



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:30 AM UTC

PDB ID : 7VZW / pdb_00007vzw
EMDB ID : EMD-32231
Title : Active state CI from Q10 dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-16
Resolution : 3.20 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:

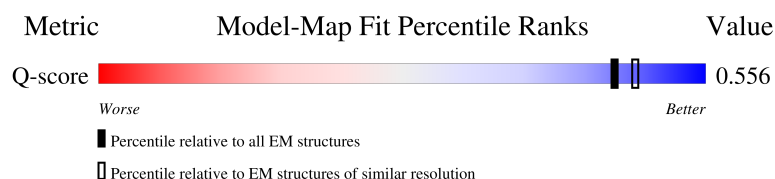
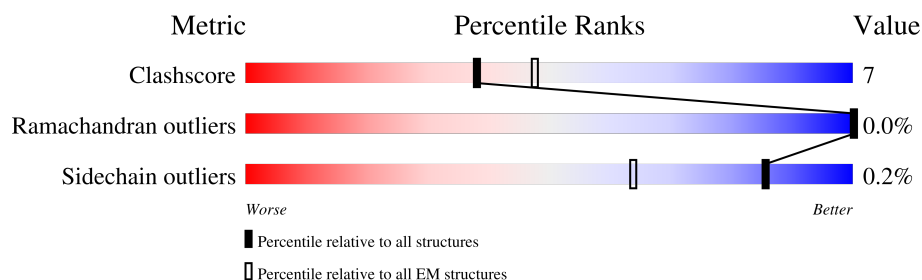
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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% 19%
2	B	176	 82% 18%
3	C	156	 83% 16%
4	E	115	 80% 20%

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

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

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 68165 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
			3326	2101	593	612	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
			694	447	103	139	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1735	1123	298	312	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	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2706	1779	419	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
			4816	3193	746	826	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
			1291	861	188	229	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
			1526	978	279	261	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		

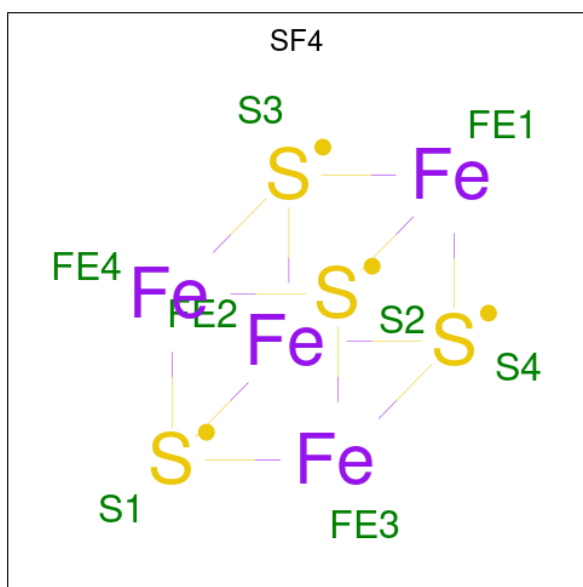
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

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

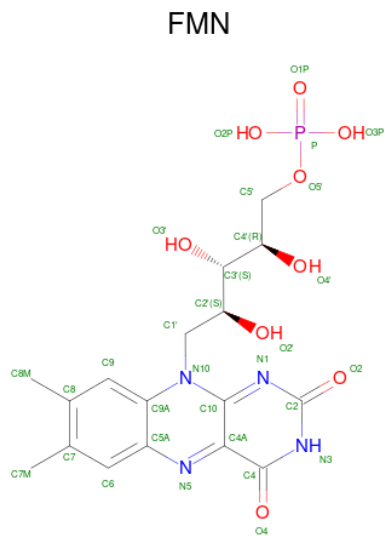
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2579	1643	438	488	10		

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



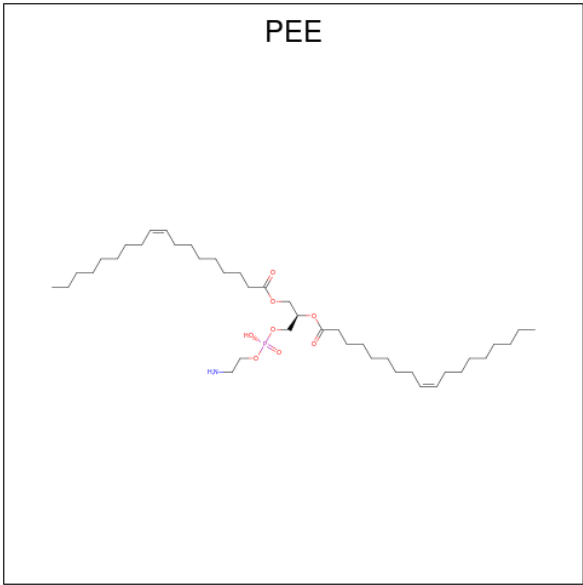
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- 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
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



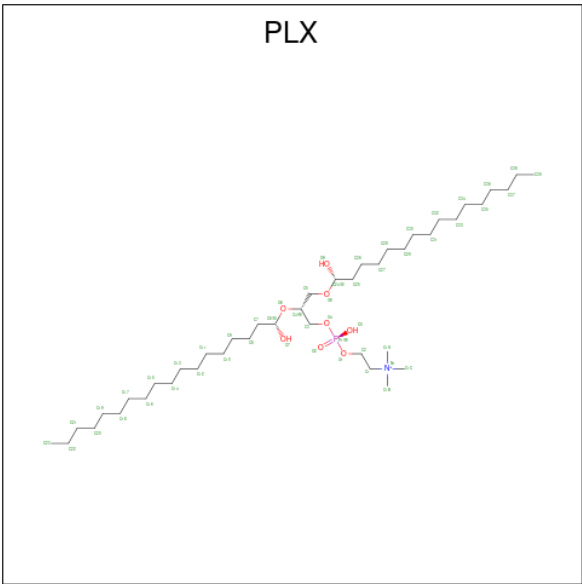
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total 51	C 41	N 1	O 8	P 1	0
47	C	1	Total 47	C 37	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
47	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
47	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
47	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	s	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 48 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).



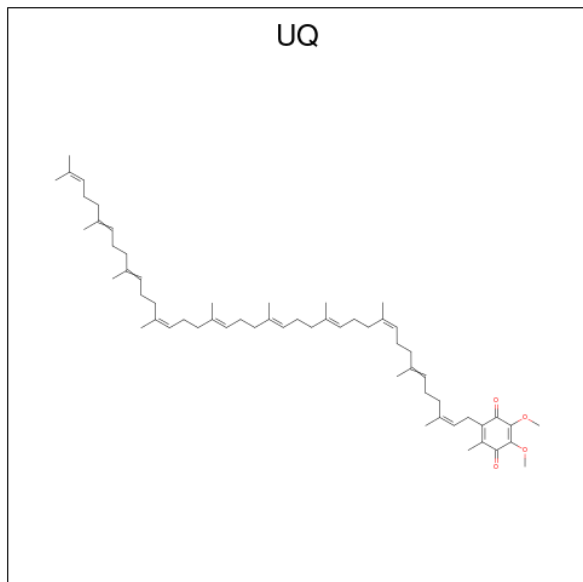
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	N	1	Total	C	N	O	P	0
			52	42	1	8	1	

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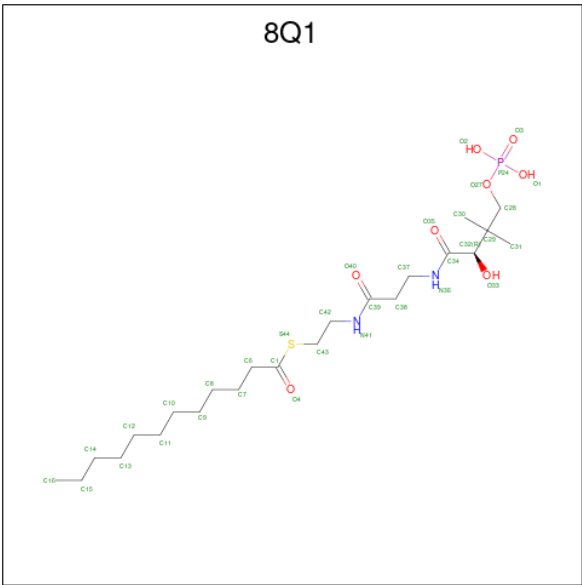
Mol	Chain	Residues	Atoms					AltConf
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	n	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



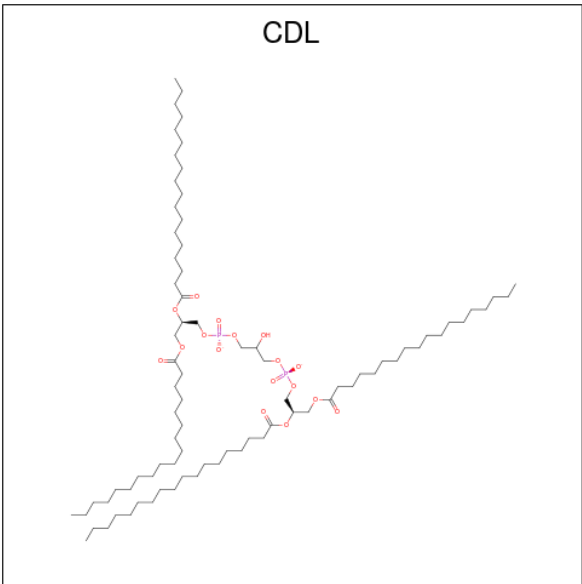
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			63	59	4	
49	J	1	Total	C	O	0
			33	29	4	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



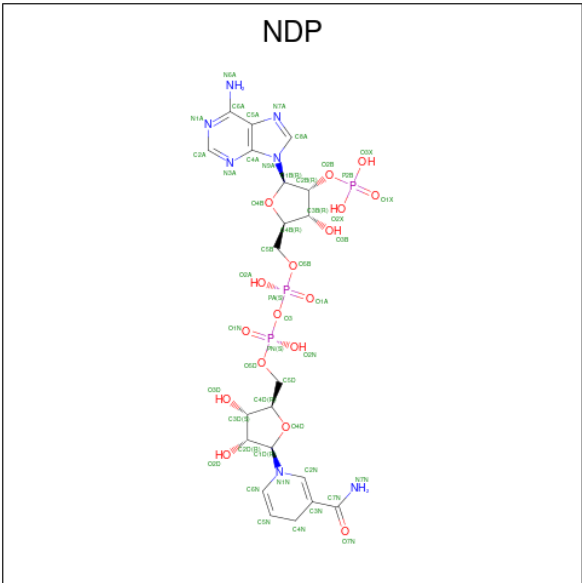
Mol	Chain	Residues	Atoms				AltConf
51	I	1	Total	C	O	P	0
			51	32	17	2	

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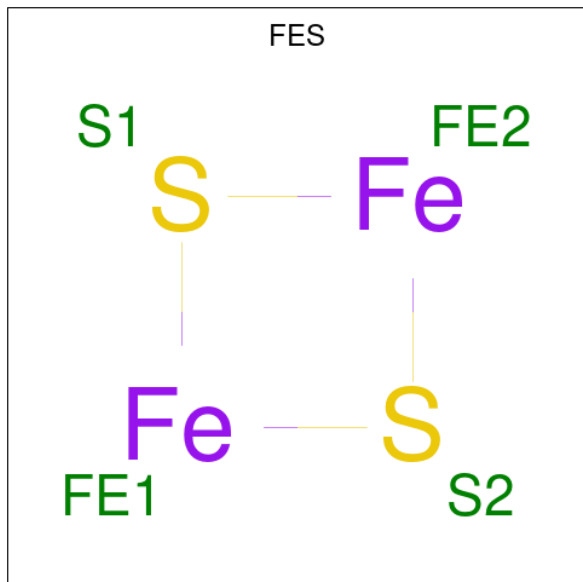
Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total	C	O	P	0
			94	75	17	2	
51	V	1	Total	C	O	P	0
			100	81	17	2	
51	a	1	Total	C	O	P	0
			100	81	17	2	
51	l	1	Total	C	O	P	0
			99	80	17	2	
51	l	1	Total	C	O	P	0
			100	81	17	2	
51	m	1	Total	C	O	P	0
			100	81	17	2	
51	n	1	Total	C	O	P	0
			55	36	17	2	
51	r	1	Total	C	O	P	0
			100	81	17	2	
51	s	1	Total	C	O	P	0
			89	70	17	2	

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



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

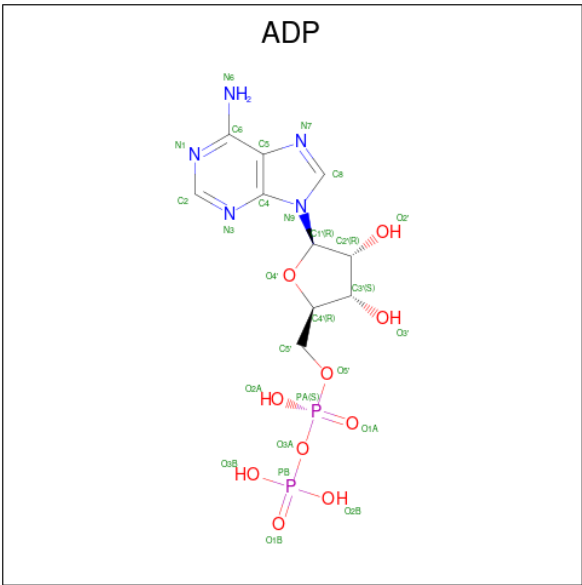
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

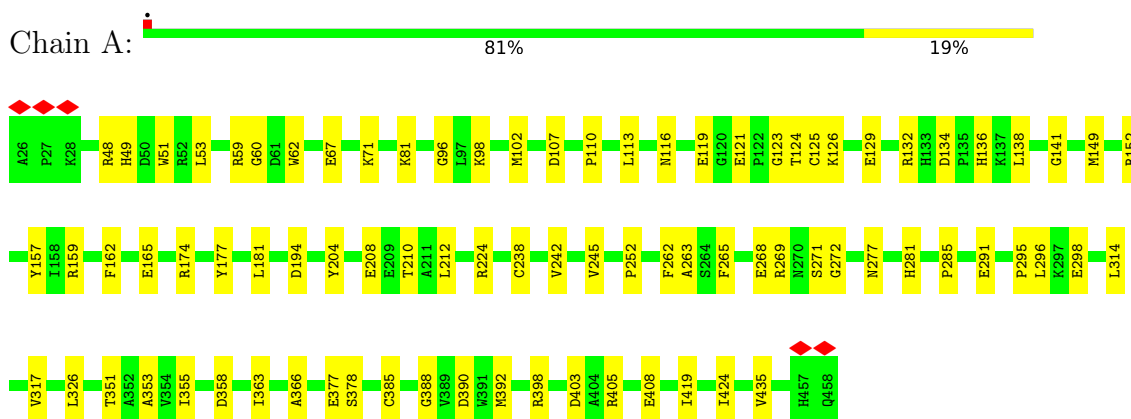


Mol	Chain	Residues	Atoms					AltConf
56	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

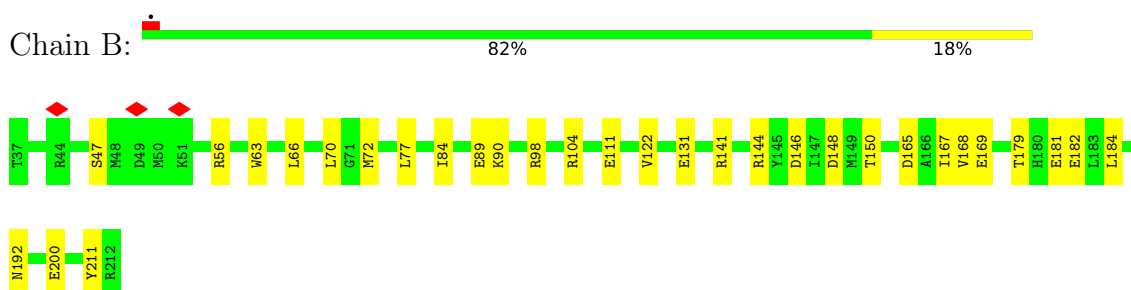
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

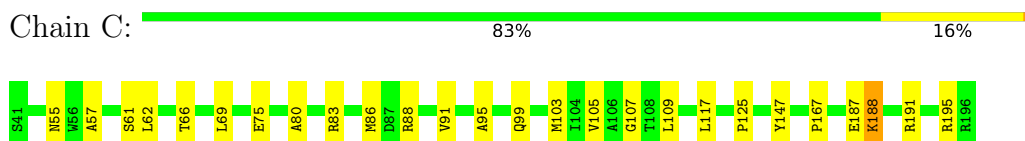
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



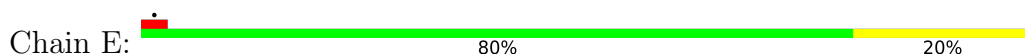
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

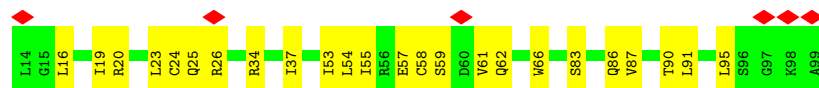


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6





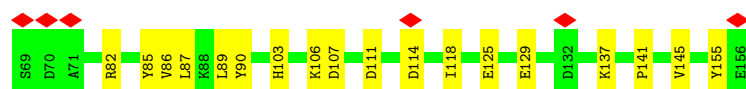
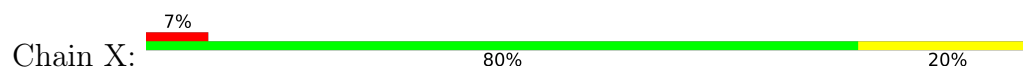
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



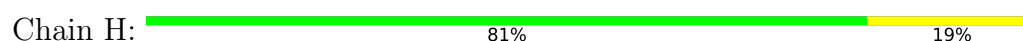
- Molecule 6: Acyl carrier protein



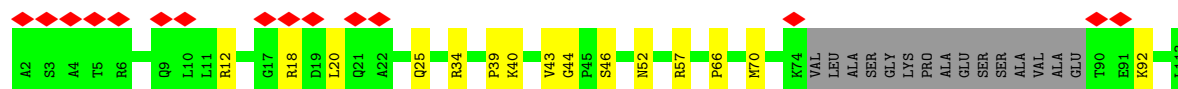
- Molecule 6: Acyl carrier protein



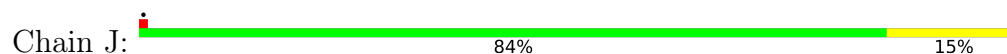
- Molecule 7: Complex I subunit B13

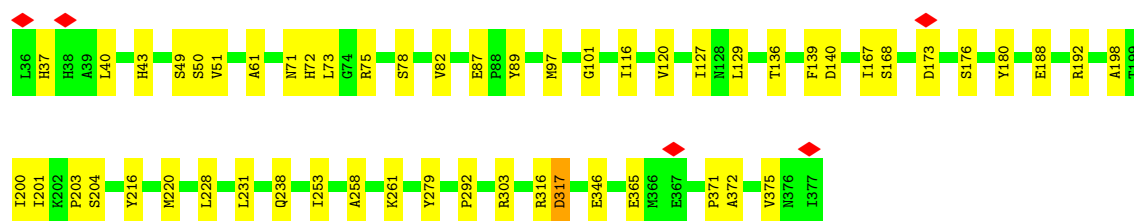


- Molecule 8: Complex I-B14.5a

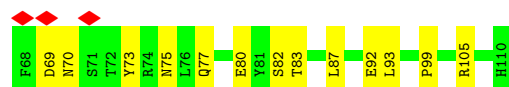


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

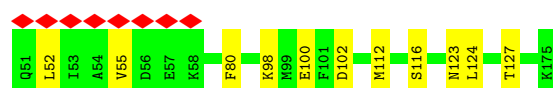
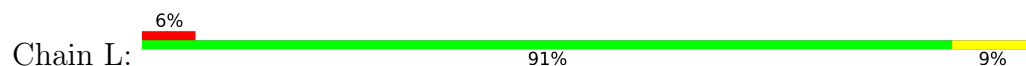




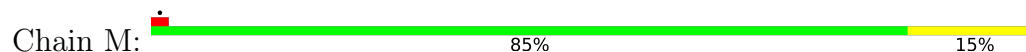
• Molecule 10: Complex I-9kD



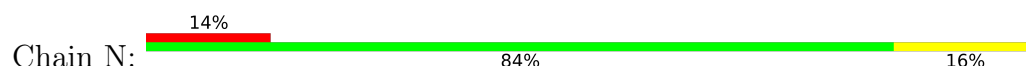
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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



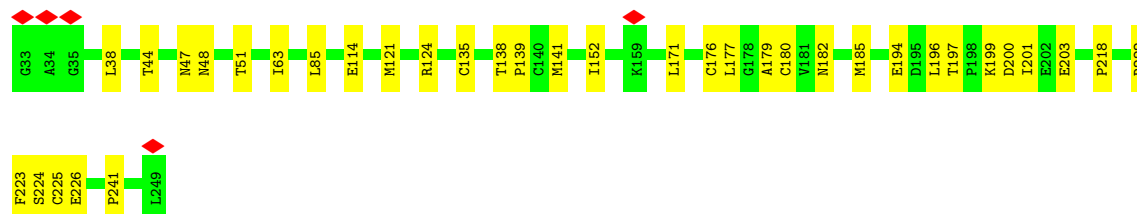
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





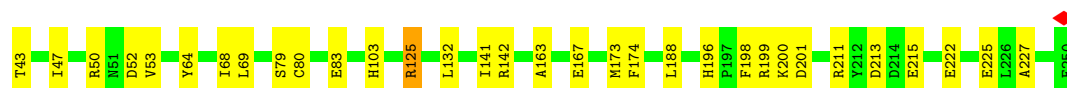
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O: 83% 17%



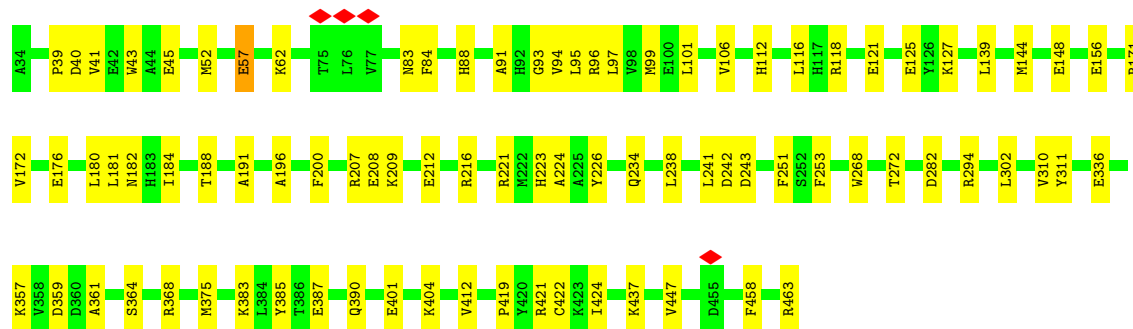
- Molecule 15: Complex I-30kD

Chain P: 85% 15%



- Molecule 16: Complex I-49kD

Chain Q: 80% 20%



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

Chain S: 89% 11%

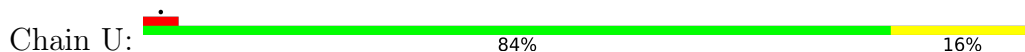


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

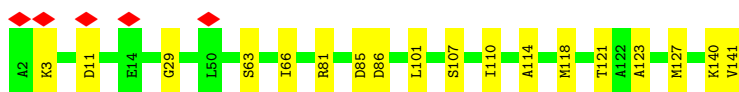
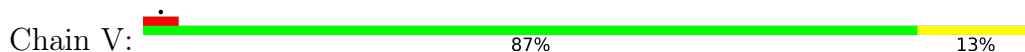
Chain T: 7% 90% 10%



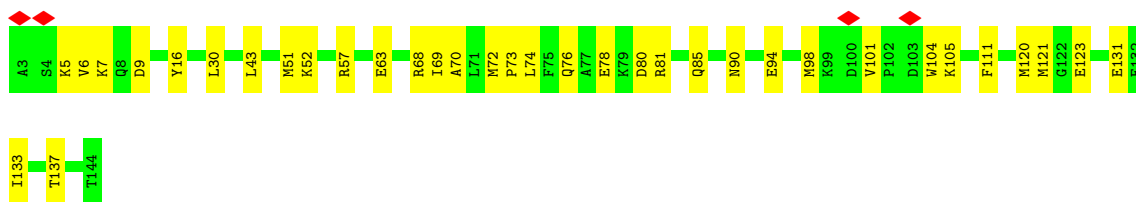
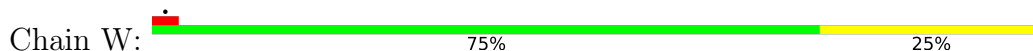
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



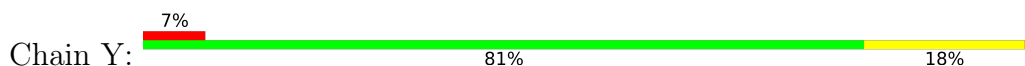
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



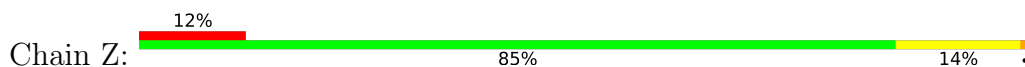
- Molecule 21: Complex I-B16.6



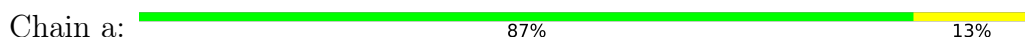
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

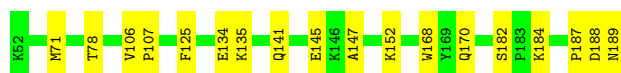


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

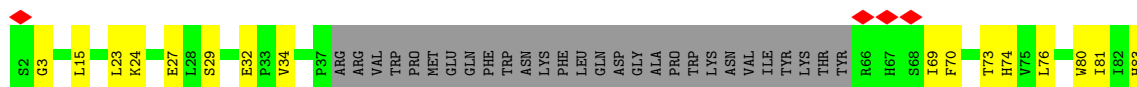


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

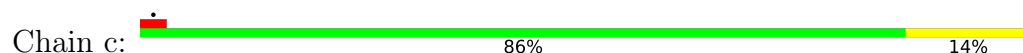




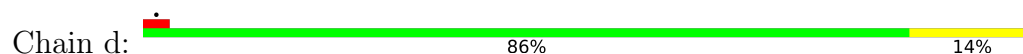
- Molecule 25: Complex I-B17



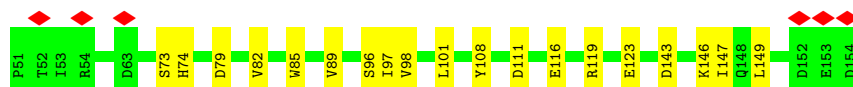
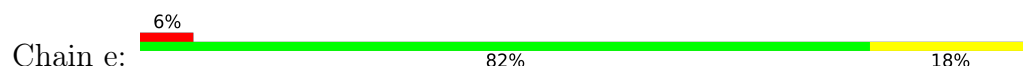
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



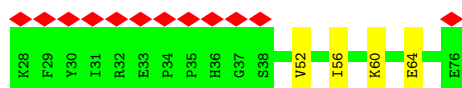
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



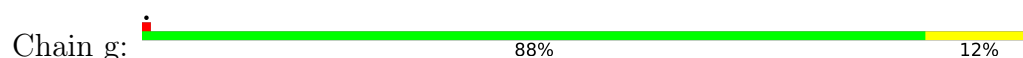
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

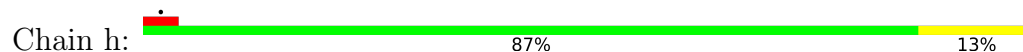


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

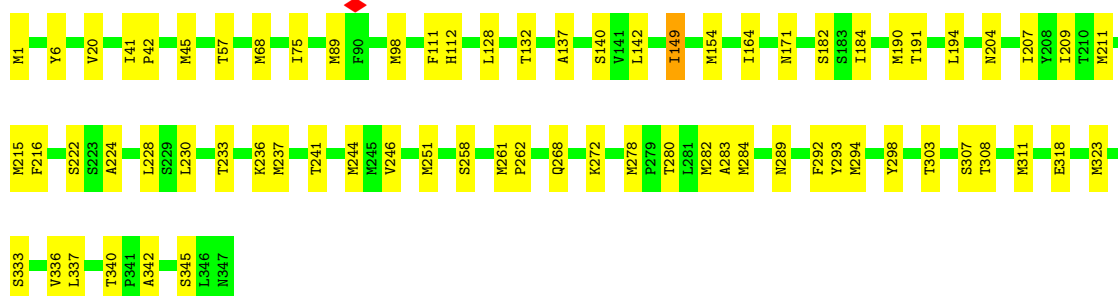
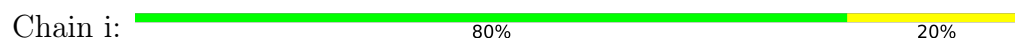




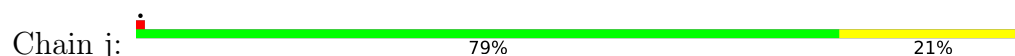
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



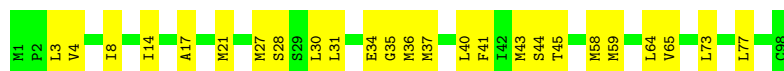
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



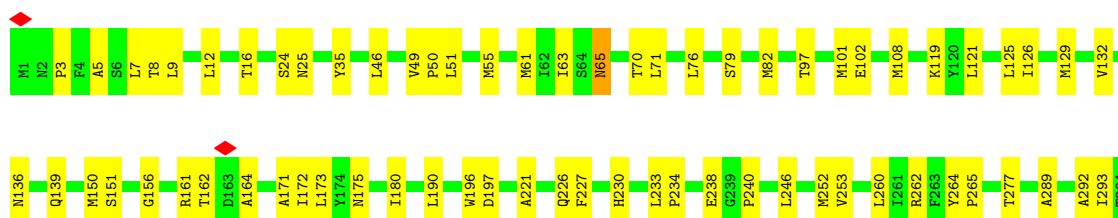
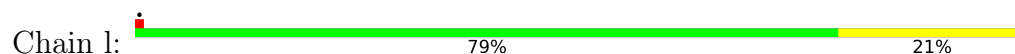
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

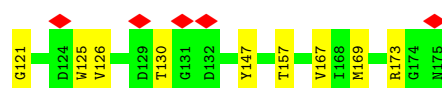
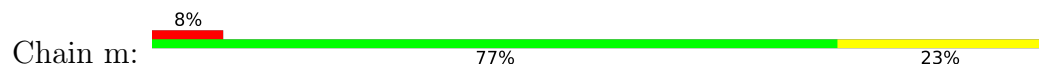


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

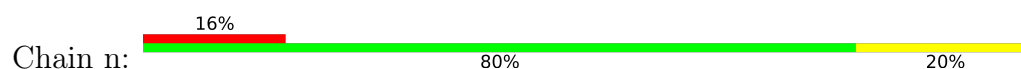




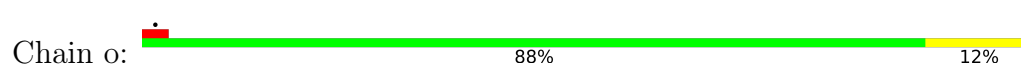
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



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



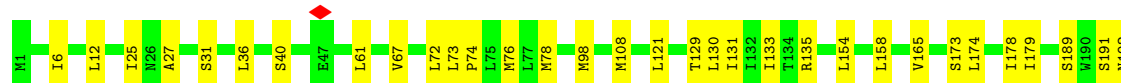
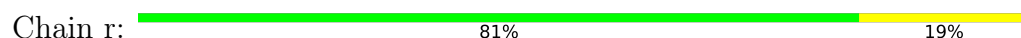
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

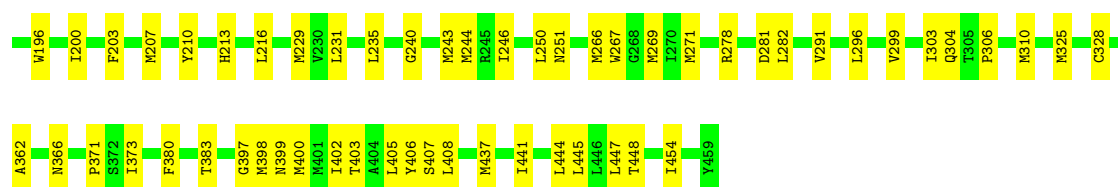


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



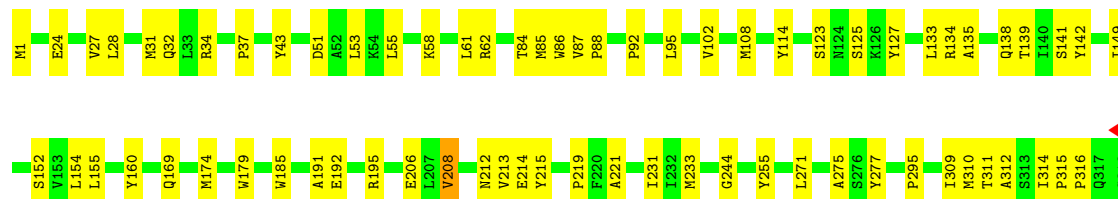
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4





- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 78% 22%



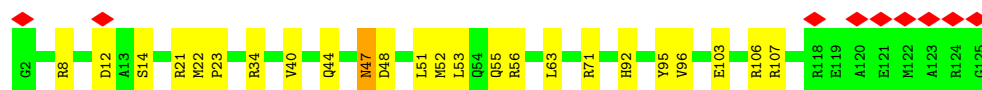
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 87% 13%



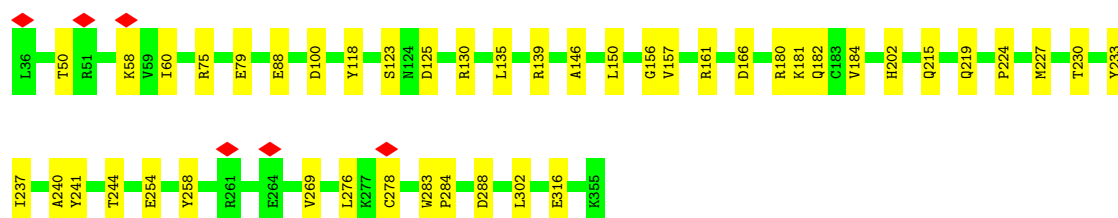
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 7% 81% 19%



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

Chain w: 86% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128783	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	0.217	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0219	Depositor
Map size ($\text{\AA}$)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: SF4, CDL, FES, 2MR, FMN, ZN, UQ, ADP, 8Q1, NDP, MG, PLX, PEE

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	0.15	0/3402	0.30	0/4598
2	B	0.19	0/1443	0.31	0/1952
3	C	0.17	0/1279	0.26	0/1730
4	E	0.14	0/995	0.26	0/1340
5	F	0.15	0/698	0.36	0/940
6	G	0.16	0/702	0.45	0/952
6	X	0.14	0/705	0.31	0/954
7	H	0.15	0/929	0.34	0/1258
8	I	0.14	0/798	0.35	0/1079
9	J	0.14	0/2828	0.29	0/3834
10	K	0.12	0/377	0.26	0/509
11	L	0.16	0/1039	0.28	0/1403
12	M	0.15	0/5384	0.28	0/7295
13	N	0.12	0/1245	0.28	0/1694
14	O	0.14	0/1711	0.31	0/2328
15	P	0.20	0/1786	0.42	1/2432 (0.0%)
16	Q	0.18	0/3538	0.32	0/4796
17	S	0.16	0/581	0.38	0/781
18	T	0.13	0/755	0.25	0/1018
19	U	0.12	0/664	0.24	0/912
20	V	0.13	0/1042	0.24	0/1411
21	W	0.15	0/1192	0.30	0/1610
22	Y	0.13	0/610	0.29	0/836
23	Z	0.15	0/660	0.33	0/892
24	a	0.17	0/1184	0.31	0/1603
25	b	0.14	0/844	0.31	0/1149
26	c	0.14	0/1371	0.29	0/1875
27	d	0.13	0/1494	0.27	0/2015
28	e	0.14	0/891	0.30	0/1210
29	f	0.12	0/386	0.25	0/523
30	g	0.14	0/1031	0.27	0/1394
31	h	0.15	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.18	0/2769	0.33	0/3764
33	j	0.16	0/938	0.30	0/1281
34	k	0.18	0/759	0.30	0/1029
35	l	0.16	0/4947	0.33	0/6728
36	m	0.18	0/1323	0.36	0/1797
37	n	0.13	0/491	0.26	0/663
38	o	0.15	0/1092	0.32	0/1481
39	p	0.13	0/1582	0.25	0/2145
40	r	0.17	0/3723	0.30	0/5078
41	s	0.18	0/2581	0.35	0/3529
42	u	0.14	0/1436	0.30	0/1938
43	v	0.14	0/1052	0.34	0/1411
44	w	0.15	0/2639	0.37	0/3575
All	All	0.16	0/67785	0.31	1/91932 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	125	ARG	N-CA-C	8.81	120.88	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3326	0	3288	67	0
2	B	1412	0	1363	26	0
3	C	1248	0	1254	21	0
4	E	971	0	975	18	0
5	F	687	0	700	14	0
6	G	690	0	669	24	0
6	X	694	0	674	14	0
7	H	910	0	950	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	780	0	808	13	0
9	J	2751	0	2773	36	0
10	K	366	0	338	12	0
11	L	1016	0	1016	9	0
12	M	5296	0	5326	70	0
13	N	1204	0	1162	17	0
14	O	1671	0	1673	27	0
15	P	1735	0	1691	27	0
16	Q	3459	0	3396	61	0
17	S	566	0	561	6	0
18	T	741	0	702	9	0
19	U	643	0	642	12	0
20	V	1021	0	1025	11	0
21	W	1161	0	1144	33	0
22	Y	584	0	529	10	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	18	0
25	b	819	0	835	20	0
26	c	1315	0	1208	18	0
27	d	1461	0	1429	17	0
28	e	867	0	817	14	0
29	f	378	0	356	2	0
30	g	1000	0	994	14	0
31	h	867	0	871	12	0
32	i	2706	0	2863	55	0
33	j	914	0	951	24	0
34	k	748	0	799	21	0
35	l	4816	0	4955	85	0
36	m	1291	0	1265	47	0
37	n	479	0	486	12	0
38	o	1062	0	1072	10	0
39	p	1526	0	1462	10	0
40	r	3631	0	3839	64	0
41	s	2508	0	2607	63	0
42	u	1398	0	1374	20	0
43	v	1028	0	982	20	0
44	w	2579	0	2534	34	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	B	51	0	82	4	0
47	C	47	0	71	0	0
47	Q	47	0	71	1	0
47	U	51	0	82	4	0
47	W	41	0	59	1	0
47	l	137	0	205	9	0
47	r	51	0	82	2	0
47	s	41	0	59	3	0
48	C	52	0	88	2	0
48	N	52	0	88	2	0
48	g	52	0	88	5	0
48	j	104	0	176	3	0
48	n	52	0	88	4	0
48	r	52	0	88	5	0
49	C	63	0	90	5	0
49	J	33	0	39	2	0
50	G	35	0	0	5	0
50	X	35	0	0	1	0
51	I	51	0	46	3	0
51	V	194	0	294	8	0
51	a	100	0	156	5	0
51	l	199	0	307	19	0
51	m	100	0	156	9	0
51	n	55	0	54	1	0
51	r	100	0	156	7	0
51	s	89	0	125	5	0
52	J	48	0	25	3	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	T	1	0	0	0	0
56	w	27	0	11	1	0
All	All	68165	0	68947	1010	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 (1010) 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)
6:G:112:SER:CB	50:G:201:8Q1:O1	1.70	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.68	1.16
36:m:64:MET:HE2	36:m:64:MET:HA	1.38	1.05
36:m:65:LEU:HD11	41:s:139:THR:HG21	1.39	1.03
15:P:173:MET:O	15:P:196:HIS:HB3	1.63	0.98
44:w:50:THR:HG23	44:w:288:ASP:OD1	1.65	0.96
35:l:383:MET:HE3	35:l:384:PRO:HD2	1.52	0.90
32:i:68:MET:HG3	34:k:36:MET:HE3	1.54	0.90
1:A:124:THR:HG22	1:A:353:ALA:HB2	1.56	0.86
44:w:50:THR:CG2	44:w:288:ASP:OD1	2.24	0.84
1:A:126:LYS:N	1:A:277:ASN:HD21	1.79	0.81
36:m:64:MET:HA	36:m:64:MET:CE	2.12	0.79
20:V:66:ILE:HD11	20:V:101:LEU:HB2	1.65	0.79
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.64	0.78
36:m:64:MET:HE2	36:m:64:MET:CA	2.12	0.78
36:m:65:LEU:HD11	41:s:139:THR:CG2	2.15	0.77
6:G:112:SER:CB	50:G:201:8Q1:P24	2.73	0.76
34:k:21:MET:HB3	51:m:201:CDL:HB61	1.69	0.75
1:A:138:LEU:HD13	1:A:245:VAL:HG23	1.68	0.74
24:a:188:ASP:OD1	42:u:47:ARG:NH2	2.21	0.73
36:m:65:LEU:HD23	36:m:65:LEU:C	2.14	0.73
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.21	0.73
31:h:80:LYS:NZ	36:m:1:MET:SD	2.61	0.72
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.21	0.72
5:F:25:GLN:OE1	5:F:26:ARG:NH2	2.23	0.71
40:r:269:MET:HE1	40:r:296:LEU:HD13	1.72	0.71
2:B:47:SER:O	2:B:56:ARG:NH2	2.24	0.71
43:v:51:LEU:O	43:v:52:MET:HG2	1.90	0.71
1:A:398:ARG:HG2	1:A:403:ASP:HB3	1.73	0.71
35:l:8:THR:HB	35:l:82:MET:HE2	1.72	0.71
36:m:55:MET:O	36:m:59:ILE:HG12	1.90	0.71
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.72	0.71
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.71	0.70
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.72	0.70
22:Y:72:ARG:NH1	22:Y:76:ASP:OD1	2.24	0.70
40:r:191:SER:HB3	47:r:501:PEE:H3	1.74	0.70
32:i:89:MET:HE1	32:i:98:MET:HE3	1.74	0.69
36:m:65:LEU:CD1	41:s:139:THR:HG21	2.19	0.69
41:s:62:ARG:NH2	47:s:401:PEE:O1P	2.25	0.69
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.27	0.68
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.75	0.68
20:V:140:LYS:HG3	20:V:141:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:67:VAL:O	36:m:71:THR:HG23	1.93	0.68
16:Q:52:MET:O	32:i:171:ASN:ND2	2.27	0.68
2:B:77:LEU:HB2	41:s:31:MET:HG2	1.75	0.68
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.21	0.68
30:g:52:ARG:NH1	32:i:318:GLU:OE2	2.26	0.67
15:P:173:MET:HE2	15:P:188:LEU:HB2	1.77	0.67
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.75	0.67
11:L:98:LYS:NZ	11:L:127:THR:OG1	2.28	0.67
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.75	0.67
3:C:147:TYR:HH	15:P:198:PHE:HE1	1.42	0.67
12:M:29:SER:OG	12:M:30:ASN:N	2.28	0.66
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.27	0.66
21:W:121:MET:HB2	36:m:130:THR:HG22	1.75	0.66
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.27	0.66
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.28	0.66
33:j:79:SER:HA	33:j:87:MET:HE2	1.76	0.66
51:l:703:CDL:H712	51:l:703:CDL:H312	1.78	0.66
48:C:303:PLX:H211	49:C:304:UQ:H551	1.78	0.66
1:A:285:PRO:O	14:O:222:ARG:NH2	2.29	0.66
30:g:36:MET:HE1	48:g:201:PLX:H393	1.78	0.66
51:r:503:CDL:H401	51:r:503:CDL:H221	1.78	0.65
41:s:27:VAL:HG13	41:s:31:MET:HE3	1.78	0.65
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.30	0.65
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.78	0.65
1:A:51:TRP:NE1	10:K:77:GLN:OE1	2.27	0.65
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.79	0.65
4:E:17:VAL:HG21	11:L:55:VAL:HG12	1.78	0.64
12:M:472:PRO:O	12:M:510:TRP:NE1	2.24	0.64
51:l:702:CDL:H312	51:l:702:CDL:H742	1.79	0.64
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.27	0.64
34:k:27:MET:HG2	36:m:71:THR:HG22	1.79	0.64
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.30	0.64
4:E:37:ARG:HG2	6:G:120:MET:SD	2.38	0.64
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.30	0.64
35:l:119:LYS:NZ	51:l:702:CDL:OA3	2.30	0.64
35:l:541:ASN:HD22	47:l:704:PEE:H60	1.63	0.64
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.78	0.64
2:B:165:ASP:OD2	16:Q:368:ARG:NH2	2.31	0.64
33:j:63:LEU:HD21	36:m:63:GLY:HA2	1.79	0.64
16:Q:387:GLU:OE2	16:Q:390:GLN:NE2	2.31	0.63
40:r:210:TYR:O	40:r:213:HIS:ND1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:98:VAL:HG22	40:r:36:LEU:HB2	1.81	0.62
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.81	0.62
35:l:150:MET:HE3	35:l:150:MET:HA	1.81	0.62
36:m:25:SER:O	36:m:27:ILE:N	2.32	0.62
6:G:134:ASP:HA	6:G:137:LYS:HD3	1.81	0.62
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.40	0.62
31:h:2:PRO:HA	32:i:140:SER:HB2	1.81	0.62
35:l:585:LYS:NZ	51:m:201:CDL:OB3	2.33	0.62
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.81	0.62
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.62
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.81	0.62
18:T:51:ARG:HG2	18:T:54:ARG:HH21	1.62	0.62
24:a:170:GLN:NE2	42:u:151:ASN:OD1	2.32	0.62
51:s:402:CDL:H321	51:s:402:CDL:HB61	1.81	0.61
44:w:227:MET:SD	44:w:227:MET:N	2.73	0.61
9:J:136:THR:HG23	9:J:139:PHE:H	1.65	0.61
35:l:407:TRP:O	35:l:411:MET:HG2	2.00	0.61
40:r:129:THR:HG21	40:r:235:LEU:HD11	1.83	0.61
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.82	0.61
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.33	0.61
22:Y:93:THR:HG22	22:Y:96:GLU:HG2	1.82	0.61
27:d:99:ASP:OD1	27:d:142:ARG:NH1	2.33	0.61
1:A:378:SER:OG	1:A:385:CYS:SG	2.59	0.61
35:l:79:SER:O	35:l:139:GLN:NE2	2.34	0.61
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.83	0.61
25:b:109:THR:HG22	25:b:116:VAL:HG12	1.81	0.61
29:f:60:LYS:NZ	29:f:64:GLU:OE2	2.24	0.61
51:l:702:CDL:H452	40:r:445:LEU:HB3	1.82	0.61
51:I:201:CDL:H512	51:I:201:CDL:H722	1.83	0.61
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.83	0.61
28:e:119:ARG:O	28:e:123:GLU:HG3	2.01	0.60
38:o:28:GLU:CD	38:o:28:GLU:H	2.09	0.60
20:V:123:ALA:O	20:V:127:MET:HG3	2.00	0.60
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.33	0.60
18:T:47:ASP:OD1	18:T:48:GLY:N	2.34	0.60
1:A:125:CYS:H	1:A:277:ASN:ND2	1.99	0.60
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.82	0.60
27:d:69:ARG:NH2	37:n:46:LYS:O	2.33	0.60
9:J:71:ASN:HB2	9:J:97:MET:HE2	1.83	0.60
10:K:82:SER:OG	10:K:83:THR:N	2.34	0.60
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE1	1:A:129:GLU:HA	2.02	0.60
1:A:123:GLY:N	14:O:180:CYS:SG	2.75	0.59
51:l:702:CDL:H391	40:r:371:PRO:HD2	1.84	0.59
14:O:38:LEU:O	14:O:124:ARG:NH2	2.35	0.59
19:U:30:ILE:HD11	33:j:96:ILE:HD11	1.83	0.59
44:w:75:ARG:O	44:w:79:GLU:HG2	2.02	0.59
19:U:9:LEU:HD11	47:U:101:PEE:H68	1.83	0.59
35:l:346:ILE:HG12	35:l:366:MET:HE1	1.83	0.59
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.85	0.59
25:b:123:PHE:HB3	43:v:40:VAL:HG11	1.85	0.59
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.84	0.59
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.85	0.59
21:W:90:ASN:ND2	21:W:123:GLU:O	2.36	0.59
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.85	0.59
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.35	0.59
1:A:126:LYS:N	1:A:277:ASN:ND2	2.50	0.58
42:u:83:THR:HA	42:u:86:TRP:CD1	2.38	0.58
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.84	0.58
2:B:72:MET:HE1	8:I:18:ARG:HH12	1.69	0.58
13:N:68:MET:HG3	13:N:69:ASN:H	1.68	0.58
5:F:91:LEU:O	5:F:95:LEU:HD12	2.04	0.58
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.36	0.58
21:W:120:MET:HE1	31:h:73:MET:HG2	1.85	0.58
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.68	0.58
32:i:268:GLN:HA	40:r:165:VAL:HG11	1.84	0.58
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.69	0.58
51:l:702:CDL:H521	48:r:502:PLX:H211	1.84	0.58
14:O:135:CYS:HB2	14:O:177:LEU:HD12	1.86	0.58
17:S:51:ASP:OD2	42:u:22:SER:OG	2.20	0.58
44:w:118:TYR:OH	56:w:401:ADP:O2'	2.21	0.58
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.37	0.58
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.37	0.58
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.85	0.58
6:X:125:GLU:OE1	22:Y:44:TYR:OH	2.20	0.58
28:e:85:TRP:O	28:e:89:VAL:HG13	2.04	0.58
44:w:202:HIS:HE2	44:w:283:TRP:CG	2.21	0.58
1:A:119:GLU:O	1:A:159:ARG:NH1	2.36	0.58
2:B:144:ARG:NH1	2:B:146:ASP:OD2	2.37	0.58
24:a:168:TRP:HB3	30:g:3:MET:HB2	1.85	0.58
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.37	0.58
39:p:56:ASP:HB3	39:p:59:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:38:ILE:O	7:H:45:ARG:NH1	2.36	0.57
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.85	0.57
6:G:94:ASP:OD1	6:G:94:ASP:N	2.35	0.57
41:s:28:LEU:HD22	41:s:275:ALA:HB2	1.85	0.57
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.87	0.57
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.84	0.57
1:A:152:ARG:NH2	10:K:99:PRO:O	2.36	0.57
6:G:141:PRO:O	6:G:145:VAL:HG23	2.03	0.57
15:P:43:THR:HA	15:P:47:ILE:HD12	1.84	0.57
25:b:24:LYS:NZ	25:b:27:GLU:OE1	2.30	0.57
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.21	0.57
1:A:263:ALA:HA	1:A:271:SER:HB3	1.87	0.57
26:c:96:ASP:OD2	26:c:96:ASP:N	2.35	0.57
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.35	0.57
35:l:227:PHE:O	35:l:230:HIS:ND1	2.35	0.57
43:v:103:GLU:O	43:v:107:ARG:HG2	2.05	0.57
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.87	0.56
48:g:201:PLX:H361	48:g:201:PLX:H311	1.87	0.56
5:F:24:CYS:N	5:F:58:CYS:SG	2.78	0.56
15:P:173:MET:HB3	15:P:198:PHE:HB2	1.88	0.56
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.28	0.56
44:w:230:THR:HG23	44:w:233:TYR:H	1.69	0.56
47:B:303:PEE:H59	41:s:277:TYR:HE2	1.70	0.56
12:M:650:SER:OG	12:M:652:ASN:ND2	2.37	0.56
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.38	0.56
15:P:211:ARG:NE	15:P:222:GLU:OE1	2.38	0.56
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.87	0.56
21:W:51:MET:HE2	41:s:311:THR:HB	1.88	0.56
1:A:123:GLY:HA2	14:O:180:CYS:SG	2.45	0.56
12:M:666:GLN:NE2	12:M:670:GLU:OE1	2.38	0.56
2:B:111:GLU:O	2:B:141:ARG:NH1	2.39	0.56
18:T:108:THR:HG22	18:T:119:ARG:HB2	1.87	0.56
32:i:258:SER:HB2	32:i:336:VAL:HG12	1.88	0.56
40:r:403:THR:HA	40:r:406:TYR:CE2	2.41	0.56
1:A:123:GLY:CA	14:O:180:CYS:SG	2.94	0.56
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.41	0.55
39:p:119:PHE:O	39:p:123:GLU:HG2	2.06	0.55
41:s:125:SER:OG	41:s:214:GLU:OE1	2.24	0.55
10:K:80:GLU:OE2	10:K:80:GLU:N	2.40	0.55
51:V:202:CDL:H591	51:V:202:CDL:H192	1.87	0.55
3:C:55:ASN:ND2	3:C:187:GLU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:NH1	10:K:70:ASN:O	2.40	0.55
26:c:110:ASP:OD2	40:r:278:ARG:NE	2.35	0.55
25:b:29:SER:H	25:b:32:GLU:HG3	1.72	0.55
30:g:2:THR:OG1	30:g:5:SER:OG	2.20	0.55
44:w:258:TYR:CE2	44:w:269:VAL:HG13	2.42	0.55
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.88	0.55
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.89	0.55
16:Q:357:LYS:HD3	16:Q:364:SER:HB2	1.89	0.55
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.89	0.55
27:d:159:GLN:O	27:d:163:MET:HG3	2.06	0.55
31:h:69:ARG:O	31:h:73:MET:HG3	2.07	0.55
49:C:304:UQ:H412	41:s:51:ASP:HB3	1.88	0.55
6:X:107:ASP:OD1	6:X:107:ASP:N	2.34	0.55
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.89	0.55
1:A:405:ARG:H	1:A:408:GLU:HG3	1.72	0.54
16:Q:57:GLU:OE2	35:l:579:ASN:ND2	2.40	0.54
21:W:94:GLU:HG3	31:h:79:ILE:HD13	1.89	0.54
44:w:202:HIS:NE2	44:w:283:TRP:CG	2.75	0.54
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.89	0.54
21:W:76:GLN:NE2	21:W:80:ASP:OD1	2.40	0.54
29:f:52:VAL:O	29:f:56:ILE:HG23	2.07	0.54
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.89	0.54
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.90	0.54
14:O:179:ALA:HB3	14:O:185:MET:SD	2.48	0.54
16:Q:84:PHE:HB2	16:Q:99:MET:HE2	1.89	0.54
35:l:71:LEU:HD21	40:r:380:PHE:CZ	2.42	0.54
4:E:27:GLU:O	4:E:31:ARG:HG3	2.07	0.54
27:d:6:ASP:OD2	27:d:8:ASP:N	2.37	0.54
42:u:32:TYR:HE2	42:u:40:ASN:HD21	1.56	0.54
44:w:283:TRP:HB2	44:w:284:PRO:HD3	1.90	0.54
12:M:389:THR:O	12:M:390:THR:OG1	2.24	0.54
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.90	0.54
25:b:81:ILE:HG23	47:l:705:PEE:H58	1.90	0.54
51:l:702:CDL:H412	51:l:702:CDL:H602	1.89	0.54
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.90	0.54
35:l:295:GLN:O	35:l:425:ARG:NH1	2.41	0.54
37:n:39:ARG:NH1	37:n:57:TRP:O	2.35	0.54
1:A:116:ASN:ND2	46:A:502:FMN:O3'	2.40	0.53
14:O:182:ASN:ND2	14:O:194:GLU:OE1	2.41	0.53
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.89	0.53
42:u:139:GLU:OE2	42:u:139:GLU:N	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:201:CDL:H712	51:a:201:CDL:H172	1.90	0.53
44:w:240:ALA:O	44:w:244:THR:OG1	2.24	0.53
52:J:401:NDP:N7N	52:J:401:NDP:O2N	2.41	0.53
35:l:51:LEU:O	35:l:55:MET:HG3	2.09	0.53
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.41	0.53
22:Y:76:ASP:O	35:l:385:TYR:OH	2.27	0.53
32:i:112:HIS:CE1	32:i:164:ILE:HG21	2.44	0.53
34:k:30:LEU:O	34:k:34:GLU:HG3	2.08	0.53
6:G:112:SER:CA	50:G:201:8Q1:O1	2.51	0.53
7:H:44:TYR:O	7:H:48:THR:HG22	2.08	0.53
15:P:163:ALA:O	15:P:167:GLU:HG3	2.08	0.53
20:V:110:ILE:HD11	47:l:701:PEE:H1	1.89	0.53
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.41	0.53
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.91	0.53
35:l:136:ASN:HA	35:l:197:ASP:HA	1.90	0.53
36:m:82:VAL:HG13	36:m:84:VAL:H	1.72	0.53
40:r:174:LEU:HD23	40:r:179:ILE:HD11	1.90	0.53
12:M:150:ARG:HG2	12:M:150:ARG:HH11	1.73	0.53
26:c:169:GLU:HB3	43:v:53:LEU:HD11	1.90	0.53
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.89	0.53
1:A:49:HIS:O	1:A:59:ARG:NH1	2.42	0.53
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.42	0.53
3:C:147:TYR:OH	15:P:198:PHE:HE1	1.91	0.53
12:M:250:SER:OG	12:M:251:ILE:N	2.41	0.53
6:X:155:TYR:CE1	25:b:23:LEU:HB3	2.43	0.53
26:c:31:HIS:N	38:o:61:GLU:OE2	2.42	0.53
27:d:70:ARG:NH1	27:d:91:GLN:OE1	2.41	0.53
8:I:25:GLN:O	16:Q:209:LYS:NZ	2.25	0.52
31:h:93:THR:O	31:h:93:THR:OG1	2.25	0.52
40:r:306:PRO:O	40:r:310:MET:HG3	2.09	0.52
12:M:464:GLN:O	12:M:468:GLU:HG3	2.09	0.52
15:P:174:PHE:O	15:P:199:ARG:NH2	2.28	0.52
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.31	0.52
43:v:47:ASN:C	43:v:47:ASN:ND2	2.68	0.52
8:I:18:ARG:HD3	16:Q:253:PHE:CE2	2.45	0.52
39:p:57:MET:HE2	39:p:57:MET:HA	1.91	0.52
51:s:402:CDL:H221	51:s:402:CDL:H552	1.90	0.52
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.91	0.52
14:O:138:THR:HG22	14:O:139:PRO:HD3	1.91	0.52
35:l:419:THR:HA	35:l:422:TYR:CE2	2.45	0.52
1:A:129:GLU:OE2	14:O:225:CYS:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:66:PRO:HB3	15:P:79:SER:HA	1.92	0.52
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.92	0.52
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.24	0.52
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.90	0.52
33:j:16:LEU:O	33:j:20:ILE:HG13	2.10	0.52
33:j:39:CYS:SG	41:s:127:TYR:OH	2.65	0.52
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.91	0.52
3:C:88:ARG:HA	41:s:37:PRO:HA	1.91	0.52
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.91	0.52
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.42	0.52
25:b:34:VAL:HG22	39:p:114:MET:HA	1.92	0.52
35:l:190:LEU:HD12	40:r:383:THR:HG21	1.91	0.52
12:M:388:ASN:ND2	12:M:513:MET:O	2.39	0.52
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.92	0.52
44:w:283:TRP:N	44:w:284:PRO:CD	2.73	0.52
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.75	0.52
6:G:112:SER:N	50:G:201:8Q1:O1	2.42	0.52
12:M:398:ASP:OD1	12:M:398:ASP:N	2.43	0.52
30:g:3:MET:HG3	30:g:4:MET:HG2	1.91	0.52
31:h:59:GLU:N	31:h:59:GLU:OE2	2.43	0.52
36:m:88:THR:HG23	51:m:201:CDL:H521	1.92	0.52
4:E:52:LEU:HD22	4:E:104:MET:HE2	1.92	0.51
8:I:40:LYS:HB3	21:W:7:LYS:H	1.75	0.51
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.92	0.51
40:r:251:ASN:HD21	40:r:304:GLN:HE22	1.57	0.51
25:b:83:HIS:HD2	27:d:45:VAL:HG21	1.74	0.51
41:s:213:VAL:HG13	41:s:214:GLU:HG2	1.92	0.51
43:v:52:MET:HB2	43:v:55:GLN:HG3	1.93	0.51
7:H:94:MET:SD	7:H:99:PRO:HG3	2.50	0.51
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.75	0.51
40:r:67:VAL:HG12	48:r:502:PLX:H362	1.92	0.51
1:A:159:ARG:NH2	14:O:176:CYS:O	2.42	0.51
11:L:116:SER:OG	15:P:227:ALA:O	2.27	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.51
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.75	0.51
41:s:215:TYR:HD2	41:s:219:PRO:HB2	1.75	0.51
16:Q:241:LEU:HG	21:W:9:ASP:OD1	2.11	0.51
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.43	0.51
26:c:33:THR:HG23	26:c:35:ASP:OD2	2.10	0.51
28:e:97:ILE:O	28:e:101:LEU:HB2	2.11	0.51
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:61:LEU:HD22	40:r:244:MET:HE2	1.93	0.51
40:r:189:SER:OG	40:r:192:ASN:OD1	2.28	0.51
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.93	0.51
23:Z:30:GLU:O	23:Z:34:GLU:HG3	2.10	0.51
51:l:702:CDL:H861	51:l:702:CDL:H572	1.92	0.51
40:r:373:ILE:HG21	40:r:454:ILE:HD11	1.93	0.51
40:r:437:MET:O	40:r:441:ILE:HG22	2.10	0.51
44:w:180:ARG:NH2	44:w:182:GLN:OE1	2.43	0.51
6:G:136:GLU:OE2	6:G:136:GLU:N	2.37	0.51
6:X:103:HIS:HB3	6:X:106:LYS:HB2	1.93	0.51
24:a:125:PHE:HE1	48:n:101:PLX:H251	1.76	0.51
36:m:2:THR:HG1	36:m:125:TRP:CD1	2.27	0.51
36:m:57:PHE:O	36:m:61:LEU:HG	2.11	0.51
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.93	0.50
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.46	0.50
38:o:75:ASN:O	38:o:79:ASN:ND2	2.41	0.50
5:F:24:CYS:O	5:F:34:ARG:NH1	2.44	0.50
7:H:26:ILE:O	7:H:30:LYS:HG3	2.11	0.50
24:a:187:PRO:HB2	42:u:47:ARG:HH21	1.76	0.50
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.92	0.50
33:j:73:LEU:O	41:s:160:TYR:OH	2.26	0.50
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.92	0.50
20:V:11:ASP:N	20:V:11:ASP:OD1	2.44	0.50
32:i:215:MET:HE1	32:i:244:MET:HG3	1.92	0.50
34:k:41:PHE:O	34:k:45:THR:HG22	2.10	0.50
32:i:132:THR:HG23	32:i:209:ILE:HG12	1.94	0.50
40:r:31:SER:HB2	40:r:74:PRO:HG3	1.94	0.50
5:F:23:LEU:HD13	5:F:37:ILE:HD12	1.94	0.50
9:J:37:HIS:NE2	18:T:48:GLY:O	2.45	0.50
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.93	0.50
32:i:154:MET:HE2	32:i:191:THR:HG23	1.94	0.50
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.94	0.50
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.44	0.50
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.29	0.50
47:W:201:PEE:H59	41:s:108:MET:HE1	1.94	0.50
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.94	0.50
30:g:15:PHE:HB2	48:g:201:PLX:H6	1.94	0.50
36:m:61:LEU:O	41:s:114:TYR:OH	2.21	0.50
12:M:163:LYS:O	12:M:171:THR:OG1	2.30	0.50
22:Y:43:ARG:NH1	22:Y:47:PHE:O	2.45	0.50
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.47	0.49
21:W:57:ARG:HB3	41:s:316:PRO:HG2	1.93	0.49
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.93	0.49
35:l:65:ASN:ND2	35:l:65:ASN:H	2.10	0.49
36:m:55:MET:HE1	36:m:58:LEU:HD23	1.94	0.49
23:Z:25:GLU:HA	23:Z:30:GLU:OE1	2.12	0.49
44:w:202:HIS:CD2	44:w:283:TRP:CD1	3.00	0.49
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.94	0.49
23:Z:29:LEU:HA	23:Z:32:VAL:HG12	1.93	0.49
35:l:108:MET:HE3	35:l:240:PRO:HB3	1.95	0.49
37:n:29:ARG:NH2	48:n:101:PLX:O3	2.30	0.49
43:v:12:ASP:OD1	43:v:14:SER:OG	2.30	0.49
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.48	0.49
1:A:125:CYS:H	1:A:277:ASN:HD22	1.60	0.49
30:g:14:GLN:NE2	30:g:17:PRO:HA	2.27	0.49
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.36	0.49
9:J:375:VAL:HG23	9:J:375:VAL:O	2.12	0.49
12:M:493:VAL:HG12	12:M:513:MET:HE1	1.94	0.49
35:l:517:SER:HB3	51:l:703:CDL:HA32	1.94	0.49
24:a:141:GLN:O	24:a:145:GLU:HG3	2.13	0.49
36:m:34:ILE:HG12	36:m:64:MET:HG3	1.93	0.49
36:m:65:LEU:C	36:m:65:LEU:CD2	2.86	0.49
40:r:27:ALA:O	40:r:31:SER:OG	2.25	0.49
40:r:203:PHE:O	40:r:207:MET:HG2	2.11	0.49
9:J:73:LEU:O	9:J:78:SER:OG	2.29	0.49
24:a:182:SER:O	24:a:184:LYS:NZ	2.37	0.49
43:v:47:ASN:C	43:v:47:ASN:HD22	2.21	0.49
9:J:75:ARG:NH1	15:P:213:ASP:OD2	2.46	0.49
28:e:79:ASP:HB3	28:e:82:VAL:HG12	1.93	0.49
35:l:71:LEU:HG	40:r:310:MET:HE1	1.94	0.49
35:l:156:GLY:HA2	35:l:164:ALA:HB1	1.94	0.49
35:l:573:MET:HE3	47:l:701:PEE:H26	1.94	0.49
40:r:243:MET:HA	40:r:246:ILE:HG22	1.95	0.49
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.95	0.49
3:C:80:ALA:HB2	3:C:86:MET:HE2	1.95	0.48
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.94	0.48
21:W:98:MET:HG3	21:W:104:TRP:CD1	2.48	0.48
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.95	0.48
36:m:88:THR:HG1	51:m:201:CDL:H1O1	1.59	0.48
31:h:84:ASP:HA	31:h:87:ILE:HG12	1.95	0.48
32:i:233:THR:HG23	32:i:241:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:71:LEU:O	36:m:147:TYR:OH	2.27	0.48
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.96	0.48
3:C:95:ALA:HB1	41:s:208:VAL:HG23	1.95	0.48
12:M:512:VAL:O	12:M:514:ASN:ND2	2.46	0.48
27:d:140:GLN:O	27:d:144:SER:HB3	2.13	0.48
33:j:28:ASN:O	33:j:33:LYS:NZ	2.39	0.48
39:p:62:GLN:O	39:p:66:GLN:HG3	2.13	0.48
41:s:85:MET:HE2	41:s:233:MET:HE2	1.94	0.48
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.44	0.48
20:V:29:GLY:O	20:V:63:SER:HB3	2.12	0.48
6:X:111:ASP:OD2	6:X:111:ASP:N	2.46	0.48
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.28	0.48
41:s:152:SER:HA	41:s:155:LEU:HD12	1.95	0.48
5:F:61:VAL:HG23	5:F:62:GLN:H	1.78	0.48
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.45	0.48
33:j:61:THR:HG21	33:j:105:GLU:OE2	2.13	0.48
41:s:138:GLN:NE2	41:s:191:ALA:O	2.41	0.48
41:s:149:ILE:HG21	41:s:185:TRP:HB2	1.95	0.48
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.94	0.48
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.94	0.48
1:A:98:LYS:NZ	1:A:242:VAL:O	2.34	0.48
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.96	0.48
1:A:390:ASP:OD2	12:M:202:ASN:ND2	2.47	0.48
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.47	0.48
15:P:200:LYS:NZ	16:Q:125:GLU:OE1	2.30	0.48
51:m:201:CDL:H161	51:m:201:CDL:H191	1.66	0.48
5:F:86:GLN:O	5:F:90:THR:HG23	2.13	0.48
7:H:11:LEU:HD12	7:H:14:LEU:HD22	1.95	0.48
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.94	0.48
21:W:120:MET:O	21:W:121:MET:HB3	2.13	0.48
24:a:78:THR:HB	28:e:96:SER:OG	2.14	0.48
35:l:289:ALA:O	35:l:293:ILE:HG23	2.14	0.48
40:r:31:SER:HB3	40:r:73:LEU:HD23	1.96	0.48
7:H:48:THR:HA	7:H:51:ILE:HG12	1.95	0.48
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.96	0.48
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.95	0.48
18:T:64:GLU:OE2	18:T:64:GLU:HA	2.14	0.48
26:c:58:ARG:NH2	26:c:60:GLU:OE2	2.47	0.48
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.95	0.48
38:o:20:PRO:HB3	39:p:65:ARG:HH12	1.78	0.48
1:A:48:ARG:HH11	10:K:70:ASN:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.96	0.48
51:I:201:CDL:H111	51:I:201:CDL:H142	1.66	0.48
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.95	0.48
20:V:107:SER:HB3	20:V:110:ILE:HB	1.96	0.48
32:i:182:SER:HB2	32:i:293:TYR:OH	2.14	0.48
32:i:280:THR:O	32:i:284:MET:HG2	2.14	0.48
51:l:702:CDL:H621	51:l:702:CDL:H432	1.96	0.48
13:N:73:THR:HG21	13:N:81:MET:HE1	1.96	0.47
14:O:199:LYS:O	14:O:203:GLU:HG3	2.14	0.47
51:l:703:CDL:H612	51:l:703:CDL:H641	1.64	0.47
39:p:50:GLU:HG2	39:p:51:HIS:CD2	2.49	0.47
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.79	0.47
11:L:124:LEU:HD21	15:P:201:ASP:O	2.13	0.47
21:W:120:MET:O	21:W:120:MET:HG2	2.12	0.47
52:J:401:NDP:H2N	52:J:401:NDP:H2D	1.72	0.47
12:M:77:MET:HE1	12:M:117:MET:HG2	1.94	0.47
17:S:50:ARG:O	17:S:54:ILE:HG23	2.13	0.47
6:X:82:ARG:O	6:X:86:VAL:HG12	2.14	0.47
44:w:125:ASP:O	44:w:130:ARG:NH2	2.47	0.47
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.31	0.47
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.96	0.47
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.50	0.47
12:M:29:SER:HG	12:M:30:ASN:H	1.60	0.47
14:O:44:THR:HG23	14:O:47:ASN:H	1.79	0.47
20:V:3:LYS:HB2	20:V:3:LYS:HE2	1.68	0.47
27:d:164:LEU:HD23	28:e:149:LEU:HD13	1.96	0.47
40:r:366:ASN:ND2	40:r:407:SER:OG	2.41	0.47
12:M:215:MET:HG3	12:M:714:VAL:HG12	1.95	0.47
24:a:187:PRO:HB2	42:u:47:ARG:HE	1.80	0.47
32:i:190:MET:HG2	32:i:204:ASN:HB3	1.95	0.47
38:o:9:SER:OG	38:o:10:ARG:N	2.47	0.47
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.97	0.47
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.97	0.47
18:T:51:ARG:HG2	18:T:54:ARG:NH2	2.28	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.50	0.47
37:n:30:ARG:HG3	37:n:30:ARG:HH11	1.80	0.47
40:r:216:LEU:HD22	40:r:291:VAL:HG23	1.97	0.47
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.95	0.47
2:B:104:ARG:HD2	2:B:168:VAL:HG21	1.96	0.47
47:B:303:PEE:H55	47:B:303:PEE:H61	1.75	0.47
4:E:48:HIS:NE2	9:J:365:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:92:LYS:HD2	8:I:92:LYS:HA	1.64	0.47
12:M:347:ASP:OD1	12:M:347:ASP:N	2.39	0.47
12:M:501:ARG:HH21	12:M:665:PHE:HD2	1.60	0.47
19:U:52:ASN:OD1	19:U:52:ASN:N	2.47	0.47
26:c:149:ILE:HG13	26:c:150:TYR:HD1	1.79	0.47
32:i:342:ALA:O	32:i:345:SER:OG	2.30	0.47
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.97	0.47
40:r:398:MET:O	40:r:402:ILE:HG13	2.14	0.47
41:s:87:VAL:HG23	41:s:88:PRO:HD3	1.96	0.47
44:w:150:LEU:HD12	44:w:156:GLY:HA2	1.95	0.47
44:w:202:HIS:CD2	44:w:283:TRP:CG	3.03	0.47
2:B:63:TRP:HE1	47:B:303:PEE:H1	1.80	0.47
9:J:140:ASP:N	9:J:140:ASP:OD1	2.45	0.47
15:P:173:MET:CE	15:P:188:LEU:HB2	2.44	0.47
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.48	0.47
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.97	0.47
24:a:135:LYS:HD2	37:n:32:ASP:OD1	2.15	0.47
25:b:108:ASP:OD1	43:v:71:ARG:NH1	2.33	0.47
3:C:61:SER:O	3:C:61:SER:OG	2.31	0.47
6:G:80:LYS:HE2	6:G:100:VAL:HG21	1.97	0.47
9:J:37:HIS:O	9:J:40:LEU:N	2.37	0.47
9:J:303:ARG:HB2	9:J:316:ARG:HD3	1.97	0.47
12:M:264:SER:HB2	12:M:272:ARG:HG2	1.97	0.47
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.97	0.47
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.30	0.47
33:j:20:ILE:HG12	48:j:201:PLX:H142	1.95	0.47
35:l:151:SER:HB2	35:l:252:MET:HE2	1.97	0.47
1:A:102:MET:HE2	1:A:149:MET:HB3	1.97	0.46
30:g:36:MET:HE3	30:g:36:MET:HB3	1.76	0.46
35:l:132:VAL:O	35:l:262:ARG:NH2	2.47	0.46
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.96	0.46
16:Q:144:MET:O	16:Q:148:GLU:HG2	2.15	0.46
35:l:277:THR:HG23	35:l:314:MET:HG3	1.96	0.46
35:l:401:MET:SD	35:l:482:MET:HG2	2.55	0.46
6:G:135:ALA:HA	6:G:138:LEU:HD13	1.96	0.46
10:K:69:ASP:N	10:K:69:ASP:OD1	2.49	0.46
27:d:106:ILE:HG13	27:d:135:VAL:HG21	1.96	0.46
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.96	0.46
1:A:388:GLY:HA3	1:A:419:ILE:HD11	1.98	0.46
5:F:83:SER:O	5:F:87:VAL:HG12	2.14	0.46
21:W:120:MET:HE2	36:m:126:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:298:TYR:O	32:i:303:THR:OG1	2.32	0.46
32:i:311:MET:HE2	32:i:311:MET:HB2	1.86	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.16	0.46
41:s:85:MET:HE2	41:s:233:MET:CE	2.46	0.46
4:E:30:ARG:O	4:E:34:GLU:HG3	2.15	0.46
8:I:43:VAL:HG23	8:I:44:GLY:H	1.81	0.46
15:P:198:PHE:CE2	16:Q:121:GLU:HB2	2.50	0.46
51:V:202:CDL:H721	51:V:202:CDL:H752	1.61	0.46
6:X:141:PRO:O	6:X:145:VAL:HG12	2.15	0.46
30:g:7:ARG:HH21	30:g:91:ASP:CG	2.24	0.46
34:k:3:LEU:HD23	36:m:121:GLY:HA2	1.97	0.46
38:o:17:THR:O	38:o:23:TYR:OH	2.25	0.46
15:P:173:MET:O	15:P:196:HIS:CB	2.51	0.46
32:i:230:LEU:HD21	32:i:244:MET:HE3	1.96	0.46
35:l:171:ALA:O	35:l:175:ASN:ND2	2.49	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.97	0.46
40:r:154:LEU:HD23	40:r:154:LEU:HA	1.80	0.46
40:r:447:LEU:HD11	48:r:502:PLX:H393	1.98	0.46
41:s:139:THR:HA	41:s:142:TYR:CE2	2.50	0.46
5:F:25:GLN:NE2	5:F:57:GLU:OE2	2.49	0.46
6:G:93:ILE:HG21	6:G:98:LEU:HD13	1.97	0.46
9:J:258:ALA:HA	9:J:261:LYS:HG3	1.98	0.46
26:c:154:GLN:HG3	35:l:401:MET:HB3	1.98	0.46
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.98	0.46
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.97	0.46
33:j:103:ALA:O	33:j:107:THR:HG23	2.15	0.46
40:r:108:MET:HB3	40:r:121:LEU:HD13	1.97	0.46
9:J:43:HIS:O	9:J:50:SER:OG	2.24	0.46
16:Q:88:HIS:HB3	16:Q:91:ALA:HB2	1.97	0.46
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.96	0.46
21:W:111:PHE:CE2	31:h:65:GLU:HG3	2.50	0.46
35:l:392:LYS:HE2	35:l:416:THR:HG23	1.98	0.46
35:l:541:ASN:ND2	47:l:704:PEE:H60	2.30	0.46
35:l:561:ILE:HG13	35:l:562:LEU:H	1.81	0.46
41:s:135:ALA:O	41:s:139:THR:HG22	2.16	0.46
7:H:55:LYS:O	7:H:59:VAL:HG23	2.16	0.46
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.51	0.46
33:j:33:LYS:HG2	41:s:61:LEU:HD21	1.97	0.46
43:v:92:HIS:O	43:v:96:VAL:HG23	2.15	0.46
1:A:424:ILE:HG12	12:M:76:ARG:NH2	2.30	0.46
9:J:50:SER:OG	9:J:51:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:83:GLN:NE2	26:c:97:LEU:O	2.45	0.46
9:J:87:GLU:HG3	9:J:89:TYR:H	1.81	0.45
12:M:395:GLU:OE2	12:M:417:ARG:HD2	2.16	0.45
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.98	0.45
32:i:294:MET:HE2	40:r:130:LEU:HD21	1.98	0.45
40:r:269:MET:HE2	40:r:399:ASN:ND2	2.31	0.45
41:s:92:PRO:HB3	41:s:255:TYR:CD2	2.52	0.45
44:w:202:HIS:NE2	44:w:283:TRP:CD2	2.83	0.45
1:A:174:ARG:NH1	10:K:92:GLU:OE1	2.50	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.16	0.45
13:N:41:GLU:OE1	13:N:47:LYS:NZ	2.49	0.45
23:Z:75:PHE:O	23:Z:79:VAL:HG22	2.16	0.45
32:i:68:MET:HE1	34:k:37:MET:HG2	1.98	0.45
32:i:307:SER:OG	32:i:308:THR:N	2.49	0.45
35:l:121:LEU:HD22	35:l:246:LEU:HD23	1.98	0.45
51:r:503:CDL:H741	51:r:503:CDL:H772	1.42	0.45
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.99	0.45
8:I:52:ASN:OD1	8:I:57:ARG:NE	2.49	0.45
51:V:201:CDL:H341	51:V:201:CDL:H371	1.70	0.45
34:k:44:SER:OG	34:k:59:MET:SD	2.73	0.45
40:r:131:ILE:O	40:r:135:ARG:HB3	2.16	0.45
1:A:268:GLU:OE2	1:A:269:ARG:NH1	2.49	0.45
4:E:71:ALA:HB1	50:G:201:8Q1:O33	2.17	0.45
12:M:301:ARG:HA	12:M:301:ARG:HD2	1.76	0.45
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.97	0.45
19:U:38:TYR:HD1	19:U:41:TYR:HD2	1.63	0.45
23:Z:58:ALA:O	35:l:434:LYS:NZ	2.49	0.45
27:d:120:SER:HB3	43:v:56:ARG:HH22	1.81	0.45
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.98	0.45
51:m:201:CDL:H222	51:m:201:CDL:H331	1.98	0.45
1:A:67:GLU:O	1:A:71:LYS:HG2	2.16	0.45
2:B:90:LYS:HG2	13:N:91:HIS:NE2	2.32	0.45
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.52	0.45
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.99	0.45
12:M:186:ALA:HA	12:M:190:ALA:HB3	1.99	0.45
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.98	0.45
38:o:106:LYS:O	38:o:110:ASP:OD1	2.35	0.45
40:r:267:TRP:HE1	40:r:271:MET:HE2	1.81	0.45
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.51	0.45
51:s:402:CDL:H331	51:s:402:CDL:H362	1.81	0.45
8:I:34:ARG:HA	8:I:34:ARG:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:U:101:PEE:H26	41:s:295:PRO:HB3	1.99	0.45
21:W:133:ILE:O	21:W:137:THR:HG23	2.17	0.45
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.52	0.45
38:o:53:ASP:HB3	38:o:56:ARG:HG2	1.98	0.45
41:s:61:LEU:HD12	41:s:61:LEU:HA	1.78	0.45
41:s:233:MET:SD	41:s:233:MET:C	3.00	0.45
20:V:114:ALA:O	20:V:118:MET:HB2	2.17	0.45
21:W:74:LEU:O	21:W:78:GLU:HG3	2.17	0.45
21:W:105:LYS:HE2	21:W:105:LYS:HB3	1.66	0.45
25:b:29:SER:HB2	25:b:32:GLU:HG2	1.99	0.45
51:m:201:CDL:H462	51:m:201:CDL:H432	1.70	0.45
3:C:103:MET:HE3	3:C:105:VAL:HG22	1.98	0.45
9:J:180:TYR:HB2	9:J:317:ASP:OD1	2.16	0.45
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.52	0.45
6:X:89:LEU:O	6:X:89:LEU:HD23	2.17	0.45
32:i:230:LEU:O	32:i:233:THR:HG22	2.17	0.45
36:m:3:MET:HB2	36:m:5:ILE:HG12	1.99	0.45
41:s:169:GLN:HG3	41:s:244:GLY:HA3	1.99	0.45
43:v:22:MET:HG2	43:v:23:PRO:HA	1.98	0.45
1:A:326:LEU:HD22	1:A:363:ILE:HD11	1.98	0.45
2:B:167:ILE:HG23	2:B:167:ILE:O	2.17	0.45
5:F:54:LEU:C	5:F:55:ILE:HD13	2.41	0.45
12:M:371:VAL:HB	12:M:482:GLN:HG3	1.99	0.45
12:M:525:ALA:O	12:M:530:TYR:HB2	2.17	0.45
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.99	0.45
43:v:21:ARG:HB2	43:v:21:ARG:NH1	2.32	0.45
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.00	0.44
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.98	0.44
26:c:93:ASP:OD1	38:o:44:LYS:NZ	2.44	0.44
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.45	0.44
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.98	0.44
1:A:134:ASP:OD2	1:A:134:ASP:N	2.49	0.44
3:C:99:GLN:NE2	41:s:212:ASN:O	2.50	0.44
12:M:94:MET:HE2	12:M:94:MET:HB2	1.82	0.44
48:N:201:PLX:H22	48:N:201:PLX:H1C3	1.78	0.44
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.99	0.44
34:k:17:ALA:O	34:k:21:MET:HG2	2.17	0.44
36:m:64:MET:CE	36:m:64:MET:CA	2.86	0.44
40:r:98:MET:HE1	51:r:503:CDL:H191	1.98	0.44
43:v:44:GLN:NE2	43:v:48:ASP:OD1	2.50	0.44
1:A:110:PRO:O	1:A:238:CYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:OD1	1:A:277:ASN:N	2.50	0.44
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.44	0.44
13:N:73:THR:HG22	13:N:73:THR:O	2.17	0.44
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.99	0.44
26:c:149:ILE:HG13	26:c:150:TYR:CD1	2.52	0.44
28:e:111:ASP:OD2	28:e:116:GLU:HG3	2.17	0.44
33:j:73:LEU:N	33:j:74:PRO:HD2	2.32	0.44
33:j:73:LEU:HD23	33:j:73:LEU:HA	1.81	0.44
4:E:45:ASN:O	4:E:49:LEU:HD13	2.18	0.44
17:S:4:GLU:HG2	41:s:43:TYR:HD1	1.82	0.44
25:b:15:LEU:HD13	39:p:170:ILE:HG21	1.97	0.44
32:i:154:MET:HE2	32:i:191:THR:CG2	2.47	0.44
32:i:278:MET:O	32:i:282:MET:HG3	2.18	0.44
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.99	0.44
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.81	0.44
32:i:246:VAL:HG11	51:r:503:CDL:H392	1.99	0.44
33:j:63:LEU:HD23	33:j:63:LEU:HA	1.82	0.44
42:u:153:GLU:OE2	42:u:153:GLU:HA	2.18	0.44
3:C:69:LEU:HB2	3:C:107:GLY:HA3	2.00	0.44
12:M:117:MET:HE2	12:M:143:SER:HB2	1.99	0.44
19:U:53:TYR:HB2	21:W:72:MET:SD	2.57	0.44
25:b:97:VAL:HG22	35:l:63:ILE:HG23	1.98	0.44
36:m:30:GLY:O	36:m:34:ILE:HG13	2.18	0.44
9:J:167:ILE:HD13	9:J:201:ILE:HB	2.00	0.44
12:M:150:ARG:HG2	12:M:150:ARG:NH1	2.33	0.44
47:U:101:PEE:H35	47:U:101:PEE:H30	1.74	0.44
21:W:98:MET:SD	21:W:101:VAL:HG21	2.58	0.44
48:g:201:PLX:H102	48:g:201:PLX:H71	1.59	0.44
32:i:142:LEU:HD22	32:i:149:ILE:HD11	1.99	0.44
35:l:538:THR:HG22	47:l:704:PEE:H59	2.00	0.44
6:G:132:ASP:O	6:G:133:ILE:HG22	2.18	0.44
10:K:87:LEU:HD13	14:O:85:LEU:HD13	2.00	0.44
19:U:46:ASN:HD21	41:s:314:ILE:HD12	1.81	0.44
51:a:201:CDL:H852	48:r:502:PLX:H232	1.99	0.44
32:i:1:MET:HE3	32:i:6:TYR:HD1	1.82	0.44
40:r:267:TRP:NE1	40:r:271:MET:HE2	2.32	0.44
2:B:148:ASP:OD1	2:B:150:THR:OG1	2.30	0.44
47:B:303:PEE:H38	19:U:25:ILE:HG12	2.00	0.44
49:C:304:UQ:HM52	16:Q:93:GLY:HA2	1.98	0.44
12:M:124:HIS:HB3	16:Q:375:MET:HE3	2.00	0.44
12:M:308:ARG:NH2	12:M:578:PRO:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.47	0.44
32:i:323:MET:SD	32:i:323:MET:N	2.90	0.44
14:O:197:THR:OG1	14:O:200:ASP:OD2	2.36	0.43
16:Q:383:LYS:HD2	16:Q:383:LYS:HA	1.84	0.43
6:X:137:LYS:HA	25:b:3:GLY:HA2	2.00	0.43
26:c:35:ASP:OD2	26:c:35:ASP:N	2.36	0.43
27:d:85:MET:HE2	27:d:85:MET:HB3	1.86	0.43
30:g:32:ARG:O	30:g:36:MET:HG2	2.17	0.43
32:i:215:MET:HG2	32:i:251:MET:HE1	1.99	0.43
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.53	0.43
40:r:229:MET:HE2	40:r:328:CYS:SG	2.57	0.43
3:C:57:ALA:HB1	41:s:53:LEU:HB3	2.00	0.43
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.00	0.43
22:Y:43:ARG:HA	22:Y:43:ARG:HD3	1.85	0.43
26:c:115:ASN:OD1	35:l:162:THR:HG23	2.17	0.43
35:l:180:ILE:HG12	40:r:397:GLY:HA3	1.99	0.43
36:m:64:MET:HE2	36:m:64:MET:N	2.33	0.43
40:r:74:PRO:O	40:r:78:MET:HG3	2.18	0.43
51:I:201:CDL:HA31	13:N:6:VAL:HG21	1.99	0.43
12:M:251:ILE:HG13	12:M:604:GLN:HB3	2.00	0.43
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.26	0.43
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.01	0.43
16:Q:127:LYS:O	16:Q:419:PRO:HD2	2.19	0.43
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.54	0.43
32:i:57:THR:HA	34:k:77:LEU:HD13	2.00	0.43
33:j:90:MET:HE3	33:j:90:MET:HA	2.00	0.43
35:l:9:LEU:HD23	35:l:9:LEU:HA	1.88	0.43
37:n:34:LYS:NZ	51:n:102:CDL:HA22	2.33	0.43
1:A:204:TYR:HB3	1:A:377:GLU:HB3	2.00	0.43
1:A:262:PHE:CE2	1:A:272:GLY:HA3	2.53	0.43
5:F:19:ILE:HB	5:F:53:ILE:HG23	2.00	0.43
6:G:126:PHE:CE1	6:G:148:ILE:HG21	2.53	0.43
11:L:102:ASP:OD1	11:L:102:ASP:N	2.52	0.43
12:M:51:GLN:HA	12:M:54:GLU:HG2	2.01	0.43
12:M:329:MET:HG2	12:M:565:PHE:CG	2.53	0.43
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.30	0.43
51:V:201:CDL:H751	51:V:201:CDL:H381	1.99	0.43
33:j:18:VAL:HG12	47:s:401:PEE:H16	1.99	0.43
35:l:362:LEU:HD22	35:l:366:MET:HE2	2.00	0.43
3:C:191:ARG:O	3:C:195:ARG:HG3	2.19	0.43
9:J:231:LEU:HD23	9:J:231:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:161:TYR:HB2	26:c:165:ASP:HA	2.01	0.43
32:i:207:ILE:HD12	32:i:262:PRO:HG3	1.99	0.43
41:s:134:ARG:NH1	41:s:206:GLU:OE2	2.40	0.43
44:w:224:PRO:HA	44:w:227:MET:HE1	1.99	0.43
6:G:79:ILE:HG22	6:G:145:VAL:HG13	1.99	0.43
15:P:52:ASP:OD1	15:P:53:VAL:N	2.51	0.43
26:c:184:TYR:HB3	43:v:34:ARG:HB3	2.00	0.43
33:j:56:PHE:HB2	36:m:70:TYR:OH	2.19	0.43
40:r:266:MET:O	40:r:269:MET:HG2	2.18	0.43
40:r:325:MET:HE2	40:r:362:ALA:HB2	2.00	0.43
41:s:142:TYR:CZ	41:s:192:GLU:HG2	2.54	0.43
43:v:103:GLU:OE2	43:v:106:ARG:NE	2.45	0.43
1:A:81:LYS:HG2	1:A:96:GLY:HA3	2.00	0.43
1:A:107:ASP:OD1	1:A:107:ASP:N	2.52	0.43
34:k:35:GLY:HA3	36:m:20:PHE:HZ	1.84	0.43
48:n:101:PLX:H1C3	48:n:101:PLX:H22	1.76	0.43
40:r:240:GLY:O	40:r:244:MET:HG3	2.19	0.43
1:A:210:THR:HB	1:A:224:ARG:H	1.84	0.43
12:M:47:THR:O	12:M:96:VAL:HG22	2.18	0.43
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.19	0.43
16:Q:121:GLU:HG2	16:Q:422:CYS:O	2.19	0.43
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.23	0.43
27:d:26:LEU:HD23	27:d:26:LEU:HA	1.88	0.43
35:l:517:SER:OG	35:l:518:GLN:N	2.51	0.43
3:C:66:THR:HG23	49:C:304:UQ:H102	2.01	0.43
5:F:16:LEU:HD21	5:F:19:ILE:HD11	2.00	0.43
6:G:89:LEU:HD12	6:G:89:LEU:HA	1.87	0.43
6:G:113:LEU:O	6:G:117:GLU:HG3	2.19	0.43
49:J:402:UQ:H201	49:J:402:UQ:H221	1.66	0.43
35:l:161:ARG:NH2	35:l:238:GLU:OE2	2.52	0.43
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.01	0.43
41:s:123:SER:HB3	41:s:214:GLU:HG3	2.01	0.43
4:E:14:GLY:O	4:E:15:THR:OG1	2.28	0.42
12:M:476:LEU:HD21	12:M:481:LEU:HD21	2.00	0.42
12:M:676:ASN:OD1	12:M:676:ASN:N	2.51	0.42
22:Y:65:MET:HE1	35:l:378:LEU:HD12	2.01	0.42
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.54	0.42
35:l:297:ASP:O	35:l:301:ILE:HG13	2.20	0.42
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.54	0.42
51:l:702:CDL:H801	48:r:502:PLX:H202	2.01	0.42
36:m:65:LEU:HD23	36:m:65:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:HB2	1:A:212:LEU:HD21	2.00	0.42
8:I:46:SER:O	8:I:52:ASN:ND2	2.50	0.42
12:M:59:GLN:HG2	12:M:62:ARG:NH2	2.34	0.42
6:X:137:LYS:HE2	6:X:137:LYS:HB3	1.89	0.42
24:a:145:GLU:OE2	42:u:163:HIS:NE2	2.45	0.42
35:l:12:LEU:HD22	35:l:129:MET:HB3	2.01	0.42
35:l:557:TRP:O	35:l:561:ILE:HG12	2.18	0.42
51:s:402:CDL:H141	51:s:402:CDL:H171	1.70	0.42
44:w:181:LYS:O	44:w:184:VAL:HG22	2.19	0.42
1:A:366:ALA:HA	14:O:141:MET:HE1	2.00	0.42
2:B:70:LEU:HG	41:s:277:TYR:OH	2.19	0.42
4:E:40:TYR:HB3	6:G:120:MET:HE1	2.01	0.42
16:Q:83:ASN:O	41:s:127:TYR:OH	2.36	0.42
19:U:32:LEU:HB3	41:s:310:MET:SD	2.60	0.42
31:h:83:ARG:O	31:h:87:ILE:HG23	2.18	0.42
32:i:45:MET:HE2	32:i:45:MET:HB3	1.85	0.42
51:l:703:CDL:H382	51:l:703:CDL:H351	1.62	0.42
36:m:45:LEU:CD2	36:m:50:SER:HA	2.49	0.42
44:w:123:SER:OG	44:w:125:ASP:OD1	2.22	0.42
44:w:254:GLU:OE2	44:w:278:CYS:HA	2.19	0.42
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.28	0.42
12:M:367:CYS:HB3	12:M:533:GLY:O	2.20	0.42
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.54	0.42
1:A:53:LEU:HB2	1:A:136:HIS:CE1	2.54	0.42
1:A:358:ASP:OD1	1:A:358:ASP:N	2.48	0.42
4:E:14:GLY:O	11:L:52:LEU:HD11	2.19	0.42
4:E:70:ASN:OD1	4:E:70:ASN:N	2.52	0.42
7:H:76:GLN:HB2	7:H:79:GLU:OE1	2.19	0.42
12:M:382:ARG:HE	12:M:527:ASP:CG	2.27	0.42
12:M:413:LEU:HD13	12:M:413:LEU:HA	1.93	0.42
14:O:152:ILE:HG21	14:O:171:LEU:HD13	2.01	0.42
16:Q:62:LYS:HA	16:Q:62:LYS:HD3	1.76	0.42
34:k:4:VAL:O	34:k:8:ILE:HG12	2.19	0.42
47:r:501:PEE:H75	47:r:501:PEE:H69	1.96	0.42
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.52	0.42
1:A:121:GLU:HG2	1:A:351:THR:HG21	2.02	0.42
3:C:188:LYS:HE2	3:C:188:LYS:HB3	1.73	0.42
12:M:509:ASP:OD2	12:M:509:ASP:N	2.41	0.42
51:V:202:CDL:H852	35:l:558:LEU:HD21	2.00	0.42
6:X:114:ASP:O	6:X:118:ILE:HG13	2.20	0.42
22:Y:83:HIS:O	22:Y:83:HIS:ND1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:a:201:CDL:H511	47:l:705:PEE:H52	2.01	0.42
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.54	0.42
44:w:100:ASP:OD1	44:w:100:ASP:N	2.37	0.42
44:w:215:GLN:O	44:w:219:GLN:HG2	2.20	0.42
4:E:22:SER:HB3	4:E:27:GLU:HB2	2.00	0.42
6:G:110:LEU:HB3	6:G:114:ASP:HB2	2.02	0.42
9:J:49:SER:HB2	15:P:225:GLU:HG2	2.02	0.42
9:J:192:ARG:HA	9:J:192:ARG:HD3	1.91	0.42
9:J:204:SER:OG	9:J:238:GLN:O	2.38	0.42
13:N:144:TYR:CE1	13:N:145:LYS:HD2	2.55	0.42
21:W:131:GLU:CD	21:W:131:GLU:H	2.28	0.42
35:l:16:THR:HG22	35:l:126:ILE:HD13	2.02	0.42
40:r:72:LEU:HD12	40:r:72:LEU:HA	1.82	0.42
40:r:196:TRP:CD1	40:r:250:LEU:HD13	2.55	0.42
40:r:445:LEU:HA	40:r:448:THR:HG22	2.02	0.42
4:E:87:LYS:HB2	4:E:87:LYS:HE3	1.95	0.42
12:M:197:THR:O	14:O:114:GLU:HG2	2.20	0.42
14:O:63:ILE:HG13	14:O:85:LEU:HD23	2.02	0.42
37:n:46:LYS:HB2	37:n:46:LYS:HE3	1.79	0.42
41:s:84:THR:O	41:s:87:VAL:HG22	2.19	0.42
41:s:86:TRP:NE1	41:s:233:MET:HB2	2.33	0.42
9:J:204:SER:OG	9:J:204:SER:O	2.36	0.42
12:M:543:LYS:HE3	12:M:543:LYS:HB3	1.85	0.42
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.32	0.42
21:W:98:MET:HG3	21:W:104:TRP:NE1	2.35	0.42
24:a:106:VAL:HA	24:a:107:PRO:HD3	1.93	0.42
24:a:170:GLN:HB2	30:g:6:GLY:O	2.20	0.42
30:g:87:LEU:HD12	30:g:87:LEU:HA	1.89	0.42
33:j:88:LEU:HD13	41:s:309:ILE:HD12	2.00	0.42
35:l:504:LEU:HD11	51:l:703:CDL:H311	2.02	0.42
47:l:704:PEE:H55	40:r:405:LEU:HD13	2.00	0.42
39:p:5:ALA:HB1	39:p:152:GLU:HB2	2.01	0.42
51:r:503:CDL:H872	51:r:503:CDL:H841	1.76	0.42
41:s:315:PRO:HA	41:s:316:PRO:HD3	1.93	0.42
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.79	0.42
47:Q:501:PEE:H61	47:Q:501:PEE:H37	2.01	0.42
6:X:87:LEU:HA	6:X:87:LEU:HD23	1.85	0.42
51:a:201:CDL:H512	47:l:705:PEE:H13	2.02	0.42
25:b:111:LEU:HD23	25:b:111:LEU:HA	1.88	0.42
32:i:268:GLN:HG3	42:u:168:PHE:HZ	1.85	0.42
34:k:64:LEU:HD23	34:k:64:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:24:PRO:HB3	36:m:89:VAL:HG11	2.02	0.42
51:m:201:CDL:H652	51:m:201:CDL:H622	1.96	0.42
47:s:401:PEE:H31	51:s:402:CDL:H222	2.01	0.42
42:u:68:LEU:HD23	42:u:68:LEU:HA	1.83	0.42
5:F:59:SER:O	5:F:61:VAL:N	2.53	0.41
16:Q:180:LEU:HD23	16:Q:180:LEU:HA	1.89	0.41
25:b:76:LEU:HD12	25:b:76:LEU:HA	1.86	0.41
32:i:75:ILE:HD12	34:k:40:LEU:HD22	2.02	0.41
34:k:14:ILE:HG23	51:m:201:CDL:H751	2.01	0.41
35:l:293:ILE:HG21	35:l:418:LEU:HD22	2.02	0.41
51:l:702:CDL:H202	51:l:702:CDL:H231	1.86	0.41
40:r:299:VAL:O	40:r:303:ILE:HG23	2.20	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.02	0.41
12:M:278:HIS:CE1	12:M:281:ILE:HD12	2.55	0.41
22:Y:94:ASP:OD1	22:Y:99:ILE:HB	2.19	0.41
35:l:260:LEU:HD23	35:l:260:LEU:HA	1.82	0.41
51:l:702:CDL:H342	51:l:702:CDL:H372	1.61	0.41
48:n:101:PLX:H82	40:r:40:SER:HB2	2.02	0.41
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.39	0.41
8:I:70:MET:HE3	8:I:70:MET:O	2.20	0.41
13:N:85:GLU:HG2	13:N:86:TRP:H	1.85	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.41
19:U:42:ALA:HB2	41:s:312:ALA:HA	2.02	0.41
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.02	0.41
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.01	0.41
1:A:281:HIS:ND1	1:A:358:ASP:OD1	2.53	0.41
4:E:81:LEU:HD23	4:E:81:LEU:HA	1.89	0.41
12:M:343:GLY:O	12:M:521:SER:OG	2.32	0.41
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.41
15:P:125:ARG:NH2	15:P:199:ARG:HG2	2.35	0.41
18:T:84:ILE:HD12	18:T:84:ILE:HA	1.90	0.41
19:U:15:LYS:HB3	19:U:15:LYS:HE2	1.83	0.41
51:V:202:CDL:H111	51:V:202:CDL:H351	2.01	0.41
28:e:73:SER:O	28:e:74:HIS:HB2	2.20	0.41
32:i:261:MET:HE1	32:i:336:VAL:HG13	2.02	0.41
32:i:337:LEU:O	32:i:340:THR:OG1	2.30	0.41
34:k:28:SER:HB3	36:m:23:LYS:HG2	2.02	0.41
41:s:138:GLN:O	41:s:141:SER:OG	2.31	0.41
6:G:104:PHE:HA	6:G:108:LEU:HB2	2.02	0.41
6:G:119:ILE:O	6:G:122:MET:HB2	2.21	0.41
9:J:216:TYR:O	9:J:220:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:632:MET:H	12:M:632:MET:HG2	1.63	0.41
17:S:52:ARG:HE	17:S:52:ARG:HB3	1.78	0.41
40:r:76:MET:HG2	40:r:229:MET:SD	2.61	0.41
40:r:200:ILE:HD13	40:r:200:ILE:HA	1.91	0.41
48:C:303:PLX:H122	48:C:303:PLX:H92	1.65	0.41
7:H:76:GLN:O	7:H:78:GLU:N	2.54	0.41
14:O:121:MET:HB3	14:O:121:MET:HE2	1.84	0.41
33:j:69:ILE:O	33:j:73:LEU:HG	2.21	0.41
48:j:202:PLX:H132	48:j:202:PLX:H161	1.71	0.41
34:k:58:MET:HE2	34:k:58:MET:HB3	1.98	0.41
35:l:24:SER:OG	35:l:25:ASN:N	2.51	0.41
51:l:702:CDL:H611	51:l:702:CDL:H581	1.66	0.41
41:s:1:MET:HE3	41:s:1:MET:HB3	1.91	0.41
41:s:102:VAL:HG21	41:s:154:LEU:HD11	2.03	0.41
3:C:187:GLU:HB2	9:J:87:GLU:OE1	2.19	0.41
6:G:133:ILE:HD12	6:G:133:ILE:HA	1.81	0.41
7:H:35:LEU:HA	7:H:38:ILE:HD12	2.03	0.41
48:j:202:PLX:H22	48:j:202:PLX:H1C3	1.76	0.41
51:l:702:CDL:H611	51:l:702:CDL:H811	2.03	0.41
41:s:174:MET:HE2	41:s:174:MET:HB2	1.93	0.41
44:w:58:LYS:O	44:w:60:ILE:HG13	2.19	0.41
4:E:119:LEU:HA	4:E:119:LEU:HD12	1.82	0.41
20:V:118:MET:HA	20:V:121:THR:HG22	2.02	0.41
51:V:201:CDL:H352	51:V:201:CDL:H322	1.47	0.41
51:a:201:CDL:OB4	28:e:108:TYR:OH	2.34	0.41
30:g:14:GLN:O	30:g:15:PHE:HB3	2.21	0.41
32:i:98:MET:HE2	32:i:98:MET:HB2	1.86	0.41
35:l:305:SER:HB2	35:l:422:TYR:CE1	2.56	0.41
37:n:27:LEU:HD12	40:r:6:ILE:HD11	2.03	0.41
42:u:113:ASP:OD1	42:u:113:ASP:C	2.63	0.41
44:w:135:LEU:HD23	44:w:135:LEU:HA	1.94	0.41
44:w:237:ILE:O	44:w:241:TYR:HB2	2.19	0.41
44:w:283:TRP:N	44:w:284:PRO:HD2	2.35	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.41
49:C:304:UQ:H13	49:C:304:UQ:H171	1.90	0.41
4:E:81:LEU:O	4:E:85:LYS:HG3	2.20	0.41
6:G:91:ASP:OD2	6:G:92:LYS:N	2.53	0.41
9:J:228:LEU:O	9:J:292:PRO:HA	2.21	0.41
12:M:331:GLN:NE2	12:M:630:ALA:O	2.53	0.41
19:U:26:GLY:HA3	47:U:101:PEE:H37	2.03	0.41
21:W:5:LYS:HG2	21:W:6:VAL:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:77:CYS:SG	27:d:84:CYS:HB3	2.60	0.41
48:g:201:PLX:HG1	48:g:201:PLX:H122	1.78	0.41
32:i:228:LEU:HD23	32:i:228:LEU:HA	1.92	0.41
32:i:246:VAL:HG21	51:r:503:CDL:H361	2.03	0.41
35:l:327:LEU:O	35:l:331:MET:HG2	2.21	0.41
40:r:281:ASP:OD1	40:r:282:LEU:N	2.51	0.41
43:v:53:LEU:HA	43:v:53:LEU:HD12	1.76	0.41
44:w:276:LEU:HD23	44:w:276:LEU:HA	1.90	0.41
1:A:355:ILE:HD13	14:O:139:PRO:HG3	2.03	0.41
9:J:116:ILE:O	9:J:120:VAL:HG22	2.21	0.41
12:M:47:THR:HG23	12:M:51:GLN:HB2	2.03	0.41
36:m:45:LEU:HD23	36:m:50:SER:HA	2.02	0.41
38:o:50:GLN:O	38:o:56:ARG:HD3	2.21	0.41
44:w:146:ALA:HB1	44:w:157:VAL:HG21	2.03	0.41
2:B:98:ARG:HB3	2:B:169:GLU:OE2	2.21	0.40
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.38	0.40
3:C:109:LEU:HD13	3:C:117:LEU:HD13	2.03	0.40
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.57	0.40
21:W:73:PRO:HG2	42:u:40:ASN:HB3	2.04	0.40
24:a:189:ASN:OD1	24:a:189:ASN:C	2.64	0.40
32:i:222:SER:O	32:i:224:ALA:N	2.54	0.40
51:l:702:CDL:HA62	51:l:702:CDL:H511	2.01	0.40
39:p:176:GLU:HG2	39:p:177:ARG:HG2	2.04	0.40
9:J:61:ALA:HB3	9:J:82:VAL:HG13	2.03	0.40
13:N:72:ASP:OD1	13:N:73:THR:N	2.55	0.40
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	2.02	0.40
19:U:54:PRO:HD3	21:W:69:ILE:HD13	2.02	0.40
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.86	0.40
21:W:52:LYS:HB3	21:W:52:LYS:HE3	1.60	0.40
25:b:69:ILE:O	25:b:73:THR:HG22	2.21	0.40
44:w:302:LEU:HD23	44:w:302:LEU:HA	1.84	0.40
15:P:50:ARG:NH2	15:P:80:CYS:SG	2.94	0.40
15:P:64:TYR:OH	15:P:103:HIS:NE2	2.43	0.40
25:b:70:PHE:O	25:b:74:HIS:HB2	2.21	0.40
27:d:73:ASP:OD2	27:d:75:THR:N	2.41	0.40
31:h:38:LYS:O	31:h:42:GLU:HG3	2.22	0.40
32:i:268:GLN:NE2	32:i:272:LYS:HE3	2.36	0.40
33:j:92:LEU:O	33:j:96:ILE:HG12	2.22	0.40
36:m:26:PRO:HB2	36:m:71:THR:HG21	2.03	0.40
1:A:124:THR:HG21	1:A:351:THR:HG21	2.04	0.40
7:H:19:THR:O	7:H:19:THR:OG1	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:J:402:UQ:H153	49:J:402:UQ:H171	1.80	0.40
51:V:202:CDL:H842	51:V:202:CDL:H811	1.91	0.40
21:W:30:LEU:HD23	21:W:30:LEU:HA	1.84	0.40
22:Y:61:PHE:HA	22:Y:64:THR:HG22	2.03	0.40
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.79	0.40
28:e:119:ARG:HA	28:e:119:ARG:HD3	1.78	0.40
28:e:143:ASP:HB2	28:e:146:LYS:HE3	2.02	0.40
35:l:420:ALA:O	35:l:424:THR:HG22	2.22	0.40
40:r:400:MET:HE2	40:r:400:MET:HB3	1.87	0.40
1:A:265:PHE:HB3	1:A:291:GLU:HG3	2.03	0.40
1:A:392:MET:HE3	1:A:435:VAL:HG21	2.04	0.40
2:B:181:GLU:OE2	9:J:101:GLY:N	2.52	0.40
12:M:124:HIS:CD2	16:Q:375:MET:HE3	2.57	0.40
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.03	0.40
13:N:96:ASP:HA	13:N:97:PRO:HD3	1.95	0.40
48:N:201:PLX:H312	48:N:201:PLX:H342	1.77	0.40
16:Q:184:ILE:HG21	16:Q:207:ARG:HG3	2.03	0.40
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.56	0.40
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.56	0.40
32:i:258:SER:HB3	32:i:333:SER:O	2.22	0.40
35:l:97:THR:O	35:l:101:MET:HG3	2.22	0.40
35:l:253:VAL:HB	35:l:310:LEU:HD11	2.04	0.40
40:r:12:LEU:HD23	40:r:12:LEU:HA	1.98	0.40
40:r:178:ILE:HD13	40:r:178:ILE:HA	1.89	0.40
51:r:503:CDL:H381	51:r:503:CDL:H781	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	417 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	42
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	101 (92%)	8 (7%)	1 (1%)	14	47
8	I	93/112 (83%)	78 (84%)	15 (16%)	0	100	100
9	J	340/342 (99%)	327 (96%)	13 (4%)	0	100	100
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
12	M	688/690 (100%)	660 (96%)	28 (4%)	0	100	100
13	N	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
14	O	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	415 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
18	T	94/96 (98%)	94 (100%)	0	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%)	138 (99%)	2 (1%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	91 (97%)	3 (3%)	0	100	100
26	c	154/156 (99%)	142 (92%)	12 (8%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	96 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
33	j	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
34	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
35	l	604/606 (100%)	571 (94%)	33 (6%)	0	100	100
36	m	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	21	56
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
41	s	316/318 (99%)	303 (96%)	12 (4%)	1 (0%)	36	68
42	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
43	v	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	307 (96%)	11 (4%)	0	100	100
All	All	8174/8312 (98%)	7859 (96%)	311 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
36	m	26	PRO
7	H	77	ILE
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	345/346 (100%)	345 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	75/81 (93%)	75 (100%)	0	100	100
6	X	76/81 (94%)	75 (99%)	1 (1%)	61	78
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	88
10	K	42/42 (100%)	42 (100%)	0	100	100
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	580 (100%)	0	100	100
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	82
14	O	183/183 (100%)	182 (100%)	1 (0%)	81	85
15	P	189/190 (100%)	189 (100%)	0	100	100
16	Q	370/370 (100%)	368 (100%)	2 (0%)	81	85
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	100 (99%)	1 (1%)	68	80
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	62/62 (100%)	61 (98%)	1 (2%)	55	75
23	Z	62/62 (100%)	61 (98%)	1 (2%)	55	75
24	a	121/121 (100%)	120 (99%)	1 (1%)	73	82
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	310/311 (100%)	309 (100%)	1 (0%)	86	88
33	j	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	536 (99%)	4 (1%)	76	83
36	m	130/141 (92%)	130 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	157/159 (99%)	157 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	275/275 (100%)	275 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	80
44	w	280/283 (99%)	280 (100%)	0	100	100
All	All	7151/7240 (99%)	7134 (100%)	17 (0%)	85	89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	188	LYS
9	J	317	ASP
13	N	80	SER
14	O	224	SER
16	Q	57	GLU
16	Q	101	LEU
20	V	85	ASP
6	X	129	GLU
22	Y	76	ASP
23	Z	30	GLU
24	a	71	MET
32	i	149	ILE
35	l	65	ASN
35	l	70	THR
35	l	391	SER
35	l	503	GLU
43	v	47	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	244	ASN
1	A	277	ASN
1	A	422	HIS
4	E	45	ASN
9	J	278	GLN
9	J	356	HIS
11	L	71	HIS
11	L	92	ASN
12	M	425	ASN
12	M	569	GLN
12	M	652	ASN
13	N	13	GLN
13	N	135	GLN
14	O	69	ASN
14	O	90	ASN
14	O	131	HIS
14	O	191	ASN
15	P	55	HIS
15	P	82	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	36	GLN
17	S	61	HIS
20	V	129	GLN
6	X	142	GLN
22	Y	49	GLN
23	Z	21	GLN
23	Z	91	GLN
25	b	26	GLN
26	c	84	GLN
26	c	94	HIS
26	c	127	ASN
29	f	62	HIS
30	g	119	HIS
31	h	21	GLN
35	l	23	ASN
35	l	59	GLN
35	l	135	ASN
35	l	165	ASN
35	l	175	ASN
35	l	194	ASN
35	l	199	GLN

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Mol	Chain	Res	Type
35	l	296	ASN
35	l	309	GLN
35	l	444	ASN
35	l	447	ASN
35	l	470	ASN
36	m	175	ASN
38	o	126	ASN
39	p	75	GLN
39	p	78	GLN
40	r	20	HIS
40	r	304	GLN
44	w	215	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	1.98	1 (10%)	5,13,15	5.97	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	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.63	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	12.22	130.68	119.48
16	Q	118	2MR	CD-NE-CZ	4.01	130.90	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.36	130.86	123.65

There are no chirality outliers.

All (2) 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

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 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\# Z > 2$
47	PEE	I	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.10	3 (7%)
49	UQ	J	402	-	33,33,63	3.52	9 (27%)	42,43,79	2.71	14 (33%)
47	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PLX	j	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-		
56	ADP	w	401	-	28,29,29	3.16	9 (32%)	43,45,45	1.91	9 (20%)
47	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
50	8Q1	X	201	6	32,34,34	1.61	6 (18%)	39,43,43	1.53	7 (17%)
48	PLX	C	303	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	1 (1%)
50	8Q1	G	201	-	32,34,34	1.60	6 (18%)	39,43,43	1.62	6 (15%)
51	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
47	PEE	Q	501	-	46,46,50	1.22	6 (13%)	49,51,55	1.05	3 (6%)
48	PLX	n	101	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)
52	NDP	J	401	-	51,52,52	4.27	25 (49%)	71,80,80	2.19	14 (19%)
47	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
51	CDL	n	102	-	54,54,99	1.38	8 (14%)	60,66,111	1.10	4 (6%)
45	SF4	M	801	12	0,12,12	-	-	-		
49	UQ	C	304	-	63,63,63	3.74	15 (23%)	78,79,79	3.14	34 (43%)
48	PLX	N	201	-	51,51,51	1.20	5 (9%)	53,59,59	0.62	1 (1%)
51	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.88	4 (4%)
53	FES	O	301	14	0,4,4	-	-	-		
48	PLX	j	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	2 (3%)
51	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
47	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
51	CDL	m	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
47	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
51	CDL	l	702	-	98,98,99	1.11	8 (8%)	104,110,111	0.91	4 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
47	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
51	CDL	l	703	-	99,99,99	1.10	9 (9%)	105,111,111	0.87	4 (3%)
48	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.59	1 (1%)
51	CDL	s	402	-	88,88,99	1.15	8 (9%)	94,100,111	0.93	4 (4%)
47	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-		
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.24	8 (16%)
47	PEE	s	401	-	40,40,50	1.17	5 (12%)	43,45,55	1.04	2 (4%)
48	PLX	g	201	-	51,51,51	1.20	3 (5%)	53,59,59	0.66	1 (1%)
51	CDL	r	503	-	99,99,99	1.10	8 (8%)	105,111,111	0.89	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
51	CDL	I	201	-	50,50,99	1.43	8 (16%)	56,62,111	1.15	4 (7%)

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
47	PEE	l	701	-	-	26/43/43/54	-
49	UQ	J	402	-	-	15/27/51/87	0/1/1/1
47	PEE	C	302	-	-	29/50/50/54	-
48	PLX	j	202	-	-	25/55/55/55	-
56	ADP	w	401	-	-	4/16/32/32	0/3/3/3
45	SF4	A	501	1	-	-	0/6/5/5
47	PEE	B	303	-	-	21/54/54/54	-
50	8Q1	X	201	6	-	17/41/41/41	-
48	PLX	C	303	-	-	25/55/55/55	-
50	8Q1	G	201	-	-	11/41/41/41	-
51	CDL	V	202	-	-	51/110/110/110	-
47	PEE	Q	501	-	-	24/50/50/54	-
48	PLX	n	101	-	-	25/55/55/55	-
52	NDP	J	401	-	-	9/34/77/77	0/5/5/5
47	PEE	U	101	-	-	21/54/54/54	-
51	CDL	n	102	-	-	23/65/65/110	-
45	SF4	M	801	12	-	-	0/6/5/5
49	UQ	C	304	-	-	27/63/87/87	0/1/1/1
48	PLX	N	201	-	-	25/55/55/55	-
51	CDL	V	201	-	-	50/104/104/110	-
53	FES	O	301	14	-	-	0/1/1/1
48	PLX	j	201	-	-	33/55/55/55	-
51	CDL	a	201	-	-	57/110/110/110	-
47	PEE	l	705	-	-	26/49/49/54	-
51	CDL	m	201	-	-	64/110/110/110	-
47	PEE	l	704	-	-	28/54/54/54	-
51	CDL	l	702	-	-	56/109/109/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	B	302	2	-	-	0/6/5/5
47	PEE	W	201	-	-	23/44/44/54	-
51	CDL	l	703	-	-	58/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PLX	r	502	-	-	30/55/55/55	-
51	CDL	s	402	-	-	52/99/99/110	-
47	PEE	r	501	-	-	28/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
47	PEE	s	401	-	-	18/44/44/54	-
48	PLX	g	201	-	-	29/55/55/55	-
51	CDL	r	503	-	-	55/110/110/110	-
53	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
51	CDL	I	201	-	-	30/61/61/110	-

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	C3B-C2B	-13.36	1.23	1.53
52	J	401	NDP	O4D-C4D	10.62	1.68	1.45
52	J	401	NDP	C3D-C4D	-10.07	1.27	1.53
49	J	402	UQ	C18-C19	9.95	1.56	1.33
49	C	304	UQ	C18-C19	9.95	1.56	1.33
49	C	304	UQ	C13-C14	9.67	1.55	1.33
49	J	402	UQ	C13-C14	9.53	1.55	1.33
49	C	304	UQ	C23-C24	9.40	1.54	1.33
49	J	402	UQ	C8-C9	9.37	1.54	1.33
49	C	304	UQ	C8-C9	9.29	1.54	1.33
49	C	304	UQ	C28-C29	9.19	1.54	1.33
56	w	401	ADP	C3'-C4'	-9.01	1.30	1.53
49	C	304	UQ	C33-C34	8.86	1.53	1.33
49	C	304	UQ	C38-C39	8.56	1.52	1.33
49	C	304	UQ	C43-C44	8.55	1.52	1.33
49	C	304	UQ	C48-C49	8.15	1.51	1.33
52	J	401	NDP	O4B-C4B	-7.96	1.27	1.45
56	w	401	ADP	O4'-C4'	7.62	1.61	1.45
49	J	402	UQ	C23-C24	7.50	1.54	1.32
52	J	401	NDP	C6N-C5N	7.29	1.55	1.33
52	J	401	NDP	C2N-C3N	7.28	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	304	UQ	C53-C54	7.07	1.53	1.32
52	J	401	NDP	PN-O3	6.41	1.66	1.59
56	w	401	ADP	PA-O3A	6.36	1.66	1.59
52	J	401	NDP	C6A-N6A	5.76	1.48	1.34
52	J	401	NDP	P2B-O2B	5.71	1.69	1.59
56	w	401	ADP	C6-N6	5.41	1.48	1.34
52	J	401	NDP	PA-O3	5.33	1.65	1.59
52	J	401	NDP	C3B-C4B	5.23	1.66	1.53
50	X	201	8Q1	C34-N36	5.11	1.45	1.33
52	J	401	NDP	O4D-C1D	-5.09	1.30	1.42
50	G	201	8Q1	C39-N41	5.07	1.45	1.33
50	X	201	8Q1	C39-N41	5.05	1.45	1.33
50	G	201	8Q1	C34-N36	4.98	1.45	1.33
52	J	401	NDP	C6N-N1N	4.97	1.49	1.37
52	J	401	NDP	O4B-C1B	4.71	1.52	1.42
52	J	401	NDP	C1B-N9A	-4.65	1.33	1.46
56	w	401	ADP	O4'-C1'	-4.61	1.31	1.42
52	J	401	NDP	O2D-C2D	-4.07	1.32	1.43
52	J	401	NDP	C7N-N7N	3.86	1.44	1.33
47	l	701	PEE	C18-C19	3.84	1.53	1.31
47	s	401	PEE	C18-C19	3.83	1.53	1.31
47	B	303	PEE	C18-C19	3.82	1.53	1.31
47	l	704	PEE	C18-C19	3.82	1.53	1.31
47	C	302	PEE	C18-C19	3.82	1.53	1.31
47	W	201	PEE	C18-C19	3.81	1.53	1.31
47	r	501	PEE	C18-C19	3.81	1.53	1.31
47	l	705	PEE	C18-C19	3.81	1.53	1.31
47	U	101	PEE	C18-C19	3.81	1.53	1.31
47	Q	501	PEE	C18-C19	3.77	1.53	1.31
47	l	701	PEE	C39-C38	3.75	1.53	1.31
47	U	101	PEE	C39-C38	3.74	1.53	1.31
47	B	303	PEE	C39-C38	3.74	1.52	1.31
47	r	501	PEE	C39-C38	3.73	1.52	1.31
47	C	302	PEE	C39-C38	3.73	1.52	1.31
47	l	705	PEE	C39-C38	3.73	1.52	1.31
47	l	704	PEE	C39-C38	3.71	1.52	1.31
47	Q	501	PEE	C39-C38	3.70	1.52	1.31
51	V	201	CDL	OA8-CA7	3.50	1.43	1.33
51	V	202	CDL	OA8-CA7	3.46	1.43	1.33
51	s	402	CDL	OA8-CA7	3.46	1.43	1.33
51	n	102	CDL	OA8-CA7	3.45	1.43	1.33
51	I	201	CDL	OA8-CA7	3.44	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	l	702	CDL	OA8-CA7	3.43	1.43	1.33
51	r	503	CDL	OA8-CA7	3.42	1.43	1.33
51	l	703	CDL	OA8-CA7	3.40	1.43	1.33
51	m	201	CDL	OA8-CA7	3.38	1.43	1.33
56	w	401	ADP	C8-N9	-3.38	1.31	1.37
51	a	201	CDL	OA8-CA7	3.37	1.43	1.33
46	A	502	FMN	C4A-N5	3.36	1.38	1.30
52	J	401	NDP	C8A-N9A	-3.32	1.31	1.37
56	w	401	ADP	O2'-C2'	-3.22	1.35	1.43
52	J	401	NDP	C5A-N7A	-3.13	1.33	1.39
51	V	201	CDL	OA6-CA5	3.09	1.43	1.34
51	m	201	CDL	OA6-CA5	3.06	1.42	1.34
51	I	201	CDL	OB6-CB5	3.03	1.42	1.34
51	a	201	CDL	OB6-CB5	3.02	1.42	1.34
51	r	503	CDL	OB6-CB5	3.01	1.42	1.34
51	l	702	CDL	OB6-CB5	3.01	1.42	1.34
51	V	202	CDL	OB6-CB5	3.01	1.42	1.34
51	m	201	CDL	OB6-CB5	3.00	1.42	1.34
51	m	201	CDL	OB8-CB7	3.00	1.42	1.33
51	s	402	CDL	OB6-CB5	3.00	1.42	1.34
51	n	102	CDL	OB8-CB7	3.00	1.42	1.33
51	a	201	CDL	OB8-CB7	2.99	1.42	1.33
51	V	201	CDL	OB6-CB5	2.98	1.42	1.34
51	s	402	CDL	OA6-CA5	2.97	1.42	1.34
51	I	201	CDL	OB8-CB7	2.97	1.42	1.33
51	I	201	CDL	OA6-CA5	2.97	1.42	1.34
51	l	703	CDL	OB6-CB5	2.96	1.42	1.34
51	l	702	CDL	OB8-CB7	2.96	1.42	1.33
51	n	102	CDL	OA6-CA5	2.95	1.42	1.34
51	r	503	CDL	OB8-CB7	2.94	1.41	1.33
51	V	201	CDL	OB8-CB7	2.94	1.41	1.33
51	V	202	CDL	OA6-CA5	2.93	1.42	1.34
51	l	703	CDL	OB8-CB7	2.93	1.41	1.33
52	J	401	NDP	C7N-C3N	2.93	1.55	1.48
51	n	102	CDL	OB6-CB5	2.93	1.42	1.34
48	C	303	PLX	O6-C4	-2.92	1.40	1.44
48	n	101	PLX	O6-C4	-2.92	1.40	1.44
48	g	201	PLX	O6-C4	-2.91	1.40	1.44
56	w	401	ADP	O3'-C3'	2.91	1.50	1.43
51	l	703	CDL	OA6-CA5	2.90	1.42	1.34
51	a	201	CDL	OA6-CA5	2.90	1.42	1.34
52	J	401	NDP	O3D-C3D	2.89	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	V	202	CDL	OB8-CB7	2.89	1.41	1.33
51	l	702	CDL	OA6-CA5	2.88	1.42	1.34
51	s	402	CDL	OB8-CB7	2.87	1.41	1.33
51	r	503	CDL	OA6-CA5	2.82	1.42	1.34
48	N	201	PLX	O6-C4	-2.79	1.41	1.44
48	r	502	PLX	O6-C4	-2.75	1.41	1.44
49	J	402	UQ	C6-C1	2.74	1.54	1.46
48	j	202	PLX	O6-C4	-2.71	1.41	1.44
49	C	304	UQ	C6-C1	2.69	1.54	1.46
51	l	703	CDL	OA6-CA4	-2.66	1.40	1.46
47	W	201	PEE	O2-C2	-2.66	1.40	1.46
51	l	702	CDL	OA6-CA4	-2.64	1.40	1.46
47	C	302	PEE	O2-C2	-2.64	1.40	1.46
51	r	503	CDL	OA6-CA4	-2.64	1.40	1.46
48	j	201	PLX	O6-C4	-2.63	1.41	1.44
47	l	704	PEE	O2-C2	-2.63	1.40	1.46
47	r	501	PEE	O2-C2	-2.62	1.40	1.46
51	n	102	CDL	OA6-CA4	-2.61	1.40	1.46
47	Q	501	PEE	O2-C2	-2.59	1.40	1.46
47	l	701	PEE	O2-C2	-2.59	1.40	1.46
47	B	303	PEE	O2-C2	-2.59	1.40	1.46
47	l	705	PEE	O2-C2	-2.59	1.40	1.46
51	a	201	CDL	OA6-CA4	-2.58	1.40	1.46
47	s	401	PEE	O2-C2	-2.56	1.40	1.46
51	V	202	CDL	OA6-CA4	-2.56	1.40	1.46
51	s	402	CDL	OA6-CA4	-2.54	1.40	1.46
51	I	201	CDL	OA6-CA4	-2.54	1.40	1.46
47	U	101	PEE	O2-C2	-2.54	1.40	1.46
48	j	202	PLX	C7-C6	2.51	1.56	1.50
52	J	401	NDP	O2B-C2B	2.49	1.52	1.44
47	l	701	PEE	O3-C30	2.48	1.40	1.33
47	B	303	PEE	O3-C30	2.47	1.40	1.33
47	s	401	PEE	O3-C30	2.45	1.40	1.33
47	r	501	PEE	O3-C30	2.44	1.40	1.33
51	n	102	CDL	OB6-CB4	-2.44	1.40	1.46
47	U	101	PEE	O3-C30	2.43	1.40	1.33
47	C	302	PEE	O3-C30	2.43	1.40	1.33
47	l	705	PEE	O3-C30	2.42	1.40	1.33
50	X	201	8Q1	O40-C39	-2.41	1.18	1.23
47	l	704	PEE	O3-C30	2.40	1.40	1.33
47	Q	501	PEE	O3-C30	2.39	1.40	1.33
51	V	201	CDL	OB6-CB4	-2.39	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	401	ADP	C5-N7	-2.39	1.34	1.39
51	s	402	CDL	OB6-CB4	-2.38	1.41	1.46
50	G	201	8Q1	O35-C34	-2.38	1.18	1.23
51	l	703	CDL	OB6-CB4	-2.38	1.41	1.46
51	m	201	CDL	OB6-CB4	-2.38	1.41	1.46
50	G	201	8Q1	O40-C39	-2.38	1.18	1.23
48	r	502	PLX	C7-C6	2.37	1.55	1.50
48	j	201	PLX	C7-C6	2.37	1.55	1.50
50	X	201	8Q1	C1-S44	2.36	1.81	1.76
48	g	201	PLX	C7-C6	2.36	1.55	1.50
51	n	102	CDL	PB2-OB2	2.35	1.68	1.59
47	W	201	PEE	O3-C30	2.35	1.40	1.33
51	V	202	CDL	OB6-CB4	-2.35	1.41	1.46
50	G	201	8Q1	C1-S44	2.35	1.81	1.76
46	A	502	FMN	C10-N1	2.34	1.37	1.33
50	X	201	8Q1	O35-C34	-2.34	1.18	1.23
48	N	201	PLX	C7-C6	2.33	1.55	1.50
51	r	503	CDL	OB6-CB4	-2.32	1.41	1.46
51	a	201	CDL	OB6-CB4	-2.31	1.41	1.46
48	n	101	PLX	C7-C6	2.31	1.55	1.50
51	I	201	CDL	OB6-CB4	-2.31	1.41	1.46
51	m	201	CDL	OA6-CA4	-2.31	1.41	1.46
47	l	704	PEE	O3-C3	-2.31	1.40	1.45
49	J	402	UQ	C7-C8	2.30	1.54	1.50
51	V	201	CDL	PB2-OB2	2.29	1.68	1.59
47	l	704	PEE	O2-C10	2.29	1.40	1.34
48	C	303	PLX	C7-C6	2.28	1.55	1.50
51	l	702	CDL	OB6-CB4	-2.27	1.41	1.46
47	r	501	PEE	O2-C10	2.27	1.40	1.34
49	C	304	UQ	C7-C8	2.27	1.54	1.50
51	V	202	CDL	PB2-OB2	2.26	1.68	1.59
47	B	303	PEE	O2-C10	2.26	1.40	1.34
47	l	701	PEE	O2-C10	2.26	1.40	1.34
47	l	705	PEE	O2-C10	2.25	1.40	1.34
51	I	201	CDL	PB2-OB2	2.25	1.68	1.59
51	a	201	CDL	PB2-OB2	2.24	1.68	1.59
47	U	101	PEE	O2-C10	2.24	1.40	1.34
47	W	201	PEE	O3-C3	-2.24	1.40	1.45
52	J	401	NDP	C2D-C3D	2.24	1.59	1.53
51	V	202	CDL	PB2-OB5	2.23	1.68	1.59
47	s	401	PEE	O2-C10	2.23	1.40	1.34
51	I	201	CDL	PB2-OB5	2.23	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	l	703	CDL	PB2-OB2	2.22	1.68	1.59
51	m	201	CDL	PB2-OB2	2.22	1.68	1.59
51	r	503	CDL	PB2-OB2	2.22	1.68	1.59
51	l	702	CDL	PB2-OB2	2.22	1.68	1.59
51	V	201	CDL	PB2-OB5	2.21	1.68	1.59
47	Q	501	PEE	O3-C3	-2.21	1.40	1.45
51	l	702	CDL	PB2-OB5	2.21	1.68	1.59
51	m	201	CDL	PB2-OB5	2.21	1.68	1.59
51	V	201	CDL	OA6-CA4	-2.21	1.41	1.46
47	C	302	PEE	O2-C10	2.21	1.40	1.34
51	a	201	CDL	PB2-OB5	2.20	1.68	1.59
48	N	201	PLX	P1-O4	2.19	1.68	1.59
47	U	101	PEE	O3-C3	-2.19	1.40	1.45
51	s	402	CDL	PB2-OB2	2.19	1.68	1.59
47	W	201	PEE	O2-C10	2.18	1.40	1.34
47	s	401	PEE	O3-C3	-2.18	1.40	1.45
51	n	102	CDL	PB2-OB5	2.18	1.67	1.59
48	j	202	PLX	P1-O4	2.18	1.67	1.59
52	J	401	NDP	O7N-C7N	-2.18	1.19	1.24
47	Q	501	PEE	O2-C10	2.18	1.40	1.34
48	g	201	PLX	P1-O4	2.17	1.67	1.59
49	C	304	UQ	O2-CM2	-2.16	1.40	1.45
51	r	503	CDL	PB2-OB5	2.16	1.67	1.59
47	l	705	PEE	O3-C3	-2.16	1.40	1.45
51	l	703	CDL	PB2-OB5	2.15	1.67	1.59
48	n	101	PLX	P1-O4	2.15	1.67	1.59
47	C	302	PEE	O3-C3	-2.15	1.40	1.45
48	C	303	PLX	P1-O4	2.13	1.67	1.59
49	C	304	UQ	O4-C4	-2.13	1.18	1.23
49	J	402	UQ	O4-C4	-2.12	1.18	1.23
48	r	502	PLX	P1-O4	2.12	1.67	1.59
48	j	202	PLX	P1-O1	2.11	1.67	1.59
47	l	701	PEE	O3-C3	-2.10	1.40	1.45
49	C	304	UQ	O3-CM3	-2.10	1.40	1.45
48	N	201	PLX	P1-O1	2.09	1.67	1.59
47	B	303	PEE	O3-C3	-2.09	1.40	1.45
47	r	501	PEE	O3-C3	-2.09	1.40	1.45
52	J	401	NDP	PA-O5B	2.09	1.67	1.59
48	j	201	PLX	P1-O4	2.09	1.67	1.59
48	r	502	PLX	P1-O1	2.08	1.67	1.59
51	s	402	CDL	PB2-OB5	2.08	1.67	1.59
48	n	101	PLX	P1-O1	2.07	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	402	UQ	O3-CM3	-2.06	1.40	1.45
50	X	201	8Q1	C6-C1	2.05	1.52	1.50
50	G	201	8Q1	C6-C1	2.04	1.52	1.50
49	J	402	UQ	C21-C19	2.04	1.55	1.51
48	C	303	PLX	P1-O1	2.03	1.67	1.59
48	r	502	PLX	C1-C2	2.02	1.57	1.51
48	j	201	PLX	P1-O1	2.02	1.67	1.59
48	N	201	PLX	C1-C2	2.01	1.57	1.51
51	V	201	CDL	C11-CA5	2.01	1.56	1.50
51	l	703	CDL	C11-CA5	2.00	1.56	1.50

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C3N-C2N-N1N	-7.85	111.67	123.20
49	J	402	UQ	C7-C8-C9	-7.77	113.44	126.83
49	C	304	UQ	C7-C8-C9	-7.61	113.72	126.83
49	C	304	UQ	C42-C43-C44	-6.90	111.84	127.62
52	J	401	NDP	C1D-N1N-C2N	-6.70	110.10	121.14
49	J	402	UQ	C12-C13-C14	-6.59	112.53	127.62
49	C	304	UQ	C47-C48-C49	-6.59	112.54	127.62
49	C	304	UQ	C37-C38-C39	-6.38	113.02	127.62
52	J	401	NDP	C6N-N1N-C2N	-6.25	112.63	119.32
49	C	304	UQ	C22-C23-C24	-6.23	113.36	127.62
49	C	304	UQ	C27-C28-C29	-6.22	113.38	127.62
49	J	402	UQ	C17-C18-C19	-6.16	113.52	127.62
49	C	304	UQ	C12-C13-C14	-6.08	113.72	127.62
49	C	304	UQ	C17-C18-C19	-6.07	113.74	127.62
49	C	304	UQ	C32-C33-C34	-6.02	113.85	127.62
50	G	201	8Q1	C6-C1-S44	6.02	120.57	113.40
52	J	401	NDP	C5A-C4A-N3A	-5.65	118.94	126.72
56	w	401	ADP	C5-C4-N3	-5.36	119.34	126.72
50	X	201	8Q1	C6-C1-S44	5.30	119.71	113.40
52	J	401	NDP	C1D-N1N-C6N	-5.12	109.94	120.77
49	C	304	UQ	C30-C29-C28	-4.71	111.54	123.63
56	w	401	ADP	N3-C2-N1	-4.57	121.66	128.58
49	C	304	UQ	C45-C44-C43	-4.53	111.99	123.63
49	J	402	UQ	C22-C23-C24	-4.42	112.89	127.64
49	C	304	UQ	C20-C19-C18	-4.35	112.46	123.63
49	C	304	UQ	C50-C49-C48	-4.26	112.70	123.63
49	C	304	UQ	C10-C9-C8	-4.22	112.78	123.63
49	C	304	UQ	C52-C53-C54	-4.21	113.60	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	401	ADP	N3-C4-N9	4.21	134.32	127.17
49	C	304	UQ	C40-C39-C38	-4.20	112.85	123.63
49	J	402	UQ	C10-C9-C8	-4.20	112.85	123.63
47	s	401	PEE	O2-C10-C11	4.16	120.47	111.48
52	J	401	NDP	N3A-C2A-N1A	-4.14	122.32	128.58
51	l	702	CDL	OB6-CB5-C51	4.13	120.41	111.48
49	C	304	UQ	C25-C24-C23	-4.11	113.07	123.63
51	m	201	CDL	OB6-CB5-C51	4.09	120.34	111.48
49	J	402	UQ	C15-C14-C13	-4.08	113.14	123.63
49	J	402	UQ	C20-C19-C18	-4.07	113.19	123.63
52	J	401	NDP	N3A-C4A-N9A	4.06	134.08	127.17
51	I	201	CDL	OB6-CB5-C51	4.06	120.27	111.48
49	C	304	UQ	C31-C29-C28	-4.06	112.06	121.17
47	B	303	PEE	O2-C10-C11	4.03	120.21	111.48
47	C	302	PEE	O2-C10-C11	4.01	120.16	111.48
47	U	101	PEE	O2-C10-C11	4.01	120.15	111.48
51	s	402	CDL	OA6-CA5-C11	3.99	120.12	111.48
51	V	201	CDL	OA6-CA5-C11	3.99	120.11	111.48
47	r	501	PEE	O2-C10-C11	3.99	120.11	111.48
47	W	201	PEE	O2-C10-C11	3.98	120.10	111.48
51	l	702	CDL	OA6-CA5-C11	3.98	120.09	111.48
51	s	402	CDL	OB6-CB5-C51	3.98	120.08	111.48
47	Q	501	PEE	O2-C10-C11	3.97	120.07	111.48
49	C	304	UQ	C41-C39-C38	-3.96	112.28	121.17
51	a	201	CDL	OB6-CB5-C51	3.96	120.04	111.48
51	I	201	CDL	OA6-CA5-C11	3.95	120.04	111.48
51	a	201	CDL	OA6-CA5-C11	3.95	120.03	111.48
51	V	202	CDL	OB6-CB5-C51	3.95	120.02	111.48
51	r	503	CDL	OA6-CA5-C11	3.94	120.01	111.48
47	l	705	PEE	O2-C10-C11	3.94	120.01	111.48
51	V	202	CDL	OA6-CA5-C11	3.93	119.98	111.48
49	J	402	UQ	C21-C19-C18	-3.93	112.35	121.17
47	l	701	PEE	O2-C10-C11	3.90	119.92	111.48
51	n	102	CDL	OB6-CB5-C51	3.90	119.92	111.48
49	C	304	UQ	C51-C49-C48	-3.90	112.41	121.17
51	n	102	CDL	OA6-CA5-C11	3.90	119.91	111.48
49	C	304	UQ	C35-C34-C33	-3.89	113.64	123.63
47	l	704	PEE	O2-C10-C11	3.88	119.88	111.48
49	J	402	UQ	C11-C9-C8	-3.86	112.49	121.17
51	V	201	CDL	OB6-CB5-C51	3.86	119.82	111.48
51	r	503	CDL	OB6-CB5-C51	3.82	119.75	111.48
50	G	201	8Q1	O4-C1-C6	-3.81	119.58	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	304	UQ	C36-C34-C33	-3.81	112.62	121.17
49	C	304	UQ	C21-C19-C18	-3.79	112.66	121.17
49	C	304	UQ	C15-C14-C13	-3.78	113.91	123.63
51	l	703	CDL	OA6-CA5-C11	3.74	119.57	111.48
51	l	703	CDL	OB6-CB5-C51	3.72	119.52	111.48
49	C	304	UQ	C46-C44-C43	-3.70	112.87	121.17
51	m	201	CDL	OA6-CA5-C11	3.66	119.40	111.48
52	J	401	NDP	C2A-N3A-C4A	3.62	120.67	111.83
49	J	402	UQ	C16-C14-C13	-3.59	113.10	121.17
49	C	304	UQ	C11-C9-C8	-3.55	113.19	121.17
56	w	401	ADP	C2-N3-C4	3.55	120.49	111.83
56	w	401	ADP	N9-C8-N7	-3.51	108.95	113.94
50	X	201	8Q1	O4-C1-C6	-3.49	119.95	123.98
49	C	304	UQ	C26-C24-C23	-3.47	113.38	121.17
49	C	304	UQ	C16-C14-C13	-3.45	113.43	121.17
49	C	304	UQ	C55-C54-C53	-3.34	112.64	122.66
46	A	502	FMN	C4-N3-C2	-3.33	119.73	125.64
49	J	402	UQ	C26-C24-C23	-3.29	112.77	122.66
49	J	402	UQ	C25-C24-C23	-3.26	112.88	122.66
56	w	401	ADP	C4-N9-C8	3.20	109.10	105.74
56	w	401	ADP	C5-N7-C8	3.16	108.42	103.45
52	J	401	NDP	C4A-C5A-N7A	-3.13	107.00	110.58
52	J	401	NDP	N9A-C8A-N7A	-3.12	109.51	113.94
50	G	201	8Q1	C37-C38-C39	3.06	117.49	112.39
52	J	401	NDP	C5A-N7A-C8A	3.02	108.20	103.45
56	w	401	ADP	C4-C5-N7	-2.97	107.18	110.58
49	C	304	UQ	C56-C54-C53	-2.96	113.77	122.66
51	m	201	CDL	OB8-CB7-C71	2.93	120.76	111.83
51	n	102	CDL	OA8-CA7-C31	2.90	119.95	111.15
51	r	503	CDL	OB8-CB7-C71	2.87	120.59	111.83
47	B	303	PEE	O3-C30-C31	2.86	120.56	111.83
51	l	702	CDL	OA8-CA7-C31	2.86	120.55	111.83
49	C	304	UQ	CM5-C5-C6	-2.85	119.76	124.45
47	r	501	PEE	O3-C30-C31	2.84	120.48	111.83
47	Q	501	PEE	O3-C30-C31	2.83	120.45	111.83
51	a	201	CDL	OB8-CB7-C71	2.81	120.41	111.83
51	l	703	CDL	OB8-CB7-C71	2.78	120.32	111.83
51	V	202	CDL	OB8-CB7-C71	2.76	120.26	111.83
47	l	701	PEE	O3-C30-C31	2.75	120.22	111.83
51	V	201	CDL	OB8-CB7-C71	2.75	120.21	111.83
47	s	401	PEE	O3-C30-C31	2.73	120.16	111.83
51	s	402	CDL	OA8-CA7-C31	2.72	120.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	l	702	CDL	OB8-CB7-C71	2.72	120.13	111.83
51	I	201	CDL	OA8-CA7-C31	2.72	120.12	111.83
51	m	201	CDL	OA8-CA7-C31	2.72	120.12	111.83
51	I	201	CDL	OB8-CB7-C71	2.71	120.08	111.83
47	l	704	PEE	O3-C30-C31	2.70	120.06	111.83
47	U	101	PEE	O3-C30-C31	2.70	120.06	111.83
47	l	705	PEE	O3-C30-C31	2.69	120.04	111.83
47	W	201	PEE	O3-C30-C31	2.68	120.00	111.83
47	C	302	PEE	O3-C30-C31	2.67	119.98	111.83
49	C	304	UQ	C7-C6-C5	-2.67	120.31	124.89
51	V	202	CDL	OA8-CA7-C31	2.66	119.95	111.83
51	a	201	CDL	OA8-CA7-C31	2.66	119.94	111.83
51	r	503	CDL	OA8-CA7-C31	2.66	119.94	111.83
51	s	402	CDL	OB8-CB7-C71	2.64	119.89	111.83
46	A	502	FMN	C4A-C4-N3	2.64	119.97	113.25
51	n	102	CDL	OB8-CB7-C71	2.64	119.88	111.83
51	l	703	CDL	OA8-CA7-C31	2.60	119.77	111.83
46	A	502	FMN	C4A-C10-N10	2.58	120.18	116.48
51	V	201	CDL	OA8-CA7-C31	2.58	119.69	111.83
48	g	201	PLX	C1A-N1-C1	2.57	120.13	109.91
52	J	401	NDP	C2B-C1B-N9A	-2.56	109.53	113.75
56	w	401	ADP	C4'-O4'-C1'	-2.54	103.86	109.47
49	J	402	UQ	CM5-C5-C6	-2.54	120.28	124.45
50	X	201	8Q1	C37-C38-C39	2.51	116.58	112.39
49	J	402	UQ	C7-C6-C5	-2.49	120.61	124.89
48	j	202	PLX	C1A-N1-C1	2.48	119.77	109.91
46	A	502	FMN	O4-C4-C4A	-2.48	119.99	126.53
48	r	502	PLX	C1A-N1-C1	2.47	119.74	109.91
50	X	201	8Q1	C38-C39-N41	2.47	120.84	116.34
52	J	401	NDP	C4A-N9A-C8A	2.45	108.31	105.74
48	N	201	PLX	C1A-N1-C1	2.45	119.64	109.91
48	n	101	PLX	C1A-N1-C1	2.39	119.43	109.91
46	A	502	FMN	C5A-C9A-N10	2.34	120.08	117.97
48	j	201	PLX	C1A-N1-C1	2.31	119.10	109.91
48	C	303	PLX	C1A-N1-C1	2.30	119.07	109.91
46	A	502	FMN	C10-C4A-N5	-2.30	120.11	124.81
47	l	701	PEE	C20-C19-C18	-2.29	112.65	126.42
50	X	201	8Q1	C43-S44-C1	2.24	108.47	101.84
50	G	201	8Q1	O4-C1-S44	-2.23	119.84	122.68
50	G	201	8Q1	C43-S44-C1	2.20	108.35	101.84
50	X	201	8Q1	C42-N41-C39	-2.20	118.73	122.82
50	G	201	8Q1	C38-C39-N41	2.16	120.28	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	502	FMN	C9A-C5A-N5	-2.10	120.22	122.45
46	A	502	FMN	C4A-C10-N1	-2.09	119.46	124.59
50	X	201	8Q1	C32-C34-N36	2.08	120.44	116.48
52	J	401	NDP	P2B-O2B-C2B	-2.07	117.92	123.43
49	C	304	UQ	C6-C5-C4	2.02	120.76	119.17
49	C	304	UQ	C20-C19-C21	-2.02	111.73	115.23
48	j	201	PLX	C2-C1-N1	-2.01	109.36	115.82
47	Q	501	PEE	C2-O2-C10	-2.01	112.98	117.80

There are no chirality outliers.

All (1020) 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	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
47	B	303	PEE	C11-C10-O2-C2
47	C	302	PEE	C11-C10-O2-C2
47	C	302	PEE	C1-O3P-P-O2P
47	C	302	PEE	C1-O3P-P-O1P
47	C	302	PEE	C1-O3P-P-O4P
47	Q	501	PEE	C11-C10-O2-C2
47	U	101	PEE	C1-O3P-P-O2P
47	U	101	PEE	C1-O3P-P-O1P
47	U	101	PEE	C1-O3P-P-O4P
47	W	201	PEE	C4-O4P-P-O3P
47	W	201	PEE	C4-O4P-P-O2P
47	W	201	PEE	C4-O4P-P-O1P
47	l	701	PEE	C11-C10-O2-C2
47	l	701	PEE	C1-O3P-P-O2P
47	l	701	PEE	C1-O3P-P-O1P
47	l	701	PEE	C1-O3P-P-O4P
47	l	701	PEE	C4-O4P-P-O3P
47	l	701	PEE	C4-O4P-P-O2P
47	l	701	PEE	C4-O4P-P-O1P
47	l	704	PEE	O3P-C1-C2-O2
47	r	501	PEE	C1-O3P-P-O1P
47	r	501	PEE	C1-O3P-P-O4P
47	s	401	PEE	C4-O4P-P-O2P
48	C	303	PLX	N1-C1-C2-O1
48	C	303	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
48	N	201	PLX	O7-C6-O6-C4
48	N	201	PLX	C2-O1-P1-O4
48	N	201	PLX	C2-O1-P1-O2
48	N	201	PLX	C2-O1-P1-O3
48	N	201	PLX	O9-C24-O8-C5
48	g	201	PLX	C2-O1-P1-O4
48	g	201	PLX	C2-O1-P1-O3
48	j	201	PLX	O7-C6-O6-C4
48	j	201	PLX	C3-O4-P1-O1
48	j	201	PLX	C3-O4-P1-O3
48	j	201	PLX	O9-C24-C25-C26
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	C25-C24-O8-C5
48	n	101	PLX	C3-O4-P1-O1
48	n	101	PLX	C3-O4-P1-O3
48	r	502	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O2
49	C	304	UQ	C12-C13-C14-C16
49	C	304	UQ	C16-C17-C18-C19
49	C	304	UQ	C17-C18-C19-C20
49	C	304	UQ	C17-C18-C19-C21
49	C	304	UQ	C22-C23-C24-C26
49	C	304	UQ	C27-C28-C29-C31
49	C	304	UQ	C37-C38-C39-C40
49	C	304	UQ	C42-C43-C44-C45
49	C	304	UQ	C42-C43-C44-C46
49	C	304	UQ	C47-C48-C49-C51
49	J	402	UQ	C7-C8-C9-C10
49	J	402	UQ	C12-C13-C14-C15
49	J	402	UQ	C12-C13-C14-C16
49	J	402	UQ	C14-C16-C17-C18
49	J	402	UQ	C17-C18-C19-C21
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	C42-C43-S44-C1
50	G	201	8Q1	C28-O27-P24-O3
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C42-C43-S44-C1
51	I	201	CDL	CB2-C1-CA2-OA2
51	I	201	CDL	O1-C1-CB2-OB2
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA3
51	I	201	CDL	CB2-OB2-PB2-OB3
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB3
51	V	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA2-OA2-PA1-OA5
51	V	201	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	CB2-OB2-PB2-OB3
51	V	201	CDL	CB2-OB2-PB2-OB5
51	V	201	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	CB3-OB5-PB2-OB3
51	V	201	CDL	CB3-OB5-PB2-OB4
51	V	202	CDL	CA3-OA5-PA1-OA2
51	V	202	CDL	CA3-OA5-PA1-OA3
51	V	202	CDL	CB2-OB2-PB2-OB3
51	V	202	CDL	C51-CB5-OB6-CB4
51	a	201	CDL	O1-C1-CA2-OA2
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	OB7-CB5-OB6-CB4
51	l	702	CDL	O1-C1-CA2-OA2
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CB3-OB5-PB2-OB2
51	l	702	CDL	CB3-OB5-PB2-OB3
51	l	703	CDL	CA2-OA2-PA1-OA4
51	l	703	CDL	CA2-OA2-PA1-OA5
51	l	703	CDL	CA3-OA5-PA1-OA2
51	l	703	CDL	CA3-OA5-PA1-OA4
51	l	703	CDL	CB2-OB2-PB2-OB3
51	l	703	CDL	CB2-OB2-PB2-OB4
51	l	703	CDL	CB2-OB2-PB2-OB5
51	m	201	CDL	CB2-C1-CA2-OA2
51	m	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	CA2-OA2-PA1-OA4
51	m	201	CDL	CA2-OA2-PA1-OA5
51	m	201	CDL	CA3-OA5-PA1-OA2
51	m	201	CDL	CA3-OA5-PA1-OA3
51	m	201	CDL	CB3-OB5-PB2-OB2
51	m	201	CDL	CB3-OB5-PB2-OB3
51	m	201	CDL	CB3-OB5-PB2-OB4
51	n	102	CDL	O1-C1-CB2-OB2
51	n	102	CDL	CA2-C1-CB2-OB2
51	n	102	CDL	CA2-OA2-PA1-OA5
51	r	503	CDL	CA2-OA2-PA1-OA3
51	r	503	CDL	CA2-OA2-PA1-OA5
51	r	503	CDL	CA3-OA5-PA1-OA2
51	r	503	CDL	CA3-OA5-PA1-OA3
51	r	503	CDL	CB2-OB2-PB2-OB3
51	r	503	CDL	CB2-OB2-PB2-OB4
51	r	503	CDL	CB2-OB2-PB2-OB5
51	r	503	CDL	CB3-OB5-PB2-OB2
51	r	503	CDL	CB3-OB5-PB2-OB3
51	r	503	CDL	CB3-OB5-PB2-OB4
51	r	503	CDL	C51-CB5-OB6-CB4
51	s	402	CDL	CB2-C1-CA2-OA2
51	s	402	CDL	CA2-OA2-PA1-OA3
51	s	402	CDL	CA2-OA2-PA1-OA4
51	s	402	CDL	CA2-OA2-PA1-OA5
51	s	402	CDL	CB3-OB5-PB2-OB2
51	s	402	CDL	CB3-OB5-PB2-OB4
51	s	402	CDL	OB6-CB4-CB6-OB8
52	J	401	NDP	O4D-C1D-N1N-C6N
56	w	401	ADP	C5'-O5'-PA-O2A
51	s	402	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	OA9-CA7-OA8-CA6
47	B	303	PEE	O4-C10-O2-C2
47	C	302	PEE	O4-C10-O2-C2
47	Q	501	PEE	O4-C10-O2-C2
47	l	701	PEE	O4-C10-O2-C2
47	l	704	PEE	O4-C10-O2-C2
51	V	201	CDL	OA7-CA5-OA6-CA4
51	V	202	CDL	OB7-CB5-OB6-CB4
51	r	503	CDL	OB7-CB5-OB6-CB4
49	J	402	UQ	C22-C23-C24-C26
51	s	402	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
47	l	704	PEE	C11-C10-O2-C2
51	a	201	CDL	C51-CB5-OB6-CB4
47	l	704	PEE	O5-C30-O3-C3
51	V	201	CDL	C71-CB7-OB8-CB6
51	l	702	CDL	C31-CA7-OA8-CA6
49	C	304	UQ	C7-C8-C9-C10
49	C	304	UQ	C27-C28-C29-C30
47	U	101	PEE	C17-C18-C19-C20
49	J	402	UQ	C7-C8-C9-C11
47	Q	501	PEE	O5-C30-O3-C3
51	s	402	CDL	OB7-CB5-OB6-CB4
51	I	201	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CB2-OB2
51	l	703	CDL	O1-C1-CA2-OA2
51	l	703	CDL	O1-C1-CB2-OB2
51	r	503	CDL	O1-C1-CA2-OA2
51	s	402	CDL	O1-C1-CA2-OA2
51	s	402	CDL	O1-C1-CB2-OB2
47	l	704	PEE	C31-C30-O3-C3
47	U	101	PEE	C11-C10-O2-C2
47	l	705	PEE	C11-C10-O2-C2
51	m	201	CDL	C11-CA5-OA6-CA4
51	s	402	CDL	C51-CB5-OB6-CB4
47	Q	501	PEE	C31-C30-O3-C3
49	J	402	UQ	C12-C11-C9-C10
49	J	402	UQ	C15-C14-C16-C17
47	U	101	PEE	O4-C10-O2-C2
49	J	402	UQ	C9-C11-C12-C13
49	J	402	UQ	C19-C21-C22-C23
51	n	102	CDL	C1-CB2-OB2-PB2
51	V	201	CDL	OB9-CB7-OB8-CB6
49	C	304	UQ	C47-C48-C49-C50
47	B	303	PEE	C17-C18-C19-C20
47	W	201	PEE	C17-C18-C19-C20
47	l	705	PEE	C37-C38-C39-C40
51	m	201	CDL	C73-C74-C75-C76
49	C	304	UQ	C52-C53-C54-C55
51	r	503	CDL	C74-C75-C76-C77
47	l	705	PEE	O4-C10-O2-C2
51	m	201	CDL	OA7-CA5-OA6-CA4
51	I	201	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	CB2-C1-CA2-OA2
51	r	503	CDL	CB2-C1-CA2-OA2
51	s	402	CDL	CA2-C1-CB2-OB2
47	U	101	PEE	C31-C30-O3-C3
47	W	201	PEE	C31-C30-O3-C3
47	l	701	PEE	C31-C30-O3-C3
51	n	102	CDL	C74-C75-C76-C77
48	C	303	PLX	C9-C10-C11-C12
48	g	201	PLX	C9-C10-C11-C12
51	V	201	CDL	C32-C33-C34-C35
51	V	201	CDL	C59-C60-C61-C62
51	V	202	CDL	C11-C12-C13-C14
51	V	202	CDL	C32-C33-C34-C35
48	g	201	PLX	C2-C1-N1-C1A
51	s	402	CDL	C37-C38-C39-C40
49	C	304	UQ	C43-C44-C46-C47
49	C	304	UQ	C48-C49-C51-C52
49	J	402	UQ	C18-C19-C21-C22
48	g	201	PLX	C7-C8-C9-C10
51	l	702	CDL	C55-C56-C57-C58
48	C	303	PLX	C33-C34-C35-C36
48	j	202	PLX	C13-C14-C15-C16
51	V	202	CDL	CB7-C71-C72-C73
47	U	101	PEE	O5-C30-O3-C3
51	V	201	CDL	C62-C63-C64-C65
51	I	201	CDL	OA5-CA3-CA4-OA6
51	m	201	CDL	OA5-CA3-CA4-OA6
48	g	201	PLX	O6-C4-C5-O8
51	l	702	CDL	CA7-C31-C32-C33
51	l	703	CDL	C35-C36-C37-C38
47	l	701	PEE	C17-C18-C19-C20
51	a	201	CDL	CA5-C11-C12-C13
49	C	304	UQ	C32-C33-C34-C36
47	l	701	PEE	O5-C30-O3-C3
51	l	702	CDL	C34-C35-C36-C37
51	l	703	CDL	C71-CB7-OB8-CB6
51	l	702	CDL	C58-C59-C60-C61
51	l	702	CDL	CB5-C51-C52-C53
51	l	702	CDL	CB7-C71-C72-C73
49	C	304	UQ	C34-C36-C37-C38
48	N	201	PLX	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
48	g	201	PLX	C2-C1-N1-C1B
51	r	503	CDL	CA5-C11-C12-C13
51	s	402	CDL	CA7-C31-C32-C33
51	I	201	CDL	CB7-C71-C72-C73
51	a	201	CDL	CA7-C31-C32-C33
51	l	703	CDL	CB7-C71-C72-C73
51	l	702	CDL	C16-C17-C18-C19
51	l	702	CDL	C32-C33-C34-C35
51	s	402	CDL	C14-C15-C16-C17
47	U	101	PEE	C30-C31-C32-C33
51	s	402	CDL	CB7-C71-C72-C73
47	l	704	PEE	C37-C38-C39-C40
47	W	201	PEE	O5-C30-O3-C3
51	l	703	CDL	C17-C18-C19-C20
51	l	702	CDL	C71-CB7-OB8-CB6
47	l	701	PEE	C10-C11-C12-C13
51	l	703	CDL	OB9-CB7-OB8-CB6
51	l	703	CDL	CA2-C1-CB2-OB2
47	l	705	PEE	C31-C30-O3-C3
51	V	202	CDL	C71-CB7-OB8-CB6
51	m	201	CDL	C36-C37-C38-C39
51	V	201	CDL	C31-CA7-OA8-CA6
49	C	304	UQ	C25-C24-C26-C27
48	j	201	PLX	O8-C24-C25-C26
48	n	101	PLX	O8-C24-C25-C26
47	W	201	PEE	C11-C10-O2-C2
51	V	201	CDL	C51-CB5-OB6-CB4
47	W	201	PEE	O4-C10-O2-C2
51	m	201	CDL	O1-C1-CA2-OA2
51	a	201	CDL	C71-CB7-OB8-CB6
51	m	201	CDL	CA4-CA3-OA5-PA1
51	V	202	CDL	OB9-CB7-OB8-CB6
51	l	703	CDL	C51-C52-C53-C54
47	r	501	PEE	C10-C11-C12-C13
51	r	503	CDL	C60-C61-C62-C63
51	I	201	CDL	C11-C12-C13-C14
51	V	201	CDL	OB7-CB5-OB6-CB4
51	s	402	CDL	C31-C32-C33-C34
48	C	303	PLX	O6-C4-C5-O8
51	V	202	CDL	C72-C73-C74-C75
51	s	402	CDL	C33-C34-C35-C36
51	l	702	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C11-C12-C13-C14
47	r	501	PEE	C13-C14-C15-C16
47	r	501	PEE	C40-C41-C42-C43
48	C	303	PLX	C25-C26-C27-C28
48	N	201	PLX	C14-C15-C16-C17
48	N	201	PLX	C29-C30-C31-C32
51	V	201	CDL	C37-C38-C39-C40
51	V	202	CDL	C14-C15-C16-C17
51	a	201	CDL	C17-C18-C19-C20
51	l	702	CDL	C14-C15-C16-C17
51	l	703	CDL	C55-C56-C57-C58
51	s	402	CDL	C75-C76-C77-C78
47	r	501	PEE	C17-C18-C19-C20
47	s	401	PEE	C23-C24-C25-C26
48	g	201	PLX	C27-C28-C29-C30
48	j	201	PLX	C30-C31-C32-C33
48	j	201	PLX	C31-C32-C33-C34
48	r	502	PLX	C13-C14-C15-C16
51	a	201	CDL	C75-C76-C77-C78
51	r	503	CDL	C57-C58-C59-C60
48	C	303	PLX	O7-C6-C7-C8
48	C	303	PLX	O9-C24-C25-C26
48	g	201	PLX	O9-C24-C25-C26
48	r	502	PLX	O9-C24-C25-C26
47	l	705	PEE	C31-C32-C33-C34
48	j	201	PLX	C7-C8-C9-C10
48	j	201	PLX	C28-C29-C30-C31
48	j	202	PLX	C31-C32-C33-C34
48	r	502	PLX	C25-C26-C27-C28
51	V	201	CDL	C74-C75-C76-C77
51	m	201	CDL	C32-C33-C34-C35
51	m	201	CDL	C60-C61-C62-C63
51	r	503	CDL	C32-C33-C34-C35
47	s	401	PEE	C13-C14-C15-C16
48	g	201	PLX	C11-C12-C13-C14
51	V	202	CDL	C33-C34-C35-C36
51	a	201	CDL	C62-C63-C64-C65
51	l	702	CDL	C75-C76-C77-C78
51	r	503	CDL	C11-C12-C13-C14
51	I	201	CDL	CA7-C31-C32-C33
51	l	702	CDL	C11-C12-C13-C14
47	W	201	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C59-C60-C61-C62
51	a	201	CDL	C33-C34-C35-C36
47	r	501	PEE	C11-C10-O2-C2
51	V	202	CDL	O1-C1-CA2-OA2
52	J	401	NDP	C3B-C4B-C5B-O5B
47	U	101	PEE	C23-C24-C25-C26
48	g	201	PLX	C25-C26-C27-C28
51	V	201	CDL	C31-C32-C33-C34
51	V	201	CDL	C33-C34-C35-C36
51	a	201	CDL	C60-C61-C62-C63
51	a	201	CDL	C73-C74-C75-C76
51	r	503	CDL	C35-C36-C37-C38
47	l	705	PEE	O5-C30-O3-C3
51	V	201	CDL	C52-C53-C54-C55
51	l	702	CDL	C71-C72-C73-C74
48	C	303	PLX	C17-C18-C19-C20
48	n	101	PLX	C27-C28-C29-C30
47	l	705	PEE	C22-C23-C24-C25
48	g	201	PLX	C32-C33-C34-C35
51	m	201	CDL	C55-C56-C57-C58
51	l	702	CDL	CB2-C1-CA2-OA2
51	s	402	CDL	C71-CB7-OB8-CB6
48	n	101	PLX	C3-C4-C5-O8
51	m	201	CDL	CB3-CB4-CB6-OB8
48	C	303	PLX	C27-C28-C29-C30
48	n	101	PLX	C13-C14-C15-C16
48	r	502	PLX	C10-C11-C12-C13
50	G	201	8Q1	C12-C13-C14-C15
51	V	202	CDL	C35-C36-C37-C38
51	V	202	CDL	CA7-C31-C32-C33
47	l	704	PEE	C31-C32-C33-C34
47	l	705	PEE	C33-C34-C35-C36
48	g	201	PLX	C13-C14-C15-C16
48	j	201	PLX	C13-C14-C15-C16
48	j	201	PLX	C9-C10-C11-C12
48	j	202	PLX	C7-C8-C9-C10
48	n	101	PLX	C10-C11-C12-C13
48	n	101	PLX	C31-C32-C33-C34
48	r	502	PLX	C30-C31-C32-C33
51	l	702	CDL	C18-C19-C20-C21
51	l	702	CDL	C52-C53-C54-C55
51	l	702	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	C14-C15-C16-C17
51	V	201	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	OB9-CB7-OB8-CB6
48	C	303	PLX	C11-C12-C13-C14
48	j	202	PLX	C28-C29-C30-C31
48	n	101	PLX	C14-C15-C16-C17
48	r	502	PLX	C27-C28-C29-C30
51	V	202	CDL	C37-C38-C39-C40
51	m	201	CDL	C14-C15-C16-C17
51	r	503	CDL	C62-C63-C64-C65
47	W	201	PEE	C13-C14-C15-C16
51	m	201	CDL	C13-C14-C15-C16
48	g	201	PLX	C2-C1-N1-C1C
47	r	501	PEE	C31-C32-C33-C34
51	m	201	CDL	C34-C35-C36-C37
48	C	303	PLX	C7-C8-C9-C10
48	N	201	PLX	C27-C28-C29-C30
48	j	202	PLX	C16-C17-C18-C19
47	r	501	PEE	C39-C40-C41-C42
51	m	201	CDL	C75-C76-C77-C78
51	s	402	CDL	C71-C72-C73-C74
51	s	402	CDL	C73-C74-C75-C76
47	l	701	PEE	C11-C12-C13-C14
48	C	303	PLX	C14-C15-C16-C17
50	X	201	8Q1	C10-C11-C12-C13
51	m	201	CDL	C59-C60-C61-C62
51	n	102	CDL	C71-C72-C73-C74
51	V	202	CDL	C42-C43-C44-C45
51	V	202	CDL	C82-C83-C84-C85
51	l	703	CDL	C79-C80-C81-C82
47	C	302	PEE	C42-C43-C44-C45
48	n	101	PLX	C9-C10-C11-C12
47	r	501	PEE	O4-C10-O2-C2
48	j	202	PLX	C14-C15-C16-C17
47	Q	501	PEE	C21-C22-C23-C24
48	g	201	PLX	C14-C15-C16-C17
48	j	201	PLX	C32-C33-C34-C35
48	j	202	PLX	C25-C26-C27-C28
50	X	201	8Q1	C11-C12-C13-C14
51	V	202	CDL	C74-C75-C76-C77
51	l	703	CDL	C11-C12-C13-C14
51	l	703	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	C79-C80-C81-C82
48	N	201	PLX	C33-C34-C35-C36
48	j	202	PLX	C33-C34-C35-C36
48	r	502	PLX	C11-C10-C9-C8
51	r	503	CDL	C41-C42-C43-C44
51	s	402	CDL	C82-C83-C84-C85
48	j	201	PLX	C11-C12-C13-C14
51	r	503	CDL	C75-C76-C77-C78
51	s	402	CDL	C52-C53-C54-C55
51	s	402	CDL	C17-C18-C19-C20
51	s	402	CDL	CB5-C51-C52-C53
49	J	402	UQ	C11-C12-C13-C14
47	W	201	PEE	C12-C13-C14-C15
51	V	202	CDL	C52-C53-C54-C55
51	n	102	CDL	C52-C53-C54-C55
51	n	102	CDL	C55-C56-C57-C58
48	g	201	PLX	C28-C29-C30-C31
48	j	202	PLX	C9-C10-C11-C12
51	V	202	CDL	C75-C76-C77-C78
51	a	201	CDL	C37-C38-C39-C40
47	s	401	PEE	C11-C10-O2-C2
51	l	702	CDL	C51-CB5-OB6-CB4
51	V	202	CDL	C17-C18-C19-C20
51	r	503	CDL	C31-C32-C33-C34
51	r	503	CDL	C43-C44-C45-C46
47	s	401	PEE	O4-C10-O2-C2
51	a	201	CDL	C31-C32-C33-C34
51	m	201	CDL	C61-C62-C63-C64
47	Q	501	PEE	C19-C20-C21-C22
47	W	201	PEE	C15-C16-C17-C18
51	r	503	CDL	C14-C15-C16-C17
48	j	202	PLX	C12-C13-C14-C15
51	s	402	CDL	OB9-CB7-OB8-CB6
48	r	502	PLX	C14-C15-C16-C17
51	l	702	CDL	C74-C75-C76-C77
51	l	702	CDL	C35-C36-C37-C38
47	B	303	PEE	C10-C11-C12-C13
51	V	202	CDL	CB5-C51-C52-C53
51	r	503	CDL	CA7-C31-C32-C33
51	l	702	CDL	C62-C63-C64-C65
51	m	201	CDL	C11-C12-C13-C14
47	W	201	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OB5-CB3-CB4-OB6
48	N	201	PLX	C10-C11-C12-C13
48	j	201	PLX	C14-C15-C16-C17
48	g	201	PLX	C12-C13-C14-C15
51	V	201	CDL	C34-C35-C36-C37
51	a	201	CDL	C38-C39-C40-C41
51	V	202	CDL	C73-C74-C75-C76
51	r	503	CDL	C71-C72-C73-C74
48	n	101	PLX	O6-C4-C5-O8
51	V	202	CDL	OA6-CA4-CA6-OA8
51	l	703	CDL	OA6-CA4-CA6-OA8
51	m	201	CDL	OB6-CB4-CB6-OB8
47	B	303	PEE	C31-C32-C33-C34
48	g	201	PLX	C30-C31-C32-C33
51	V	201	CDL	C55-C56-C57-C58
51	V	201	CDL	C58-C59-C60-C61
51	a	201	CDL	C52-C53-C54-C55
51	a	201	CDL	C71-C72-C73-C74
51	l	702	CDL	C59-C60-C61-C62
51	l	703	CDL	C37-C38-C39-C40
51	m	201	CDL	C71-C72-C73-C74
47	B	303	PEE	C36-C37-C38-C39
47	r	501	PEE	C36-C37-C38-C39
51	l	702	CDL	C56-C57-C58-C59
48	g	201	PLX	C33-C34-C35-C36
48	j	201	PLX	C25-C26-C27-C28
48	j	202	PLX	C27-C28-C29-C30
51	V	201	CDL	C71-C72-C73-C74
51	a	201	CDL	C15-C16-C17-C18
51	l	703	CDL	C59-C60-C61-C62
51	V	202	CDL	CB2-C1-CA2-OA2
47	r	501	PEE	C21-C22-C23-C24
51	l	703	CDL	C82-C83-C84-C85
48	j	202	PLX	C29-C30-C31-C32
48	j	201	PLX	C33-C34-C35-C36
51	r	503	CDL	C37-C38-C39-C40
47	l	704	PEE	C11-C12-C13-C14
48	r	502	PLX	C28-C29-C30-C31
51	l	703	CDL	C31-C32-C33-C34
50	X	201	8Q1	O33-C32-C34-O35
47	l	704	PEE	C43-C44-C45-C46
47	r	501	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	C25-C26-C27-C28
51	l	703	CDL	C32-C33-C34-C35
51	m	201	CDL	C37-C38-C39-C40
51	a	201	CDL	C21-C22-C23-C24
47	s	401	PEE	C19-C20-C21-C22
51	V	201	CDL	C14-C15-C16-C17
51	l	702	CDL	C37-C38-C39-C40
51	s	402	CDL	C51-C52-C53-C54
47	C	302	PEE	O3P-C1-C2-C3
47	Q	501	PEE	O3P-C1-C2-C3
47	l	704	PEE	O3P-C1-C2-C3
51	V	201	CDL	OB5-CB3-CB4-CB6
51	r	503	CDL	C73-C74-C75-C76
52	J	401	NDP	O4B-C4B-C5B-O5B
47	W	201	PEE	C24-C25-C26-C27
51	l	703	CDL	C51-CB5-OB6-CB4
48	n	101	PLX	C7-C8-C9-C10
51	V	202	CDL	C13-C14-C15-C16
47	C	302	PEE	C1-C2-C3-O3
47	W	201	PEE	C1-C2-C3-O3
47	l	705	PEE	C1-C2-C3-O3
48	g	201	PLX	C3-C4-C5-O8
48	j	201	PLX	C3-C4-C5-O8
48	j	202	PLX	C3-C4-C5-O8
51	I	201	CDL	CA3-CA4-CA6-OA8
51	s	402	CDL	C55-C56-C57-C58
48	j	202	PLX	C11-C12-C13-C14
51	m	201	CDL	C16-C17-C18-C19
51	m	201	CDL	C71-CB7-OB8-CB6
51	r	503	CDL	C71-CB7-OB8-CB6
47	l	704	PEE	C30-C31-C32-C33
48	j	201	PLX	C27-C28-C29-C30
51	l	703	CDL	C74-C75-C76-C77
51	m	201	CDL	C18-C19-C20-C21
48	C	303	PLX	C18-C19-C20-C21
47	r	501	PEE	C14-C15-C16-C17
51	l	703	CDL	CA7-C31-C32-C33
49	C	304	UQ	C13-C14-C16-C17
48	C	303	PLX	C10-C11-C12-C13
48	N	201	PLX	C28-C29-C30-C31
51	V	202	CDL	C62-C63-C64-C65
51	l	703	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
51	m	201	CDL	C17-C18-C19-C20
51	s	402	CDL	C54-C55-C56-C57
51	l	703	CDL	C75-C76-C77-C78
51	s	402	CDL	C35-C36-C37-C38
47	s	401	PEE	C22-C23-C24-C25
48	N	201	PLX	C7-C8-C9-C10
51	s	402	CDL	C59-C60-C61-C62
51	m	201	CDL	CA6-CA4-OA6-CA5
48	N	201	PLX	C25-C26-C27-C28
51	m	201	CDL	C33-C34-C35-C36
51	n	102	CDL	C73-C74-C75-C76
51	s	402	CDL	C36-C37-C38-C39
49	C	304	UQ	C52-C53-C54-C56
47	B	303	PEE	C35-C36-C37-C38
47	B	303	PEE	C39-C40-C41-C42
47	l	701	PEE	C35-C36-C37-C38
51	a	201	CDL	C11-C12-C13-C14
47	W	201	PEE	C10-C11-C12-C13
51	a	201	CDL	CA2-C1-CB2-OB2
47	l	705	PEE	O3P-C1-C2-O2
47	s	401	PEE	O3P-C1-C2-O2
48	r	502	PLX	C18-C19-C20-C21
51	l	702	CDL	C63-C64-C65-C66
48	g	201	PLX	C10-C11-C12-C13
51	l	703	CDL	C61-C62-C63-C64
51	s	402	CDL	C40-C41-C42-C43
47	s	401	PEE	C31-C32-C33-C34
48	r	502	PLX	C11-C12-C13-C14
51	r	503	CDL	C83-C84-C85-C86
51	n	102	CDL	C75-C76-C77-C78
51	V	202	CDL	C41-C42-C43-C44
51	m	201	CDL	C19-C20-C21-C22
48	n	101	PLX	C29-C30-C31-C32
47	l	704	PEE	O2-C2-C3-O3
47	l	705	PEE	O2-C2-C3-O3
51	V	201	CDL	C72-C73-C74-C75
51	r	503	CDL	C42-C43-C44-C45
47	B	303	PEE	C34-C35-C36-C37
50	X	201	8Q1	C6-C7-C8-C9
51	m	201	CDL	C52-C53-C54-C55
51	V	202	CDL	C64-C65-C66-C67
51	V	202	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
47	U	101	PEE	C36-C37-C38-C39
48	N	201	PLX	C12-C13-C14-C15
47	l	704	PEE	C19-C20-C21-C22
50	G	201	8Q1	C30-C29-C32-O33
47	l	701	PEE	C32-C33-C34-C35
51	I	201	CDL	C71-C72-C73-C74
51	r	503	CDL	C84-C85-C86-C87
47	r	501	PEE	C11-C12-C13-C14
51	a	201	CDL	C36-C37-C38-C39
51	r	503	CDL	CB7-C71-C72-C73
47	B	303	PEE	C42-C43-C44-C45
51	r	503	CDL	C64-C65-C66-C67
47	B	303	PEE	C31-C30-O3-C3
47	C	302	PEE	C32-C33-C34-C35
47	s	401	PEE	C14-C15-C16-C17
48	C	303	PLX	C30-C31-C32-C33
48	r	502	PLX	C31-C32-C33-C34
51	r	503	CDL	C54-C55-C56-C57
51	r	503	CDL	C77-C78-C79-C80
47	U	101	PEE	C38-C39-C40-C41
47	U	101	PEE	C34-C35-C36-C37
51	V	202	CDL	C34-C35-C36-C37
51	r	503	CDL	C1-CB2-OB2-PB2
47	l	705	PEE	C13-C14-C15-C16
47	s	401	PEE	C11-C12-C13-C14
51	V	201	CDL	C54-C55-C56-C57
51	a	201	CDL	C32-C33-C34-C35
47	r	501	PEE	O3P-C1-C2-C3
51	I	201	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	OB5-CB3-CB4-CB6
51	m	201	CDL	OA5-CA3-CA4-CA6
51	r	503	CDL	CB5-C51-C52-C53
51	m	201	CDL	OB9-CB7-OB8-CB6
51	r	503	CDL	OB9-CB7-OB8-CB6
51	m	201	CDL	C84-C85-C86-C87
47	Q	501	PEE	C34-C35-C36-C37
48	g	201	PLX	C11-C10-C9-C8
51	m	201	CDL	C20-C21-C22-C23
51	m	201	CDL	C15-C16-C17-C18
51	l	702	CDL	OB7-CB5-OB6-CB4
47	B	303	PEE	C12-C13-C14-C15
47	Q	501	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
48	n	101	PLX	C26-C27-C28-C29
47	Q	501	PEE	C1-C2-C3-O3
47	r	501	PEE	C1-C2-C3-O3
48	C	303	PLX	C3-C4-C5-O8
51	l	703	CDL	CA3-CA4-CA6-OA8
51	n	102	CDL	CA3-CA4-CA6-OA8
51	l	702	CDL	C36-C37-C38-C39
51	l	702	CDL	C24-C25-C26-C27
51	r	503	CDL	C33-C34-C35-C36
48	n	101	PLX	C28-C29-C30-C31
51	V	202	CDL	C40-C41-C42-C43
51	l	703	CDL	C62-C63-C64-C65
51	a	201	CDL	C22-C23-C24-C25
47	U	101	PEE	O3P-C1-C2-O2
48	N	201	PLX	O4-C3-C4-O6
48	n	101	PLX	O4-C3-C4-O6
51	l	702	CDL	OB5-CB3-CB4-OB6
51	m	201	CDL	OB5-CB3-CB4-OB6
47	l	701	PEE	C14-C15-C16-C17
48	N	201	PLX	C16-C17-C18-C19
51	V	201	CDL	C1-CB2-OB2-PB2
51	a	201	CDL	C35-C36-C37-C38
51	m	201	CDL	C35-C36-C37-C38
48	j	201	PLX	C34-C35-C36-C37
51	s	402	CDL	C84-C85-C86-C87
51	V	201	CDL	C21-C22-C23-C24
51	m	201	CDL	C41-C42-C43-C44
51	s	402	CDL	C34-C35-C36-C37
48	r	502	PLX	O6-C4-C5-O8
51	I	201	CDL	OA6-CA4-CA6-OA8
51	n	102	CDL	OA6-CA4-CA6-OA8
51	a	201	CDL	C84-C85-C86-C87
51	l	703	CDL	C44-C45-C46-C47
51	l	703	CDL	C12-C13-C14-C15
49	C	304	UQ	C12-C11-C9-C8
47	B	303	PEE	C38-C39-C40-C41
48	C	303	PLX	O8-C24-C25-C26
48	j	202	PLX	O6-C6-C7-C8
48	j	201	PLX	C35-C36-C37-C38
47	l	704	PEE	C21-C22-C23-C24
51	V	202	CDL	C24-C25-C26-C27
48	N	201	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
47	B	303	PEE	C23-C24-C25-C26
48	n	101	PLX	C16-C17-C18-C19
48	n	101	PLX	C11-C12-C13-C14
51	a	201	CDL	C82-C83-C84-C85
51	m	201	CDL	C82-C83-C84-C85
47	Q	501	PEE	C18-C19-C20-C21
47	r	501	PEE	C38-C39-C40-C41
47	r	501	PEE	C15-C16-C17-C18
48	C	303	PLX	C36-C37-C38-C39
47	W	201	PEE	O3P-C1-C2-C3
47	l	705	PEE	O3P-C1-C2-C3
48	n	101	PLX	O4-C3-C4-C5
51	I	201	CDL	OB5-CB3-CB4-CB6
47	r	501	PEE	C20-C21-C22-C23
51	m	201	CDL	C39-C40-C41-C42
48	n	101	PLX	C30-C31-C32-C33
51	r	503	CDL	C59-C60-C61-C62
47	Q	501	PEE	C24-C25-C26-C27
51	l	703	CDL	C12-C11-CA5-OA6
48	j	201	PLX	C10-C11-C12-C13
51	I	201	CDL	C52-C53-C54-C55
47	C	302	PEE	C43-C44-C45-C46
51	l	703	CDL	OB7-CB5-OB6-CB4
51	m	201	CDL	C64-C65-C66-C67
47	B	303	PEE	O5-C30-O3-C3
51	l	703	CDL	C64-C65-C66-C67
51	I	201	CDL	C71-CB7-OB8-CB6
47	Q	501	PEE	O3P-C1-C2-O2
47	l	701	PEE	O3P-C1-C2-O2
48	r	502	PLX	O4-C3-C4-O6
51	I	201	CDL	OB5-CB3-CB4-OB6
51	V	201	CDL	OA5-CA3-CA4-OA6
47	s	401	PEE	C12-C13-C14-C15
48	r	502	PLX	C3-C4-C5-O8
51	V	202	CDL	CA3-CA4-CA6-OA8
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-C34
48	j	201	PLX	C11-C10-C9-C8
51	m	201	CDL	C43-C44-C45-C46
51	V	201	CDL	C75-C76-C77-C78
47	C	302	PEE	O2-C2-C3-O3
47	Q	501	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	OB6-CB4-CB6-OB8
47	l	704	PEE	C32-C33-C34-C35
48	C	303	PLX	C35-C36-C37-C38
51	l	702	CDL	C21-C22-C23-C24
48	j	201	PLX	N1-C1-C2-O1
48	r	502	PLX	C7-C8-C9-C10
51	a	201	CDL	O1-C1-CB2-OB2
48	j	201	PLX	C12-C13-C14-C15
48	C	303	PLX	C13-C14-C15-C16
51	n	102	CDL	C54-C55-C56-C57
51	I	201	CDL	OB9-CB7-OB8-CB6
48	j	201	PLX	C26-C27-C28-C29
51	r	503	CDL	C51-C52-C53-C54
48	g	201	PLX	C31-C32-C33-C34
47	l	701	PEE	C13-C14-C15-C16
48	g	201	PLX	C25-C24-O8-C5
51	n	102	CDL	C71-CB7-OB8-CB6
47	l	705	PEE	C23-C24-C25-C26
47	Q	501	PEE	C11-C12-C13-C14
51	V	202	CDL	C71-C72-C73-C74
52	J	401	NDP	C2D-C1D-N1N-C2N
47	U	101	PEE	O3P-C1-C2-C3
47	l	701	PEE	O3P-C1-C2-C3
47	s	401	PEE	O3P-C1-C2-C3
48	N	201	PLX	O4-C3-C4-C5
48	r	502	PLX	O4-C3-C4-C5
51	V	201	CDL	OA5-CA3-CA4-CA6
51	a	201	CDL	OB5-CB3-CB4-CB6
50	X	201	8Q1	C28-C29-C32-C34
52	J	401	NDP	O4D-C4D-C5D-O5D
51	n	102	CDL	OB9-CB7-OB8-CB6
47	C	302	PEE	O3P-C1-C2-O2
47	r	501	PEE	O3P-C1-C2-O2
51	a	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	OB5-CB3-CB4-OB6
51	l	703	CDL	OA5-CA3-CA4-OA6
51	l	703	CDL	OB5-CB3-CB4-OB6
51	I	201	CDL	C51-C52-C53-C54
48	r	502	PLX	C34-C35-C36-C37
51	l	702	CDL	C82-C83-C84-C85
47	Q	501	PEE	C10-C11-C12-C13
47	r	501	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
48	j	201	PLX	O6-C4-C5-O8
48	j	202	PLX	O6-C4-C5-O8
51	r	503	CDL	C56-C57-C58-C59
50	X	201	8Q1	C13-C14-C15-C16
47	l	704	PEE	C1-C2-C3-O3
51	m	201	CDL	CA3-CA4-CA6-OA8
51	s	402	CDL	CB3-CB4-CB6-OB8
47	l	704	PEE	C34-C35-C36-C37
51	m	201	CDL	C58-C59-C60-C61
51	m	201	CDL	C62-C63-C64-C65
47	U	101	PEE	C24-C25-C26-C27
48	r	502	PLX	C36-C37-C38-C39
51	l	703	CDL	C73-C74-C75-C76
47	C	302	PEE	C4-O4P-P-O3P
47	C	302	PEE	C4-O4P-P-O2P
47	Q	501	PEE	C4-O4P-P-O3P
47	Q	501	PEE	C4-O4P-P-O2P
47	W	201	PEE	C1-O3P-P-O1P
47	W	201	PEE	C1-O3P-P-O4P
47	l	705	PEE	C1-O3P-P-O2P
47	l	705	PEE	C1-O3P-P-O1P
47	l	705	PEE	C1-O3P-P-O4P
47	r	501	PEE	C1-O3P-P-O2P
47	s	401	PEE	C4-O4P-P-O3P
47	s	401	PEE	C4-O4P-P-O1P
48	g	201	PLX	C3-O4-P1-O2
48	j	201	PLX	C3-C4-O6-C6
48	j	201	PLX	C5-C4-O6-C6
48	j	201	PLX	C2-O1-P1-O3
48	r	502	PLX	C3-O4-P1-O3
51	I	201	CDL	CA3-OA5-PA1-OA2
51	I	201	CDL	CB3-OB5-PB2-OB2
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB2-OB2-PB2-OB5
51	V	202	CDL	CB3-OB5-PB2-OB2
51	V	202	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB2-OB2-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	CB3-OB5-PB2-OB2
51	a	201	CDL	CB3-OB5-PB2-OB3
51	l	702	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CA3-OA5-PA1-OA3
51	m	201	CDL	CA3-OA5-PA1-OA4
51	n	102	CDL	CA2-OA2-PA1-OA4
51	n	102	CDL	CB3-OB5-PB2-OB2
51	n	102	CDL	CB3-OB5-PB2-OB3
51	r	503	CDL	CA2-OA2-PA1-OA4
51	s	402	CDL	CA3-OA5-PA1-OA2
51	s	402	CDL	CA3-OA5-PA1-OA3
51	s	402	CDL	CA3-OA5-PA1-OA4
52	J	401	NDP	C5D-O5D-PN-O1N
56	w	401	ADP	C5'-O5'-PA-O1A
56	w	401	ADP	C5'-O5'-PA-O3A
51	a	201	CDL	C58-C59-C60-C61
47	s	401	PEE	C24-C25-C26-C27
48	j	202	PLX	C18-C19-C20-C21
51	V	202	CDL	C12-C13-C14-C15
51	r	503	CDL	C13-C14-C15-C16
47	l	705	PEE	C11-C12-C13-C14
47	l	704	PEE	C1-C2-O2-C10
51	V	201	CDL	CA6-CA4-OA6-CA5
51	a	201	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	OA5-CA3-CA4-CA6
48	N	201	PLX	C30-C31-C32-C33
47	U	101	PEE	C16-C17-C18-C19
48	j	202	PLX	O4-C3-C4-O6
51	a	201	CDL	C14-C15-C16-C17
51	s	402	CDL	C12-C13-C14-C15
51	s	402	CDL	C11-C12-C13-C14
48	r	502	PLX	C35-C36-C37-C38
51	m	201	CDL	C42-C43-C44-C45
51	V	202	CDL	C58-C59-C60-C61
47	W	201	PEE	O2-C2-C3-O3
51	s	402	CDL	OA6-CA4-CA6-OA8
47	l	701	PEE	C18-C19-C20-C21
48	n	101	PLX	C12-C13-C14-C15
47	C	302	PEE	C12-C13-C14-C15
47	C	302	PEE	C15-C16-C17-C18
47	l	704	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C30-C29-C32-O33
51	s	402	CDL	C72-C71-CB7-OB8
47	C	302	PEE	C13-C14-C15-C16
48	n	101	PLX	C15-C16-C17-C18
47	l	705	PEE	C34-C35-C36-C37
51	V	202	CDL	C32-C31-CA7-OA8
51	l	703	CDL	C43-C44-C45-C46
51	m	201	CDL	C74-C75-C76-C77
48	n	101	PLX	O7-C6-C7-C8
48	g	201	PLX	O6-C6-C7-C8
52	J	401	NDP	C2B-O2B-P2B-O3X
48	r	502	PLX	C15-C16-C17-C18
51	V	202	CDL	C60-C61-C62-C63
47	l	705	PEE	C18-C19-C20-C21
51	V	201	CDL	CA4-CA3-OA5-PA1
49	J	402	UQ	C21-C22-C23-C24
48	C	303	PLX	C28-C29-C30-C31
47	B	303	PEE	C44-C45-C46-C47
47	l	705	PEE	C16-C17-C18-C19
51	l	702	CDL	C73-C74-C75-C76
51	V	202	CDL	C54-C55-C56-C57
51	m	201	CDL	C31-C32-C33-C34
47	B	303	PEE	C21-C22-C23-C24
51	l	703	CDL	C15-C16-C17-C18
49	C	304	UQ	C40-C39-C41-C42
51	l	703	CDL	C33-C34-C35-C36
47	r	501	PEE	C37-C38-C39-C40
47	l	704	PEE	C42-C43-C44-C45
51	l	703	CDL	C41-C42-C43-C44
48	C	303	PLX	C29-C30-C31-C32
51	a	201	CDL	C74-C75-C76-C77
51	r	503	CDL	C15-C16-C17-C18
47	l	704	PEE	C15-C16-C17-C18
47	r	501	PEE	C33-C34-C35-C36
51	V	202	CDL	C31-C32-C33-C34
47	l	704	PEE	C23-C24-C25-C26
51	I	201	CDL	C31-C32-C33-C34
47	W	201	PEE	C16-C17-C18-C19
49	C	304	UQ	C39-C41-C42-C43
51	s	402	CDL	CA3-CA4-CA6-OA8
47	B	303	PEE	C13-C14-C15-C16
47	l	704	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
48	C	303	PLX	C6-C7-C8-C9
51	V	201	CDL	CA7-C31-C32-C33
51	n	102	CDL	OB5-CB3-CB4-OB6
47	r	501	PEE	C12-C13-C14-C15
51	l	703	CDL	C39-C40-C41-C42
47	C	302	PEE	C38-C39-C40-C41
51	a	201	CDL	C44-C45-C46-C47
48	j	201	PLX	C16-C17-C18-C19
51	l	702	CDL	C20-C21-C22-C23
47	l	704	PEE	C16-C17-C18-C19
47	s	401	PEE	C18-C19-C20-C21
51	r	503	CDL	OA6-CA4-CA6-OA8
52	J	401	NDP	O4D-C1D-N1N-C2N
51	m	201	CDL	C77-C78-C79-C80
51	r	503	CDL	C52-C53-C54-C55
48	j	201	PLX	C29-C30-C31-C32
51	l	702	CDL	C41-C42-C43-C44
48	N	201	PLX	O8-C24-C25-C26
48	j	202	PLX	C24-C25-C26-C27
51	l	703	CDL	C36-C37-C38-C39
51	l	702	CDL	C54-C55-C56-C57
47	l	704	PEE	C39-C40-C41-C42
48	g	201	PLX	C36-C37-C38-C39
51	V	201	CDL	C53-C54-C55-C56
48	g	201	PLX	O7-C6-C7-C8
48	r	502	PLX	O7-C6-C7-C8
47	C	302	PEE	C33-C34-C35-C36
51	l	702	CDL	C76-C77-C78-C79
48	r	502	PLX	C16-C17-C18-C19
47	l	705	PEE	C38-C39-C40-C41
51	r	503	CDL	C72-C71-CB7-OB8
51	s	402	CDL	C15-C16-C17-C18
47	l	704	PEE	C13-C14-C15-C16
47	l	705	PEE	C15-C16-C17-C18
51	l	702	CDL	C44-C45-C46-C47
48	j	202	PLX	C30-C31-C32-C33
51	V	201	CDL	C64-C65-C66-C67
51	l	702	CDL	OB5-CB3-CB4-CB6
51	m	201	CDL	OB5-CB3-CB4-CB6
48	N	201	PLX	O6-C4-C5-O8
51	V	202	CDL	C16-C17-C18-C19
49	J	402	UQ	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C5'-O5'-P-O3P
47	B	303	PEE	C16-C17-C18-C19
47	C	302	PEE	C18-C19-C20-C21
47	l	701	PEE	C38-C39-C40-C41
47	U	101	PEE	C41-C42-C43-C44
47	l	704	PEE	C3-C2-O2-C10
47	s	401	PEE	C16-C17-C18-C19
47	Q	501	PEE	C15-C16-C17-C18
47	B	303	PEE	C11-C12-C13-C14
51	n	102	CDL	CB7-C71-C72-C73
48	r	502	PLX	C29-C30-C31-C32
51	l	702	CDL	C22-C23-C24-C25
47	Q	501	PEE	C36-C37-C38-C39
47	W	201	PEE	C18-C19-C20-C21
48	N	201	PLX	C3-C4-C5-O8
51	l	702	CDL	C51-C52-C53-C54
51	l	702	CDL	C60-C61-C62-C63
51	s	402	CDL	C57-C58-C59-C60
47	C	302	PEE	C16-C17-C18-C19
47	r	501	PEE	C16-C17-C18-C19
51	a	201	CDL	C16-C17-C18-C19
48	N	201	PLX	C1-C2-O1-P1
50	X	201	8Q1	C31-C29-C32-C34
48	C	303	PLX	O6-C6-C7-C8
48	r	502	PLX	C33-C34-C35-C36
47	C	302	PEE	C20-C21-C22-C23
51	r	503	CDL	C39-C40-C41-C42
47	C	302	PEE	C44-C45-C46-C47
51	a	201	CDL	C64-C65-C66-C67
48	j	202	PLX	C7-C6-O6-C4
48	g	201	PLX	C6-C7-C8-C9
51	l	702	CDL	C72-C71-CB7-OB8
47	Q	501	PEE	C22-C23-C24-C25
51	V	202	CDL	C44-C45-C46-C47
51	n	102	CDL	C72-C71-CB7-OB8
51	s	402	CDL	C12-C11-CA5-OA6
47	U	101	PEE	C19-C20-C21-C22
51	m	201	CDL	C53-C54-C55-C56
47	l	701	PEE	O3-C30-C31-C32
56	w	401	ADP	PB-O3A-PA-O2A
47	U	101	PEE	O2-C10-C11-C12
51	I	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
51	l	703	CDL	C72-C71-CB7-OB8
51	a	201	CDL	C12-C13-C14-C15
51	a	201	CDL	C41-C42-C43-C44
51	r	503	CDL	C21-C22-C23-C24
47	C	302	PEE	O3-C30-C31-C32
48	N	201	PLX	C26-C27-C28-C29
48	r	502	PLX	C19-C20-C21-C22
50	X	201	8Q1	C29-C32-C34-O35
51	V	202	CDL	C39-C40-C41-C42
47	Q	501	PEE	C23-C24-C25-C26
51	a	201	CDL	C51-C52-C53-C54
51	s	402	CDL	C74-C75-C76-C77
51	l	703	CDL	C56-C57-C58-C59
51	V	201	CDL	C40-C41-C42-C43
47	C	302	PEE	O2-C10-C11-C12
51	a	201	CDL	C43-C44-C45-C46
51	V	201	CDL	CB3-CB4-CB6-OB8
48	j	201	PLX	C25-C24-O8-C5
48	r	502	PLX	C26-C27-C28-C29
47	l	701	PEE	O2-C2-C3-O3
47	l	705	PEE	O3-C30-C31-C32
51	a	201	CDL	C32-C31-CA7-OA8
48	j	202	PLX	O4-C3-C4-C5
51	V	201	CDL	CB2-C1-CA2-OA2
49	C	304	UQ	C30-C29-C31-C32
47	Q	501	PEE	C20-C21-C22-C23
49	C	304	UQ	C33-C34-C36-C37
51	m	201	CDL	C54-C55-C56-C57
47	C	302	PEE	C35-C36-C37-C38
47	C	302	PEE	C34-C35-C36-C37
51	m	201	CDL	C44-C45-C46-C47
51	l	703	CDL	C12-C11-CA5-OA7
50	X	201	8Q1	C29-C32-C34-N36
51	n	102	CDL	C72-C71-CB7-OB9
51	a	201	CDL	C13-C14-C15-C16
47	l	701	PEE	O2-C10-C11-C12
51	a	201	CDL	C12-C11-CA5-OA6
47	W	201	PEE	C34-C35-C36-C37
47	B	303	PEE	C18-C19-C20-C21
47	C	302	PEE	O5-C30-C31-C32
51	s	402	CDL	C12-C11-CA5-OA7
48	j	202	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
52	J	401	NDP	C3D-C4D-C5D-O5D
51	V	201	CDL	C57-C58-C59-C60
47	U	101	PEE	O4-C10-C11-C12
47	l	701	PEE	O5-C30-C31-C32
47	l	704	PEE	C14-C15-C16-C17
47	l	705	PEE	C14-C15-C16-C17
48	n	101	PLX	C6-C7-C8-C9
51	a	201	CDL	C53-C54-C55-C56
47	C	302	PEE	O4-C10-C11-C12
51	l	702	CDL	C72-C71-CB7-OB9
49	C	304	UQ	C45-C44-C46-C47
51	a	201	CDL	C76-C77-C78-C79
47	Q	501	PEE	C2-C1-O3P-P
51	I	201	CDL	C72-C71-CB7-OB9
51	l	703	CDL	C72-C71-CB7-OB9
47	l	705	PEE	O5-C30-C31-C32
51	r	503	CDL	C82-C83-C84-C85
48	j	201	PLX	O4-C3-C4-C5
51	n	102	CDL	OB5-CB3-CB4-CB6
51	a	201	CDL	C32-C31-CA7-OA9
51	m	201	CDL	C12-C11-CA5-OA6
51	a	201	CDL	C12-C11-CA5-OA7
47	r	501	PEE	C18-C19-C20-C21
47	l	701	PEE	O4-C10-C11-C12
51	l	703	CDL	C80-C81-C82-C83

There are no ring outliers.

34 monomers are involved in 116 short contacts:

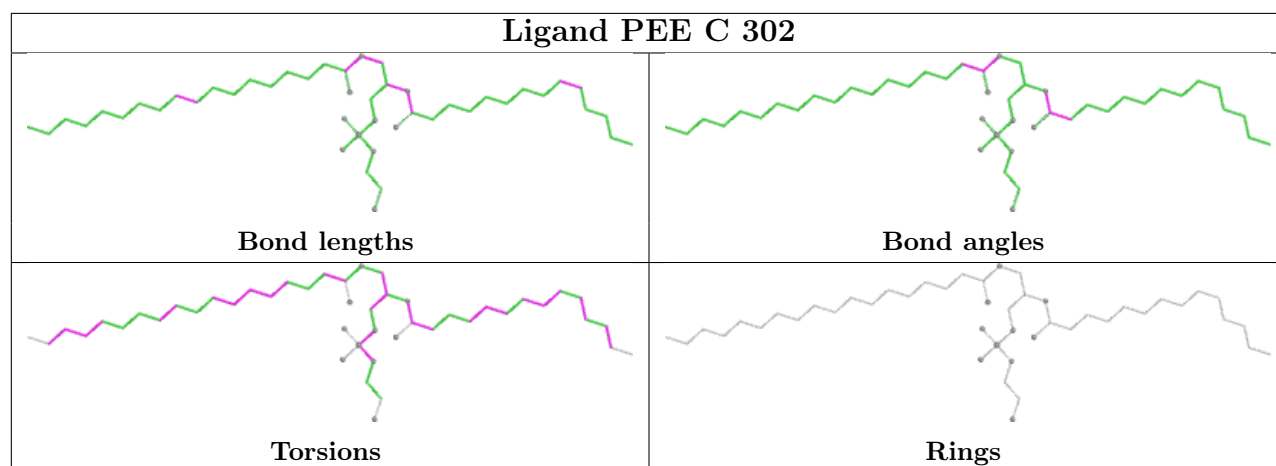
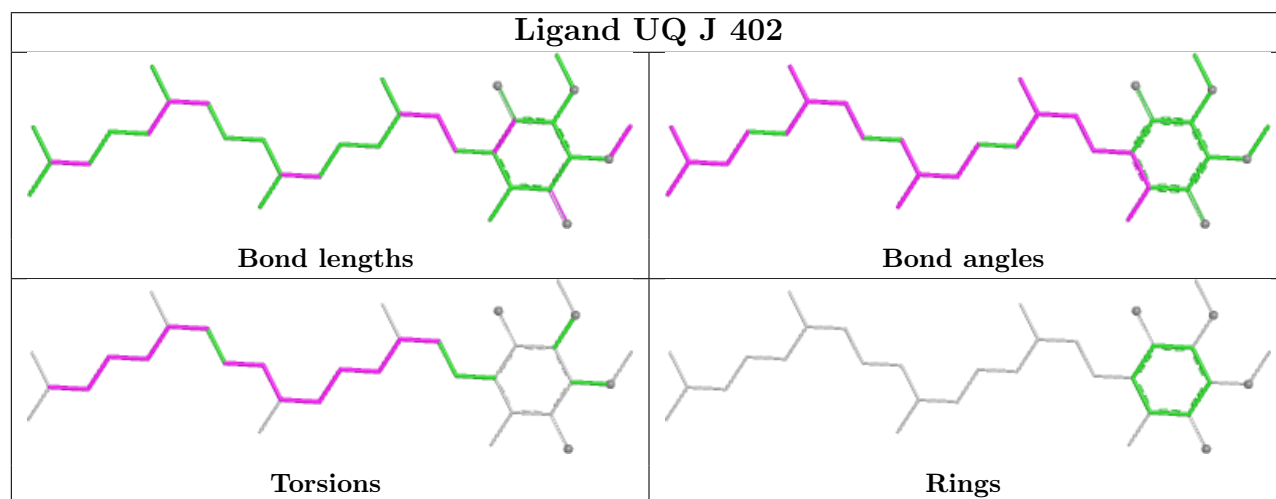
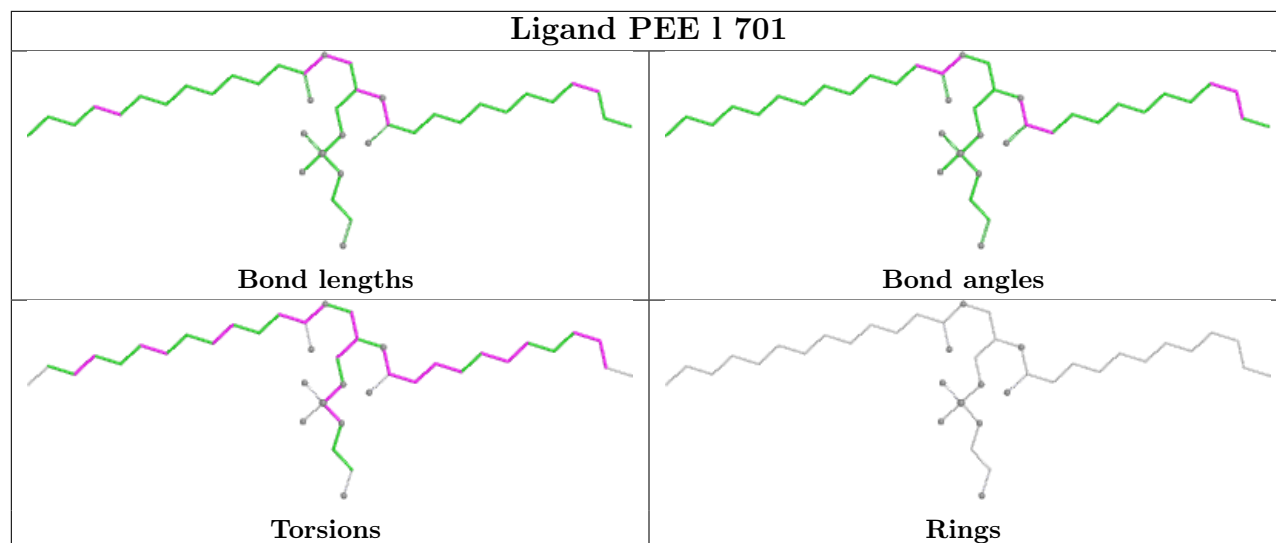
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	l	701	PEE	2	0
49	J	402	UQ	2	0
48	j	202	PLX	2	0
45	A	501	SF4	1	0
56	w	401	ADP	1	0
47	B	303	PEE	4	0
50	X	201	8Q1	1	0
48	C	303	PLX	2	0
50	G	201	8Q1	5	0
51	V	202	CDL	5	0
47	Q	501	PEE	1	0
48	n	101	PLX	4	0

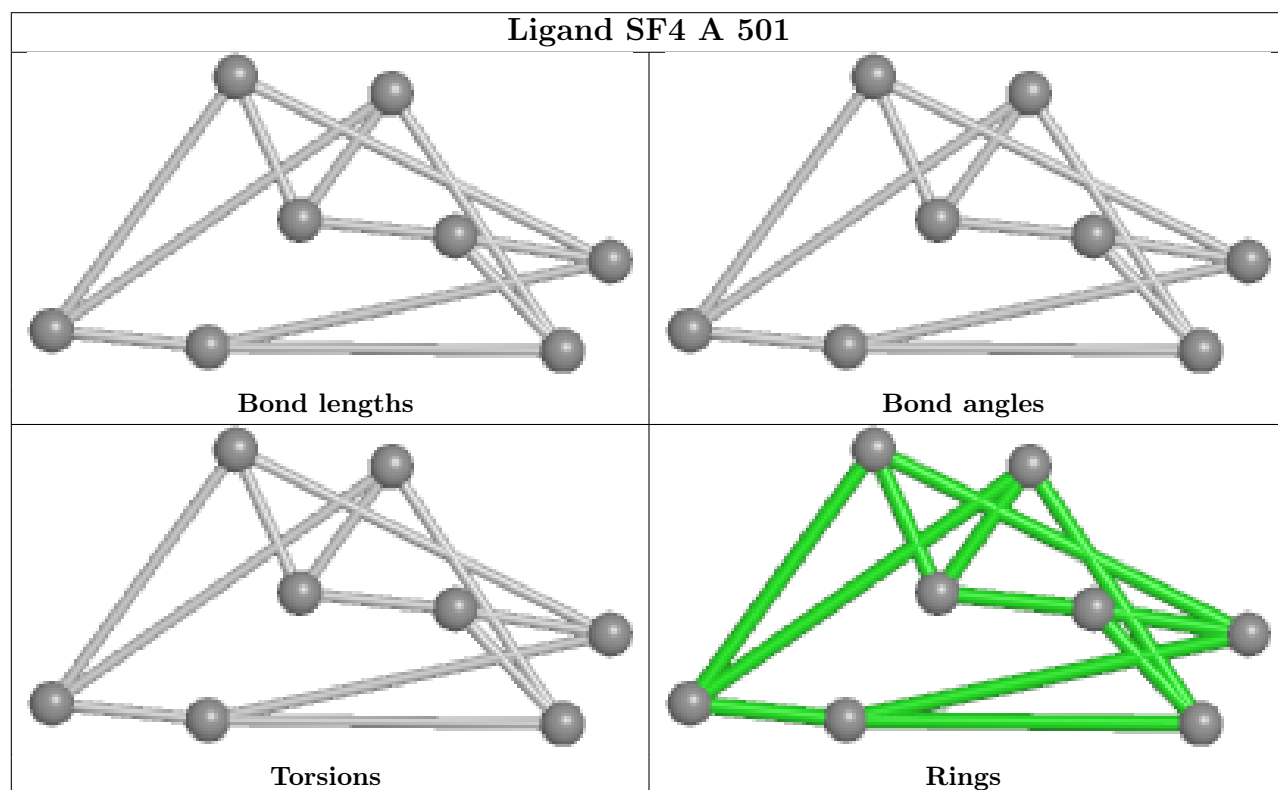
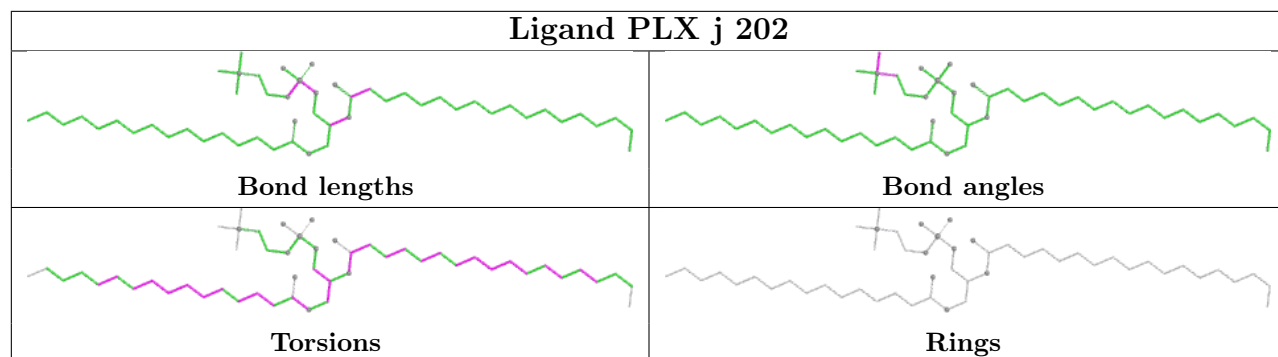
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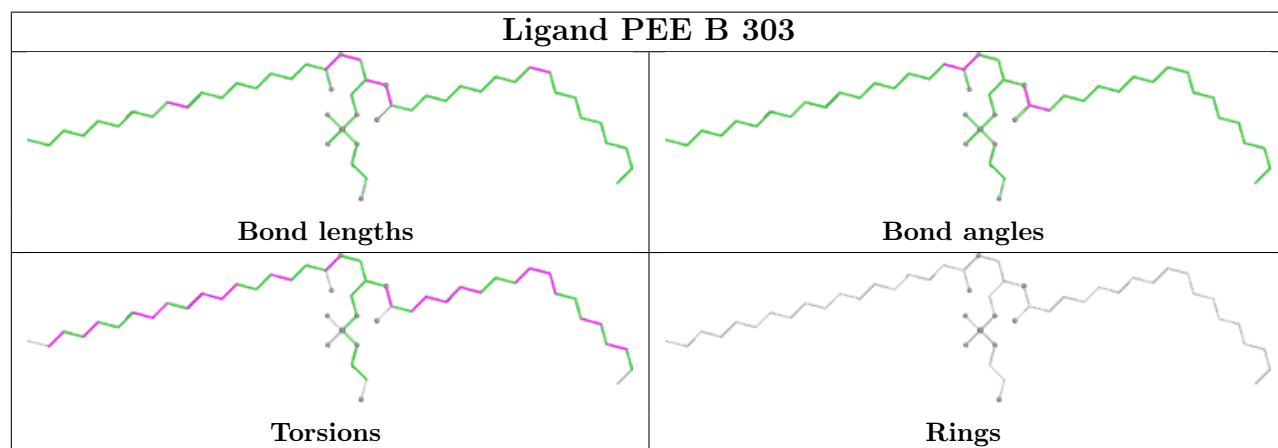
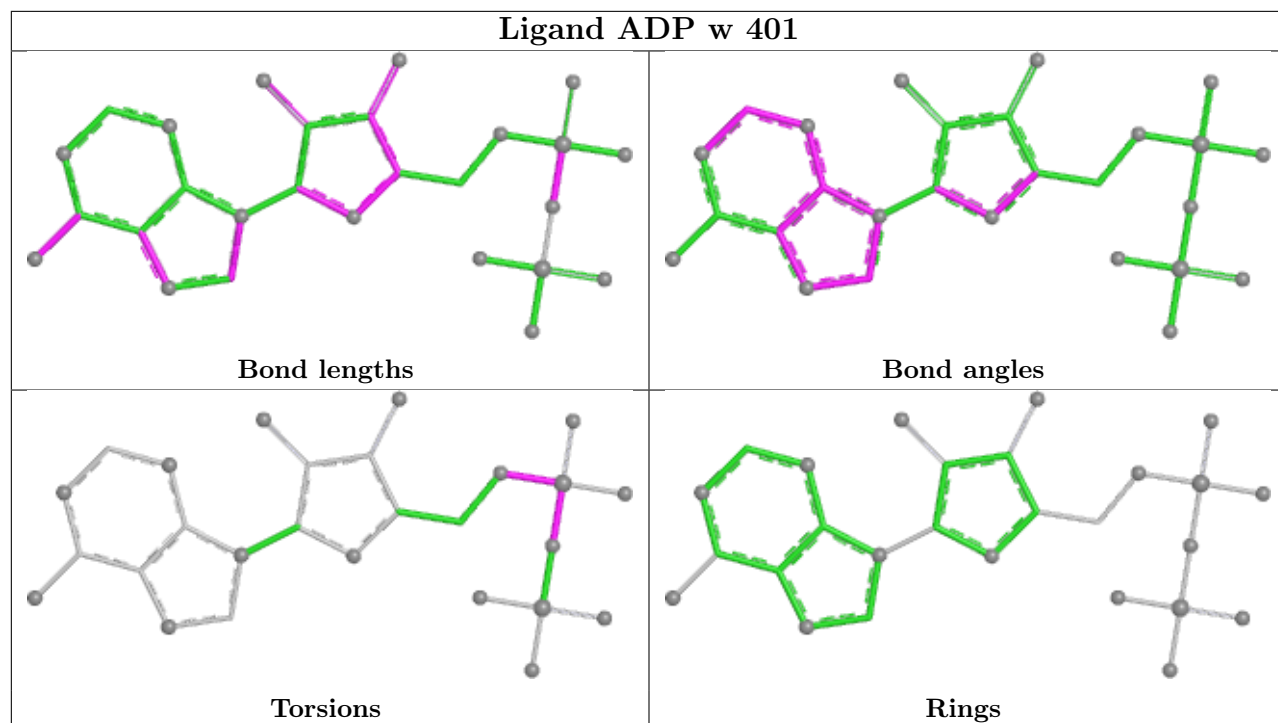
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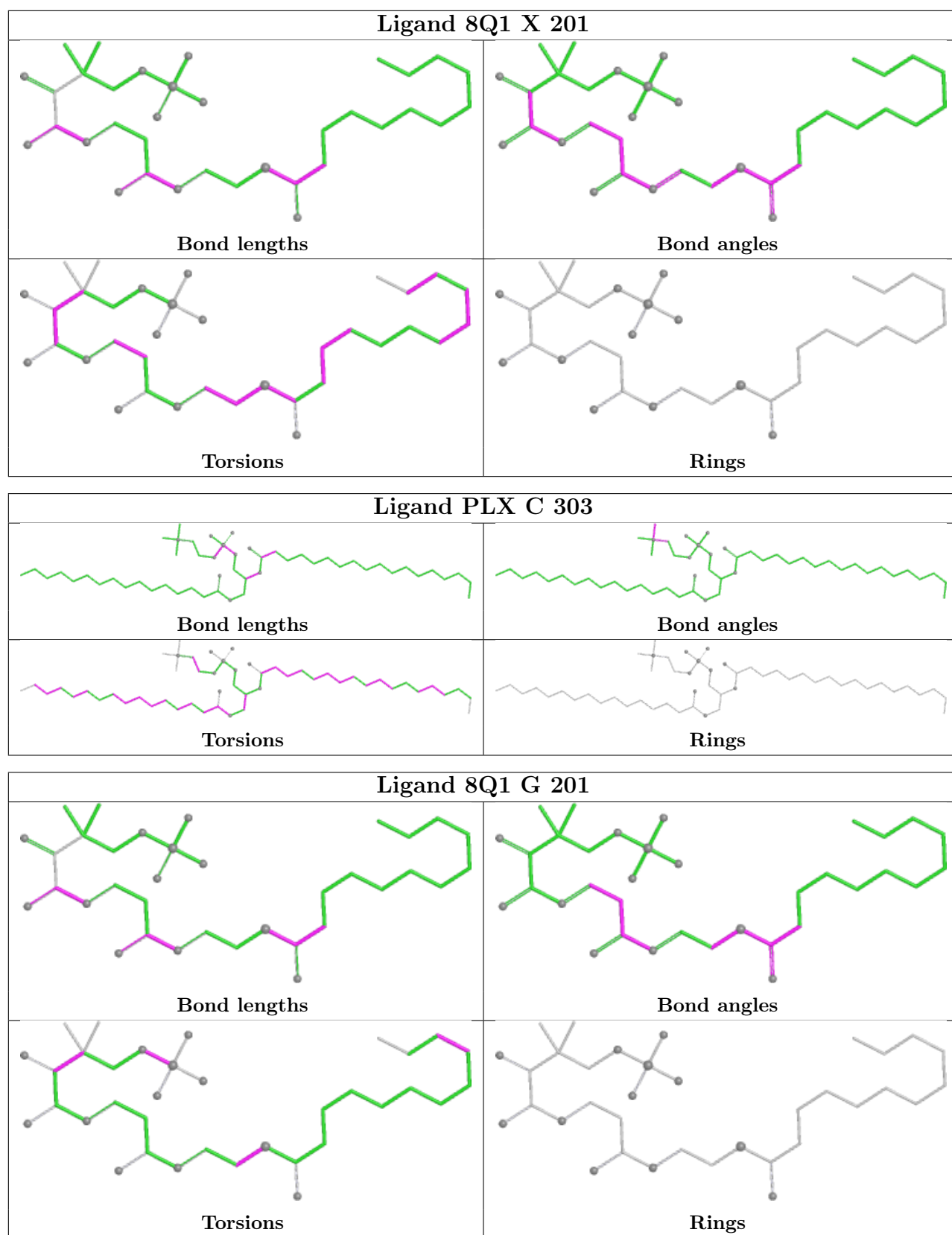
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	J	401	NDP	3	0
47	U	101	PEE	4	0
51	n	102	CDL	1	0
49	C	304	UQ	5	0
48	N	201	PLX	2	0
51	V	201	CDL	3	0
48	j	201	PLX	1	0
51	a	201	CDL	5	0
47	l	705	PEE	3	0
51	m	201	CDL	9	0
47	l	704	PEE	4	0
51	l	702	CDL	14	0
47	W	201	PEE	1	0
51	l	703	CDL	5	0
48	r	502	PLX	5	0
51	s	402	CDL	5	0
47	r	501	PEE	2	0
46	A	502	FMN	3	0
47	s	401	PEE	3	0
48	g	201	PLX	5	0
51	r	503	CDL	7	0
51	I	201	CDL	3	0

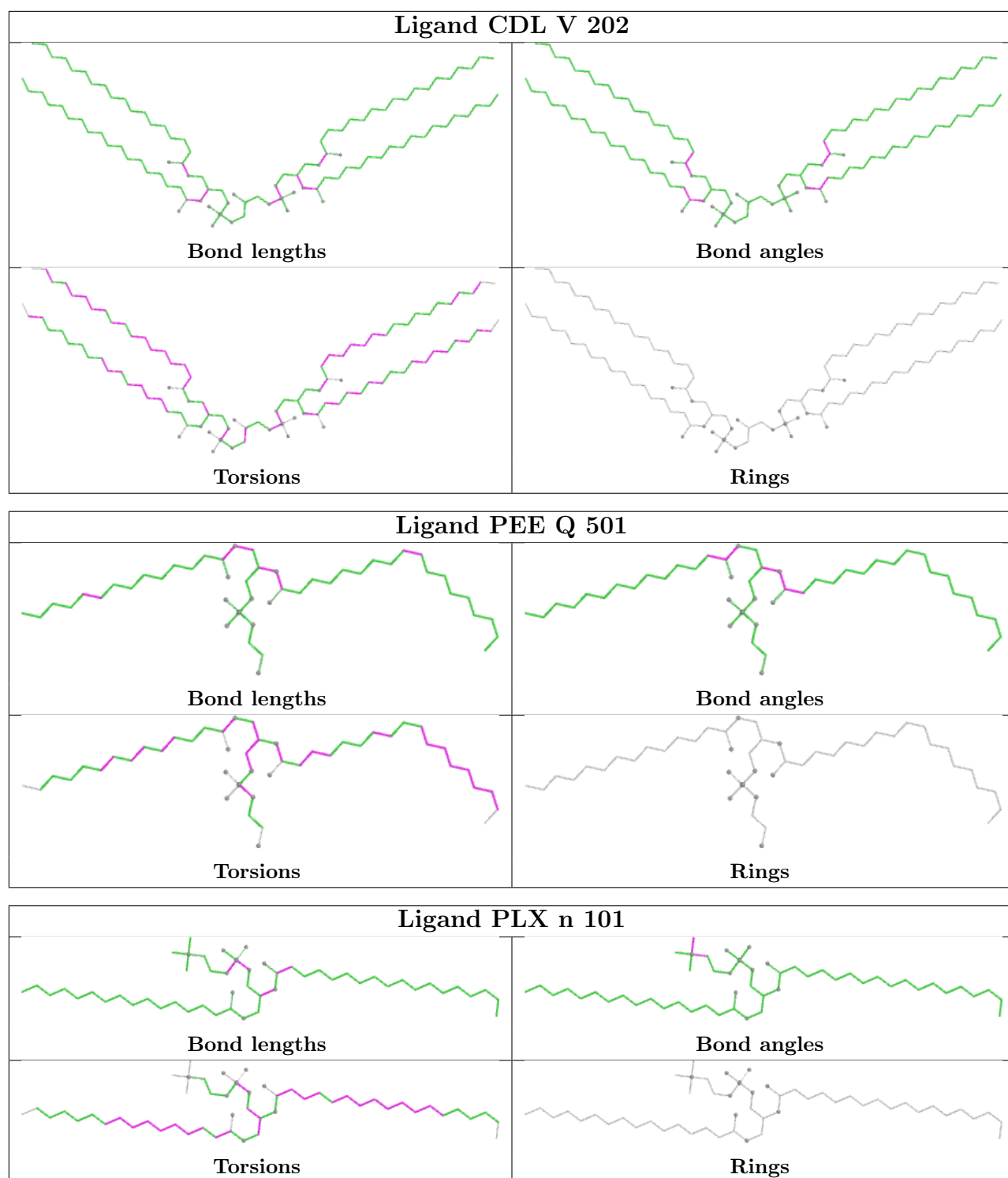
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



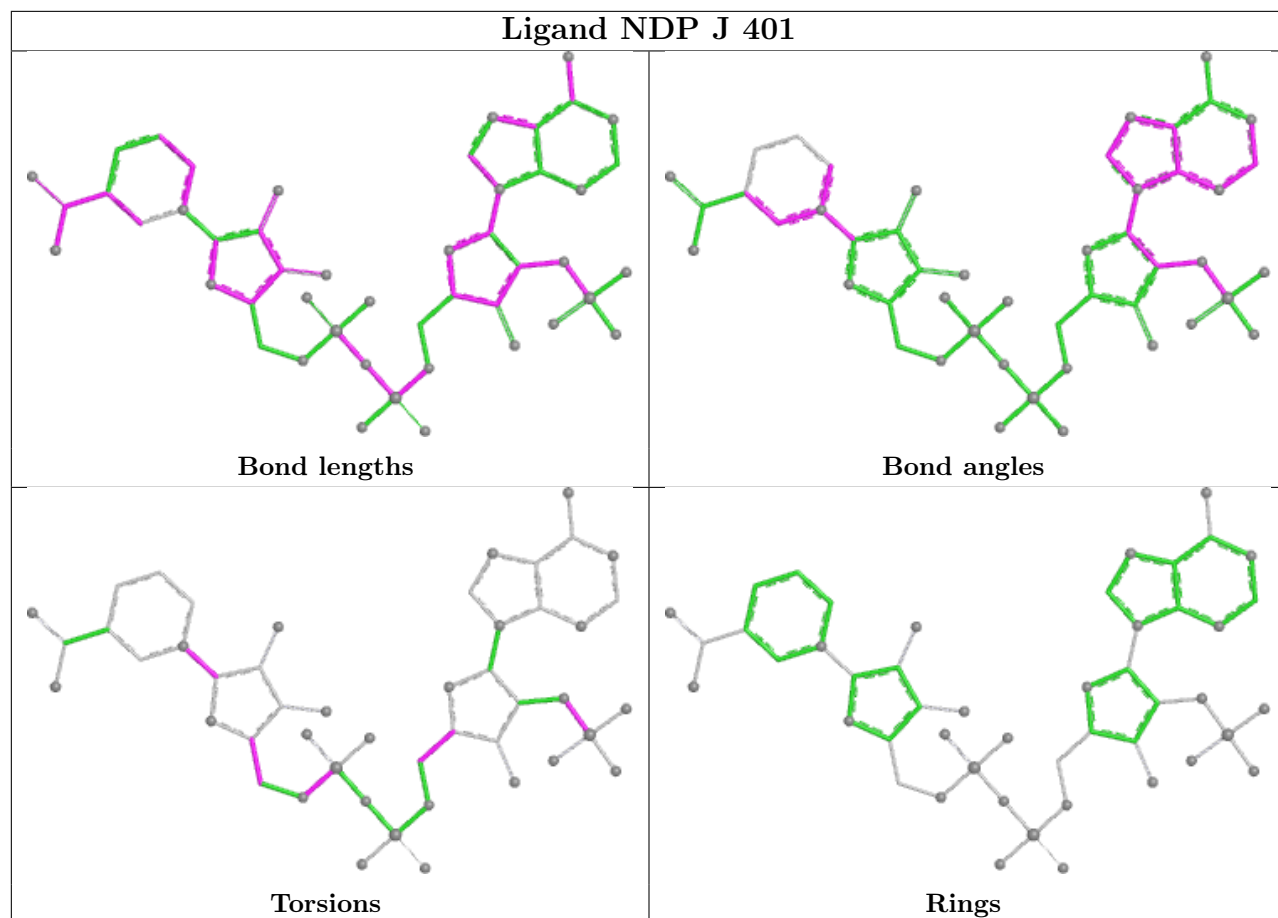




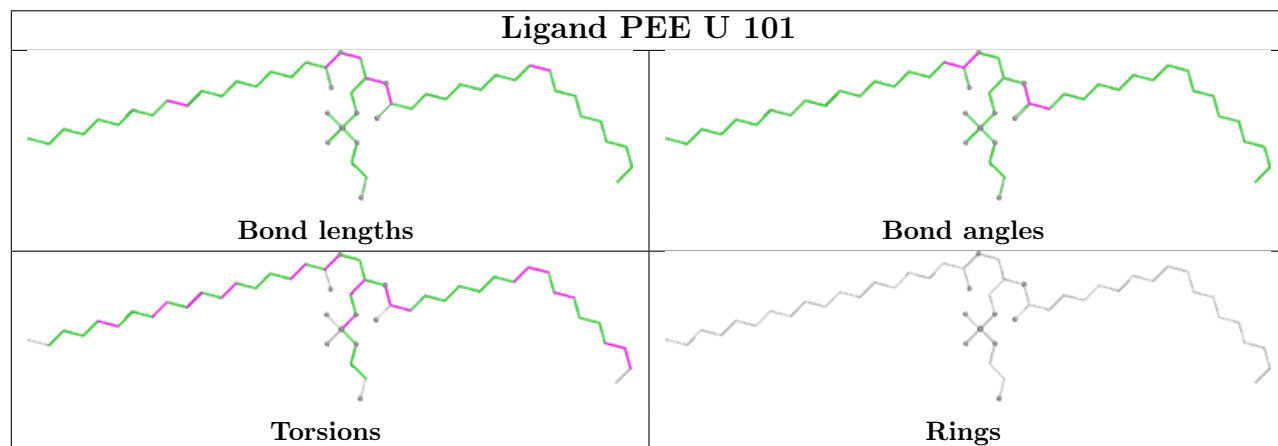




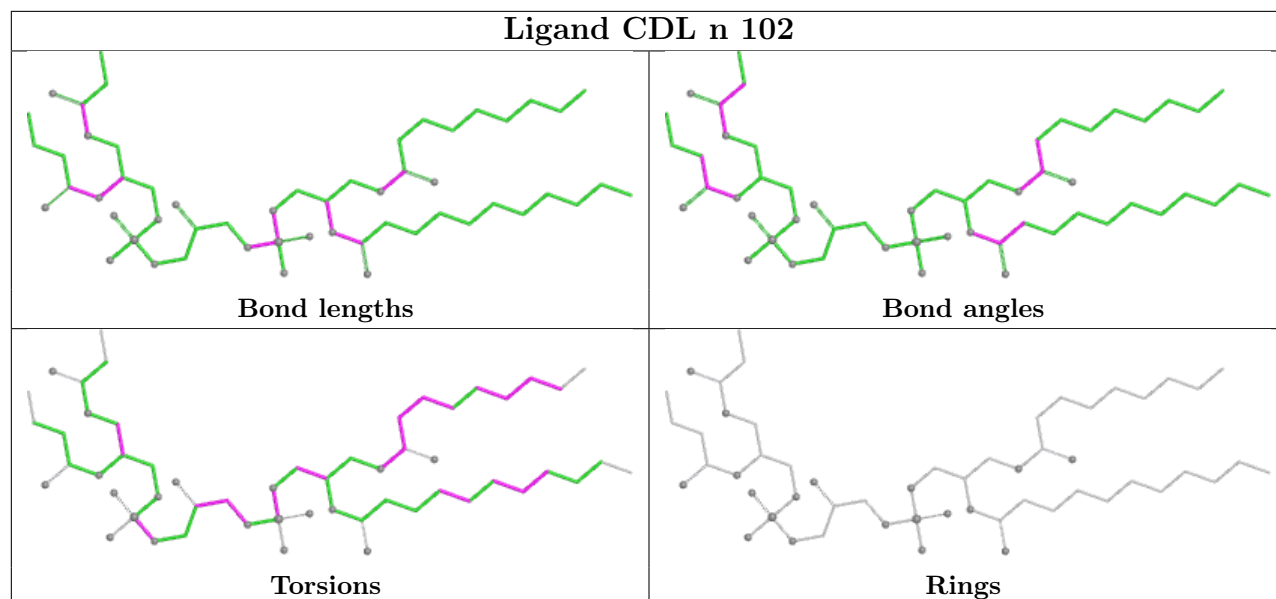
Ligand NDP J 401



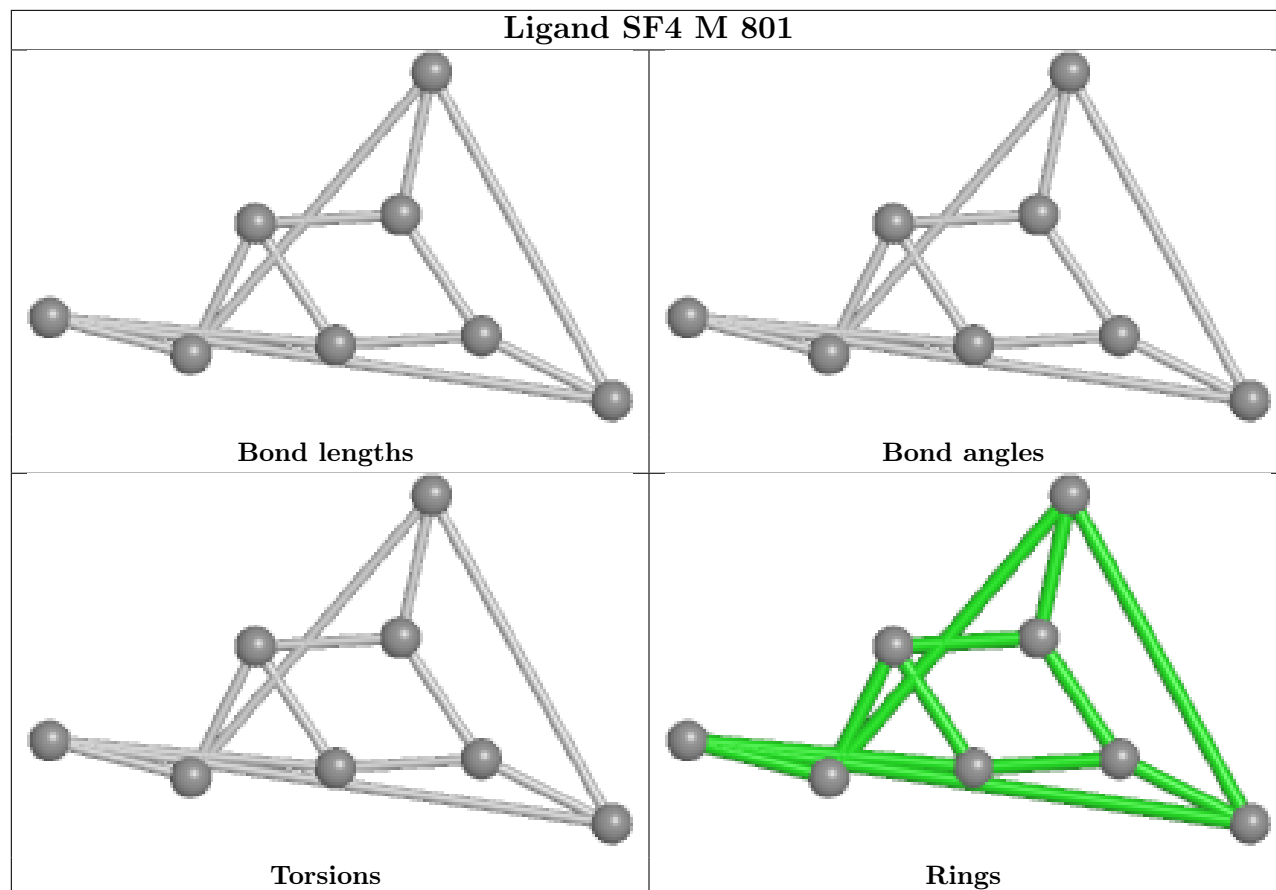
Ligand PEE U 101

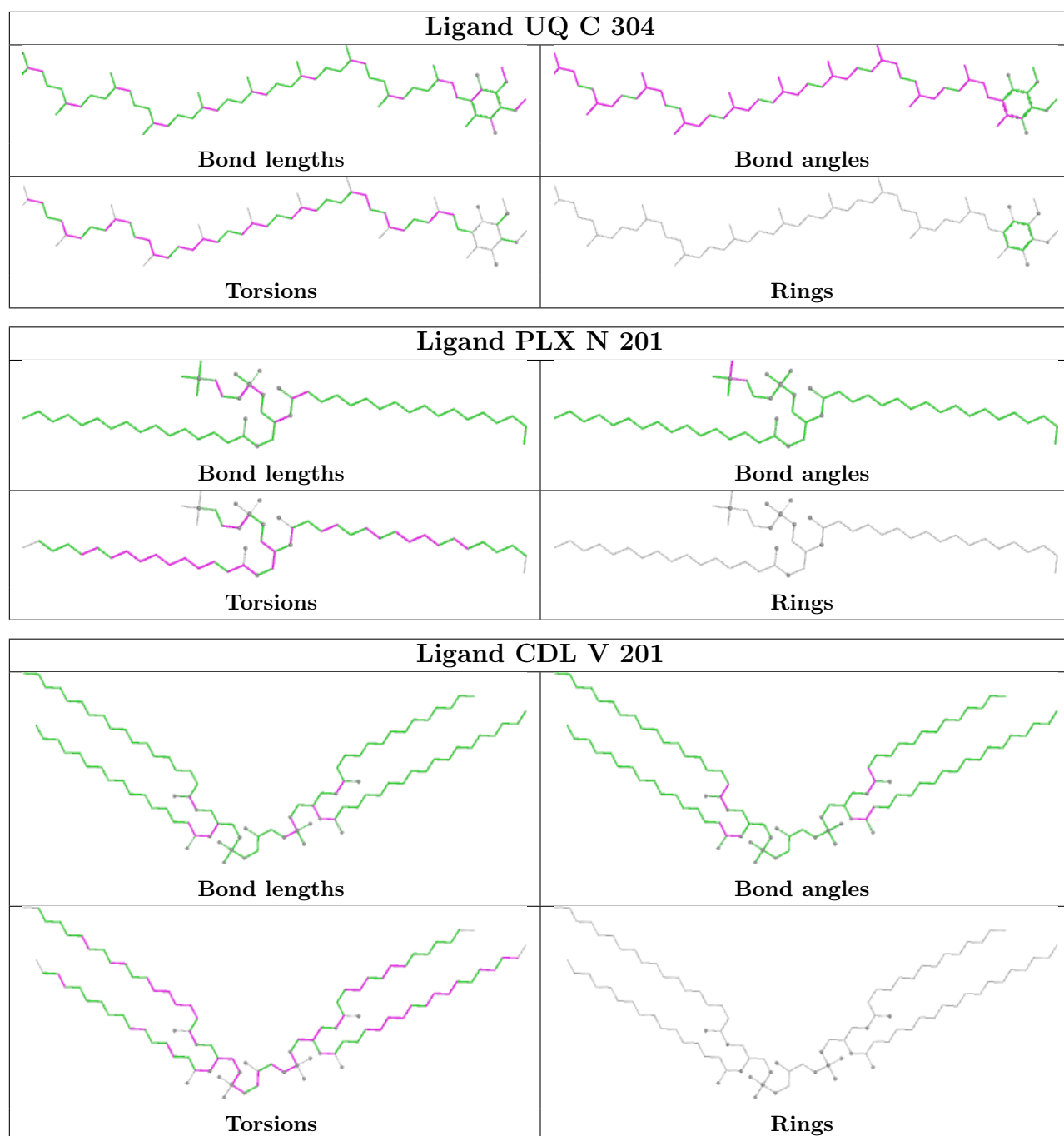


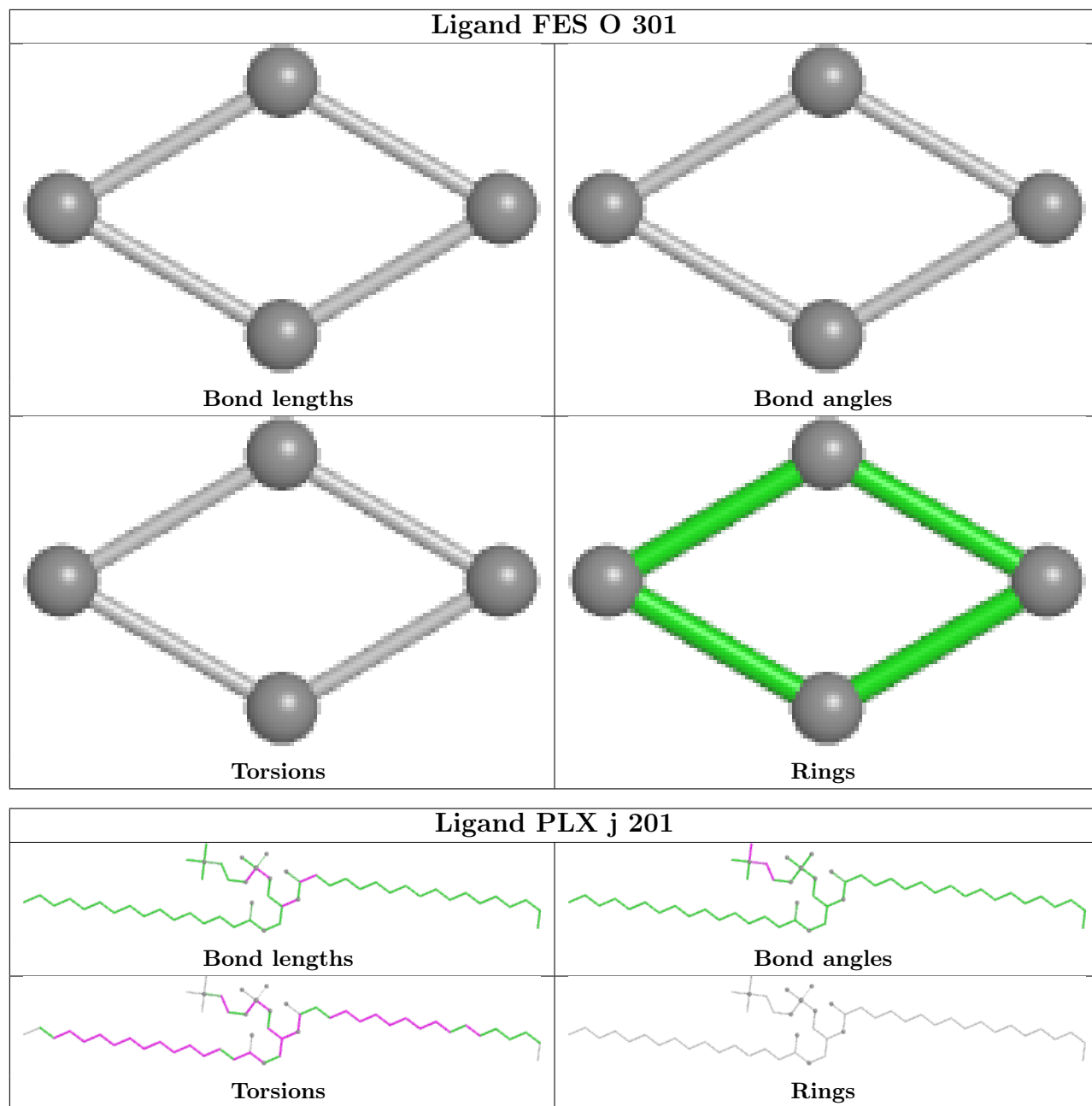
Ligand CDL n 102

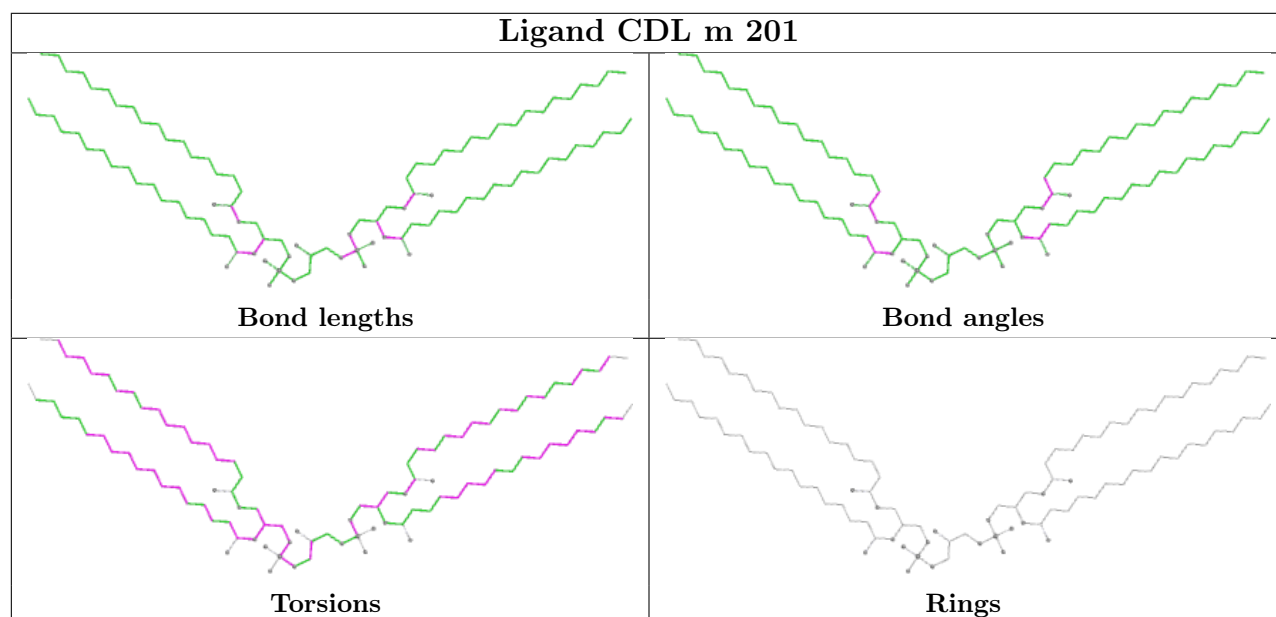
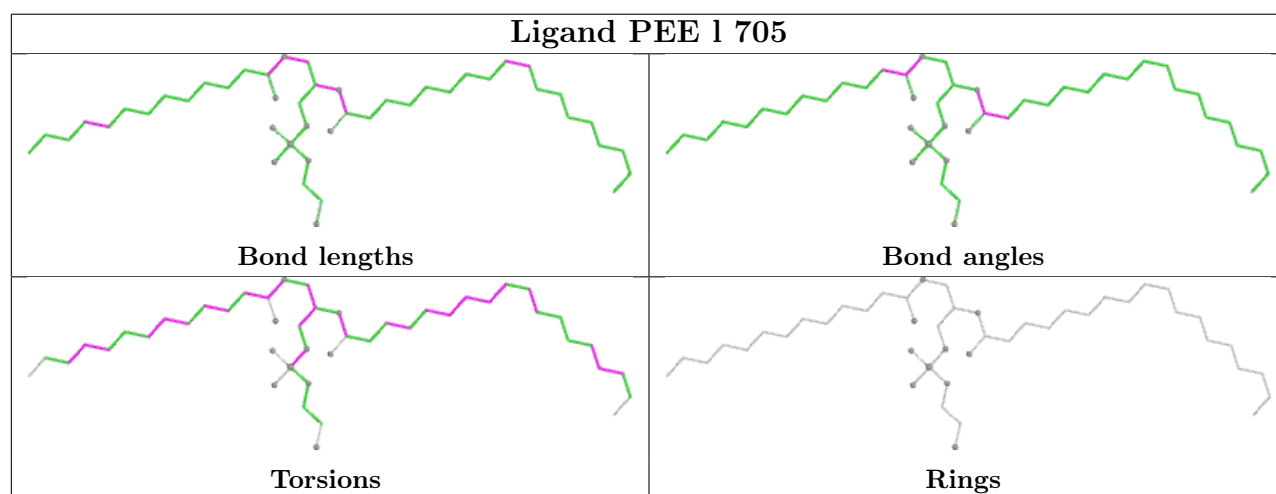
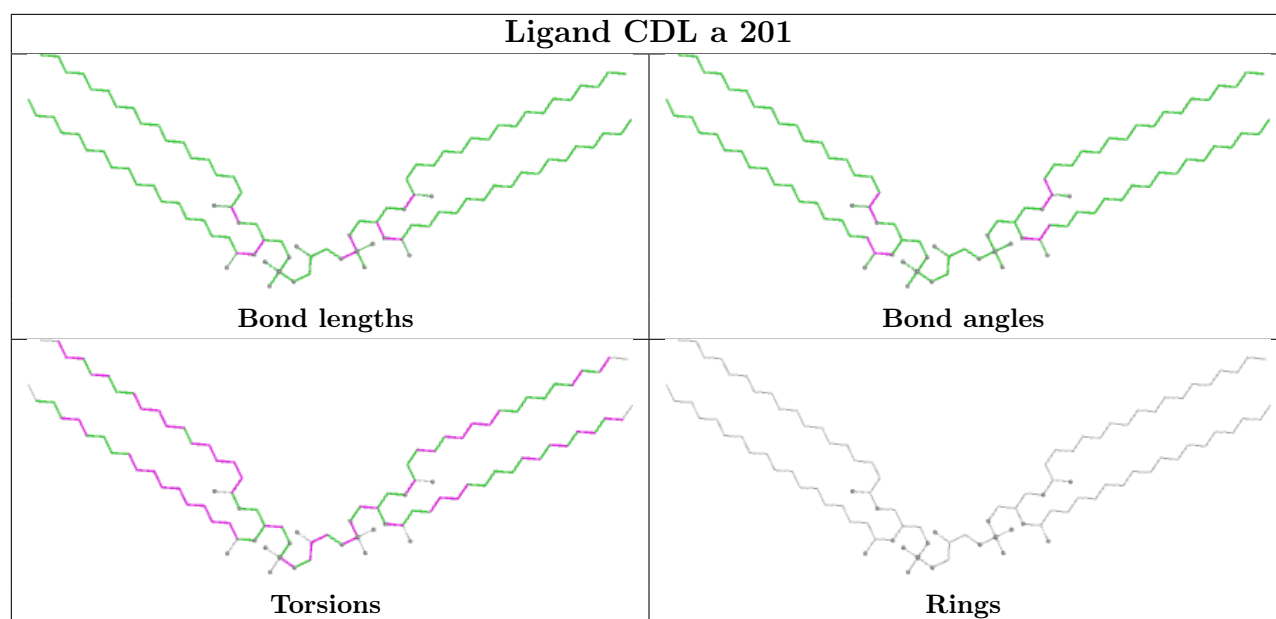


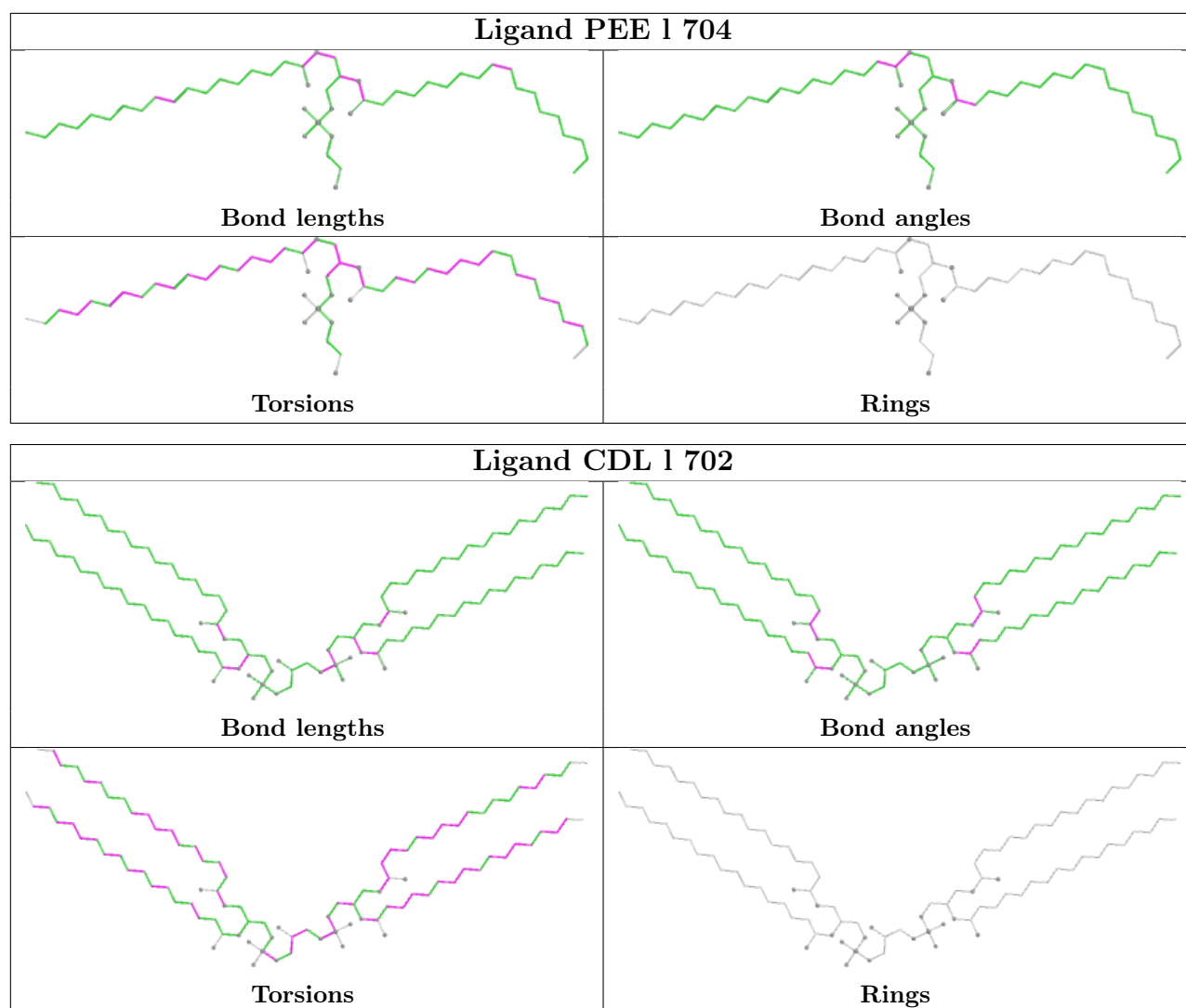
Ligand SF4 M 801

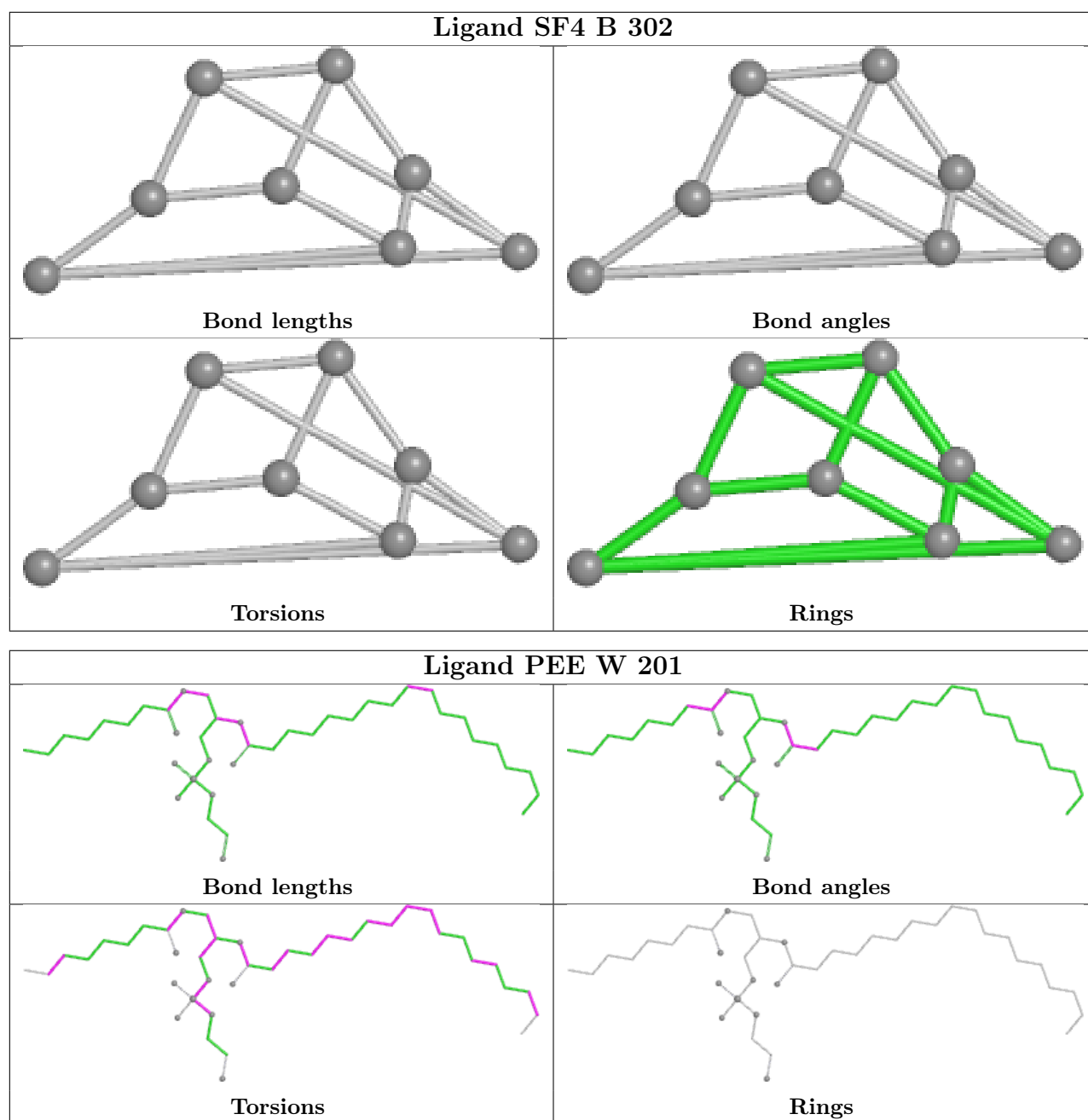


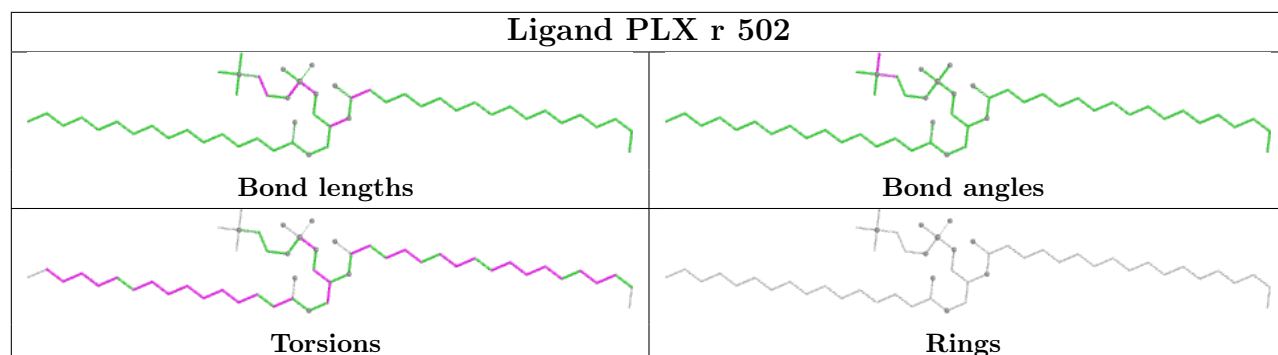
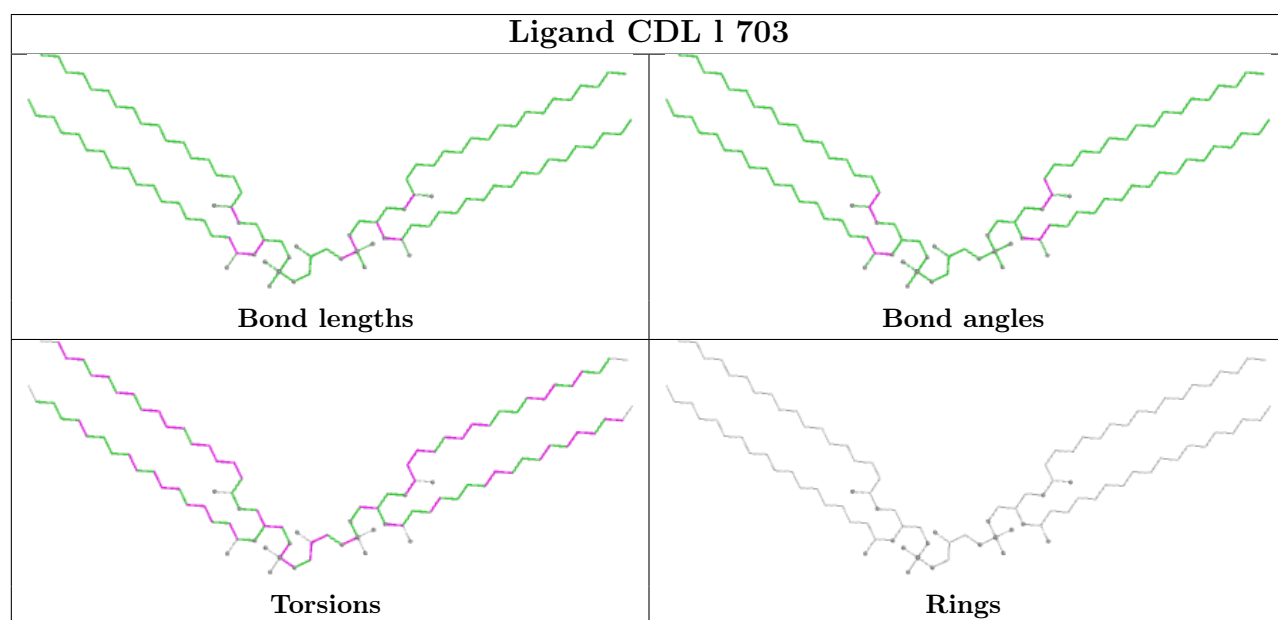
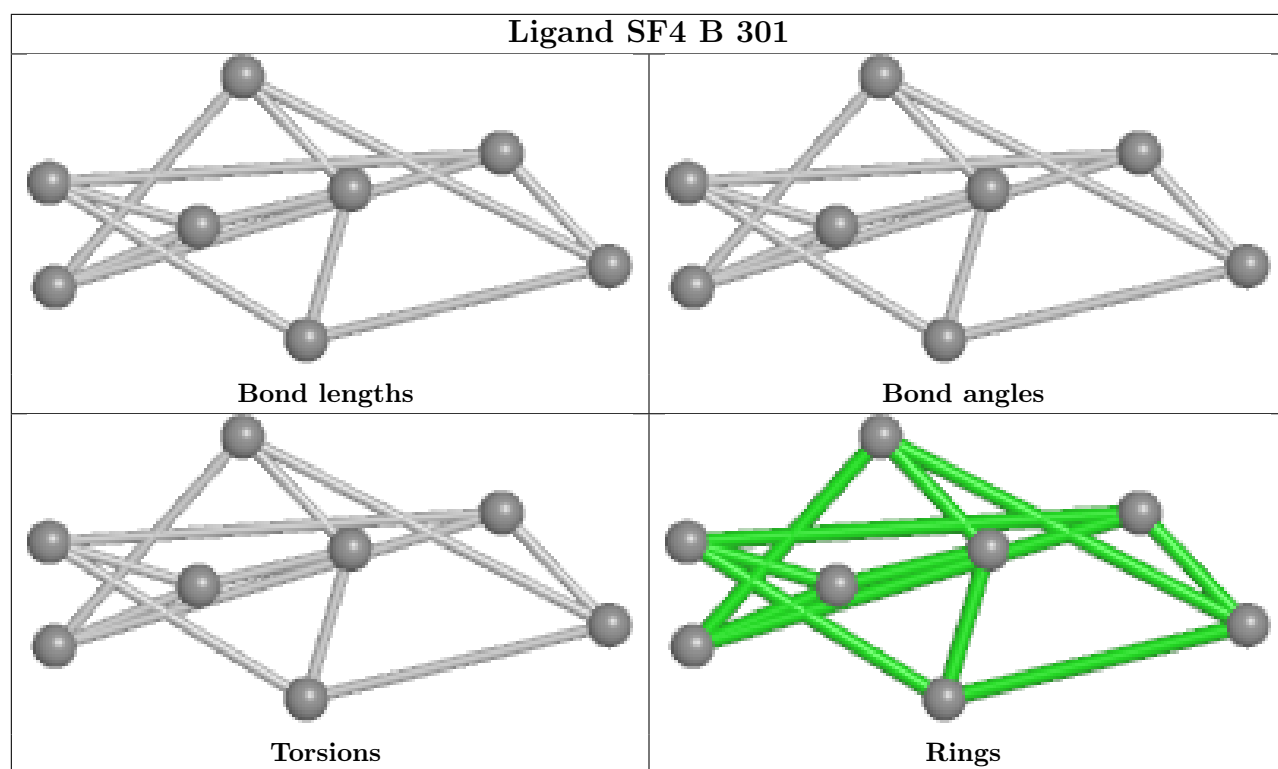


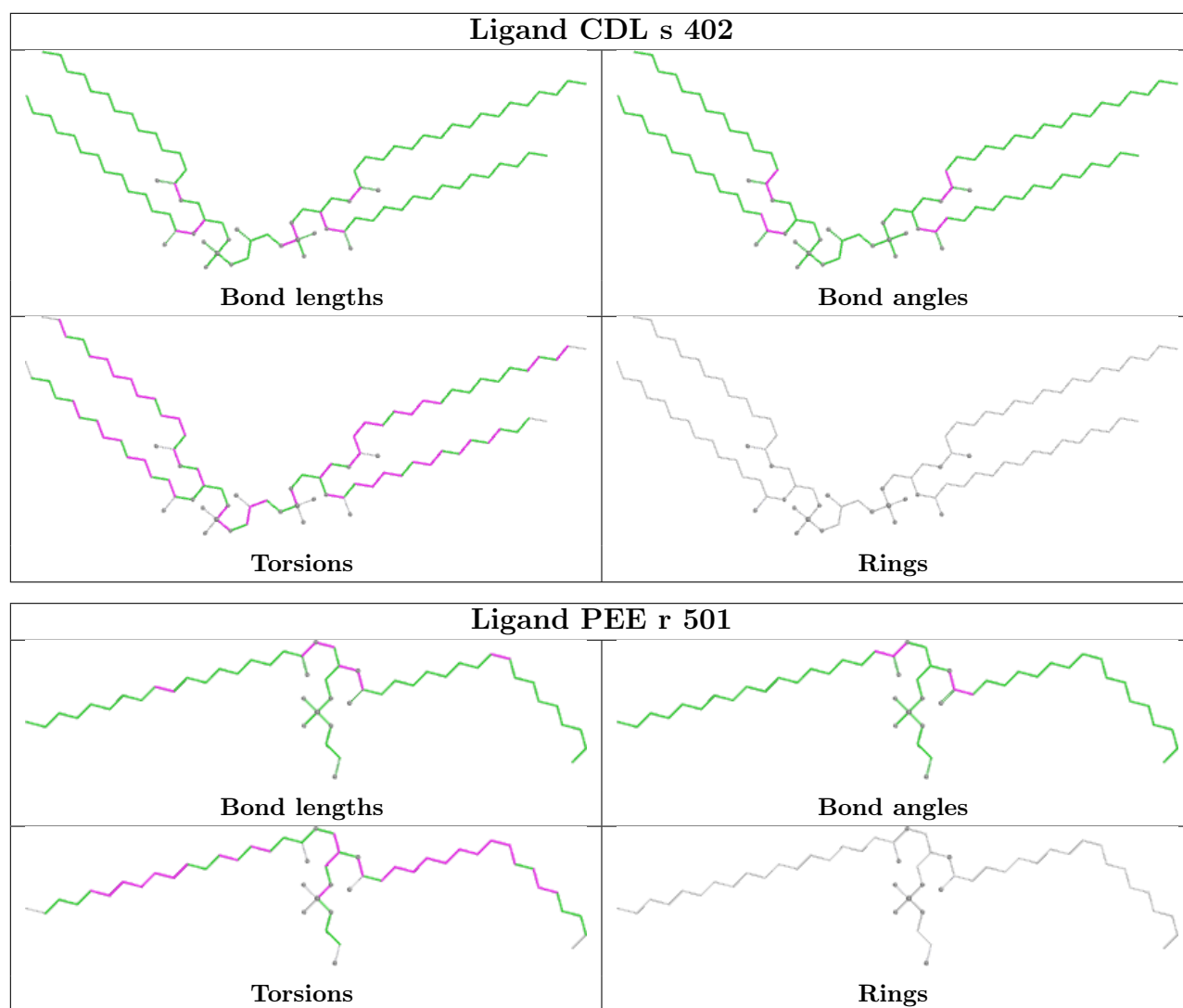


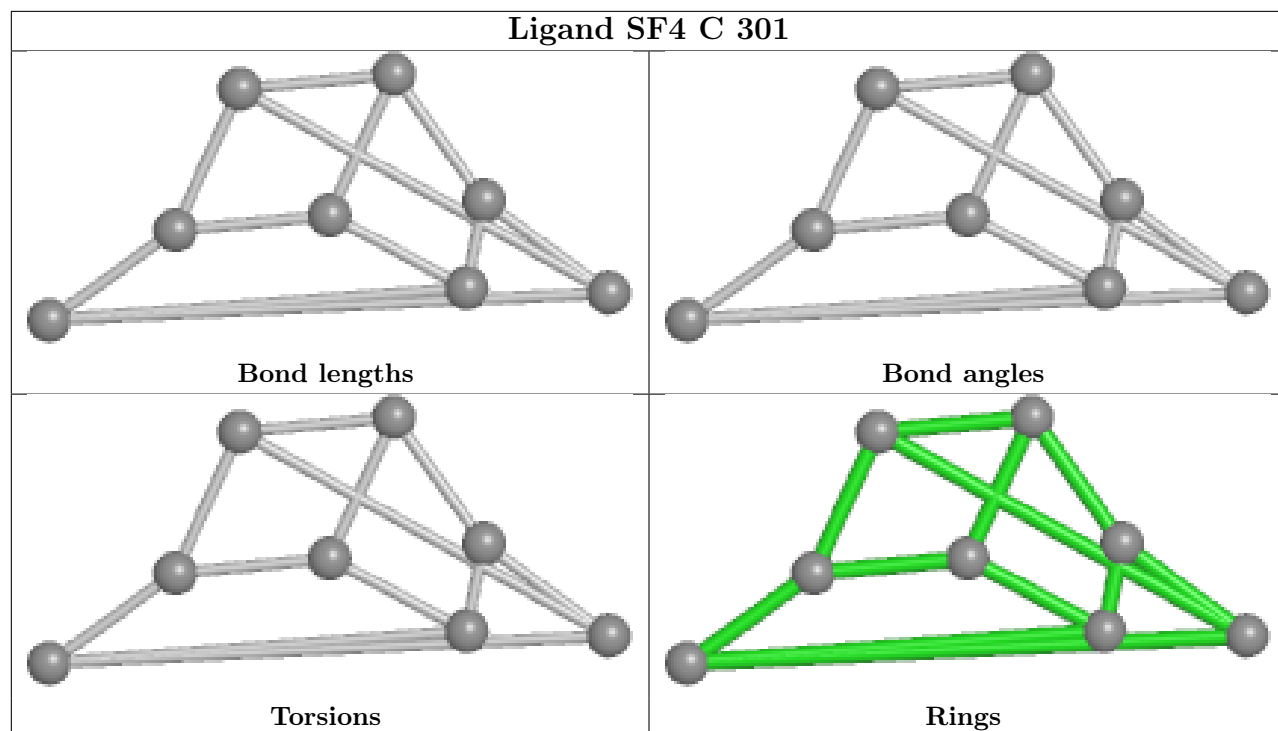


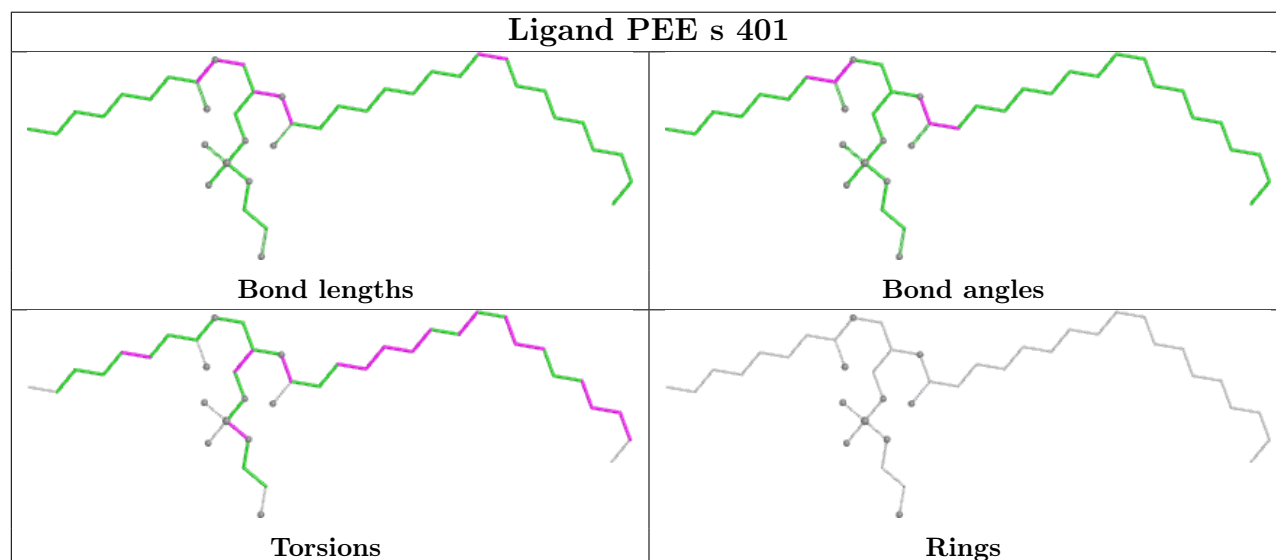
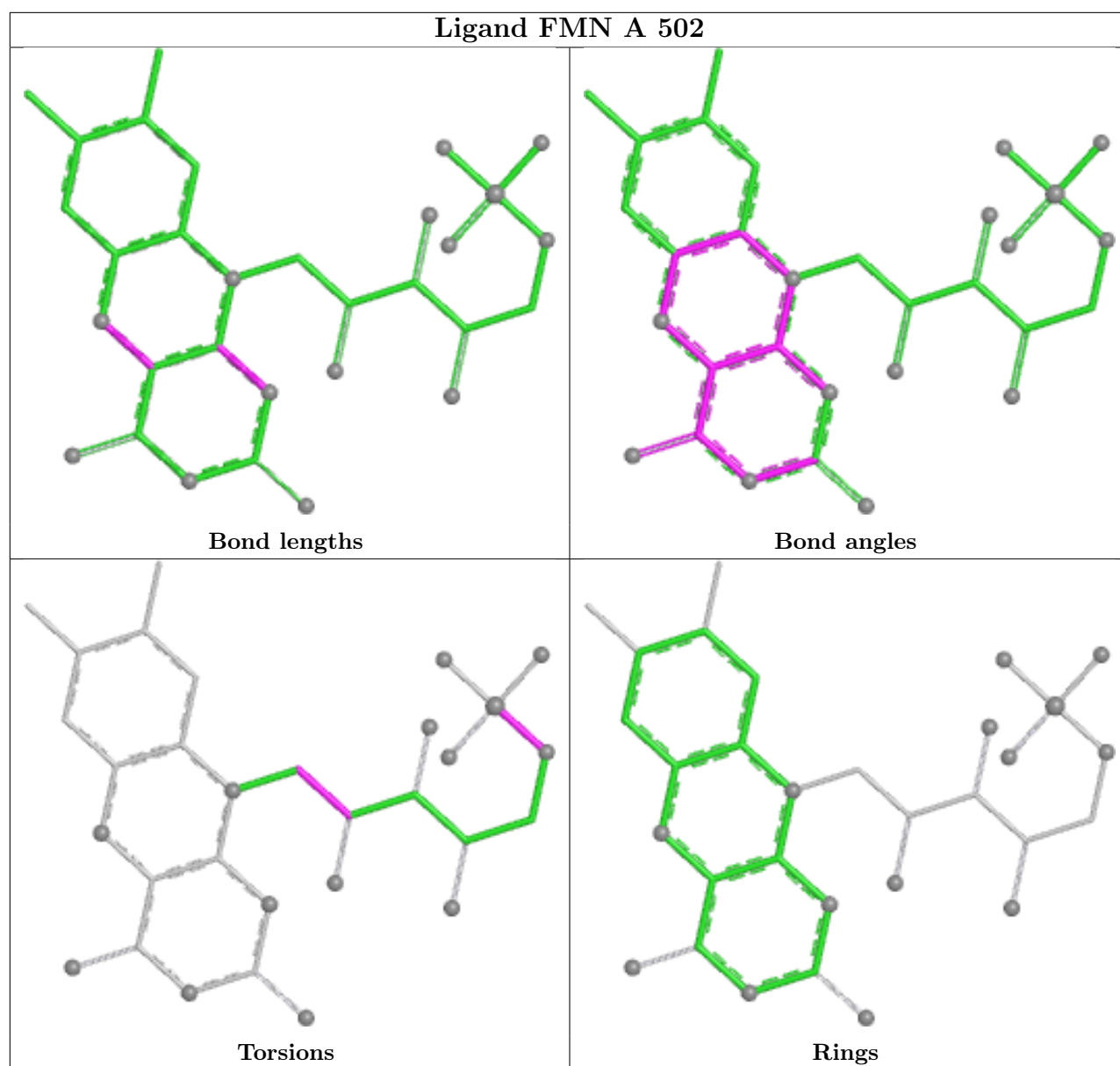


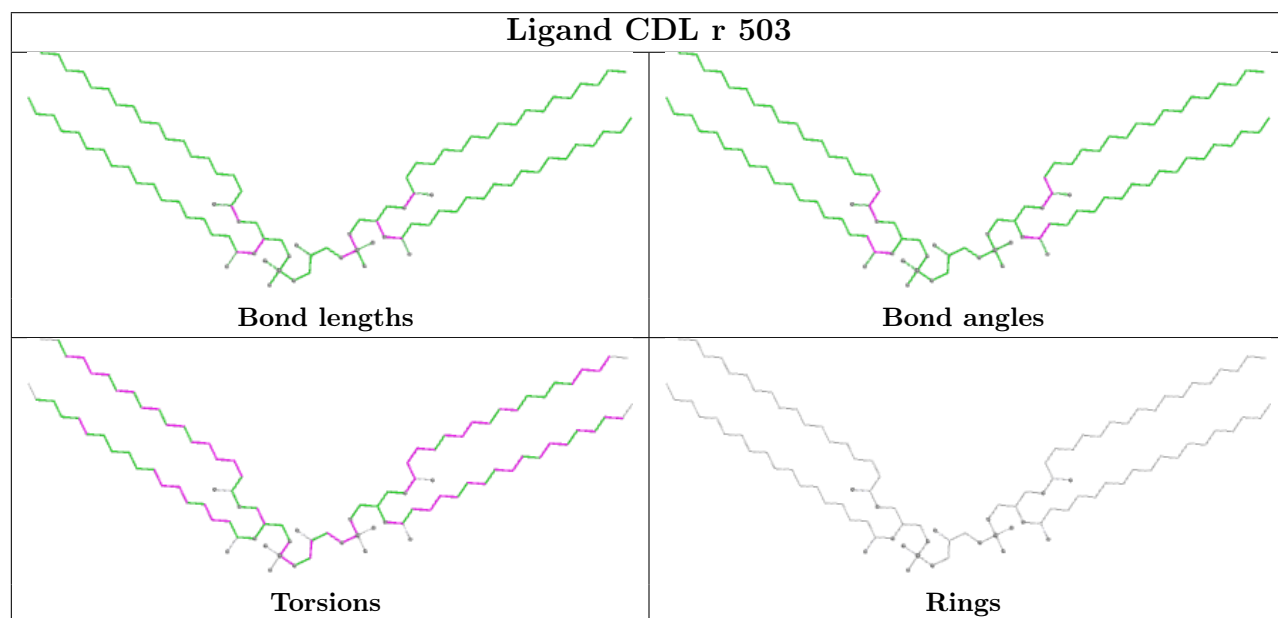
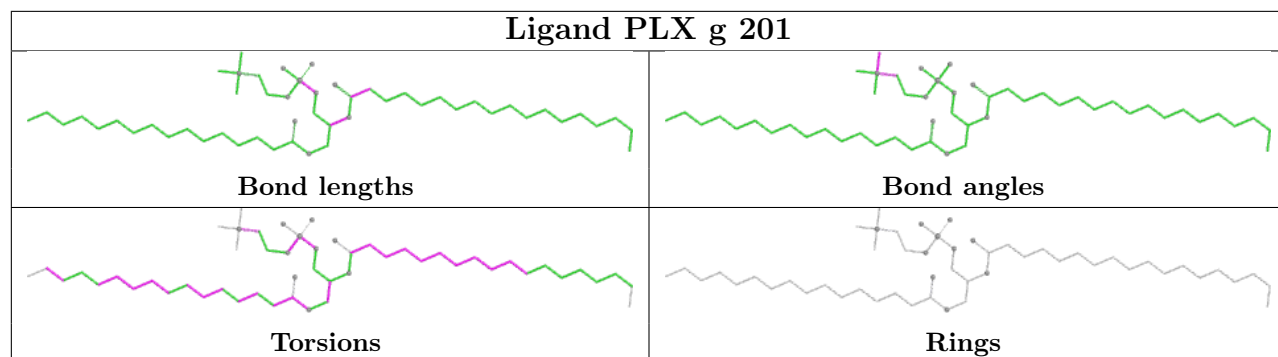


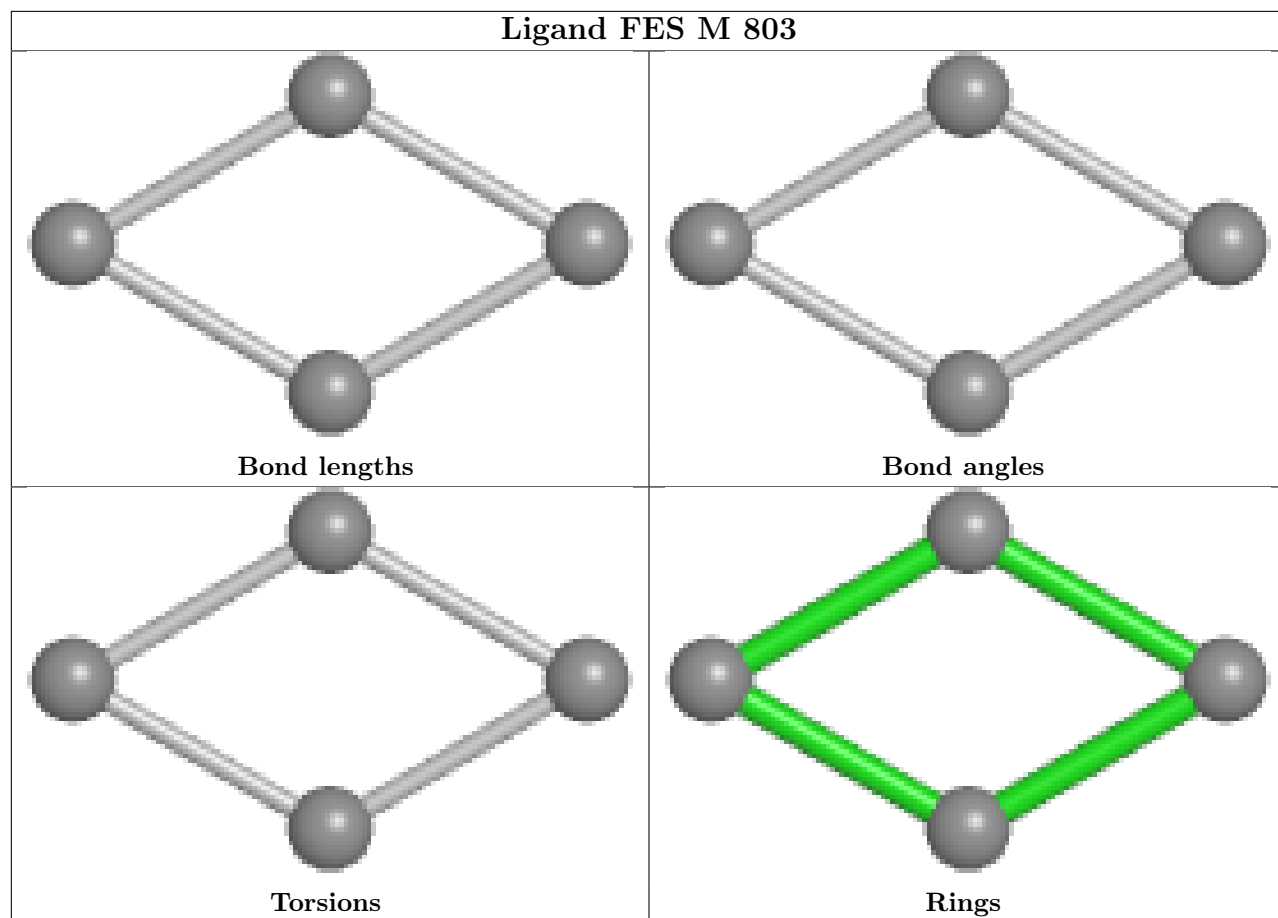


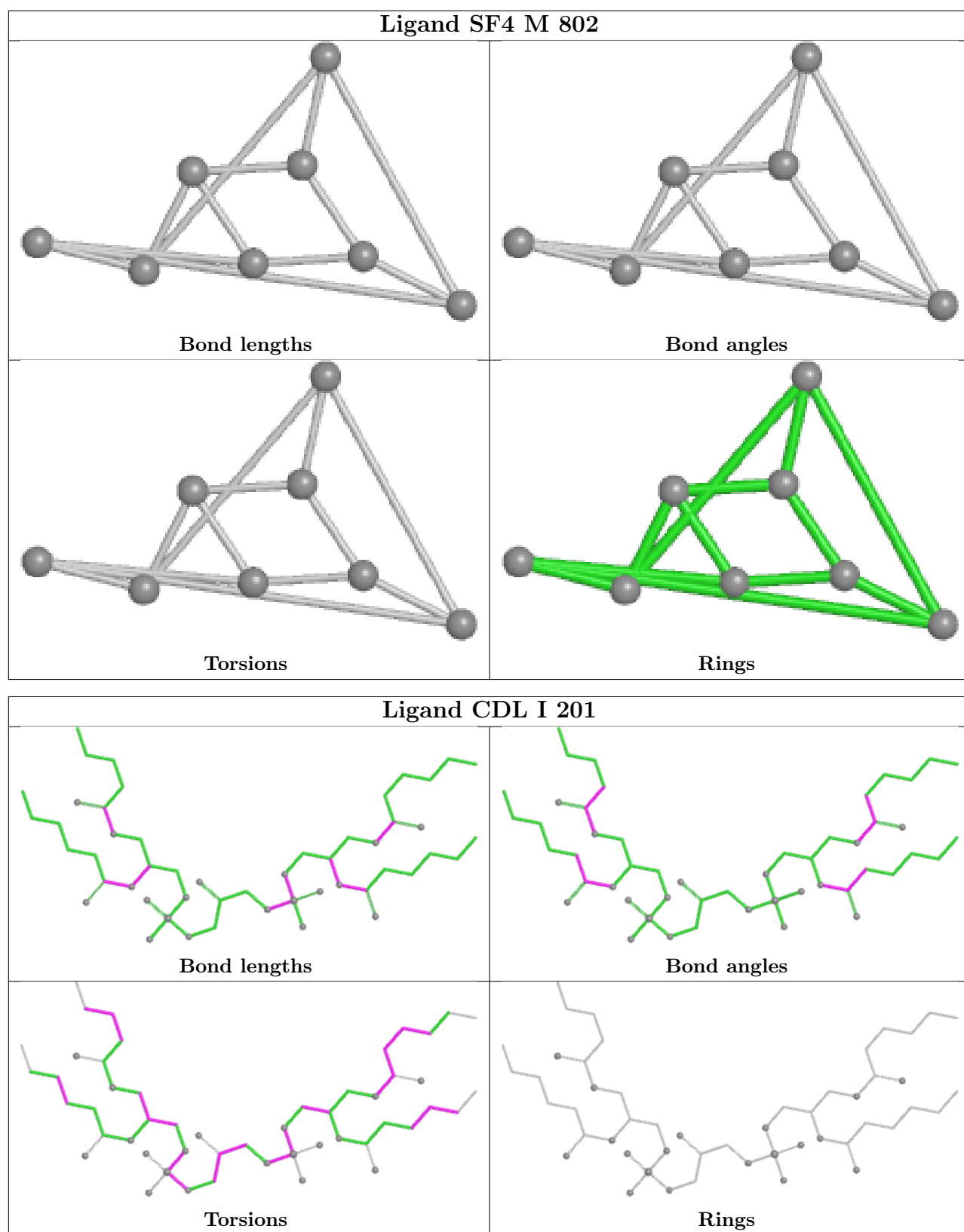












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

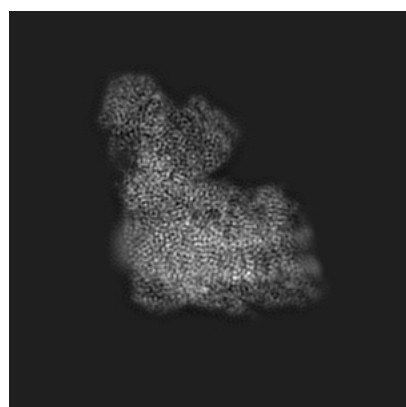
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32231. These allow visual inspection of the internal detail of the map and identification of artifacts.

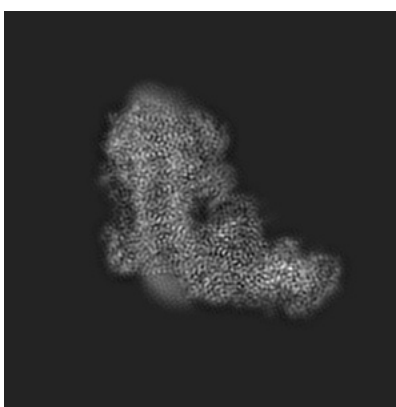
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

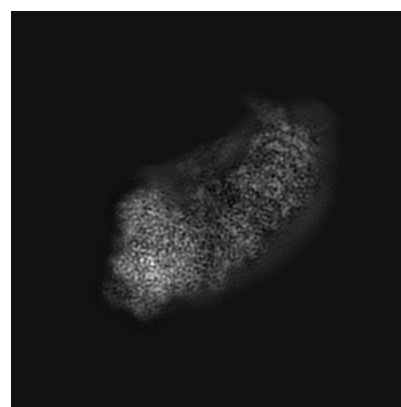
6.1.1 Primary map



X



Y

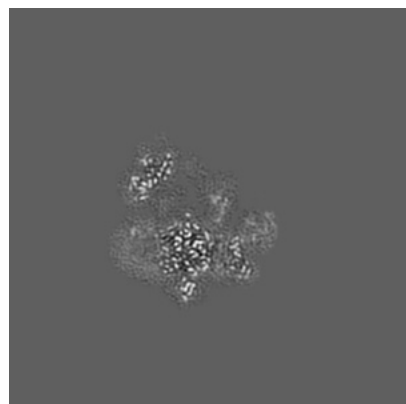


Z

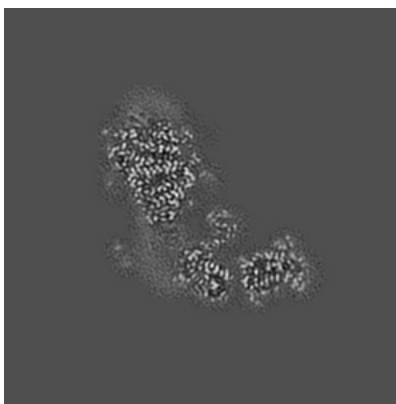
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

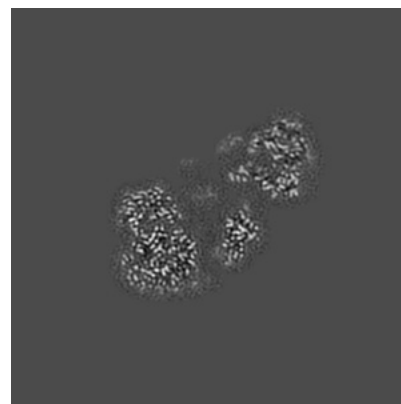
6.2.1 Primary map



X Index: 165



Y Index: 165

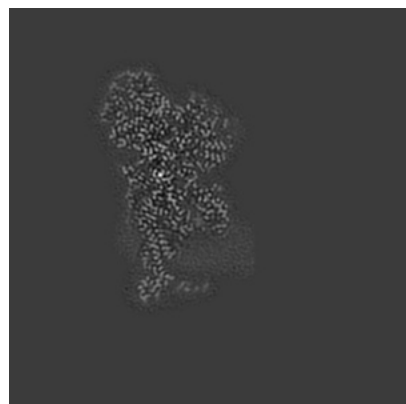


Z Index: 165

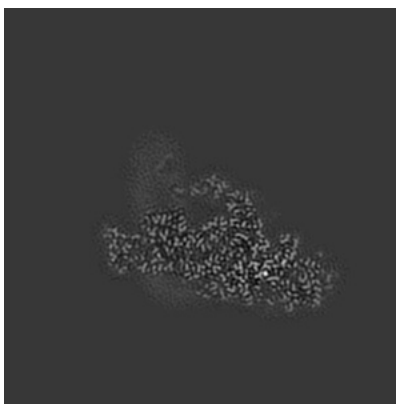
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

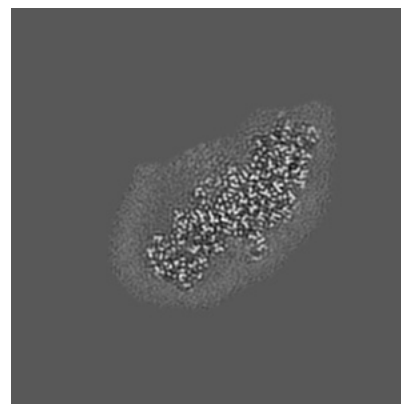
6.3.1 Primary map



X Index: 115



Y Index: 120

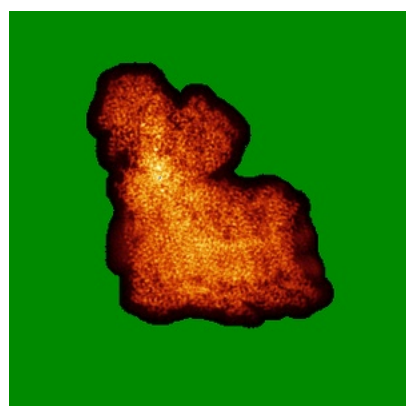


Z Index: 136

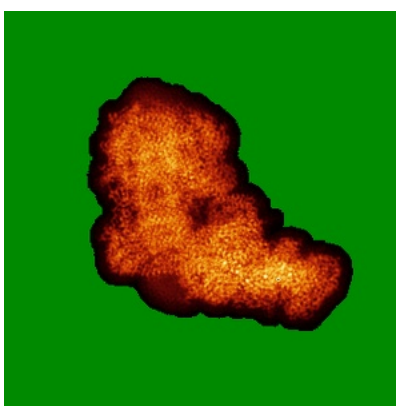
The images above show the largest variance slices of the map in three orthogonal directions.

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

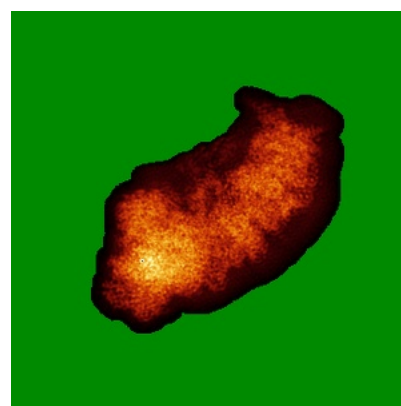
6.4.1 Primary map



X



Y

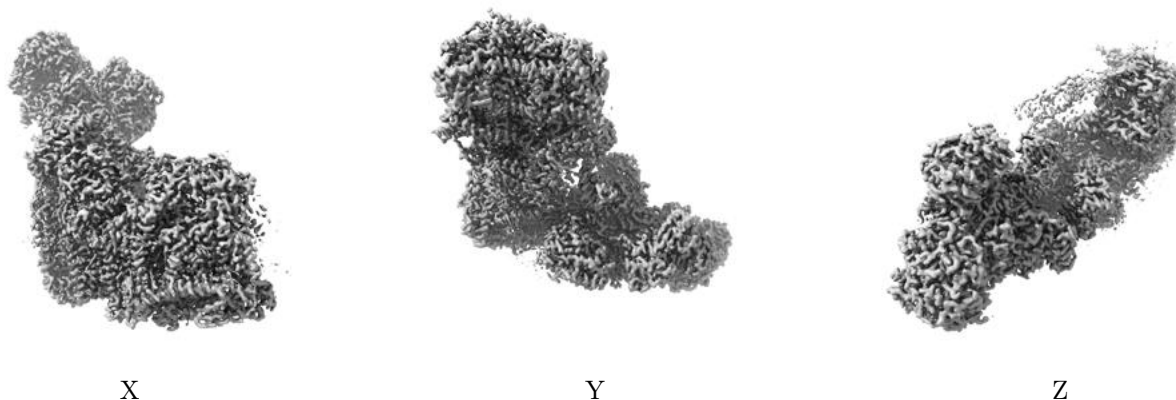


Z

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 0.0219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

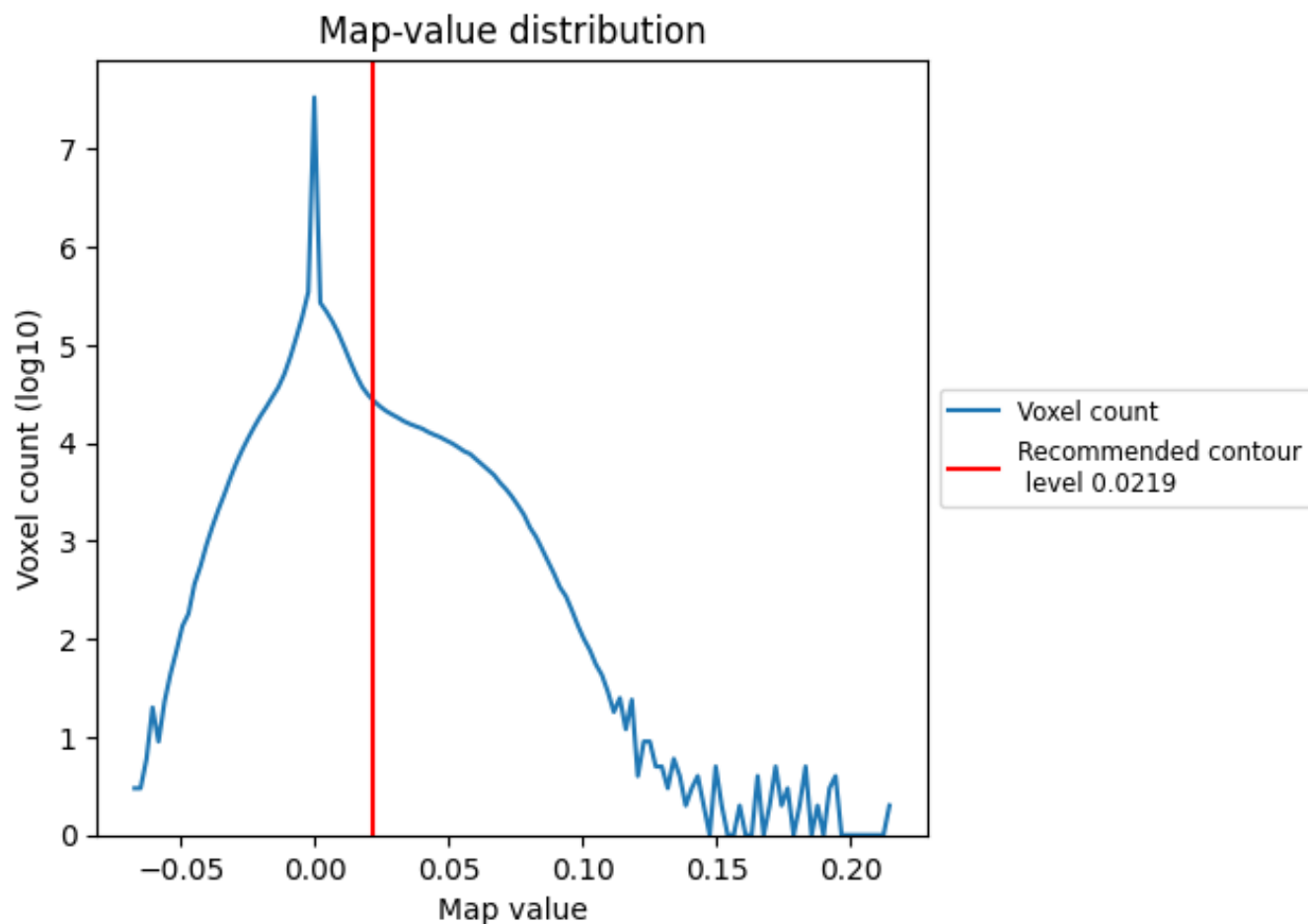
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

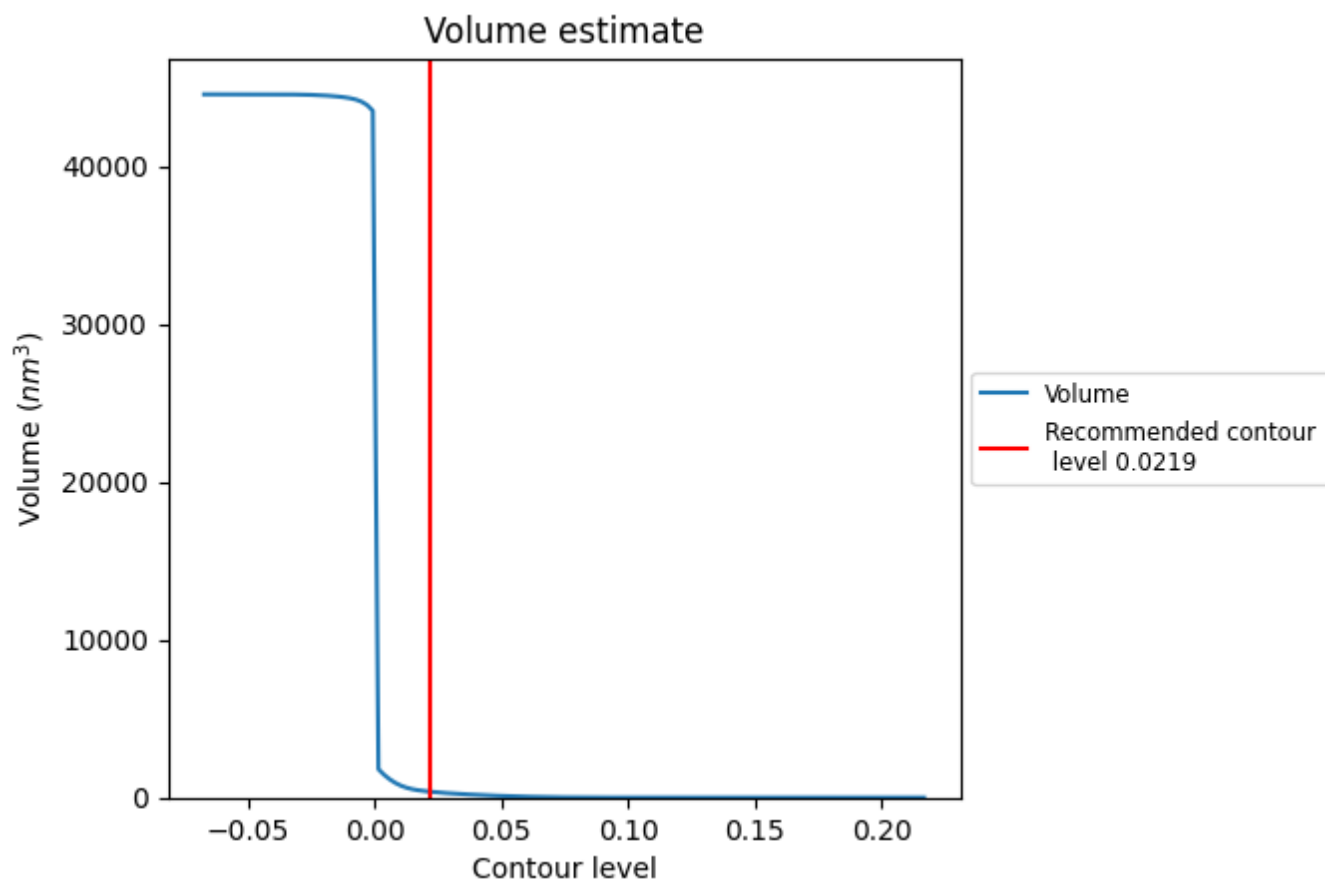
This section contains the results of statistical analysis of the map.

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.

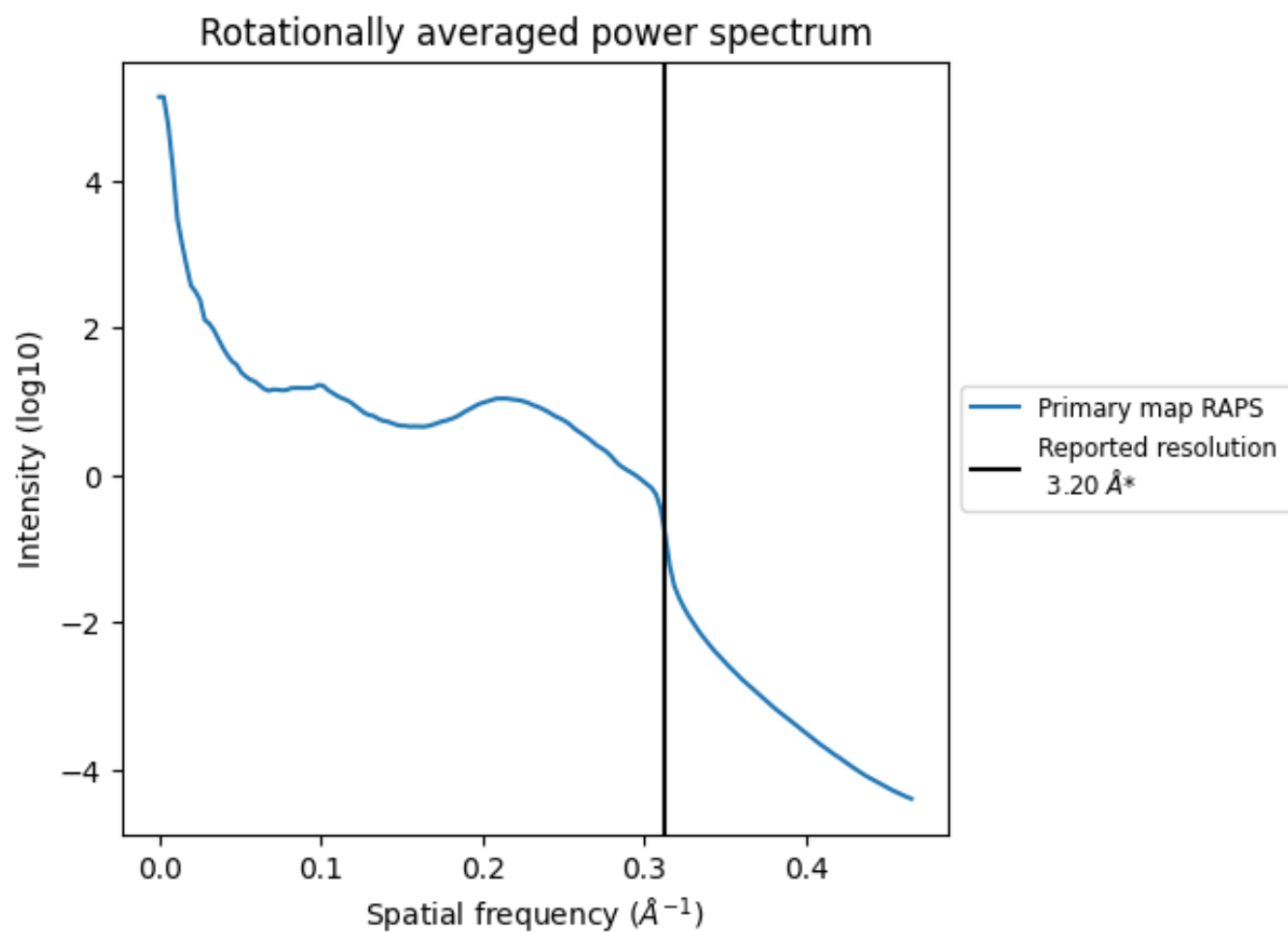
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369 nm³; this corresponds to an approximate mass of 333 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 0.312 Å⁻¹

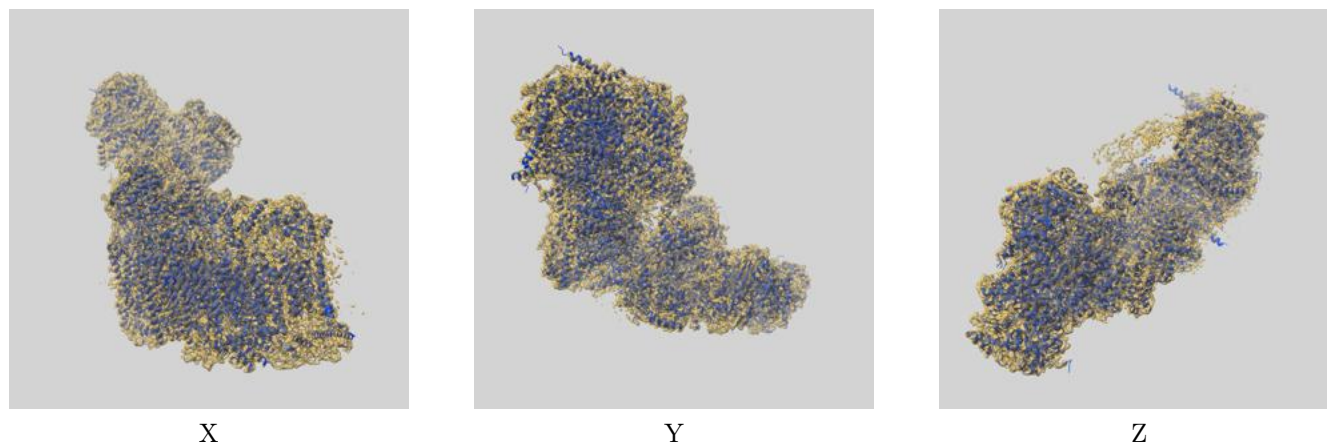
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

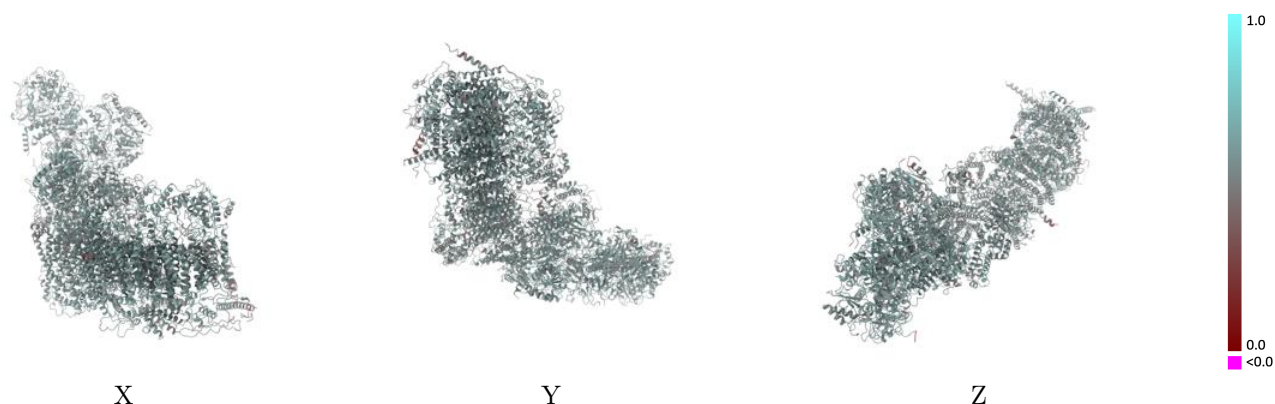
This section contains information regarding the fit between EMDB map EMD-32231 and PDB model 7VZW. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



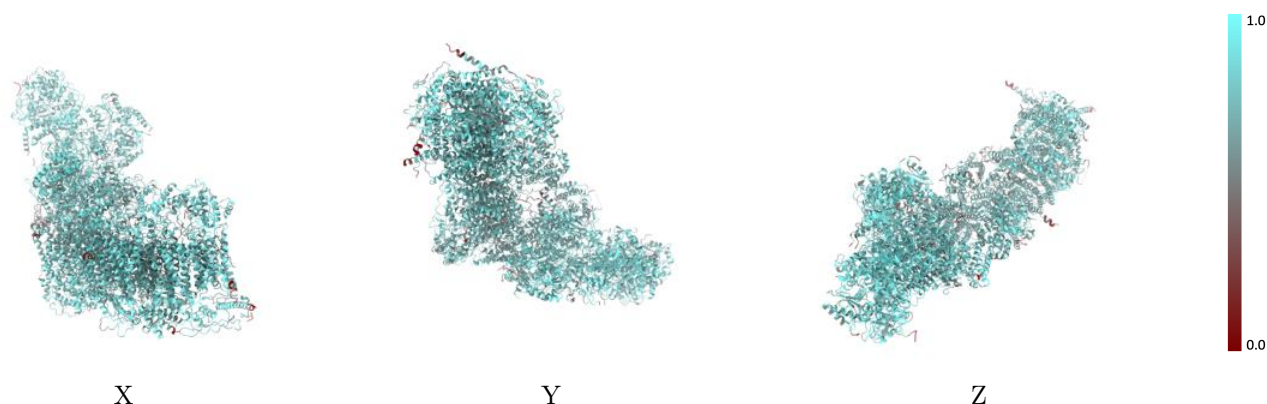
The images above show the 3D surface view of the map at the recommended contour level 0.0219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



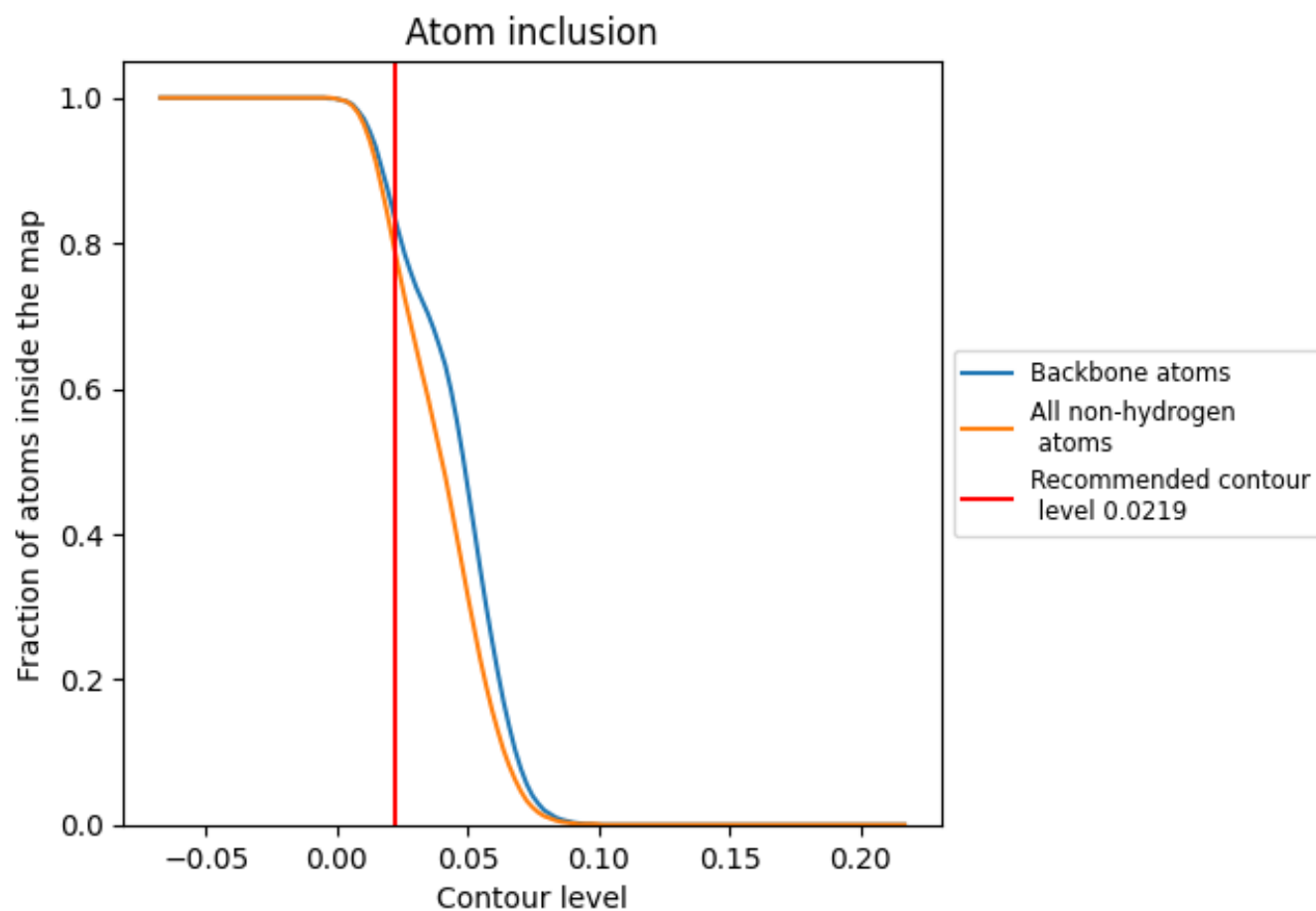
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0219).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.0219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.5560
A	 0.8090	 0.5550
B	 0.8760	 0.5770
C	 0.8200	 0.5770
E	 0.7940	 0.5580
F	 0.7470	 0.5250
G	 0.6060	 0.4690
H	 0.8000	 0.5550
I	 0.6690	 0.5400
J	 0.8230	 0.5670
K	 0.7660	 0.5480
L	 0.8020	 0.5690
M	 0.8320	 0.5670
N	 0.6990	 0.5500
O	 0.7990	 0.5510
P	 0.8660	 0.5840
Q	 0.8440	 0.5780
S	 0.8370	 0.5610
T	 0.7780	 0.5660
U	 0.7470	 0.5470
V	 0.6890	 0.5340
W	 0.7800	 0.5530
X	 0.7360	 0.5300
Y	 0.7380	 0.5210
Z	 0.6620	 0.5100
a	 0.8010	 0.5640
b	 0.7560	 0.5340
c	 0.7830	 0.5500
d	 0.7650	 0.5350
e	 0.7550	 0.5430
f	 0.6680	 0.5220
g	 0.8020	 0.5610
h	 0.7740	 0.5400
i	 0.8400	 0.5670
j	 0.7490	 0.5570



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Chain	Atom inclusion	Q-score
k	 0.8320	 0.5700
l	 0.7840	 0.5550
m	 0.7350	 0.5330
n	 0.6510	 0.5200
o	 0.7690	 0.5480
p	 0.8040	 0.5530
r	 0.8170	 0.5680
s	 0.8210	 0.5640
u	 0.8030	 0.5530
v	 0.7570	 0.5280
w	 0.7820	 0.5470