	5,13,15	5.96	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.69	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.08	130.55	119.48
16	Q	118	2MR	CD-NE-CZ	4.33	131.50	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.38	130.91	123.65

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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$
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
45	SF4	M	802	12	0,12,12	-	-	-		
52	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.24	14 (19%)
56	CDL	s	401	-	88,88,99	1.17	9 (10%)	94,100,111	0.95	5 (5%)
56	CDL	l	702	-	91,91,99	1.14	9 (9%)	97,103,111	0.88	4 (4%)
49	PLX	e	201	-	51,51,51	1.22	5 (9%)	53,59,59	0.53	0
48	PEE	V	203	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
48	PEE	l	703	-	50,50,50	1.18	6 (12%)	53,55,55	0.94	2 (3%)
49	PLX	J	403	-	51,51,51	1.23	4 (7%)	53,59,59	0.59	1 (1%)
49	PLX	a	202	-	51,51,51	1.22	5 (9%)	53,59,59	0.61	1 (1%)
56	CDL	i	401	-	86,86,99	1.17	8 (9%)	92,98,111	0.90	4 (4%)
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.68	11 (17%)
48	PEE	l	704	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
58	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.96	9 (20%)
48	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.02	2 (4%)
56	CDL	l	701	-	98,98,99	1.12	8 (8%)	104,110,111	0.88	4 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
56	CDL	N	201	-	50,50,99	1.43	8 (16%)	56,62,111	1.14	4 (7%)
56	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.90	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.00	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
54	FES	O	301	14	0,4,4	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
49	PLX	j	203	-	51,51,51	1.21	5 (9%)	53,59,59	0.62	1 (1%)
49	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.64	1 (1%)
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
53	UQ	J	402	-	33,33,63	3.52	9 (27%)	42,43,79	2.71	14 (33%)
56	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.85	4 (3%)
50	DCQ	C	304	-	23,23,23	1.34	3 (13%)	27,29,29	1.00	1 (3%)
51	8Q1	G	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.66	5 (12%)
48	PEE	B	303	-	50,50,50	1.19	6 (12%)	53,55,55	0.99	2 (3%)
49	PLX	C	303	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
48	PEE	j	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.03	2 (4%)
56	CDL	V	202	-	99,99,99	1.11	9 (9%)	105,111,111	0.89	5 (4%)
56	CDL	r	503	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.23	8 (16%)
51	8Q1	X	201	6	32,34,34	1.65	6 (18%)	39,43,43	1.58	8 (20%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
56	CDL	V	204	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
56	CDL	n	101	-	54,54,99	1.40	9 (16%)	60,66,111	1.10	4 (6%)
49	PLX	g	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.61	1 (1%)
54	FES	M	803	12	0,4,4	-	-	-		
53	UQ	s	402	-	38,38,63	3.64	11 (28%)	48,49,79	2.68	15 (31%)

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
48	PEE	r	501	-	-	28/54/54/54	-
52	NDP	J	401	-	-	9/34/77/77	0/5/5/5
56	CDL	s	401	-	-	50/99/99/110	-
45	SF4	M	802	12	-	-	0/6/5/5
56	CDL	l	702	-	-	56/102/102/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	e	201	-	-	35/55/55/55	-
48	PEE	V	203	-	-	23/43/43/54	-
48	PEE	l	703	-	-	25/54/54/54	-
49	PLX	J	403	-	-	32/55/55/55	-
49	PLX	a	202	-	-	27/55/55/55	-
56	CDL	i	401	-	-	46/97/97/110	-
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
48	PEE	l	704	-	-	22/49/49/54	-
58	ADP	w	401	-	-	5/16/32/32	0/3/3/3
48	PEE	C	302	-	-	26/50/50/54	-
56	CDL	l	701	-	-	56/109/109/110	-
45	SF4	A	501	1	-	-	0/6/5/5
56	CDL	N	201	-	-	34/61/61/110	-
56	CDL	V	201	-	-	61/104/104/110	-
48	PEE	W	201	-	-	20/44/44/54	-
45	SF4	B	301	2	-	-	0/6/5/5
54	FES	O	301	14	-	-	0/1/1/1
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	j	203	-	-	30/55/55/55	-
49	PLX	r	502	-	-	30/55/55/55	-
48	PEE	j	201	-	-	22/54/54/54	-
53	UQ	J	402	-	-	13/27/51/87	0/1/1/1
56	CDL	a	201	-	-	55/110/110/110	-
50	DCQ	C	304	-	-	4/14/38/38	0/1/1/1
51	8Q1	G	201	-	-	14/41/41/41	-
48	PEE	B	303	-	-	21/54/54/54	-
49	PLX	C	303	-	-	25/55/55/55	-
48	PEE	j	202	-	-	22/44/44/54	-
56	CDL	V	202	-	-	55/110/110/110	-
56	CDL	r	503	-	-	61/110/110/110	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
51	8Q1	X	201	6	-	7/41/41/41	-
45	SF4	B	302	2	-	-	0/6/5/5
56	CDL	V	204	-	-	65/110/110/110	-
45	SF4	C	301	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	CDL	n	101	-	-	28/65/65/110	-
49	PLX	g	201	-	-	32/55/55/55	-
54	FES	M	803	12	-	-	0/1/1/1
53	UQ	s	402	-	-	13/33/57/87	0/1/1/1

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-13.29	1.23	1.53
52	J	401	NDP	O4D-C4D	10.72	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.33	1.26	1.53
53	s	402	UQ	C18-C19	10.01	1.56	1.33
53	J	402	UQ	C18-C19	9.99	1.56	1.33
52	J	401	NDP	C3D-C4D	-9.91	1.27	1.53
53	s	402	UQ	C13-C14	9.63	1.55	1.33
53	J	402	UQ	C13-C14	9.56	1.55	1.33
53	s	402	UQ	C23-C24	9.47	1.54	1.33
47	A	503	NAI	O4B-C1B	9.41	1.63	1.42
53	J	402	UQ	C8-C9	9.29	1.54	1.33
53	s	402	UQ	C8-C9	9.29	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.27	1.26	1.45
52	J	401	NDP	O4B-C4B	-7.83	1.27	1.45
58	w	401	ADP	O4'-C4'	7.79	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.70	1.29	1.53
53	J	402	UQ	C23-C24	7.55	1.55	1.32
52	J	401	NDP	C2N-C3N	7.47	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.34	1.30	1.53
53	s	402	UQ	C28-C29	7.31	1.54	1.32
52	J	401	NDP	C6N-C5N	7.25	1.55	1.33
47	A	503	NAI	O4D-C4D	7.03	1.60	1.45
52	J	401	NDP	PN-O3	6.49	1.66	1.59
58	w	401	ADP	PA-O3A	6.42	1.66	1.59
47	A	503	NAI	PA-O3	6.23	1.66	1.59
52	J	401	NDP	P2B-O2B	6.03	1.70	1.59
47	A	503	NAI	C2D-C3D	5.92	1.69	1.53
52	J	401	NDP	C6A-N6A	5.81	1.49	1.34
52	J	401	NDP	PA-O3	5.72	1.65	1.59
47	A	503	NAI	PN-O3	5.63	1.65	1.59
47	A	503	NAI	O4D-C1D	5.60	1.54	1.42
58	w	401	ADP	C6-N6	5.47	1.48	1.34
52	J	401	NDP	C3B-C4B	5.44	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C7N-N7N	5.31	1.48	1.33
51	G	201	8Q1	C39-N41	5.23	1.45	1.33
47	A	503	NAI	C4N-C3N	-5.21	1.40	1.50
51	X	201	8Q1	C39-N41	5.19	1.45	1.33
51	X	201	8Q1	C34-N36	5.11	1.45	1.33
47	A	503	NAI	C6A-N6A	5.07	1.47	1.34
51	G	201	8Q1	C34-N36	5.03	1.45	1.33
52	J	401	NDP	C6N-N1N	5.03	1.49	1.37
52	J	401	NDP	O4D-C1D	-5.01	1.30	1.42
52	J	401	NDP	O4B-C1B	4.75	1.53	1.42
58	w	401	ADP	O4'-C1'	-4.61	1.31	1.42
52	J	401	NDP	C1B-N9A	-4.55	1.33	1.46
47	A	503	NAI	O2B-C2B	4.35	1.53	1.43
52	J	401	NDP	O2D-C2D	-3.94	1.33	1.43
48	B	303	PEE	C18-C19	3.84	1.53	1.31
48	j	201	PEE	C18-C19	3.82	1.53	1.31
48	r	501	PEE	C18-C19	3.82	1.53	1.31
48	V	203	PEE	C18-C19	3.82	1.53	1.31
48	W	201	PEE	C18-C19	3.82	1.53	1.31
52	J	401	NDP	C7N-N7N	3.81	1.44	1.33
48	C	302	PEE	C18-C19	3.81	1.53	1.31
48	j	202	PEE	C18-C19	3.81	1.53	1.31
48	l	704	PEE	C18-C19	3.81	1.53	1.31
48	l	703	PEE	C18-C19	3.80	1.53	1.31
48	B	303	PEE	C39-C38	3.75	1.53	1.31
48	r	501	PEE	C39-C38	3.74	1.52	1.31
48	j	201	PEE	C39-C38	3.74	1.52	1.31
48	C	302	PEE	C39-C38	3.73	1.52	1.31
48	V	203	PEE	C39-C38	3.72	1.52	1.31
48	l	703	PEE	C39-C38	3.72	1.52	1.31
48	l	704	PEE	C39-C38	3.71	1.52	1.31
47	A	503	NAI	C7N-C3N	3.60	1.56	1.48
56	i	401	CDL	OA8-CA7	3.51	1.43	1.33
56	l	701	CDL	OA8-CA7	3.51	1.43	1.33
56	V	204	CDL	OA8-CA7	3.48	1.43	1.33
56	n	101	CDL	OA8-CA7	3.46	1.43	1.33
56	N	201	CDL	OA8-CA7	3.46	1.43	1.33
56	a	201	CDL	OA8-CA7	3.45	1.43	1.33
56	V	201	CDL	OA8-CA7	3.45	1.43	1.33
56	l	702	CDL	OA8-CA7	3.44	1.43	1.33
56	r	503	CDL	OA8-CA7	3.43	1.43	1.33
56	s	401	CDL	OA8-CA7	3.43	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	V	202	CDL	OA8-CA7	3.39	1.43	1.33
58	w	401	ADP	C8-N9	-3.36	1.31	1.37
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.49
46	A	502	FMN	C4A-N5	3.30	1.37	1.30
58	w	401	ADP	O2'-C2'	-3.19	1.35	1.43
52	J	401	NDP	C8A-N9A	-3.14	1.32	1.37
56	V	201	CDL	OA6-CA5	3.14	1.43	1.34
56	V	204	CDL	OA6-CA5	3.13	1.43	1.34
56	r	503	CDL	OB6-CB5	3.08	1.43	1.34
56	i	401	CDL	OB6-CB5	3.07	1.43	1.34
56	s	401	CDL	OB6-CB5	3.07	1.42	1.34
56	n	101	CDL	OB8-CB7	3.05	1.42	1.33
56	l	701	CDL	OB6-CB5	3.05	1.42	1.34
56	N	201	CDL	OB6-CB5	3.05	1.42	1.34
56	s	401	CDL	OA6-CA5	3.05	1.42	1.34
56	a	201	CDL	OB6-CB5	3.05	1.42	1.34
56	n	101	CDL	OB6-CB5	3.04	1.42	1.34
52	J	401	NDP	C5A-N7A	-3.03	1.33	1.39
56	V	202	CDL	OA6-CA5	3.02	1.42	1.34
56	N	201	CDL	OB8-CB7	3.02	1.42	1.33
52	J	401	NDP	C7N-C3N	3.02	1.55	1.48
56	a	201	CDL	OB8-CB7	3.01	1.42	1.33
56	a	201	CDL	OA6-CA5	3.01	1.42	1.34
56	l	702	CDL	OA6-CA5	3.01	1.42	1.34
56	V	201	CDL	OB8-CB7	3.00	1.42	1.33
56	i	401	CDL	OA6-CA5	3.00	1.42	1.34
56	V	202	CDL	OB6-CB5	3.00	1.42	1.34
56	V	204	CDL	OB6-CB5	3.00	1.42	1.34
56	V	202	CDL	OB8-CB7	3.00	1.42	1.33
56	V	204	CDL	OB8-CB7	3.00	1.42	1.33
56	l	701	CDL	OB8-CB7	3.00	1.42	1.33
56	V	201	CDL	OB6-CB5	3.00	1.42	1.34
56	l	702	CDL	OB8-CB7	2.99	1.42	1.33
56	i	401	CDL	OB8-CB7	2.99	1.42	1.33
56	l	702	CDL	OB6-CB5	2.98	1.42	1.34
56	r	503	CDL	OB8-CB7	2.97	1.42	1.33
56	s	401	CDL	OB8-CB7	2.96	1.42	1.33
58	w	401	ADP	O3'-C3'	2.94	1.50	1.43
56	n	101	CDL	OA6-CA5	2.93	1.42	1.34
56	N	201	CDL	OA6-CA5	2.92	1.42	1.34
49	e	201	PLX	O6-C4	-2.91	1.40	1.44
56	r	503	CDL	OA6-CA5	2.91	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	O3D-C3D	2.89	1.50	1.43
56	l	701	CDL	OA6-CA5	2.88	1.42	1.34
49	a	202	PLX	O6-C4	-2.87	1.40	1.44
49	g	201	PLX	O6-C4	-2.85	1.41	1.44
49	J	403	PLX	O6-C4	-2.83	1.41	1.44
53	J	402	UQ	C6-C1	2.77	1.54	1.46
53	s	402	UQ	C6-C1	2.75	1.54	1.46
49	C	303	PLX	O6-C4	-2.73	1.41	1.44
49	j	203	PLX	O6-C4	-2.68	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.67	1.33	1.37
48	r	501	PEE	O2-C2	-2.61	1.40	1.46
49	r	502	PLX	O6-C4	-2.61	1.41	1.44
56	l	701	CDL	OA6-CA4	-2.60	1.40	1.46
56	n	101	CDL	OA6-CA4	-2.60	1.40	1.46
48	W	201	PEE	O2-C2	-2.59	1.40	1.46
48	j	202	PEE	O2-C2	-2.58	1.40	1.46
56	a	201	CDL	OA6-CA4	-2.58	1.40	1.46
48	C	302	PEE	O2-C2	-2.58	1.40	1.46
56	r	503	CDL	OA6-CA4	-2.57	1.40	1.46
46	A	502	FMN	C10-N1	2.57	1.38	1.33
48	B	303	PEE	O2-C2	-2.57	1.40	1.46
56	N	201	CDL	OA6-CA4	-2.57	1.40	1.46
56	i	401	CDL	OA6-CA4	-2.55	1.40	1.46
52	J	401	NDP	O2B-C2B	2.55	1.52	1.44
48	j	201	PEE	O2-C2	-2.54	1.40	1.46
53	s	402	UQ	C7-C8	2.52	1.54	1.50
51	X	201	8Q1	C1-S44	2.51	1.82	1.76
56	l	702	CDL	OA6-CA4	-2.51	1.40	1.46
48	l	704	PEE	O2-C2	-2.50	1.40	1.46
56	V	202	CDL	OA6-CA4	-2.50	1.40	1.46
48	l	703	PEE	O2-C2	-2.50	1.40	1.46
56	s	401	CDL	OA6-CA4	-2.50	1.40	1.46
49	j	203	PLX	C7-C6	2.49	1.55	1.50
48	B	303	PEE	O3-C30	2.47	1.40	1.33
48	V	203	PEE	O2-C2	-2.46	1.40	1.46
47	A	503	NAI	C6N-C5N	2.45	1.40	1.33
48	V	203	PEE	O3-C30	2.43	1.40	1.33
51	G	201	8Q1	C1-S44	2.43	1.82	1.76
51	X	201	8Q1	C6-C1	2.43	1.53	1.50
48	j	201	PEE	O3-C30	2.42	1.40	1.33
48	l	703	PEE	O3-C30	2.42	1.40	1.33
48	j	202	PEE	O3-C30	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	PN-O5D	2.42	1.68	1.59
48	W	201	PEE	O3-C30	2.42	1.40	1.33
49	C	303	PLX	C7-C6	2.42	1.55	1.50
49	J	403	PLX	C7-C6	2.41	1.55	1.50
48	l	704	PEE	O3-C30	2.41	1.40	1.33
58	w	401	ADP	C5-N7	-2.41	1.34	1.39
48	r	501	PEE	O3-C30	2.40	1.40	1.33
56	l	702	CDL	OB6-CB4	-2.40	1.41	1.46
48	C	302	PEE	O3-C30	2.40	1.40	1.33
47	A	503	NAI	C5B-C4B	2.39	1.58	1.51
56	V	202	CDL	OB6-CB4	-2.38	1.41	1.46
48	V	203	PEE	O2-C10	2.36	1.41	1.34
56	V	204	CDL	OA6-CA4	-2.36	1.41	1.46
49	a	202	PLX	C7-C6	2.36	1.55	1.50
56	n	101	CDL	OB6-CB4	-2.36	1.41	1.46
52	J	401	NDP	C2D-C3D	2.35	1.59	1.53
48	l	703	PEE	O2-C10	2.35	1.40	1.34
47	A	503	NAI	O3B-C3B	-2.34	1.37	1.43
49	r	502	PLX	C7-C6	2.33	1.55	1.50
49	e	201	PLX	C7-C6	2.33	1.55	1.50
48	l	704	PEE	O2-C10	2.33	1.40	1.34
51	X	201	8Q1	O40-C39	-2.33	1.18	1.23
50	C	304	DCQ	C6-C5	2.33	1.53	1.46
56	V	204	CDL	OB6-CB4	-2.32	1.41	1.46
48	W	201	PEE	O2-C10	2.32	1.40	1.34
51	G	201	8Q1	O35-C34	-2.31	1.19	1.23
51	G	201	8Q1	O40-C39	-2.31	1.18	1.23
56	V	201	CDL	PB2-OB2	2.31	1.68	1.59
56	a	201	CDL	OB6-CB4	-2.30	1.41	1.46
56	l	701	CDL	OB6-CB4	-2.30	1.41	1.46
50	C	304	DCQ	O4-C4M	-2.30	1.40	1.45
49	g	201	PLX	C7-C6	2.30	1.55	1.50
56	s	401	CDL	OB6-CB4	-2.29	1.41	1.46
56	V	201	CDL	OB6-CB4	-2.29	1.41	1.46
48	B	303	PEE	O2-C10	2.28	1.40	1.34
56	n	101	CDL	PB2-OB2	2.28	1.68	1.59
51	X	201	8Q1	O35-C34	-2.28	1.19	1.23
56	N	201	CDL	OB6-CB4	-2.27	1.41	1.46
56	N	201	CDL	PB2-OB5	2.26	1.68	1.59
48	C	302	PEE	O2-C10	2.26	1.40	1.34
56	N	201	CDL	PB2-OB2	2.26	1.68	1.59
56	a	201	CDL	PB2-OB2	2.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	i	401	CDL	PB2-OB5	2.25	1.68	1.59
56	V	202	CDL	PB2-OB2	2.25	1.68	1.59
48	j	201	PEE	O2-C10	2.25	1.40	1.34
56	s	401	CDL	PB2-OB2	2.25	1.68	1.59
56	n	101	CDL	PB2-OB5	2.24	1.68	1.59
48	j	202	PEE	O2-C10	2.24	1.40	1.34
56	r	503	CDL	OB6-CB4	-2.24	1.41	1.46
56	r	503	CDL	PB2-OB2	2.24	1.68	1.59
56	V	201	CDL	PB2-OB5	2.24	1.68	1.59
56	i	401	CDL	PB2-OB2	2.23	1.68	1.59
49	J	403	PLX	P1-O4	2.23	1.68	1.59
56	r	503	CDL	PB2-OB5	2.23	1.68	1.59
56	l	702	CDL	PB2-OB2	2.23	1.68	1.59
48	r	501	PEE	O2-C10	2.23	1.40	1.34
56	i	401	CDL	OB6-CB4	-2.23	1.41	1.46
56	V	204	CDL	PB2-OB2	2.22	1.68	1.59
56	l	701	CDL	PB2-OB5	2.22	1.68	1.59
56	l	701	CDL	PB2-OB2	2.21	1.68	1.59
48	V	203	PEE	O3-C3	-2.20	1.40	1.45
53	J	402	UQ	C7-C8	2.20	1.54	1.50
48	W	201	PEE	O3-C3	-2.20	1.40	1.45
50	C	304	DCQ	O3-C3M	-2.20	1.40	1.45
56	a	201	CDL	PB2-OB5	2.20	1.68	1.59
49	j	203	PLX	P1-O4	2.19	1.68	1.59
56	s	401	CDL	PB2-OB5	2.19	1.68	1.59
49	g	201	PLX	P1-O4	2.18	1.67	1.59
56	V	202	CDL	PB2-OB5	2.18	1.67	1.59
56	V	204	CDL	PB2-OB5	2.18	1.67	1.59
49	C	303	PLX	P1-O4	2.18	1.67	1.59
49	e	201	PLX	P1-O4	2.17	1.67	1.59
56	l	702	CDL	PB2-OB5	2.17	1.67	1.59
48	l	703	PEE	O3-C3	-2.17	1.40	1.45
48	B	303	PEE	O3-C3	-2.17	1.40	1.45
48	C	302	PEE	O3-C3	-2.16	1.40	1.45
48	r	501	PEE	O3-C3	-2.16	1.40	1.45
56	V	201	CDL	OA6-CA4	-2.15	1.41	1.46
53	s	402	UQ	O4-C4	-2.15	1.18	1.23
49	a	202	PLX	P1-O4	2.15	1.67	1.59
49	r	502	PLX	P1-O4	2.14	1.67	1.59
53	J	402	UQ	C21-C19	2.14	1.55	1.51
49	r	502	PLX	C25-C24	2.13	1.55	1.50
52	J	401	NDP	O7N-C7N	-2.13	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	s	402	UQ	O3-CM3	-2.13	1.40	1.45
48	l	704	PEE	O3-C3	-2.13	1.40	1.45
52	J	401	NDP	PA-O5B	2.13	1.67	1.59
49	e	201	PLX	P1-O1	2.12	1.67	1.59
48	j	202	PEE	O3-C3	-2.12	1.40	1.45
48	j	201	PEE	O3-C3	-2.11	1.40	1.45
53	J	402	UQ	O4-C4	-2.11	1.18	1.23
49	j	203	PLX	P1-O1	2.11	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.11	1.35	1.39
49	J	403	PLX	P1-O1	2.11	1.67	1.59
49	C	303	PLX	P1-O1	2.10	1.67	1.59
56	V	201	CDL	C11-CA5	2.07	1.56	1.50
49	a	202	PLX	P1-O1	2.07	1.67	1.59
49	r	502	PLX	P1-O1	2.07	1.67	1.59
49	g	201	PLX	P1-O1	2.07	1.67	1.59
53	s	402	UQ	C21-C19	2.06	1.55	1.51
51	G	201	8Q1	C6-C1	2.06	1.52	1.50
53	J	402	UQ	O3-CM3	-2.06	1.40	1.45
56	V	202	CDL	C11-CA5	2.05	1.56	1.50
53	s	402	UQ	C5-C4	2.03	1.54	1.47
49	e	201	PLX	C1-C2	2.03	1.57	1.51
56	s	401	CDL	C11-CA5	2.03	1.56	1.50
49	a	202	PLX	C25-C24	2.02	1.55	1.50
49	g	201	PLX	C25-C24	2.02	1.54	1.50
56	l	702	CDL	C11-CA5	2.01	1.56	1.50
56	n	101	CDL	C11-CA5	2.00	1.56	1.50
49	j	203	PLX	C1-C2	2.00	1.57	1.51

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C7-C8-C9	-7.77	113.45	126.83
52	J	401	NDP	C3N-C2N-N1N	-7.59	112.06	123.20
52	J	401	NDP	C1D-N1N-C2N	-7.27	109.16	121.14
53	s	402	UQ	C7-C8-C9	-6.81	115.10	126.83
52	J	401	NDP	C6N-N1N-C2N	-6.61	112.24	119.32
51	G	201	8Q1	C6-C1-S44	6.52	121.17	113.40
53	J	402	UQ	C12-C13-C14	-6.31	113.19	127.62
53	J	402	UQ	C17-C18-C19	-6.21	113.40	127.62
53	s	402	UQ	C12-C13-C14	-6.06	113.74	127.62
53	s	402	UQ	C22-C23-C24	-5.94	114.02	127.62
53	s	402	UQ	C17-C18-C19	-5.88	114.16	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	X	201	8Q1	C6-C1-S44	5.78	120.29	113.40
52	J	401	NDP	C5A-C4A-N3A	-5.68	118.89	126.72
52	J	401	NDP	C1D-N1N-C6N	-5.58	108.96	120.77
58	w	401	ADP	C5-C4-N3	-5.41	119.27	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.37	119.32	126.72
58	w	401	ADP	N3-C2-N1	-4.67	121.51	128.58
53	s	402	UQ	C10-C9-C8	-4.57	111.89	123.63
47	A	503	NAI	N3A-C2A-N1A	-4.47	121.81	128.58
53	J	402	UQ	C10-C9-C8	-4.47	112.16	123.63
56	s	401	CDL	OA6-CA5-C11	4.38	120.96	111.48
53	s	402	UQ	C27-C28-C29	-4.37	113.08	127.64
53	s	402	UQ	C25-C24-C23	-4.33	112.51	123.63
58	w	401	ADP	N3-C4-N9	4.29	134.46	127.17
53	J	402	UQ	C22-C23-C24	-4.27	113.40	127.64
53	J	402	UQ	C15-C14-C13	-4.22	112.79	123.63
52	J	401	NDP	N3A-C2A-N1A	-4.20	122.23	128.58
56	V	201	CDL	OB6-CB5-C51	4.16	120.48	111.48
53	J	402	UQ	C20-C19-C18	-4.11	113.07	123.63
56	N	201	CDL	OB6-CB5-C51	4.11	120.37	111.48
48	j	202	PEE	O2-C10-C11	4.05	120.25	111.48
51	G	201	8Q1	O4-C1-C6	-4.05	119.31	123.98
56	V	204	CDL	OB6-CB5-C51	4.04	120.22	111.48
56	V	202	CDL	OA6-CA5-C11	4.04	120.22	111.48
48	C	302	PEE	O2-C10-C11	4.03	120.20	111.48
52	J	401	NDP	N3A-C4A-N9A	4.02	134.00	127.17
48	B	303	PEE	O2-C10-C11	3.98	120.09	111.48
56	r	503	CDL	OA6-CA5-C11	3.97	120.06	111.48
56	s	401	CDL	OB6-CB5-C51	3.97	120.06	111.48
48	V	203	PEE	O2-C10-C11	3.95	120.03	111.48
56	a	201	CDL	OB6-CB5-C51	3.95	120.02	111.48
56	i	401	CDL	OB6-CB5-C51	3.95	120.02	111.48
56	n	101	CDL	OA6-CA5-C11	3.94	120.00	111.48
56	l	701	CDL	OA6-CA5-C11	3.92	119.97	111.48
53	J	402	UQ	C16-C14-C13	-3.92	112.37	121.17
56	V	202	CDL	OB6-CB5-C51	3.91	119.95	111.48
56	r	503	CDL	OB6-CB5-C51	3.91	119.95	111.48
48	l	704	PEE	O2-C10-C11	3.91	119.94	111.48
56	l	702	CDL	OA6-CA5-C11	3.91	119.93	111.48
53	s	402	UQ	C20-C19-C18	-3.90	113.61	123.63
56	n	101	CDL	OB6-CB5-C51	3.89	119.90	111.48
48	r	501	PEE	O2-C10-C11	3.85	119.82	111.48
53	s	402	UQ	C15-C14-C13	-3.85	113.74	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	V	201	CDL	OA6-CA5-C11	3.85	119.81	111.48
48	j	201	PEE	O2-C10-C11	3.84	119.79	111.48
56	N	201	CDL	OA6-CA5-C11	3.84	119.78	111.48
56	l	701	CDL	OB6-CB5-C51	3.81	119.73	111.48
47	A	503	NAI	N3A-C4A-N9A	3.80	133.63	127.17
56	i	401	CDL	OA6-CA5-C11	3.78	119.66	111.48
48	W	201	PEE	O2-C10-C11	3.76	119.62	111.48
48	l	703	PEE	O2-C10-C11	3.73	119.54	111.48
53	s	402	UQ	C21-C19-C18	-3.69	112.88	121.17
47	A	503	NAI	C2A-N3A-C4A	3.67	120.80	111.83
52	J	401	NDP	C2A-N3A-C4A	3.67	120.80	111.83
53	s	402	UQ	C11-C9-C8	-3.66	112.95	121.17
53	J	402	UQ	C11-C9-C8	-3.64	113.00	121.17
58	w	401	ADP	N9-C8-N7	-3.62	108.80	113.94
56	l	702	CDL	OB6-CB5-C51	3.61	119.29	111.48
53	s	402	UQ	C16-C14-C13	-3.60	113.08	121.17
58	w	401	ADP	C2-N3-C4	3.58	120.58	111.83
56	a	201	CDL	OA6-CA5-C11	3.54	119.13	111.48
51	X	201	8Q1	O4-C1-C6	-3.47	119.97	123.98
53	J	402	UQ	C21-C19-C18	-3.44	113.44	121.17
47	A	503	NAI	C4A-C5A-N7A	-3.40	106.69	110.58
47	A	503	NAI	C5A-N7A-C8A	3.38	108.77	103.45
53	s	402	UQ	C26-C24-C23	-3.38	113.58	121.17
56	V	204	CDL	OA6-CA5-C11	3.37	118.77	111.48
51	G	201	8Q1	C37-C38-C39	3.37	118.00	112.39
47	A	503	NAI	N9A-C8A-N7A	-3.34	109.20	113.94
58	w	401	ADP	C5-N7-C8	3.29	108.62	103.45
46	A	502	FMN	C4-N3-C2	-3.27	119.83	125.64
58	w	401	ADP	C4-N9-C8	3.27	109.17	105.74
53	s	402	UQ	C30-C29-C28	-3.25	112.91	122.66
52	J	401	NDP	C4A-C5A-N7A	-3.24	106.88	110.58
53	J	402	UQ	C26-C24-C23	-3.22	112.99	122.66
53	s	402	UQ	C31-C29-C28	-3.22	113.00	122.66
53	J	402	UQ	C25-C24-C23	-3.15	113.19	122.66
52	J	401	NDP	N9A-C8A-N7A	-3.14	109.48	113.94
52	J	401	NDP	C5A-N7A-C8A	3.10	108.32	103.45
47	A	503	NAI	C3D-C2D-C1D	3.08	107.30	101.46
58	w	401	ADP	C4-C5-N7	-3.01	107.14	110.58
47	A	503	NAI	C2D-C3D-C4D	2.98	108.36	102.61
56	n	101	CDL	OA8-CA7-C31	2.93	120.06	111.15
48	B	303	PEE	O3-C30-C31	2.92	120.73	111.83
56	V	204	CDL	OB8-CB7-C71	2.91	120.71	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	l	701	CDL	OA8-CA7-C31	2.88	120.61	111.83
53	J	402	UQ	C7-C6-C5	-2.85	120.00	124.89
56	V	204	CDL	OA8-CA7-C31	2.85	120.53	111.83
56	N	201	CDL	OB8-CB7-C71	2.79	120.35	111.83
56	i	401	CDL	OA8-CA7-C31	2.78	120.31	111.83
56	V	201	CDL	OB8-CB7-C71	2.78	120.30	111.83
56	a	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
56	n	101	CDL	OB8-CB7-C71	2.77	120.27	111.83
56	r	503	CDL	OB8-CB7-C71	2.74	120.20	111.83
48	l	704	PEE	O3-C30-C31	2.74	120.20	111.83
48	r	501	PEE	O3-C30-C31	2.74	120.18	111.83
48	V	203	PEE	O3-C30-C31	2.73	120.15	111.83
48	l	703	PEE	O3-C30-C31	2.72	120.13	111.83
56	V	202	CDL	OB8-CB7-C71	2.71	120.10	111.83
56	l	701	CDL	OB8-CB7-C71	2.71	120.09	111.83
56	a	201	CDL	OA8-CA7-C31	2.71	120.09	111.83
51	X	201	8Q1	C37-C38-C39	2.70	116.89	112.39
56	i	401	CDL	OB8-CB7-C71	2.68	120.02	111.83
48	j	202	PEE	O3-C30-C31	2.68	120.01	111.83
56	r	503	CDL	OA8-CA7-C31	2.67	119.97	111.83
56	V	201	CDL	OA8-CA7-C31	2.65	119.93	111.83
46	A	502	FMN	C4A-C4-N3	2.65	119.99	113.25
56	N	201	CDL	OA8-CA7-C31	2.65	119.90	111.83
56	l	702	CDL	OB8-CB7-C71	2.64	119.88	111.83
56	l	702	CDL	OA8-CA7-C31	2.64	119.88	111.83
48	j	201	PEE	O3-C30-C31	2.63	119.87	111.83
56	s	401	CDL	OA8-CA7-C31	2.63	119.85	111.83
48	C	302	PEE	O3-C30-C31	2.63	119.84	111.83
58	w	401	ADP	C4'-O4'-C1'	-2.62	103.68	109.47
51	X	201	8Q1	C43-S44-C1	2.61	109.56	101.84
48	W	201	PEE	O3-C30-C31	2.61	119.79	111.83
56	s	401	CDL	OB8-CB7-C71	2.59	119.73	111.83
56	V	202	CDL	OA8-CA7-C31	2.58	119.70	111.83
51	X	201	8Q1	C38-C39-N41	2.58	121.04	116.34
50	C	304	DCQ	C1M-C1-C6	-2.57	120.22	124.45
49	r	502	PLX	C1A-N1-C1	2.56	120.08	109.91
46	A	502	FMN	O4-C4-C4A	-2.55	119.79	126.53
53	J	402	UQ	CM5-C5-C6	-2.54	120.28	124.45
51	G	201	8Q1	O4-C1-S44	-2.49	119.52	122.68
49	a	202	PLX	C1A-N1-C1	2.47	119.74	109.91
47	A	503	NAI	C4A-N9A-C8A	2.44	108.30	105.74
49	j	203	PLX	C1A-N1-C1	2.42	119.55	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C4A-C10-N10	2.40	119.91	116.48
49	g	201	PLX	C1A-N1-C1	2.39	119.42	109.91
49	J	403	PLX	C1A-N1-C1	2.36	119.30	109.91
52	J	401	NDP	C4A-N9A-C8A	2.36	108.22	105.74
49	C	303	PLX	C1A-N1-C1	2.35	119.24	109.91
48	V	203	PEE	C20-C19-C18	-2.32	112.44	126.42
51	X	201	8Q1	O4-C1-S44	-2.32	119.74	122.68
46	A	502	FMN	C5A-C9A-N10	2.29	120.04	117.97
46	A	502	FMN	C4A-C10-N1	-2.26	119.04	124.59
56	s	401	CDL	CA4-OA6-CA5	-2.20	112.54	117.80
46	A	502	FMN	C10-C4A-N5	-2.19	120.34	124.81
47	A	503	NAI	C4D-O4D-C1D	-2.19	104.63	109.47
51	G	201	8Q1	C43-S44-C1	2.15	108.21	101.84
46	A	502	FMN	C9A-C5A-N5	-2.14	120.18	122.45
51	X	201	8Q1	C42-N41-C39	-2.14	118.84	122.82
56	V	201	CDL	CB4-OB6-CB5	-2.11	112.74	117.80
52	J	401	NDP	C2B-C1B-N9A	-2.09	110.31	113.75
52	J	401	NDP	P2B-O2B-C2B	-2.05	117.96	123.43
51	X	201	8Q1	C32-C34-N36	2.02	120.32	116.48
56	V	202	CDL	CB4-OB6-CB5	-2.00	113.01	117.80

There are no chirality outliers.

All (1066) 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'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	A	503	NAI	PN-O3-PA-O5B
48	C	302	PEE	C1-O3P-P-O1P
48	V	203	PEE	C1-O3P-P-O2P
48	V	203	PEE	C1-O3P-P-O4P
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O4P
48	j	202	PEE	C11-C10-O2-C2
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	l	703	PEE	C4-O4P-P-O3P
48	l	704	PEE	C1-O3P-P-O1P
48	l	704	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	O6-C6-C7-C8
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	C2-O1-P1-O4
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	C2-O1-P1-O3
49	C	303	PLX	N1-C1-C2-O1
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O7-C6-C7-C8
49	J	403	PLX	C7-C6-O6-C4
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-O4-P1-O1
49	J	403	PLX	C3-O4-P1-O2
49	J	403	PLX	C3-O4-P1-O3
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C3-O4-P1-O3
49	a	202	PLX	O9-C24-C25-C26
49	e	201	PLX	O7-C6-O6-C4
49	e	201	PLX	O9-C24-O8-C5
49	e	201	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O2
49	g	201	PLX	C2-O1-P1-O3
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	O6-C6-C7-C8
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	O9-C24-C25-C26
51	G	201	8Q1	O4-C1-S44-C43
51	G	201	8Q1	C6-C1-S44-C43
51	G	201	8Q1	O27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	G	201	8Q1	O27-C28-C29-C31
51	G	201	8Q1	O27-C28-C29-C32
51	G	201	8Q1	N41-C42-C43-S44
51	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
51	X	201	8Q1	C42-C43-S44-C1
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C15
53	J	402	UQ	C16-C17-C18-C19
53	J	402	UQ	C17-C18-C19-C21
53	J	402	UQ	C22-C23-C24-C26
53	s	402	UQ	C7-C8-C9-C10
53	s	402	UQ	C7-C8-C9-C11
53	s	402	UQ	C22-C23-C24-C26
56	N	201	CDL	CA3-OA5-PA1-OA3
56	N	201	CDL	CB2-OB2-PB2-OB3
56	N	201	CDL	CB2-OB2-PB2-OB4
56	N	201	CDL	CB2-OB2-PB2-OB5
56	N	201	CDL	CB3-OB5-PB2-OB3
56	V	201	CDL	CA2-OA2-PA1-OA5
56	V	201	CDL	CA3-OA5-PA1-OA2
56	V	201	CDL	CA3-OA5-PA1-OA3
56	V	201	CDL	CA3-OA5-PA1-OA4
56	V	201	CDL	C11-CA5-OA6-CA4
56	V	201	CDL	CB2-OB2-PB2-OB3
56	V	201	CDL	CB2-OB2-PB2-OB5
56	V	201	CDL	CB3-OB5-PB2-OB2
56	V	201	CDL	CB3-OB5-PB2-OB3
56	V	201	CDL	CB3-OB5-PB2-OB4
56	V	202	CDL	CB2-C1-CA2-OA2
56	V	202	CDL	CA2-OA2-PA1-OA5
56	V	202	CDL	CA3-OA5-PA1-OA2
56	V	202	CDL	CA3-OA5-PA1-OA3
56	V	202	CDL	CB2-OB2-PB2-OB3
56	V	202	CDL	CB2-OB2-PB2-OB5
56	V	202	CDL	CB3-OB5-PB2-OB2
56	V	202	CDL	CB3-OB5-PB2-OB3
56	V	204	CDL	CA2-OA2-PA1-OA3
56	V	204	CDL	CA3-OA5-PA1-OA2
56	V	204	CDL	CA3-OA5-PA1-OA4
56	V	204	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
56	V	204	CDL	CB2-OB2-PB2-OB3
56	V	204	CDL	CB2-OB2-PB2-OB4
56	V	204	CDL	CB2-OB2-PB2-OB5
56	a	201	CDL	CA2-OA2-PA1-OA3
56	a	201	CDL	CA2-OA2-PA1-OA4
56	a	201	CDL	CA2-OA2-PA1-OA5
56	a	201	CDL	CB2-OB2-PB2-OB3
56	a	201	CDL	CB2-OB2-PB2-OB4
56	a	201	CDL	CB2-OB2-PB2-OB5
56	a	201	CDL	CB3-OB5-PB2-OB3
56	i	401	CDL	O1-C1-CB2-OB2
56	i	401	CDL	CA2-C1-CB2-OB2
56	i	401	CDL	CA2-OA2-PA1-OA3
56	i	401	CDL	CA2-OA2-PA1-OA4
56	i	401	CDL	CA2-OA2-PA1-OA5
56	i	401	CDL	CA3-OA5-PA1-OA3
56	i	401	CDL	OA9-CA7-OA8-CA6
56	i	401	CDL	C31-CA7-OA8-CA6
56	l	701	CDL	CB2-C1-CA2-OA2
56	l	701	CDL	O1-C1-CB2-OB2
56	l	701	CDL	CA2-OA2-PA1-OA3
56	l	701	CDL	CA2-OA2-PA1-OA4
56	l	701	CDL	CA2-OA2-PA1-OA5
56	l	701	CDL	OA5-CA3-CA4-OA6
56	l	701	CDL	OA9-CA7-OA8-CA6
56	l	701	CDL	C31-CA7-OA8-CA6
56	l	701	CDL	CB2-OB2-PB2-OB4
56	l	701	CDL	CB2-OB2-PB2-OB5
56	l	702	CDL	O1-C1-CA2-OA2
56	l	702	CDL	O1-C1-CB2-OB2
56	l	702	CDL	CA2-C1-CB2-OB2
56	l	702	CDL	CA2-OA2-PA1-OA4
56	l	702	CDL	CA2-OA2-PA1-OA5
56	l	702	CDL	CB2-OB2-PB2-OB3
56	l	702	CDL	CB2-OB2-PB2-OB4
56	l	702	CDL	CB2-OB2-PB2-OB5
56	l	702	CDL	OB6-CB4-CB6-OB8
56	n	101	CDL	CA2-OA2-PA1-OA4
56	n	101	CDL	CA2-OA2-PA1-OA5
56	n	101	CDL	CA3-OA5-PA1-OA2
56	n	101	CDL	CA3-OA5-PA1-OA3
56	n	101	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
56	n	101	CDL	CB2-OB2-PB2-OB4
56	n	101	CDL	CB2-OB2-PB2-OB5
56	n	101	CDL	CB3-OB5-PB2-OB2
56	n	101	CDL	CB3-OB5-PB2-OB3
56	n	101	CDL	CB3-OB5-PB2-OB4
56	r	503	CDL	O1-C1-CA2-OA2
56	r	503	CDL	CA3-OA5-PA1-OA3
56	r	503	CDL	CB2-OB2-PB2-OB3
56	r	503	CDL	CB2-OB2-PB2-OB4
56	r	503	CDL	CB2-OB2-PB2-OB5
56	r	503	CDL	CB3-OB5-PB2-OB2
56	r	503	CDL	CB3-OB5-PB2-OB3
56	r	503	CDL	CB3-OB5-PB2-OB4
56	s	401	CDL	CA2-OA2-PA1-OA3
56	s	401	CDL	C31-CA7-OA8-CA6
56	s	401	CDL	C51-CB5-OB6-CB4
58	w	401	ADP	C5'-O5'-PA-O2A
58	w	401	ADP	C5'-O5'-PA-O3A
56	s	401	CDL	OA9-CA7-OA8-CA6
48	B	303	PEE	O4-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	j	202	PEE	O4-C10-O2-C2
56	V	201	CDL	OA7-CA5-OA6-CA4
56	s	401	CDL	OB7-CB5-OB6-CB4
50	C	304	DCQ	C6-C7-C8-C9
48	j	201	PEE	C11-C10-O2-C2
53	s	402	UQ	C18-C19-C21-C22
53	s	402	UQ	C23-C24-C26-C27
53	J	402	UQ	C17-C18-C19-C20
48	V	203	PEE	C17-C18-C19-C20
53	J	402	UQ	C12-C13-C14-C16
53	s	402	UQ	C17-C18-C19-C21
56	l	702	CDL	C35-C36-C37-C38
56	N	201	CDL	O1-C1-CA2-OA2
56	N	201	CDL	O1-C1-CB2-OB2
56	V	202	CDL	O1-C1-CA2-OA2
56	V	204	CDL	O1-C1-CB2-OB2
56	n	101	CDL	O1-C1-CA2-OA2
48	B	303	PEE	C11-C10-O2-C2
48	V	203	PEE	C11-C10-O2-C2
48	l	703	PEE	C11-C10-O2-C2
48	l	704	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C11-C10-O2-C2
56	N	201	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	C11-C12-C13-C14
58	w	401	ADP	O4'-C4'-C5'-O5'
53	J	402	UQ	C12-C11-C9-C8
48	V	203	PEE	O4-C10-O2-C2
53	J	402	UQ	C14-C16-C17-C18
53	s	402	UQ	C14-C16-C17-C18
49	r	502	PLX	C7-C8-C9-C10
53	J	402	UQ	C22-C23-C24-C25
53	s	402	UQ	C27-C28-C29-C31
48	W	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
49	J	403	PLX	C9-C10-C11-C12
48	l	703	PEE	O4-C10-O2-C2
48	r	501	PEE	O4-C10-O2-C2
56	V	201	CDL	CA2-C1-CB2-OB2
56	l	701	CDL	CA2-C1-CB2-OB2
56	n	101	CDL	CB2-C1-CA2-OA2
56	s	401	CDL	CA2-C1-CB2-OB2
56	V	201	CDL	C71-CB7-OB8-CB6
56	V	202	CDL	C31-CA7-OA8-CA6
49	j	203	PLX	C13-C14-C15-C16
56	s	401	CDL	C14-C15-C16-C17
56	l	702	CDL	C71-C72-C73-C74
49	g	201	PLX	C7-C8-C9-C10
49	r	502	PLX	C9-C10-C11-C12
56	r	503	CDL	C76-C77-C78-C79
53	J	402	UQ	C13-C14-C16-C17
53	s	402	UQ	C13-C14-C16-C17
49	j	203	PLX	C28-C29-C30-C31
56	N	201	CDL	CB5-C51-C52-C53
56	l	701	CDL	CA5-C11-C12-C13
56	V	204	CDL	O1-C1-CA2-OA2
56	i	401	CDL	O1-C1-CA2-OA2
56	l	701	CDL	O1-C1-CA2-OA2
56	s	401	CDL	O1-C1-CB2-OB2
56	V	201	CDL	C59-C60-C61-C62
56	V	202	CDL	C17-C18-C19-C20
56	V	202	CDL	C37-C38-C39-C40
56	V	202	CDL	C76-C77-C78-C79
48	l	704	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
56	N	201	CDL	OB7-CB5-OB6-CB4
48	r	501	PEE	O3P-C1-C2-O2
56	N	201	CDL	OA5-CA3-CA4-OA6
56	V	201	CDL	OB5-CB3-CB4-OB6
56	s	401	CDL	OA5-CA3-CA4-OA6
56	i	401	CDL	OB6-CB4-CB6-OB8
48	l	703	PEE	C31-C30-O3-C3
56	n	101	CDL	CB5-C51-C52-C53
49	r	502	PLX	C11-C12-C13-C14
56	V	204	CDL	C58-C59-C60-C61
48	B	303	PEE	C17-C18-C19-C20
48	l	704	PEE	C37-C38-C39-C40
56	V	201	CDL	OB9-CB7-OB8-CB6
52	J	401	NDP	O4D-C4D-C5D-O5D
48	j	201	PEE	C31-C30-O3-C3
49	J	403	PLX	C25-C26-C27-C28
56	r	503	CDL	C74-C75-C76-C77
56	N	201	CDL	CA7-C31-C32-C33
56	a	201	CDL	CB7-C71-C72-C73
56	i	401	CDL	CB5-C51-C52-C53
56	l	701	CDL	CB5-C51-C52-C53
56	V	202	CDL	OA9-CA7-OA8-CA6
56	V	202	CDL	C51-CB5-OB6-CB4
56	V	201	CDL	CA5-C11-C12-C13
56	n	101	CDL	CB7-C71-C72-C73
56	s	401	CDL	CA5-C11-C12-C13
56	l	701	CDL	C58-C59-C60-C61
49	g	201	PLX	C9-C10-C11-C12
56	l	702	CDL	C51-C52-C53-C54
56	V	201	CDL	O1-C1-CB2-OB2
56	V	202	CDL	O1-C1-CB2-OB2
56	a	201	CDL	O1-C1-CA2-OA2
56	r	503	CDL	O1-C1-CB2-OB2
48	V	203	PEE	C30-C31-C32-C33
48	l	703	PEE	O5-C30-O3-C3
56	V	204	CDL	C43-C44-C45-C46
56	l	701	CDL	C55-C56-C57-C58
56	V	204	CDL	C36-C37-C38-C39
56	a	201	CDL	C71-CB7-OB8-CB6
56	n	101	CDL	C75-C76-C77-C78
52	J	401	NDP	C2D-C1D-N1N-C6N
56	a	201	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
56	V	201	CDL	C32-C33-C34-C35
56	V	202	CDL	OB7-CB5-OB6-CB4
56	N	201	CDL	CB2-C1-CA2-OA2
56	V	202	CDL	CA2-C1-CB2-OB2
56	V	204	CDL	CB2-C1-CA2-OA2
56	a	201	CDL	CB2-C1-CA2-OA2
56	i	401	CDL	CB2-C1-CA2-OA2
56	l	702	CDL	CB2-C1-CA2-OA2
56	r	503	CDL	CB2-C1-CA2-OA2
56	l	701	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C34-C35-C36-C37
56	V	202	CDL	C33-C34-C35-C36
56	l	701	CDL	C16-C17-C18-C19
56	V	201	CDL	C34-C35-C36-C37
56	V	204	CDL	C13-C14-C15-C16
48	j	201	PEE	O5-C30-O3-C3
49	a	202	PLX	C34-C35-C36-C37
56	s	401	CDL	CB7-C71-C72-C73
49	j	203	PLX	O6-C6-C7-C8
56	V	204	CDL	C11-CA5-OA6-CA4
56	r	503	CDL	C51-CB5-OB6-CB4
56	V	204	CDL	OA7-CA5-OA6-CA4
56	r	503	CDL	OB7-CB5-OB6-CB4
48	r	501	PEE	C17-C18-C19-C20
48	W	201	PEE	C31-C30-O3-C3
56	i	401	CDL	CB7-C71-C72-C73
56	V	201	CDL	C53-C54-C55-C56
56	l	702	CDL	C51-CB5-OB6-CB4
48	j	202	PEE	C31-C30-O3-C3
49	g	201	PLX	C27-C28-C29-C30
56	V	204	CDL	C55-C56-C57-C58
56	l	701	CDL	C75-C76-C77-C78
48	B	303	PEE	C20-C21-C22-C23
48	j	202	PEE	C23-C24-C25-C26
49	a	202	PLX	C10-C11-C12-C13
56	V	204	CDL	C71-C72-C73-C74
56	i	401	CDL	C37-C38-C39-C40
56	i	401	CDL	C76-C77-C78-C79
56	n	101	CDL	C74-C75-C76-C77
56	s	401	CDL	C73-C74-C75-C76
48	B	303	PEE	C13-C14-C15-C16
49	g	201	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
56	V	202	CDL	C34-C35-C36-C37
56	V	204	CDL	C32-C33-C34-C35
56	V	204	CDL	C59-C60-C61-C62
56	s	401	CDL	C18-C19-C20-C21
56	s	401	CDL	C52-C53-C54-C55
49	C	303	PLX	O9-C24-C25-C26
49	J	403	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
48	r	501	PEE	C31-C32-C33-C34
49	J	403	PLX	C12-C13-C14-C15
49	a	202	PLX	C13-C14-C15-C16
49	j	203	PLX	C7-C8-C9-C10
49	j	203	PLX	C27-C28-C29-C30
49	r	502	PLX	C28-C29-C30-C31
56	V	201	CDL	C37-C38-C39-C40
56	V	202	CDL	C56-C57-C58-C59
56	V	204	CDL	C11-C12-C13-C14
56	V	204	CDL	C56-C57-C58-C59
56	V	204	CDL	C73-C74-C75-C76
56	V	204	CDL	C76-C77-C78-C79
56	l	701	CDL	C52-C53-C54-C55
56	r	503	CDL	C75-C76-C77-C78
48	r	501	PEE	C11-C12-C13-C14
49	J	403	PLX	C27-C28-C29-C30
49	r	502	PLX	C27-C28-C29-C30
49	r	502	PLX	C11-C10-C9-C8
56	a	201	CDL	OB9-CB7-OB8-CB6
48	C	302	PEE	C11-C10-O2-C2
48	j	202	PEE	C14-C15-C16-C17
56	V	204	CDL	C78-C79-C80-C81
56	l	702	CDL	C15-C16-C17-C18
56	V	204	CDL	CA7-C31-C32-C33
58	w	401	ADP	C3'-C4'-C5'-O5'
48	W	201	PEE	C12-C13-C14-C15
48	j	202	PEE	C11-C12-C13-C14
49	j	203	PLX	C25-C26-C27-C28
56	V	202	CDL	C15-C16-C17-C18
56	l	701	CDL	C51-C52-C53-C54
56	l	701	CDL	C62-C63-C64-C65
56	l	701	CDL	OB9-CB7-OB8-CB6
49	a	202	PLX	C9-C10-C11-C12
49	e	201	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
56	r	503	CDL	C43-C44-C45-C46
56	r	503	CDL	C71-C72-C73-C74
56	s	401	CDL	C15-C16-C17-C18
49	r	502	PLX	C33-C34-C35-C36
56	r	503	CDL	C59-C60-C61-C62
48	W	201	PEE	C13-C14-C15-C16
49	a	202	PLX	C7-C8-C9-C10
49	g	201	PLX	C13-C14-C15-C16
56	V	202	CDL	C75-C76-C77-C78
56	a	201	CDL	C21-C22-C23-C24
56	a	201	CDL	C35-C36-C37-C38
56	i	401	CDL	C81-C82-C83-C84
56	s	401	CDL	C34-C35-C36-C37
56	l	702	CDL	OB7-CB5-OB6-CB4
49	j	203	PLX	C14-C15-C16-C17
56	V	202	CDL	C59-C60-C61-C62
56	n	101	CDL	C71-C72-C73-C74
48	B	303	PEE	C31-C30-O3-C3
56	l	702	CDL	C71-CB7-OB8-CB6
49	e	201	PLX	C13-C14-C15-C16
56	V	201	CDL	C56-C57-C58-C59
56	l	701	CDL	C56-C57-C58-C59
56	l	702	CDL	C75-C76-C77-C78
56	r	503	CDL	C62-C63-C64-C65
48	C	302	PEE	C11-C12-C13-C14
49	C	303	PLX	C9-C10-C11-C12
49	J	403	PLX	C10-C11-C12-C13
49	a	202	PLX	C12-C13-C14-C15
49	e	201	PLX	C11-C10-C9-C8
49	g	201	PLX	C33-C34-C35-C36
49	j	203	PLX	C9-C10-C11-C12
49	r	502	PLX	C31-C32-C33-C34
56	V	201	CDL	C71-C72-C73-C74
56	l	701	CDL	C59-C60-C61-C62
56	l	702	CDL	C21-C22-C23-C24
56	n	101	CDL	C54-C55-C56-C57
56	r	503	CDL	C41-C42-C43-C44
56	s	401	CDL	C71-C72-C73-C74
51	X	201	8Q1	C12-C13-C14-C15
49	j	203	PLX	C16-C17-C18-C19
56	a	201	CDL	C36-C37-C38-C39
56	l	701	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
56	r	503	CDL	C33-C34-C35-C36
56	r	503	CDL	C55-C56-C57-C58
49	g	201	PLX	C2-C1-N1-C1A
48	j	201	PEE	C22-C23-C24-C25
49	g	201	PLX	C30-C31-C32-C33
56	V	204	CDL	C18-C19-C20-C21
48	W	201	PEE	O5-C30-O3-C3
51	G	201	8Q1	C11-C12-C13-C14
56	V	202	CDL	C41-C42-C43-C44
56	s	401	CDL	C32-C33-C34-C35
56	a	201	CDL	C11-CA5-OA6-CA4
56	N	201	CDL	C31-CA7-OA8-CA6
49	j	203	PLX	C12-C13-C14-C15
56	V	201	CDL	C54-C55-C56-C57
49	g	201	PLX	C10-C11-C12-C13
56	r	503	CDL	C15-C16-C17-C18
48	r	501	PEE	C30-C31-C32-C33
56	i	401	CDL	C14-C15-C16-C17
56	r	503	CDL	C16-C17-C18-C19
56	s	401	CDL	C35-C36-C37-C38
48	j	202	PEE	O5-C30-O3-C3
48	V	203	PEE	C32-C33-C34-C35
48	C	302	PEE	O4-C10-O2-C2
56	V	202	CDL	C55-C56-C57-C58
48	r	501	PEE	C33-C34-C35-C36
56	V	201	CDL	C21-C22-C23-C24
56	a	201	CDL	C34-C35-C36-C37
56	l	701	CDL	C72-C73-C74-C75
56	l	701	CDL	CA7-C31-C32-C33
48	V	203	PEE	C31-C30-O3-C3
56	V	201	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C23-C24-C25-C26
48	l	704	PEE	C14-C15-C16-C17
49	g	201	PLX	C11-C12-C13-C14
49	r	502	PLX	C13-C14-C15-C16
56	i	401	CDL	C59-C60-C61-C62
56	l	701	CDL	C35-C36-C37-C38
56	n	101	CDL	C73-C74-C75-C76
48	j	201	PEE	C21-C22-C23-C24
56	r	503	CDL	C34-C35-C36-C37
49	r	502	PLX	C30-C31-C32-C33
50	C	304	DCQ	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
56	V	201	CDL	C52-C53-C54-C55
49	j	203	PLX	C11-C12-C13-C14
56	r	503	CDL	C82-C83-C84-C85
49	g	201	PLX	C25-C26-C27-C28
56	V	204	CDL	C39-C40-C41-C42
56	V	201	CDL	C51-CB5-OB6-CB4
56	s	401	CDL	CA7-C31-C32-C33
56	i	401	CDL	C55-C56-C57-C58
56	r	503	CDL	C81-C82-C83-C84
48	B	303	PEE	C35-C36-C37-C38
48	j	202	PEE	C15-C16-C17-C18
56	V	204	CDL	C64-C65-C66-C67
48	j	202	PEE	C22-C23-C24-C25
49	C	303	PLX	C17-C18-C19-C20
56	l	701	CDL	C36-C37-C38-C39
47	A	503	NAI	O4B-C4B-C5B-O5B
49	a	202	PLX	C11-C12-C13-C14
49	e	201	PLX	C17-C18-C19-C20
49	g	201	PLX	C12-C13-C14-C15
49	j	203	PLX	C33-C34-C35-C36
56	V	202	CDL	C52-C53-C54-C55
56	V	202	CDL	C74-C75-C76-C77
49	g	201	PLX	C2-C1-N1-C1B
49	r	502	PLX	C12-C13-C14-C15
56	V	204	CDL	C81-C82-C83-C84
56	l	702	CDL	C55-C56-C57-C58
56	s	401	CDL	C37-C38-C39-C40
48	B	303	PEE	O5-C30-O3-C3
56	l	702	CDL	OB9-CB7-OB8-CB6
56	n	101	CDL	C51-C52-C53-C54
56	r	503	CDL	C14-C15-C16-C17
56	s	401	CDL	C19-C20-C21-C22
48	B	303	PEE	C10-C11-C12-C13
56	V	201	CDL	OB7-CB5-OB6-CB4
56	a	201	CDL	OA7-CA5-OA6-CA4
48	l	703	PEE	O3P-C1-C2-O2
49	j	203	PLX	C30-C31-C32-C33
49	g	201	PLX	C32-C33-C34-C35
56	s	401	CDL	C59-C60-C61-C62
49	J	403	PLX	C33-C34-C35-C36
56	V	202	CDL	C19-C20-C21-C22
56	V	204	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
48	V	203	PEE	C10-C11-C12-C13
56	V	202	CDL	C83-C84-C85-C86
56	a	201	CDL	C62-C63-C64-C65
49	g	201	PLX	O6-C4-C5-O8
56	V	202	CDL	OB6-CB4-CB6-OB8
56	l	701	CDL	OA6-CA4-CA6-OA8
56	r	503	CDL	OB6-CB4-CB6-OB8
48	W	201	PEE	C21-C22-C23-C24
49	C	303	PLX	C10-C11-C12-C13
56	V	204	CDL	C37-C38-C39-C40
56	V	204	CDL	C51-C52-C53-C54
56	l	702	CDL	C74-C75-C76-C77
56	V	201	CDL	C14-C15-C16-C17
48	j	201	PEE	C36-C37-C38-C39
49	J	403	PLX	C28-C29-C30-C31
49	e	201	PLX	C26-C27-C28-C29
56	V	201	CDL	C76-C77-C78-C79
56	i	401	CDL	C73-C74-C75-C76
56	l	702	CDL	C59-C60-C61-C62
56	r	503	CDL	C32-C33-C34-C35
49	J	403	PLX	C11-C10-C9-C8
49	J	403	PLX	C32-C33-C34-C35
56	V	201	CDL	C75-C76-C77-C78
56	a	201	CDL	C20-C21-C22-C23
56	i	401	CDL	C77-C78-C79-C80
56	s	401	CDL	C75-C76-C77-C78
48	r	501	PEE	C23-C24-C25-C26
56	i	401	CDL	C75-C76-C77-C78
49	r	502	PLX	C25-C26-C27-C28
48	C	302	PEE	C44-C45-C46-C47
56	a	201	CDL	C61-C62-C63-C64
56	n	101	CDL	C55-C56-C57-C58
48	V	203	PEE	O5-C30-O3-C3
56	N	201	CDL	OA9-CA7-OA8-CA6
49	a	202	PLX	C31-C32-C33-C34
56	V	201	CDL	C41-C42-C43-C44
56	s	401	CDL	C82-C83-C84-C85
48	l	703	PEE	C13-C14-C15-C16
56	N	201	CDL	C11-C12-C13-C14
56	l	702	CDL	C11-C12-C13-C14
48	C	302	PEE	C41-C42-C43-C44
56	V	201	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
56	l	702	CDL	C62-C63-C64-C65
48	r	501	PEE	O3P-C1-C2-C3
56	V	204	CDL	OA5-CA3-CA4-CA6
56	a	201	CDL	OB5-CB3-CB4-CB6
56	s	401	CDL	OA5-CA3-CA4-CA6
49	e	201	PLX	C27-C28-C29-C30
49	r	502	PLX	C14-C15-C16-C17
56	r	503	CDL	C37-C38-C39-C40
56	V	201	CDL	OA9-CA7-OA8-CA6
51	G	201	8Q1	C12-C13-C14-C15
56	l	701	CDL	C11-C12-C13-C14
56	s	401	CDL	C54-C55-C56-C57
56	V	202	CDL	C39-C40-C41-C42
49	J	403	PLX	O8-C24-C25-C26
56	l	702	CDL	C14-C15-C16-C17
48	C	302	PEE	C12-C13-C14-C15
56	V	201	CDL	C73-C74-C75-C76
56	a	201	CDL	C60-C61-C62-C63
56	r	503	CDL	C71-CB7-OB8-CB6
48	V	203	PEE	C33-C34-C35-C36
56	V	202	CDL	C60-C61-C62-C63
56	l	702	CDL	CA7-C31-C32-C33
48	C	302	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
48	j	202	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
49	e	201	PLX	C3-C4-C5-O8
49	g	201	PLX	C3-C4-C5-O8
56	N	201	CDL	CA3-CA4-CA6-OA8
56	V	202	CDL	CB3-CB4-CB6-OB8
48	r	501	PEE	C15-C16-C17-C18
49	J	403	PLX	C34-C35-C36-C37
48	l	704	PEE	C21-C22-C23-C24
49	r	502	PLX	C16-C17-C18-C19
56	V	201	CDL	C63-C64-C65-C66
48	l	703	PEE	C11-C12-C13-C14
49	g	201	PLX	C2-C1-N1-C1C
56	V	202	CDL	CA7-C31-C32-C33
56	s	401	CDL	C55-C56-C57-C58
49	g	201	PLX	C36-C37-C38-C39
49	C	303	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C5'-O5'-P-O1P
56	V	204	CDL	C53-C54-C55-C56
48	l	704	PEE	C31-C32-C33-C34
56	i	401	CDL	C62-C63-C64-C65
48	C	302	PEE	C42-C43-C44-C45
48	j	202	PEE	C21-C22-C23-C24
56	l	702	CDL	C52-C53-C54-C55
56	r	503	CDL	C13-C14-C15-C16
48	l	703	PEE	C15-C16-C17-C18
48	W	201	PEE	C22-C23-C24-C25
49	C	303	PLX	C33-C34-C35-C36
56	V	201	CDL	CA7-C31-C32-C33
48	j	202	PEE	C31-C32-C33-C34
51	G	201	8Q1	C6-C7-C8-C9
56	i	401	CDL	C12-C13-C14-C15
49	a	202	PLX	C16-C17-C18-C19
56	a	201	CDL	C11-C12-C13-C14
56	r	503	CDL	C84-C85-C86-C87
56	V	202	CDL	OB5-CB3-CB4-OB6
47	A	503	NAI	C3B-C4B-C5B-O5B
56	V	204	CDL	C17-C18-C19-C20
56	V	204	CDL	C71-CB7-OB8-CB6
49	J	403	PLX	C11-C12-C13-C14
49	C	303	PLX	C11-C10-C9-C8
49	a	202	PLX	C25-C26-C27-C28
56	r	503	CDL	C58-C59-C60-C61
49	C	303	PLX	C28-C29-C30-C31
49	e	201	PLX	C30-C31-C32-C33
56	V	202	CDL	C62-C63-C64-C65
48	l	703	PEE	C32-C33-C34-C35
56	l	701	CDL	C37-C38-C39-C40
56	a	201	CDL	C84-C85-C86-C87
49	C	303	PLX	C14-C15-C16-C17
47	A	503	NAI	C2D-C1D-N1N-C2N
48	j	202	PEE	C12-C13-C14-C15
48	l	703	PEE	C21-C22-C23-C24
56	V	204	CDL	C52-C53-C54-C55
56	l	702	CDL	C73-C74-C75-C76
48	j	201	PEE	C44-C45-C46-C47
48	r	501	PEE	C24-C25-C26-C27
56	r	503	CDL	C17-C18-C19-C20
56	V	204	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
48	j	202	PEE	C30-C31-C32-C33
48	j	202	PEE	C24-C25-C26-C27
53	s	402	UQ	C12-C11-C9-C10
56	l	701	CDL	C82-C83-C84-C85
56	a	201	CDL	C31-CA7-OA8-CA6
56	i	401	CDL	C71-CB7-OB8-CB6
56	l	701	CDL	CB7-C71-C72-C73
56	V	204	CDL	C34-C35-C36-C37
56	i	401	CDL	C35-C36-C37-C38
48	B	303	PEE	C38-C39-C40-C41
49	C	303	PLX	C26-C27-C28-C29
56	s	401	CDL	C39-C40-C41-C42
56	V	202	CDL	C54-C55-C56-C57
56	l	701	CDL	C74-C75-C76-C77
49	C	303	PLX	C7-C8-C9-C10
49	a	202	PLX	C11-C10-C9-C8
56	a	201	CDL	C14-C15-C16-C17
56	s	401	CDL	C40-C41-C42-C43
48	l	703	PEE	O3P-C1-C2-C3
49	J	403	PLX	O4-C3-C4-C5
56	N	201	CDL	OA5-CA3-CA4-CA6
56	N	201	CDL	OB5-CB3-CB4-CB6
56	V	201	CDL	OB5-CB3-CB4-CB6
56	i	401	CDL	OB5-CB3-CB4-CB6
56	l	702	CDL	OA5-CA3-CA4-CA6
56	V	201	CDL	C44-C45-C46-C47
56	l	702	CDL	C36-C37-C38-C39
56	r	503	CDL	OB9-CB7-OB8-CB6
52	J	401	NDP	O4B-C4B-C5B-O5B
52	J	401	NDP	C3D-C4D-C5D-O5D
56	s	401	CDL	C17-C18-C19-C20
48	C	302	PEE	C32-C33-C34-C35
48	r	501	PEE	C12-C13-C14-C15
56	a	201	CDL	C12-C13-C14-C15
56	N	201	CDL	C52-C53-C54-C55
48	l	704	PEE	C12-C13-C14-C15
56	l	701	CDL	C81-C82-C83-C84
56	V	204	CDL	C75-C76-C77-C78
48	l	703	PEE	C31-C32-C33-C34
48	l	704	PEE	C1-C2-C3-O3
49	r	502	PLX	C3-C4-C5-O8
51	X	201	8Q1	O33-C32-C34-N36

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Mol	Chain	Res	Type	Atoms
56	i	401	CDL	CB3-CB4-CB6-OB8
56	l	701	CDL	CA3-CA4-CA6-OA8
56	r	503	CDL	CB3-CB4-CB6-OB8
56	s	401	CDL	CB3-CB4-CB6-OB8
56	r	503	CDL	C64-C65-C66-C67
49	e	201	PLX	C11-C12-C13-C14
56	i	401	CDL	CA5-C11-C12-C13
56	i	401	CDL	C64-C65-C66-C67
56	a	201	CDL	C71-C72-C73-C74
49	g	201	PLX	C14-C15-C16-C17
49	j	203	PLX	C17-C18-C19-C20
56	V	202	CDL	C73-C74-C75-C76
56	V	204	CDL	C21-C22-C23-C24
49	e	201	PLX	C15-C16-C17-C18
56	a	201	CDL	CA5-C11-C12-C13
56	r	503	CDL	CA5-C11-C12-C13
49	e	201	PLX	O4-C3-C4-O6
56	i	401	CDL	OB5-CB3-CB4-OB6
56	l	701	CDL	OB5-CB3-CB4-OB6
56	n	101	CDL	OA5-CA3-CA4-OA6
49	a	202	PLX	C15-C16-C17-C18
48	l	703	PEE	C44-C45-C46-C47
56	l	701	CDL	C14-C15-C16-C17
48	W	201	PEE	C10-C11-C12-C13
56	V	204	CDL	OB9-CB7-OB8-CB6
49	e	201	PLX	C16-C17-C18-C19
56	l	702	CDL	C12-C13-C14-C15
56	r	503	CDL	CA7-C31-C32-C33
48	C	302	PEE	O2-C2-C3-O3
48	W	201	PEE	O2-C2-C3-O3
49	e	201	PLX	O6-C4-C5-O8
49	r	502	PLX	O6-C4-C5-O8
56	V	204	CDL	OB6-CB4-CB6-OB8
56	l	701	CDL	OB6-CB4-CB6-OB8
56	s	401	CDL	OB6-CB4-CB6-OB8
52	J	401	NDP	C3B-C4B-C5B-O5B
51	X	201	8Q1	C9-C10-C11-C12
47	A	503	NAI	C2D-C1D-N1N-C6N
56	V	202	CDL	C78-C79-C80-C81
56	V	202	CDL	C84-C85-C86-C87
48	C	302	PEE	C34-C35-C36-C37
56	r	503	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	O6-C6-C7-C8
49	a	202	PLX	O8-C24-C25-C26
49	e	201	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
49	a	202	PLX	C28-C29-C30-C31
56	a	201	CDL	C72-C73-C74-C75
56	V	204	CDL	C33-C34-C35-C36
49	J	403	PLX	C30-C31-C32-C33
48	C	302	PEE	C19-C20-C21-C22
56	l	701	CDL	C21-C22-C23-C24
56	l	702	CDL	C32-C33-C34-C35
48	j	201	PEE	C38-C39-C40-C41
56	l	702	CDL	C72-C73-C74-C75
49	J	403	PLX	C36-C37-C38-C39
56	s	401	CDL	C71-CB7-OB8-CB6
48	l	704	PEE	C24-C25-C26-C27
49	J	403	PLX	C14-C15-C16-C17
56	N	201	CDL	CA2-C1-CB2-OB2
56	V	204	CDL	CA2-C1-CB2-OB2
56	a	201	CDL	CA2-C1-CB2-OB2
56	a	201	CDL	C31-C32-C33-C34
56	l	701	CDL	C71-C72-C73-C74
48	j	202	PEE	C19-C20-C21-C22
48	l	703	PEE	C24-C25-C26-C27
48	l	704	PEE	C31-C30-O3-C3
48	j	201	PEE	C30-C31-C32-C33
56	s	401	CDL	C84-C85-C86-C87
56	V	204	CDL	C82-C83-C84-C85
49	e	201	PLX	O4-C3-C4-C5
56	a	201	CDL	C38-C39-C40-C41
56	r	503	CDL	C12-C13-C14-C15
48	r	501	PEE	C36-C37-C38-C39
56	l	702	CDL	CA4-CA3-OA5-PA1
56	s	401	CDL	C56-C57-C58-C59
56	a	201	CDL	OA9-CA7-OA8-CA6
49	e	201	PLX	C24-C25-C26-C27
56	l	702	CDL	C52-C51-CB5-OB6
56	i	401	CDL	OB9-CB7-OB8-CB6
56	s	401	CDL	OB9-CB7-OB8-CB6
56	V	201	CDL	C36-C37-C38-C39
56	l	701	CDL	C80-C81-C82-C83
56	V	204	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
56	l	701	CDL	C24-C25-C26-C27
49	a	202	PLX	C27-C28-C29-C30
56	l	702	CDL	C64-C65-C66-C67
49	J	403	PLX	C24-C25-C26-C27
49	g	201	PLX	C6-C7-C8-C9
49	J	403	PLX	O4-C3-C4-O6
56	V	202	CDL	OA5-CA3-CA4-OA6
56	l	702	CDL	OA5-CA3-CA4-OA6
56	i	401	CDL	C71-C72-C73-C74
49	a	202	PLX	C3-C4-C5-O8
53	J	402	UQ	C9-C11-C12-C13
56	V	201	CDL	CA3-CA4-CA6-OA8
56	V	204	CDL	CB3-CB4-CB6-OB8
56	i	401	CDL	CA3-CA4-CA6-OA8
56	l	702	CDL	CB3-CB4-CB6-OB8
56	s	401	CDL	C11-CA5-OA6-CA4
56	a	201	CDL	CB5-C51-C52-C53
56	a	201	CDL	C44-C45-C46-C47
56	a	201	CDL	C37-C38-C39-C40
56	V	202	CDL	C64-C65-C66-C67
56	s	401	CDL	OA6-CA4-CA6-OA8
56	V	201	CDL	C11-C12-C13-C14
48	V	203	PEE	C13-C14-C15-C16
48	W	201	PEE	C23-C24-C25-C26
56	V	201	CDL	C51-C52-C53-C54
49	e	201	PLX	C2-C1-N1-C1B
48	C	302	PEE	C14-C15-C16-C17
48	l	704	PEE	O5-C30-O3-C3
48	l	704	PEE	C13-C14-C15-C16
49	J	403	PLX	N1-C1-C2-O1
48	W	201	PEE	C30-C31-C32-C33
56	l	702	CDL	C12-C11-CA5-OA6
56	a	201	CDL	O1-C1-CB2-OB2
49	g	201	PLX	C11-C10-C9-C8
49	g	201	PLX	O9-C24-C25-C26
49	e	201	PLX	C35-C36-C37-C38
49	J	403	PLX	C25-C24-O8-C5
49	a	202	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
51	X	201	8Q1	O33-C32-C34-O35
56	l	702	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
56	r	503	CDL	C44-C45-C46-C47
56	l	701	CDL	C20-C21-C22-C23
48	B	303	PEE	O3P-C1-C2-C3
56	V	202	CDL	OA5-CA3-CA4-CA6
56	l	701	CDL	OA5-CA3-CA4-CA6
56	n	101	CDL	OA5-CA3-CA4-CA6
56	s	401	CDL	OA7-CA5-OA6-CA4
48	r	501	PEE	C41-C42-C43-C44
49	r	502	PLX	C32-C33-C34-C35
56	V	202	CDL	C38-C39-C40-C41
48	r	501	PEE	C31-C30-O3-C3
56	i	401	CDL	C34-C35-C36-C37
48	W	201	PEE	C34-C35-C36-C37
56	V	204	CDL	C79-C80-C81-C82
56	l	702	CDL	C78-C79-C80-C81
56	s	401	CDL	C74-C75-C76-C77
56	V	201	CDL	CB4-CB3-OB5-PB2
49	C	303	PLX	C11-C12-C13-C14
49	g	201	PLX	O8-C24-C25-C26
48	B	303	PEE	O3P-C1-C2-O2
56	N	201	CDL	OB5-CB3-CB4-OB6
56	a	201	CDL	OB5-CB3-CB4-OB6
49	e	201	PLX	C2-C1-N1-C1C
49	e	201	PLX	C29-C30-C31-C32
52	J	401	NDP	O4D-C1D-N1N-C6N
48	j	202	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
56	N	201	CDL	OA6-CA4-CA6-OA8
56	i	401	CDL	OA6-CA4-CA6-OA8
56	l	702	CDL	CB7-C71-C72-C73
48	V	203	PEE	C1-C2-C3-O3
56	l	701	CDL	CB3-CB4-CB6-OB8
56	V	204	CDL	C77-C78-C79-C80
48	B	303	PEE	C44-C45-C46-C47
48	r	501	PEE	O5-C30-O3-C3
49	e	201	PLX	C18-C19-C20-C21
56	V	204	CDL	C44-C45-C46-C47
49	j	203	PLX	C29-C30-C31-C32
48	W	201	PEE	C24-C25-C26-C27
56	s	401	CDL	C31-C32-C33-C34
49	j	203	PLX	C32-C33-C34-C35
48	C	302	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C1-O3P-P-O4P
48	j	201	PEE	C1-O3P-P-O2P
48	l	703	PEE	C1-O3P-P-O1P
48	l	704	PEE	C1-O3P-P-O2P
48	r	501	PEE	C4-O4P-P-O2P
49	C	303	PLX	C3-O4-P1-O2
49	a	202	PLX	C5-C4-O6-C6
49	e	201	PLX	C3-C4-O6-C6
49	e	201	PLX	C5-C4-O6-C6
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O3
49	j	203	PLX	C3-O4-P1-O1
49	j	203	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	502	PLX	C2-O1-P1-O3
56	N	201	CDL	CB3-OB5-PB2-OB2
56	N	201	CDL	CB3-OB5-PB2-OB4
56	V	201	CDL	CA2-OA2-PA1-OA3
56	V	201	CDL	CB2-OB2-PB2-OB4
56	V	202	CDL	CB2-OB2-PB2-OB4
56	V	202	CDL	CB3-OB5-PB2-OB4
56	i	401	CDL	CA3-OA5-PA1-OA2
56	i	401	CDL	CB2-OB2-PB2-OB3
56	i	401	CDL	CB2-OB2-PB2-OB5
56	l	701	CDL	CB3-OB5-PB2-OB4
56	l	702	CDL	CB3-OB5-PB2-OB2
56	l	702	CDL	CB3-OB5-PB2-OB3
56	l	702	CDL	CB3-OB5-PB2-OB4
56	r	503	CDL	CA3-OA5-PA1-OA2
56	s	401	CDL	CB3-OB5-PB2-OB3
56	V	204	CDL	CB5-C51-C52-C53
56	V	204	CDL	C19-C20-C21-C22
56	V	204	CDL	CA4-CA3-OA5-PA1
56	i	401	CDL	C1-CB2-OB2-PB2
56	r	503	CDL	C1-CB2-OB2-PB2
56	r	503	CDL	CB4-CB3-OB5-PB2
56	a	201	CDL	C76-C77-C78-C79
56	a	201	CDL	C82-C83-C84-C85
48	l	703	PEE	C10-C11-C12-C13
56	r	503	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	C24-C25-C26-C27
49	j	203	PLX	C24-C25-C26-C27
48	j	201	PEE	C40-C41-C42-C43
56	V	201	CDL	C72-C73-C74-C75
48	l	703	PEE	C3-C2-O2-C10
56	a	201	CDL	CA3-CA4-OA6-CA5
56	V	201	CDL	C31-C32-C33-C34
56	V	204	CDL	C35-C36-C37-C38
56	V	202	CDL	OB5-CB3-CB4-CB6
56	V	202	CDL	C36-C37-C38-C39
48	j	201	PEE	C34-C35-C36-C37
56	V	202	CDL	CB7-C71-C72-C73
48	V	203	PEE	C34-C35-C36-C37
49	a	202	PLX	C30-C31-C32-C33
47	A	503	NAI	O4D-C1D-N1N-C2N
48	B	303	PEE	C39-C40-C41-C42
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
48	V	203	PEE	C18-C19-C20-C21
56	a	201	CDL	C24-C25-C26-C27
56	s	401	CDL	CB5-C51-C52-C53
48	r	501	PEE	C16-C17-C18-C19
48	W	201	PEE	C15-C16-C17-C18
49	e	201	PLX	C9-C10-C11-C12
49	j	203	PLX	C4-C5-O8-C24
49	e	201	PLX	C2-C1-N1-C1A
56	V	204	CDL	C54-C55-C56-C57
56	r	503	CDL	C57-C58-C59-C60
49	g	201	PLX	O6-C6-C7-C8
49	j	203	PLX	O8-C24-C25-C26
56	i	401	CDL	C36-C37-C38-C39
56	l	701	CDL	C78-C79-C80-C81
48	j	201	PEE	C41-C42-C43-C44
49	e	201	PLX	C10-C11-C12-C13
49	e	201	PLX	C28-C29-C30-C31
48	C	302	PEE	C16-C17-C18-C19
48	l	704	PEE	C18-C19-C20-C21
56	i	401	CDL	C13-C14-C15-C16
48	l	703	PEE	C19-C20-C21-C22
56	V	201	CDL	C40-C41-C42-C43
49	r	502	PLX	C18-C19-C20-C21
49	e	201	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	O4D-C1D-N1N-C6N
56	V	204	CDL	C60-C61-C62-C63
56	V	204	CDL	C52-C51-CB5-OB6
48	V	203	PEE	C35-C36-C37-C38
56	V	201	CDL	C64-C65-C66-C67
51	X	201	8Q1	C43-C42-N41-C39
53	s	402	UQ	C24-C26-C27-C28
56	n	101	CDL	C56-C57-C58-C59
56	V	204	CDL	C63-C64-C65-C66
56	s	401	CDL	C77-C78-C79-C80
56	l	702	CDL	C82-C83-C84-C85
56	V	201	CDL	CA6-CA4-OA6-CA5
48	B	303	PEE	C22-C23-C24-C25
56	r	503	CDL	C52-C53-C54-C55
56	r	503	CDL	C72-C71-CB7-OB8
48	B	303	PEE	C21-C22-C23-C24
53	s	402	UQ	C22-C23-C24-C25
56	n	101	CDL	C32-C31-CA7-OA8
48	j	202	PEE	C18-C19-C20-C21
49	r	502	PLX	C4-C3-O4-P1
56	V	201	CDL	CA4-CA3-OA5-PA1
56	V	202	CDL	C77-C78-C79-C80
56	N	201	CDL	CB7-C71-C72-C73
56	r	503	CDL	C21-C22-C23-C24
49	e	201	PLX	C12-C13-C14-C15
50	C	304	DCQ	C10-C11-C12-C13
56	n	101	CDL	C52-C53-C54-C55
56	V	202	CDL	C44-C45-C46-C47
56	r	503	CDL	CA2-C1-CB2-OB2
48	l	703	PEE	C30-C31-C32-C33
52	J	401	NDP	C2B-O2B-P2B-O1X
56	i	401	CDL	C12-C11-CA5-OA6
56	l	701	CDL	C18-C19-C20-C21
48	r	501	PEE	C20-C21-C22-C23
56	V	204	CDL	C15-C16-C17-C18
52	J	401	NDP	PN-O3-PA-O1A
56	r	503	CDL	C53-C54-C55-C56
48	l	704	PEE	C30-C31-C32-C33
56	V	201	CDL	C38-C39-C40-C41
51	G	201	8Q1	C1-C6-C7-C8
48	V	203	PEE	C2-C1-O3P-P
56	i	401	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
56	n	101	CDL	C32-C31-CA7-OA9
56	a	201	CDL	C54-C55-C56-C57
56	s	401	CDL	CA3-CA4-CA6-OA8
49	a	202	PLX	C33-C34-C35-C36
48	C	302	PEE	O5-C30-O3-C3
48	l	703	PEE	C36-C37-C38-C39
49	g	201	PLX	O7-C6-C7-C8
56	r	503	CDL	C77-C78-C79-C80
56	i	401	CDL	C33-C34-C35-C36
56	V	201	CDL	C43-C44-C45-C46
48	l	703	PEE	C38-C39-C40-C41
56	V	202	CDL	C32-C31-CA7-OA8
49	C	303	PLX	C25-C26-C27-C28
48	V	203	PEE	C37-C38-C39-C40
56	l	701	CDL	C34-C35-C36-C37
49	g	201	PLX	C20-C21-C22-C23
48	r	501	PEE	C21-C22-C23-C24
56	l	702	CDL	C18-C19-C20-C21
49	J	403	PLX	C6-C7-C8-C9
48	C	302	PEE	O3P-C1-C2-C3
56	l	701	CDL	OB5-CB3-CB4-CB6
48	l	703	PEE	O2-C2-C3-O3
56	r	503	CDL	OA6-CA4-CA6-OA8
51	X	201	8Q1	C11-C12-C13-C14
48	V	203	PEE	C31-C32-C33-C34
53	s	402	UQ	C12-C13-C14-C15
49	J	403	PLX	C4-C5-O8-C24
48	B	303	PEE	C18-C19-C20-C21
48	j	202	PEE	C16-C17-C18-C19
56	N	201	CDL	OB9-CB7-OB8-CB6
56	V	201	CDL	C57-C58-C59-C60
49	C	303	PLX	C31-C32-C33-C34
56	a	201	CDL	C80-C81-C82-C83
48	C	302	PEE	C31-C30-O3-C3
56	s	401	CDL	C72-C71-CB7-OB8
56	r	503	CDL	C54-C55-C56-C57
48	C	302	PEE	C18-C19-C20-C21
48	C	302	PEE	C38-C39-C40-C41
48	V	203	PEE	C38-C39-C40-C41
48	r	501	PEE	C18-C19-C20-C21
48	l	703	PEE	C1-C2-C3-O3
49	j	203	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	C43-C44-C45-C46
48	B	303	PEE	C16-C17-C18-C19
48	C	302	PEE	C36-C37-C38-C39
48	j	201	PEE	C16-C17-C18-C19
48	l	704	PEE	C36-C37-C38-C39
49	j	203	PLX	C10-C11-C12-C13
49	j	203	PLX	O6-C4-C5-O8
48	l	703	PEE	C16-C17-C18-C19
48	l	704	PEE	C38-C39-C40-C41
56	V	204	CDL	C57-C58-C59-C60
56	r	503	CDL	C56-C57-C58-C59
56	N	201	CDL	C52-C51-CB5-OB6
56	V	202	CDL	C80-C81-C82-C83
56	l	702	CDL	OB5-CB3-CB4-CB6
51	G	201	8Q1	C9-C10-C11-C12
49	j	203	PLX	C19-C20-C21-C22
49	j	203	PLX	C7-C6-O6-C4
56	r	503	CDL	C79-C80-C81-C82
48	l	704	PEE	C20-C21-C22-C23
48	V	203	PEE	C16-C17-C18-C19
48	W	201	PEE	C18-C19-C20-C21
48	W	201	PEE	C33-C34-C35-C36
49	e	201	PLX	C34-C35-C36-C37
56	a	201	CDL	C32-C33-C34-C35
56	N	201	CDL	C71-CB7-OB8-CB6
48	C	302	PEE	C17-C18-C19-C20
53	J	402	UQ	C19-C21-C22-C23
50	C	304	DCQ	C11-C10-C9-C8
56	a	201	CDL	C57-C58-C59-C60
49	C	303	PLX	C18-C19-C20-C21
48	W	201	PEE	C16-C17-C18-C19
56	l	702	CDL	C61-C62-C63-C64
56	s	401	CDL	C72-C73-C74-C75
56	i	401	CDL	C79-C80-C81-C82
48	C	302	PEE	O3-C30-C31-C32
56	V	204	CDL	C12-C11-CA5-OA6
56	V	201	CDL	C12-C11-CA5-OA6
52	J	401	NDP	C2B-O2B-P2B-O2X
56	l	702	CDL	C77-C78-C79-C80
48	W	201	PEE	C14-C15-C16-C17
56	N	201	CDL	C12-C11-CA5-OA6
56	s	401	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
56	V	201	CDL	OB6-CB4-CB6-OB8
56	s	401	CDL	C33-C34-C35-C36
56	N	201	CDL	C72-C71-CB7-OB8
48	j	201	PEE	C19-C20-C21-C22
56	V	201	CDL	C55-C56-C57-C58
56	a	201	CDL	C73-C74-C75-C76
56	l	702	CDL	C33-C34-C35-C36
56	l	701	CDL	C12-C11-CA5-OA6
48	j	201	PEE	C11-C12-C13-C14
56	V	202	CDL	C71-C72-C73-C74
56	a	201	CDL	C12-C11-CA5-OA6
56	r	503	CDL	C32-C31-CA7-OA8
56	l	701	CDL	C60-C61-C62-C63
49	g	201	PLX	C15-C16-C17-C18
56	l	702	CDL	C52-C51-CB5-OB7
56	l	702	CDL	OB5-CB3-CB4-OB6
56	V	204	CDL	C20-C21-C22-C23
56	l	702	CDL	C12-C11-CA5-OA7
48	V	203	PEE	C11-C12-C13-C14
56	a	201	CDL	C40-C41-C42-C43
56	a	201	CDL	C52-C53-C54-C55
56	V	201	CDL	C12-C11-CA5-OA7
49	a	202	PLX	C24-C25-C26-C27
48	C	302	PEE	O5-C30-C31-C32
56	n	101	CDL	C52-C51-CB5-OB6
49	J	403	PLX	O9-C24-O8-C5
56	N	201	CDL	C12-C11-CA5-OA7
56	l	702	CDL	C54-C55-C56-C57
48	V	203	PEE	O2-C2-C3-O3
56	N	201	CDL	C52-C51-CB5-OB7
48	l	704	PEE	C16-C17-C18-C19
56	N	201	CDL	C72-C71-CB7-OB9
56	r	503	CDL	C32-C31-CA7-OA9
49	J	403	PLX	C31-C32-C33-C34
56	V	204	CDL	C12-C11-CA5-OA7
58	w	401	ADP	PB-O3A-PA-O2A
56	a	201	CDL	C64-C65-C66-C67
56	l	701	CDL	C76-C77-C78-C79
48	r	501	PEE	C38-C39-C40-C41
48	r	501	PEE	O2-C10-C11-C12
56	a	201	CDL	C12-C11-CA5-OA7

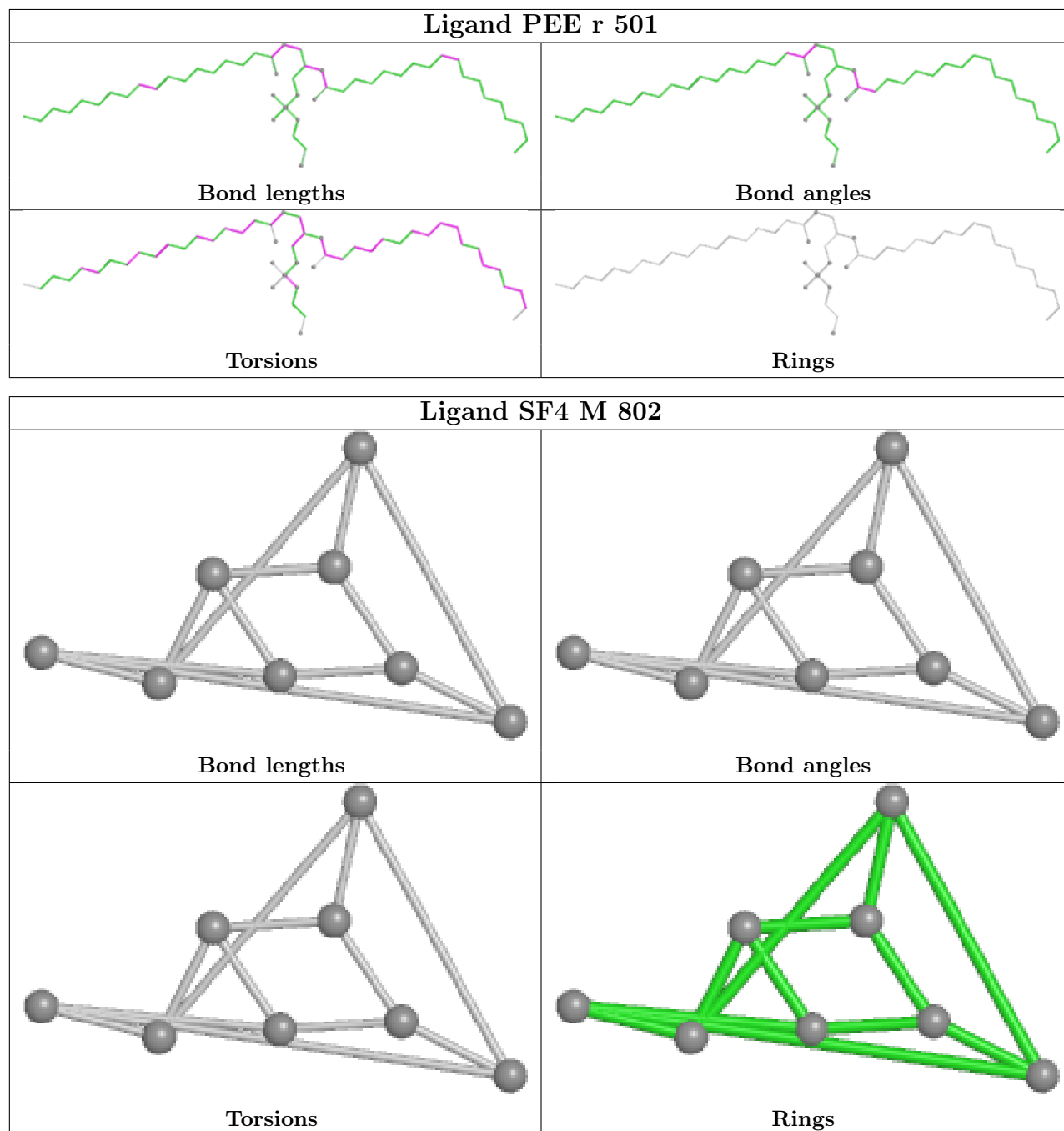
There are no ring outliers.

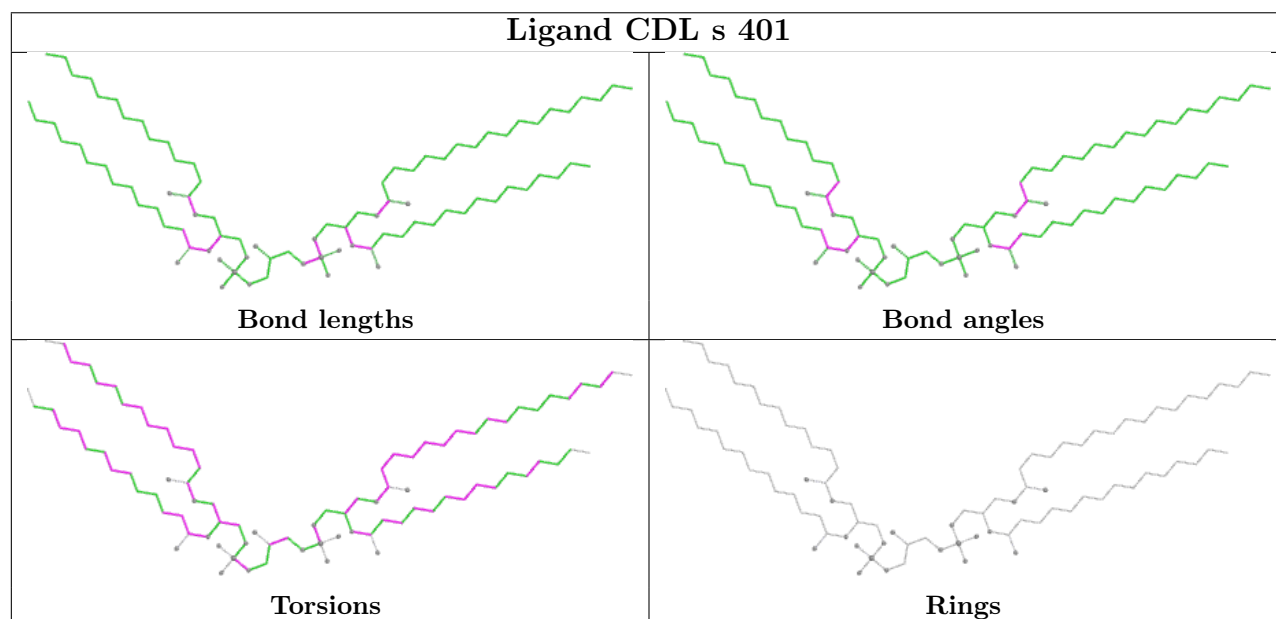
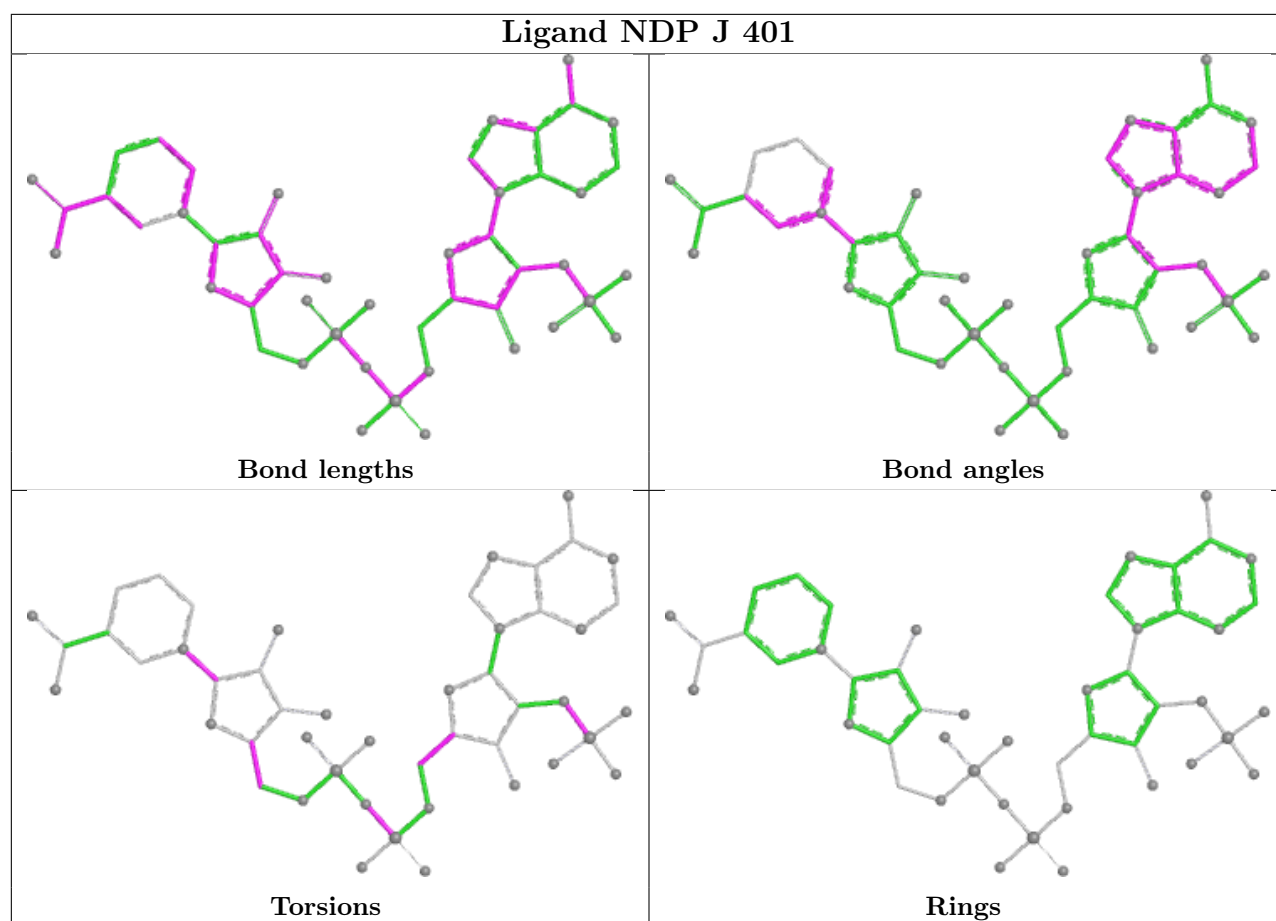
34 monomers are involved in 150 short contacts:

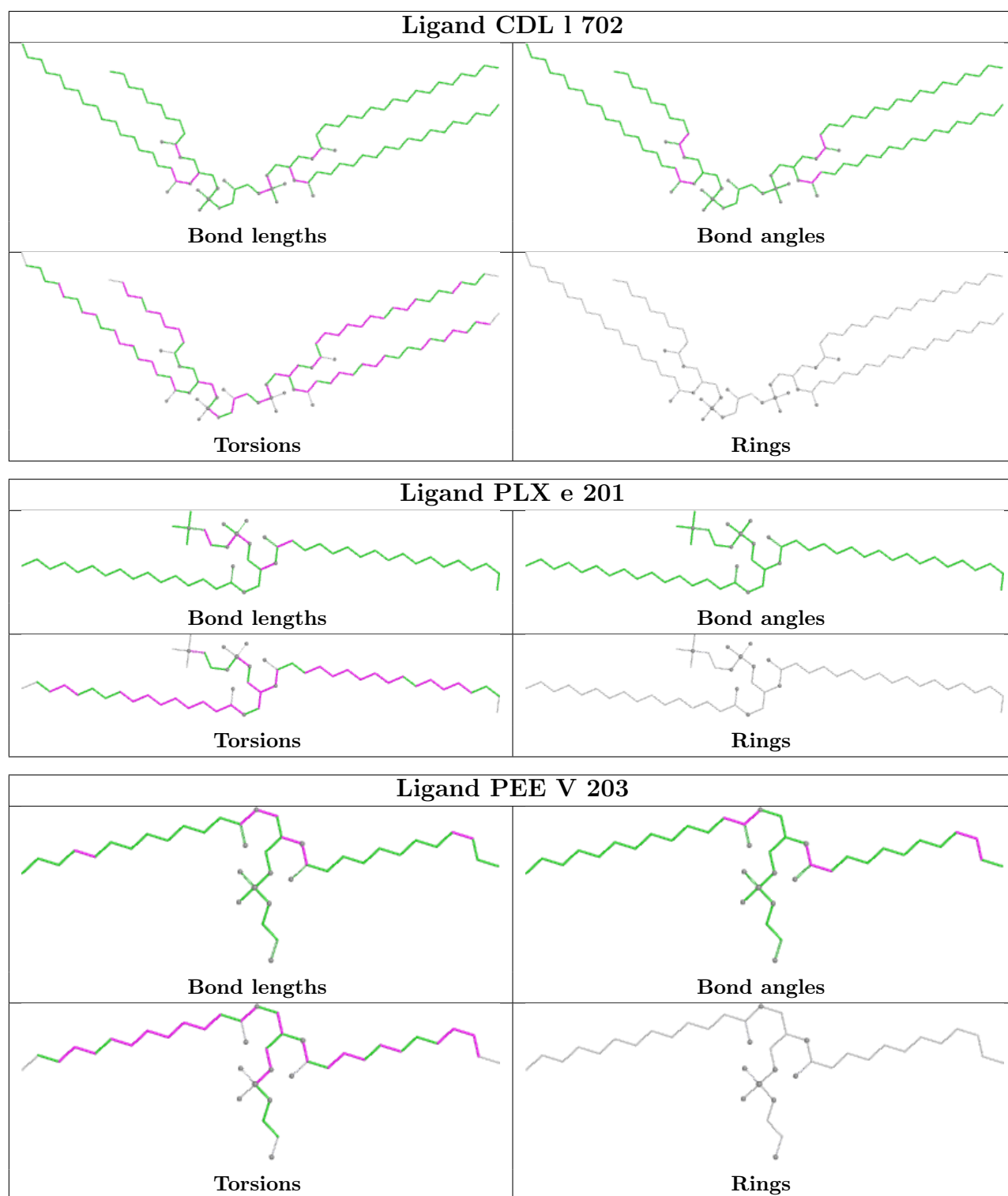
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	r	501	PEE	8	0
52	J	401	NDP	2	0
56	s	401	CDL	5	0
56	l	702	CDL	5	0
49	e	201	PLX	5	0
48	V	203	PEE	2	0
48	l	703	PEE	2	0
49	J	403	PLX	8	0
49	a	202	PLX	2	0
56	i	401	CDL	4	0
47	A	503	NAI	7	0
48	l	704	PEE	4	0
58	w	401	ADP	2	0
48	C	302	PEE	3	0
56	l	701	CDL	14	0
45	A	501	SF4	1	0
56	V	201	CDL	5	0
49	j	203	PLX	5	0
49	r	502	PLX	6	0
48	j	201	PEE	5	0
53	J	402	UQ	1	0
56	a	201	CDL	7	0
50	C	304	DCQ	2	0
48	B	303	PEE	5	0
49	C	303	PLX	4	0
48	j	202	PEE	3	0
56	V	202	CDL	10	0
56	r	503	CDL	10	0
46	A	502	FMN	5	0
45	C	301	SF4	1	0
56	V	204	CDL	10	0
56	n	101	CDL	1	0
49	g	201	PLX	3	0
53	s	402	UQ	2	0

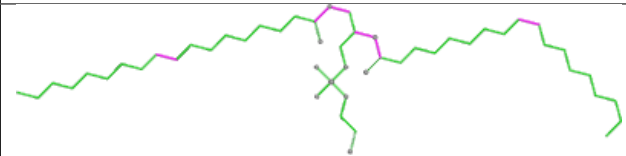
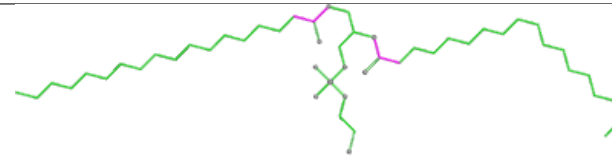
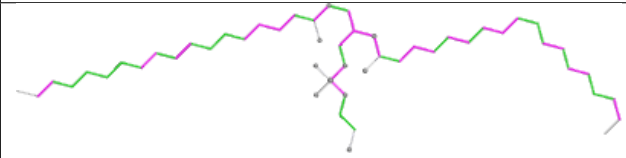
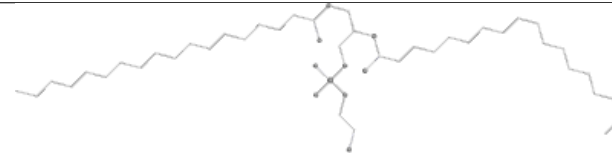
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

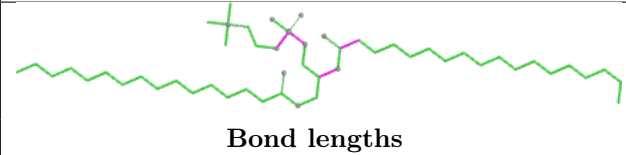
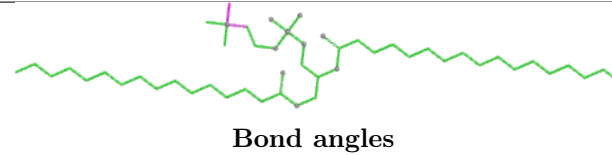
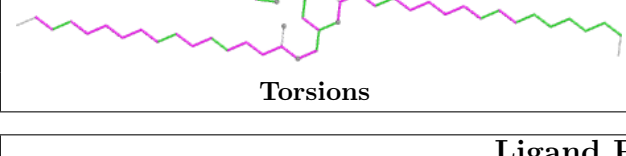
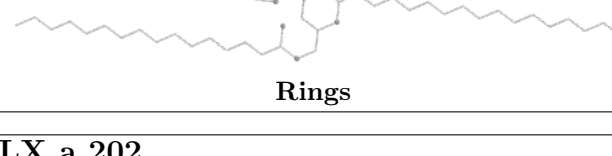
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

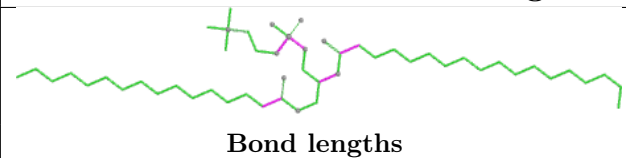
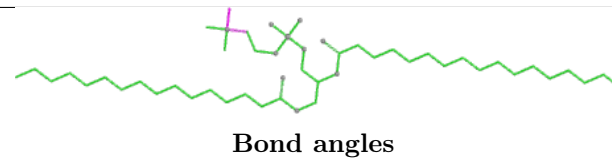
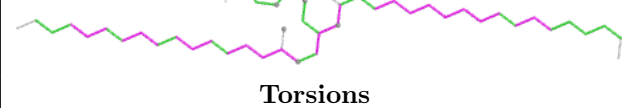


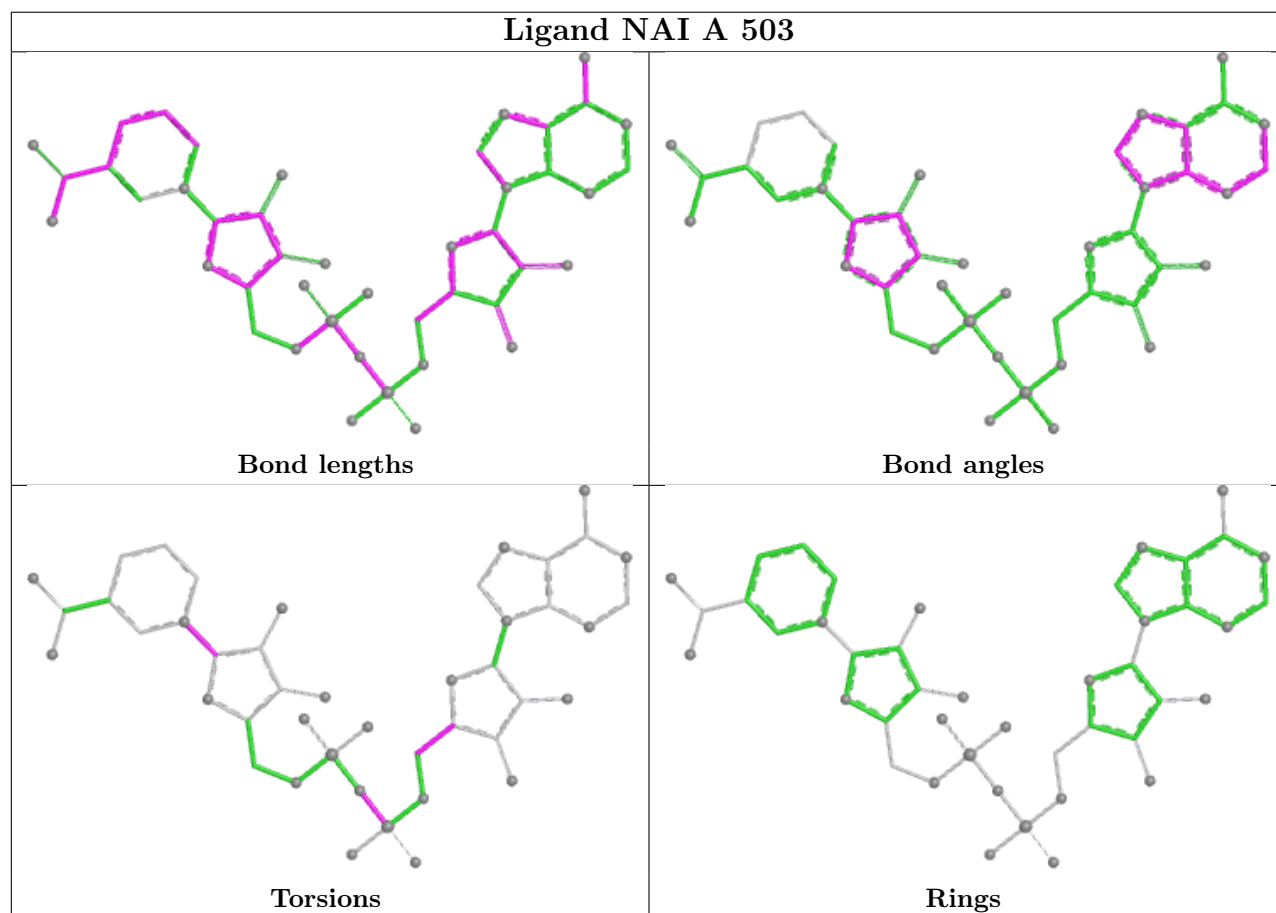
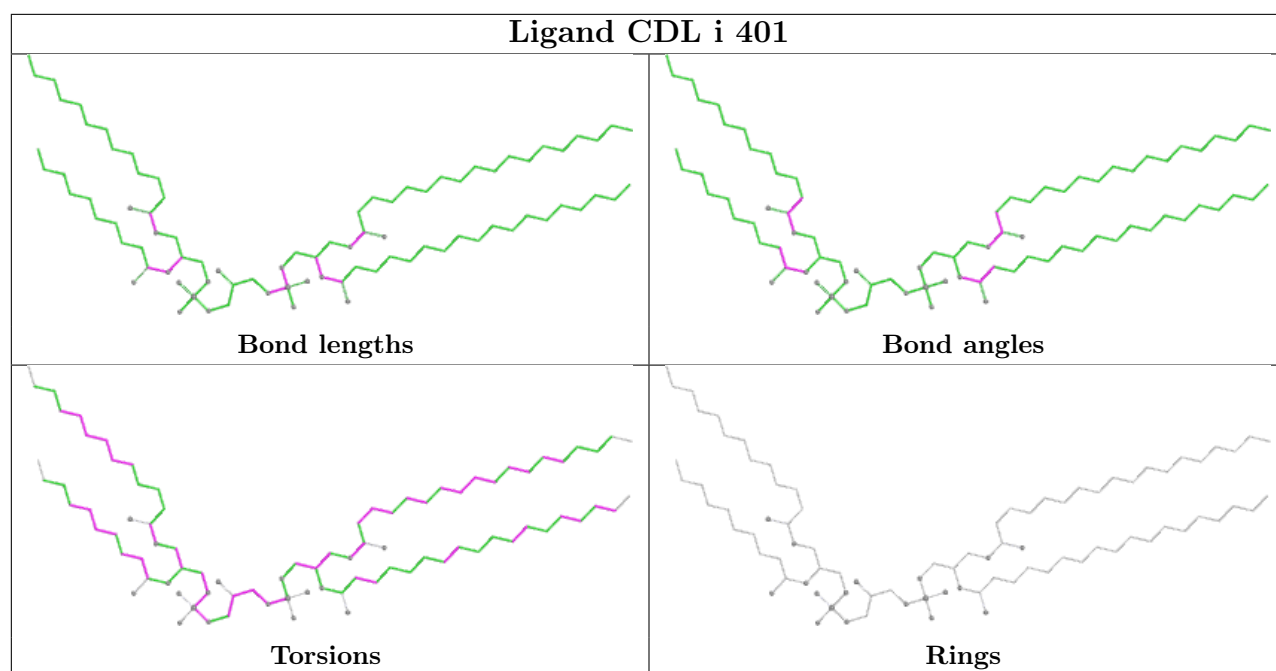


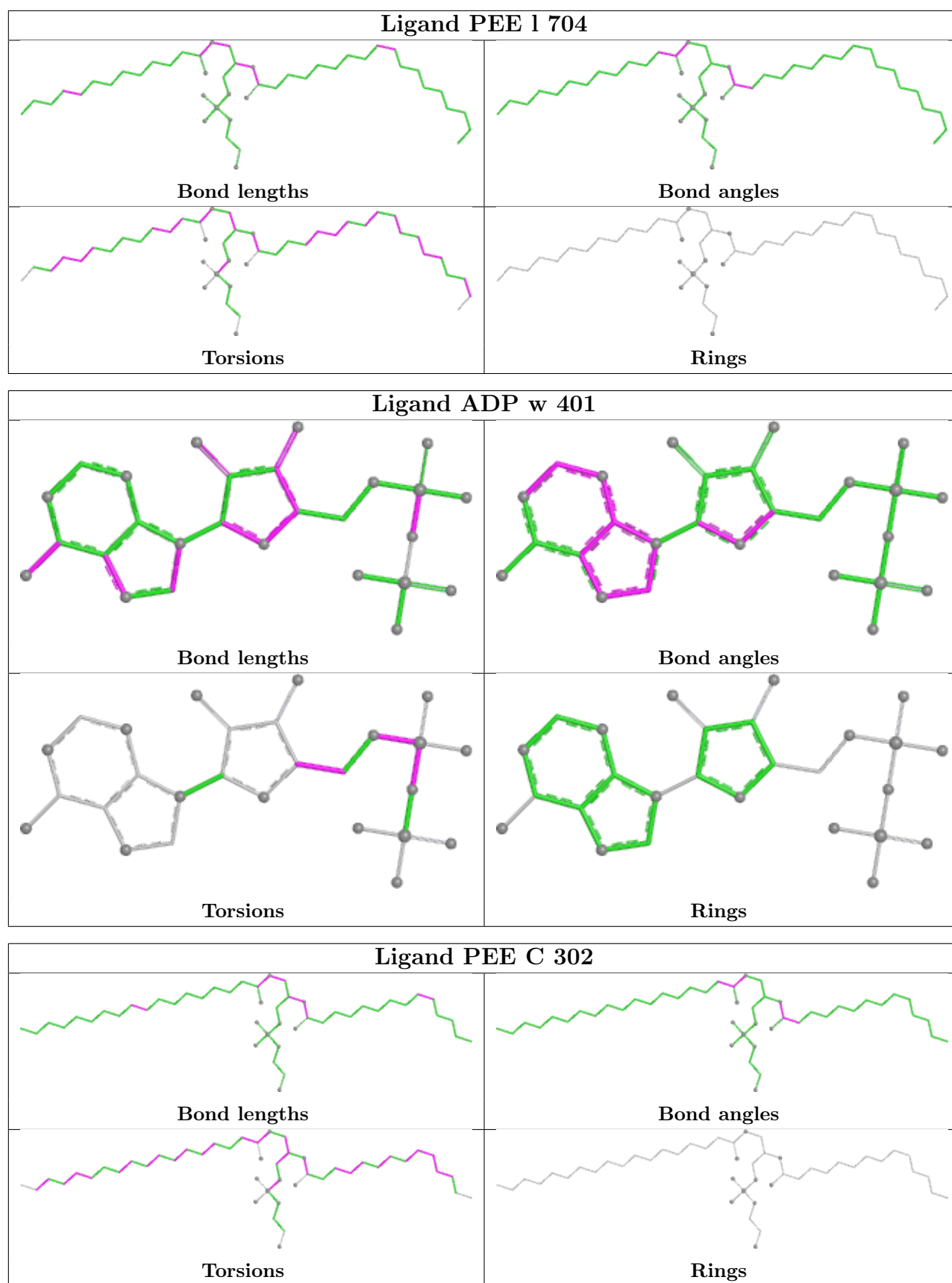


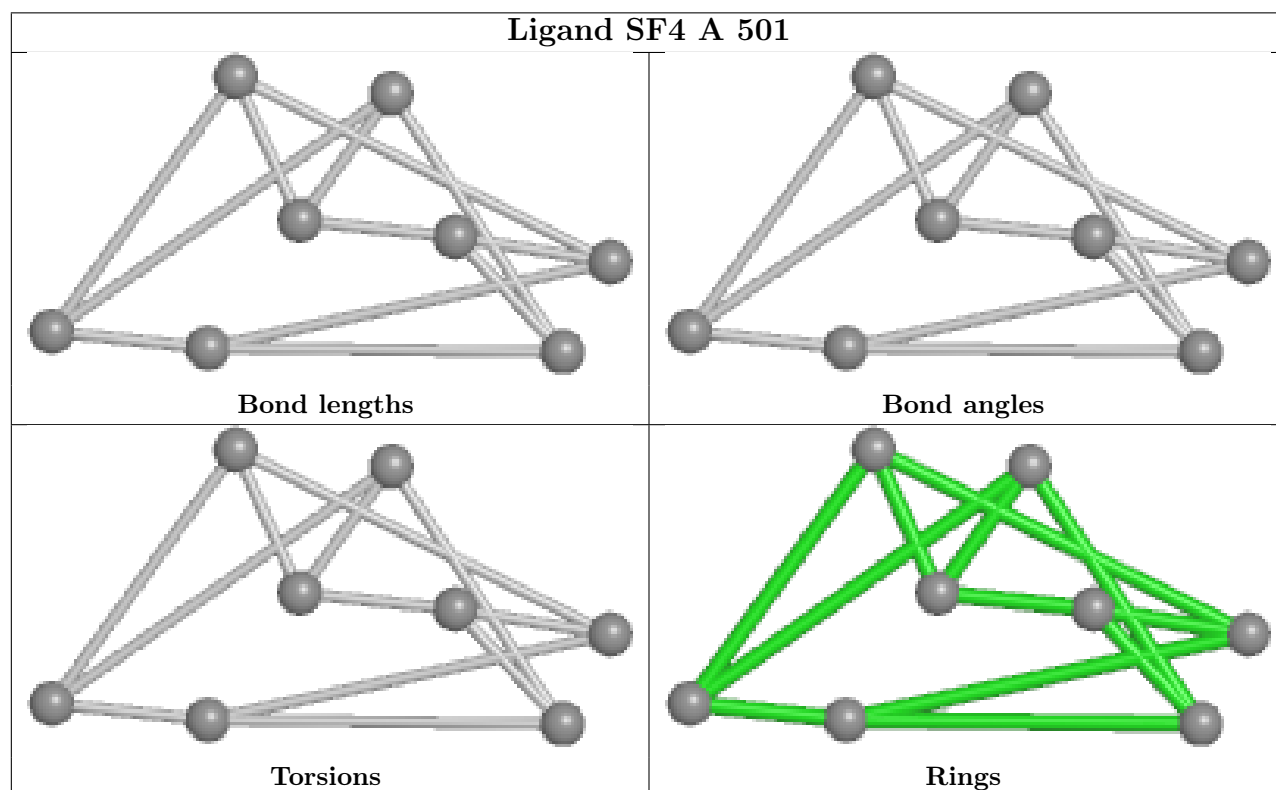
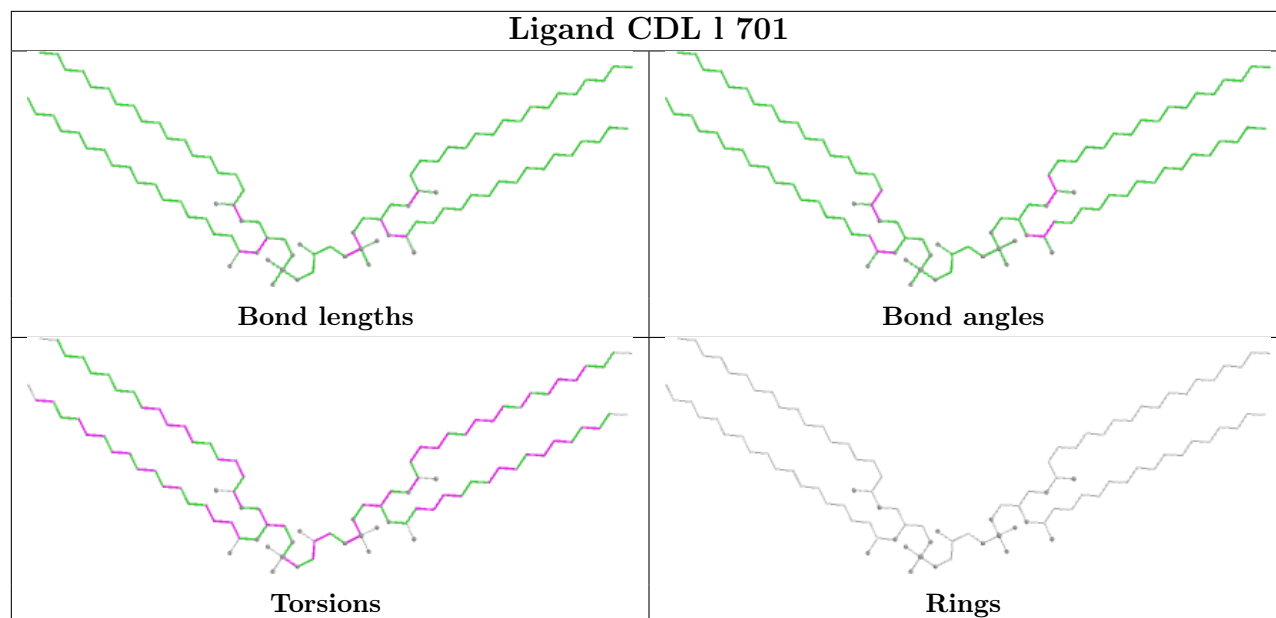
Ligand PEE 1 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

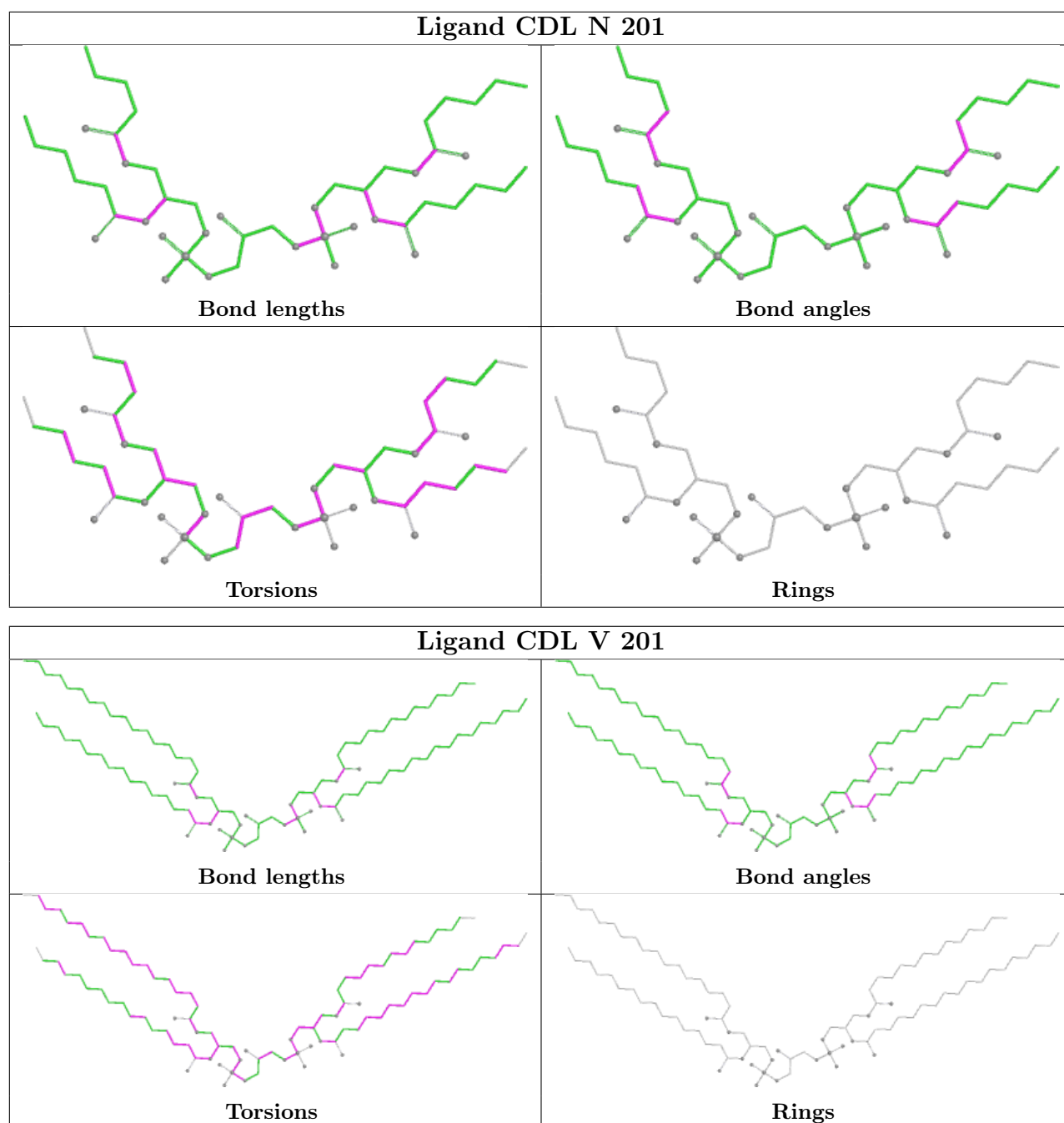
Ligand PLX J 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

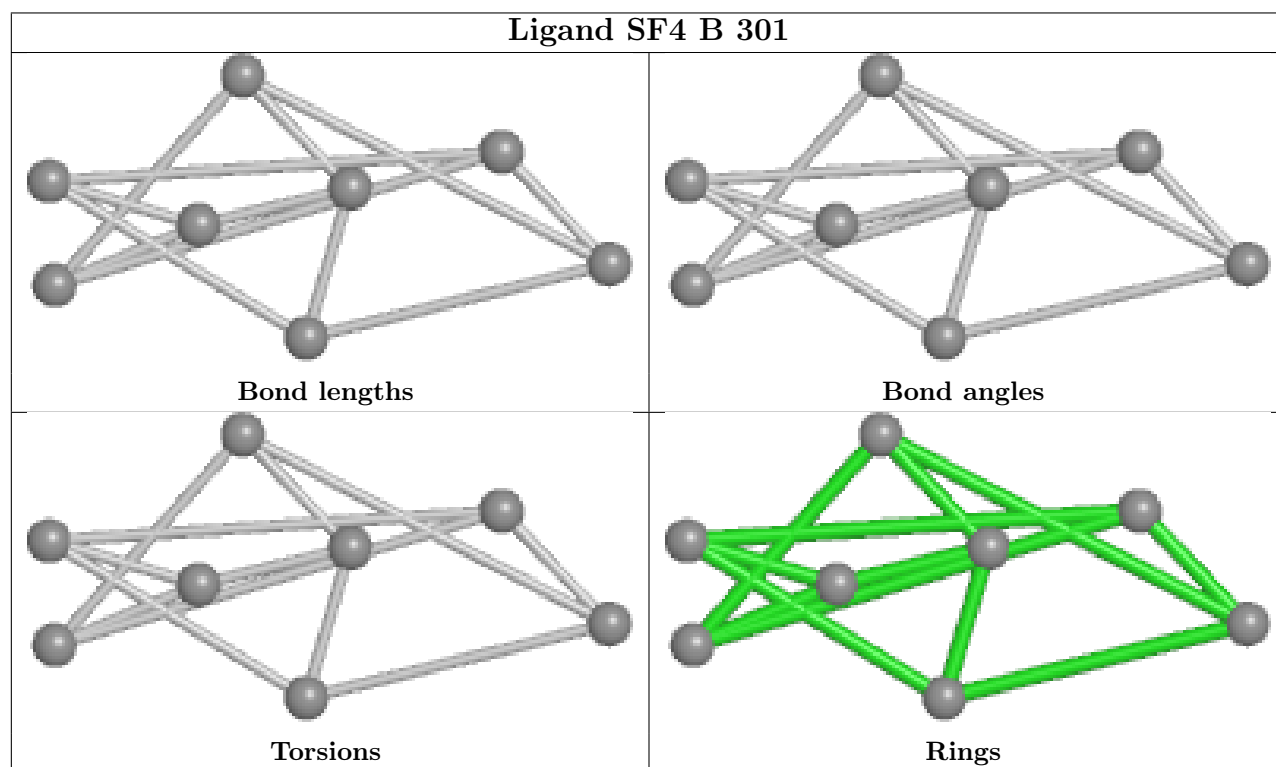
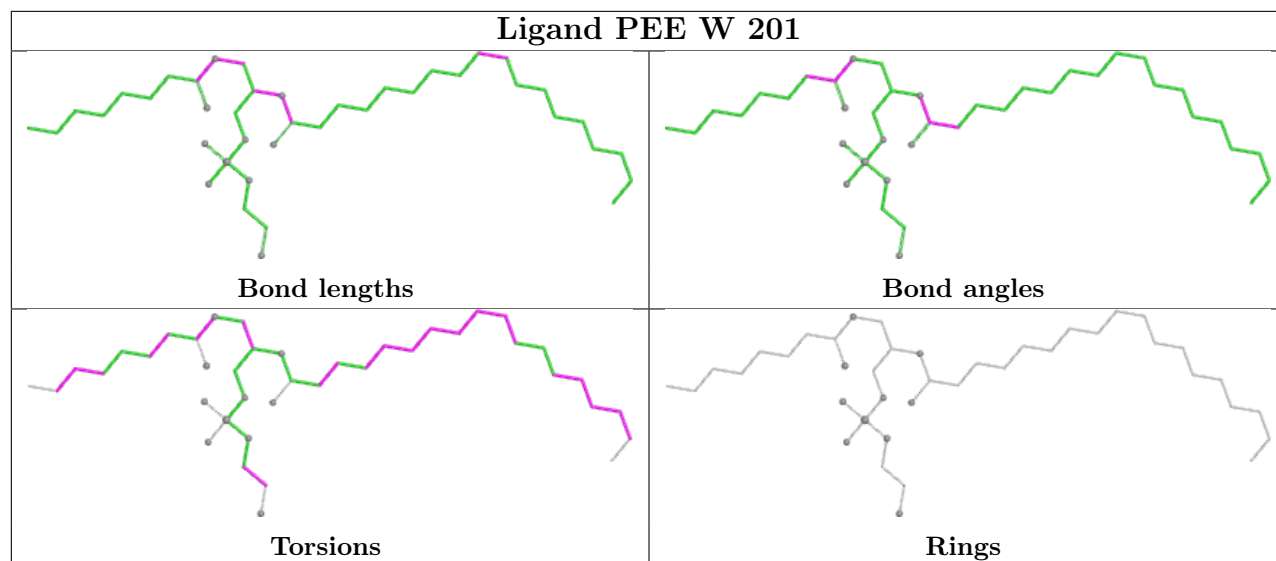
Ligand PLX a 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

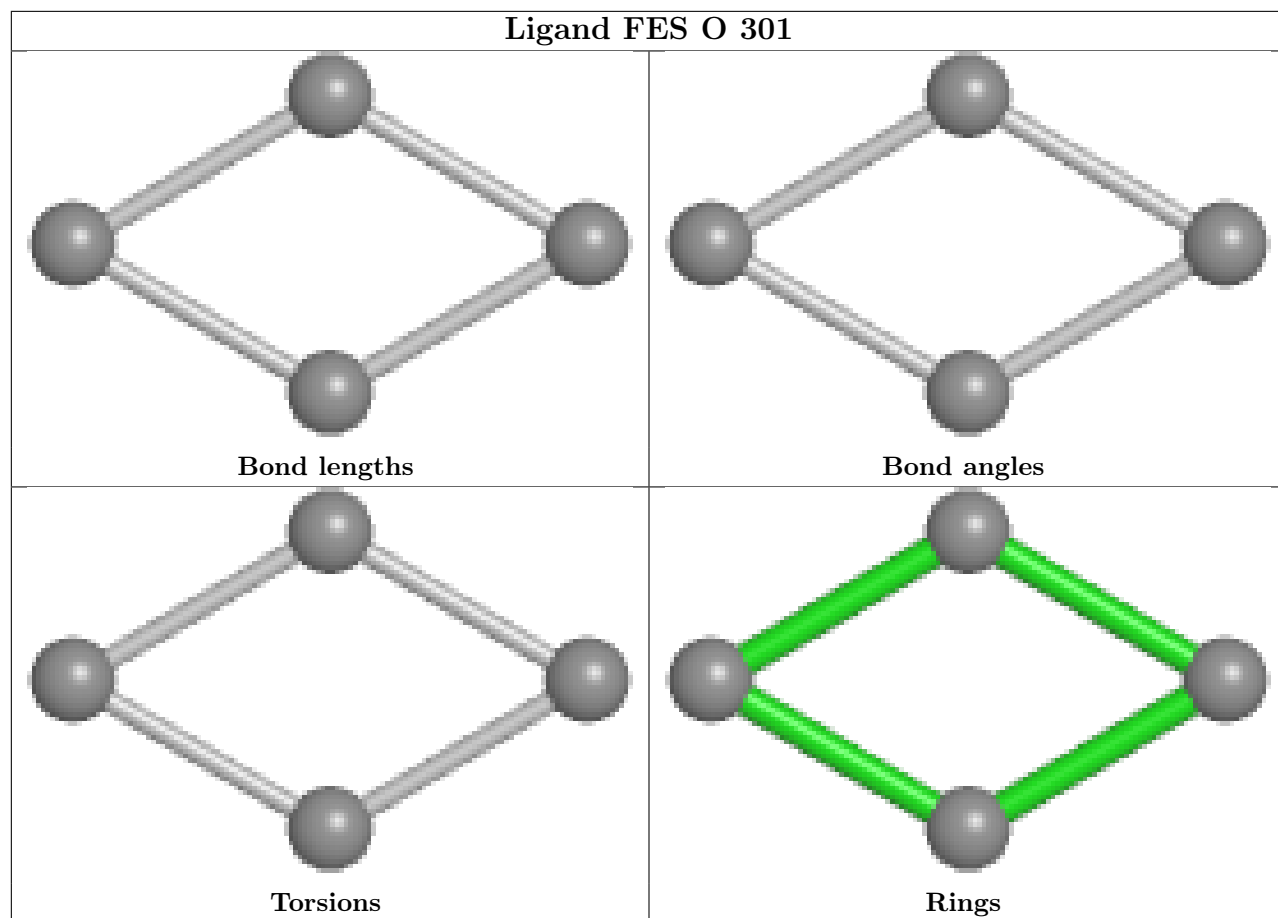


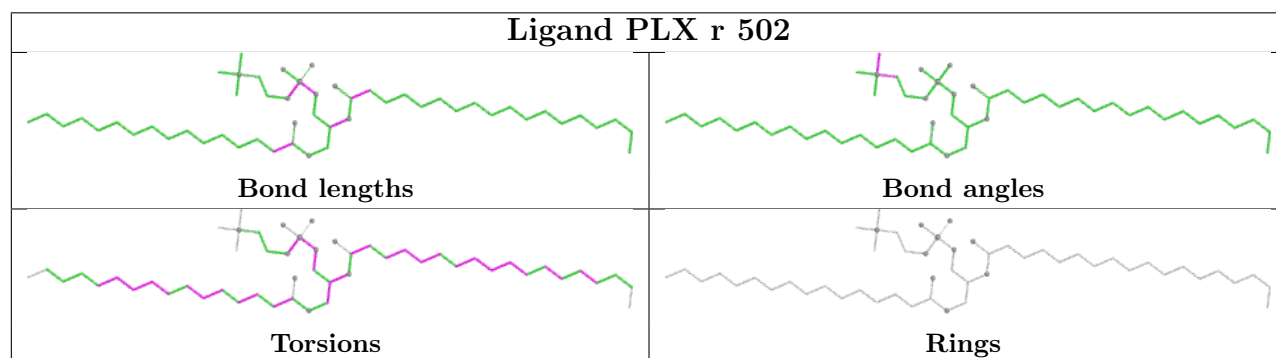
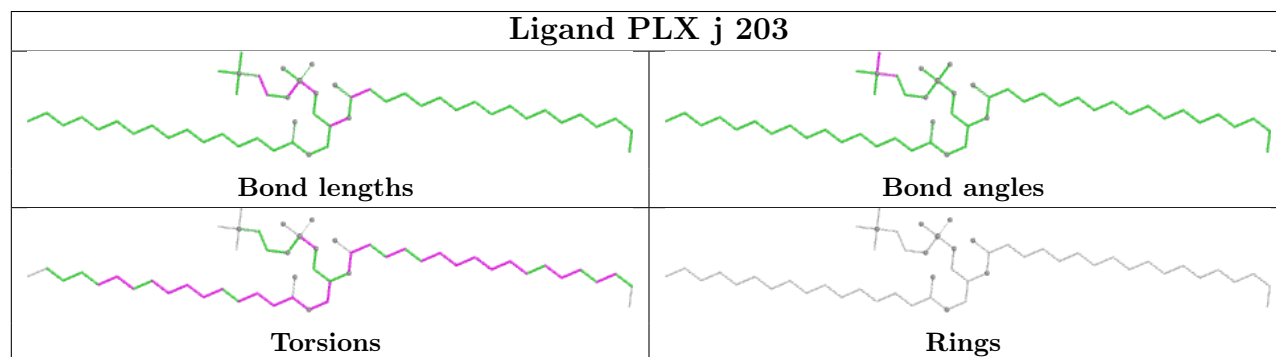
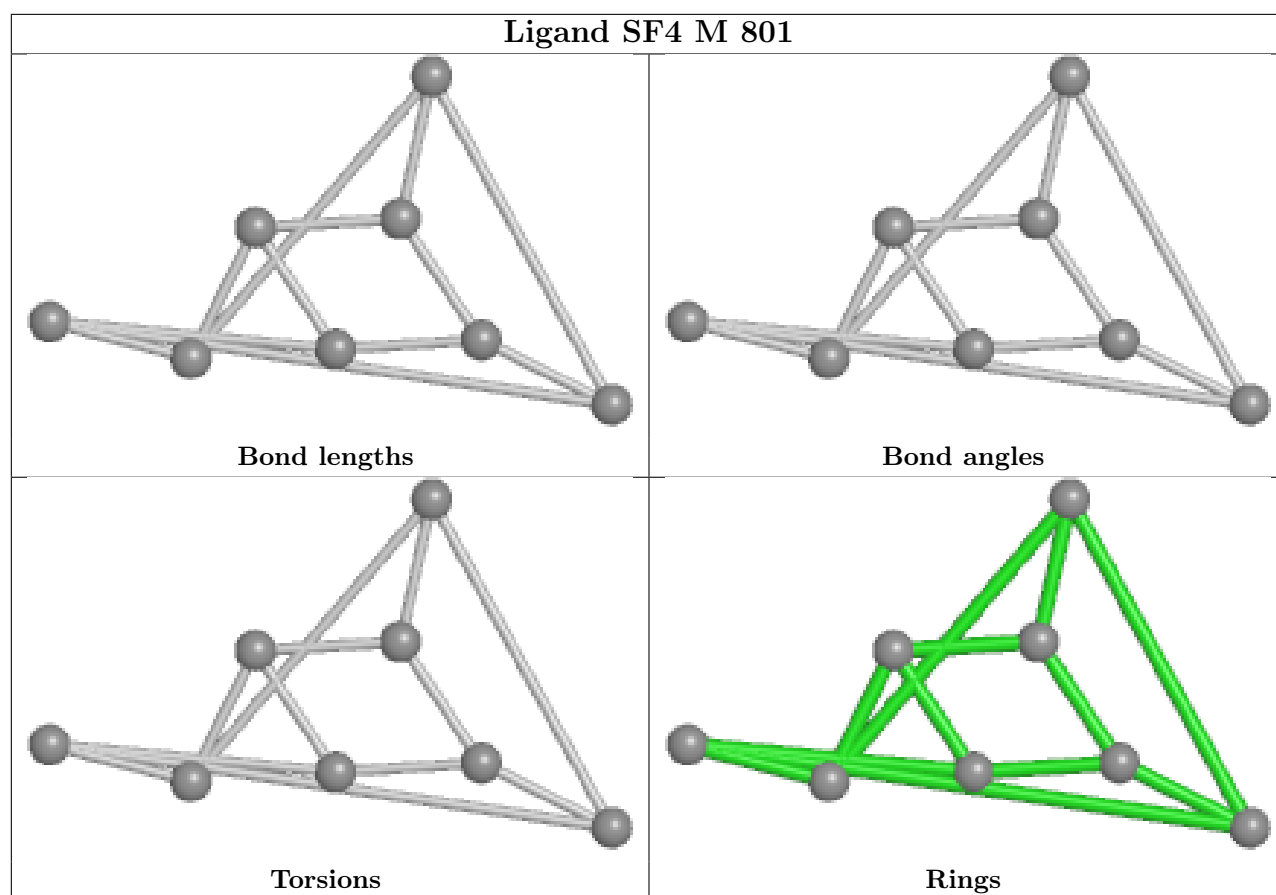


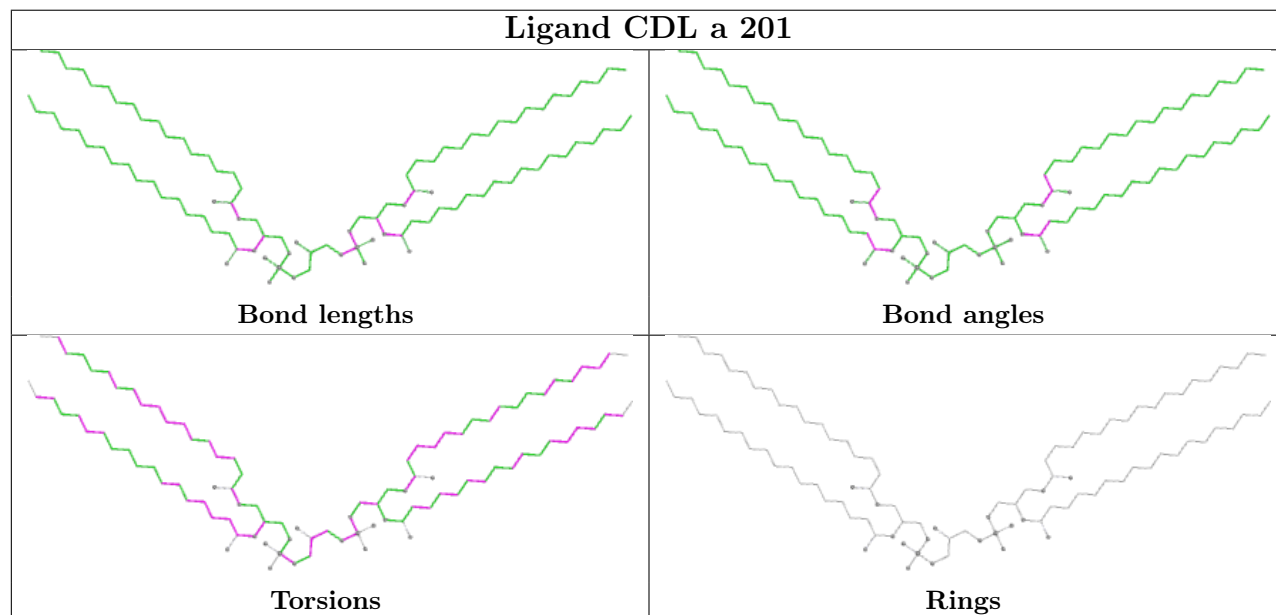
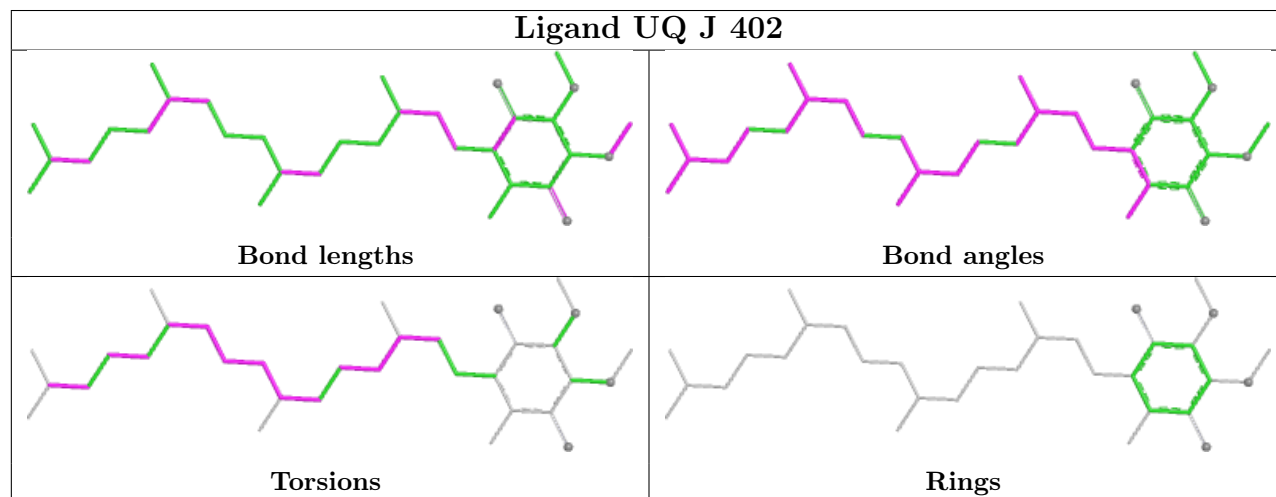
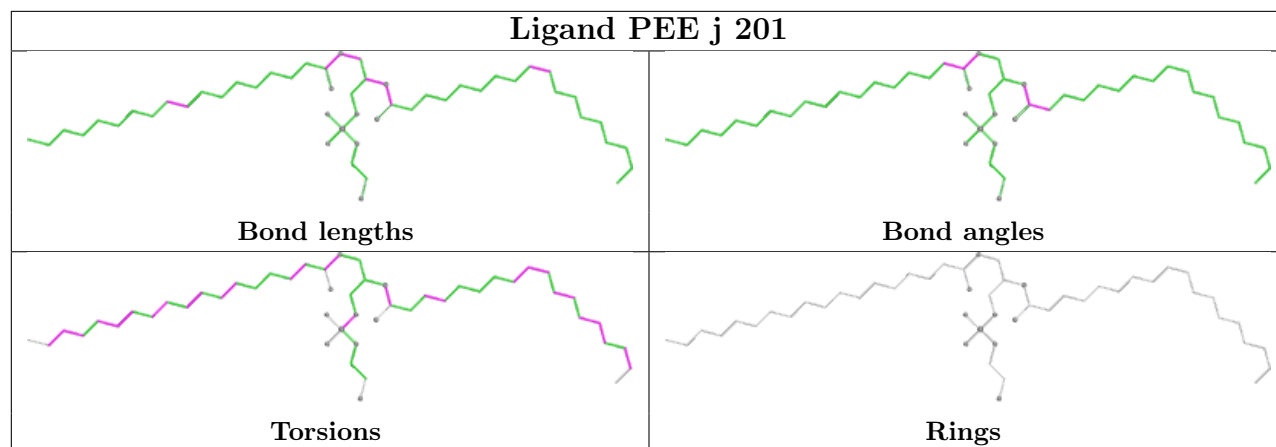


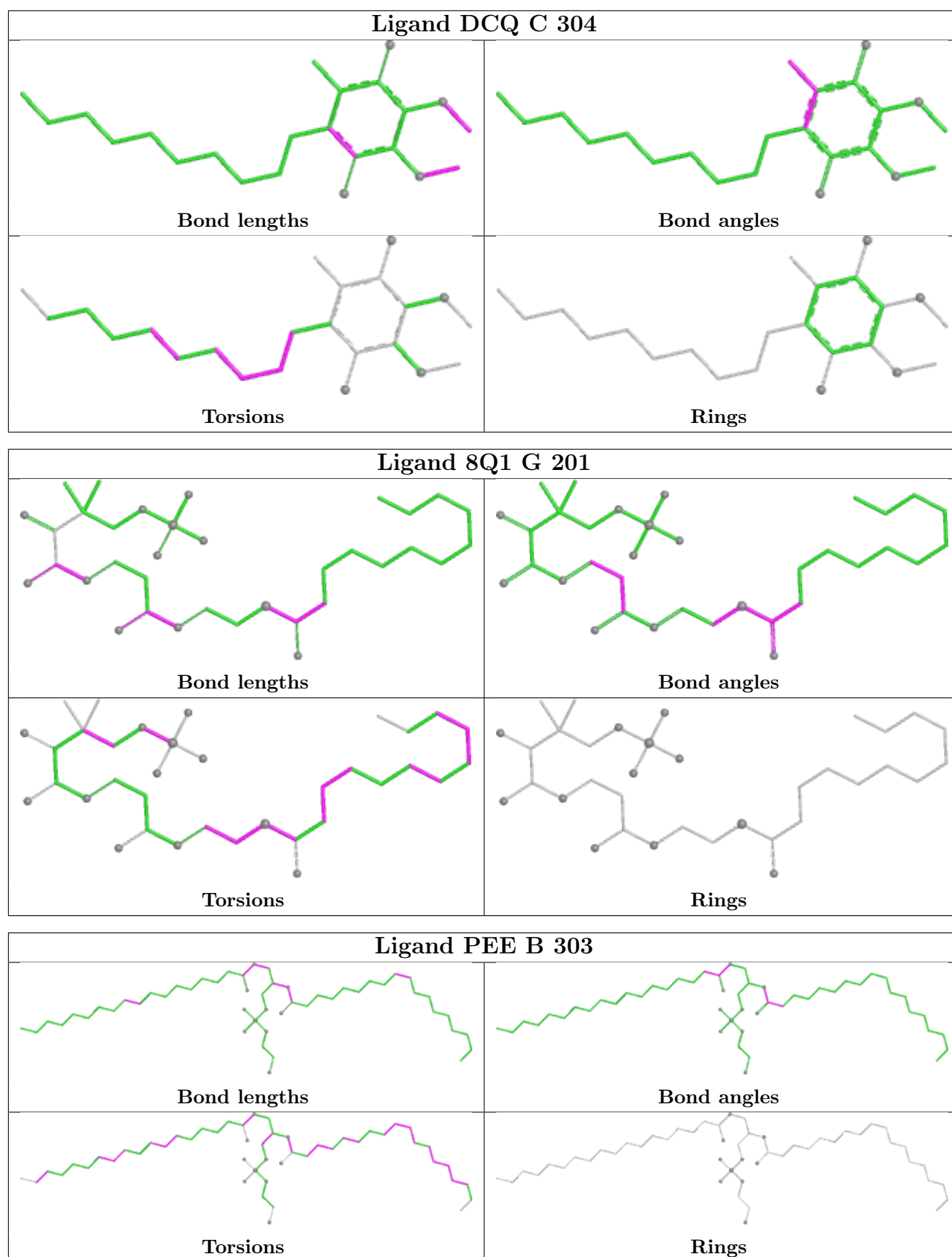


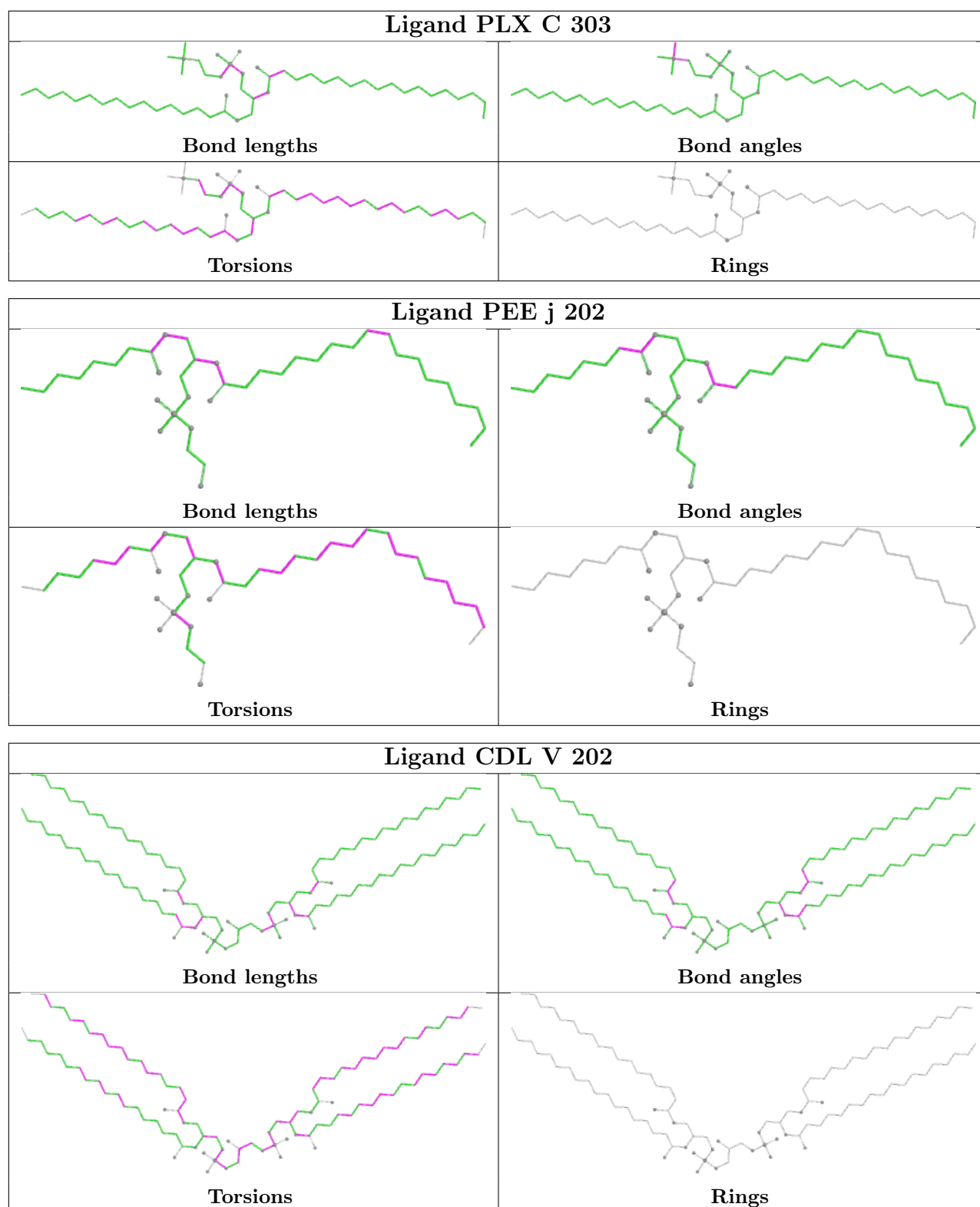


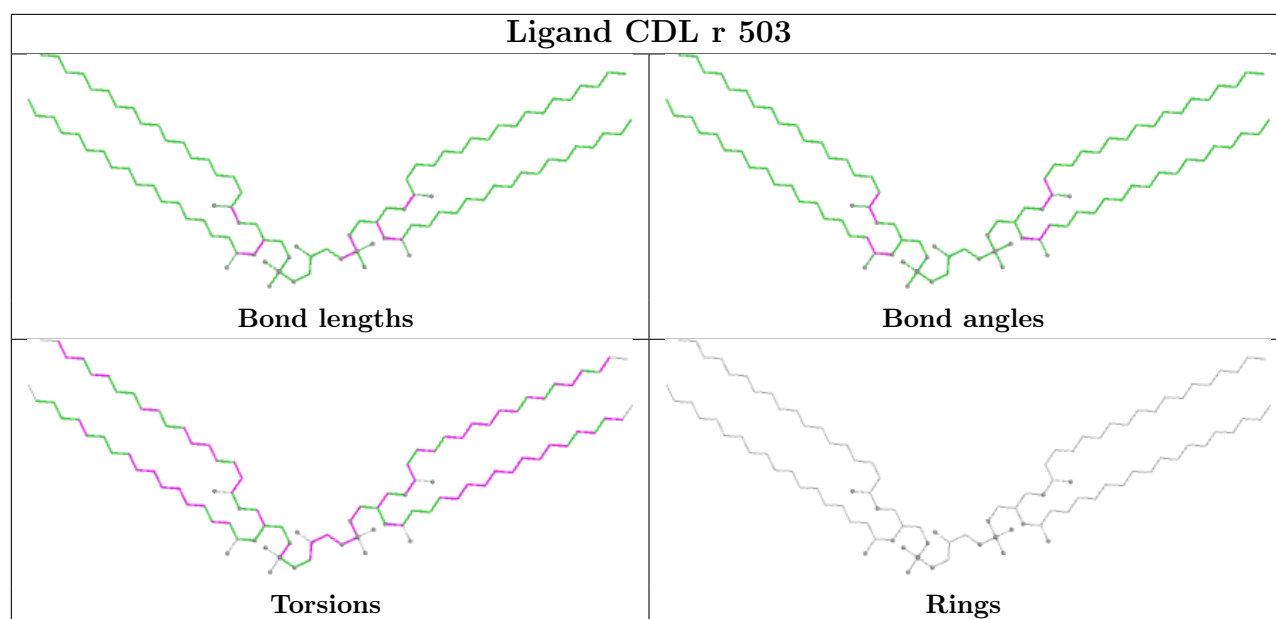


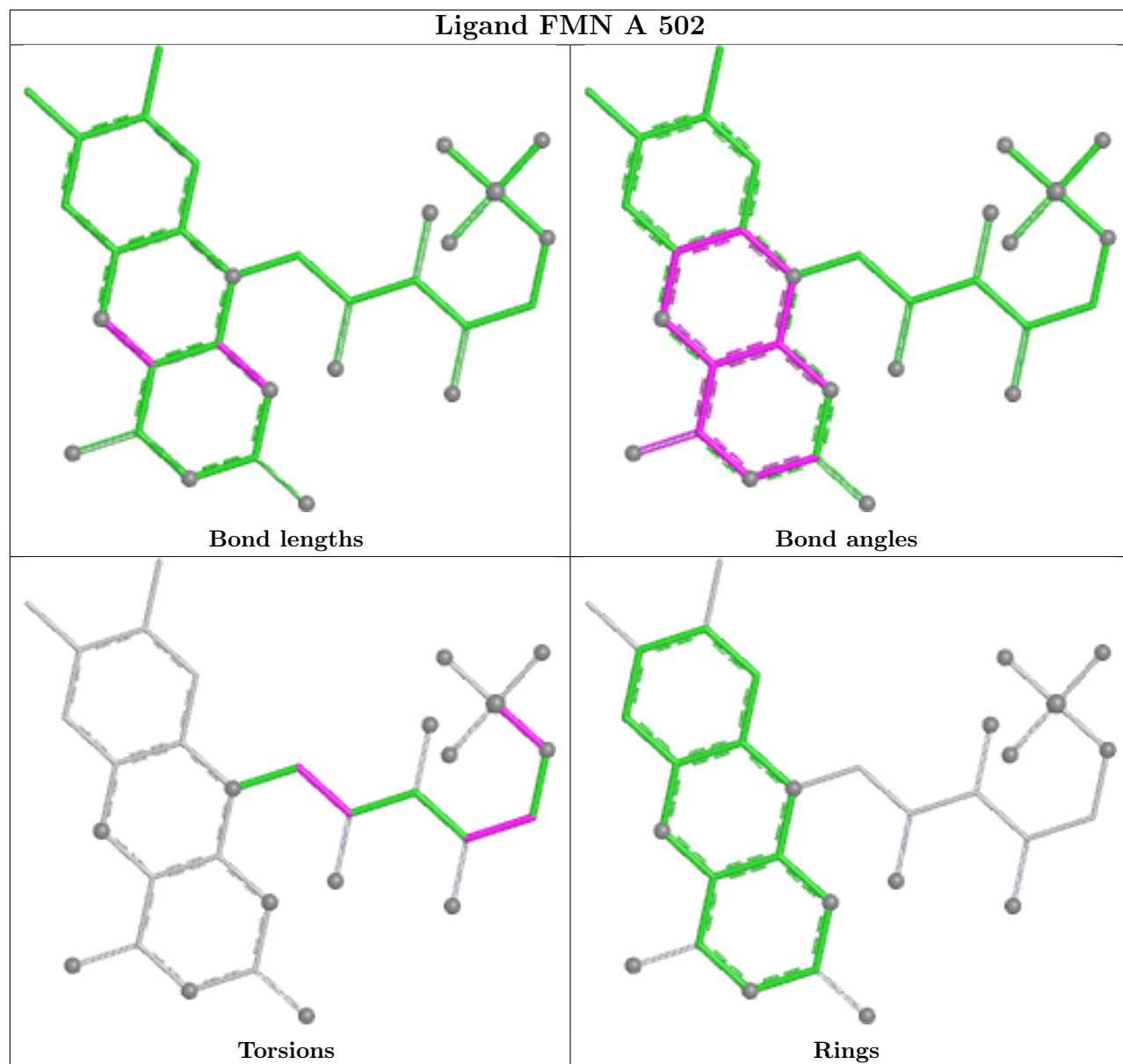


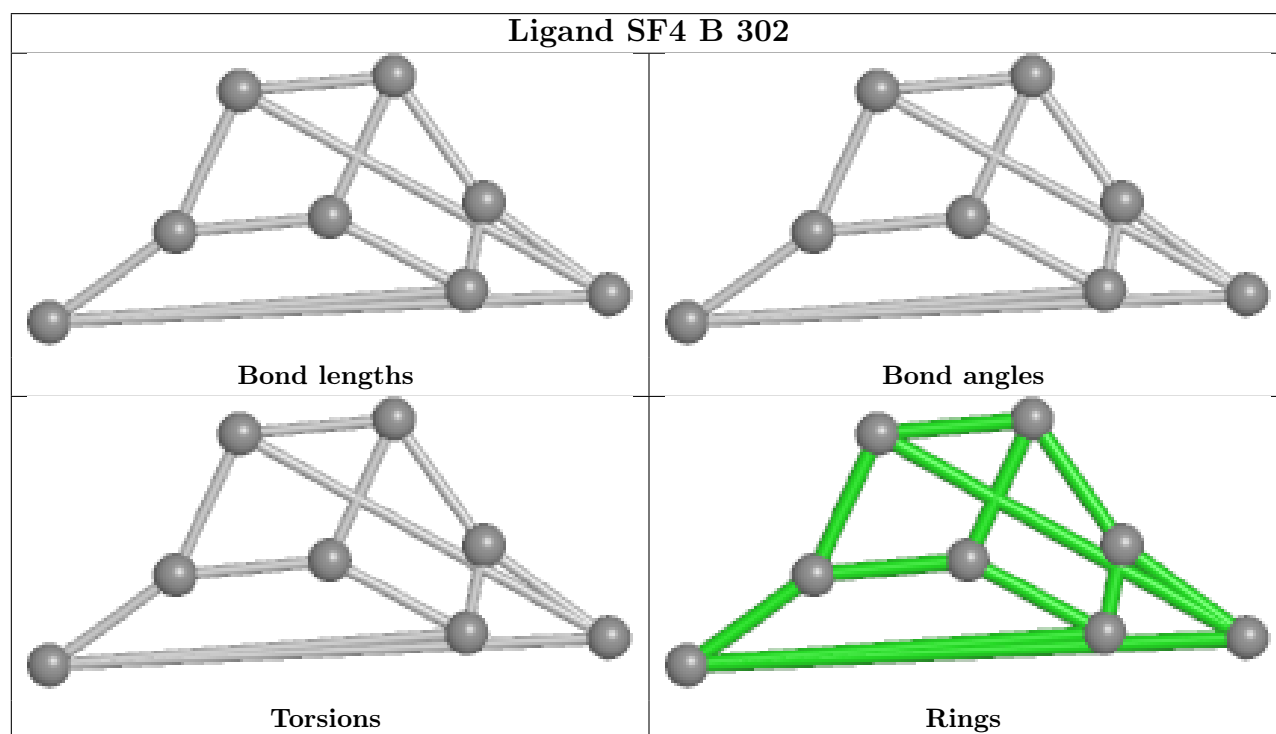
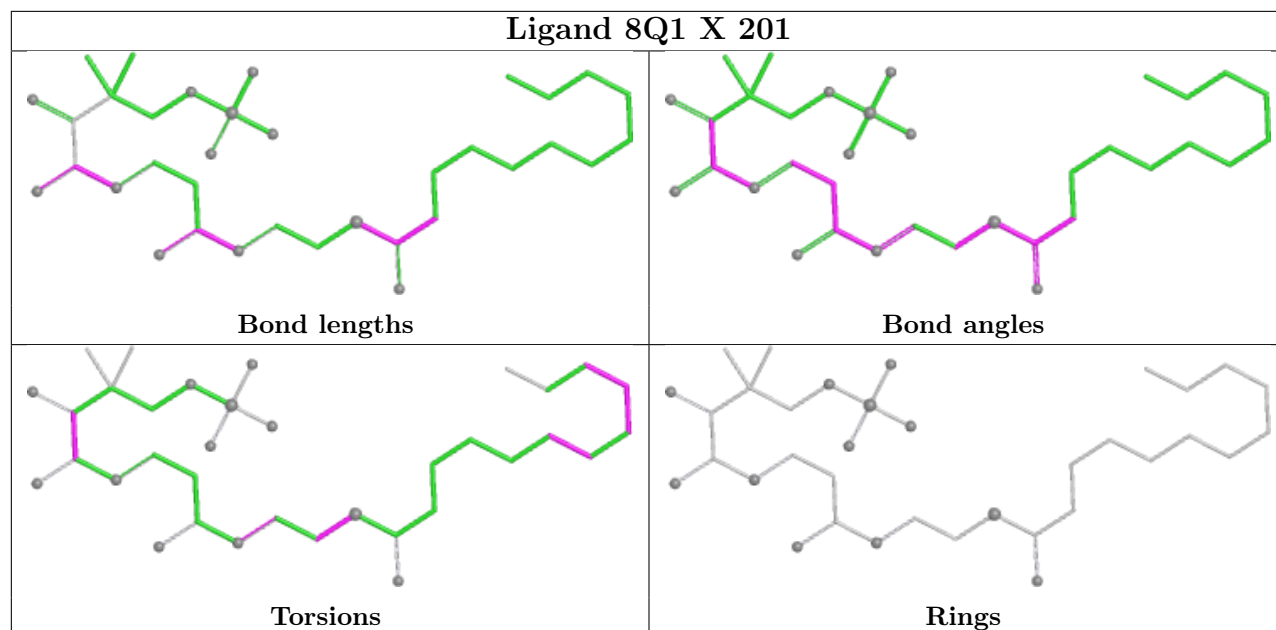


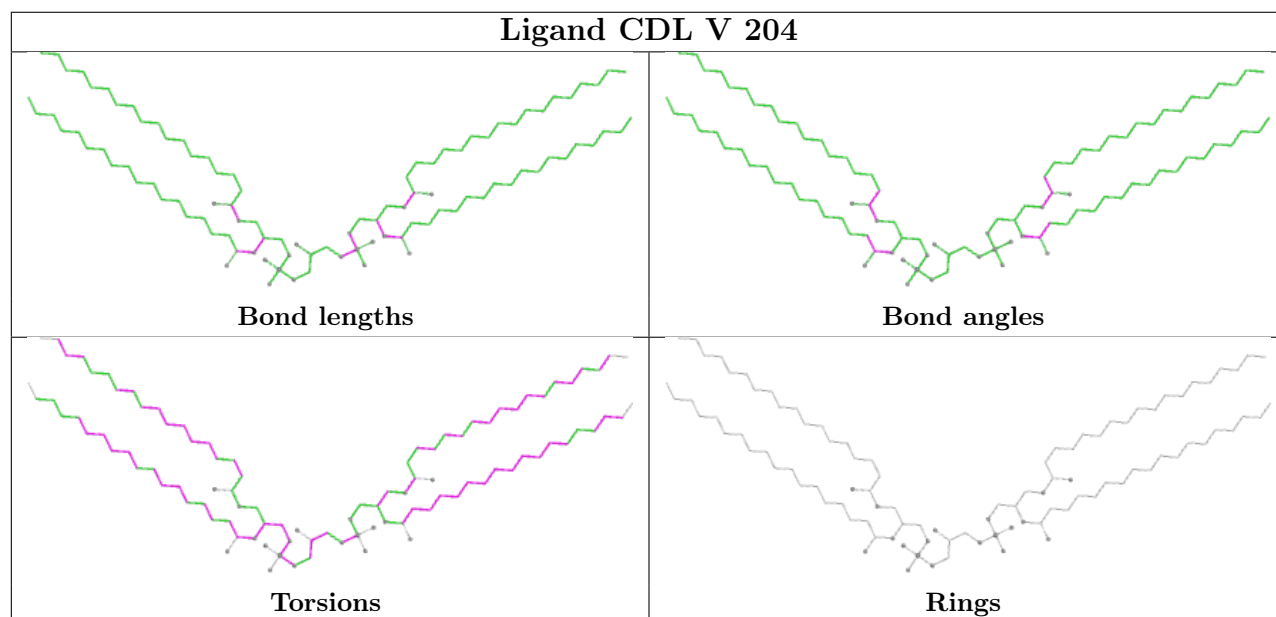
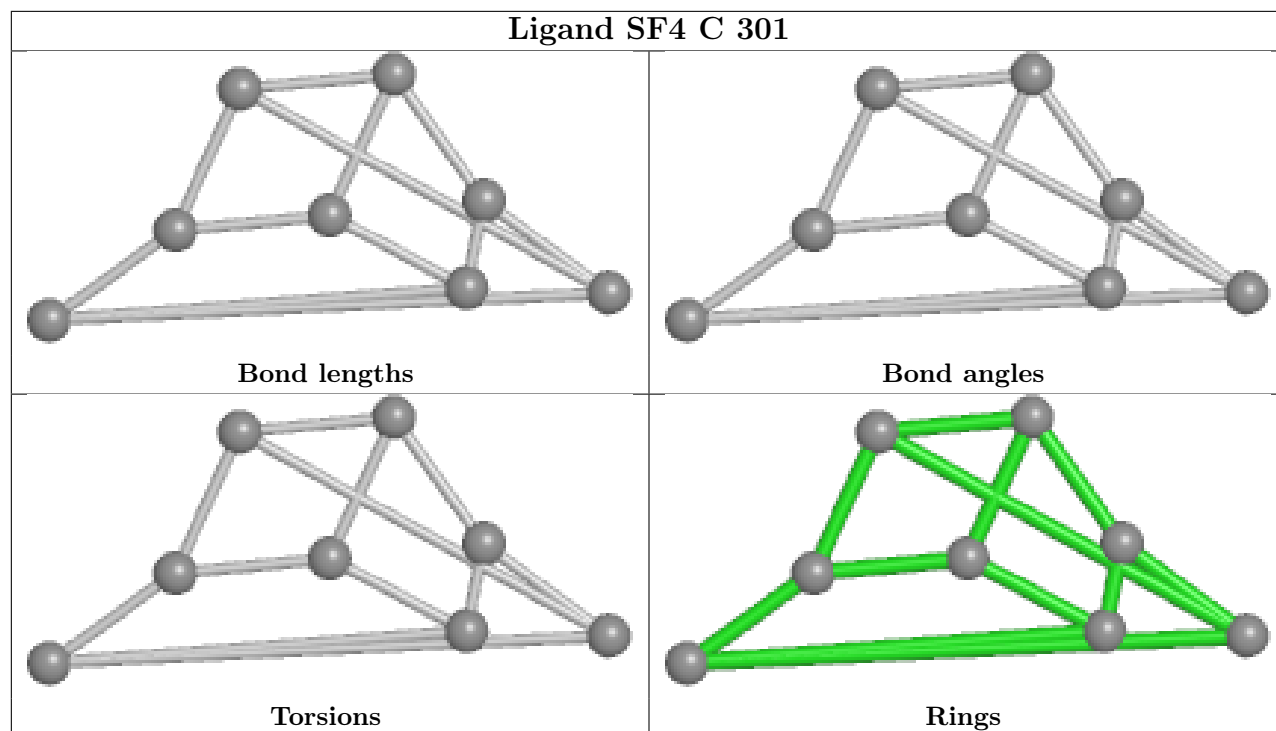


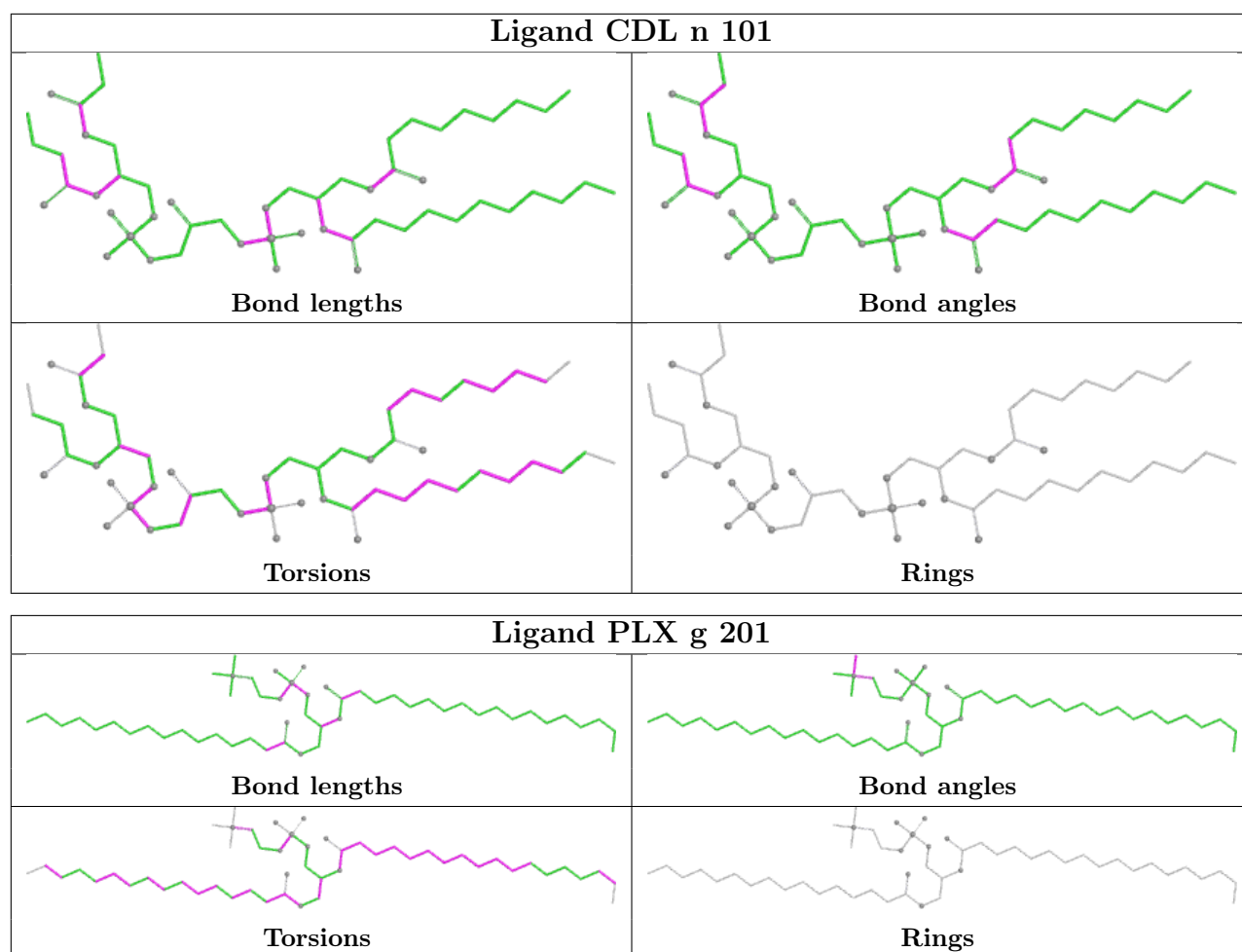


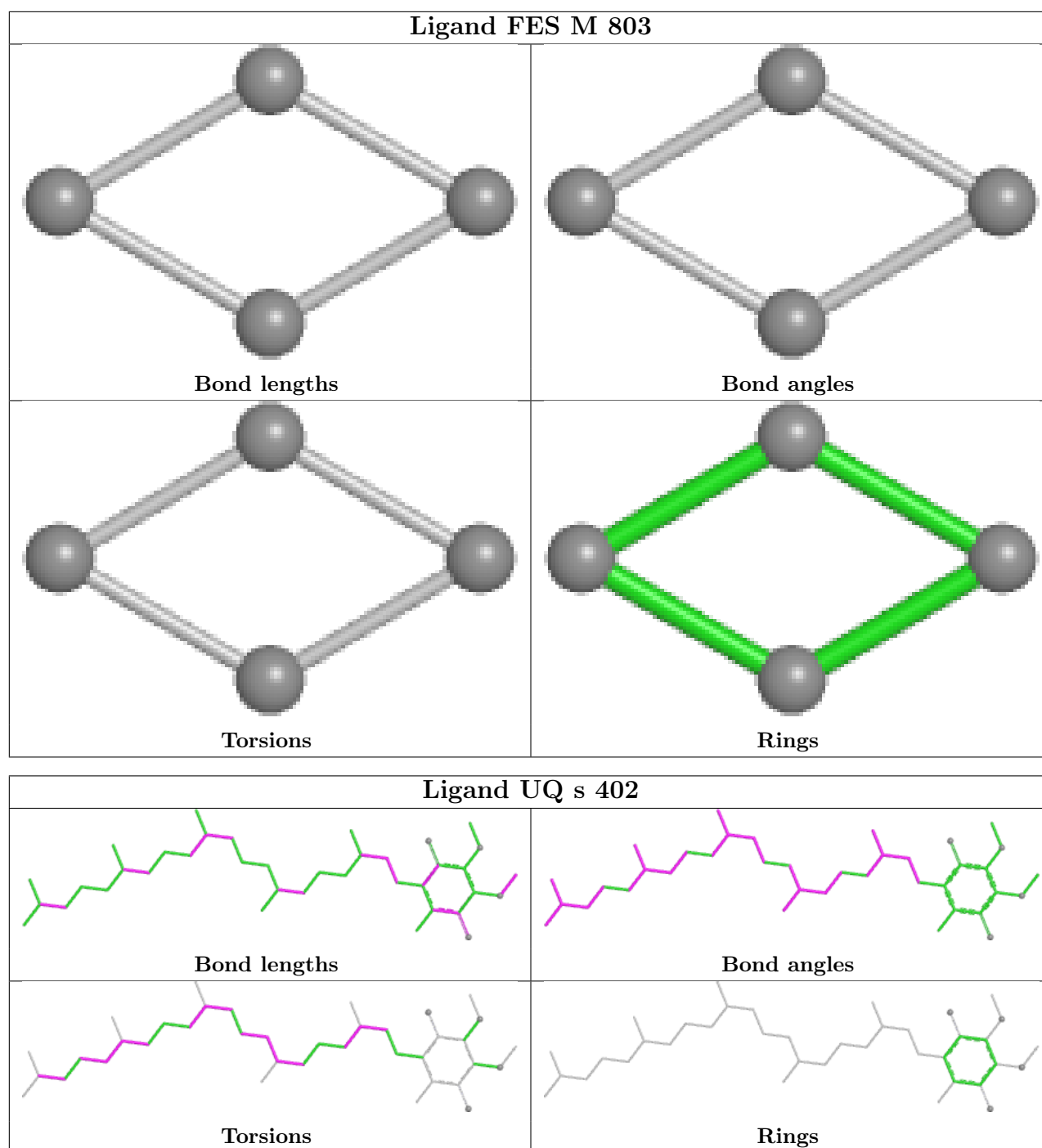












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

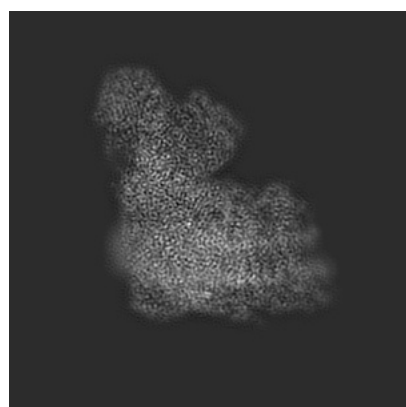
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32267. These allow visual inspection of the internal detail of the map and identification of artifacts.

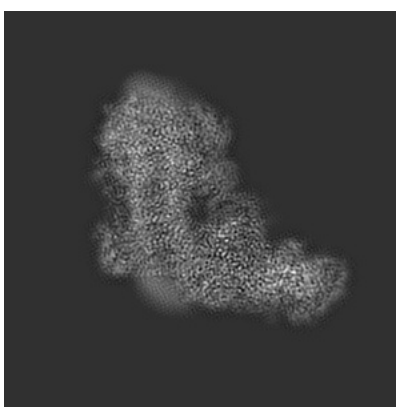
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

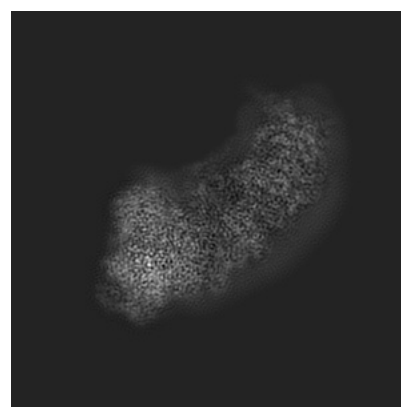
6.1.1 Primary map



X



Y

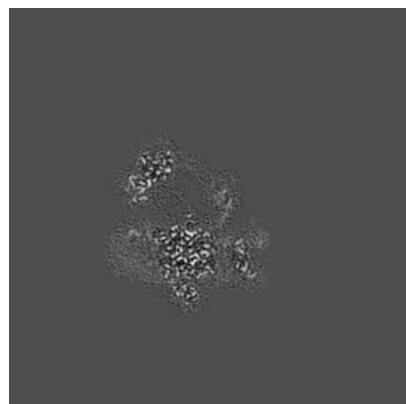


Z

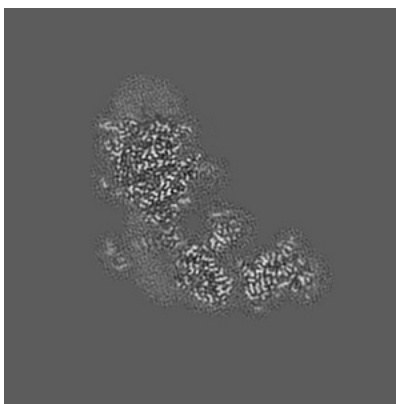
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

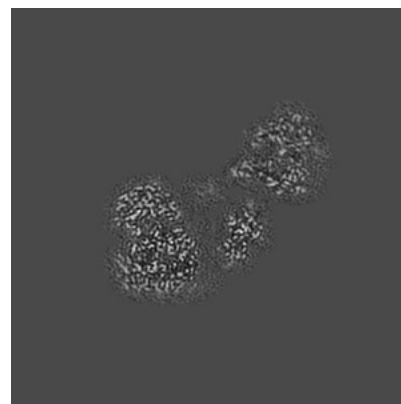
6.2.1 Primary map



X Index: 155



Y Index: 155

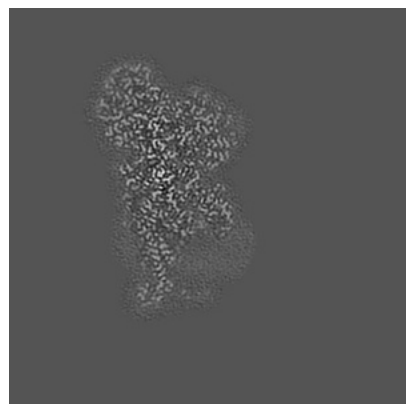


Z Index: 155

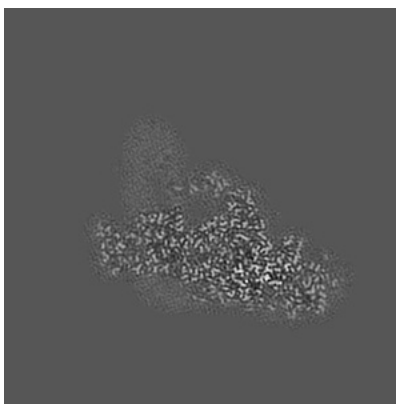
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

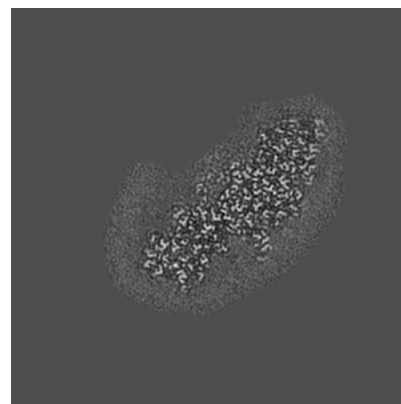
6.3.1 Primary map



X Index: 106



Y Index: 112

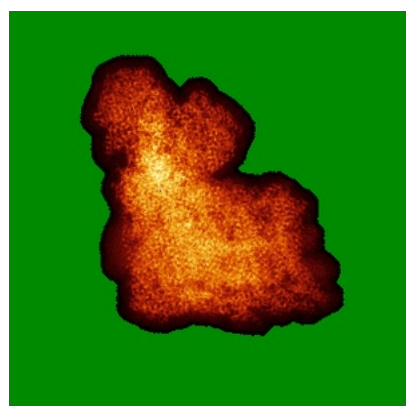


Z Index: 126

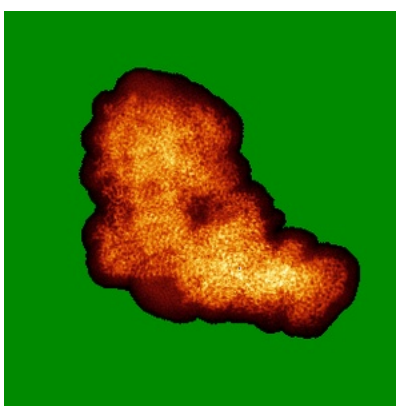
The images above show the largest variance slices of the map in three orthogonal directions.

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

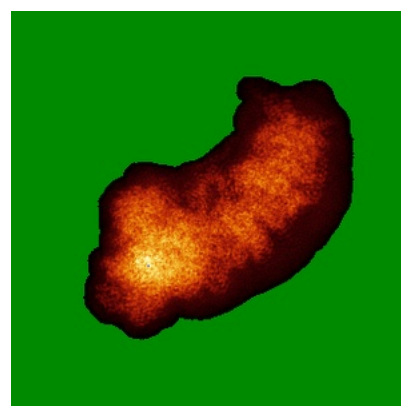
6.4.1 Primary map



X



Y

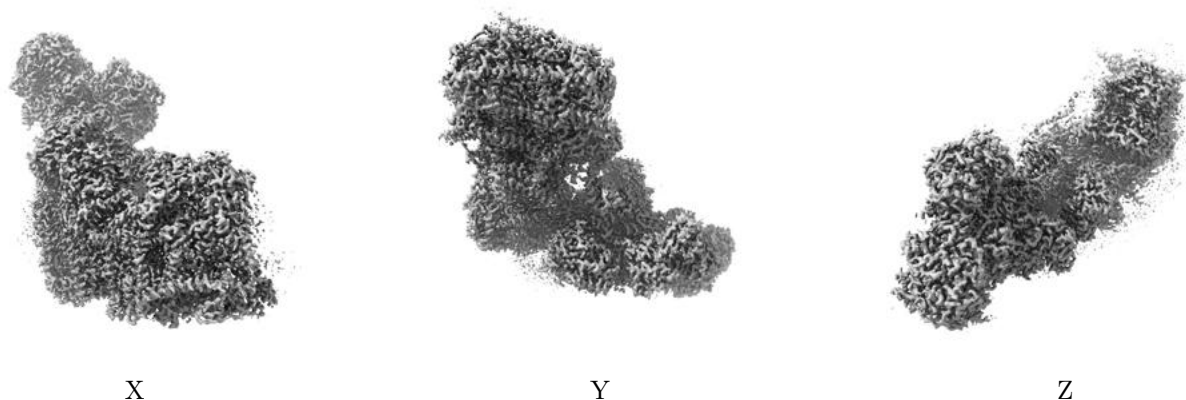


Z

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 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

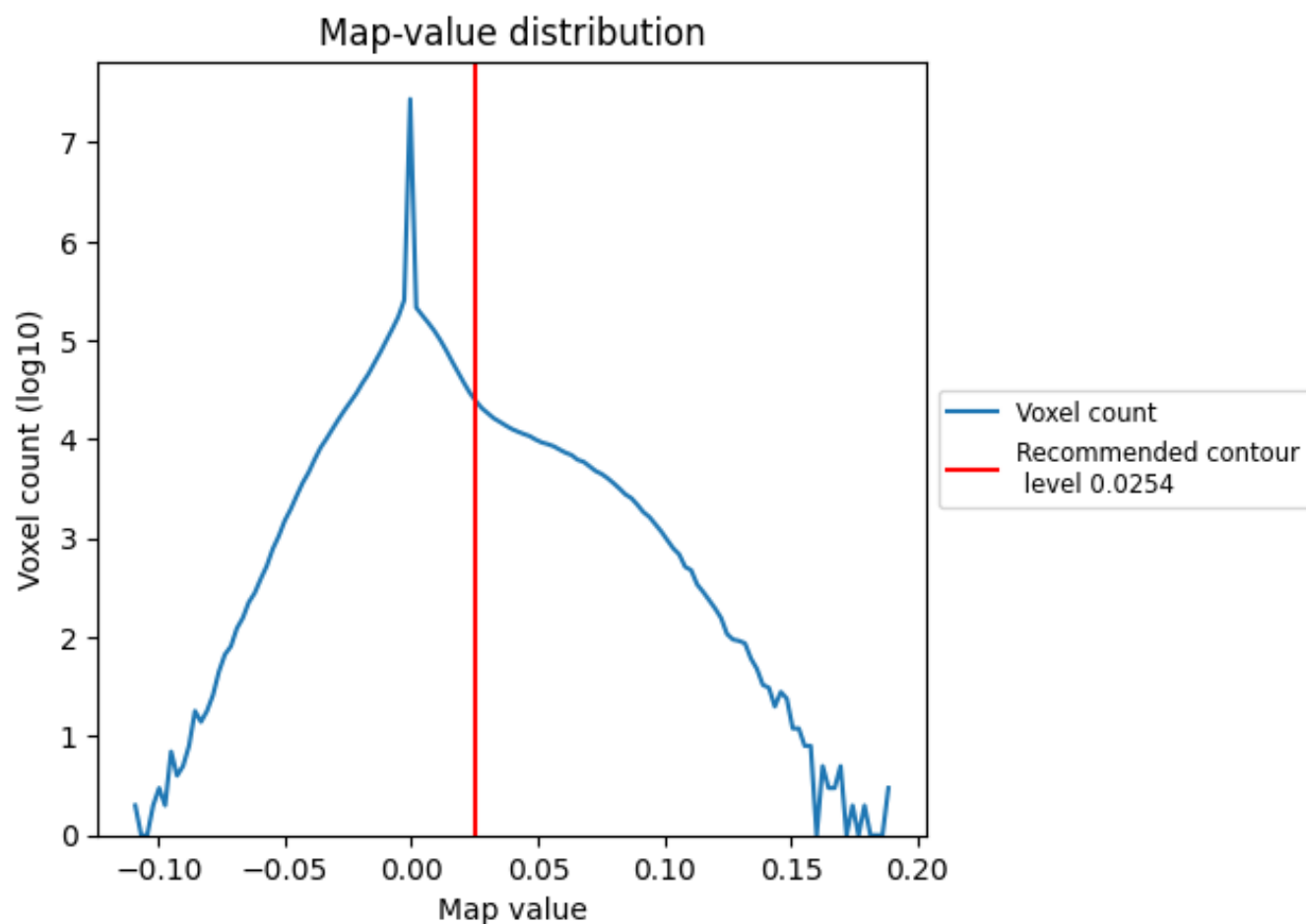
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

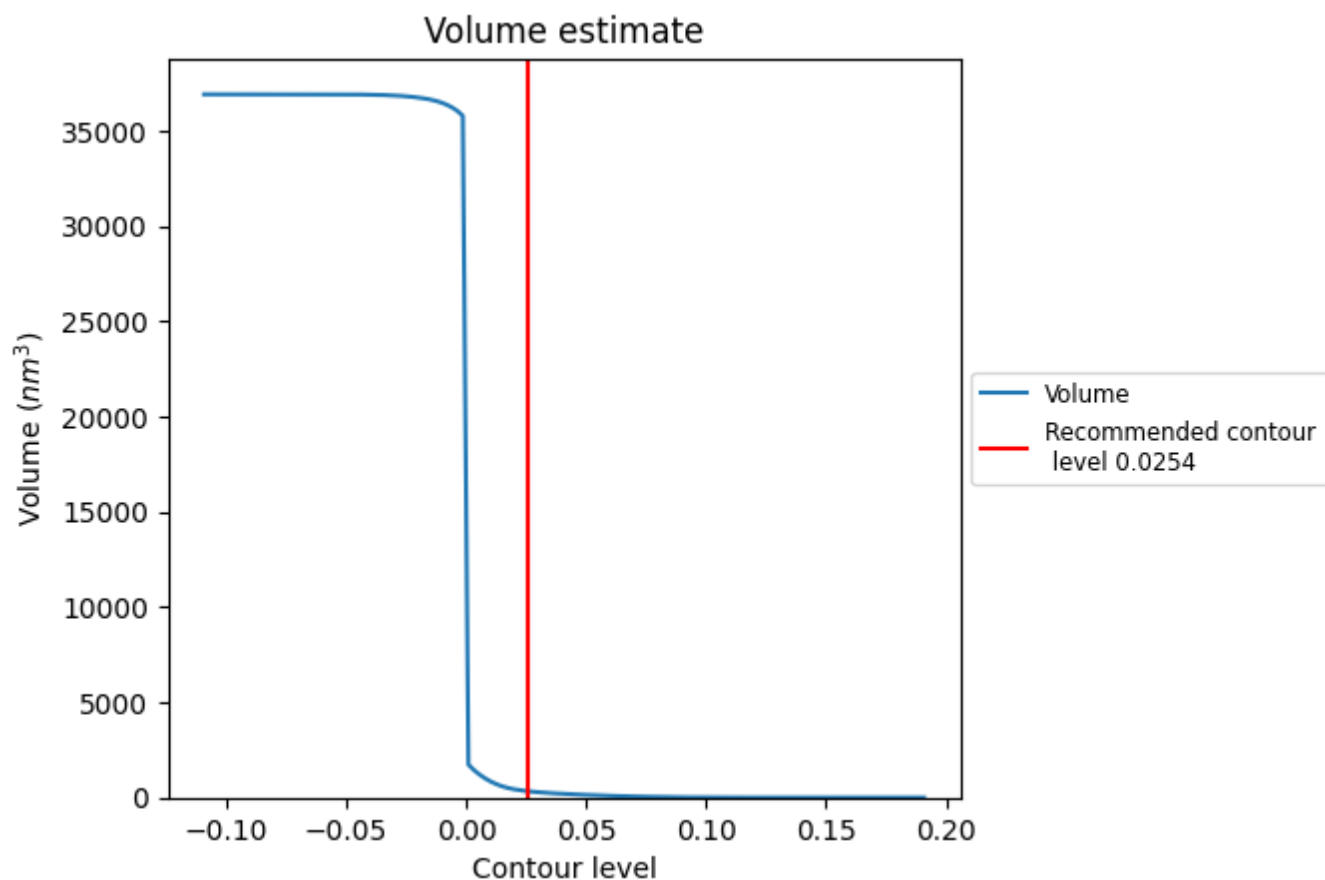
This section contains the results of statistical analysis of the map.

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.

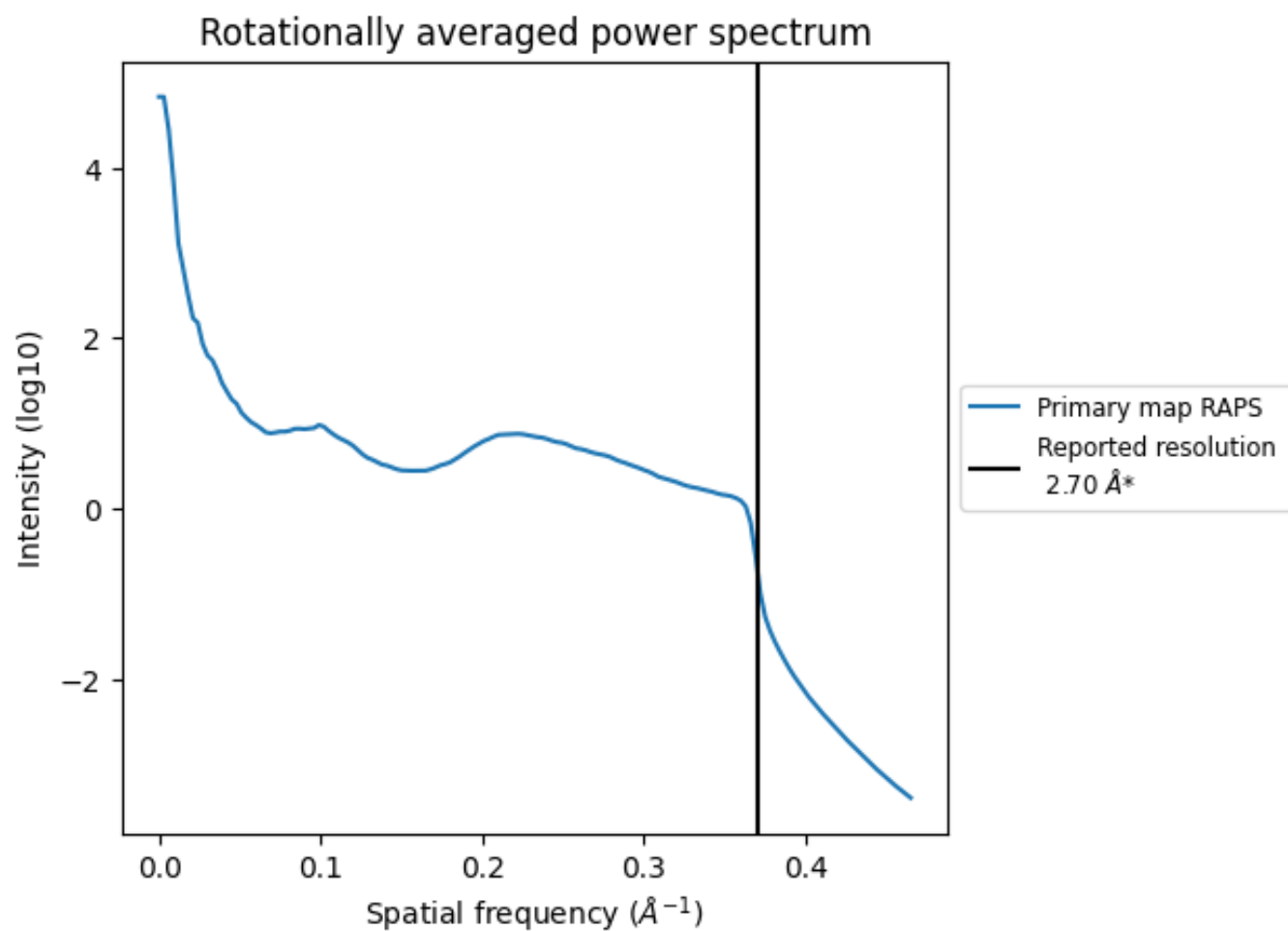
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 0.370 Å⁻¹

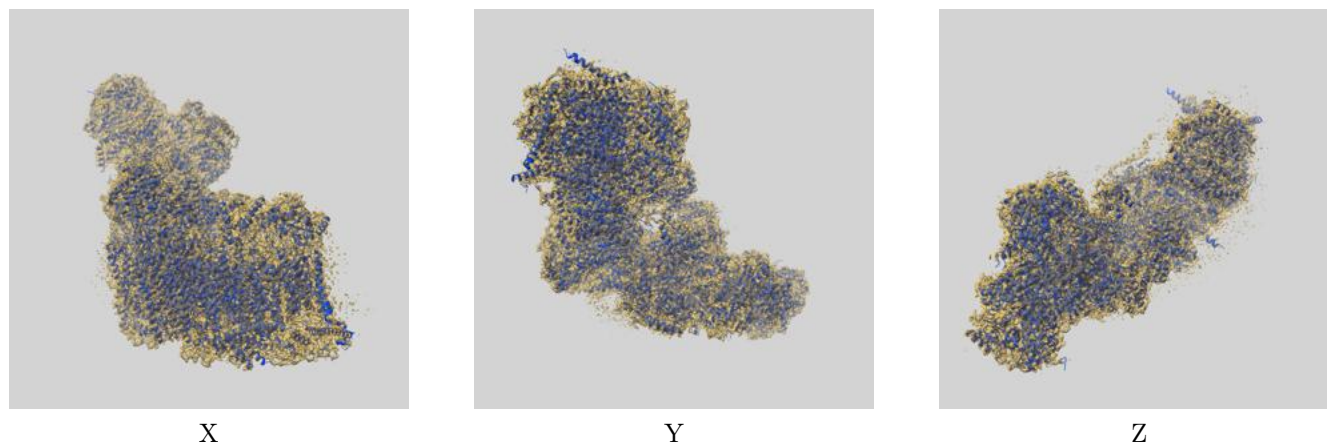
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

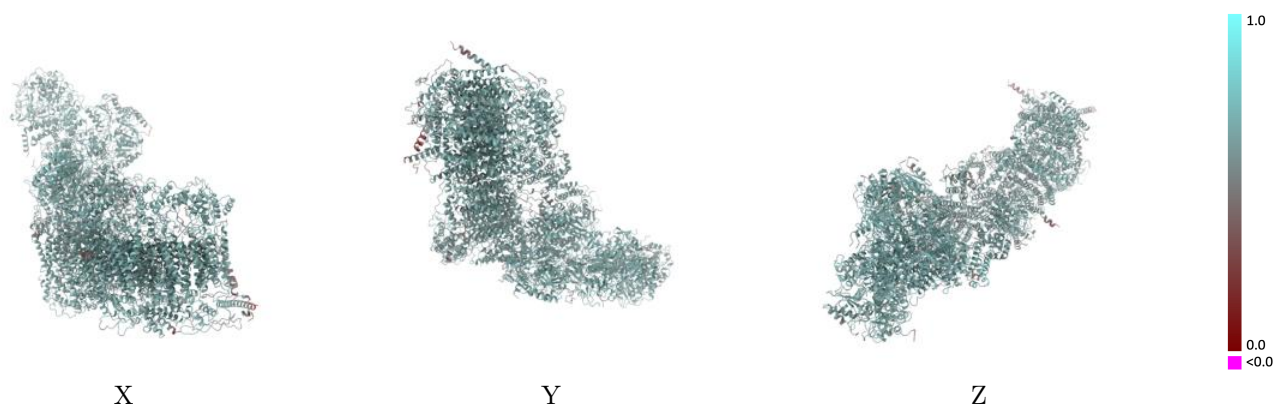
This section contains information regarding the fit between EMDB map EMD-32267 and PDB model 7W2Y. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



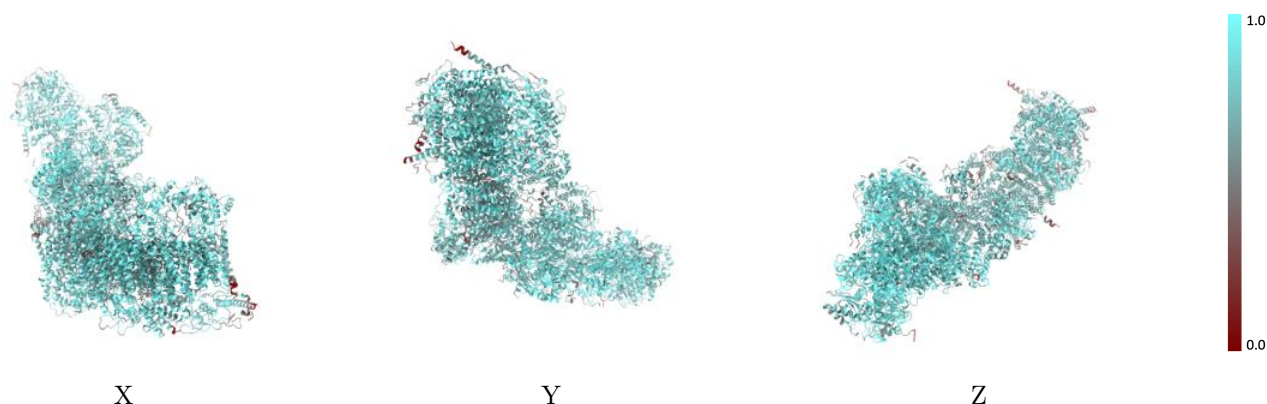
The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



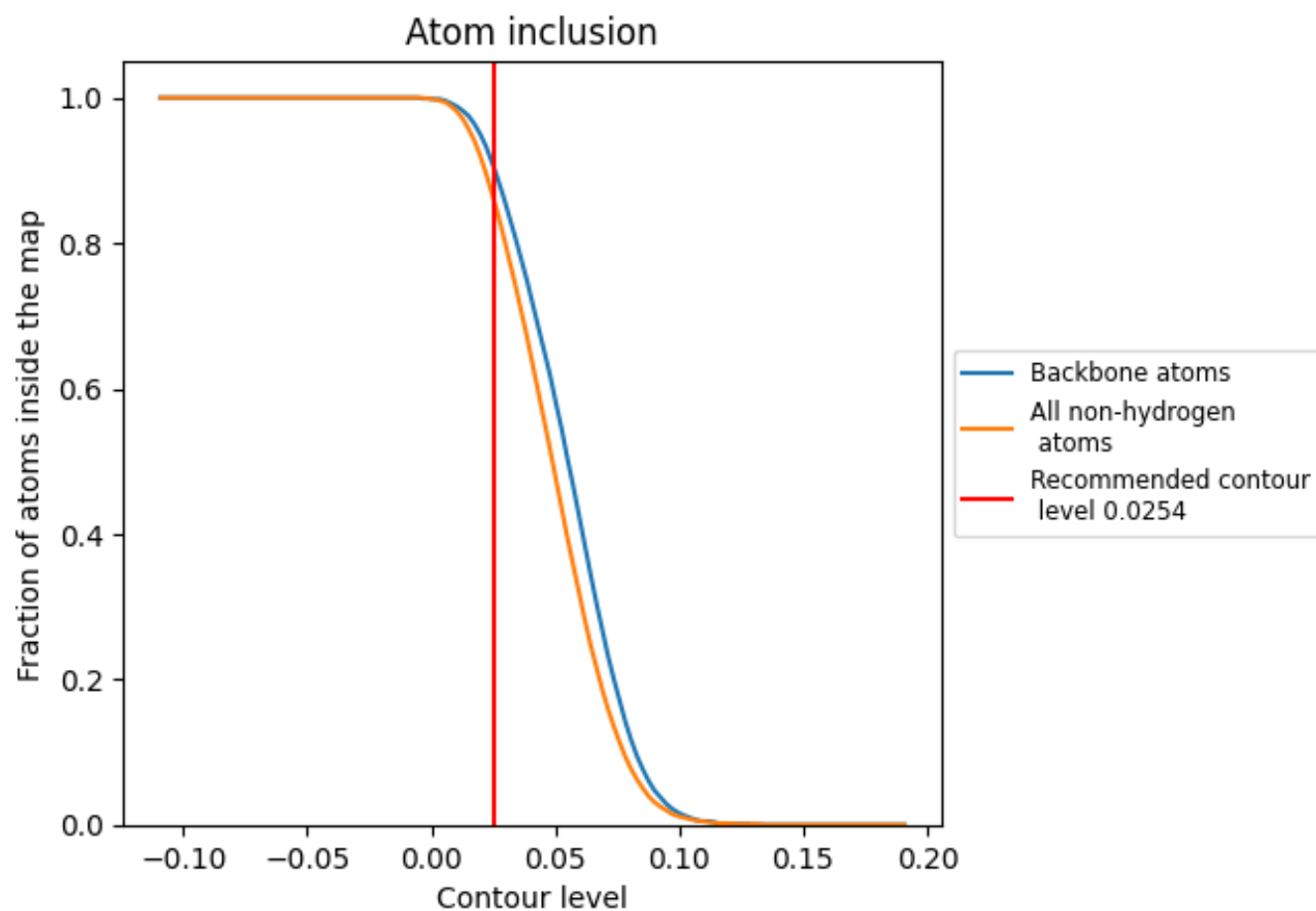
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0254).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.0254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.6260
A	 0.8670	 0.6190
B	 0.9370	 0.6610
C	 0.9270	 0.6570
E	 0.8800	 0.6400
F	 0.7930	 0.5900
G	 0.6270	 0.5350
H	 0.8740	 0.6320
I	 0.7340	 0.5900
J	 0.8890	 0.6350
K	 0.7800	 0.5930
L	 0.8880	 0.6480
M	 0.9090	 0.6420
N	 0.7340	 0.6060
O	 0.8300	 0.6090
P	 0.9550	 0.6680
Q	 0.9510	 0.6610
S	 0.9020	 0.6380
T	 0.8090	 0.6220
U	 0.8280	 0.6060
V	 0.6860	 0.5850
W	 0.8310	 0.6140
X	 0.7850	 0.6040
Y	 0.7190	 0.5620
Z	 0.6460	 0.5530
a	 0.8400	 0.6290
b	 0.7830	 0.5940
c	 0.8370	 0.6170
d	 0.7840	 0.6000
e	 0.7780	 0.5960
f	 0.6570	 0.5620
g	 0.8640	 0.6260
h	 0.8560	 0.6130
i	 0.9280	 0.6510
j	 0.8500	 0.6340



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Chain	Atom inclusion	Q-score
k	 0.9300	 0.6460
l	 0.8630	 0.6290
m	 0.8110	 0.6060
n	 0.6920	 0.5690
o	 0.8380	 0.6270
p	 0.8500	 0.6220
r	 0.9110	 0.6410
s	 0.9180	 0.6480
u	 0.8520	 0.6170
v	 0.7270	 0.5640
w	 0.8580	 0.6220