



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID : 7V2H / pdb_00007v2h
EMDB ID : EMD-31645
Title : Active state complex I from DQ-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-09
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

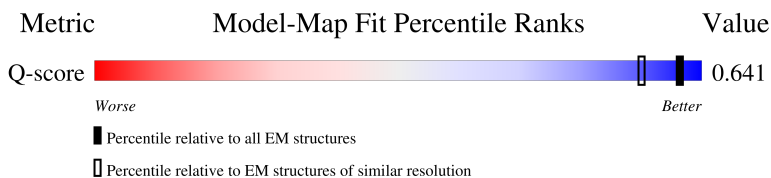
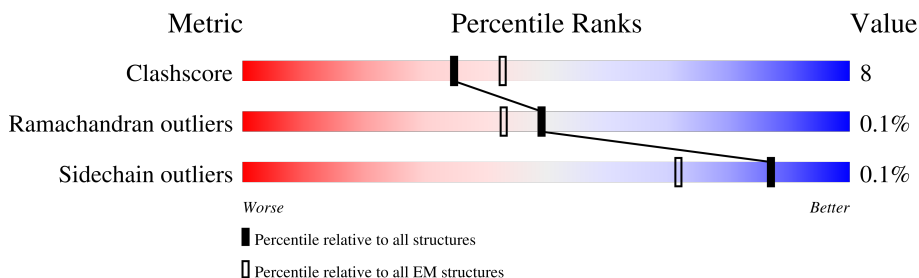
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	 83% 17%
2	B	176	 84% 16%
3	C	156	 87% 13%
4	E	115	 91% 9%

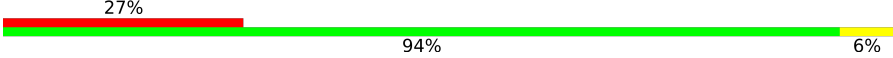
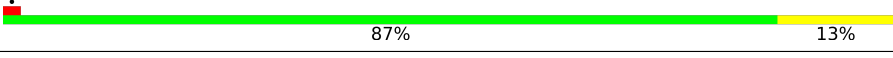
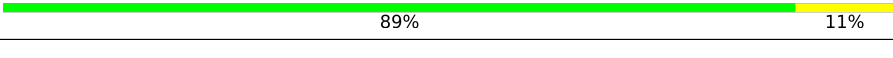
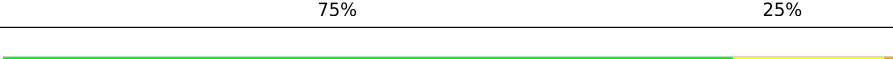
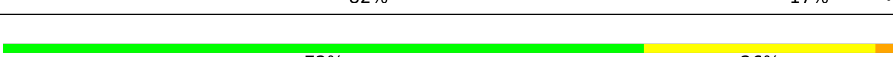
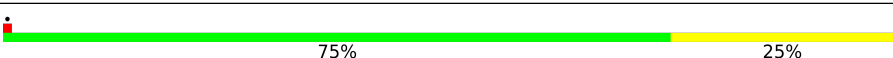
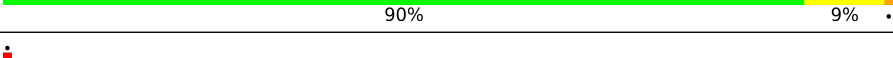
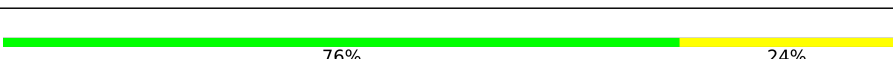
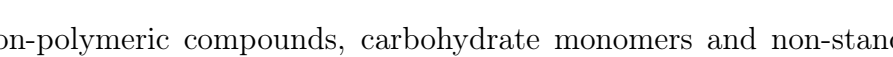
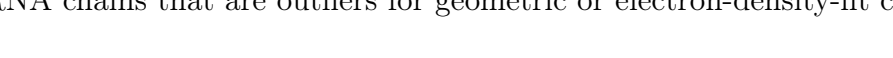
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	PEE	l	720	-	-	X	-
55	CDL	V	201	-	-	X	-
55	CDL	V	203	-	-	X	-
55	CDL	a	201	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 68293 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

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

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

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			693	447	103	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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 NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	6		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1277	852	187	225	13		

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

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

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

4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

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

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

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

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

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

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

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

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

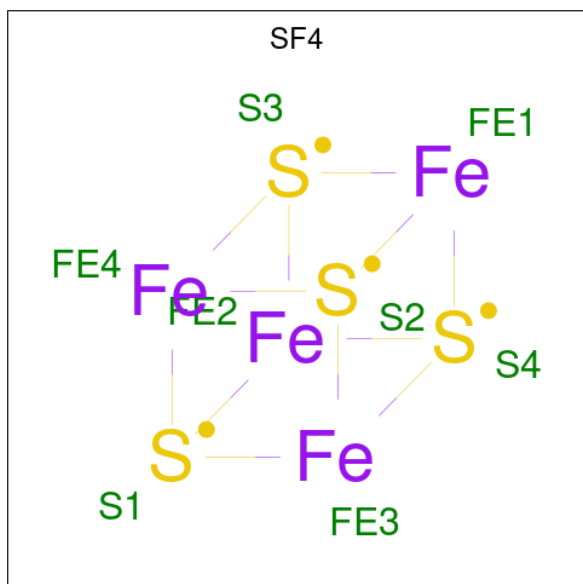
There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



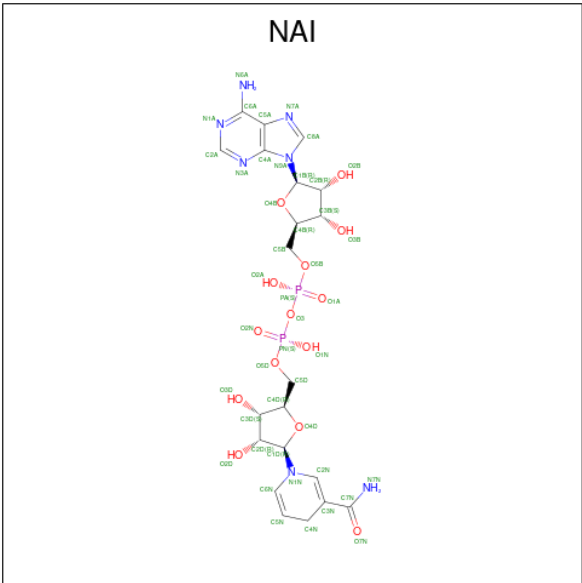
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



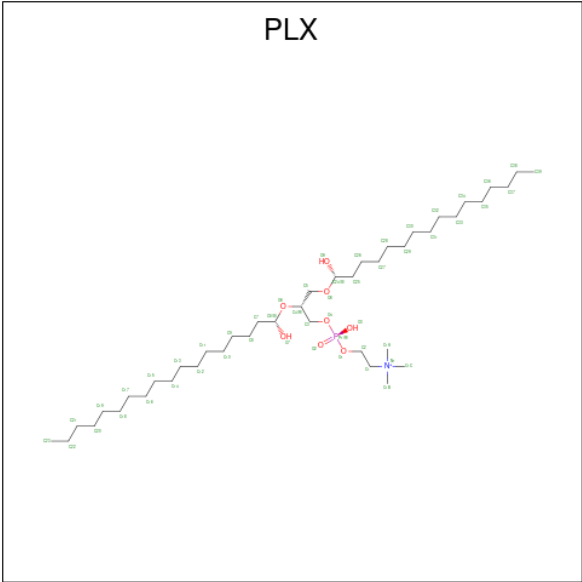
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



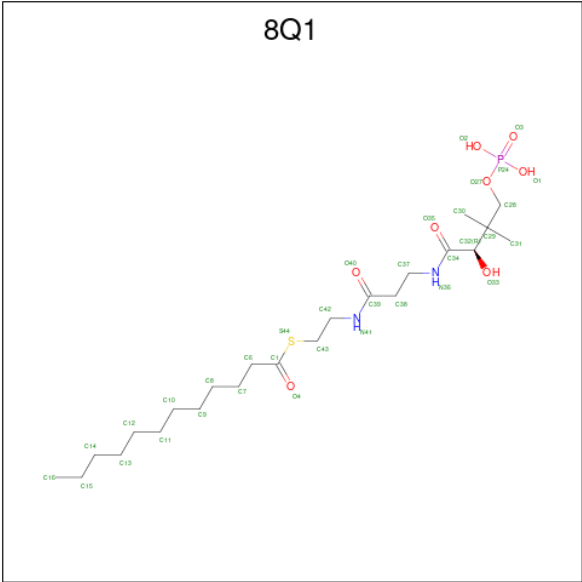
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



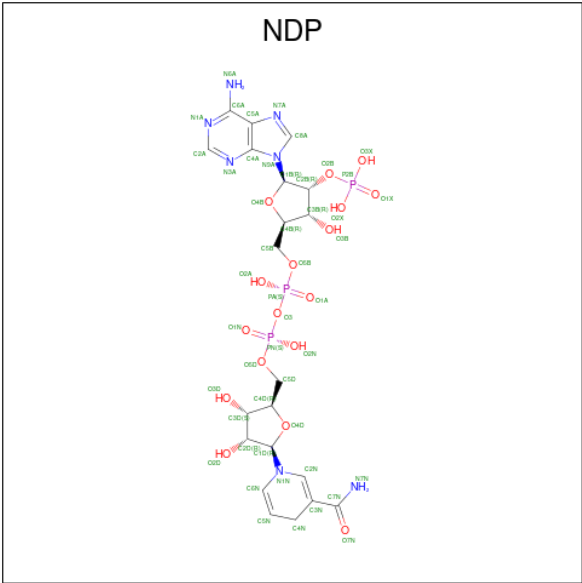
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	n	1	Total	C	N	O	P	0
			52	42	1	8	1	

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



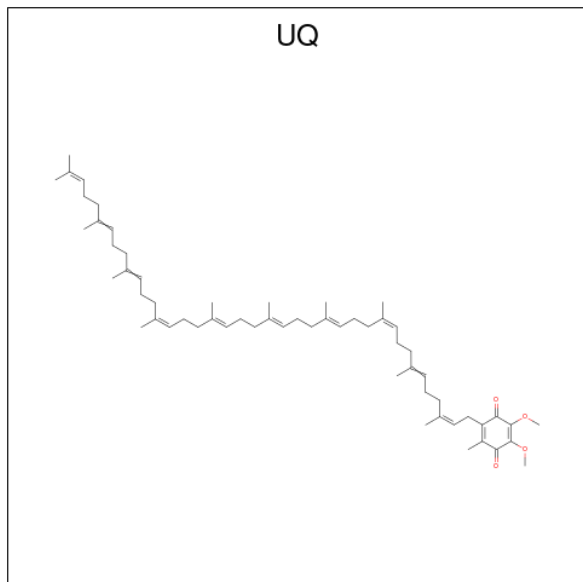
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is 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).



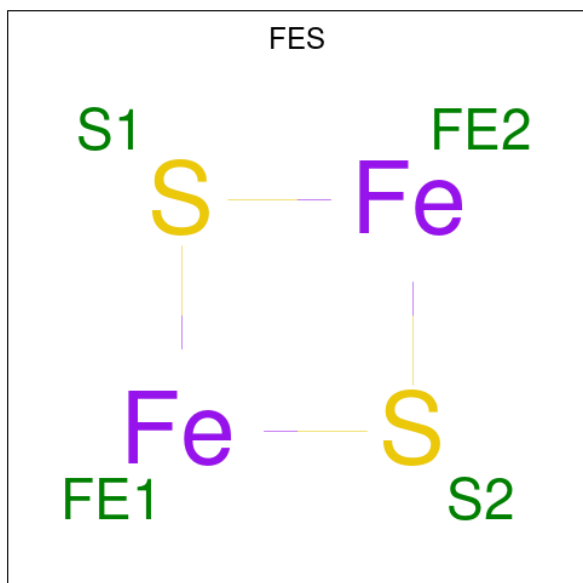
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

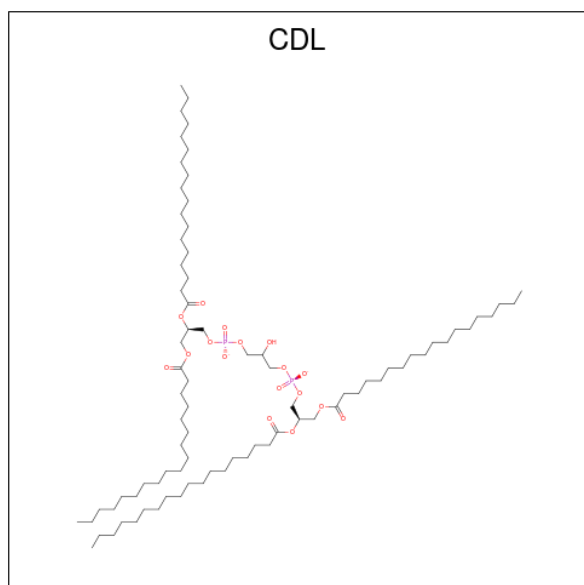


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

- 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 CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



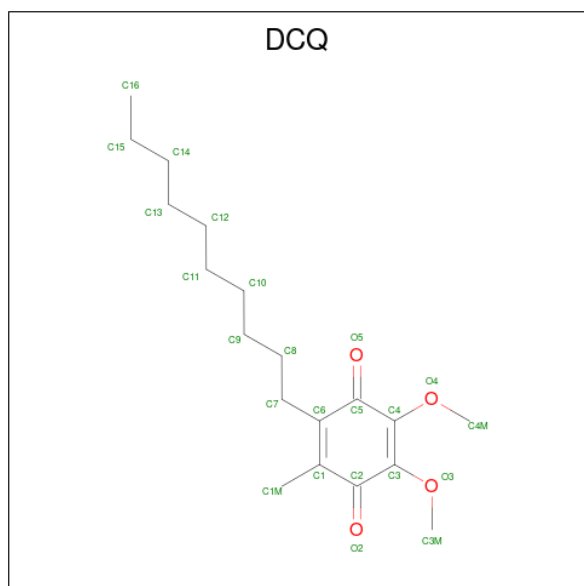
Mol	Chain	Residues	Atoms				AltConf
55	N	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	V	1	Total	C	O	P	0
			100	81	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	i	1	Total	C	O	P	0
			87	68	17	2	
55	k	1	Total	C	O	P	0
			100	81	17	2	

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

- Molecule 56 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$) (labeled as "Ligand of Interest" by depositor).

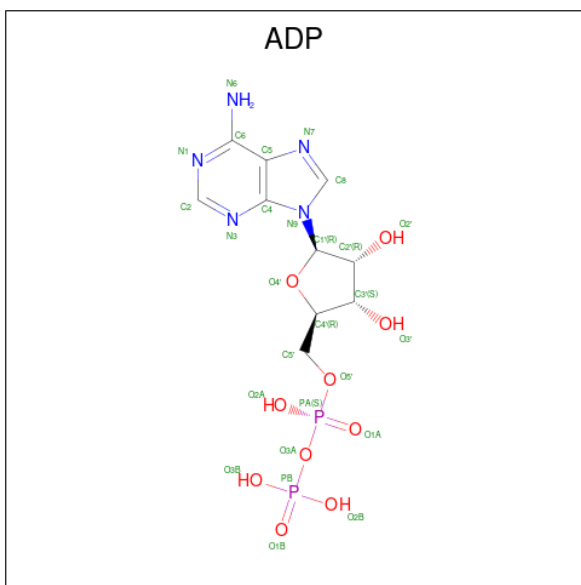


Mol	Chain	Residues	Atoms				AltConf
56	Q	1	Total	C	O		0
			23	19	4		

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

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

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

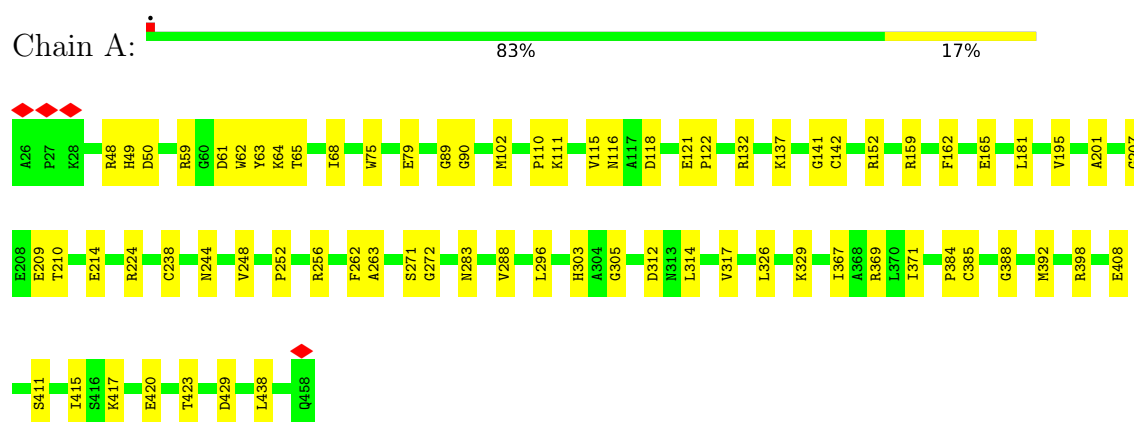


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

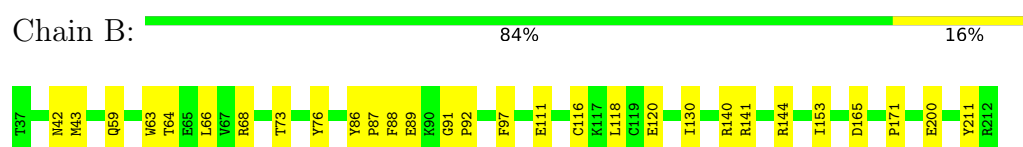
3 Residue-property plots [i](#)

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.

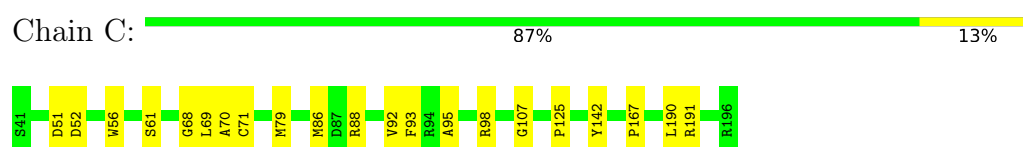
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



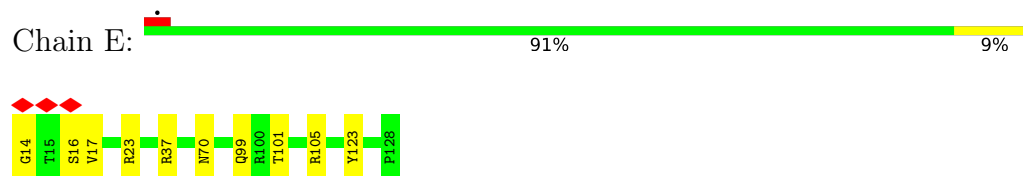
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



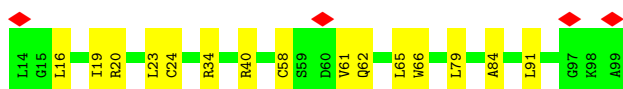
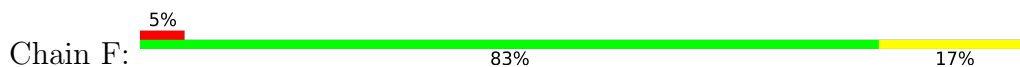
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



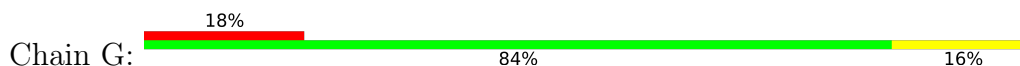
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



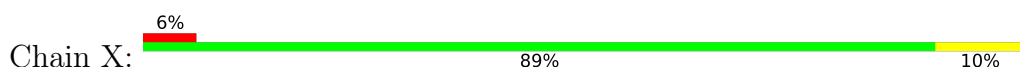
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



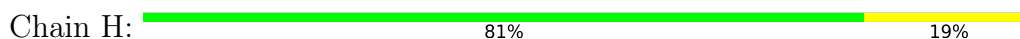
- Molecule 6: Acyl carrier protein, mitochondrial



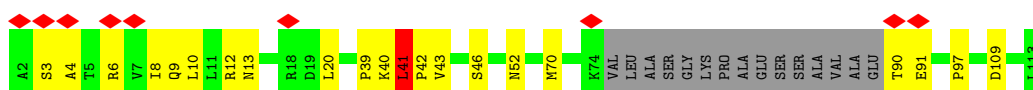
- Molecule 6: Acyl carrier protein, mitochondrial



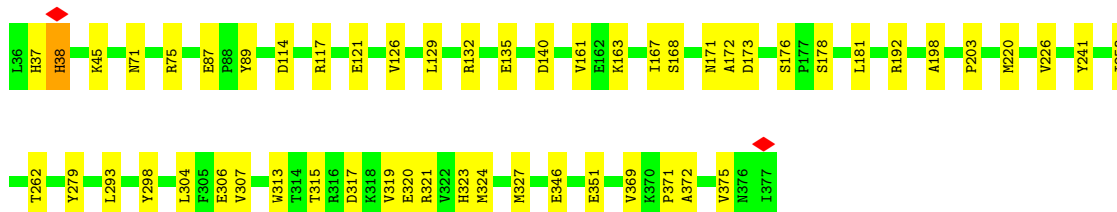
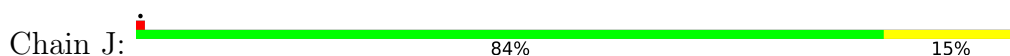
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



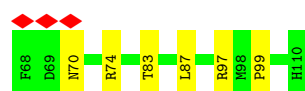
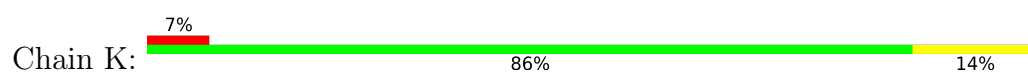
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



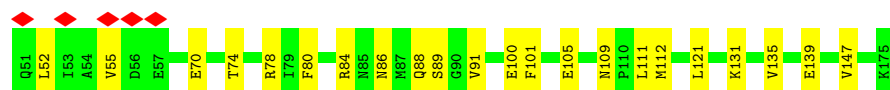
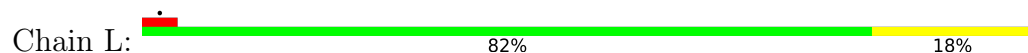
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



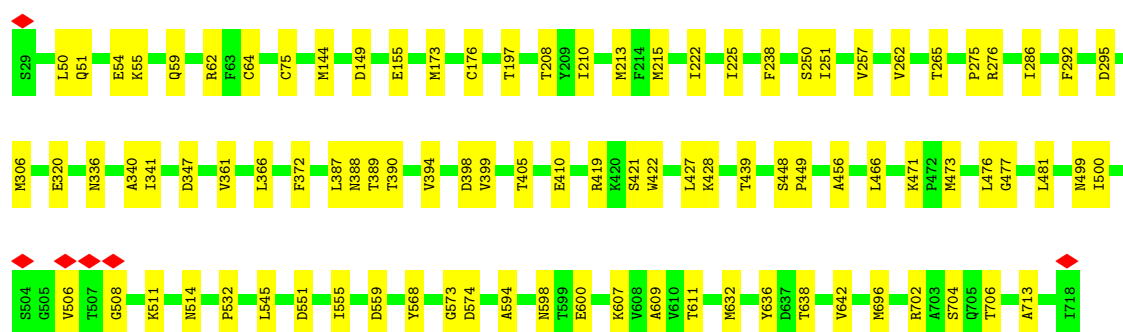
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



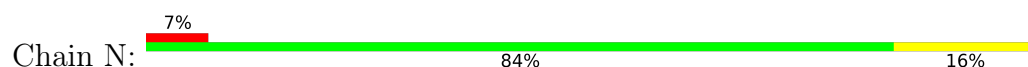
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



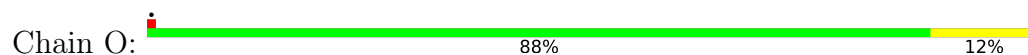
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



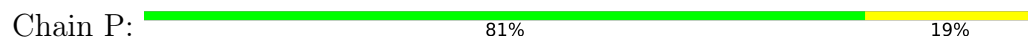
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

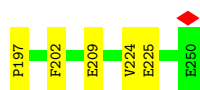


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

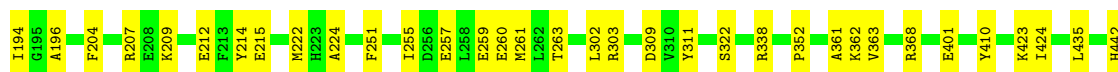
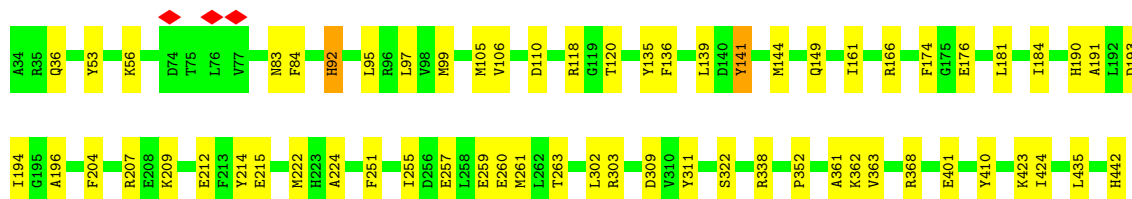
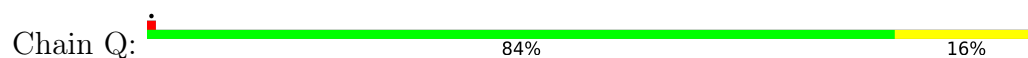


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

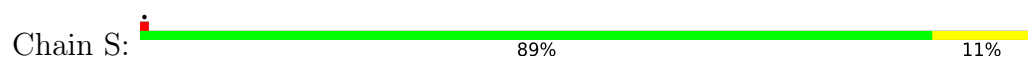




- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



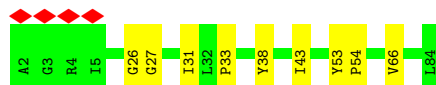
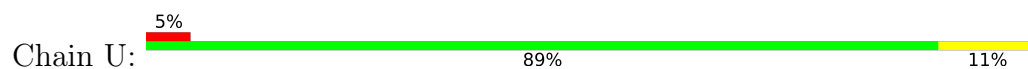
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



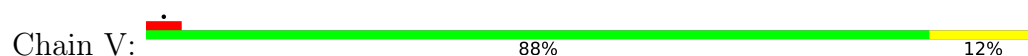
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



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



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W: 

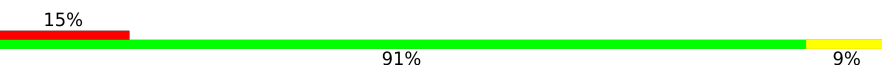


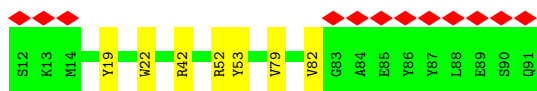
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 



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

Chain Z: 



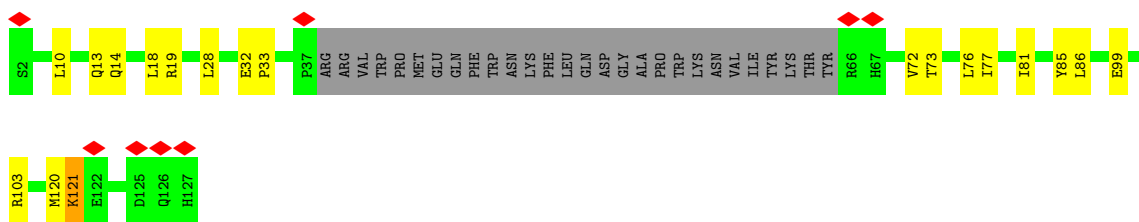
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 

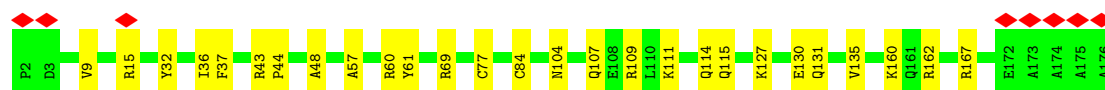
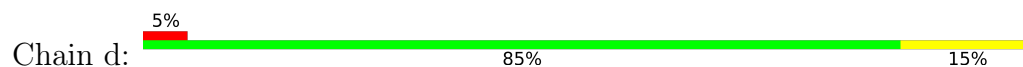


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

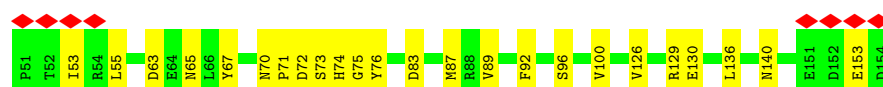
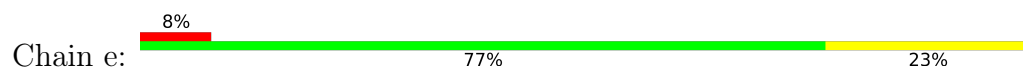
Chain c: 



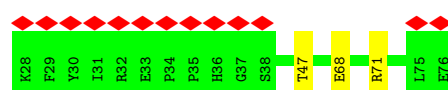
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



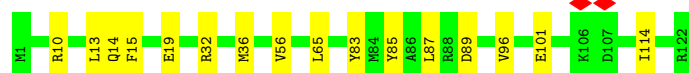
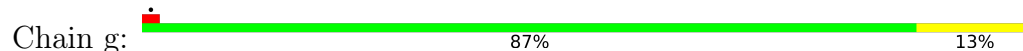
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



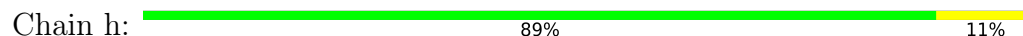
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



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



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

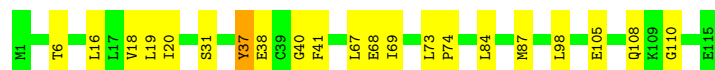
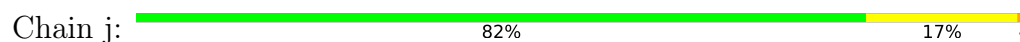


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2





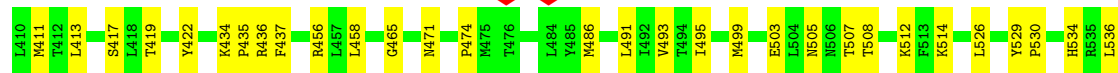
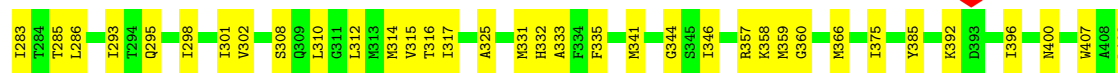
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



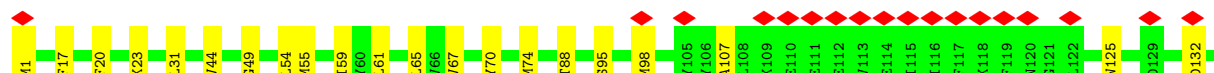
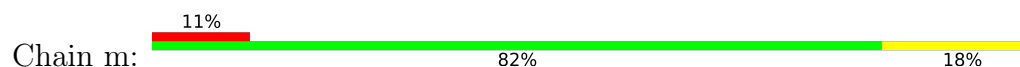
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



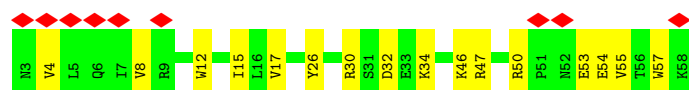
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



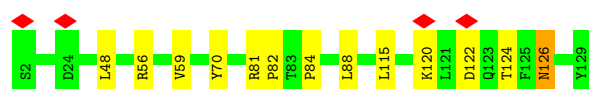
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



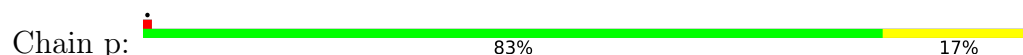
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



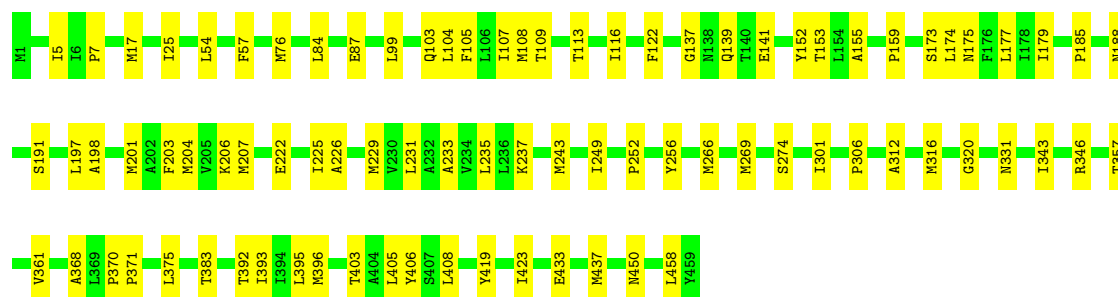
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



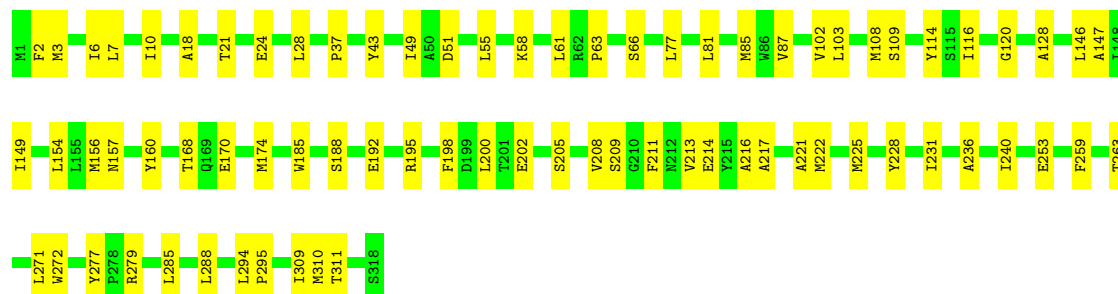
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

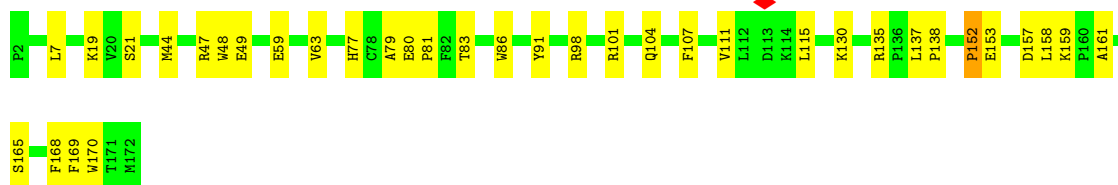


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



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

Chain u:  79% 20%



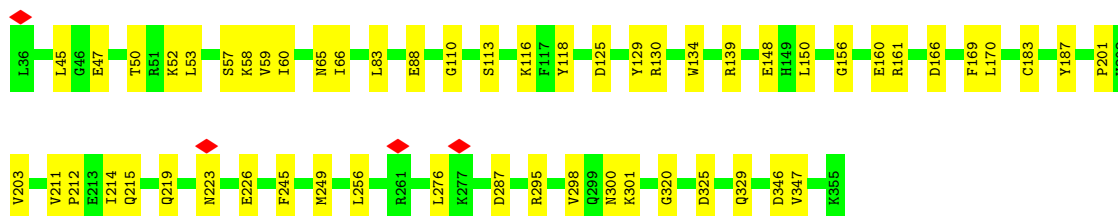
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  12% 82% 17%



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

Chain w:  83% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	462013	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	0.263	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0239	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	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: FES, FMN, PLX, DCQ, SF4, 2MR, 8Q1, PEE, ZN, NAI, CDL, NDP, MG, ADP, UQ

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	0.14	0/3406	0.35	0/4603
2	B	0.14	0/1443	0.35	0/1952
3	C	0.17	0/1279	0.39	0/1730
4	E	0.11	0/995	0.30	0/1340
5	F	0.12	0/698	0.34	0/940
6	G	0.19	0/705	0.46	0/956
6	X	0.14	0/704	0.41	0/953
7	H	0.18	0/929	0.48	0/1258
8	I	0.20	0/798	0.62	3/1079 (0.3%)
9	J	0.14	0/2828	0.36	0/3834
10	K	0.09	0/377	0.28	0/509
11	L	0.11	0/1039	0.29	0/1403
12	M	0.14	0/5384	0.37	0/7295
13	N	0.12	0/1245	0.32	0/1694
14	O	0.14	0/1711	0.39	0/2328
15	P	0.13	0/1789	0.32	0/2436
16	Q	0.30	3/3538 (0.1%)	0.37	1/4796 (0.0%)
17	S	0.14	0/581	0.44	0/781
18	T	0.14	0/755	0.38	0/1018
19	U	0.10	0/664	0.26	0/912
20	V	0.13	0/1042	0.30	0/1411
21	W	0.13	0/1192	0.29	0/1610
22	Y	0.11	0/610	0.33	0/836
23	Z	0.08	0/660	0.29	0/892
24	a	0.12	0/1184	0.33	0/1603
25	b	0.14	0/844	0.39	0/1149
26	c	0.15	0/1371	0.39	0/1875
27	d	0.11	0/1494	0.28	0/2015
28	e	0.11	0/891	0.32	0/1210
29	f	0.11	0/386	0.33	0/523
30	g	0.12	0/1036	0.28	0/1401
31	h	0.12	0/889	0.33	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.39	1/3768 (0.0%)
33	j	0.16	0/938	0.48	2/1281 (0.2%)
34	k	0.21	0/759	0.56	3/1029 (0.3%)
35	l	0.15	0/4929	0.38	0/6704
36	m	0.15	0/1309	0.39	0/1780
37	n	0.11	0/491	0.29	0/663
38	o	0.17	0/1092	0.42	0/1481
39	p	0.11	0/1590	0.27	0/2155
40	r	0.15	0/3723	0.36	0/5078
41	s	0.21	0/2581	0.50	3/3529 (0.1%)
42	u	0.17	0/1436	0.44	1/1938 (0.1%)
43	v	0.12	0/1052	0.37	0/1411
44	w	0.11	0/2642	0.33	0/3580
All	All	0.16	3/67782 (0.0%)	0.37	14/91929 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	1
25	b	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	193	ASP	C-N	10.40	1.47	1.33
16	Q	92	HIS	C-N	-8.91	1.22	1.33
16	Q	141	TYR	C-N	-6.94	1.24	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	41	LEU	CA-C-N	7.79	127.80	119.78
8	I	41	LEU	C-N-CA	7.79	127.80	119.78
8	I	43	VAL	N-CA-C	6.59	117.24	110.05
34	k	24	SER	N-CA-C	6.29	118.13	111.28
16	Q	224	ALA	N-CA-C	6.27	118.11	111.28
41	s	217	ALA	N-CA-C	6.15	118.47	108.08
41	s	200	LEU	N-CA-C	5.88	117.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	324	LYS	N-CA-C	5.74	117.53	111.28
33	j	37	TYR	N-CA-C	5.53	117.54	108.52
42	u	169	PHE	N-CA-C	5.52	118.23	111.82
34	k	25	HIS	N-CA-C	5.37	118.30	109.76
41	s	217	ALA	CB-CA-C	-5.35	110.42	116.63
34	k	22	TYR	N-CA-C	5.18	117.69	109.24
33	j	31	SER	N-CA-C	5.02	116.76	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	P	44	ARG	Peptide
25	b	121	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	54	0
2	B	1412	0	1363	23	0
3	C	1248	0	1254	20	0
4	E	971	0	975	9	0
5	F	687	0	700	9	0
6	G	693	0	671	14	0
6	X	693	0	671	7	0
7	H	910	0	950	13	0
8	I	780	0	808	25	0
9	J	2751	0	2773	40	0
10	K	366	0	338	6	0
11	L	1016	0	1016	18	0
12	M	5296	0	5327	60	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	17	0
15	P	1738	0	1693	25	0
16	Q	3459	0	3396	52	0
17	S	566	0	561	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	T	741	0	702	6	0
19	U	643	0	642	9	0
20	V	1021	0	1025	20	0
21	W	1161	0	1144	19	0
22	Y	584	0	529	10	0
23	Z	641	0	620	6	0
24	a	1151	0	1164	17	0
25	b	819	0	835	24	0
26	c	1315	0	1208	19	0
27	d	1461	0	1429	25	0
28	e	867	0	817	23	0
29	f	378	0	356	2	0
30	g	1005	0	999	14	0
31	h	867	0	871	12	0
32	i	2710	0	2874	61	0
33	j	914	0	951	21	0
34	k	748	0	799	22	0
35	l	4800	0	4939	119	0
36	m	1277	0	1239	30	0
37	n	479	0	486	13	0
38	o	1062	0	1072	13	0
39	p	1534	0	1470	20	0
40	r	3631	0	3839	69	0
41	s	2508	0	2607	67	0
42	u	1398	0	1374	26	0
43	v	1028	0	982	17	0
44	w	2582	0	2531	39	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
47	A	44	0	27	6	0
48	C	47	0	71	6	0
48	U	51	0	82	4	0
48	V	91	0	136	18	0
48	j	41	0	59	7	0
48	l	144	0	222	48	0
48	m	41	0	59	9	0
48	s	51	0	82	5	0
49	C	52	0	88	5	0
49	V	52	0	88	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	e	52	0	88	19	0
49	i	52	0	88	4	0
49	j	104	0	176	16	0
49	n	52	0	88	0	0
50	G	35	0	0	1	0
50	X	35	0	0	1	0
51	J	48	0	26	3	0
52	J	33	0	39	5	0
52	s	38	0	47	3	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	N	51	0	46	11	0
55	V	194	0	294	46	0
55	a	100	0	156	21	0
55	i	87	0	124	4	0
55	k	100	0	156	7	0
55	l	199	0	305	25	0
55	m	89	0	125	7	0
55	n	55	0	54	6	0
55	r	100	0	156	4	0
56	Q	23	0	30	8	0
57	T	1	0	0	0	0
58	w	27	0	11	6	0
All	All	68293	0	69069	1096	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 8.

All (1096) 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)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.23
49:e:201:PLX:H151	55:l:712:CDL:H802	1.20	1.19
16:Q:92:HIS:ND1	56:Q:501:DCQ:H3MB	1.61	1.15
55:a:201:CDL:H642	55:a:201:CDL:H602	1.16	1.13
55:V:203:CDL:H342	55:V:203:CDL:H111	1.11	1.08
48:l:718:PEE:H34	48:l:718:PEE:H42	1.16	1.07
55:V:203:CDL:H372	55:V:203:CDL:H322	1.13	1.07
55:V:203:CDL:H152	55:V:203:CDL:H351	1.35	1.06
8:I:40:LYS:HB3	21:W:7:LYS:H	1.18	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:202:PEE:H33	48:m:202:PEE:H42	1.38	1.04
6:G:103:HIS:N	6:G:107:ASP:OD2	1.91	1.03
55:l:712:CDL:H242	48:l:720:PEE:H34	1.39	1.03
55:V:203:CDL:H111	55:V:203:CDL:C34	1.90	1.01
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.42	1.00
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.09	1.00
49:e:201:PLX:O2	48:l:720:PEE:H10	1.60	1.00
1:A:121:GLU:HG2	47:A:503:NAI:H42N	1.40	1.00
55:V:203:CDL:H242	55:V:203:CDL:H451	1.44	1.00
55:a:201:CDL:H251	55:a:201:CDL:H211	1.48	0.96
55:V:203:CDL:H322	55:V:203:CDL:C37	1.95	0.95
55:a:201:CDL:H871	55:a:201:CDL:H832	1.48	0.95
48:j:201:PEE:H31	55:m:201:CDL:H222	1.48	0.93
6:G:103:HIS:H	6:G:107:ASP:CG	1.76	0.93
48:V:202:PEE:H33	48:V:202:PEE:H71	1.49	0.91
49:e:201:PLX:H181	55:l:712:CDL:H801	1.53	0.91
49:j:202:PLX:H371	49:j:202:PLX:H331	1.53	0.90
55:V:203:CDL:H362	55:V:203:CDL:H401	1.56	0.88
49:e:201:PLX:H151	55:l:712:CDL:C80	2.04	0.87
33:j:20:ILE:HD11	49:j:202:PLX:H201	1.53	0.87
55:V:201:CDL:H321	35:l:576:MET:HE1	1.56	0.86
26:c:116:ARG:HG2	48:l:719:PEE:H49	1.57	0.86
48:V:202:PEE:H47	40:r:155:ALA:HB3	1.56	0.86
55:n:102:CDL:H581	55:n:102:CDL:H541	1.57	0.85
20:V:59:TYR:CD1	55:V:201:CDL:H112	2.11	0.85
41:s:288:LEU:HD11	48:s:401:PEE:H7	1.59	0.84
55:V:201:CDL:C32	35:l:576:MET:HE1	2.07	0.84
55:N:202:CDL:H532	55:N:202:CDL:OA9	1.78	0.83
55:V:201:CDL:H321	35:l:576:MET:CE	2.09	0.82
41:s:288:LEU:CD1	48:s:401:PEE:H7	2.09	0.82
55:a:201:CDL:H642	55:a:201:CDL:C60	2.03	0.82
49:e:201:PLX:C15	55:l:712:CDL:H802	2.06	0.81
49:j:202:PLX:H371	49:j:202:PLX:C33	2.10	0.81
48:l:718:PEE:H34	48:l:718:PEE:C25	2.06	0.80
48:m:202:PEE:H33	48:m:202:PEE:C25	2.11	0.80
32:i:295:ARG:NH2	48:l:718:PEE:O2P	2.10	0.80
48:V:202:PEE:H40	48:V:202:PEE:H79	1.63	0.80
9:J:220:MET:HE2	9:J:226:VAL:HG13	1.64	0.80
48:l:718:PEE:H42	48:l:718:PEE:C21	2.06	0.80
16:Q:141:TYR:CE1	56:Q:501:DCQ:H4M	2.17	0.79
48:l:718:PEE:H36	48:l:718:PEE:H28	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:34:LYS:NZ	55:n:102:CDL:HB22	1.98	0.79
55:a:201:CDL:H111	48:l:720:PEE:H60	1.63	0.79
37:n:34:LYS:HZ3	55:n:102:CDL:HB22	1.47	0.78
8:I:8:ILE:HD11	55:N:202:CDL:H111	1.64	0.77
49:j:202:PLX:H6	49:j:202:PLX:O4	1.84	0.77
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.64	0.77
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.65	0.77
4:E:70:ASN:O	50:G:201:8Q1:C38	2.33	0.76
55:a:201:CDL:H871	55:a:201:CDL:C83	2.15	0.76
1:A:121:GLU:HG2	47:A:503:NAI:C4N	2.17	0.75
49:e:201:PLX:H21	48:l:720:PEE:H2	1.69	0.75
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.67	0.75
25:b:103:ARG:HH12	43:v:67:LEU:HD13	1.52	0.74
1:A:50:ASP:O	1:A:59:ARG:NH2	2.20	0.74
41:s:156:MET:HB3	41:s:174:MET:HE3	1.69	0.74
24:a:95:GLU:CD	55:a:201:CDL:H1O1	1.95	0.74
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.69	0.74
35:l:257:VAL:HG13	35:l:317:ILE:HD11	1.70	0.74
55:l:712:CDL:H242	48:l:720:PEE:C21	2.17	0.73
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.71	0.73
48:m:202:PEE:C1	48:m:202:PEE:H10	2.19	0.73
35:l:103:PHE:HB2	35:l:341:MET:HE3	1.69	0.73
33:j:73:LEU:HD12	36:m:55:MET:HE1	1.69	0.72
34:k:79:VAL:HG22	36:m:74:MET:HE1	1.71	0.72
21:W:94:GLU:OE2	21:W:104:TRP:NE1	2.23	0.72
25:b:85:TYR:OH	48:l:720:PEE:H15	1.89	0.72
55:V:203:CDL:H401	55:V:203:CDL:C36	2.16	0.72
48:m:202:PEE:H10	48:m:202:PEE:H2	1.72	0.72
49:j:202:PLX:H331	49:j:202:PLX:C37	2.20	0.72
8:I:40:LYS:HB3	21:W:7:LYS:N	2.01	0.72
49:e:201:PLX:H21	48:l:720:PEE:C1	2.19	0.71
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.72	0.71
35:l:228:GLY:HA3	48:l:719:PEE:H38	1.73	0.71
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.26	0.71
48:l:718:PEE:H28	48:l:718:PEE:C22	2.21	0.70
48:V:202:PEE:H40	48:V:202:PEE:C46	2.21	0.70
55:V:203:CDL:H392	38:o:88:LEU:HD21	1.72	0.70
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.74	0.70
1:A:152:ARG:NH2	10:K:99:PRO:O	2.25	0.70
9:J:132:ARG:HH21	51:J:401:NDP:H51A	1.55	0.69
34:k:23:ARG:HG3	36:m:23:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:r:714:CDL:H221	55:r:714:CDL:H401	1.74	0.69
44:w:125:ASP:O	44:w:130:ARG:NH2	2.26	0.69
44:w:139:ARG:HH12	58:w:401:ADP:N6	1.85	0.69
8:I:6:ARG:HH21	8:I:10:LEU:HD11	1.57	0.69
48:V:207:PEE:H8	48:V:207:PEE:O2P	1.92	0.69
24:a:95:GLU:CD	55:a:201:CDL:O1	2.36	0.69
24:a:78:THR:HG21	28:e:96:SER:HA	1.74	0.69
8:I:9:GLN:O	8:I:13:ASN:ND2	2.26	0.69
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.73	0.69
44:w:47:GLU:OE2	44:w:52:LYS:NZ	2.26	0.69
38:o:126:ASN:N	38:o:126:ASN:HD22	1.89	0.68
40:r:231:LEU:HD23	40:r:235:LEU:HD12	1.76	0.68
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.26	0.68
55:a:201:CDL:H382	27:d:48:ALA:HB2	1.75	0.68
3:C:95:ALA:HB1	41:s:208:VAL:HG13	1.76	0.68
7:H:101:GLU:HB3	7:H:102:PRO:HD2	1.74	0.68
5:F:16:LEU:HD21	5:F:19:ILE:HD11	1.76	0.68
16:Q:141:TYR:HE1	56:Q:501:DCQ:H4M	1.56	0.68
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.76	0.67
44:w:118:TYR:OH	58:w:401:ADP:O3'	2.06	0.67
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.11	0.67
5:F:65:LEU:HB2	5:F:79:LEU:HD11	1.77	0.67
35:l:419:THR:HA	35:l:422:TYR:CE2	2.30	0.67
48:l:718:PEE:H37	48:l:718:PEE:H60	1.77	0.66
6:X:91:ASP:OD2	23:Z:42:ARG:NH1	2.27	0.66
34:k:44:SER:HB2	34:k:59:MET:HE1	1.78	0.66
55:m:201:CDL:H871	48:m:202:PEE:H47	1.78	0.66
40:r:403:THR:HA	40:r:406:TYR:CE2	2.29	0.66
20:V:36:VAL:HG22	55:V:201:CDL:H742	1.77	0.66
35:l:495:ILE:HG22	35:l:499:MET:HE2	1.76	0.66
55:l:713:CDL:H422	55:l:713:CDL:H621	1.78	0.65
16:Q:92:HIS:ND1	56:Q:501:DCQ:C3M	2.51	0.65
35:l:69:MET:HE3	35:l:76:LEU:HD12	1.78	0.65
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.77	0.65
35:l:68:TRP:CZ3	35:l:69:MET:HE2	2.32	0.65
14:O:38:LEU:O	14:O:124:ARG:NH2	2.29	0.65
43:v:51:LEU:O	43:v:52:MET:HG3	1.97	0.65
35:l:67:HIS:O	48:l:720:PEE:H12	1.98	0.64
12:M:555:ILE:HG23	12:M:559:ASP:HB2	1.80	0.64
40:r:370:PRO:HG3	40:r:375:LEU:HD13	1.80	0.64
8:I:3:SER:O	55:N:202:CDL:HA22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:342:ALA:HB3	49:i:705:PLX:H332	1.80	0.64
2:B:42:ASN:O	2:B:43:MET:HE2	1.97	0.64
41:s:24:GLU:OE2	41:s:228:TYR:OH	2.10	0.64
35:l:286:LEU:HD13	35:l:411:MET:SD	2.37	0.63
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.81	0.63
19:U:26:GLY:HA3	48:U:101:PEE:H37	1.80	0.63
41:s:277:TYR:HE2	48:s:401:PEE:H59	1.63	0.63
11:L:109:ASN:ND2	11:L:111:LEU:O	2.29	0.63
32:i:69:MET:CE	32:i:100:MET:HE3	2.29	0.63
36:m:61:LEU:O	41:s:114:TYR:OH	2.16	0.63
41:s:277:TYR:CE2	48:s:401:PEE:H59	2.33	0.63
33:j:20:ILE:HD11	49:j:202:PLX:C20	2.28	0.63
16:Q:53:TYR:OH	32:i:295:ARG:NH2	2.32	0.63
5:F:24:CYS:N	5:F:58:CYS:SG	2.72	0.63
41:s:156:MET:HB3	41:s:174:MET:CE	2.28	0.63
41:s:18:ALA:O	41:s:21:THR:OG1	2.17	0.63
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.80	0.62
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.79	0.62
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.62
21:W:120:MET:HB3	21:W:123:GLU:HG3	1.82	0.62
34:k:37:MET:HG2	34:k:67:ALA:HB2	1.82	0.62
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.32	0.62
32:i:218:LEU:HB3	32:i:244:MET:HE2	1.80	0.62
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.80	0.62
55:V:203:CDL:H342	55:V:203:CDL:C11	2.07	0.62
25:b:85:TYR:CZ	48:l:720:PEE:H15	2.35	0.62
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.82	0.62
32:i:97:MET:HA	32:i:100:MET:HE2	1.80	0.62
48:j:201:PEE:H40	41:s:77:LEU:HD12	1.82	0.62
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.82	0.61
55:n:102:CDL:H581	55:n:102:CDL:C54	2.30	0.61
55:N:202:CDL:H711	41:s:43:TYR:OH	2.01	0.61
55:a:201:CDL:H572	48:l:720:PEE:H20	1.82	0.61
8:I:40:LYS:CG	21:W:6:VAL:HA	2.30	0.61
14:O:182:ASN:HB3	14:O:194:GLU:HB2	1.82	0.61
2:B:76:TYR:OH	16:Q:257:GLU:OE1	2.15	0.61
11:L:84:ARG:NH1	11:L:88:GLN:O	2.33	0.61
55:a:201:CDL:H211	55:a:201:CDL:C25	2.24	0.61
49:e:201:PLX:H122	55:l:712:CDL:H632	1.83	0.61
9:J:117:ARG:O	9:J:121:GLU:HG3	2.01	0.61
55:V:203:CDL:H211	55:V:203:CDL:H442	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:201:PLX:H1C3	49:e:201:PLX:O1	2.00	0.61
49:e:201:PLX:C2	48:l:720:PEE:H3	2.30	0.61
9:J:317:ASP:OD2	9:J:321:ARG:NH1	2.34	0.61
32:i:100:MET:HE1	35:l:599:MET:HE3	1.83	0.61
20:V:113:ALA:CB	48:V:207:PEE:H53	2.31	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
55:V:201:CDL:H322	35:l:576:MET:HE1	1.83	0.61
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.82	0.61
48:V:202:PEE:H22	40:r:198:ALA:HB2	1.83	0.60
34:k:33:LEU:HA	34:k:36:MET:HE3	1.82	0.60
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.83	0.60
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.83	0.60
55:a:201:CDL:H771	28:e:100:VAL:HA	1.84	0.60
35:l:359:MET:O	35:l:436:ARG:NH2	2.34	0.60
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.31	0.60
55:V:201:CDL:OA8	55:V:201:CDL:H331	2.01	0.60
1:A:48:ARG:NH1	10:K:70:ASN:O	2.34	0.60
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.83	0.60
49:e:201:PLX:P1	48:l:720:PEE:H10	2.40	0.60
32:i:207:ILE:HD11	32:i:261:MET:HE2	1.84	0.60
11:L:70:GLU:O	11:L:74:THR:OG1	2.19	0.59
55:k:101:CDL:H521	36:m:88:THR:HG23	1.84	0.59
35:l:599:MET:O	35:l:603:ASN:HB3	2.03	0.59
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.35	0.59
1:A:102:MET:O	1:A:111:LYS:NZ	2.35	0.59
9:J:298:TYR:CD2	9:J:319:VAL:HG13	2.37	0.59
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.83	0.59
35:l:512:LYS:HZ1	35:l:514:LYS:HE2	1.68	0.59
1:A:89:GLY:O	47:A:503:NAI:H2N	2.02	0.59
42:u:77:HIS:CE1	42:u:115:LEU:HD21	2.37	0.59
55:a:201:CDL:H602	55:a:201:CDL:C64	2.09	0.59
28:e:126:VAL:O	28:e:130:GLU:HG2	2.03	0.59
41:s:7:LEU:HD23	41:s:10:ILE:HD11	1.84	0.59
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.84	0.59
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.22	0.59
35:l:66:TRP:CD1	48:l:720:PEE:O4P	2.56	0.59
40:r:153:THR:HG23	40:r:206:LYS:HD3	1.85	0.59
9:J:178:SER:OG	9:J:317:ASP:OD1	2.20	0.58
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.37	0.58
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.84	0.58
49:e:201:PLX:C2	48:l:720:PEE:C1	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.86	0.58
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.85	0.58
6:G:103:HIS:H	6:G:107:ASP:CB	2.15	0.58
8:I:4:ALA:HA	55:N:202:CDL:HA22	1.85	0.58
35:l:545:SER:OG	40:r:274:SER:O	2.18	0.58
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.44	0.58
9:J:304:LEU:HD11	49:j:202:PLX:H291	1.85	0.58
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.44	0.58
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.85	0.58
34:k:3:LEU:HD11	36:m:107:ALA:HB1	1.85	0.58
48:l:720:PEE:O2P	48:l:720:PEE:N	2.26	0.58
26:c:164:ASN:HA	26:c:181:VAL:HB	1.85	0.58
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.85	0.58
13:N:132:LYS:NZ	13:N:136:GLU:OE1	2.34	0.58
48:V:207:PEE:H8	48:V:207:PEE:P	2.43	0.58
36:m:31:LEU:HD21	55:m:201:CDL:H542	1.86	0.58
44:w:58:LYS:O	44:w:60:ILE:HG13	2.04	0.58
1:A:210:THR:HB	1:A:224:ARG:HG3	1.86	0.58
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.85	0.58
11:L:111:LEU:HG	11:L:112:MET:HG2	1.85	0.58
24:a:166:GLY:O	24:a:170:GLN:NE2	2.33	0.58
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.68	0.58
39:p:35:ASP:OD1	39:p:36:LYS:N	2.35	0.58
9:J:87:GLU:HG3	9:J:89:TYR:H	1.69	0.57
48:V:202:PEE:H47	40:r:155:ALA:CB	2.31	0.57
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.86	0.57
35:l:66:TRP:NE1	48:l:720:PEE:O4P	2.37	0.57
41:s:24:GLU:HG3	41:s:271:LEU:CD2	2.25	0.57
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.86	0.57
20:V:35:ILE:HD12	55:V:201:CDL:H802	1.86	0.57
55:m:201:CDL:H182	55:m:201:CDL:H362	1.86	0.57
8:I:40:LYS:CB	21:W:7:LYS:H	2.05	0.57
9:J:293:LEU:HD23	9:J:298:TYR:HB2	1.86	0.57
55:l:713:CDL:H121	55:l:713:CDL:H322	1.87	0.57
36:m:95:SER:HA	36:m:98:MET:HE2	1.87	0.57
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.86	0.57
48:V:202:PEE:H34	40:r:201:MET:HG3	1.87	0.57
55:r:714:CDL:H232	55:r:714:CDL:H782	1.87	0.57
35:l:206:ASN:HB3	35:l:207:GLU:OE1	2.04	0.57
55:m:201:CDL:H552	55:m:201:CDL:H202	1.86	0.57
3:C:93:PHE:CE2	56:Q:501:DCQ:H12	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:203:CDL:H362	55:V:203:CDL:C40	2.20	0.57
16:Q:259:GLU:OE2	21:W:23:ARG:NE	2.38	0.57
12:M:306:MET:HE1	13:N:139:PRO:HG3	1.87	0.56
30:g:89:ASP:OD2	42:u:161:ALA:HB1	2.04	0.56
41:s:205:SER:OG	41:s:279:ARG:NH1	2.34	0.56
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.32	0.56
39:p:121:LYS:NZ	39:p:124:GLN:OE1	2.27	0.56
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.39	0.56
32:i:69:MET:HE1	32:i:100:MET:HE3	1.85	0.56
39:p:159:LYS:HG2	39:p:160:GLU:H	1.68	0.56
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.87	0.56
1:A:262:PHE:CE2	1:A:272:GLY:HA3	2.41	0.56
25:b:81:ILE:HD13	48:l:720:PEE:H65	1.86	0.56
40:r:104:LEU:HG	40:r:108:MET:HE2	1.88	0.56
43:v:8:ARG:NH2	43:v:18:ASP:OD1	2.39	0.56
2:B:171:PRO:HG3	2:B:200:GLU:HG2	1.86	0.56
3:C:98:ARG:HD2	41:s:61:LEU:HD21	1.88	0.56
12:M:59:GLN:HE21	12:M:62:ARG:HH12	1.53	0.56
25:b:73:THR:HA	25:b:77:ILE:HD12	1.88	0.56
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.86	0.56
8:I:40:LYS:HG2	21:W:6:VAL:HA	1.87	0.56
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.88	0.56
40:r:84:LEU:HD22	40:r:87:GLU:HG3	1.87	0.56
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.41	0.56
55:V:203:CDL:H152	55:V:203:CDL:C35	2.24	0.56
48:V:207:PEE:P	48:V:207:PEE:C3	2.94	0.56
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.87	0.56
41:s:209:SER:HB3	41:s:213:VAL:HB	1.88	0.56
19:U:26:GLY:HA3	48:U:101:PEE:C23	2.37	0.55
1:A:214:GLU:OE2	1:A:224:ARG:HD3	2.06	0.55
12:M:466:LEU:HD13	12:M:500:ILE:HD11	1.88	0.55
42:u:152:PRO:O	42:u:153:GLU:HG2	2.06	0.55
12:M:456:ALA:O	12:M:499:ASN:ND2	2.39	0.55
26:c:96:ASP:OD1	26:c:96:ASP:N	2.37	0.55
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.55
40:r:343:ILE:O	40:r:346:ARG:NH1	2.38	0.55
22:Y:71:TRP:CD1	22:Y:72:ARG:HH21	2.24	0.55
34:k:19:LEU:HD22	34:k:36:MET:HE1	1.89	0.55
9:J:171:ASN:HA	9:J:327:MET:HE3	1.89	0.55
48:V:202:PEE:H2	40:r:191:SER:HB3	1.88	0.55
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.38	0.55
12:M:636:TYR:CD2	12:M:642:VAL:HG22	2.41	0.55
20:V:67:GLY:HA2	55:V:201:CDL:H221	1.89	0.55
35:l:245:ALA:O	35:l:249:SER:OG	2.21	0.55
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.89	0.55
3:C:68:GLY:HA3	56:Q:501:DCQ:H8	1.88	0.54
55:N:202:CDL:C75	55:N:202:CDL:C55	2.86	0.54
48:V:202:PEE:H25	40:r:159:PRO:HB3	1.89	0.54
32:i:93:VAL:HA	35:l:603:ASN:HD21	1.71	0.54
42:u:83:THR:HA	42:u:86:TRP:CD1	2.41	0.54
3:C:190:LEU:HD22	48:C:311:PEE:H14	1.88	0.54
11:L:86:ASN:O	11:L:86:ASN:ND2	2.40	0.54
12:M:213:MET:HB3	12:M:215:MET:HG2	1.89	0.54
13:N:68:MET:HG2	13:N:69:ASN:H	1.72	0.54
24:a:90:ASN:OD1	55:a:201:CDL:HB22	2.07	0.54
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.89	0.54
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.72	0.54
55:l:712:CDL:H591	55:l:712:CDL:H332	1.90	0.54
25:b:10:LEU:HD12	25:b:13:GLN:HE21	1.73	0.54
49:e:201:PLX:O1	49:e:201:PLX:H1A2	2.07	0.54
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.90	0.54
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.90	0.54
41:s:236:ALA:HB1	41:s:259:PHE:HZ	1.73	0.54
26:c:67:ASP:O	38:o:81:ARG:NH2	2.41	0.54
55:l:712:CDL:H432	55:l:712:CDL:H621	1.88	0.54
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.40	0.54
43:v:18:ASP:OD2	43:v:21:ARG:NH1	2.41	0.54
5:F:61:VAL:HG23	5:F:62:GLN:H	1.73	0.53
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.89	0.53
55:V:201:CDL:H511	35:l:576:MET:O	2.08	0.53
30:g:19:GLU:HG2	42:u:158:LEU:HD22	1.91	0.53
34:k:37:MET:HG2	34:k:67:ALA:CB	2.38	0.53
55:l:712:CDL:HA62	55:l:712:CDL:H722	1.88	0.53
48:l:718:PEE:H30	40:r:152:TYR:CE1	2.42	0.53
4:E:17:VAL:HG21	11:L:55:VAL:HG22	1.91	0.53
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.89	0.53
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.91	0.53
55:V:201:CDL:C32	35:l:576:MET:CE	2.78	0.53
25:b:85:TYR:HD1	48:l:720:PEE:H52	1.74	0.53
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.42	0.53
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.90	0.53

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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	0.53
8:I:3:SER:O	55:N:202:CDL:H1	2.09	0.53
48:C:311:PEE:H31	49:C:312:PLX:C39	2.39	0.53
27:d:131:GLN:O	27:d:135:VAL:HG23	2.09	0.53
12:M:389:THR:HB	12:M:473:MET:HE3	1.92	0.52
30:g:85:TYR:CZ	42:u:165:SER:HB2	2.45	0.52
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.27	0.52
40:r:122:PHE:HZ	40:r:206:LYS:HG3	1.74	0.52
48:l:719:PEE:C11	48:l:719:PEE:H7	2.38	0.52
40:r:188:ASN:OD1	40:r:256:TYR:OH	2.26	0.52
9:J:168:SER:O	9:J:203:PRO:HD2	2.09	0.52
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.44	0.52
32:i:203:LEU:HD11	32:i:261:MET:HE3	1.92	0.52
2:B:73:THR:OG1	41:s:272:TRP:NE1	2.39	0.52
13:N:65:THR:O	13:N:73:THR:OG1	2.25	0.52
33:j:68:GLU:HG3	33:j:98:LEU:HD13	1.91	0.52
1:A:61:ASP:OD1	1:A:137:LYS:NZ	2.42	0.52
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.32	0.52
3:C:92:VAL:HG11	52:s:402:UQ:H103	1.92	0.52
55:V:203:CDL:HB4	38:o:82:PRO:HB2	1.91	0.52
48:j:201:PEE:H26	55:m:201:CDL:H162	1.91	0.52
20:V:115:CYS:SG	55:V:203:CDL:H671	2.49	0.52
43:v:22:MET:HG2	43:v:23:PRO:HA	1.91	0.52
20:V:40:SER:HA	55:V:201:CDL:CB6	2.40	0.52
30:g:15:PHE:HB2	49:i:705:PLX:H6	1.91	0.52
13:N:129:THR:HA	18:T:43:GLN:HG2	1.90	0.52
17:S:31:ASN:OD1	17:S:60:TYR:OH	2.21	0.52
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.91	0.52
44:w:287:ASP:OD1	44:w:287:ASP:N	2.42	0.52
27:d:69:ARG:NH2	37:n:46:LYS:O	2.36	0.52
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.92	0.52
42:u:157:ASP:HB3	42:u:159:LYS:NZ	2.24	0.52
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.42	0.51
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.91	0.51
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.92	0.51
2:B:43:MET:HE3	16:Q:322:SER:HB2	1.92	0.51
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.45	0.51
8:I:40:LYS:H	21:W:7:LYS:HB3	1.75	0.51
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.33	0.51
11:L:112:MET:SD	13:N:126:PRO:HB2	2.50	0.51
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:133:LEU:O	26:c:137:VAL:HG23	2.10	0.51
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.91	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.51
12:M:50:LEU:HD11	12:M:62:ARG:HH21	1.75	0.51
48:V:202:PEE:H33	48:V:202:PEE:C42	2.31	0.51
55:V:203:CDL:OA7	55:V:203:CDL:HA61	2.09	0.51
32:i:258:SER:OG	32:i:336:VAL:HG12	2.11	0.51
16:Q:166:ARG:NH1	16:Q:352:PRO:O	2.39	0.51
25:b:85:TYR:HE1	48:l:720:PEE:O5	1.93	0.51
55:i:401:CDL:H141	55:i:401:CDL:H341	1.93	0.51
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.46	0.51
48:l:719:PEE:H7	48:l:719:PEE:H14	1.92	0.51
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.45	0.51
1:A:49:HIS:HA	10:K:74:ARG:HD3	1.93	0.51
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.92	0.51
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.93	0.51
31:h:21:GLN:HA	34:k:53:PHE:CE1	2.45	0.51
48:m:202:PEE:H59	41:s:108:MET:HE1	1.93	0.51
55:n:102:CDL:H741	55:n:102:CDL:C53	2.40	0.51
40:r:203:PHE:O	40:r:207:MET:HG2	2.10	0.51
55:V:203:CDL:H262	55:V:203:CDL:H471	1.92	0.51
50:X:201:8Q1:C8	39:p:47:ARG:NH1	2.74	0.51
55:a:201:CDL:H832	55:a:201:CDL:C87	2.27	0.51
27:d:15:ARG:HH11	27:d:15:ARG:HG2	1.76	0.51
3:C:79:MET:SD	3:C:86:MET:HB3	2.50	0.51
12:M:638:THR:O	12:M:642:VAL:HG23	2.11	0.51
55:a:201:CDL:H191	55:a:201:CDL:H732	1.91	0.51
25:b:81:ILE:HG23	48:l:720:PEE:H58	1.93	0.51
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.93	0.51
38:o:115:LEU:HG	38:o:120:LYS:O	2.11	0.51
2:B:144:ARG:NH1	11:L:112:MET:O	2.41	0.51
4:E:101:THR:O	4:E:105:ARG:HG3	2.10	0.51
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.93	0.51
26:c:168:LEU:HA	26:c:172:GLY:HA2	1.93	0.51
32:i:340:THR:HB	42:u:170:TRP:CH2	2.46	0.51
9:J:132:ARG:NH2	51:J:401:NDP:H51A	2.24	0.50
9:J:320:GLU:O	9:J:324:MET:HG3	2.12	0.50
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.93	0.50
20:V:40:SER:HA	55:V:201:CDL:HB62	1.91	0.50
26:c:162:PRO:HG3	43:v:39:MET:HE2	1.94	0.50
31:h:94:PRO:HG2	31:h:99:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:8:THR:HG23	55:i:401:CDL:H791	1.92	0.50
55:n:102:CDL:H741	55:n:102:CDL:H531	1.94	0.50
15:P:43:THR:HA	15:P:47:ILE:HD12	1.94	0.50
33:j:19:LEU:HD11	48:j:201:PEE:H52	1.93	0.50
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.47	0.50
44:w:211:VAL:HA	44:w:214:ILE:HD12	1.94	0.50
6:G:69:SER:HB2	16:Q:56:LYS:HG3	1.93	0.50
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.50
48:l:718:PEE:C22	48:l:718:PEE:C18	2.86	0.50
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.77	0.50
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.93	0.50
35:l:11:THR:HG21	35:l:47:SER:HB3	1.94	0.50
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.93	0.50
36:m:1:MET:HE2	36:m:125:TRP:HE1	1.76	0.50
7:H:94:MET:SD	7:H:99:PRO:HG3	2.51	0.50
24:a:108:GLU:HB2	24:a:111:GLU:HG3	1.93	0.50
31:h:21:GLN:HB3	31:h:37:GLU:OE1	2.11	0.50
42:u:44:MET:SD	42:u:48:TRP:HZ3	2.34	0.50
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.46	0.50
20:V:35:ILE:CD1	55:V:201:CDL:H802	2.41	0.50
55:a:201:CDL:H541	48:l:720:PEE:H16	1.93	0.50
33:j:69:ILE:HD13	41:s:147:ALA:HB3	1.94	0.50
35:l:176:ARG:HA	35:l:179:ASP:HB2	1.92	0.50
1:A:283:ASN:ND2	1:A:305:GLY:O	2.45	0.50
25:b:99:GLU:HG2	35:l:61:MET:HG3	1.92	0.50
40:r:433:GLU:O	40:r:437:MET:HG2	2.12	0.50
3:C:51:ASP:HB2	3:C:191:ARG:HH21	1.77	0.50
55:V:201:CDL:H512	35:l:580:GLN:HE22	1.76	0.50
25:b:81:ILE:HD13	48:l:720:PEE:C39	2.40	0.50
1:A:411:SER:O	1:A:415:ILE:HG12	2.10	0.49
7:H:76:GLN:O	7:H:78:GLU:N	2.45	0.49
18:T:54:ARG:O	18:T:58:ARG:NH2	2.43	0.49
19:U:38:TYR:HB2	41:s:310:MET:O	2.11	0.49
25:b:13:GLN:NE2	25:b:14:GLN:HG3	2.27	0.49
49:e:201:PLX:C18	55:l:712:CDL:H801	2.34	0.49
12:M:388:ASN:HB3	12:M:511:LYS:HD3	1.92	0.49
35:l:503:GLU:O	35:l:507:THR:HG23	2.12	0.49
39:p:27:LEU:HD21	39:p:40:PHE:HB3	1.93	0.49
40:r:57:PHE:HD1	40:r:113:THR:HG22	1.77	0.49
12:M:336:ASN:O	12:M:336:ASN:ND2	2.44	0.49
35:l:227:PHE:O	35:l:230:HIS:ND1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:720:PEE:H5	48:l:720:PEE:P	2.33	0.49
39:p:168:TRP:O	39:p:172:THR:OG1	2.22	0.49
41:s:170:GLU:CD	42:u:98:ARG:HH12	2.20	0.49
1:A:75:TRP:O	1:A:79:GLU:HG2	2.13	0.49
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.47	0.49
42:u:80:GLU:HB2	42:u:81:PRO:HD3	1.94	0.49
14:O:242:GLY:HA2	14:O:245:VAL:HG23	1.93	0.49
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.95	0.49
26:c:127:ASN:O	26:c:131:LYS:HD2	2.13	0.49
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.78	0.49
35:l:12:LEU:HD22	35:l:129:MET:HB3	1.95	0.49
35:l:166:THR:CG2	48:l:719:PEE:H2	2.42	0.49
40:r:174:LEU:HA	40:r:179:ILE:HD11	1.95	0.49
41:s:24:GLU:HG2	41:s:28:LEU:HD13	1.93	0.49
41:s:209:SER:HB3	41:s:213:VAL:CB	2.42	0.49
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.95	0.49
8:I:109:ASP:OD2	21:W:21:TYR:OH	2.28	0.49
26:c:166:LEU:HB3	26:c:169:GLU:HB2	1.95	0.49
30:g:10:ARG:NH2	32:i:347:ASN:O	2.45	0.49
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.94	0.49
27:d:107:GLN:HB3	27:d:111:LYS:NZ	2.27	0.49
31:h:32:ARG:HH11	31:h:32:ARG:HG2	1.77	0.49
41:s:81:LEU:O	41:s:85:MET:HG2	2.13	0.49
1:A:384:PRO:HB2	1:A:423:THR:CG2	2.43	0.49
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.94	0.49
26:c:48:ARG:NH2	26:c:63:GLU:OE1	2.42	0.49
33:j:67:LEU:HD22	36:m:59:ILE:HD12	1.95	0.49
48:m:202:PEE:C1	48:m:202:PEE:C4	2.90	0.49
40:r:105:PHE:O	40:r:109:THR:OG1	2.22	0.49
1:A:116:ASN:ND2	1:A:207:GLY:O	2.33	0.49
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.93	0.49
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.48	0.49
12:M:372:PHE:H	12:M:532:PRO:HB2	1.77	0.49
55:l:712:CDL:H311	55:l:712:CDL:H561	1.95	0.49
41:s:236:ALA:HB1	41:s:259:PHE:CZ	2.48	0.49
3:C:56:TRP:CE2	49:C:312:PLX:H91	2.48	0.48
22:Y:76:ASP:O	35:l:385:TYR:OH	2.20	0.48
24:a:135:LYS:NZ	37:n:32:ASP:OD1	2.31	0.48
55:k:101:CDL:H782	55:k:101:CDL:H592	1.94	0.48
16:Q:136:PHE:HA	16:Q:139:LEU:HG	1.95	0.48
19:U:27:GLY:O	19:U:31:ILE:HG12	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:V:203:CDL:H322	55:V:203:CDL:C36	2.42	0.48
35:l:474:PRO:HD2	43:v:67:LEU:HD21	1.94	0.48
20:V:95:CYS:HA	20:V:115:CYS:HA	1.94	0.48
32:i:34:GLU:OE2	32:i:67:SER:OG	2.20	0.48
32:i:146:SER:O	32:i:149:ILE:HG12	2.13	0.48
35:l:566:THR:O	35:l:570:GLN:HG2	2.13	0.48
1:A:262:PHE:CZ	1:A:272:GLY:HA3	2.48	0.48
3:C:88:ARG:HA	41:s:37:PRO:HA	1.96	0.48
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.94	0.48
27:d:162:ARG:NH2	28:e:140:ASN:OD1	2.38	0.48
28:e:92:PHE:O	28:e:96:SER:HB2	2.14	0.48
33:j:18:VAL:HG12	48:j:201:PEE:H16	1.94	0.48
35:l:599:MET:HA	35:l:603:ASN:HB2	1.94	0.48
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.35	0.48
12:M:399:VAL:HG22	12:M:428:LYS:HB3	1.94	0.48
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.43	0.48
28:e:63:ASP:N	28:e:63:ASP:OD1	2.46	0.48
40:r:266:MET:O	40:r:269:MET:HG2	2.12	0.48
41:s:109:SER:OG	41:s:192:GLU:OE2	2.31	0.48
11:L:89:SER:O	12:M:59:GLN:NE2	2.42	0.48
12:M:51:GLN:O	12:M:54:GLU:HG2	2.14	0.48
12:M:390:THR:HA	12:M:600:GLU:HG2	1.94	0.48
55:V:203:CDL:H782	35:l:557:TRP:CE3	2.49	0.48
26:c:116:ARG:CG	48:l:719:PEE:H49	2.37	0.48
30:g:32:ARG:O	30:g:36:MET:HG2	2.13	0.48
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.95	0.48
48:C:311:PEE:H31	49:C:312:PLX:H393	1.94	0.48
15:P:148:ASP:OD1	15:P:151:THR:OG1	2.22	0.48
25:b:85:TYR:CD1	48:l:720:PEE:H52	2.49	0.48
32:i:172:GLN:HB2	32:i:178:ILE:HG13	1.95	0.48
35:l:561:ILE:HG13	35:l:562:LEU:H	1.77	0.48
15:P:147:THR:HB	15:P:153:ILE:HD11	1.94	0.48
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.96	0.48
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.95	0.48
55:l:713:CDL:H172	55:l:713:CDL:H802	1.96	0.48
43:v:66:LEU:O	43:v:70:LYS:HG2	2.14	0.48
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.96	0.48
35:l:417:SER:OG	35:l:493:VAL:HG13	2.13	0.48
2:B:153:ILE:CG2	3:C:142:TYR:HB2	2.44	0.48
9:J:220:MET:HE2	9:J:226:VAL:CG1	2.39	0.48
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:j:203:PLX:H251	36:m:151:THR:HG21	1.96	0.48
55:l:713:CDL:H861	55:l:713:CDL:H201	1.95	0.48
37:n:4:VAL:HG22	37:n:8:VAL:HG23	1.95	0.48
38:o:56:ARG:C	38:o:56:ARG:HD2	2.39	0.48
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.96	0.48
1:A:388:GLY:O	1:A:392:MET:HG3	2.14	0.47
9:J:375:VAL:HG23	9:J:375:VAL:O	2.14	0.47
15:P:122:ARG:NH1	15:P:127:GLU:OE1	2.38	0.47
22:Y:97:LEU:HD22	43:v:107:ARG:HH11	1.78	0.47
25:b:32:GLU:HB3	39:p:115:TYR:CD1	2.49	0.47
27:d:160:LYS:NZ	30:g:114:ILE:O	2.46	0.47
31:h:21:GLN:HA	34:k:53:PHE:HE1	1.79	0.47
32:i:285:THR:HA	48:l:718:PEE:H67	1.96	0.47
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.96	0.47
35:l:250:SER:HB2	35:l:333:ALA:HA	1.96	0.47
35:l:505:ASN:O	35:l:508:THR:HG22	2.13	0.47
44:w:88:GLU:N	44:w:160:GLU:HG3	2.29	0.47
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.49	0.47
55:a:201:CDL:H201	55:a:201:CDL:H752	1.95	0.47
32:i:149:ILE:HD11	32:i:195:PRO:HB3	1.96	0.47
41:s:149:ILE:HG21	41:s:185:TRP:HB2	1.95	0.47
41:s:214:GLU:OE1	41:s:214:GLU:HA	2.15	0.47
43:v:70:LYS:HD2	43:v:80:CYS:SG	2.54	0.47
12:M:59:GLN:HE21	12:M:62:ARG:NH1	2.12	0.47
12:M:257:VAL:O	12:M:598:ASN:OD1	2.32	0.47
16:Q:450:ILE:HA	16:Q:453:THR:HG22	1.96	0.47
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.95	0.47
55:a:201:CDL:H521	48:l:720:PEE:H14	1.95	0.47
21:W:91:LEU:HD22	42:u:7:LEU:HD12	1.97	0.47
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.79	0.47
31:h:80:LYS:NZ	36:m:1:MET:HE3	2.30	0.47
1:A:115:VAL:HG22	1:A:248:VAL:HG21	1.97	0.47
6:G:90:TYR:CE2	6:G:92:LYS:HB2	2.50	0.47
15:P:51:ASN:HB3	15:P:82:ASN:ND2	2.29	0.47
15:P:52:ASP:O	15:P:56:LYS:HG3	2.14	0.47
55:V:201:CDL:OA7	55:V:201:CDL:HA31	2.13	0.47
48:V:202:PEE:C45	40:r:201:MET:HE2	2.44	0.47
6:G:103:HIS:O	6:G:107:ASP:HB2	2.14	0.47
9:J:298:TYR:HD2	9:J:319:VAL:HG13	1.80	0.47
16:Q:97:LEU:HG	16:Q:99:MET:HG3	1.97	0.47
19:U:33:PRO:HA	41:s:310:MET:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:68:ARG:HD2	36:m:135:PHE:CZ	2.49	0.47
28:e:53:ILE:HG22	28:e:55:LEU:H	1.79	0.47
35:l:27:TYR:O	35:l:115:ASN:ND2	2.44	0.47
35:l:331:MET:SD	35:l:465:GLY:HA2	2.55	0.47
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.49	0.47
1:A:63:TYR:CD2	1:A:64:LYS:HG2	2.50	0.47
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.97	0.47
21:W:51:MET:HE2	41:s:311:THR:HB	1.96	0.47
26:c:140:MET:HE2	35:l:283:ILE:HG13	1.97	0.47
30:g:101:GLU:CD	30:g:101:GLU:H	2.22	0.47
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.96	0.47
49:j:202:PLX:H371	49:j:202:PLX:C32	2.44	0.47
35:l:71:LEU:N	35:l:71:LEU:HD22	2.29	0.47
55:l:712:CDL:H582	55:l:712:CDL:H791	1.95	0.47
40:r:225:ILE:HD13	40:r:331:ASN:HB2	1.95	0.47
44:w:169:PHE:CD2	58:w:401:ADP:N6	2.83	0.47
16:Q:141:TYR:HE1	56:Q:501:DCQ:C4M	2.27	0.47
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.97	0.47
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.96	0.47
49:j:202:PLX:H92	49:j:202:PLX:H122	1.79	0.47
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.49	0.47
55:l:712:CDL:H391	40:r:371:PRO:HD2	1.96	0.47
37:n:26:TYR:CZ	37:n:30:ARG:HD2	2.50	0.47
37:n:54:GLU:HG2	37:n:55:VAL:HG22	1.96	0.47
39:p:132:SER:O	39:p:136:GLU:HG3	2.15	0.47
41:s:228:TYR:HA	41:s:231:ILE:HD12	1.97	0.47
9:J:114:ASP:HA	9:J:117:ARG:HG2	1.97	0.47
30:g:83:TYR:CZ	30:g:87:LEU:HD11	2.49	0.47
12:M:361:VAL:HG22	12:M:632:MET:HE1	1.97	0.47
14:O:179:ALA:HB3	14:O:185:MET:HG2	1.97	0.47
49:V:205:PLX:H92	49:V:205:PLX:H121	1.50	0.47
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.96	0.46
12:M:144:MET:O	16:Q:362:LYS:HE3	2.14	0.46
15:P:157:VAL:HG21	15:P:182:PRO:HD3	1.95	0.46
28:e:72:ASP:OD1	28:e:72:ASP:N	2.48	0.46
2:B:111:GLU:O	2:B:141:ARG:NH1	2.49	0.46
13:N:42:ASP:OD2	13:N:48:TYR:OH	2.29	0.46
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.80	0.46
17:S:63:THR:HG23	42:u:21:SER:HB2	1.96	0.46
8:I:8:ILE:HD11	55:N:202:CDL:H142	1.98	0.46
12:M:389:THR:O	12:M:390:THR:OG1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:100:MET:HE2	32:i:100:MET:HB2	1.81	0.46
48:l:718:PEE:H37	48:l:718:PEE:C37	2.44	0.46
55:r:714:CDL:H351	55:r:714:CDL:H201	1.96	0.46
41:s:116:ILE:HD12	41:s:211:PHE:CZ	2.50	0.46
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.48	0.46
40:r:76:MET:HE2	40:r:99:LEU:HD22	1.98	0.46
40:r:185:PRO:HB3	40:r:252:PRO:HD3	1.97	0.46
40:r:392:THR:O	40:r:396:MET:HG2	2.16	0.46
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.51	0.46
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.97	0.46
10:K:87:LEU:HD22	14:O:66:ILE:HD11	1.97	0.46
11:L:105:GLU:HA	12:M:611:THR:HG21	1.97	0.46
12:M:295:ASP:OD1	12:M:704:SER:OG	2.23	0.46
27:d:127:LYS:O	27:d:130:GLU:HG3	2.15	0.46
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.16	0.46
32:i:72:MET:HE3	32:i:76:ILE:HG13	1.98	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.16	0.46
35:l:310:LEU:O	35:l:314:MET:HG2	2.15	0.46
41:s:157:ASN:OD1	41:s:168:THR:OG1	2.24	0.46
41:s:209:SER:HB3	41:s:213:VAL:HA	1.96	0.46
48:s:401:PEE:H61	48:s:401:PEE:H55	1.69	0.46
49:V:205:PLX:H72	49:V:205:PLX:H101	1.70	0.46
25:b:120:MET:HE3	43:v:61:HIS:HB2	1.97	0.46
49:e:201:PLX:H252	40:r:450:ASN:HB2	1.97	0.46
34:k:24:SER:O	34:k:89:TYR:HA	2.14	0.46
3:C:86:MET:HE1	3:C:93:PHE:CD2	2.50	0.46
9:J:135:GLU:HG2	9:J:140:ASP:HA	1.98	0.46
9:J:298:TYR:CE2	9:J:323:HIS:HE1	2.33	0.46
20:V:131:GLU:OE1	40:r:191:SER:OG	2.28	0.46
22:Y:44:TYR:O	22:Y:45:ARG:HB2	2.16	0.46
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.97	0.46
12:M:696:MET:HG2	12:M:702:ARG:HA	1.97	0.46
20:V:38:ALA:HB2	55:k:101:CDL:H251	1.97	0.46
27:d:114:GLN:OE1	35:l:199:GLN:HG3	2.16	0.46
55:l:712:CDL:H342	55:l:712:CDL:H372	1.63	0.46
6:G:138:LEU:O	6:G:139:MET:HE2	2.15	0.46
32:i:128:LEU:O	32:i:132:THR:OG1	2.24	0.46
49:i:705:PLX:H102	49:i:705:PLX:H71	1.49	0.46
42:u:79:ALA:O	42:u:83:THR:OG1	2.23	0.46
48:C:311:PEE:H82	48:C:311:PEE:H74	1.73	0.46
20:V:115:CYS:SG	55:V:203:CDL:C67	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:222:SER:O	32:i:224:ALA:N	2.48	0.46
32:i:243:LEU:HD22	32:i:330:ILE:HG21	1.97	0.46
36:m:165:VAL:O	36:m:168:ILE:HG12	2.16	0.46
40:r:122:PHE:CZ	40:r:206:LYS:HG3	2.51	0.46
2:B:116:CYS:SG	2:B:118:LEU:HG	2.56	0.45
21:W:36:PHE:O	21:W:40:ILE:HG12	2.16	0.45
26:c:169:GLU:OE1	26:c:169:GLU:N	2.48	0.45
28:e:55:LEU:HD21	44:w:320:GLY:HA3	1.99	0.45
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.98	0.45
35:l:293:ILE:HD12	55:l:713:CDL:H521	1.97	0.45
48:m:202:PEE:H42	48:m:202:PEE:C21	2.18	0.45
2:B:43:MET:HE3	16:Q:322:SER:CB	2.46	0.45
52:J:402:UQ:H102	48:j:201:PEE:O2P	2.16	0.45
11:L:84:ARG:HD3	11:L:91:VAL:HG12	1.98	0.45
12:M:197:THR:O	14:O:114:GLU:HG2	2.16	0.45
12:M:341:ILE:HG13	12:M:545:LEU:HD11	1.98	0.45
48:V:207:PEE:O3	35:l:568:PHE:HE2	1.98	0.45
1:A:263:ALA:HA	1:A:271:SER:HB3	1.98	0.45
55:V:201:CDL:H602	55:V:201:CDL:H571	1.76	0.45
32:i:237:MET:SD	32:i:319:HIS:NE2	2.86	0.45
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.52	0.45
48:m:202:PEE:C25	48:m:202:PEE:C21	2.86	0.45
1:A:195:VAL:O	10:K:97:ARG:NH1	2.48	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.73	0.45
7:H:35:LEU:HD23	7:H:38:ILE:HD12	1.97	0.45
8:I:70:MET:SD	15:P:63:GLN:HG2	2.56	0.45
6:X:100:VAL:O	6:X:141:PRO:HD2	2.16	0.45
49:e:201:PLX:C25	40:r:450:ASN:HB2	2.47	0.45
48:j:201:PEE:H40	41:s:77:LEU:CD1	2.46	0.45
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.98	0.45
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.98	0.45
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.31	0.45
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.98	0.45
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.51	0.45
41:s:198:PHE:CD1	41:s:285:LEU:HD13	2.52	0.45
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.99	0.45
16:Q:174:PHE:HD1	16:Q:214:TYR:HE1	1.65	0.45
27:d:167:ARG:NE	28:e:153:GLU:OE1	2.35	0.45
32:i:11:MET:HG2	55:i:401:CDL:H581	1.99	0.45
34:k:75:LEU:O	34:k:79:VAL:HG23	2.17	0.45
55:k:101:CDL:H611	55:k:101:CDL:H581	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.51	0.45
48:U:101:PEE:H59	48:U:101:PEE:H64	1.66	0.45
21:W:82:ARG:NH1	31:h:106:PRO:O	2.50	0.45
23:Z:79:VAL:HA	23:Z:82:VAL:HG22	1.99	0.45
37:n:17:VAL:HG13	40:r:7:PRO:HB3	1.99	0.45
40:r:175:ASN:O	40:r:179:ILE:HG12	2.15	0.45
44:w:256:LEU:HD11	44:w:276:LEU:HD11	1.97	0.45
1:A:398:ARG:HH22	1:A:408:GLU:CD	2.25	0.45
2:B:59:GLN:HG3	2:B:64:THR:OG1	2.17	0.45
15:P:44:ARG:HB2	15:P:45:PRO:HD3	1.98	0.45
18:T:79:VAL:O	18:T:121:PRO:HD3	2.17	0.45
27:d:37:PHE:CD1	35:l:3:PRO:HB3	2.52	0.45
32:i:139:LEU:HD13	32:i:190:MET:HE1	1.98	0.45
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.99	0.45
35:l:10:THR:O	35:l:14:ILE:HG23	2.16	0.45
35:l:295:GLN:HB2	35:l:301:ILE:HG12	1.98	0.45
35:l:557:TRP:O	35:l:561:ILE:HG12	2.17	0.45
44:w:325:ASP:O	44:w:329:GLN:HG2	2.17	0.45
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.98	0.45
6:G:136:GLU:O	6:G:139:MET:HE3	2.16	0.45
9:J:241:TYR:OH	9:J:351:GLU:OE2	2.29	0.45
12:M:340:ALA:HB3	12:M:366:LEU:HD13	1.98	0.45
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.98	0.45
16:Q:184:ILE:HD11	16:Q:251:PHE:CE1	2.52	0.45
32:i:307:SER:OG	32:i:308:THR:N	2.50	0.45
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.51	0.45
39:p:22:ARG:NH2	39:p:68:GLU:OE1	2.50	0.45
43:v:14:SER:O	43:v:109:LEU:HD21	2.16	0.45
1:A:209:GLU:OE1	47:A:503:NAI:O3B	2.32	0.44
7:H:108:PRO:HG2	15:P:124:ASN:ND2	2.31	0.44
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.16	0.44
49:e:201:PLX:H22	48:l:720:PEE:H9	1.99	0.44
32:i:277:ILE:O	32:i:281:LEU:HG	2.16	0.44
55:k:101:CDL:H131	55:k:101:CDL:H161	1.80	0.44
35:l:80:PHE:HB3	35:l:82:MET:HE2	1.98	0.44
55:l:712:CDL:H142	55:l:712:CDL:H331	1.99	0.44
6:G:103:HIS:N	6:G:107:ASP:HB2	2.31	0.44
10:K:83:THR:HG23	14:O:88:ARG:HH11	1.82	0.44
14:O:242:GLY:HA2	14:O:245:VAL:CG2	2.48	0.44
28:e:65:ASN:HD21	28:e:67:TYR:HB2	1.82	0.44
8:I:41:LEU:HA	8:I:42:PRO:HD2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:43:GLN:C	18:T:43:GLN:CD	2.85	0.44
26:c:116:ARG:HA	48:l:719:PEE:H49	1.99	0.44
32:i:168:GLY:HA3	32:i:181:TYR:CE1	2.52	0.44
49:j:203:PLX:H132	49:j:203:PLX:H161	1.51	0.44
48:l:718:PEE:H30	40:r:152:TYR:CD1	2.52	0.44
9:J:71:ASN:O	9:J:75:ARG:HG3	2.18	0.44
14:O:245:VAL:HG12	14:O:246:GLN:O	2.17	0.44
16:Q:435:LEU:HA	16:Q:454:GLN:HE22	1.83	0.44
35:l:558:LEU:HD23	35:l:561:ILE:HD11	1.98	0.44
55:m:201:CDL:H771	55:m:201:CDL:H801	1.83	0.44
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.52	0.44
1:A:122:PRO:HA	14:O:176:CYS:SG	2.58	0.44
3:C:98:ARG:HB3	41:s:216:ALA:HB2	1.99	0.44
4:E:16:SER:O	4:E:16:SER:OG	2.29	0.44
8:I:3:SER:O	55:N:202:CDL:CA2	2.65	0.44
32:i:81:SER:O	32:i:83:GLN:N	2.48	0.44
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.99	0.44
32:i:200:MET:SD	32:i:265:MET:HB3	2.58	0.44
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.50	0.44
40:r:76:MET:HE3	40:r:226:ALA:O	2.18	0.44
40:r:269:MET:HE1	40:r:396:MET:SD	2.58	0.44
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.58	0.44
1:A:326:LEU:HD23	1:A:367:ILE:HD11	2.00	0.44
8:I:46:SER:O	8:I:52:ASN:ND2	2.51	0.44
16:Q:259:GLU:HG3	16:Q:263:THR:OG1	2.17	0.44
16:Q:261:MET:HE3	16:Q:261:MET:HB3	1.87	0.44
32:i:217:MET:HE2	32:i:326:LEU:HB2	2.00	0.44
37:n:12:TRP:O	37:n:15:ILE:HG12	2.17	0.44
40:r:312:ALA:O	40:r:316:MET:HG3	2.18	0.44
5:F:40:ARG:HH12	5:F:84:ALA:C	2.26	0.44
6:G:103:HIS:H	6:G:107:ASP:HB2	1.80	0.44
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.00	0.44
33:j:73:LEU:N	33:j:74:PRO:HD2	2.33	0.44
40:r:141:GLU:HB2	40:r:222:GLU:OE2	2.18	0.44
6:G:104:PHE:HB2	6:G:105:MET:HE3	2.00	0.44
9:J:38:HIS:CE1	13:N:132:LYS:HE3	2.53	0.44
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.83	0.44
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.99	0.44
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.00	0.44
35:l:312:LEU:HA	35:l:315:VAL:HG22	1.99	0.44
40:r:197:LEU:O	40:r:201:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:r:714:CDL:H791	55:r:714:CDL:H761	1.60	0.44
42:u:83:THR:HA	42:u:86:TRP:NE1	2.33	0.44
49:C:312:PLX:H141	41:s:49:ILE:HG21	2.00	0.43
11:L:78:ARG:HD3	12:M:607:LYS:HE2	2.00	0.43
12:M:506:VAL:HG12	12:M:508:GLY:H	1.82	0.43
55:V:203:CDL:C39	38:o:88:LEU:HD21	2.46	0.43
6:X:89:LEU:HD21	23:Z:19:TYR:HB2	1.99	0.43
22:Y:100:LEU:HB3	22:Y:104:GLU:OE1	2.18	0.43
31:h:2:PRO:HA	32:i:140:SER:HB2	2.00	0.43
49:j:203:PLX:H311	49:j:203:PLX:H282	1.51	0.43
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.42	0.43
44:w:215:GLN:O	44:w:219:GLN:OE1	2.36	0.43
12:M:551:ASP:OD2	12:M:568:TYR:OH	2.29	0.43
34:k:27:MET:HE1	36:m:70:TYR:HB3	2.00	0.43
35:l:400:ASN:HB3	35:l:486:MET:CE	2.49	0.43
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.99	0.43
40:r:57:PHE:CD1	40:r:113:THR:HG22	2.53	0.43
1:A:59:ARG:HG2	14:O:238:PRO:HB2	1.99	0.43
3:C:61:SER:OG	41:s:51:ASP:OD1	2.30	0.43
8:I:4:ALA:HA	55:N:202:CDL:CA2	2.48	0.43
33:j:37:TYR:CD1	33:j:37:TYR:C	2.96	0.43
34:k:4:VAL:O	34:k:8:ILE:HG12	2.17	0.43
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.53	0.43
35:l:530:PRO:O	35:l:534:HIS:HB2	2.17	0.43
36:m:65:LEU:N	41:s:114:TYR:OH	2.51	0.43
52:s:402:UQ:H152	52:s:402:UQ:H121	1.81	0.43
44:w:139:ARG:NH1	58:w:401:ADP:HN61	1.93	0.43
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.52	0.43
12:M:51:GLN:O	12:M:55:LYS:HG3	2.18	0.43
16:Q:190:HIS:O	16:Q:194:ILE:HD12	2.18	0.43
6:X:105:MET:HE1	6:X:112:SER:HA	1.99	0.43
24:a:63:TYR:OH	28:e:71:PRO:O	2.31	0.43
35:l:42:TYR:HA	35:l:45:THR:HG22	2.00	0.43
41:s:102:VAL:HG21	41:s:154:LEU:HD11	2.00	0.43
9:J:307:VAL:HG23	49:j:202:PLX:H272	2.00	0.43
12:M:398:ASP:OD2	12:M:471:LYS:N	2.50	0.43
14:O:151:ALA:HB2	14:O:198:PRO:HB3	2.00	0.43
20:V:108:TYR:CE2	55:V:203:CDL:HA32	2.53	0.43
27:d:104:ASN:OD1	35:l:73:THR:O	2.36	0.43
29:f:68:GLU:OE2	29:f:71:ARG:NH2	2.52	0.43
55:i:401:CDL:H382	55:i:401:CDL:H411	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:346:ARG:O	40:r:419:TYR:HA	2.19	0.43
1:A:367:ILE:O	1:A:371:ILE:HG12	2.19	0.43
9:J:132:ARG:HE	51:J:401:NDP:H8A	1.83	0.43
9:J:315:THR:O	9:J:319:VAL:HG23	2.18	0.43
12:M:405:THR:HB	12:M:477:GLY:HA3	2.01	0.43
55:N:202:CDL:H711	41:s:43:TYR:HH	1.83	0.43
28:e:87:MET:HE3	28:e:87:MET:HB3	1.89	0.43
32:i:88:LYS:HG2	32:i:148:SER:HB2	2.01	0.43
44:w:245:PHE:O	44:w:249:MET:HG2	2.19	0.43
1:A:90:GLY:HA3	47:A:503:NAI:H1D	2.00	0.43
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.01	0.43
16:Q:161:ILE:HD13	16:Q:363:VAL:HG11	2.00	0.43
24:a:176:LYS:HE3	31:h:45:HIS:ND1	2.33	0.43
55:a:201:CDL:H432	27:d:44:PRO:HB3	2.00	0.43
28:e:70:ASN:HB3	28:e:73:SER:HB3	2.01	0.43
35:l:491:LEU:O	35:l:495:ILE:HG12	2.19	0.43
42:u:19:LYS:HE3	42:u:19:LYS:HB3	1.84	0.43
44:w:45:LEU:O	44:w:45:LEU:HD12	2.19	0.43
1:A:384:PRO:HB2	1:A:423:THR:HG22	2.01	0.43
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.54	0.43
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.01	0.43
27:d:32:TYR:O	27:d:36:ILE:HG12	2.19	0.43
28:e:55:LEU:HD21	44:w:320:GLY:CA	2.49	0.43
35:l:226:GLN:OE1	35:l:314:MET:HG3	2.18	0.43
35:l:230:HIS:N	35:l:231:PRO:HD3	2.34	0.43
40:r:5:ILE:HG23	40:r:104:LEU:HD11	2.00	0.43
11:L:135:VAL:O	11:L:139:GLU:HG3	2.19	0.43
12:M:421:SER:OG	12:M:427:LEU:HD22	2.19	0.43
15:P:173:MET:HE1	15:P:189:THR:HG23	2.01	0.43
48:U:101:PEE:H35	48:U:101:PEE:H30	1.62	0.43
21:W:128:ARG:NH1	31:h:102:GLU:OE1	2.25	0.43
27:d:15:ARG:HG2	27:d:15:ARG:NH1	2.33	0.43
32:i:190:MET:CE	32:i:205:LEU:HB2	2.49	0.43
32:i:261:MET:HB2	32:i:337:LEU:HD12	2.00	0.43
32:i:320:THR:OG1	44:w:300:ASN:HA	2.19	0.43
35:l:561:ILE:HG13	35:l:562:LEU:N	2.34	0.43
1:A:118:ASP:O	1:A:159:ARG:HD2	2.18	0.43
2:B:68:ARG:NE	16:Q:260:GLU:OE2	2.51	0.43
7:H:35:LEU:HD22	7:H:45:ARG:HA	2.01	0.43
19:U:54:PRO:HD3	21:W:69:ILE:HD13	2.01	0.43
26:c:36:MET:HA	26:c:36:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:201:PLX:H181	55:l:712:CDL:C80	2.38	0.43
39:p:159:LYS:HG2	39:p:160:GLU:N	2.34	0.43
44:w:50:THR:HA	44:w:53:LEU:HD23	2.01	0.43
3:C:52:ASP:HB3	49:C:312:PLX:H251	2.00	0.42
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	2.01	0.42
24:a:139:ILE:HG23	40:r:54:LEU:HD23	2.00	0.42
40:r:266:MET:HB3	40:r:395:LEU:HD13	2.01	0.42
11:L:101:PHE:CE2	11:L:121:LEU:HD13	2.54	0.42
12:M:551:ASP:OD1	12:M:574:ASP:HB3	2.19	0.42
20:V:141:VAL:HG22	20:V:141:VAL:O	2.19	0.42
55:V:201:CDL:H562	55:V:201:CDL:H531	1.56	0.42
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.42
23:Z:52:ARG:HD3	35:l:435:PRO:O	2.19	0.42
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.54	0.42
28:e:74:HIS:NE2	28:e:87:MET:HE2	2.34	0.42
35:l:346:ILE:HA	35:l:366:MET:HE1	2.01	0.42
35:l:407:TRP:O	35:l:411:MET:HG2	2.19	0.42
43:v:113:LYS:HE3	43:v:113:LYS:HB3	1.91	0.42
4:E:23:ARG:NH2	11:L:52:LEU:O	2.45	0.42
9:J:313:TRP:CE2	52:J:402:UQ:H72	2.54	0.42
12:M:208:THR:OG1	12:M:210:ILE:O	2.31	0.42
27:d:43:ARG:HB3	27:d:44:PRO:HD3	2.01	0.42
27:d:57:ALA:HA	27:d:60:ARG:HH21	1.84	0.42
31:h:32:ARG:HG2	31:h:32:ARG:NH1	2.34	0.42
31:h:36:PHE:CD1	31:h:62:ASP:HB3	2.54	0.42
32:i:155:LEU:HD22	32:i:278:MET:SD	2.59	0.42
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.99	0.42
34:k:57:ASN:HB3	36:m:143:ILE:HG13	2.01	0.42
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.41	0.42
55:l:713:CDL:H641	55:l:713:CDL:H612	1.76	0.42
36:m:141:MET:HE2	36:m:141:MET:HA	2.00	0.42
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.52	0.42
27:d:111:LYS:HE3	35:l:197:ASP:OD2	2.19	0.42
28:e:73:SER:O	28:e:75:GLY:N	2.53	0.42
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.01	0.42
55:k:101:CDL:H652	55:k:101:CDL:H622	1.69	0.42
41:s:3:MET:HE3	41:s:3:MET:HB3	1.94	0.42
48:C:311:PEE:H52	48:C:311:PEE:O5	2.20	0.42
9:J:172:ALA:HA	9:J:181:LEU:HB3	2.02	0.42
55:l:712:CDL:H202	55:l:712:CDL:H231	1.96	0.42
41:s:240:ILE:HG13	41:s:259:PHE:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:107:PHE:O	42:u:111:VAL:HG22	2.19	0.42
44:w:59:VAL:HG12	44:w:201:PRO:HB3	2.02	0.42
7:H:37:GLN:HB2	7:H:95:LEU:HD11	2.01	0.42
8:I:90:THR:OG1	8:I:91:GLU:N	2.52	0.42
52:J:402:UQ:H202	52:J:402:UQ:H221	1.91	0.42
12:M:419:ARG:NH1	12:M:439:THR:O	2.51	0.42
20:V:140:LYS:HB2	20:V:140:LYS:HE2	1.87	0.42
22:Y:78:ASP:HB3	22:Y:83:HIS:HB2	2.02	0.42
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.55	0.42
41:s:120:GLY:HA2	41:s:128:ALA:HB1	2.02	0.42
52:J:402:UQ:HM53	52:J:402:UQ:H71	1.75	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.01	0.42
55:V:203:CDL:H392	38:o:88:LEU:CD2	2.47	0.42
25:b:121:LYS:HD3	43:v:40:VAL:HA	2.01	0.42
35:l:409:LEU:O	35:l:413:LEU:HG	2.19	0.42
1:A:62:TRP:HE3	1:A:65:THR:HG21	1.85	0.42
1:A:63:TYR:CE2	1:A:64:LYS:HE3	2.53	0.42
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.01	0.42
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.85	0.42
35:l:66:TRP:HE1	48:l:720:PEE:C4	2.33	0.42
40:r:139:GLN:HB2	40:r:222:GLU:OE1	2.19	0.42
40:r:243:MET:HB3	40:r:301:ILE:HG21	2.01	0.42
7:H:50:GLN:O	7:H:54:GLU:HG3	2.19	0.42
9:J:45:LYS:HB3	15:P:225:GLU:OE2	2.19	0.42
9:J:369:VAL:HG12	9:J:369:VAL:O	2.20	0.42
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.01	0.42
30:g:13:LEU:HA	49:i:705:PLX:H32	2.01	0.42
32:i:171:ASN:HB2	35:l:574:SER:OG	2.19	0.42
35:l:316:THR:HG23	35:l:325:ALA:HB2	2.02	0.42
41:s:7:LEU:HA	41:s:10:ILE:HG12	2.01	0.42
6:G:102:SER:HA	6:G:107:ASP:OD2	2.20	0.42
44:w:223:ASN:HB3	44:w:226:GLU:HG3	2.02	0.42
12:M:262:VAL:HG23	12:M:276:ARG:HB2	2.02	0.41
13:N:85:GLU:HG2	13:N:86:TRP:N	2.35	0.41
19:U:43:ILE:HG13	33:j:84:LEU:HD12	2.02	0.41
32:i:54:GLU:HG3	34:k:93:LEU:HB3	2.01	0.41
32:i:278:MET:HG2	32:i:282:MET:SD	2.60	0.41
36:m:44:VAL:HG12	36:m:49:GLY:O	2.19	0.41
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.02	0.41
41:s:222:MET:HA	41:s:225:MET:HE3	2.02	0.41
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:292:PHE:HB3	12:M:706:THR:HG21	2.01	0.41
12:M:573:GLY:HA3	13:N:137:TRP:CG	2.55	0.41
20:V:55:ARG:O	20:V:58:ARG:HG2	2.20	0.41
22:Y:65:MET:HE2	22:Y:65:MET:HB3	1.88	0.41
25:b:28:LEU:HB3	25:b:32:GLU:HG3	2.02	0.41
25:b:72:VAL:HG23	25:b:76:LEU:HD23	2.01	0.41
27:d:77:CYS:SG	27:d:84:CYS:HB3	2.60	0.41
36:m:54:LEU:HB3	41:s:103:LEU:CD2	2.51	0.41
40:r:357:THR:O	40:r:361:VAL:HG23	2.19	0.41
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.55	0.41
5:F:61:VAL:O	5:F:62:GLN:NE2	2.49	0.41
9:J:304:LEU:O	9:J:307:VAL:HG22	2.19	0.41
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.35	0.41
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	2.01	0.41
42:u:101:ARG:NH1	42:u:104:GLN:OE1	2.49	0.41
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.56	0.41
44:w:346:ASP:OD1	44:w:347:VAL:HG13	2.20	0.41
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41
9:J:163:LYS:NZ	9:J:253:ILE:O	2.40	0.41
22:Y:43:ARG:HD3	22:Y:48:PRO:HA	2.02	0.41
28:e:129:ARG:NH1	28:e:136:LEU:O	2.52	0.41
40:r:225:ILE:O	40:r:229:MET:HG3	2.20	0.41
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.02	0.41
41:s:195:ARG:HD3	41:s:231:ILE:HD11	2.02	0.41
41:s:294:LEU:HB3	41:s:295:PRO:HD3	2.02	0.41
2:B:120:GLU:HB2	2:B:130:ILE:HD12	2.01	0.41
8:I:3:SER:O	8:I:3:SER:OG	2.34	0.41
12:M:64:CYS:HB3	12:M:75:CYS:HB3	2.03	0.41
12:M:213:MET:HE1	12:M:713:ALA:O	2.20	0.41
15:P:197:PRO:HA	15:P:202:PHE:CD2	2.56	0.41
55:V:201:CDL:H322	55:V:201:CDL:H352	1.61	0.41
55:V:203:CDL:H801	55:V:203:CDL:H832	1.77	0.41
34:k:22:TYR:O	35:l:585:LYS:HE3	2.21	0.41
35:l:95:PHE:HZ	35:l:456:ARG:HG2	1.85	0.41
1:A:68:ILE:HD11	1:A:256:ARG:HG3	2.02	0.41
12:M:265:THR:HG21	12:M:609:ALA:HB1	2.02	0.41
13:N:3:LEU:O	13:N:6:VAL:HG22	2.21	0.41
14:O:100:LYS:O	14:O:104:ILE:HG12	2.20	0.41
26:c:179:GLU:OE2	26:c:179:GLU:N	2.53	0.41
33:j:73:LEU:O	41:s:160:TYR:OH	2.32	0.41
39:p:139:GLN:NE2	39:p:156:PRO:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PHE:HB2	16:Q:215:GLU:OE2	2.21	0.41
16:Q:105:MET:HE3	16:Q:105:MET:HB3	1.84	0.41
35:l:285:THR:HA	35:l:308:SER:HA	2.03	0.41
35:l:407:TRP:CE2	35:l:411:MET:HE3	2.56	0.41
48:l:718:PEE:H14	48:l:718:PEE:H1	1.84	0.41
2:B:91:GLY:HA2	2:B:92:PRO:HD3	1.93	0.41
14:O:133:GLN:HG2	14:O:172:ILE:HD11	2.03	0.41
16:Q:410:TYR:HB3	16:Q:423:LYS:HB3	2.02	0.41
55:a:201:CDL:OB3	49:e:201:PLX:H1B2	2.20	0.41
25:b:81:ILE:HG21	48:l:720:PEE:H64	2.03	0.41
32:i:183:SER:O	32:i:187:MET:HG2	2.20	0.41
35:l:357:ARG:HG2	39:p:32:VAL:HG22	2.03	0.41
42:u:59:GLU:O	42:u:63:VAL:HG23	2.20	0.41
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.61	0.41
1:A:201:ALA:HB1	14:O:121:MET:HB2	2.03	0.41
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.86	0.41
9:J:126:VAL:HG23	9:J:161:VAL:HG11	2.02	0.41
12:M:394:VAL:HG22	12:M:473:MET:HE1	2.03	0.41
14:O:140:CYS:HA	14:O:183:ALA:HB1	2.02	0.41
15:P:185:ARG:NH2	16:Q:110:ASP:OD1	2.52	0.41
21:W:54:ASN:HD22	41:s:156:MET:HE3	1.85	0.41
24:a:94:GLY:O	27:d:61:TYR:OH	2.28	0.41
26:c:145:TRP:CE2	26:c:149:ILE:HD11	2.56	0.41
27:d:9:VAL:HA	27:d:109:ARG:HH21	1.85	0.41
32:i:141:VAL:O	32:i:145:ILE:HG12	2.21	0.41
33:j:16:LEU:HD21	49:j:202:PLX:H212	2.03	0.41
33:j:87:MET:HG2	36:m:147:TYR:HB3	2.03	0.41
35:l:244:SER:O	35:l:249:SER:HB3	2.21	0.41
35:l:392:LYS:O	35:l:396:ILE:HG12	2.21	0.41
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.55	0.41
41:s:209:SER:HB3	41:s:213:VAL:CA	2.51	0.41
1:A:62:TRP:CE2	1:A:181:LEU:HD13	2.56	0.41
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.21	0.41
48:C:311:PEE:C23	49:j:202:PLX:H202	2.50	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
52:J:402:UQ:H101	52:J:402:UQ:H121	1.75	0.41
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.02	0.41
16:Q:120:THR:HG23	16:Q:135:TYR:CD1	2.56	0.41
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.28	0.41
17:S:50:ARG:O	17:S:54:ILE:HG12	2.20	0.41
55:V:203:CDL:H312	38:o:84:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:86:LEU:HB3	35:l:1:MET:HE1	2.02	0.41
35:l:51:LEU:HD22	35:l:91:PRO:HG3	2.02	0.41
41:s:146:LEU:HD12	41:s:188:SER:HB3	2.02	0.41
52:s:402:UQ:H221	52:s:402:UQ:H262	1.58	0.41
2:B:88:PHE:CZ	13:N:30:ALA:HA	2.56	0.40
12:M:173:MET:HE3	12:M:176:CYS:HB2	2.03	0.40
12:M:448:SER:HA	12:M:449:PRO:HD3	1.96	0.40
15:P:209:GLU:HB3	15:P:224:VAL:HG12	2.01	0.40
16:Q:209:LYS:HA	16:Q:212:GLU:OE2	2.21	0.40
19:U:66:VAL:O	42:u:130:LYS:HE3	2.21	0.40
20:V:59:TYR:CD1	55:V:201:CDL:C11	2.96	0.40
49:V:205:PLX:H6	49:V:205:PLX:H51	1.43	0.40
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.02	0.40
32:i:228:LEU:HD23	32:i:228:LEU:HA	1.92	0.40
49:j:203:PLX:H152	49:j:203:PLX:H341	2.02	0.40
55:l:713:CDL:H841	55:l:713:CDL:H182	2.03	0.40
39:p:127:ARG:HG2	39:p:130:ARG:HH22	1.86	0.40
40:r:204:MET:HE2	40:r:243:MET:CE	2.51	0.40
44:w:65:ASN:OD1	44:w:66:ILE:N	2.38	0.40
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.03	0.40
1:A:367:ILE:HG13	1:A:438:LEU:HD13	2.03	0.40
5:F:23:LEU:HD12	5:F:34:ARG:HG2	2.02	0.40
12:M:422:TRP:HA	12:M:427:LEU:HB3	2.02	0.40
20:V:38:ALA:HA	55:k:101:CDL:H201	2.02	0.40
48:V:202:PEE:H64	48:V:202:PEE:H59	1.89	0.40
32:i:179:MET:HE3	32:i:179:MET:HB3	1.88	0.40
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.02	0.40
35:l:281:GLY:O	35:l:285:THR:HG22	2.21	0.40
40:r:103:GLN:O	40:r:107:ILE:HG23	2.21	0.40
40:r:179:ILE:HG23	40:r:249:ILE:HG21	2.03	0.40
41:s:253:GLU:CD	41:s:253:GLU:H	2.30	0.40
44:w:116:LYS:HE3	44:w:116:LYS:HB2	1.92	0.40
4:E:99:GLN:CD	33:j:41:PHE:HD1	2.28	0.40
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.21	0.40
19:U:53:TYR:CZ	42:u:44:MET:HG3	2.56	0.40
55:V:201:CDL:H462	55:V:201:CDL:H431	1.93	0.40
48:V:202:PEE:H14	32:i:276:ILE:HG21	2.02	0.40
6:X:83:VAL:HG13	6:X:122:MET:HE3	2.03	0.40
25:b:19:ARG:HA	39:p:171:VAL:HG13	2.02	0.40
32:i:23:SER:HB2	32:i:29:ILE:HG13	2.03	0.40
33:j:105:GLU:HG2	33:j:110:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:17:ILE:HB	35:l:18:PRO:HD3	2.03	0.40
38:o:122:ASP:OD1	38:o:124:THR:HG22	2.22	0.40
41:s:259:PHE:O	41:s:263:THR:HG22	2.21	0.40
2:B:211:TYR:CE1	8:I:39:PRO:HG3	2.55	0.40
7:H:106:GLU:OE1	7:H:107:PRO:HD2	2.20	0.40
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.52	0.40
21:W:122:GLY:HA2	36:m:125:TRP:CZ3	2.56	0.40
1:A:369:ARG:HD2	1:A:369:ARG:HA	1.87	0.40
3:C:70:ALA:O	56:Q:501:DCQ:C4M	2.70	0.40
3:C:86:MET:HE1	3:C:93:PHE:CE2	2.57	0.40
5:F:91:LEU:HD23	5:F:91:LEU:HA	1.81	0.40
17:S:34:LYS:HB2	42:u:91:TYR:HA	2.03	0.40
17:S:46:ASN:ND2	36:m:132:ASP:HB3	2.37	0.40
24:a:140:LEU:HD21	40:r:177:LEU:HB3	2.03	0.40
30:g:14:GLN:O	30:g:15:PHE:HB3	2.22	0.40
32:i:234:TRP:CE3	32:i:304:MET:HG2	2.57	0.40
35:l:79:SER:OG	35:l:135:ASN:HB3	2.22	0.40
36:m:164:GLY:O	36:m:168:ILE:HG23	2.21	0.40
40:r:368:ALA:O	40:r:375:LEU:HD12	2.21	0.40
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.84	0.40
44:w:211:VAL:CG1	44:w:212:PRO:HD3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	422 (98%)	9 (2%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	107 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	H	110/112 (98%)	106 (96%)	3 (3%)	1 (1%)	14	27
8	I	93/112 (83%)	86 (92%)	7 (8%)	0	100	100
9	J	340/342 (99%)	331 (97%)	8 (2%)	1 (0%)	36	55
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	677 (98%)	11 (2%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	201 (98%)	4 (2%)	1 (0%)	24	43
16	Q	427/430 (99%)	419 (98%)	8 (2%)	0	100	100
17	S	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14	27
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	604/606 (100%)	585 (97%)	19 (3%)	0	100	100
36	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	38
40	r	457/459 (100%)	454 (99%)	3 (1%)	0	100	100
41	s	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
42	u	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	38
43	v	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8175/8314 (98%)	7932 (97%)	237 (3%)	6 (0%)	49	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	44	ARG
7	H	77	ILE
9	J	38	HIS
33	j	40	GLY
42	u	152	PRO
39	p	174	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	131 (99%)	1 (1%)	73	88
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	75/81 (93%)	74 (99%)	1 (1%)	61	82
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	84
9	J	296/296 (100%)	296 (100%)	0	100	100
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%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	370/370 (100%)	370 (100%)	0	100	100
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%)	101 (100%)	0	100	100
21	W	121/123 (98%)	121 (100%)	0	100	100
22	Y	62/62 (100%)	62 (100%)	0	100	100
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	121 (100%)	0	100	100
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	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	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	94
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/540 (99%)	536 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	m	126/141 (89%)	126 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	87
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	410 (100%)	0	100	100
41	s	275/275 (100%)	274 (100%)	1 (0%)	84	93
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/111 (94%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7150/7241 (99%)	7143 (100%)	7 (0%)	87	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	71	CYS
8	I	41	LEU
6	X	100	VAL
32	i	100	MET
35	l	71	LEU
38	o	126	ASN
41	s	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	277	ASN
1	A	284	HIS
1	A	344	GLN
1	A	346	GLN
1	A	393	ASN
3	C	111	ASN
4	E	126	HIS
6	G	142	GLN
8	I	13	ASN
8	I	29	GLN
9	J	128	ASN
9	J	295	HIS

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Mol	Chain	Res	Type
10	K	70	ASN
10	K	78	HIS
11	L	71	HIS
11	L	86	ASN
12	M	178	GLN
12	M	669	ASN
13	N	5	GLN
13	N	12	GLN
13	N	13	GLN
13	N	113	HIS
13	N	123	GLN
14	O	41	HIS
14	O	90	ASN
15	P	55	HIS
15	P	82	ASN
15	P	124	ASN
15	P	131	ASN
15	P	196	HIS
15	P	228	GLN
16	Q	79	ASN
16	Q	162	GLN
16	Q	183	HIS
16	Q	454	GLN
17	S	40	HIS
18	T	74	GLN
18	T	120	GLN
6	X	142	GLN
22	Y	57	GLN
23	Z	21	GLN
23	Z	33	GLN
24	a	189	ASN
25	b	13	GLN
26	c	84	GLN
27	d	131	GLN
28	e	86	ASN
30	g	81	GLN
30	g	90	HIS
32	i	49	ASN
32	i	120	GLN
32	i	310	ASN
34	k	57	ASN
35	l	59	GLN

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Mol	Chain	Res	Type
35	l	296	ASN
35	l	348	HIS
35	l	354	GLN
35	l	446	ASN
35	l	470	ASN
35	l	580	GLN
35	l	603	ASN
38	o	50	GLN
38	o	79	ASN
38	o	123	GLN
38	o	126	ASN
39	p	13	GLN
40	r	30	HIS
40	r	138	ASN
40	r	139	GLN
40	r	175	ASN
40	r	251	ASN
41	s	47	GLN
41	s	97	ASN
41	s	247	HIS
41	s	250	HIS
41	s	287	HIS
42	u	151	ASN
43	v	55	GLN
44	w	132	GLN
44	w	149	HIS
44	w	215	GLN
44	w	322	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.02	1 (10%)	5,13,15	5.92	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	5.80	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	12.02	130.50	119.48
16	Q	118	2MR	CD-NE-CZ	3.99	130.85	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.49	131.15	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

Of 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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$
53	FES	M	803	12	0,4,4	-	-	-		
48	PEE	l	718	-	46,46,50	1.22	6 (13%)	49,51,55	1.03	2 (4%)
55	CDL	i	401	-	86,86,99	1.17	8 (9%)	92,98,111	0.91	4 (4%)
55	CDL	k	101	-	99,99,99	1.12	9 (9%)	105,111,111	0.84	4 (3%)
51	NDP	J	401	-	51,52,52	2.45	7 (13%)	71,80,80	1.53	16 (22%)
49	PLX	i	705	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
53	FES	O	301	14	0,4,4	-	-	-		
55	CDL	m	201	-	88,88,99	1.17	8 (9%)	94,100,111	0.95	5 (5%)
56	DCQ	Q	501	-	23,23,23	1.34	5 (21%)	27,29,29	1.07	2 (7%)
52	UQ	s	402	-	38,38,63	3.63	10 (26%)	48,49,79	2.77	17 (35%)
49	PLX	j	203	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	PLX	n	101	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
50	8Q1	X	201	-	32,34,34	2.28	7 (21%)	39,43,43	1.76	11 (28%)
45	SF4	C	301	3	0,12,12	-	-	-		
48	PEE	l	719	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
52	UQ	J	402	-	33,33,63	3.52	10 (30%)	42,43,79	2.73	14 (33%)
55	CDL	a	201	-	99,99,99	0.93	4 (4%)	105,111,111	1.11	9 (8%)
55	CDL	n	102	-	54,54,99	1.25	4 (7%)	60,66,111	1.24	5 (8%)
55	CDL	r	714	-	99,99,99	1.12	8 (8%)	105,111,111	0.88	4 (3%)
49	PLX	j	202	-	51,51,51	0.60	0	53,59,59	0.67	0
48	PEE	U	101	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	8 (16%)
55	CDL	V	201	-	93,93,99	0.94	4 (4%)	99,105,111	1.13	6 (6%)
48	PEE	m	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.04	2 (4%)
55	CDL	V	203	-	99,99,99	0.91	4 (4%)	105,111,111	1.05	8 (7%)
49	PLX	C	312	-	51,51,51	1.21	4 (7%)	53,59,59	0.60	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	M	802	12	0,12,12	-	-	-		
55	CDL	N	202	-	50,50,99	1.29	4 (8%)	56,62,111	1.34	6 (10%)
45	SF4	A	501	1	0,12,12	-	-	-		
47	NAI	A	503	-	47,48,48	4.00	22 (46%)	64,73,73	1.73	12 (18%)
49	PLX	V	205	-	51,51,51	1.21	5 (9%)	53,59,59	0.63	1 (1%)
48	PEE	V	202	-	50,50,50	1.17	6 (12%)	53,55,55	0.95	2 (3%)
48	PEE	j	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.08	3 (6%)
49	PLX	e	201	-	51,51,51	0.60	0	53,59,59	0.63	0
55	CDL	l	712	-	98,98,99	1.12	8 (8%)	104,110,111	0.89	4 (3%)
48	PEE	s	401	-	50,50,50	1.19	6 (12%)	53,55,55	1.00	2 (3%)
48	PEE	V	207	-	39,39,50	1.33	6 (15%)	42,44,55	1.10	3 (7%)
55	CDL	l	713	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
50	8Q1	G	201	-	32,34,34	2.27	7 (21%)	39,43,43	1.83	13 (33%)
45	SF4	M	801	12	0,12,12	-	-	-		
48	PEE	l	720	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
58	ADP	w	401	-	28,29,29	3.15	9 (32%)	43,45,45	1.94	9 (20%)
45	SF4	B	302	2	0,12,12	-	-	-		
48	PEE	C	311	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	FES	M	803	12	-	-	0/1/1/1
48	PEE	l	718	-	-	15/50/50/54	-
55	CDL	i	401	-	-	47/97/97/110	-
55	CDL	k	101	-	-	66/110/110/110	-
51	NDP	J	401	-	-	6/34/77/77	0/5/5/5
49	PLX	i	705	-	-	31/55/55/55	-
53	FES	O	301	14	-	-	0/1/1/1
55	CDL	m	201	-	-	56/99/99/110	-
56	DCQ	Q	501	-	-	4/14/38/38	0/1/1/1
52	UQ	s	402	-	-	13/33/57/87	0/1/1/1
49	PLX	j	203	-	-	33/55/55/55	-
49	PLX	n	101	-	-	31/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	B	301	2	-	-	0/6/5/5
50	8Q1	X	201	-	-	10/41/41/41	-
45	SF4	C	301	3	-	-	0/6/5/5
48	PEE	l	719	-	-	27/54/54/54	-
52	UQ	J	402	-	-	14/27/51/87	0/1/1/1
55	CDL	a	201	-	-	38/110/110/110	-
55	CDL	n	102	-	-	26/65/65/110	-
55	CDL	r	714	-	-	60/110/110/110	-
49	PLX	j	202	-	-	26/55/55/55	-
48	PEE	U	101	-	-	27/54/54/54	-
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
55	CDL	V	201	-	-	38/104/104/110	-
48	PEE	m	202	-	-	21/44/44/54	-
55	CDL	V	203	-	-	44/110/110/110	-
49	PLX	C	312	-	-	27/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
55	CDL	N	202	-	-	29/61/61/110	-
45	SF4	A	501	1	-	-	0/6/5/5
47	NAI	A	503	-	-	5/29/72/72	0/5/5/5
49	PLX	V	205	-	-	27/55/55/55	-
48	PEE	V	202	-	-	31/54/54/54	-
48	PEE	j	201	-	-	18/44/44/54	-
49	PLX	e	201	-	-	23/55/55/55	-
55	CDL	l	712	-	-	59/109/109/110	-
48	PEE	s	401	-	-	20/54/54/54	-
48	PEE	V	207	-	-	25/43/43/54	-
55	CDL	l	713	-	-	63/110/110/110	-
50	8Q1	G	201	-	-	19/41/41/41	-
48	PEE	l	720	-	-	23/49/49/54	-
58	ADP	w	401	-	-	2/16/32/32	0/3/3/3
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	C	311	-	-	19/50/50/54	-

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	P2B-O2B	13.89	1.83	1.59
47	A	503	NAI	C3D-C4D	-10.46	1.26	1.53
52	s	402	UQ	C18-C19	9.99	1.56	1.33
52	J	402	UQ	C18-C19	9.95	1.56	1.33
52	s	402	UQ	C13-C14	9.64	1.55	1.33
52	J	402	UQ	C13-C14	9.55	1.55	1.33
52	s	402	UQ	C23-C24	9.43	1.54	1.33
47	A	503	NAI	O4B-C1B	9.37	1.63	1.42
52	s	402	UQ	C8-C9	9.30	1.54	1.33
52	J	402	UQ	C8-C9	9.28	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.92	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.32	1.26	1.45
50	G	201	8Q1	P24-O27	7.97	1.85	1.60
47	A	503	NAI	C2D-C1D	-7.76	1.29	1.53
58	w	401	ADP	O4'-C4'	7.70	1.62	1.45
50	X	201	8Q1	P24-O27	7.66	1.84	1.60
52	J	402	UQ	C23-C24	7.51	1.54	1.32
52	s	402	UQ	C28-C29	7.37	1.54	1.32
47	A	503	NAI	C2B-C1B	-7.33	1.30	1.53
47	A	503	NAI	O4D-C4D	6.86	1.60	1.45
58	w	401	ADP	PA-O3A	6.30	1.66	1.59
47	A	503	NAI	PA-O3	6.26	1.66	1.59
47	A	503	NAI	C2D-C3D	5.85	1.69	1.53
50	G	201	8Q1	C28-C29	5.82	1.62	1.52
50	X	201	8Q1	C28-C29	5.62	1.61	1.52
47	A	503	NAI	PN-O3	5.57	1.65	1.59
47	A	503	NAI	O4D-C1D	5.48	1.54	1.42
58	w	401	ADP	C6-N6	5.42	1.48	1.34
47	A	503	NAI	C4N-C3N	-5.36	1.39	1.50
47	A	503	NAI	C7N-N7N	5.23	1.48	1.33
47	A	503	NAI	C6A-N6A	5.07	1.47	1.34
51	J	401	NDP	PA-O3	4.91	1.64	1.59
58	w	401	ADP	O4'-C1'	-4.60	1.31	1.42
55	N	202	CDL	OB8-CB7	4.37	1.46	1.33
55	a	201	CDL	OB8-CB7	4.34	1.46	1.33
55	n	102	CDL	OA8-CA7	4.30	1.45	1.33
55	N	202	CDL	OA8-CA7	4.27	1.45	1.33
55	a	201	CDL	OA8-CA7	4.27	1.45	1.33
55	V	203	CDL	OA8-CA7	4.25	1.45	1.33
55	V	201	CDL	OA8-CA7	4.24	1.45	1.33
47	A	503	NAI	O2B-C2B	4.23	1.53	1.43
55	n	102	CDL	OB8-CB7	4.21	1.45	1.33
55	N	202	CDL	OA6-CA5	4.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	201	CDL	OB8-CB7	4.17	1.45	1.33
55	V	203	CDL	OB8-CB7	4.17	1.45	1.33
55	n	102	CDL	OB6-CB5	4.15	1.46	1.34
55	V	203	CDL	OA6-CA5	4.14	1.46	1.34
55	n	102	CDL	OA6-CA5	4.13	1.46	1.34
55	V	201	CDL	OA6-CA5	4.11	1.45	1.34
55	a	201	CDL	OB6-CB5	4.10	1.45	1.34
51	J	401	NDP	PN-O5D	4.10	1.75	1.59
50	X	201	8Q1	C1-S44	4.07	1.85	1.76
55	a	201	CDL	OA6-CA5	4.06	1.45	1.34
55	V	201	CDL	OB6-CB5	4.05	1.45	1.34
55	V	203	CDL	OB6-CB5	4.00	1.45	1.34
55	N	202	CDL	OB6-CB5	3.97	1.45	1.34
48	V	202	PEE	C18-C19	3.86	1.53	1.31
48	s	401	PEE	C18-C19	3.84	1.53	1.31
48	l	719	PEE	C18-C19	3.84	1.53	1.31
48	V	207	PEE	C18-C19	3.83	1.53	1.31
48	C	311	PEE	C18-C19	3.83	1.53	1.31
48	j	201	PEE	C18-C19	3.81	1.53	1.31
48	l	720	PEE	C18-C19	3.81	1.53	1.31
48	m	202	PEE	C18-C19	3.80	1.53	1.31
48	U	101	PEE	C18-C19	3.76	1.53	1.31
48	l	718	PEE	C18-C19	3.76	1.53	1.31
48	s	401	PEE	C39-C38	3.74	1.53	1.31
48	l	720	PEE	C39-C38	3.74	1.52	1.31
48	l	718	PEE	C39-C38	3.73	1.52	1.31
48	V	202	PEE	C39-C38	3.73	1.52	1.31
48	C	311	PEE	C39-C38	3.72	1.52	1.31
48	V	207	PEE	C39-C38	3.72	1.52	1.31
48	U	101	PEE	C39-C38	3.71	1.52	1.31
48	l	719	PEE	C39-C38	3.70	1.52	1.31
50	G	201	8Q1	C34-N36	3.54	1.41	1.33
55	i	401	CDL	OA8-CA7	3.50	1.43	1.33
50	G	201	8Q1	C1-S44	3.49	1.84	1.76
55	l	712	CDL	OA8-CA7	3.48	1.43	1.33
47	A	503	NAI	C7N-C3N	3.48	1.56	1.48
55	k	101	CDL	OA8-CA7	3.45	1.43	1.33
55	l	713	CDL	OA8-CA7	3.45	1.43	1.33
55	m	201	CDL	OA8-CA7	3.45	1.43	1.33
55	r	714	CDL	OA8-CA7	3.44	1.43	1.33
46	A	502	FMN	C4A-N5	3.40	1.38	1.30
58	w	401	ADP	C8-N9	-3.35	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C4N-C5N	-3.35	1.40	1.49
50	X	201	8Q1	C34-N36	3.33	1.41	1.33
50	X	201	8Q1	O27-C28	-3.29	1.33	1.43
50	G	201	8Q1	O27-C28	-3.25	1.33	1.43
55	k	101	CDL	OA6-CA5	3.17	1.43	1.34
51	J	401	NDP	O2B-C2B	-3.16	1.33	1.44
58	w	401	ADP	O2'-C2'	-3.06	1.35	1.43
55	r	714	CDL	OB6-CB5	3.06	1.42	1.34
55	i	401	CDL	OB6-CB5	3.05	1.42	1.34
55	l	712	CDL	OB6-CB5	3.05	1.42	1.34
55	i	401	CDL	OB8-CB7	3.03	1.42	1.33
55	l	712	CDL	OB8-CB7	3.02	1.42	1.33
55	m	201	CDL	OA6-CA5	3.02	1.42	1.34
55	i	401	CDL	OA6-CA5	3.00	1.42	1.34
55	m	201	CDL	OB6-CB5	3.00	1.42	1.34
58	w	401	ADP	O3'-C3'	3.00	1.50	1.43
55	l	713	CDL	OB6-CB5	2.99	1.42	1.34
55	k	101	CDL	OB8-CB7	2.99	1.42	1.33
55	l	713	CDL	OB8-CB7	2.99	1.42	1.33
55	r	714	CDL	OB8-CB7	2.98	1.42	1.33
55	k	101	CDL	OB6-CB5	2.98	1.42	1.34
50	G	201	8Q1	C39-N41	2.97	1.40	1.33
55	l	713	CDL	OA6-CA5	2.95	1.42	1.34
55	l	712	CDL	OA6-CA5	2.94	1.42	1.34
55	m	201	CDL	OB8-CB7	2.94	1.41	1.33
50	X	201	8Q1	C6-C1	2.91	1.53	1.50
55	r	714	CDL	OA6-CA5	2.89	1.42	1.34
49	i	705	PLX	O6-C4	-2.85	1.41	1.44
52	J	402	UQ	C6-C1	2.84	1.54	1.46
50	X	201	8Q1	C39-N41	2.84	1.40	1.33
48	s	401	PEE	O2-C2	-2.78	1.40	1.46
47	A	503	NAI	C8A-N9A	-2.77	1.32	1.37
52	s	402	UQ	C6-C1	2.76	1.54	1.46
49	C	312	PLX	O6-C4	-2.74	1.41	1.44
49	n	101	PLX	O6-C4	-2.71	1.41	1.44
49	j	203	PLX	O6-C4	-2.69	1.41	1.44
48	l	719	PEE	O2-C2	-2.65	1.40	1.46
48	C	311	PEE	O2-C2	-2.63	1.40	1.46
48	l	718	PEE	O2-C2	-2.62	1.40	1.46
48	U	101	PEE	O2-C2	-2.61	1.40	1.46
48	j	201	PEE	O2-C2	-2.61	1.40	1.46
48	m	202	PEE	O2-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	714	CDL	OA6-CA4	-2.59	1.40	1.46
49	V	205	PLX	O6-C4	-2.59	1.41	1.44
55	l	712	CDL	OA6-CA4	-2.58	1.40	1.46
51	J	401	NDP	C5A-C4A	2.55	1.43	1.39
48	l	720	PEE	O2-C2	-2.55	1.40	1.46
55	m	201	CDL	OA6-CA4	-2.54	1.40	1.46
46	A	502	FMN	C10-N1	2.54	1.38	1.33
55	i	401	CDL	OA6-CA4	-2.53	1.40	1.46
48	V	207	PEE	O2-C2	-2.51	1.40	1.46
55	l	713	CDL	OA6-CA4	-2.50	1.40	1.46
48	j	201	PEE	O3-C30	2.50	1.40	1.33
48	m	202	PEE	O3-C30	2.48	1.40	1.33
48	l	720	PEE	O3-C30	2.48	1.40	1.33
49	j	203	PLX	C7-C6	2.45	1.55	1.50
47	A	503	NAI	O3B-C3B	-2.44	1.36	1.43
49	i	705	PLX	C7-C6	2.43	1.55	1.50
48	V	207	PEE	O3-C30	2.43	1.40	1.33
48	C	311	PEE	O3-C30	2.41	1.40	1.33
58	w	401	ADP	C5-N7	-2.41	1.34	1.39
49	C	312	PLX	C7-C6	2.41	1.55	1.50
48	V	202	PEE	O2-C2	-2.40	1.41	1.46
48	l	719	PEE	O3-C30	2.40	1.40	1.33
48	s	401	PEE	O3-C30	2.40	1.40	1.33
49	V	205	PLX	C7-C6	2.39	1.55	1.50
52	s	402	UQ	C7-C8	2.39	1.54	1.50
47	A	503	NAI	C6N-C5N	2.39	1.40	1.33
48	l	718	PEE	O3-C30	2.38	1.40	1.33
55	l	713	CDL	OB6-CB4	-2.35	1.41	1.46
47	A	503	NAI	PN-O5D	2.34	1.68	1.59
55	k	101	CDL	OB6-CB4	-2.34	1.41	1.46
48	U	101	PEE	O3-C30	2.34	1.40	1.33
51	J	401	NDP	C2A-N1A	2.34	1.38	1.33
49	n	101	PLX	C7-C6	2.33	1.55	1.50
48	V	202	PEE	O3-C30	2.33	1.40	1.33
55	m	201	CDL	OB6-CB4	-2.33	1.41	1.46
50	G	201	8Q1	O33-C32	-2.32	1.38	1.42
55	l	712	CDL	OB6-CB4	-2.32	1.41	1.46
56	Q	501	DCQ	O4-C4M	-2.32	1.40	1.45
48	l	719	PEE	O3-C3	-2.30	1.40	1.45
48	V	207	PEE	O2-C10	2.30	1.40	1.34
52	J	402	UQ	C7-C8	2.29	1.54	1.50
48	m	202	PEE	O2-C10	2.28	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Q	501	DCQ	C6-C5	2.28	1.52	1.46
55	i	401	CDL	PB2-OB2	2.27	1.68	1.59
48	l	720	PEE	O2-C10	2.27	1.40	1.34
55	k	101	CDL	OA6-CA4	-2.27	1.41	1.46
55	i	401	CDL	PB2-OB5	2.27	1.68	1.59
55	l	713	CDL	PB2-OB2	2.27	1.68	1.59
55	m	201	CDL	PB2-OB2	2.26	1.68	1.59
55	r	714	CDL	OB6-CB4	-2.26	1.41	1.46
55	k	101	CDL	PB2-OB2	2.25	1.68	1.59
48	V	207	PEE	O3-C3	-2.25	1.40	1.45
55	l	712	CDL	PB2-OB5	2.24	1.68	1.59
55	l	712	CDL	PB2-OB2	2.24	1.68	1.59
49	V	205	PLX	P1-O4	2.24	1.68	1.59
56	Q	501	DCQ	O3-C3M	-2.24	1.40	1.45
55	r	714	CDL	PB2-OB2	2.24	1.68	1.59
48	U	101	PEE	O3-C3	-2.23	1.40	1.45
55	k	101	CDL	PB2-OB5	2.23	1.68	1.59
55	i	401	CDL	OB6-CB4	-2.23	1.41	1.46
47	A	503	NAI	C5B-C4B	2.23	1.58	1.51
48	l	718	PEE	O2-C10	2.22	1.40	1.34
55	r	714	CDL	PB2-OB5	2.21	1.68	1.59
48	s	401	PEE	O3-C3	-2.21	1.40	1.45
49	j	203	PLX	P1-O4	2.21	1.68	1.59
48	j	201	PEE	O2-C10	2.20	1.40	1.34
55	m	201	CDL	PB2-OB5	2.20	1.68	1.59
48	V	202	PEE	O3-C3	-2.19	1.40	1.45
48	V	202	PEE	O2-C10	2.19	1.40	1.34
55	l	713	CDL	PB2-OB5	2.19	1.68	1.59
49	C	312	PLX	P1-O4	2.18	1.67	1.59
48	U	101	PEE	O2-C10	2.18	1.40	1.34
49	i	705	PLX	P1-O4	2.17	1.67	1.59
48	C	311	PEE	O2-C10	2.17	1.40	1.34
49	n	101	PLX	P1-O4	2.16	1.67	1.59
48	C	311	PEE	O3-C3	-2.16	1.40	1.45
48	l	718	PEE	O3-C3	-2.16	1.40	1.45
48	m	202	PEE	O3-C3	-2.14	1.40	1.45
52	s	402	UQ	O4-C4	-2.14	1.18	1.23
49	V	205	PLX	P1-O1	2.12	1.67	1.59
48	l	720	PEE	O3-C3	-2.11	1.40	1.45
52	J	402	UQ	O4-C4	-2.11	1.18	1.23
52	J	402	UQ	O3-CM3	-2.10	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.10	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	s	402	UQ	O3-CM3	-2.09	1.40	1.45
49	j	203	PLX	P1-O1	2.09	1.67	1.59
51	J	401	NDP	C4A-N3A	2.08	1.38	1.34
49	n	101	PLX	P1-O1	2.08	1.67	1.59
56	Q	501	DCQ	O2-C2	-2.07	1.18	1.23
48	l	719	PEE	O2-C10	2.06	1.40	1.34
49	C	312	PLX	P1-O1	2.06	1.67	1.59
52	J	402	UQ	C21-C19	2.06	1.55	1.51
52	s	402	UQ	C21-C19	2.06	1.55	1.51
48	j	201	PEE	O3-C3	-2.05	1.40	1.45
48	s	401	PEE	O2-C10	2.05	1.40	1.34
49	V	205	PLX	C25-C24	2.04	1.55	1.50
49	i	705	PLX	P1-O1	2.03	1.67	1.59
56	Q	501	DCQ	O5-C5	-2.03	1.18	1.23
52	J	402	UQ	C5-C4	2.00	1.54	1.47
55	k	101	CDL	C11-CA5	2.00	1.56	1.50

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	s	402	UQ	C7-C8-C9	-7.61	113.72	126.83
52	J	402	UQ	C7-C8-C9	-7.39	114.11	126.83
52	J	402	UQ	C12-C13-C14	-6.50	112.76	127.62
52	J	402	UQ	C17-C18-C19	-6.32	113.17	127.62
52	s	402	UQ	C22-C23-C24	-6.24	113.34	127.62
52	s	402	UQ	C12-C13-C14	-6.05	113.77	127.62
52	s	402	UQ	C17-C18-C19	-6.00	113.89	127.62
47	A	503	NAI	C5A-C4A-N3A	-5.57	119.05	126.72
58	w	401	ADP	C5-C4-N3	-5.40	119.29	126.72
50	G	201	8Q1	C6-C1-S44	5.27	119.68	113.40
52	J	402	UQ	C10-C9-C8	-4.77	111.39	123.63
58	w	401	ADP	N3-C2-N1	-4.67	121.51	128.58
50	X	201	8Q1	C6-C1-S44	4.60	118.88	113.40
47	A	503	NAI	N3A-C2A-N1A	-4.58	121.65	128.58
55	V	201	CDL	OA6-CA5-C11	4.51	121.23	111.48
52	s	402	UQ	C10-C9-C8	-4.45	112.20	123.63
55	a	201	CDL	OB6-CB5-C51	4.37	120.92	111.48
48	j	201	PEE	O2-C10-C11	4.35	120.90	111.48
51	J	401	NDP	P2B-O2B-C2B	-4.31	111.91	123.43
52	s	402	UQ	C27-C28-C29	-4.31	113.27	127.64
58	w	401	ADP	N3-C4-N9	4.30	134.47	127.17
55	a	201	CDL	OA6-CA5-C11	4.30	120.77	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	C22-C23-C24	-4.27	113.41	127.64
52	J	402	UQ	C15-C14-C13	-4.25	112.70	123.63
55	V	201	CDL	OB6-CB5-C51	4.24	120.65	111.48
52	s	402	UQ	C25-C24-C23	-4.24	112.75	123.63
55	m	201	CDL	OA6-CA5-C11	4.23	120.63	111.48
48	s	401	PEE	O2-C10-C11	4.19	120.54	111.48
55	N	202	CDL	OA6-CA5-C11	4.17	120.50	111.48
52	J	402	UQ	C20-C19-C18	-4.16	112.95	123.63
55	V	203	CDL	OB6-CB5-C51	4.14	120.43	111.48
50	X	201	8Q1	C43-S44-C1	4.14	114.07	101.84
48	V	207	PEE	O2-C10-C11	4.08	120.30	111.48
55	V	203	CDL	OA6-CA5-C11	4.05	120.24	111.48
48	m	202	PEE	O2-C10-C11	4.03	120.19	111.48
47	A	503	NAI	N3A-C4A-N9A	4.01	133.98	127.17
55	r	714	CDL	OB6-CB5-C51	4.00	120.14	111.48
55	n	102	CDL	OA6-CA5-C11	4.00	120.12	111.48
55	l	712	CDL	OA6-CA5-C11	3.99	120.10	111.48
48	l	720	PEE	O2-C10-C11	3.96	120.06	111.48
55	r	714	CDL	OA6-CA5-C11	3.94	120.00	111.48
55	N	202	CDL	OB6-CB5-C51	3.94	120.00	111.48
48	U	101	PEE	O2-C10-C11	3.94	120.00	111.48
48	C	311	PEE	O2-C10-C11	3.93	119.99	111.48
55	i	401	CDL	OA6-CA5-C11	3.93	119.99	111.48
55	m	201	CDL	OB6-CB5-C51	3.93	119.98	111.48
55	i	401	CDL	OB6-CB5-C51	3.92	119.97	111.48
55	l	712	CDL	OB6-CB5-C51	3.91	119.94	111.48
52	s	402	UQ	C20-C19-C18	-3.90	113.61	123.63
48	l	719	PEE	O2-C10-C11	3.89	119.89	111.48
52	s	402	UQ	C15-C14-C13	-3.88	113.67	123.63
55	k	101	CDL	OB6-CB5-C51	3.87	119.86	111.48
52	s	402	UQ	C21-C19-C18	-3.87	112.48	121.17
52	J	402	UQ	C16-C14-C13	-3.86	112.51	121.17
55	l	713	CDL	OA6-CA5-C11	3.85	119.82	111.48
50	G	201	8Q1	C43-S44-C1	3.85	113.23	101.84
55	n	102	CDL	OB6-CB5-C51	3.82	119.74	111.48
47	A	503	NAI	C2A-N3A-C4A	3.81	121.14	111.83
52	s	402	UQ	C16-C14-C13	-3.77	112.70	121.17
52	s	402	UQ	C11-C9-C8	-3.77	112.70	121.17
48	V	202	PEE	O2-C10-C11	3.77	119.63	111.48
48	l	718	PEE	O2-C10-C11	3.76	119.62	111.48
52	J	402	UQ	C11-C9-C8	-3.73	112.79	121.17
55	l	713	CDL	OB6-CB5-C51	3.73	119.54	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	w	401	ADP	N9-C8-N7	-3.63	108.79	113.94
58	w	401	ADP	C2-N3-C4	3.59	120.60	111.83
52	J	402	UQ	C21-C19-C18	-3.57	113.16	121.17
52	s	402	UQ	C26-C24-C23	-3.54	113.21	121.17
51	J	401	NDP	O2B-P2B-O1X	-3.51	96.81	109.33
50	X	201	8Q1	O35-C34-N36	-3.43	115.71	122.98
50	G	201	8Q1	O35-C34-N36	-3.41	115.75	122.98
51	J	401	NDP	O3-PA-O1A	-3.41	100.44	110.70
55	k	101	CDL	OA6-CA5-C11	3.36	118.75	111.48
47	A	503	NAI	C4A-C5A-N7A	-3.35	106.75	110.58
47	A	503	NAI	C5A-N7A-C8A	3.34	108.71	103.45
58	w	401	ADP	C4-N9-C8	3.33	109.24	105.74
46	A	502	FMN	C4-N3-C2	-3.32	119.74	125.64
55	a	201	CDL	OB8-CB7-C71	3.29	121.88	111.83
47	A	503	NAI	C3D-C2D-C1D	3.29	107.69	101.46
52	s	402	UQ	C30-C29-C28	-3.29	112.78	122.66
47	A	503	NAI	N9A-C8A-N7A	-3.25	109.32	113.94
55	n	102	CDL	OB8-CB7-C71	3.25	121.75	111.83
58	w	401	ADP	C5-N7-C8	3.21	108.50	103.45
55	a	201	CDL	OA8-CA7-C31	3.20	121.58	111.83
52	J	402	UQ	C25-C24-C23	-3.18	113.12	122.66
52	J	402	UQ	C26-C24-C23	-3.15	113.21	122.66
52	s	402	UQ	C31-C29-C28	-3.13	113.25	122.66
50	X	201	8Q1	C32-C34-N36	3.11	122.38	116.48
48	l	718	PEE	O3-C30-C31	3.03	121.07	111.83
51	J	401	NDP	PA-O5B-C5B	-3.02	104.03	121.35
56	Q	501	DCQ	C1M-C1-C6	-3.00	119.52	124.45
48	l	719	PEE	O3-C30-C31	3.00	120.98	111.83
48	s	401	PEE	O3-C30-C31	2.98	120.92	111.83
52	J	402	UQ	C7-C6-C5	-2.95	119.83	124.89
55	V	203	CDL	OA8-CA7-C31	2.94	120.81	111.83
58	w	401	ADP	C4-C5-N7	-2.93	107.23	110.58
55	a	201	CDL	CB4-OB6-CB5	-2.90	110.86	117.80
50	G	201	8Q1	C37-C38-C39	2.89	117.21	112.39
55	V	201	CDL	OB8-CB7-C71	2.89	120.64	111.83
55	k	101	CDL	OA8-CA7-C31	2.87	120.58	111.83
51	J	401	NDP	PN-O5D-C5D	-2.85	105.04	121.35
55	N	202	CDL	OB8-CB7-C71	2.84	120.48	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.83	103.21	109.47
50	G	201	8Q1	O2-P24-O27	-2.83	99.29	106.67
48	V	202	PEE	O3-C30-C31	2.83	120.45	111.83
55	l	712	CDL	OA8-CA7-C31	2.82	120.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	X	201	8Q1	O2-P24-O27	-2.81	99.35	106.67
48	m	202	PEE	O3-C30-C31	2.79	120.34	111.83
55	k	101	CDL	OB8-CB7-C71	2.77	120.29	111.83
48	j	201	PEE	O3-C30-C31	2.75	120.22	111.83
55	n	102	CDL	OA8-CA7-C31	2.75	119.50	111.15
48	U	101	PEE	O3-C30-C31	2.74	120.20	111.83
55	i	401	CDL	OA8-CA7-C31	2.74	120.19	111.83
50	G	201	8Q1	O4-C1-C6	-2.73	120.83	123.98
55	m	201	CDL	OA8-CA7-C31	2.72	120.14	111.83
55	V	203	CDL	OB8-CB7-C71	2.70	120.08	111.83
48	C	311	PEE	O3-C30-C31	2.69	120.05	111.83
55	r	714	CDL	OB8-CB7-C71	2.69	120.05	111.83
55	l	712	CDL	OB8-CB7-C71	2.69	120.05	111.83
55	l	713	CDL	OB8-CB7-C71	2.69	120.05	111.83
55	i	401	CDL	OB8-CB7-C71	2.69	120.03	111.83
55	m	201	CDL	OB8-CB7-C71	2.69	120.02	111.83
46	A	502	FMN	C4A-C4-N3	2.68	120.07	113.25
55	r	714	CDL	OA8-CA7-C31	2.65	119.93	111.83
55	N	202	CDL	OA8-CA7-C31	2.65	119.92	111.83
55	N	202	CDL	CA6-CA4-CA3	-2.65	105.61	111.78
52	J	402	UQ	CM5-C5-C6	-2.64	120.11	124.45
55	l	713	CDL	OA8-CA7-C31	2.64	119.87	111.83
55	V	201	CDL	CB4-OB6-CB5	-2.63	111.50	117.80
47	A	503	NAI	C2D-C3D-C4D	2.61	107.65	102.61
55	V	201	CDL	OA8-CA7-C31	2.60	119.77	111.83
51	J	401	NDP	O2N-PN-O3	2.59	114.28	107.27
49	V	205	PLX	C1A-N1-C1	2.58	120.17	109.91
46	A	502	FMN	O4-C4-C4A	-2.57	119.74	126.53
48	l	720	PEE	O3-C30-C31	2.55	119.60	111.83
49	n	101	PLX	C1A-N1-C1	2.52	119.91	109.91
51	J	401	NDP	O3X-P2B-O2X	2.51	117.23	107.80
50	G	201	8Q1	C32-C34-N36	2.51	121.25	116.48
50	G	201	8Q1	O4-C1-S44	-2.51	119.49	122.68
55	V	203	CDL	CB4-OB6-CB5	-2.51	111.79	117.80
58	w	401	ADP	C4'-O4'-C1'	-2.51	103.93	109.47
50	X	201	8Q1	O40-C39-N41	-2.48	118.17	123.03
50	X	201	8Q1	C37-C38-C39	2.48	116.52	112.39
51	J	401	NDP	O4B-C4B-C3B	2.47	110.06	105.15
55	N	202	CDL	CB4-OB6-CB5	-2.47	111.88	117.80
49	i	705	PLX	C1A-N1-C1	2.47	119.73	109.91
46	A	502	FMN	C5A-C9A-N10	2.46	120.19	117.97
51	J	401	NDP	O2N-PN-O1N	2.46	123.87	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	X	201	8Q1	O4-C1-C6	-2.44	121.16	123.98
51	J	401	NDP	N3A-C4A-N9A	2.40	131.26	127.17
47	A	503	NAI	C4A-N9A-C8A	2.39	108.25	105.74
51	J	401	NDP	C2A-N1A-C6A	-2.39	114.81	118.73
55	m	201	CDL	CA4-OA6-CA5	-2.39	112.08	117.80
49	j	203	PLX	C1A-N1-C1	2.38	119.36	109.91
48	V	207	PEE	C20-C19-C18	-2.36	112.22	126.42
48	V	207	PEE	O3-C30-C31	2.35	119.00	111.83
46	A	502	FMN	C4A-C10-N10	2.34	119.83	116.48
49	C	312	PLX	C1A-N1-C1	2.33	119.18	109.91
52	s	402	UQ	C7-C6-C5	-2.33	120.90	124.89
51	J	401	NDP	O5D-PN-O1N	-2.30	99.81	108.94
50	G	201	8Q1	O1-P24-O2	2.30	116.44	107.80
50	X	201	8Q1	O1-P24-O2	2.28	116.35	107.80
46	A	502	FMN	C9A-C5A-N5	-2.28	120.04	122.45
48	j	201	PEE	C2-O2-C10	-2.25	112.40	117.80
52	s	402	UQ	CM5-C5-C6	-2.22	120.80	124.45
47	A	503	NAI	C6N-N1N-C2N	2.22	121.70	119.32
55	n	102	CDL	OB8-CB7-OB9	-2.22	118.07	123.63
46	A	502	FMN	C4A-C10-N1	-2.21	119.16	124.59
46	A	502	FMN	C10-C4A-N5	-2.20	120.31	124.81
51	J	401	NDP	C5A-C4A-N3A	-2.19	123.70	126.72
50	G	201	8Q1	O27-P24-O3	-2.18	100.55	106.44
51	J	401	NDP	C5B-C4B-C3B	-2.17	107.40	115.21
50	G	201	8Q1	O40-C39-N41	-2.16	118.78	123.03
55	a	201	CDL	OA8-CA7-OA9	-2.16	118.22	123.63
55	V	201	CDL	OA6-CA5-OA7	-2.16	118.66	123.70
50	G	201	8Q1	C43-C42-N41	2.15	116.90	112.41
50	X	201	8Q1	O4-C1-S44	-2.14	119.96	122.68
55	a	201	CDL	OA6-CA5-OA7	-2.11	118.78	123.70
55	a	201	CDL	OB6-CB5-OB7	-2.10	118.81	123.70
55	V	203	CDL	OB6-CB5-OB7	-2.07	118.87	123.70
51	J	401	NDP	C5D-C4D-C3D	-2.06	107.78	115.21
56	Q	501	DCQ	C7-C6-C5	2.04	120.31	116.92
50	X	201	8Q1	C38-C39-N41	2.04	120.06	116.34
50	G	201	8Q1	C42-N41-C39	2.03	126.60	122.82
55	V	203	CDL	OA8-CA7-OA9	-2.03	118.56	123.63
51	J	401	NDP	O3X-P2B-O2B	-2.02	97.98	105.85
55	a	201	CDL	OB8-CB7-OB9	-2.01	118.61	123.63
55	V	203	CDL	CA4-OA6-CA5	-2.01	112.99	117.80

There are no chirality outliers.

All (1030) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
48	U	101	PEE	C19-C20-C21-C22
48	U	101	PEE	C1-O3P-P-O2P
48	U	101	PEE	C1-O3P-P-O1P
48	U	101	PEE	C1-O3P-P-O4P
48	U	101	PEE	C4-O4P-P-O1P
48	V	202	PEE	C1-O3P-P-O2P
48	V	202	PEE	C4-O4P-P-O3P
48	V	202	PEE	C4-O4P-P-O1P
48	V	207	PEE	C11-C10-O2-C2
48	V	207	PEE	O4-C10-O2-C2
48	V	207	PEE	C1-O3P-P-O2P
48	V	207	PEE	C1-O3P-P-O1P
48	V	207	PEE	C1-O3P-P-O4P
48	V	207	PEE	C4-O4P-P-O3P
48	V	207	PEE	C39-C40-C41-C42
48	j	201	PEE	C11-C10-O2-C2
48	l	718	PEE	C11-C10-O2-C2
48	l	718	PEE	O4-C10-O2-C2
48	l	718	PEE	C1-O3P-P-O2P
48	l	718	PEE	C1-O3P-P-O1P
48	l	718	PEE	C1-O3P-P-O4P
48	l	718	PEE	O5-C30-O3-C3
48	l	718	PEE	C31-C30-O3-C3
48	l	719	PEE	C11-C10-O2-C2
48	l	720	PEE	C11-C10-O2-C2
48	m	202	PEE	C1-O3P-P-O2P
48	m	202	PEE	C1-O3P-P-O1P
48	m	202	PEE	O4P-C4-C5-N
49	C	312	PLX	O6-C4-C5-O8
49	C	312	PLX	C2-O1-P1-O4
49	C	312	PLX	C2-O1-P1-O2
49	C	312	PLX	N1-C1-C2-O1
49	C	312	PLX	O9-C24-O8-C5
49	V	205	PLX	O7-C6-C7-C8
49	V	205	PLX	O6-C6-C7-C8
49	V	205	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
49	V	205	PLX	C3-O4-P1-O2
49	V	205	PLX	C2-O1-P1-O2
49	V	205	PLX	O9-C24-C25-C26
49	e	201	PLX	C3-O4-P1-O1
49	e	201	PLX	C3-O4-P1-O3
49	e	201	PLX	C2-O1-P1-O4
49	e	201	PLX	C2-O1-P1-O3
49	e	201	PLX	N1-C1-C2-O1
49	e	201	PLX	O9-C24-C25-C26
49	i	705	PLX	C2-O1-P1-O4
49	i	705	PLX	C2-O1-P1-O2
49	i	705	PLX	C2-O1-P1-O3
49	i	705	PLX	C25-C24-O8-C5
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	j	202	PLX	C5-C4-O6-C6
49	j	202	PLX	C3-O4-P1-O1
49	j	202	PLX	C2-O1-P1-O4
49	j	202	PLX	C2-O1-P1-O2
49	j	202	PLX	N1-C1-C2-O1
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	C3-O4-P1-O1
49	j	203	PLX	C3-O4-P1-O2
49	j	203	PLX	O9-C24-O8-C5
49	j	203	PLX	O9-C24-C25-C26
49	n	101	PLX	O7-C6-O6-C4
49	n	101	PLX	C3-O4-P1-O2
49	n	101	PLX	C3-O4-P1-O3
49	n	101	PLX	C2-O1-P1-O4
49	n	101	PLX	C2-O1-P1-O3
49	n	101	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	O27-C28-C29-C30
50	G	201	8Q1	O27-C28-C29-C31
50	G	201	8Q1	C43-C42-N41-C39
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	O33-C32-C34-N36
51	J	401	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
51	J	401	NDP	O4D-C4D-C5D-O5D
52	J	402	UQ	C7-C8-C9-C11
52	J	402	UQ	C12-C13-C14-C15
52	J	402	UQ	C16-C17-C18-C19
52	J	402	UQ	C17-C18-C19-C20
52	J	402	UQ	C17-C18-C19-C21
52	s	402	UQ	C7-C8-C9-C10
52	s	402	UQ	C7-C8-C9-C11
55	N	202	CDL	O1-C1-CA2-OA2
55	N	202	CDL	CB2-C1-CA2-OA2
55	N	202	CDL	O1-C1-CB2-OB2
55	N	202	CDL	CA2-C1-CB2-OB2
55	N	202	CDL	CA2-OA2-PA1-OA4
55	N	202	CDL	CA2-OA2-PA1-OA5
55	N	202	CDL	CA3-OA5-PA1-OA2
55	N	202	CDL	CA3-OA5-PA1-OA3
55	N	202	CDL	CA3-OA5-PA1-OA4
55	N	202	CDL	CB2-OB2-PB2-OB4
55	N	202	CDL	CB2-OB2-PB2-OB5
55	N	202	CDL	CB3-OB5-PB2-OB2
55	N	202	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	CA3-OA5-PA1-OA2
55	V	201	CDL	CA3-OA5-PA1-OA4
55	V	201	CDL	CB2-OB2-PB2-OB3
55	V	201	CDL	CB2-OB2-PB2-OB4
55	V	201	CDL	CB2-OB2-PB2-OB5
55	V	201	CDL	CB3-OB5-PB2-OB2
55	V	201	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	CB3-OB5-PB2-OB4
55	V	203	CDL	CA2-C1-CB2-OB2
55	V	203	CDL	CA2-OA2-PA1-OA4
55	V	203	CDL	CA2-OA2-PA1-OA5
55	V	203	CDL	CB2-OB2-PB2-OB3
55	V	203	CDL	CB2-OB2-PB2-OB4
55	V	203	CDL	CB2-OB2-PB2-OB5
55	V	203	CDL	CB3-OB5-PB2-OB2
55	V	203	CDL	CB3-OB5-PB2-OB3
55	V	203	CDL	C51-CB5-OB6-CB4
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CB2-C1-CA2-OA2
55	i	401	CDL	CA2-OA2-PA1-OA3
55	i	401	CDL	CA2-OA2-PA1-OA4
55	i	401	CDL	CA2-OA2-PA1-OA5
55	i	401	CDL	C31-CA7-OA8-CA6
55	i	401	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CB3-OB5-PB2-OB3
55	k	101	CDL	CA3-OA5-PA1-OA2
55	k	101	CDL	CA3-OA5-PA1-OA4
55	k	101	CDL	CB2-OB2-PB2-OB3
55	k	101	CDL	CB2-OB2-PB2-OB4
55	k	101	CDL	CB2-OB2-PB2-OB5
55	k	101	CDL	CB3-OB5-PB2-OB3
55	l	712	CDL	CB2-C1-CA2-OA2
55	l	712	CDL	CA2-C1-CB2-OB2
55	l	712	CDL	OA5-CA3-CA4-OA6
55	l	712	CDL	OA9-CA7-OA8-CA6
55	l	712	CDL	C31-CA7-OA8-CA6
55	l	712	CDL	CB2-OB2-PB2-OB3
55	l	712	CDL	CB2-OB2-PB2-OB4
55	l	712	CDL	CB2-OB2-PB2-OB5
55	l	712	CDL	CB3-OB5-PB2-OB2
55	l	712	CDL	CB3-OB5-PB2-OB3
55	l	712	CDL	CB3-OB5-PB2-OB4
55	l	713	CDL	CA2-OA2-PA1-OA4
55	l	713	CDL	CA2-OA2-PA1-OA5
55	l	713	CDL	CA3-OA5-PA1-OA4
55	l	713	CDL	CB2-OB2-PB2-OB3
55	l	713	CDL	CB2-OB2-PB2-OB4
55	l	713	CDL	CB2-OB2-PB2-OB5
55	l	713	CDL	CB3-OB5-PB2-OB2
55	l	713	CDL	CB3-OB5-PB2-OB3
55	l	713	CDL	CB3-OB5-PB2-OB4
55	m	201	CDL	OA9-CA7-OA8-CA6
55	m	201	CDL	C31-CA7-OA8-CA6
55	m	201	CDL	C51-CB5-OB6-CB4
55	n	102	CDL	CA2-OA2-PA1-OA3
55	n	102	CDL	CA2-OA2-PA1-OA4
55	n	102	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
55	n	102	CDL	CA3-OA5-PA1-OA3
55	n	102	CDL	CB2-OB2-PB2-OB4
55	n	102	CDL	CB2-OB2-PB2-OB5
55	n	102	CDL	CB3-OB5-PB2-OB2
55	n	102	CDL	CB3-OB5-PB2-OB3
55	n	102	CDL	CB3-OB5-PB2-OB4
55	r	714	CDL	O1-C1-CA2-OA2
55	r	714	CDL	CA2-OA2-PA1-OA3
55	r	714	CDL	CA2-OA2-PA1-OA5
55	r	714	CDL	CA3-OA5-PA1-OA3
55	r	714	CDL	CB2-OB2-PB2-OB3
55	r	714	CDL	CB2-OB2-PB2-OB5
55	r	714	CDL	CB3-OB5-PB2-OB2
55	r	714	CDL	CB3-OB5-PB2-OB3
55	r	714	CDL	CB3-OB5-PB2-OB4
58	w	401	ADP	O4'-C4'-C5'-O5'
55	i	401	CDL	OA9-CA7-OA8-CA6
52	J	402	UQ	C22-C23-C24-C25
48	j	201	PEE	O4-C10-O2-C2
48	l	719	PEE	O4-C10-O2-C2
48	l	720	PEE	O4-C10-O2-C2
55	V	203	CDL	OB7-CB5-OB6-CB4
55	m	201	CDL	OB7-CB5-OB6-CB4
52	J	402	UQ	C12-C11-C9-C8
52	s	402	UQ	C18-C19-C21-C22
52	J	402	UQ	C22-C23-C24-C26
56	Q	501	DCQ	C6-C7-C8-C9
48	U	101	PEE	C31-C30-O3-C3
55	k	101	CDL	C62-C63-C64-C65
48	V	207	PEE	C17-C18-C19-C20
48	l	720	PEE	C37-C38-C39-C40
52	J	402	UQ	C12-C13-C14-C16
52	s	402	UQ	C17-C18-C19-C21
52	s	402	UQ	C22-C23-C24-C26
49	V	205	PLX	C9-C10-C11-C12
55	V	203	CDL	O1-C1-CB2-OB2
55	i	401	CDL	O1-C1-CB2-OB2
55	l	712	CDL	O1-C1-CB2-OB2
55	l	713	CDL	O1-C1-CB2-OB2
49	i	705	PLX	C7-C8-C9-C10
55	N	202	CDL	C11-CA5-OA6-CA4
55	N	202	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
55	r	714	CDL	C51-CB5-OB6-CB4
55	N	202	CDL	OA7-CA5-OA6-CA4
52	J	402	UQ	C14-C16-C17-C18
50	X	201	8Q1	C6-C7-C8-C9
48	U	101	PEE	O5-C30-O3-C3
55	l	713	CDL	C35-C36-C37-C38
55	N	202	CDL	C31-CA7-OA8-CA6
48	U	101	PEE	C17-C18-C19-C20
55	N	202	CDL	OA9-CA7-OA8-CA6
55	r	714	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	CA2-C1-CB2-OB2
55	i	401	CDL	CA2-C1-CB2-OB2
55	k	101	CDL	CB2-C1-CA2-OA2
55	m	201	CDL	CA2-C1-CB2-OB2
55	r	714	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	C31-C30-O3-C3
55	l	712	CDL	C71-CB7-OB8-CB6
55	l	713	CDL	C71-CB7-OB8-CB6
49	j	203	PLX	C13-C14-C15-C16
55	V	201	CDL	C53-C54-C55-C56
49	i	705	PLX	C9-C10-C11-C12
55	k	101	CDL	C60-C61-C62-C63
49	V	205	PLX	C7-C8-C9-C10
55	l	713	CDL	C41-C42-C43-C44
52	J	402	UQ	C13-C14-C16-C17
55	l	712	CDL	CB5-C51-C52-C53
55	k	101	CDL	O1-C1-CA2-OA2
55	l	712	CDL	O1-C1-CA2-OA2
55	l	713	CDL	O1-C1-CA2-OA2
55	m	201	CDL	O1-C1-CB2-OB2
49	V	205	PLX	C11-C12-C13-C14
48	V	202	PEE	C33-C34-C35-C36
49	j	203	PLX	C28-C29-C30-C31
48	j	201	PEE	O5-C30-O3-C3
55	l	712	CDL	OB9-CB7-OB8-CB6
55	l	713	CDL	OB9-CB7-OB8-CB6
55	k	101	CDL	C71-CB7-OB8-CB6
48	s	401	PEE	C11-C12-C13-C14
52	s	402	UQ	C22-C23-C24-C25
55	l	713	CDL	CA7-C31-C32-C33
52	s	402	UQ	C27-C28-C29-C31
52	s	402	UQ	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
55	l	712	CDL	C55-C56-C57-C58
49	i	705	PLX	C2-C1-N1-C1A
48	V	202	PEE	C10-C11-C12-C13
55	a	201	CDL	CB5-C51-C52-C53
55	i	401	CDL	CA7-C31-C32-C33
55	i	401	CDL	CB7-C71-C72-C73
55	l	712	CDL	CA5-C11-C12-C13
55	n	102	CDL	CB7-C71-C72-C73
55	V	201	CDL	O1-C1-CB2-OB2
55	a	201	CDL	O1-C1-CB2-OB2
55	i	401	CDL	O1-C1-CA2-OA2
55	n	102	CDL	CB5-C51-C52-C53
55	N	202	CDL	OB7-CB5-OB6-CB4
48	m	202	PEE	C17-C18-C19-C20
55	k	101	CDL	OB9-CB7-OB8-CB6
55	l	713	CDL	C51-CB5-OB6-CB4
55	l	713	CDL	C71-C72-C73-C74
55	V	203	CDL	C33-C34-C35-C36
55	l	713	CDL	C31-C32-C33-C34
55	l	713	CDL	C51-C52-C53-C54
48	U	101	PEE	C30-C31-C32-C33
55	a	201	CDL	CA2-C1-CB2-OB2
48	m	202	PEE	C31-C30-O3-C3
55	V	203	CDL	C17-C18-C19-C20
55	l	712	CDL	C58-C59-C60-C61
49	i	705	PLX	C2-C1-N1-C1B
55	k	101	CDL	C58-C59-C60-C61
51	J	401	NDP	C3D-C4D-C5D-O5D
58	w	401	ADP	C3'-C4'-C5'-O5'
55	m	201	CDL	CB7-C71-C72-C73
52	s	402	UQ	C23-C24-C26-C27
49	V	205	PLX	O8-C24-C25-C26
49	e	201	PLX	O8-C24-C25-C26
49	j	203	PLX	O6-C6-C7-C8
49	j	203	PLX	O8-C24-C25-C26
49	n	101	PLX	O8-C24-C25-C26
48	U	101	PEE	C11-C10-O2-C2
55	V	201	CDL	C11-CA5-OA6-CA4
48	U	101	PEE	O4-C10-O2-C2
55	V	201	CDL	OA7-CA5-OA6-CA4
55	l	713	CDL	OB7-CB5-OB6-CB4
48	s	401	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
55	l	712	CDL	C16-C17-C18-C19
55	k	101	CDL	O1-C1-CB2-OB2
48	l	720	PEE	C34-C35-C36-C37
55	r	714	CDL	C74-C75-C76-C77
55	N	202	CDL	CA7-C31-C32-C33
55	V	203	CDL	C37-C38-C39-C40
55	N	202	CDL	CA6-CA4-OA6-CA5
55	k	101	CDL	OA5-CA3-CA4-OA6
48	V	202	PEE	C11-C10-O2-C2
55	a	201	CDL	C11-CA5-OA6-CA4
55	V	203	CDL	C13-C14-C15-C16
48	U	101	PEE	C40-C41-C42-C43
55	N	202	CDL	C51-C52-C53-C54
48	l	720	PEE	C14-C15-C16-C17
55	l	713	CDL	C15-C16-C17-C18
48	l	720	PEE	C31-C32-C33-C34
49	V	205	PLX	C27-C28-C29-C30
55	k	101	CDL	C51-C52-C53-C54
55	r	714	CDL	C43-C44-C45-C46
55	i	401	CDL	CA5-C11-C12-C13
48	V	207	PEE	C37-C38-C39-C40
49	i	705	PLX	C12-C13-C14-C15
55	i	401	CDL	C55-C56-C57-C58
55	k	101	CDL	C18-C19-C20-C21
55	r	714	CDL	C71-C72-C73-C74
49	C	312	PLX	O7-C6-C7-C8
48	m	202	PEE	C12-C13-C14-C15
49	i	705	PLX	C27-C28-C29-C30
49	i	705	PLX	C30-C31-C32-C33
49	j	203	PLX	C11-C12-C13-C14
49	n	101	PLX	C9-C10-C11-C12
55	V	201	CDL	C52-C53-C54-C55
55	V	203	CDL	C34-C35-C36-C37
55	i	401	CDL	C14-C15-C16-C17
55	i	401	CDL	C37-C38-C39-C40
55	k	101	CDL	C76-C77-C78-C79
55	k	101	CDL	C78-C79-C80-C81
55	k	101	CDL	C81-C82-C83-C84
55	l	712	CDL	C52-C53-C54-C55
55	l	713	CDL	C37-C38-C39-C40
55	l	713	CDL	C55-C56-C57-C58
55	m	201	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
55	r	714	CDL	C55-C56-C57-C58
49	i	705	PLX	C32-C33-C34-C35
55	k	101	CDL	CA7-C31-C32-C33
49	V	205	PLX	C11-C10-C9-C8
55	k	101	CDL	C52-C53-C54-C55
55	r	714	CDL	C33-C34-C35-C36
48	V	202	PEE	C11-C12-C13-C14
48	s	401	PEE	C13-C14-C15-C16
55	l	712	CDL	C56-C57-C58-C59
55	l	712	CDL	C59-C60-C61-C62
48	C	311	PEE	C11-C10-O2-C2
55	k	101	CDL	C11-CA5-OA6-CA4
49	n	101	PLX	C11-C12-C13-C14
49	n	101	PLX	C10-C11-C12-C13
55	k	101	CDL	C11-C12-C13-C14
55	n	102	CDL	O1-C1-CB2-OB2
48	V	202	PEE	C30-C31-C32-C33
48	j	201	PEE	C11-C12-C13-C14
49	C	312	PLX	C14-C15-C16-C17
49	C	312	PLX	C9-C10-C11-C12
49	j	203	PLX	C27-C28-C29-C30
55	k	101	CDL	C55-C56-C57-C58
55	l	712	CDL	C31-C32-C33-C34
55	l	712	CDL	C62-C63-C64-C65
55	l	713	CDL	C74-C75-C76-C77
55	m	201	CDL	C71-C72-C73-C74
48	l	719	PEE	C21-C22-C23-C24
48	l	719	PEE	C31-C32-C33-C34
49	j	202	PLX	C12-C13-C14-C15
55	i	401	CDL	C59-C60-C61-C62
55	m	201	CDL	C17-C18-C19-C20
55	m	201	CDL	C34-C35-C36-C37
49	j	203	PLX	C12-C13-C14-C15
49	n	101	PLX	C14-C15-C16-C17
55	l	713	CDL	C36-C37-C38-C39
48	m	202	PEE	O5-C30-O3-C3
48	V	202	PEE	C20-C21-C22-C23
55	V	203	CDL	C11-C12-C13-C14
55	l	712	CDL	C34-C35-C36-C37
55	l	712	CDL	C35-C36-C37-C38
48	V	202	PEE	O4-C10-O2-C2
55	a	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C33-C34-C35-C36
48	l	719	PEE	C31-C30-O3-C3
55	r	714	CDL	C71-CB7-OB8-CB6
48	j	201	PEE	C23-C24-C25-C26
49	V	205	PLX	C12-C13-C14-C15
49	i	705	PLX	C13-C14-C15-C16
49	i	705	PLX	C33-C34-C35-C36
49	n	101	PLX	C31-C32-C33-C34
48	C	311	PEE	C42-C43-C44-C45
48	s	401	PEE	C34-C35-C36-C37
49	j	203	PLX	C7-C8-C9-C10
49	j	203	PLX	C25-C26-C27-C28
49	n	101	PLX	C13-C14-C15-C16
55	k	101	CDL	C14-C15-C16-C17
55	k	101	CDL	C56-C57-C58-C59
55	k	101	CDL	C59-C60-C61-C62
55	l	712	CDL	C75-C76-C77-C78
55	l	713	CDL	C21-C22-C23-C24
55	m	201	CDL	C37-C38-C39-C40
55	m	201	CDL	C73-C74-C75-C76
55	r	714	CDL	C41-C42-C43-C44
55	r	714	CDL	C53-C54-C55-C56
55	r	714	CDL	C75-C76-C77-C78
48	s	401	PEE	C20-C21-C22-C23
56	Q	501	DCQ	C7-C8-C9-C10
48	l	718	PEE	C34-C35-C36-C37
49	V	205	PLX	C33-C34-C35-C36
55	k	101	CDL	C43-C44-C45-C46
55	k	101	CDL	C73-C74-C75-C76
55	l	713	CDL	C75-C76-C77-C78
55	r	714	CDL	C34-C35-C36-C37
55	V	201	CDL	C59-C60-C61-C62
55	r	714	CDL	C56-C57-C58-C59
55	V	201	CDL	C57-C58-C59-C60
55	a	201	CDL	C83-C84-C85-C86
48	l	720	PEE	C30-C31-C32-C33
55	m	201	CDL	CA7-C31-C32-C33
48	l	719	PEE	O5-C30-O3-C3
48	j	201	PEE	C13-C14-C15-C16
49	C	312	PLX	C10-C11-C12-C13
49	n	101	PLX	C7-C8-C9-C10
55	k	101	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
55	m	201	CDL	C75-C76-C77-C78
48	V	202	PEE	C31-C32-C33-C34
48	V	207	PEE	C32-C33-C34-C35
55	l	713	CDL	C11-C12-C13-C14
48	C	311	PEE	C13-C14-C15-C16
49	i	705	PLX	C28-C29-C30-C31
49	j	203	PLX	C14-C15-C16-C17
55	k	101	CDL	C71-C72-C73-C74
48	m	202	PEE	C24-C25-C26-C27
48	m	202	PEE	C13-C14-C15-C16
55	i	401	CDL	C76-C77-C78-C79
55	m	201	CDL	C32-C33-C34-C35
55	r	714	CDL	C81-C82-C83-C84
49	j	203	PLX	C30-C31-C32-C33
55	i	401	CDL	C73-C74-C75-C76
55	r	714	CDL	C76-C77-C78-C79
48	l	719	PEE	C32-C33-C34-C35
49	n	101	PLX	C15-C16-C17-C18
55	r	714	CDL	C62-C63-C64-C65
48	V	207	PEE	C18-C19-C20-C21
48	C	311	PEE	C11-C12-C13-C14
49	C	312	PLX	C33-C34-C35-C36
49	V	205	PLX	C14-C15-C16-C17
49	n	101	PLX	C12-C13-C14-C15
55	l	712	CDL	C11-C12-C13-C14
55	l	712	CDL	C37-C38-C39-C40
55	m	201	CDL	C12-C13-C14-C15
55	m	201	CDL	C35-C36-C37-C38
48	C	311	PEE	C44-C45-C46-C47
55	V	203	CDL	C36-C37-C38-C39
48	s	401	PEE	C11-C10-O2-C2
55	k	101	CDL	C51-CB5-OB6-CB4
55	m	201	CDL	C11-CA5-OA6-CA4
48	V	207	PEE	C30-C31-C32-C33
48	j	201	PEE	C14-C15-C16-C17
48	C	311	PEE	O4-C10-O2-C2
49	C	312	PLX	C28-C29-C30-C31
56	Q	501	DCQ	C10-C11-C12-C13
48	j	201	PEE	C15-C16-C17-C18
55	r	714	CDL	CB5-C51-C52-C53
49	e	201	PLX	C29-C30-C31-C32
55	V	203	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
48	C	311	PEE	C34-C35-C36-C37
55	l	712	CDL	C74-C75-C76-C77
55	r	714	CDL	C12-C13-C14-C15
52	J	402	UQ	C12-C11-C9-C10
49	i	705	PLX	C2-C1-N1-C1C
48	V	202	PEE	C40-C41-C42-C43
55	m	201	CDL	C82-C83-C84-C85
55	r	714	CDL	C15-C16-C17-C18
55	r	714	CDL	C84-C85-C86-C87
49	V	205	PLX	C28-C29-C30-C31
55	l	712	CDL	C51-C52-C53-C54
55	i	401	CDL	C81-C82-C83-C84
55	m	201	CDL	C83-C84-C85-C86
55	k	101	CDL	C64-C65-C66-C67
55	r	714	CDL	OB9-CB7-OB8-CB6
55	k	101	CDL	C39-C40-C41-C42
55	i	401	CDL	CB5-C51-C52-C53
48	s	401	PEE	O4-C10-O2-C2
55	V	201	CDL	OB5-CB3-CB4-OB6
55	l	712	CDL	OB5-CB3-CB4-OB6
55	m	201	CDL	OA5-CA3-CA4-OA6
55	l	713	CDL	C56-C57-C58-C59
55	r	714	CDL	C13-C14-C15-C16
55	a	201	CDL	C51-CB5-OB6-CB4
49	C	312	PLX	C13-C14-C15-C16
52	s	402	UQ	C27-C28-C29-C30
55	r	714	CDL	C59-C60-C61-C62
48	s	401	PEE	C35-C36-C37-C38
55	V	201	CDL	OB6-CB4-CB6-OB8
55	i	401	CDL	OB6-CB4-CB6-OB8
55	l	712	CDL	OA6-CA4-CA6-OA8
55	l	712	CDL	OB6-CB4-CB6-OB8
48	V	202	PEE	C42-C43-C44-C45
55	m	201	CDL	C18-C19-C20-C21
48	V	207	PEE	C33-C34-C35-C36
48	U	101	PEE	C36-C37-C38-C39
48	U	101	PEE	C38-C39-C40-C41
48	V	202	PEE	C36-C37-C38-C39
48	U	101	PEE	C34-C35-C36-C37
55	r	714	CDL	C37-C38-C39-C40
55	k	101	CDL	OB7-CB5-OB6-CB4
50	X	201	8Q1	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
55	l	713	CDL	C62-C63-C64-C65
55	r	714	CDL	C14-C15-C16-C17
55	r	714	CDL	C32-C33-C34-C35
52	J	402	UQ	C7-C8-C9-C10
48	s	401	PEE	C31-C30-O3-C3
49	V	205	PLX	C31-C32-C33-C34
55	V	201	CDL	C55-C56-C57-C58
55	k	101	CDL	C17-C18-C19-C20
55	l	712	CDL	C71-C72-C73-C74
55	r	714	CDL	C82-C83-C84-C85
49	V	205	PLX	C30-C31-C32-C33
55	k	101	CDL	C32-C33-C34-C35
48	C	311	PEE	C12-C13-C14-C15
48	l	719	PEE	C13-C14-C15-C16
49	V	205	PLX	C25-C26-C27-C28
49	n	101	PLX	C16-C17-C18-C19
55	k	101	CDL	C13-C14-C15-C16
55	l	712	CDL	C72-C73-C74-C75
50	X	201	8Q1	O33-C32-C34-O35
48	l	720	PEE	C20-C21-C22-C23
49	j	202	PLX	C32-C33-C34-C35
55	m	201	CDL	C55-C56-C57-C58
48	j	201	PEE	C19-C20-C21-C22
48	s	401	PEE	C23-C24-C25-C26
49	C	312	PLX	C11-C12-C13-C14
50	G	201	8Q1	C11-C10-C9-C8
55	a	201	CDL	OA5-CA3-CA4-CA6
55	a	201	CDL	OB5-CB3-CB4-CB6
55	m	201	CDL	OA7-CA5-OA6-CA4
55	V	203	CDL	C60-C61-C62-C63
55	k	101	CDL	C15-C16-C17-C18
49	i	705	PLX	C11-C12-C13-C14
55	V	201	CDL	CA5-C11-C12-C13
55	k	101	CDL	CB5-C51-C52-C53
55	l	712	CDL	CB7-C71-C72-C73
49	C	312	PLX	O6-C6-C7-C8
50	G	201	8Q1	C11-C12-C13-C14
55	m	201	CDL	C15-C16-C17-C18
55	i	401	CDL	C77-C78-C79-C80
55	k	101	CDL	C82-C83-C84-C85
55	i	401	CDL	C34-C35-C36-C37
48	V	202	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
49	C	312	PLX	C3-C4-C5-O8
55	V	201	CDL	CB3-CB4-CB6-OB8
55	i	401	CDL	CA3-CA4-CA6-OA8
55	m	201	CDL	CB3-CB4-CB6-OB8
55	l	713	CDL	C64-C65-C66-C67
55	l	713	CDL	C73-C74-C75-C76
48	V	207	PEE	C35-C36-C37-C38
48	l	718	PEE	C35-C36-C37-C38
48	m	202	PEE	C19-C20-C21-C22
55	l	712	CDL	C36-C37-C38-C39
55	k	101	CDL	C35-C36-C37-C38
49	i	705	PLX	C10-C11-C12-C13
48	j	201	PEE	C12-C13-C14-C15
55	i	401	CDL	C54-C55-C56-C57
48	U	101	PEE	C21-C22-C23-C24
55	V	203	CDL	C59-C60-C61-C62
55	i	401	CDL	C75-C76-C77-C78
55	k	101	CDL	C37-C38-C39-C40
55	l	712	CDL	C78-C79-C80-C81
48	l	720	PEE	C12-C13-C14-C15
46	A	502	FMN	C5'-O5'-P-O1P
48	l	719	PEE	C33-C34-C35-C36
49	i	705	PLX	C25-C26-C27-C28
55	k	101	CDL	C77-C78-C79-C80
55	a	201	CDL	CA3-CA4-OA6-CA5
55	m	201	CDL	C59-C60-C61-C62
48	C	311	PEE	C19-C20-C21-C22
48	s	401	PEE	C39-C40-C41-C42
55	l	712	CDL	C82-C83-C84-C85
48	s	401	PEE	O5-C30-O3-C3
55	i	401	CDL	C71-C72-C73-C74
51	J	401	NDP	O4B-C4B-C5B-O5B
49	V	205	PLX	C13-C14-C15-C16
49	n	101	PLX	C27-C28-C29-C30
49	C	312	PLX	C16-C17-C18-C19
49	j	202	PLX	C29-C30-C31-C32
55	i	401	CDL	C35-C36-C37-C38
55	n	102	CDL	C73-C74-C75-C76
49	C	312	PLX	C11-C10-C9-C8
49	i	705	PLX	C14-C15-C16-C17
55	l	713	CDL	C59-C60-C61-C62
49	n	101	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C18-C19-C20-C21
55	k	101	CDL	OB6-CB4-CB6-OB8
55	m	201	CDL	OB6-CB4-CB6-OB8
55	m	201	CDL	C40-C41-C42-C43
48	V	202	PEE	C13-C14-C15-C16
55	r	714	CDL	C73-C74-C75-C76
49	i	705	PLX	C36-C37-C38-C39
55	k	101	CDL	C84-C85-C86-C87
55	m	201	CDL	C19-C20-C21-C22
48	C	311	PEE	C31-C30-O3-C3
55	l	713	CDL	C44-C45-C46-C47
55	l	712	CDL	C14-C15-C16-C17
48	U	101	PEE	C41-C42-C43-C44
48	V	202	PEE	C24-C25-C26-C27
48	V	202	PEE	C17-C18-C19-C20
48	s	401	PEE	C37-C38-C39-C40
50	X	201	8Q1	C29-C32-C34-O35
49	j	203	PLX	C29-C30-C31-C32
48	l	718	PEE	C11-C12-C13-C14
55	k	101	CDL	C34-C35-C36-C37
55	l	713	CDL	C33-C34-C35-C36
55	r	714	CDL	C51-C52-C53-C54
48	s	401	PEE	C38-C39-C40-C41
48	U	101	PEE	C22-C23-C24-C25
48	V	207	PEE	C2-C1-O3P-P
48	s	401	PEE	C21-C22-C23-C24
48	m	202	PEE	C33-C34-C35-C36
48	l	719	PEE	C24-C25-C26-C27
55	V	201	CDL	OB5-CB3-CB4-CB6
55	k	101	CDL	OA5-CA3-CA4-CA6
55	l	712	CDL	OB5-CB3-CB4-CB6
55	l	713	CDL	OB5-CB3-CB4-CB6
55	m	201	CDL	OA5-CA3-CA4-CA6
48	V	202	PEE	C41-C42-C43-C44
50	X	201	8Q1	C13-C14-C15-C16
49	V	205	PLX	C18-C19-C20-C21
55	i	401	CDL	C38-C39-C40-C41
48	V	202	PEE	C21-C22-C23-C24
55	l	713	CDL	C39-C40-C41-C42
50	G	201	8Q1	C12-C13-C14-C15
48	U	101	PEE	C44-C45-C46-C47
55	m	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
55	l	712	CDL	C73-C74-C75-C76
55	m	201	CDL	C39-C40-C41-C42
48	j	201	PEE	C1-C2-C3-O3
48	l	720	PEE	C1-C2-C3-O3
48	m	202	PEE	C1-C2-C3-O3
49	V	205	PLX	C3-C4-C5-O8
55	i	401	CDL	CB3-CB4-CB6-OB8
55	k	101	CDL	CB3-CB4-CB6-OB8
55	l	712	CDL	CA3-CA4-CA6-OA8
55	l	712	CDL	CB3-CB4-CB6-OB8
49	e	201	PLX	C18-C19-C20-C21
49	i	705	PLX	C11-C10-C9-C8
49	e	201	PLX	C19-C20-C21-C22
55	r	714	CDL	C64-C65-C66-C67
55	a	201	CDL	C80-C81-C82-C83
49	n	101	PLX	C28-C29-C30-C31
48	V	207	PEE	C31-C30-O3-C3
55	m	201	CDL	C84-C85-C86-C87
55	l	712	CDL	C21-C22-C23-C24
48	s	401	PEE	O3P-C1-C2-O2
55	V	203	CDL	OB5-CB3-CB4-OB6
55	i	401	CDL	OB5-CB3-CB4-OB6
48	l	719	PEE	C15-C16-C17-C18
55	V	201	CDL	C21-C22-C23-C24
55	m	201	CDL	C54-C55-C56-C57
49	e	201	PLX	O6-C4-C5-O8
55	l	713	CDL	OB6-CB4-CB6-OB8
55	r	714	CDL	OB6-CB4-CB6-OB8
55	l	712	CDL	C81-C82-C83-C84
55	l	712	CDL	CA7-C31-C32-C33
55	l	713	CDL	C14-C15-C16-C17
55	m	201	CDL	C14-C15-C16-C17
55	m	201	CDL	C38-C39-C40-C41
55	r	714	CDL	CA7-C31-C32-C33
55	V	203	CDL	C62-C63-C64-C65
48	V	207	PEE	C31-C32-C33-C34
48	C	311	PEE	C15-C16-C17-C18
48	l	719	PEE	C39-C40-C41-C42
49	j	203	PLX	C10-C11-C12-C13
52	J	402	UQ	C19-C21-C22-C23
49	j	203	PLX	C9-C10-C11-C12
55	V	203	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
55	m	201	CDL	O1-C1-CA2-OA2
55	i	401	CDL	C64-C65-C66-C67
55	a	201	CDL	C31-CA7-OA8-CA6
55	i	401	CDL	C71-CB7-OB8-CB6
55	i	401	CDL	C39-C40-C41-C42
48	C	311	PEE	C43-C44-C45-C46
48	l	720	PEE	C13-C14-C15-C16
55	l	713	CDL	CA2-C1-CB2-OB2
55	k	101	CDL	C54-C55-C56-C57
48	s	401	PEE	O3P-C1-C2-C3
55	V	203	CDL	OA5-CA3-CA4-CA6
55	i	401	CDL	OB5-CB3-CB4-CB6
55	l	713	CDL	OA5-CA3-CA4-CA6
55	i	401	CDL	C52-C53-C54-C55
55	i	401	CDL	OB9-CB7-OB8-CB6
55	i	401	CDL	C1-CB2-OB2-PB2
55	k	101	CDL	C21-C22-C23-C24
55	V	203	CDL	C75-C76-C77-C78
48	j	201	PEE	C24-C25-C26-C27
48	l	720	PEE	C39-C40-C41-C42
47	A	503	NAI	C3D-C4D-C5D-O5D
55	l	713	CDL	CB7-C71-C72-C73
55	a	201	CDL	OB7-CB5-OB6-CB4
55	V	203	CDL	C12-C13-C14-C15
55	r	714	CDL	C58-C59-C60-C61
55	V	203	CDL	CA6-CA4-OA6-CA5
55	k	101	CDL	CA6-CA4-OA6-CA5
48	C	311	PEE	O5-C30-O3-C3
55	m	201	CDL	OB9-CB7-OB8-CB6
48	V	207	PEE	O5-C30-O3-C3
48	l	719	PEE	C44-C45-C46-C47
55	V	203	CDL	OA5-CA3-CA4-OA6
55	l	713	CDL	OB5-CB3-CB4-OB6
55	k	101	CDL	C33-C34-C35-C36
55	r	714	CDL	CB3-CB4-CB6-OB8
55	l	712	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C34-C35-C36-C37
49	e	201	PLX	C13-C14-C15-C16
55	k	101	CDL	C52-C51-CB5-OB6
48	V	202	PEE	C5-C4-O4P-P
48	m	202	PEE	C5-C4-O4P-P
50	G	201	8Q1	C30-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
48	C	311	PEE	O2-C2-C3-O3
48	j	201	PEE	O2-C2-C3-O3
48	m	202	PEE	O2-C2-C3-O3
49	V	205	PLX	O6-C4-C5-O8
49	j	203	PLX	O6-C4-C5-O8
55	i	401	CDL	OA6-CA4-CA6-OA8
55	m	201	CDL	OA6-CA4-CA6-OA8
49	n	101	PLX	C17-C18-C19-C20
55	l	713	CDL	C32-C33-C34-C35
55	a	201	CDL	OA9-CA7-OA8-CA6
49	V	205	PLX	C16-C17-C18-C19
49	j	202	PLX	C2-C1-N1-C1B
55	k	101	CDL	C57-C58-C59-C60
48	U	101	PEE	C12-C13-C14-C15
55	r	714	CDL	C17-C18-C19-C20
49	i	705	PLX	C31-C32-C33-C34
55	l	712	CDL	C18-C19-C20-C21
51	J	401	NDP	O4D-C1D-N1N-C6N
49	e	201	PLX	C15-C16-C17-C18
55	m	201	CDL	C74-C75-C76-C77
55	V	201	CDL	C56-C57-C58-C59
55	n	102	CDL	C51-C52-C53-C54
49	j	202	PLX	C7-C8-C9-C10
49	j	202	PLX	O9-C24-C25-C26
55	V	201	CDL	C12-C13-C14-C15
55	V	201	CDL	C42-C43-C44-C45
55	l	713	CDL	C61-C62-C63-C64
49	i	705	PLX	C20-C21-C22-C23
49	j	202	PLX	C2-C1-N1-C1C
49	j	202	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
49	n	101	PLX	C25-C24-O8-C5
48	U	101	PEE	C42-C43-C44-C45
55	m	201	CDL	C31-C32-C33-C34
55	l	712	CDL	OA5-CA3-CA4-CA6
55	l	712	CDL	OB7-CB5-OB6-CB4
55	k	101	CDL	C19-C20-C21-C22
50	G	201	8Q1	C28-C29-C32-C34
48	l	720	PEE	C17-C18-C19-C20
55	n	102	CDL	C52-C53-C54-C55
49	j	203	PLX	C16-C17-C18-C19
55	k	101	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
55	l	713	CDL	CA4-CA3-OA5-PA1
55	r	714	CDL	C1-CB2-OB2-PB2
48	V	202	PEE	C12-C13-C14-C15
55	r	714	CDL	C11-C12-C13-C14
55	a	201	CDL	OA5-CA3-CA4-OA6
55	l	713	CDL	OA5-CA3-CA4-OA6
50	X	201	8Q1	C11-C12-C13-C14
55	r	714	CDL	C11-CA5-OA6-CA4
48	s	401	PEE	C44-C45-C46-C47
49	j	202	PLX	C10-C11-C12-C13
49	n	101	PLX	C29-C30-C31-C32
49	n	101	PLX	C25-C26-C27-C28
55	V	203	CDL	C32-C33-C34-C35
48	V	202	PEE	O2-C2-C3-O3
48	l	720	PEE	O2-C2-C3-O3
55	n	102	CDL	OA6-CA4-CA6-OA8
49	j	202	PLX	C9-C10-C11-C12
48	C	311	PEE	C1-C2-C3-O3
49	e	201	PLX	C3-C4-C5-O8
55	m	201	CDL	CA3-CA4-CA6-OA8
55	n	102	CDL	C57-C58-C59-C60
48	V	202	PEE	O5-C30-O3-C3
55	V	201	CDL	C40-C41-C42-C43
55	m	201	CDL	C56-C57-C58-C59
51	J	401	NDP	C3B-C4B-C5B-O5B
49	j	203	PLX	C26-C27-C28-C29
55	n	102	CDL	C72-C73-C74-C75
48	V	202	PEE	C1-O3P-P-O1P
48	V	202	PEE	C1-O3P-P-O4P
48	V	202	PEE	C4-O4P-P-O2P
48	V	207	PEE	C4-O4P-P-O1P
48	l	719	PEE	C1-O3P-P-O1P
48	l	720	PEE	C1-O3P-P-O2P
48	l	720	PEE	C1-O3P-P-O1P
48	l	720	PEE	C1-O3P-P-O4P
48	m	202	PEE	C1-O3P-P-O4P
48	m	202	PEE	C4-O4P-P-O1P
49	C	312	PLX	C3-O4-P1-O2
49	C	312	PLX	C2-O1-P1-O3
49	V	205	PLX	C2-O1-P1-O4
49	V	205	PLX	C2-O1-P1-O3
49	i	705	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C3-C4-O6-C6
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C2-O1-P1-O3
49	j	203	PLX	C3-O4-P1-O3
49	n	101	PLX	C3-C4-O6-C6
49	n	101	PLX	C5-C4-O6-C6
49	n	101	PLX	C3-O4-P1-O1
55	V	203	CDL	CB3-OB5-PB2-OB4
55	a	201	CDL	CA3-OA5-PA1-OA3
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	CB3-OB5-PB2-OB3
55	i	401	CDL	CA3-OA5-PA1-OA3
55	i	401	CDL	CB3-OB5-PB2-OB4
55	k	101	CDL	CA2-OA2-PA1-OA3
55	k	101	CDL	CA2-OA2-PA1-OA4
55	k	101	CDL	CA2-OA2-PA1-OA5
55	l	713	CDL	CA3-OA5-PA1-OA2
55	l	713	CDL	CA3-OA5-PA1-OA3
55	m	201	CDL	CB2-OB2-PB2-OB3
55	m	201	CDL	CB2-OB2-PB2-OB4
55	m	201	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	CB3-OB5-PB2-OB3
55	n	102	CDL	CA3-OA5-PA1-OA2
55	r	714	CDL	CA2-OA2-PA1-OA4
55	r	714	CDL	CB2-OB2-PB2-OB4
55	k	101	CDL	C44-C45-C46-C47
48	l	720	PEE	C2-C1-O3P-P
48	m	202	PEE	C34-C35-C36-C37
55	V	203	CDL	CA7-C31-C32-C33
49	n	101	PLX	C30-C31-C32-C33
49	V	205	PLX	C10-C11-C12-C13
49	e	201	PLX	C27-C28-C29-C30
55	V	201	CDL	C75-C76-C77-C78
49	e	201	PLX	C30-C31-C32-C33
48	V	202	PEE	C31-C30-O3-C3
48	l	719	PEE	C36-C37-C38-C39
49	j	203	PLX	C15-C16-C17-C18
55	a	201	CDL	OB5-CB3-CB4-OB6
49	C	312	PLX	C26-C27-C28-C29
55	r	714	CDL	C54-C55-C56-C57
55	V	203	CDL	C61-C62-C63-C64
48	U	101	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
55	l	712	CDL	C44-C45-C46-C47
55	r	714	CDL	C77-C78-C79-C80
55	r	714	CDL	OA7-CA5-OA6-CA4
48	l	718	PEE	C39-C40-C41-C42
55	r	714	CDL	C72-C71-CB7-OB8
49	j	203	PLX	C32-C33-C34-C35
55	V	203	CDL	C73-C74-C75-C76
55	V	203	CDL	C31-CA7-OA8-CA6
49	i	705	PLX	C4-C5-O8-C24
48	C	311	PEE	C41-C42-C43-C44
55	V	203	CDL	OA9-CA7-OA8-CA6
49	j	202	PLX	C27-C28-C29-C30
55	l	713	CDL	C52-C51-CB5-OB6
55	r	714	CDL	CB4-CB3-OB5-PB2
55	V	201	CDL	C76-C77-C78-C79
49	e	201	PLX	C24-C25-C26-C27
49	j	202	PLX	C24-C25-C26-C27
55	r	714	CDL	C52-C53-C54-C55
49	j	203	PLX	C17-C18-C19-C20
55	V	203	CDL	C77-C78-C79-C80
55	a	201	CDL	C38-C39-C40-C41
49	j	202	PLX	C2-C1-N1-C1A
50	X	201	8Q1	C29-C32-C34-N36
50	G	201	8Q1	C37-C38-C39-O40
48	j	201	PEE	C18-C19-C20-C21
48	l	720	PEE	C18-C19-C20-C21
55	N	202	CDL	OB6-CB4-CB6-OB8
48	l	719	PEE	C42-C43-C44-C45
47	A	503	NAI	O4D-C1D-N1N-C2N
55	m	201	CDL	C78-C79-C80-C81
48	j	201	PEE	C31-C32-C33-C34
49	C	312	PLX	C7-C8-C9-C10
49	i	705	PLX	C35-C36-C37-C38
49	C	312	PLX	C31-C32-C33-C34
48	l	719	PEE	C38-C39-C40-C41
55	N	202	CDL	CA3-CA4-CA6-OA8
48	l	718	PEE	C24-C25-C26-C27
48	V	207	PEE	C3-C2-O2-C10
48	l	719	PEE	C1-C2-O2-C10
48	l	719	PEE	C3-C2-O2-C10
55	V	201	CDL	CA6-CA4-OA6-CA5
49	j	202	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C32-C33-C34-C35
48	V	202	PEE	C38-C39-C40-C41
48	l	718	PEE	C18-C19-C20-C21
49	e	201	PLX	C35-C36-C37-C38
55	r	714	CDL	C79-C80-C81-C82
55	k	101	CDL	C36-C37-C38-C39
48	l	719	PEE	O3P-C1-C2-O2
55	n	102	CDL	OB5-CB3-CB4-OB6
55	V	201	CDL	C51-CB5-OB6-CB4
48	V	207	PEE	C16-C17-C18-C19
55	a	201	CDL	C31-C32-C33-C34
55	V	201	CDL	CB4-CB3-OB5-PB2
55	i	401	CDL	C16-C17-C18-C19
49	j	203	PLX	C34-C35-C36-C37
55	V	201	CDL	OB7-CB5-OB6-CB4
49	j	202	PLX	C11-C12-C13-C14
49	C	312	PLX	C32-C33-C34-C35
47	A	503	NAI	C2N-C3N-C7N-N7N
50	G	201	8Q1	C37-C38-C39-N41
55	l	713	CDL	C82-C83-C84-C85
48	l	719	PEE	C19-C20-C21-C22
55	l	713	CDL	CB2-C1-CA2-OA2
47	A	503	NAI	C2D-C1D-N1N-C2N
48	l	720	PEE	C16-C17-C18-C19
49	i	705	PLX	O6-C6-C7-C8
49	j	202	PLX	C28-C29-C30-C31
55	l	713	CDL	C12-C11-CA5-OA6
49	C	312	PLX	C12-C13-C14-C15
55	i	401	CDL	C62-C63-C64-C65
55	V	201	CDL	C1-CB2-OB2-PB2
55	n	102	CDL	CA3-CA4-CA6-OA8
49	C	312	PLX	O9-C24-C25-C26
55	a	201	CDL	C34-C35-C36-C37
49	j	203	PLX	C24-C25-C26-C27
49	n	101	PLX	C24-C25-C26-C27
55	k	101	CDL	C38-C39-C40-C41
52	s	402	UQ	C6-C7-C8-C9
48	V	207	PEE	C38-C39-C40-C41
55	k	101	CDL	CA2-C1-CB2-OB2
49	e	201	PLX	C2-C1-N1-C1C
55	V	203	CDL	C81-C82-C83-C84
55	V	203	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
55	l	713	CDL	C53-C54-C55-C56
48	l	719	PEE	O2-C2-C3-O3
55	V	203	CDL	OB6-CB4-CB6-OB8
55	n	102	CDL	C54-C55-C56-C57
55	V	203	CDL	C78-C79-C80-C81
48	m	202	PEE	C22-C23-C24-C25
49	i	705	PLX	C6-C7-C8-C9
55	V	201	CDL	C33-C34-C35-C36
55	a	201	CDL	C40-C41-C42-C43
55	n	102	CDL	C74-C75-C76-C77
48	l	718	PEE	C16-C17-C18-C19
48	l	718	PEE	C38-C39-C40-C41
55	r	714	CDL	C44-C45-C46-C47
55	V	203	CDL	C21-C22-C23-C24
55	l	713	CDL	C31-CA7-OA8-CA6
48	V	207	PEE	C1-C2-O2-C10
48	s	401	PEE	C18-C19-C20-C21
52	s	402	UQ	C12-C13-C14-C16
55	l	713	CDL	OA9-CA7-OA8-CA6
55	a	201	CDL	C21-C22-C23-C24
49	j	203	PLX	C3-C4-C5-O8
55	l	713	CDL	CB3-CB4-CB6-OB8
55	n	102	CDL	OA9-CA7-OA8-CA6
48	m	202	PEE	C18-C19-C20-C21
48	m	202	PEE	C16-C17-C18-C19
49	e	201	PLX	C25-C26-C27-C28
55	l	713	CDL	C78-C79-C80-C81
55	N	202	CDL	C72-C71-CB7-OB8
50	G	201	8Q1	C31-C29-C32-C34
56	Q	501	DCQ	C13-C14-C15-C16
55	n	102	CDL	O1-C1-CA2-OA2
48	j	201	PEE	C16-C17-C18-C19
48	l	719	PEE	C16-C17-C18-C19
55	V	201	CDL	C41-C42-C43-C44
49	j	203	PLX	C7-C6-O6-C4
49	n	101	PLX	C2-C1-N1-C1A
55	V	203	CDL	C43-C44-C45-C46
55	l	713	CDL	C16-C17-C18-C19
55	i	401	CDL	C12-C11-CA5-OA6
48	C	311	PEE	C18-C19-C20-C21
48	s	401	PEE	C16-C17-C18-C19
55	a	201	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
55	l	713	CDL	C12-C13-C14-C15
55	m	201	CDL	C81-C82-C83-C84
55	N	202	CDL	C52-C51-CB5-OB6
55	a	201	CDL	C32-C31-CA7-OA8
55	i	401	CDL	C51-C52-C53-C54
48	U	101	PEE	O2-C10-C11-C12
48	U	101	PEE	O3-C30-C31-C32
48	V	202	PEE	O3P-C1-C2-O2
52	s	402	UQ	C13-C14-C16-C17
55	l	712	CDL	C24-C25-C26-C27
49	j	203	PLX	C18-C19-C20-C21
48	l	720	PEE	C33-C34-C35-C36
48	l	719	PEE	C1-C2-C3-O3
49	e	201	PLX	C2-C1-N1-C1B
55	r	714	CDL	C12-C11-CA5-OA6
55	m	201	CDL	C77-C78-C79-C80
48	l	719	PEE	O3P-C1-C2-C3
55	a	201	CDL	CA5-C11-C12-C13
49	n	101	PLX	C34-C35-C36-C37
47	A	503	NAI	O4D-C4D-C5D-O5D
48	V	207	PEE	C11-C12-C13-C14
55	n	102	CDL	C31-CA7-OA8-CA6
55	k	101	CDL	C52-C51-CB5-OB7
48	m	202	PEE	O4-C10-O2-C2
49	C	312	PLX	C27-C28-C29-C30
50	X	201	8Q1	C42-C43-S44-C1
48	U	101	PEE	O5-C30-C31-C32
55	a	201	CDL	C32-C31-CA7-OA9
55	l	712	CDL	C54-C55-C56-C57
49	i	705	PLX	O8-C24-C25-C26
50	X	201	8Q1	C11-C10-C9-C8
48	U	101	PEE	C23-C24-C25-C26
55	l	713	CDL	C72-C73-C74-C75
55	l	712	CDL	C32-C33-C34-C35
48	C	311	PEE	C33-C34-C35-C36
55	m	201	CDL	C33-C34-C35-C36
48	U	101	PEE	O4-C10-C11-C12
49	e	201	PLX	O9-C24-O8-C5
49	i	705	PLX	O9-C24-O8-C5
55	N	202	CDL	C72-C71-CB7-OB9
48	V	202	PEE	C39-C40-C41-C42
55	m	201	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
55	N	202	CDL	OA6-CA4-CA6-OA8
49	C	312	PLX	C24-C25-C26-C27
55	V	203	CDL	CB2-C1-CA2-OA2
55	l	713	CDL	C32-C31-CA7-OA8
48	l	719	PEE	C20-C21-C22-C23
48	l	720	PEE	C11-C12-C13-C14
50	G	201	8Q1	O33-C32-C34-N36
55	N	202	CDL	C52-C51-CB5-OB7
55	r	714	CDL	C12-C11-CA5-OA7
55	V	201	CDL	C74-C75-C76-C77
55	l	712	CDL	C33-C34-C35-C36
55	l	712	CDL	CA4-CA3-OA5-PA1
48	l	720	PEE	O2-C10-C11-C12
49	e	201	PLX	C2-C1-N1-C1A
50	G	201	8Q1	O27-C28-C29-C32
55	m	201	CDL	C72-C71-CB7-OB8
55	a	201	CDL	C12-C11-CA5-OA6
48	V	207	PEE	C10-C11-C12-C13
55	a	201	CDL	C35-C36-C37-C38
48	C	311	PEE	O3-C30-C31-C32
48	l	719	PEE	C22-C23-C24-C25
55	m	201	CDL	C12-C11-CA5-OA7

There are no ring outliers.

37 monomers are involved in 284 short contacts:

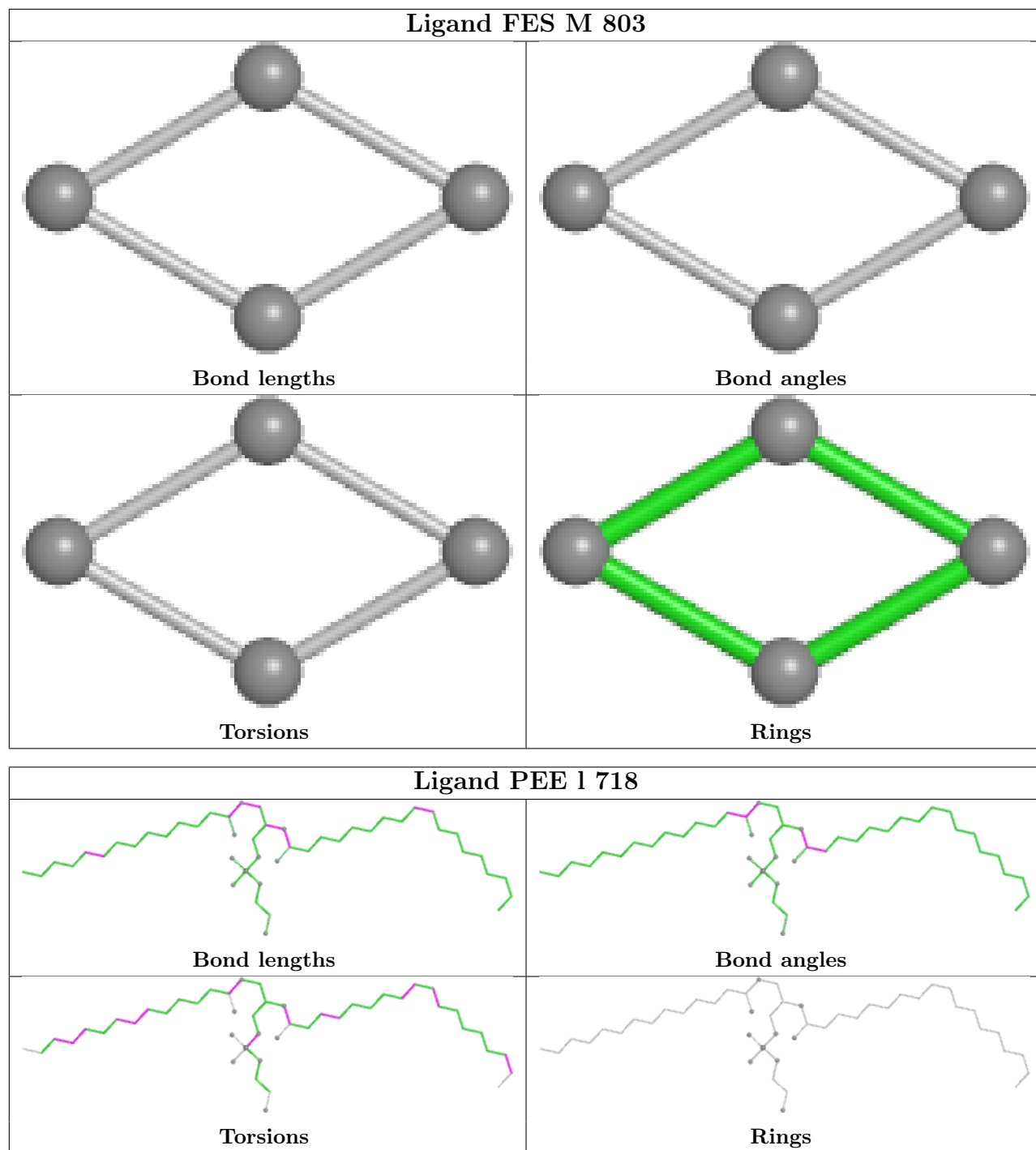
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	l	718	PEE	13	0
55	i	401	CDL	4	0
55	k	101	CDL	7	0
51	J	401	NDP	3	0
49	i	705	PLX	4	0
55	m	201	CDL	7	0
56	Q	501	DCQ	8	0
52	s	402	UQ	3	0
49	j	203	PLX	4	0
50	X	201	8Q1	1	0
48	l	719	PEE	7	0
52	J	402	UQ	5	0
55	a	201	CDL	21	0
55	n	102	CDL	6	0
55	r	714	CDL	4	0

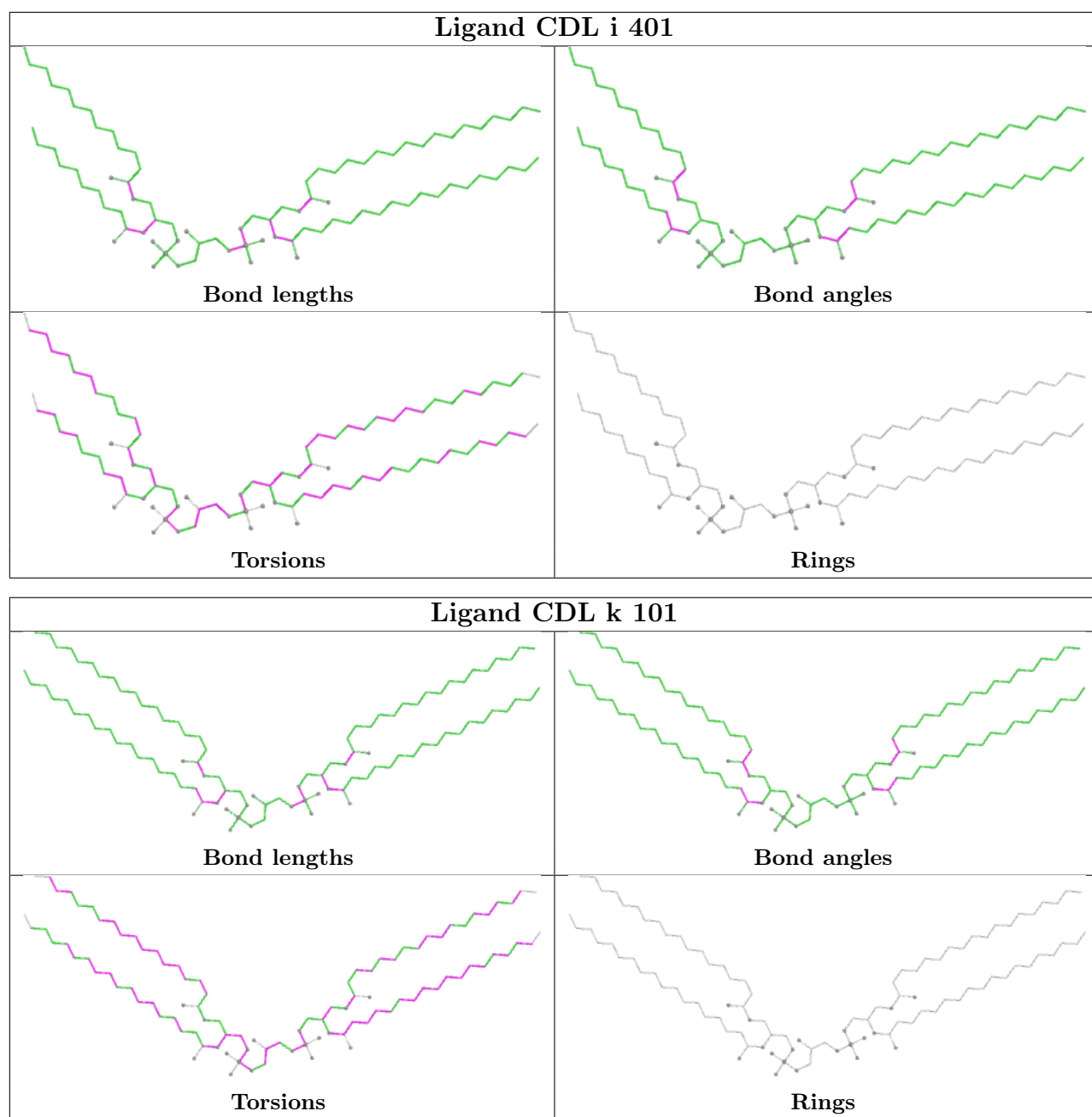
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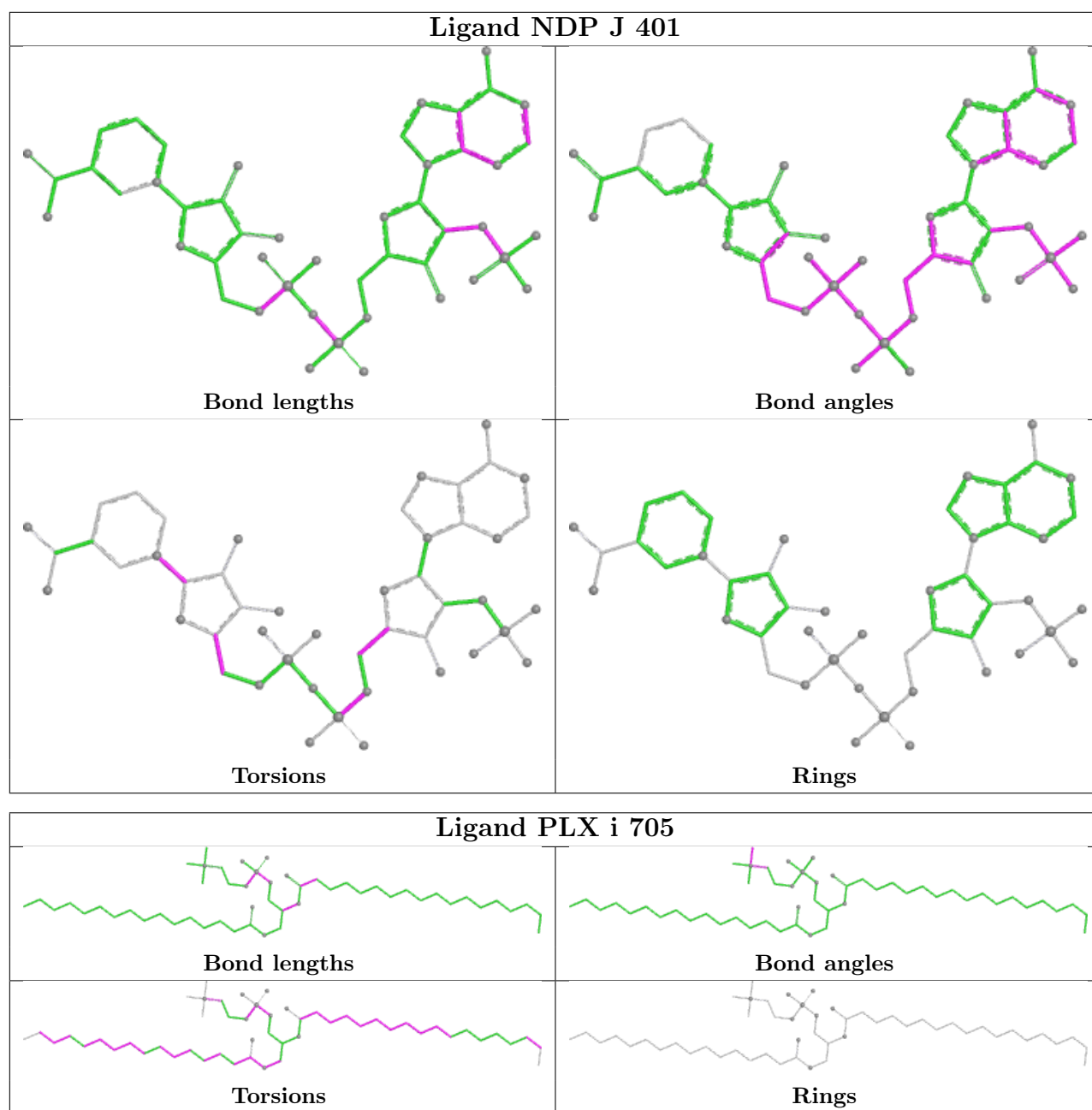
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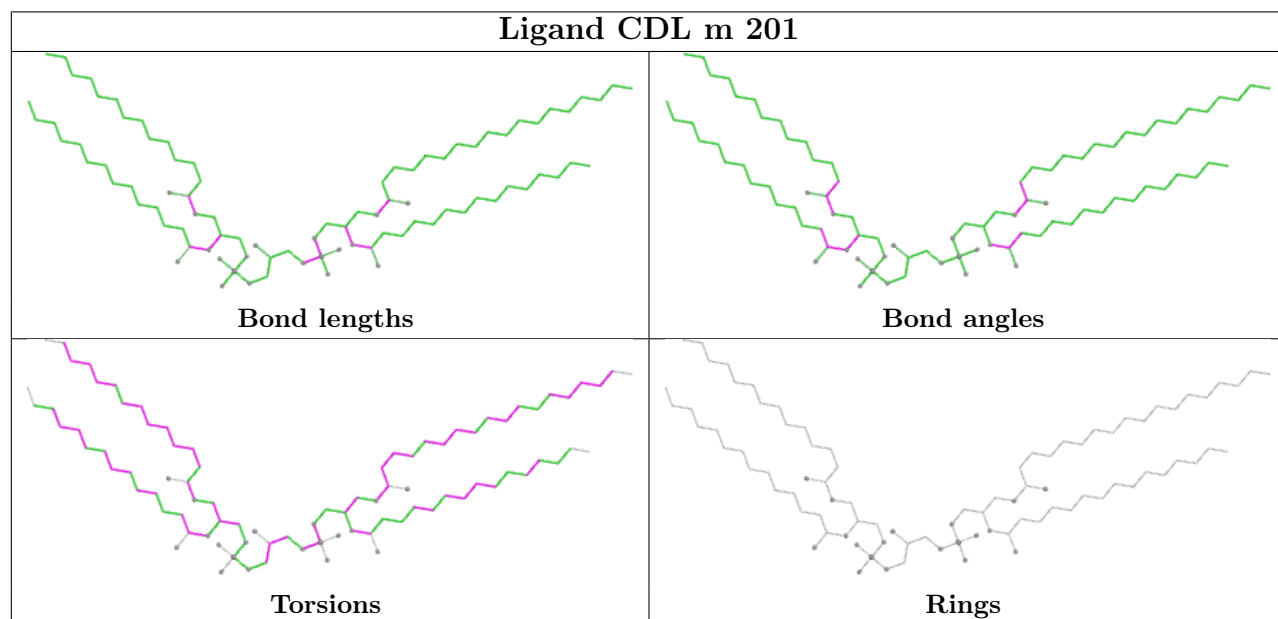
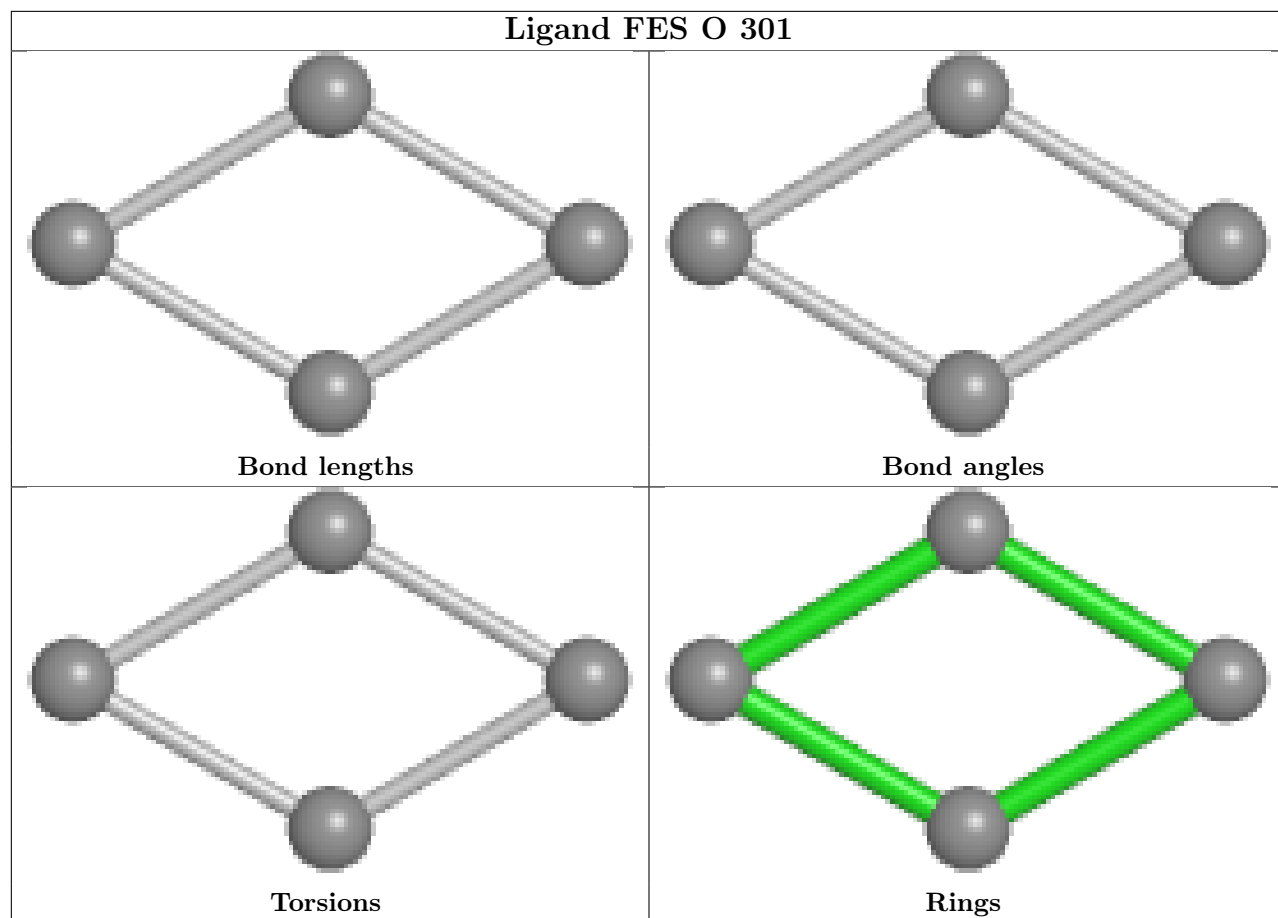
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	j	202	PLX	12	0
48	U	101	PEE	4	0
46	A	502	FMN	3	0
55	V	201	CDL	21	0
48	m	202	PEE	9	0
55	V	203	CDL	25	0
49	C	312	PLX	5	0
55	N	202	CDL	11	0
45	A	501	SF4	1	0
47	A	503	NAI	6	0
49	V	205	PLX	3	0
48	V	202	PEE	13	0
48	j	201	PEE	7	0
49	e	201	PLX	19	0
55	l	712	CDL	18	0
48	s	401	PEE	5	0
48	V	207	PEE	5	0
55	l	713	CDL	7	0
50	G	201	8Q1	1	0
48	l	720	PEE	28	0
58	w	401	ADP	6	0
48	C	311	PEE	6	0

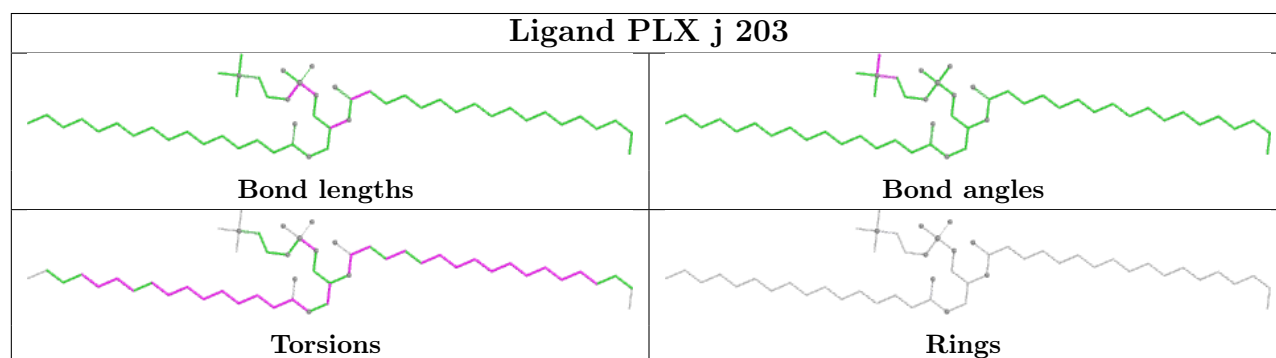
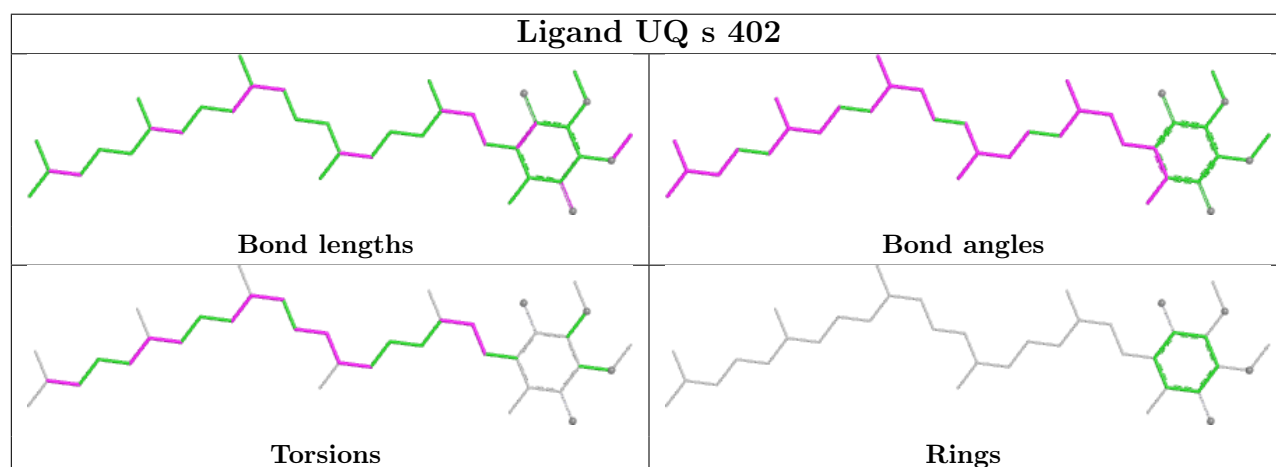
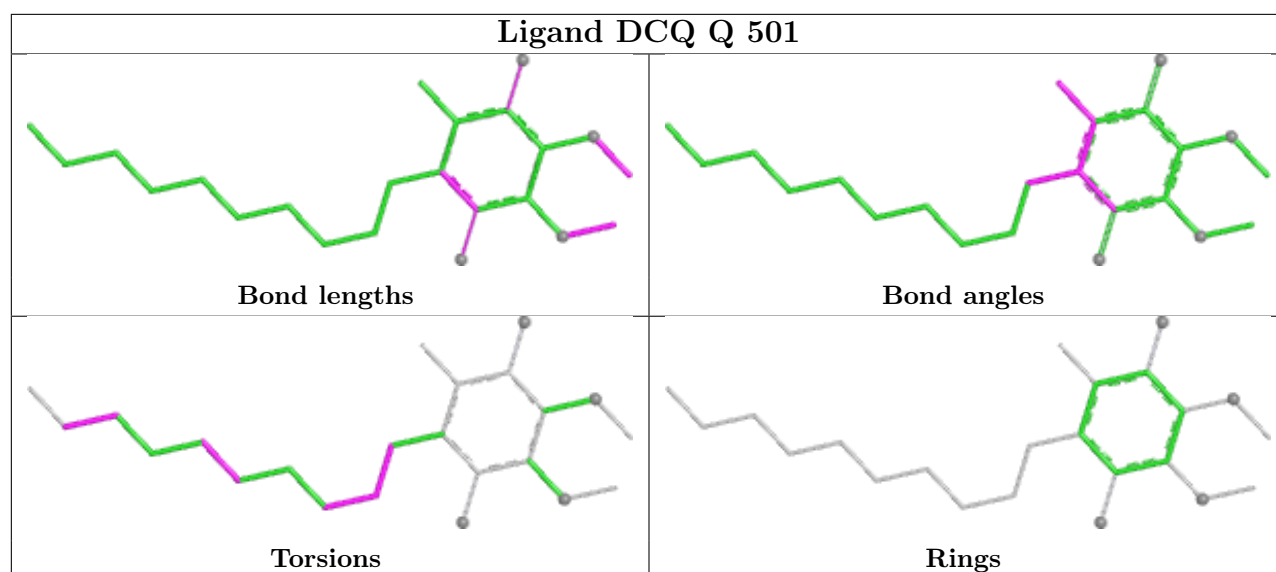
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

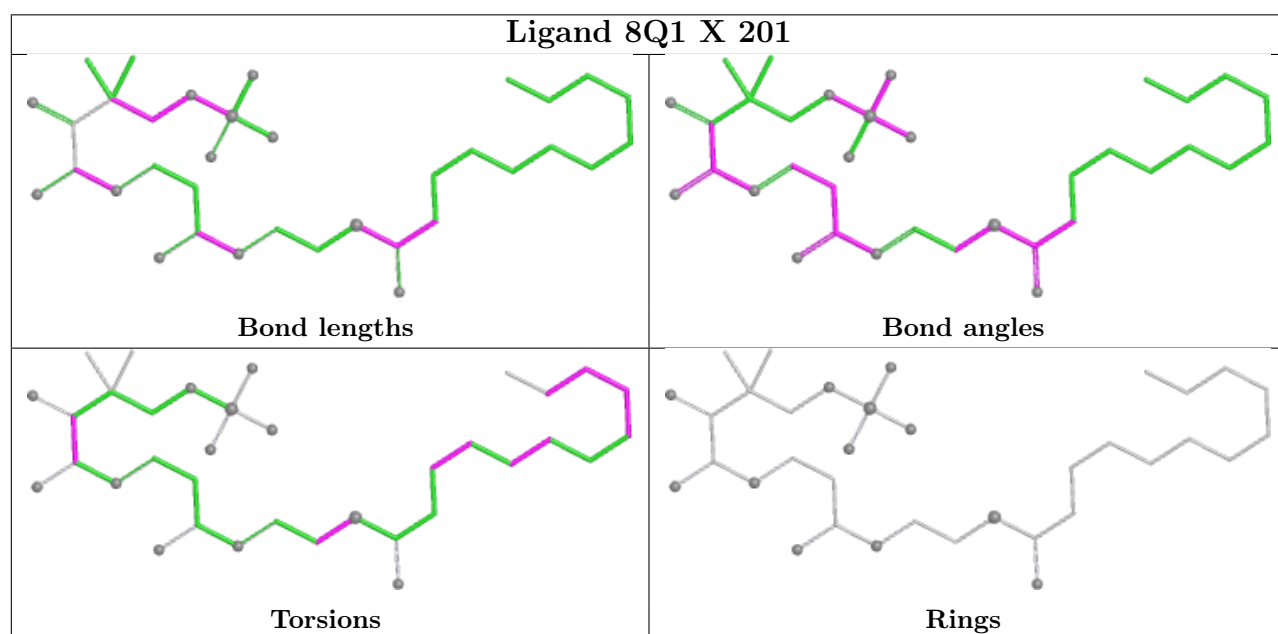
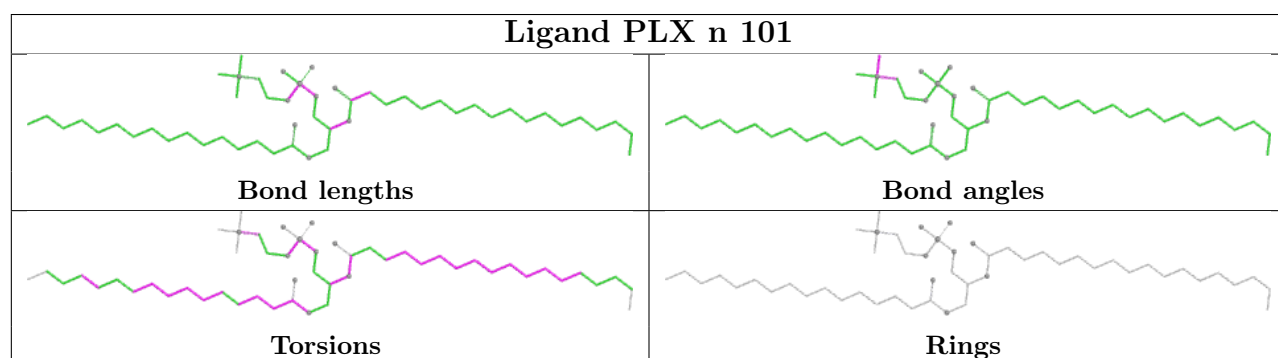
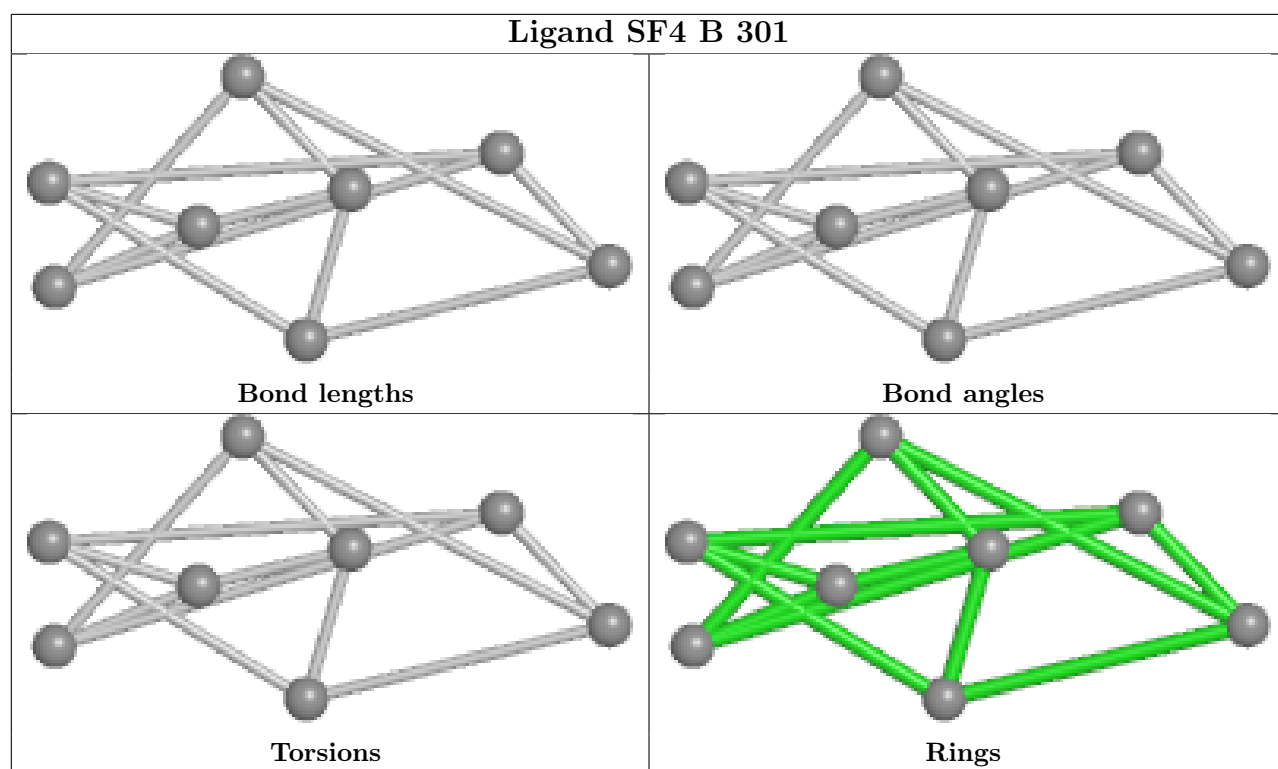


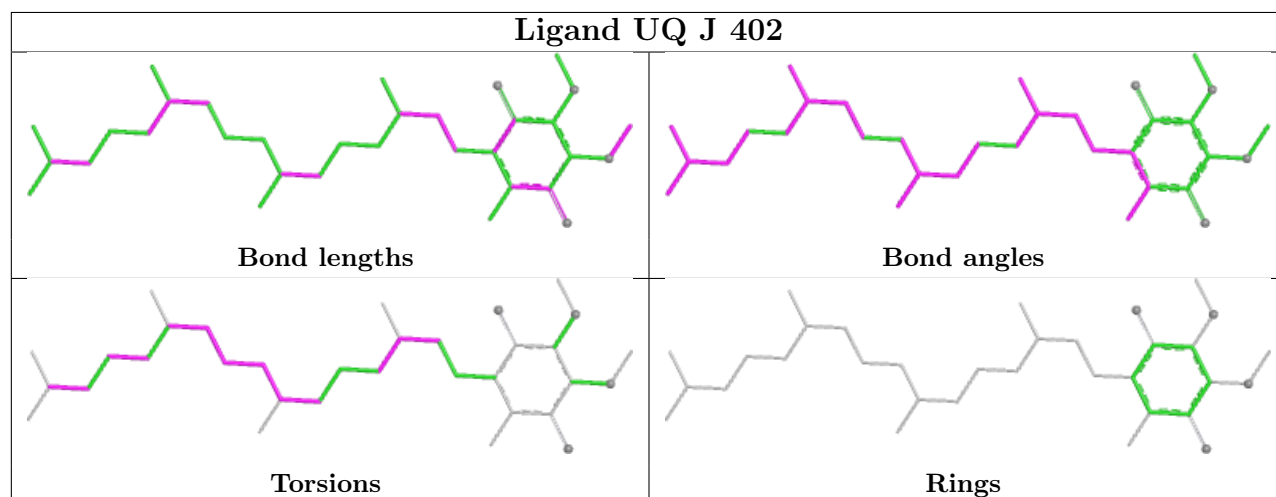
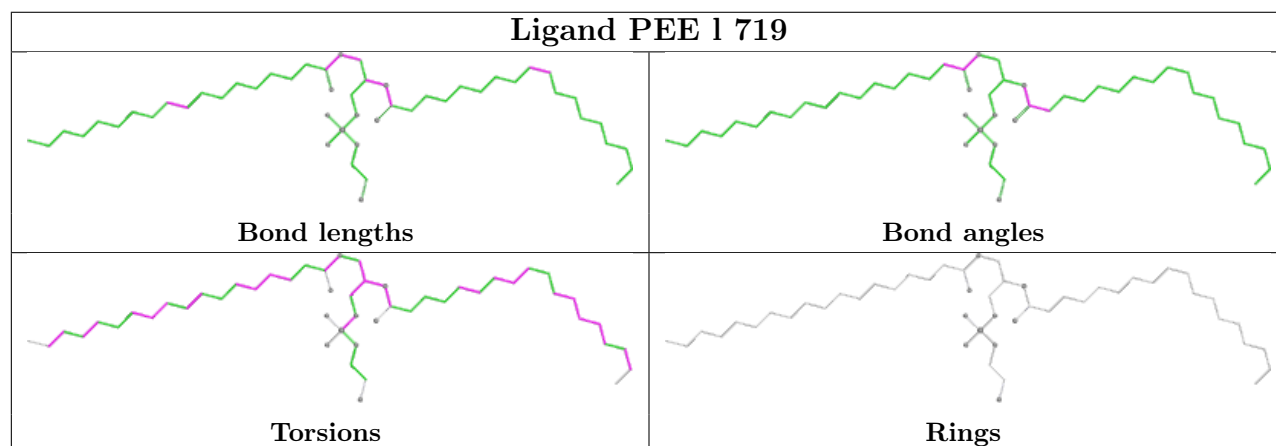
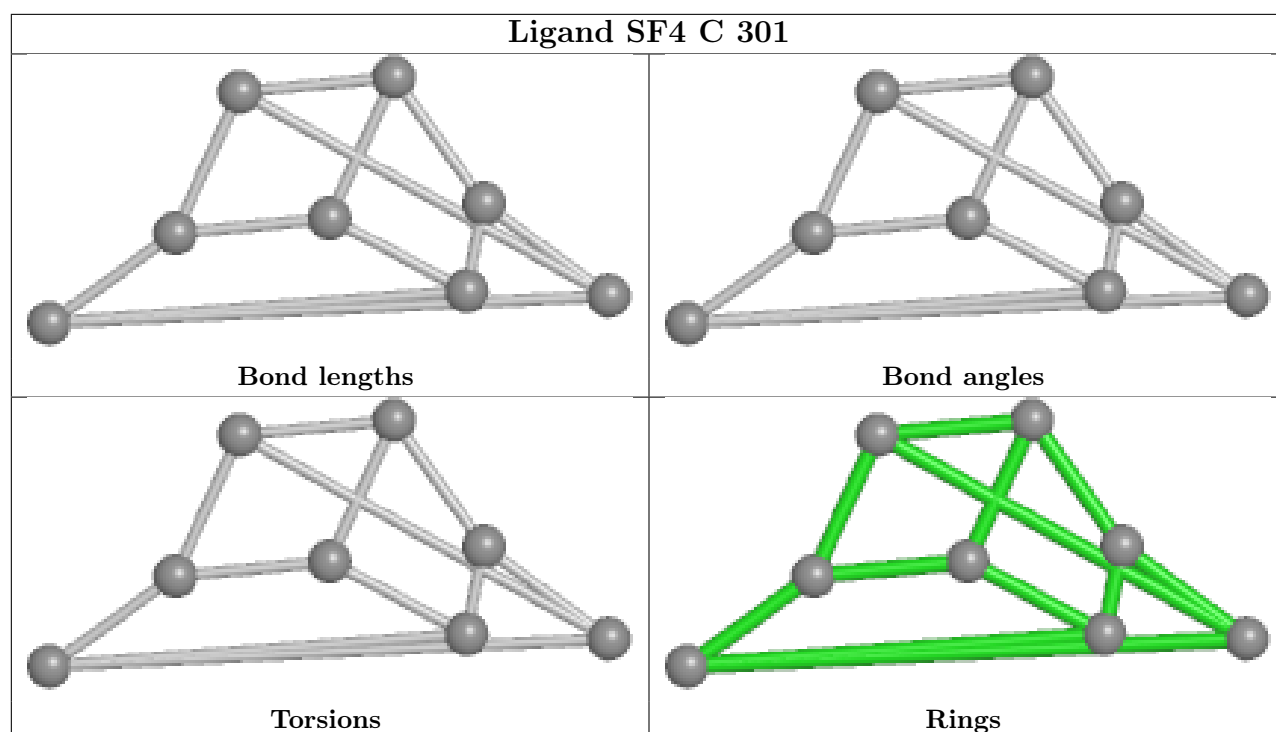


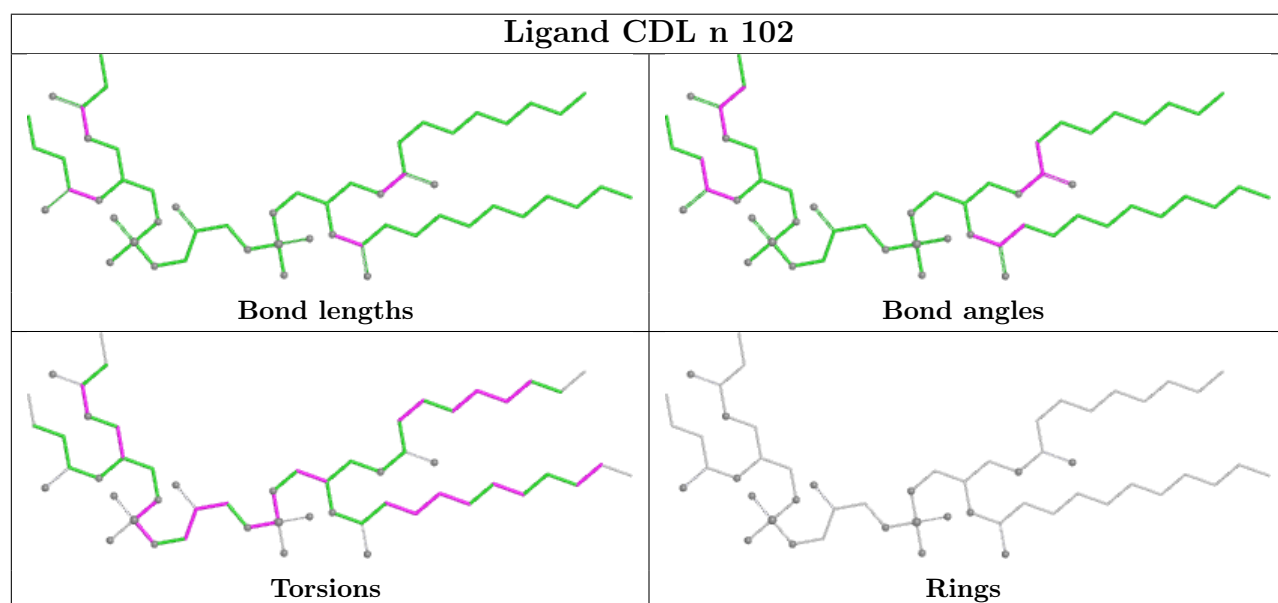
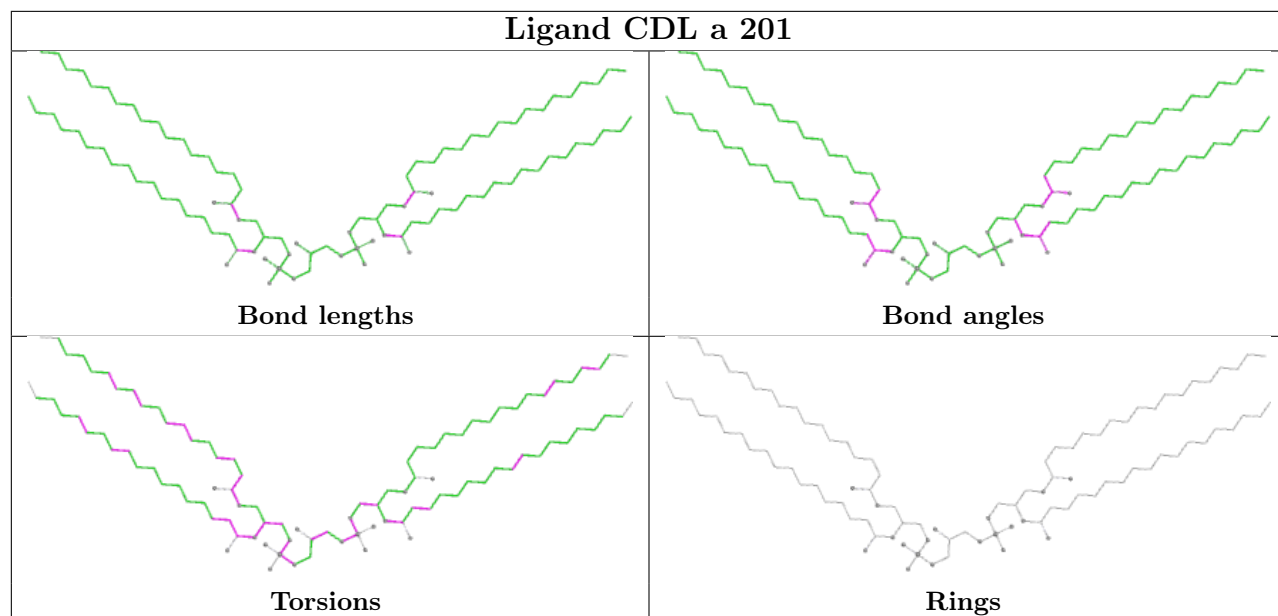


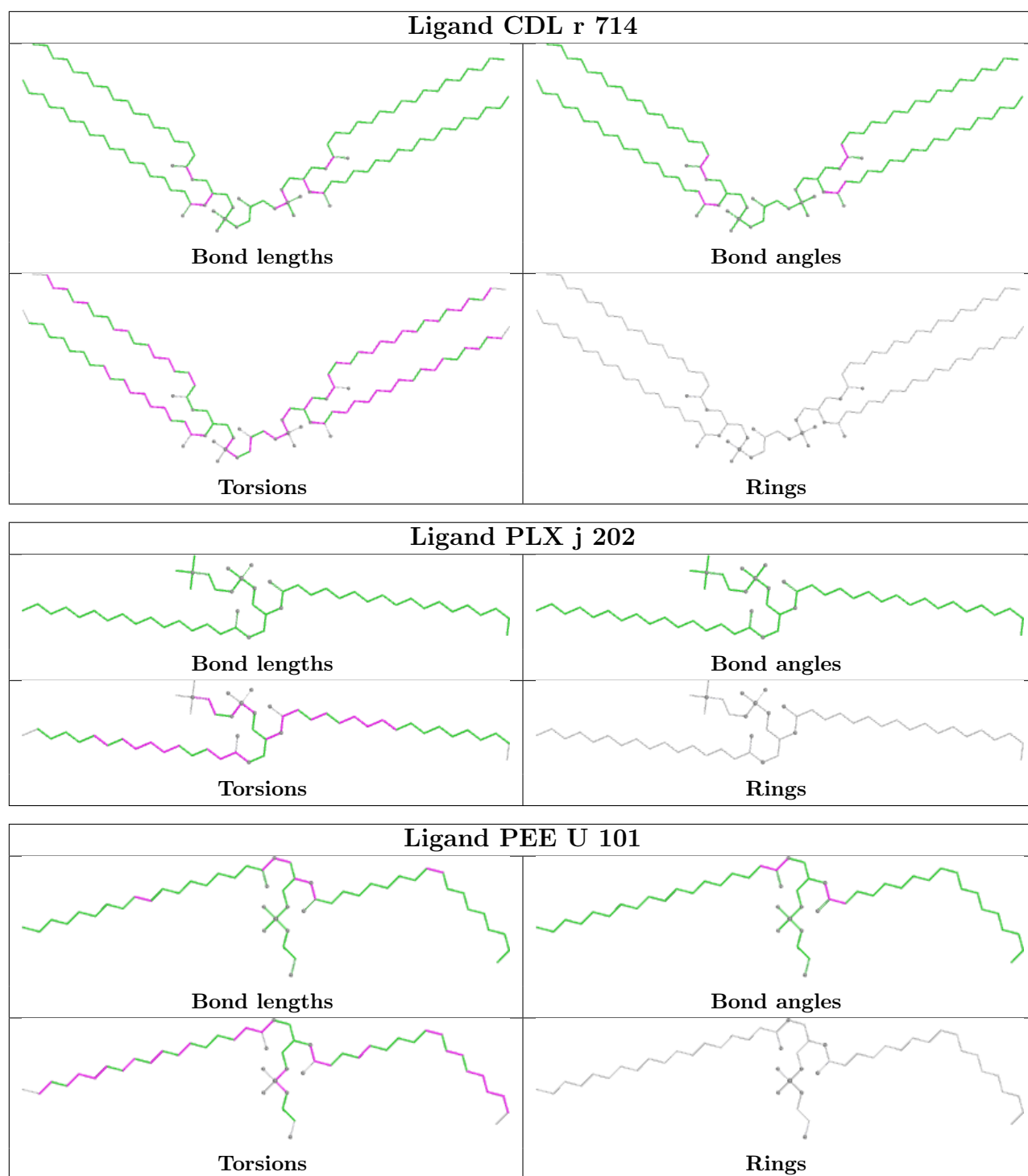


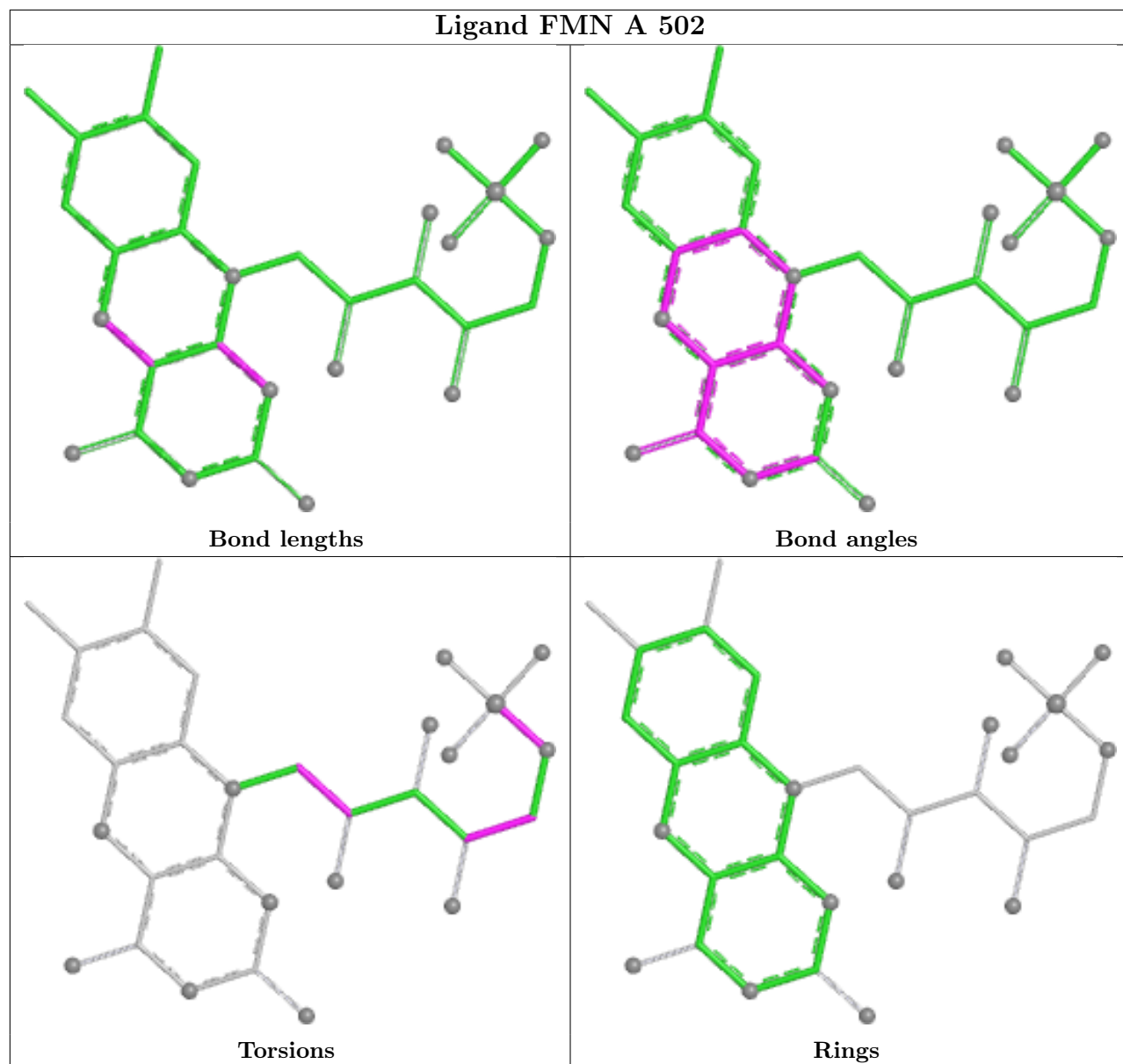


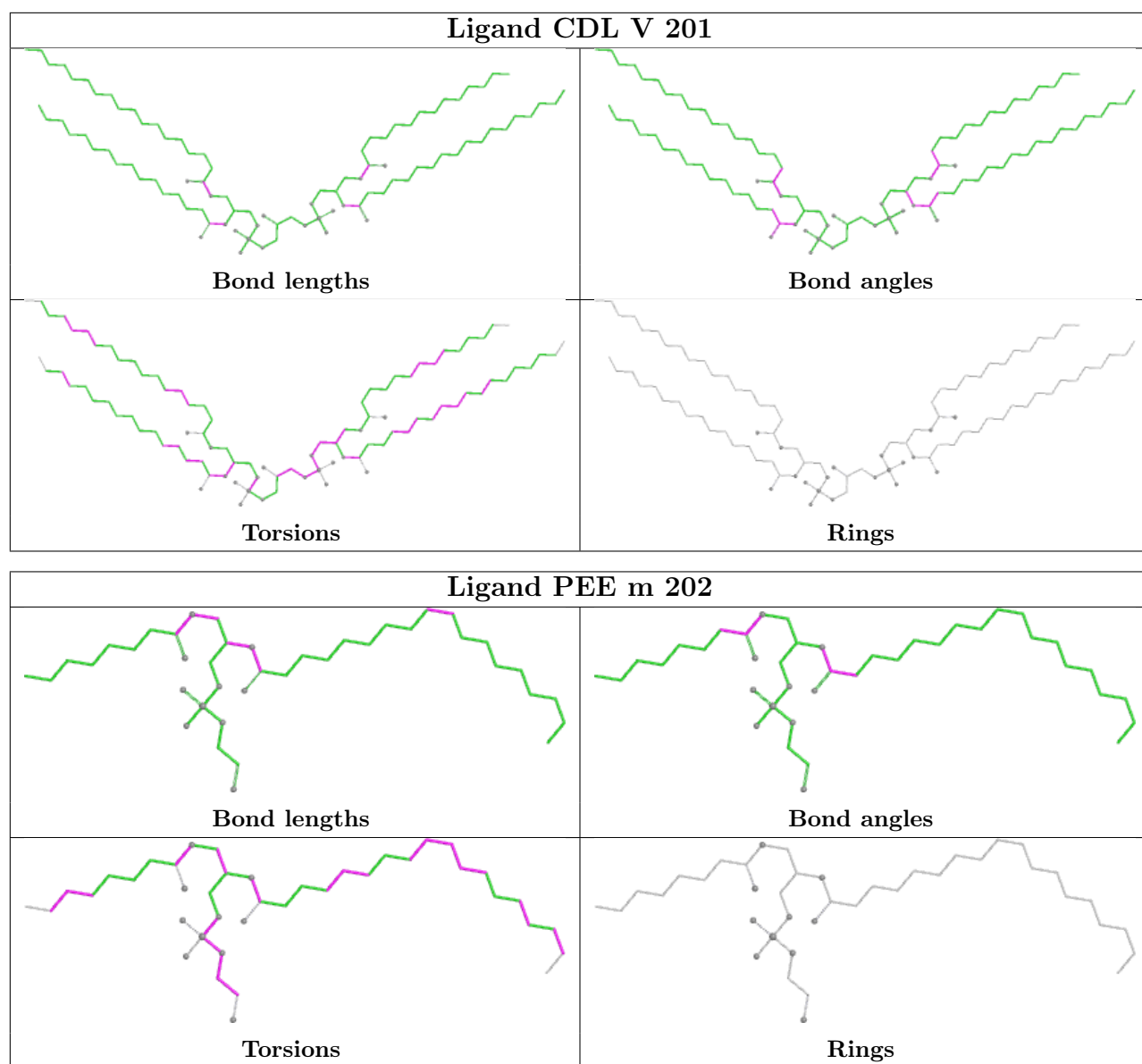


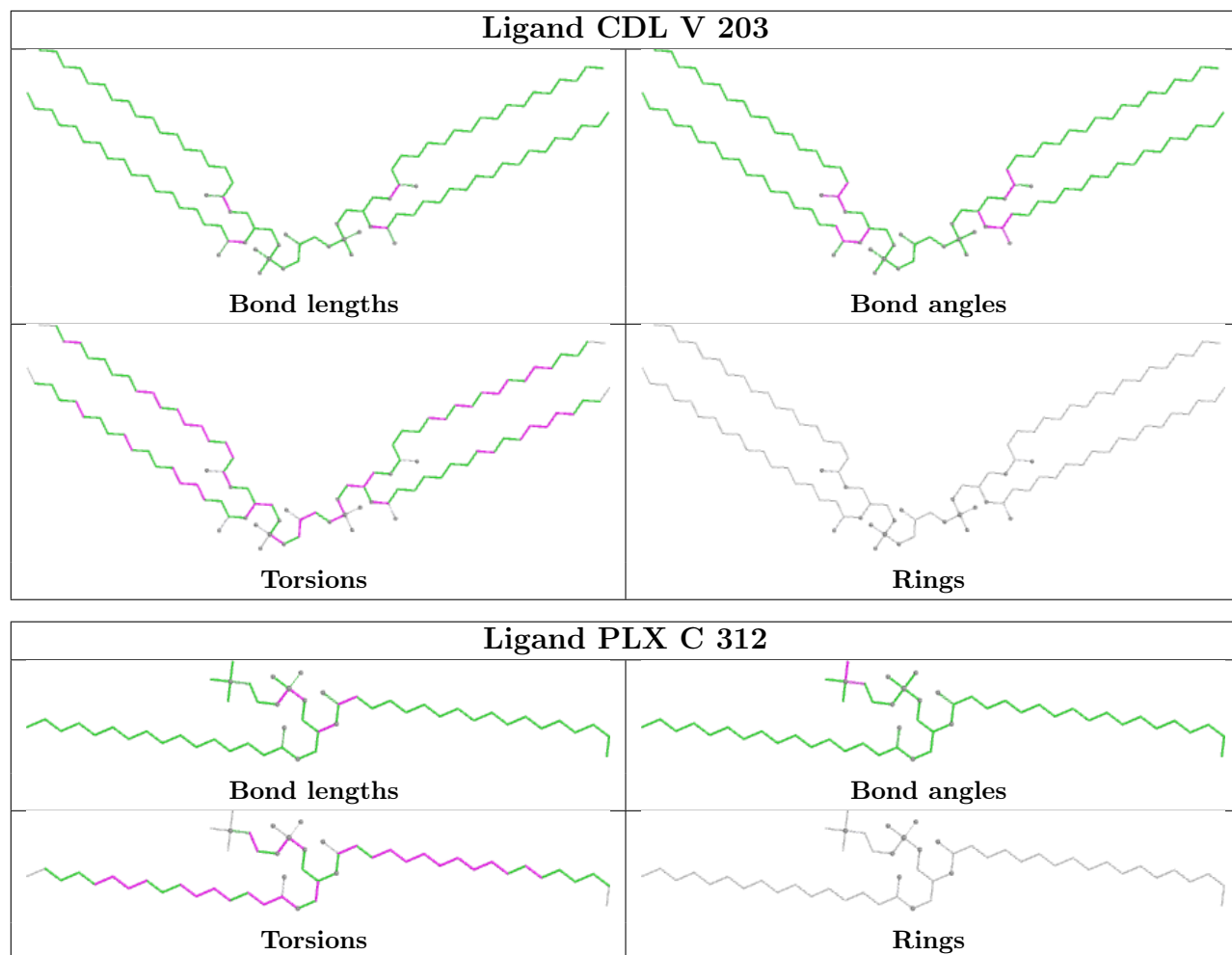




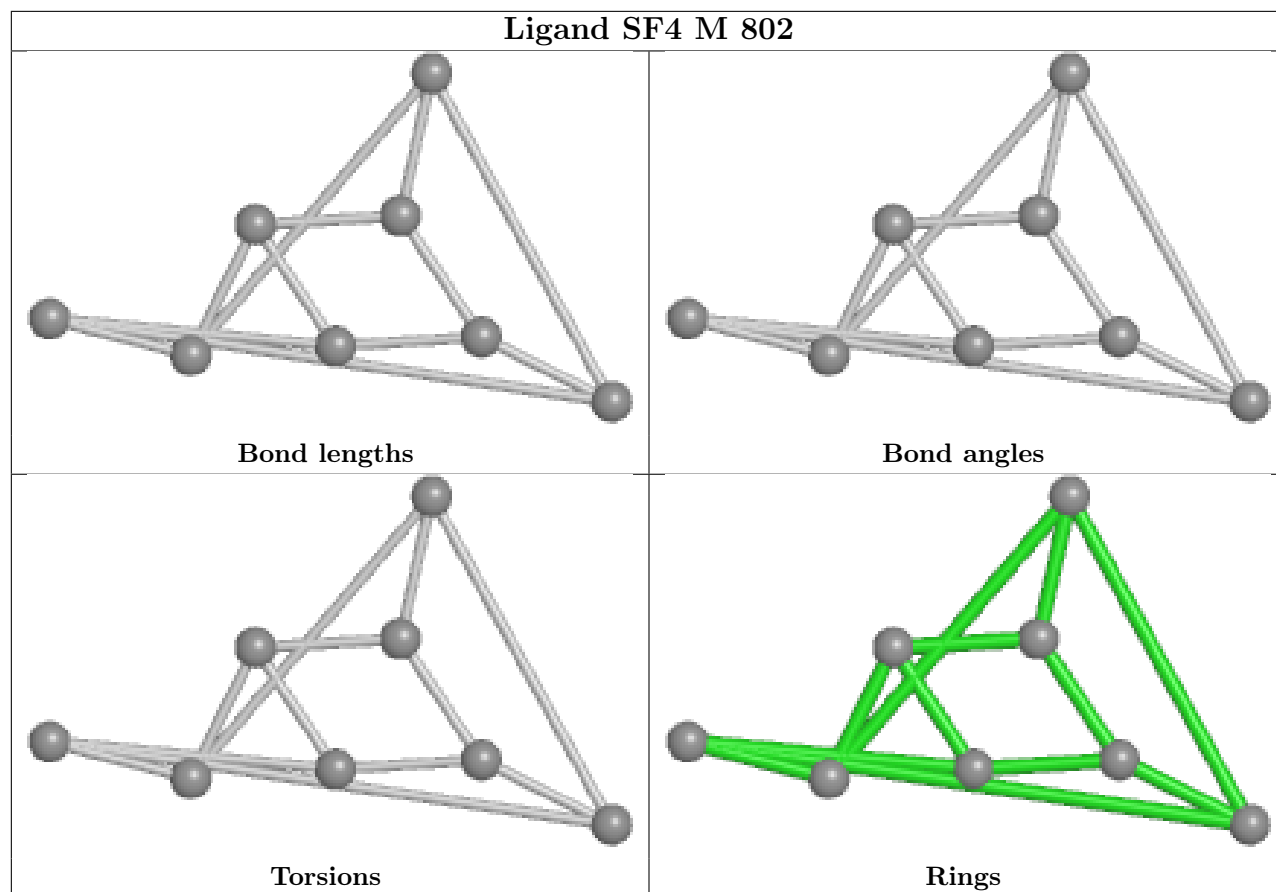




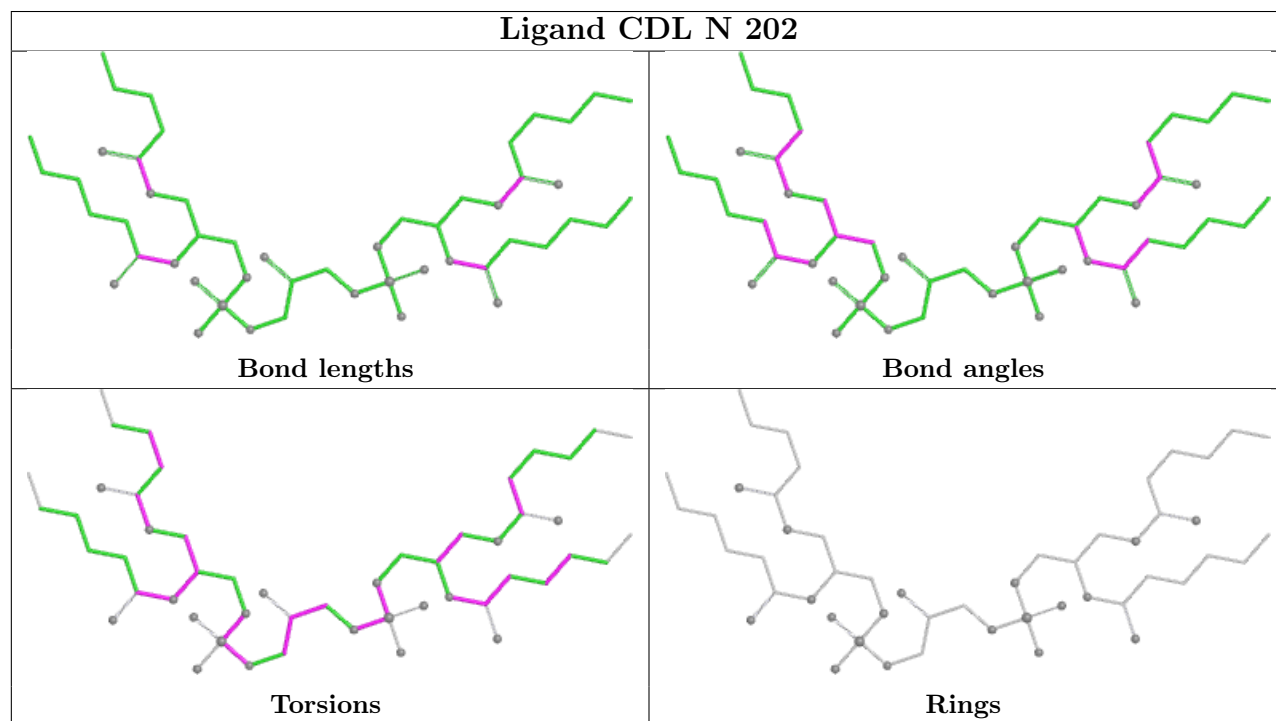


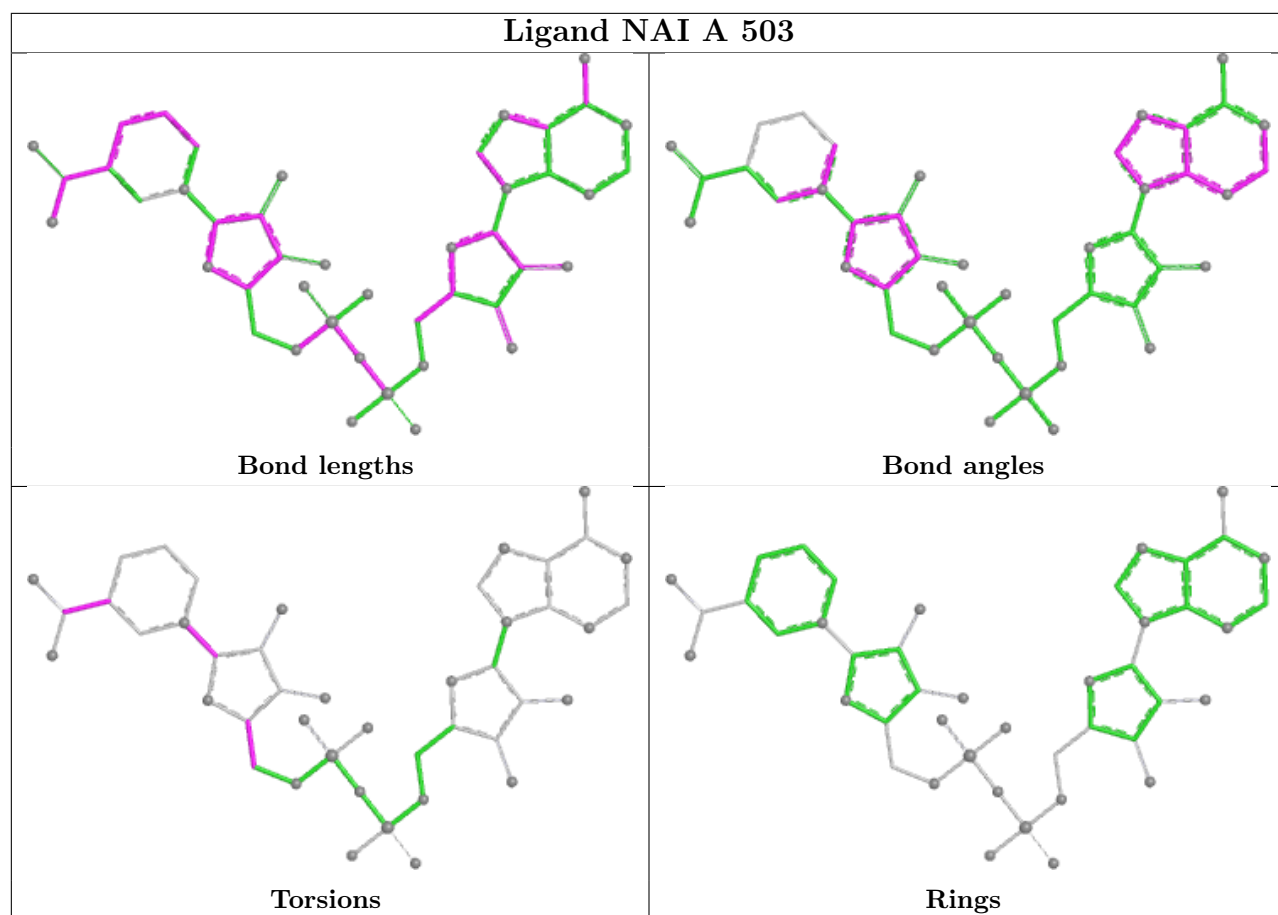
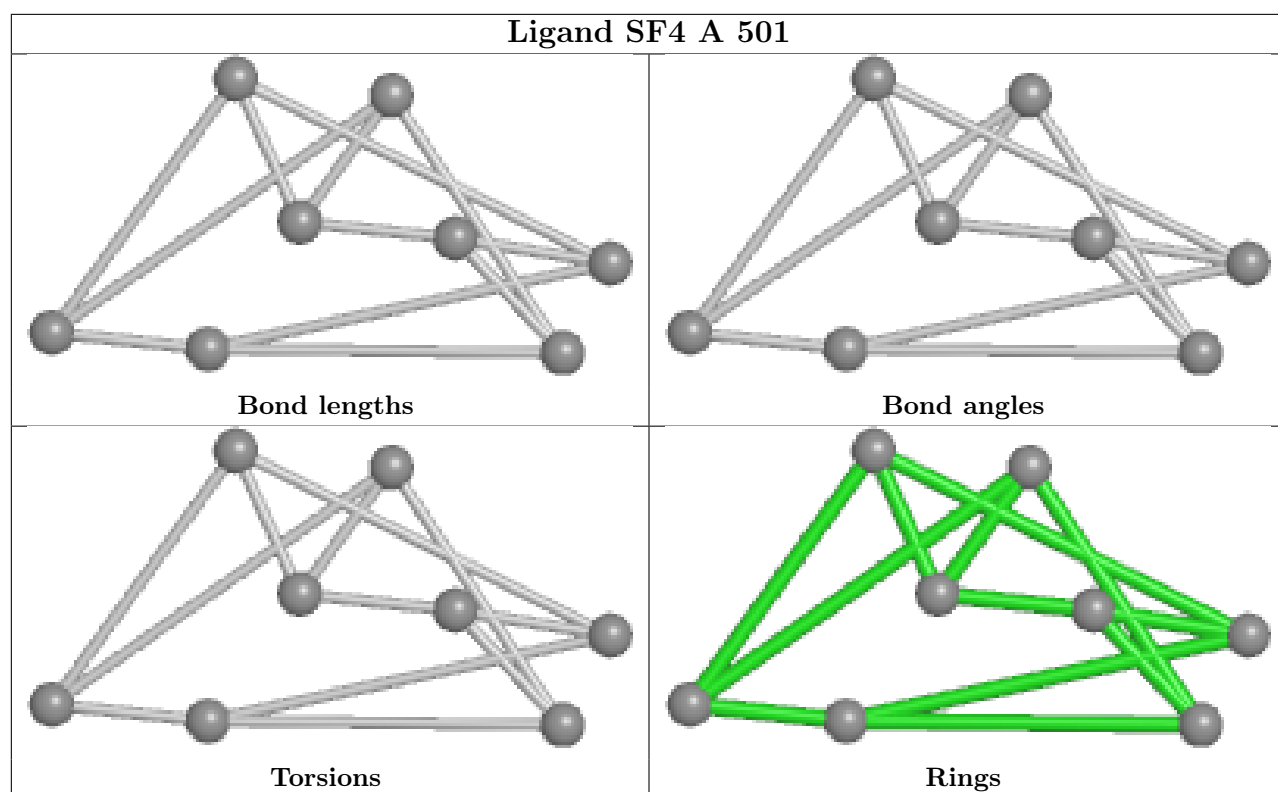


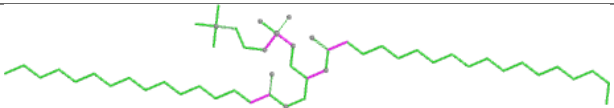
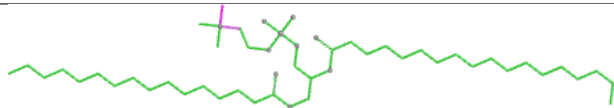
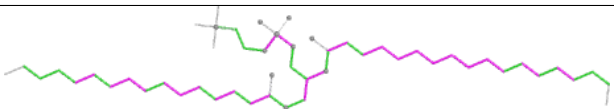
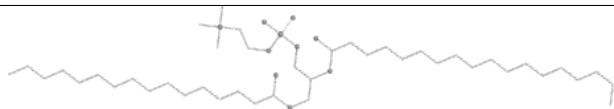
Ligand SF4 M 802

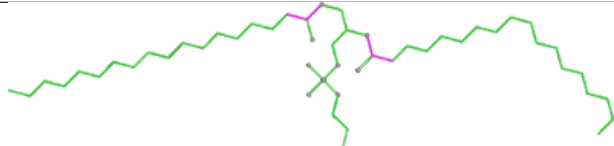
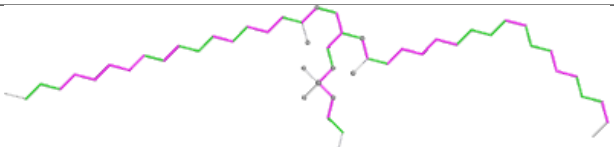
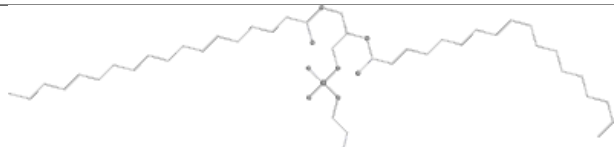


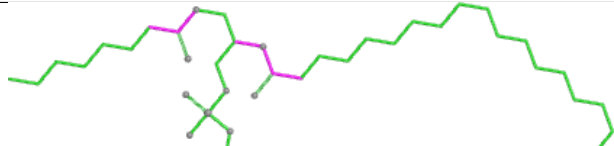
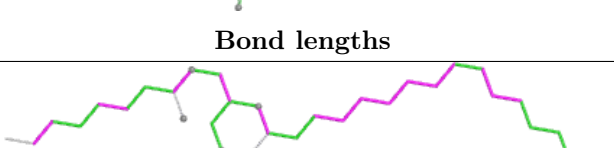
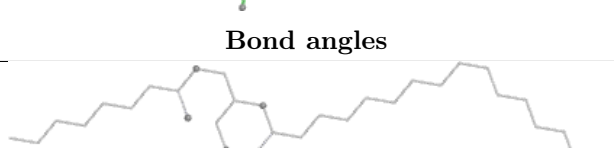
Ligand CDL N 202

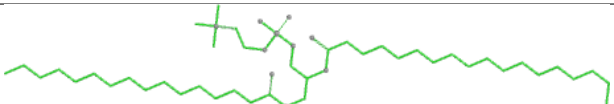
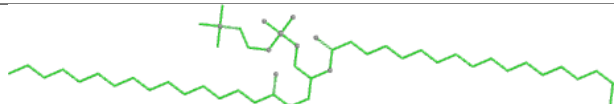
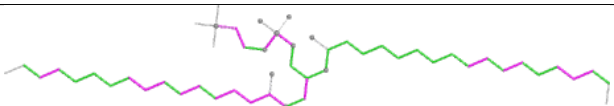
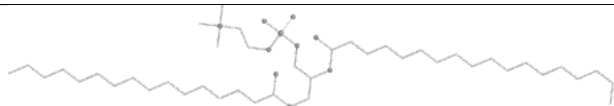


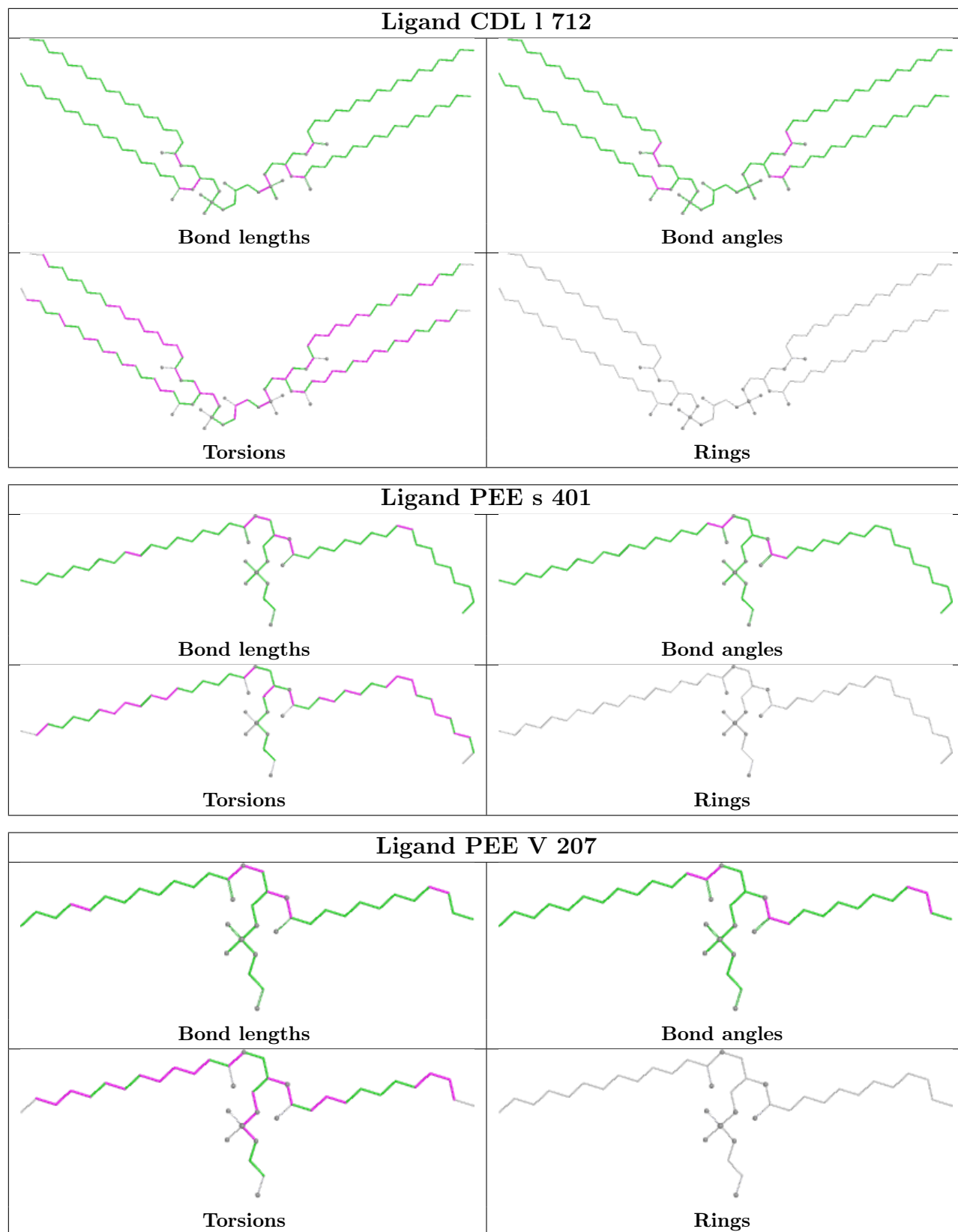


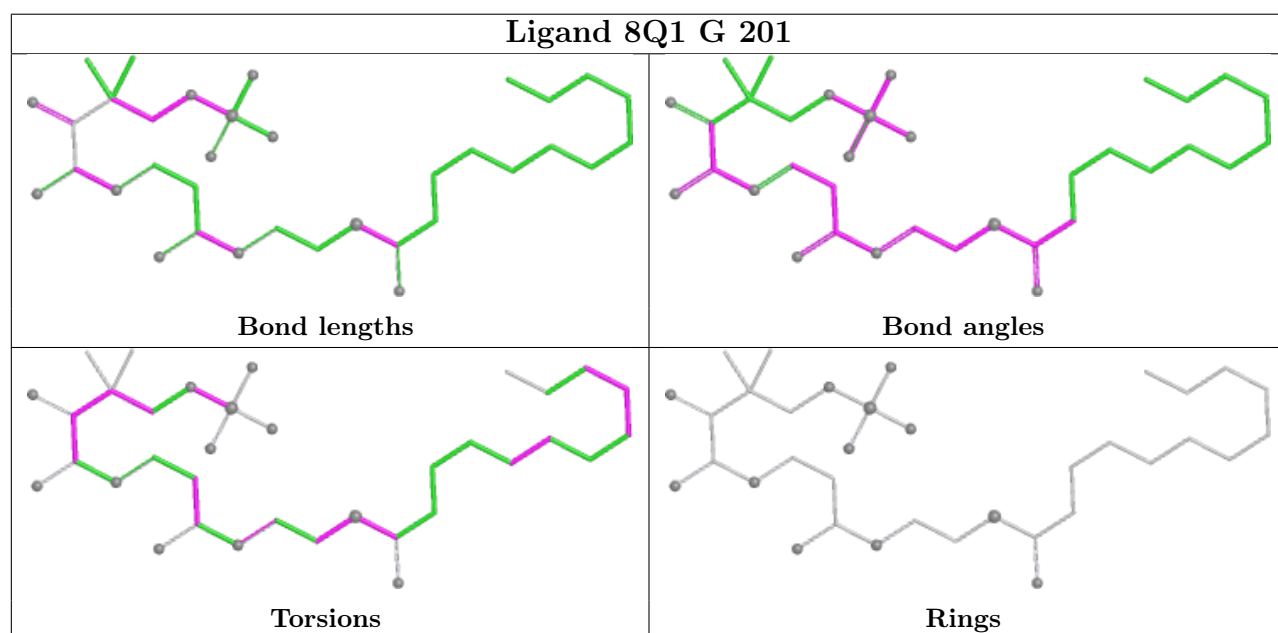
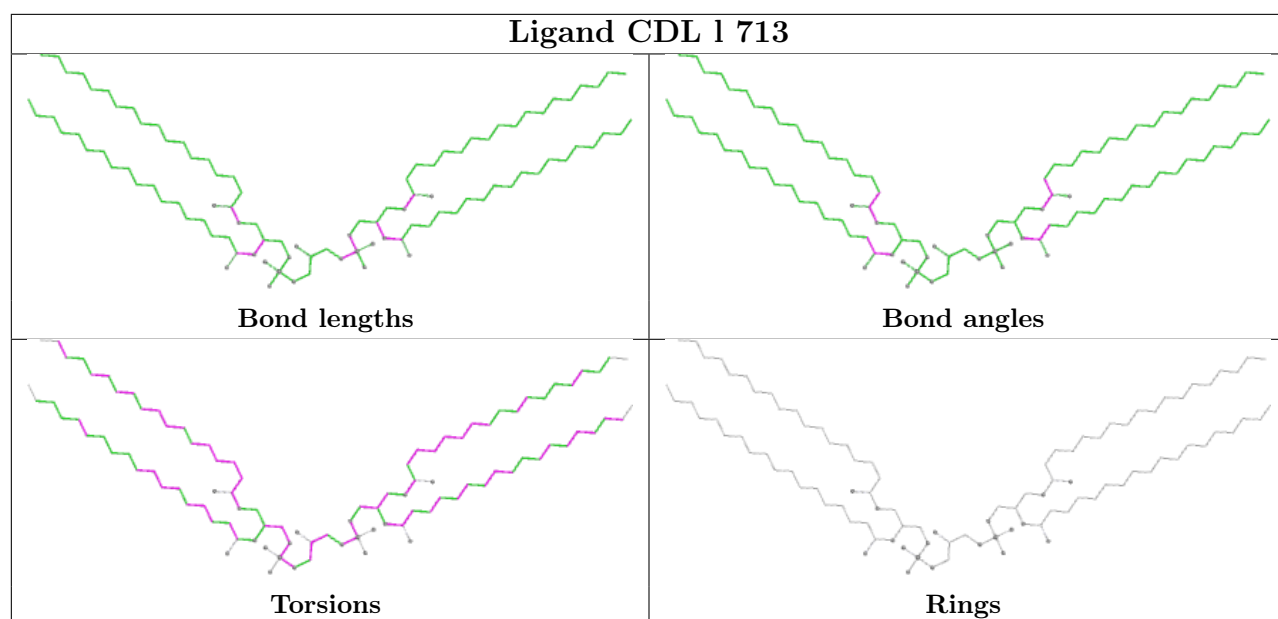
Ligand PLX V 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

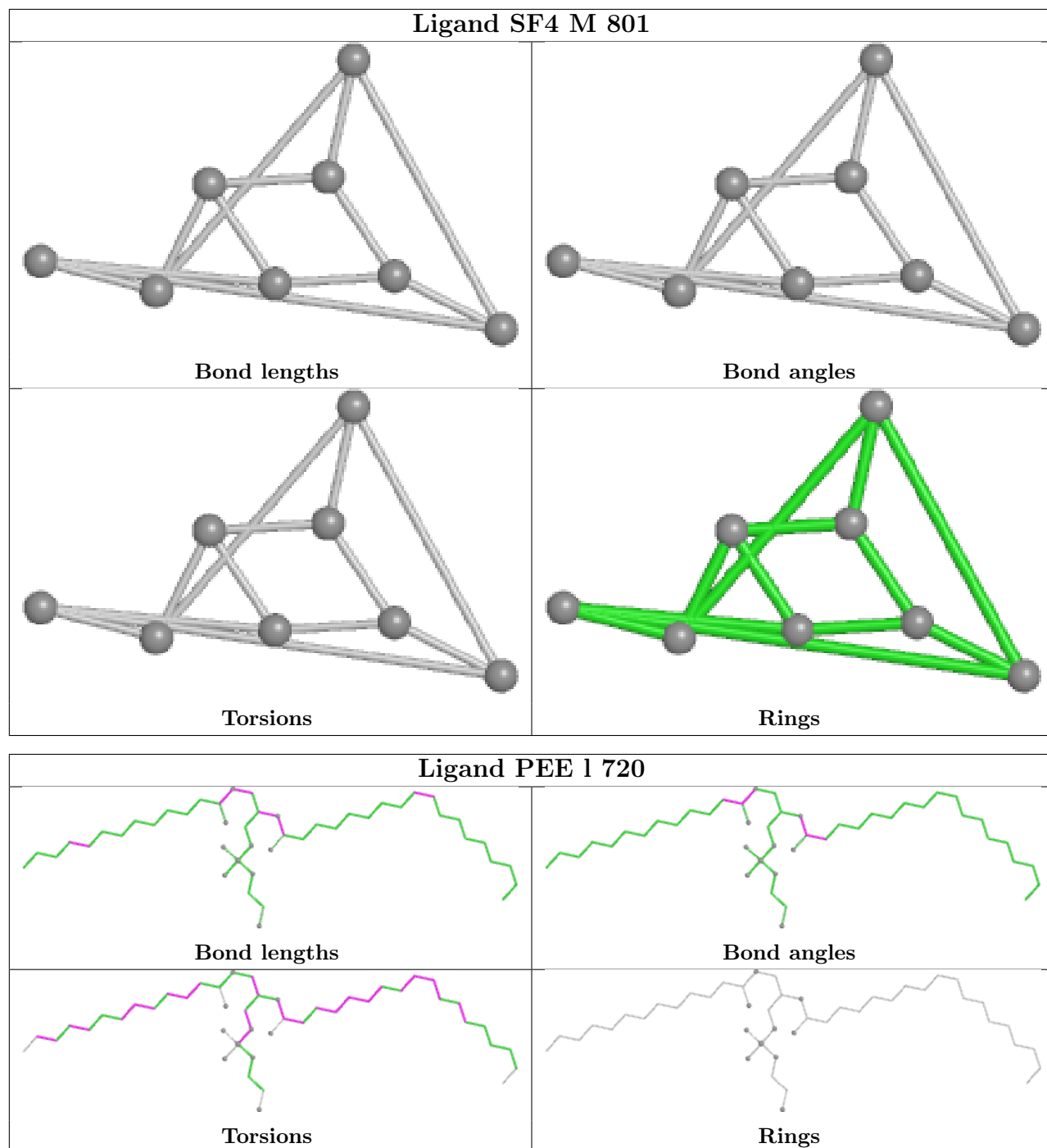
Ligand PEE V 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

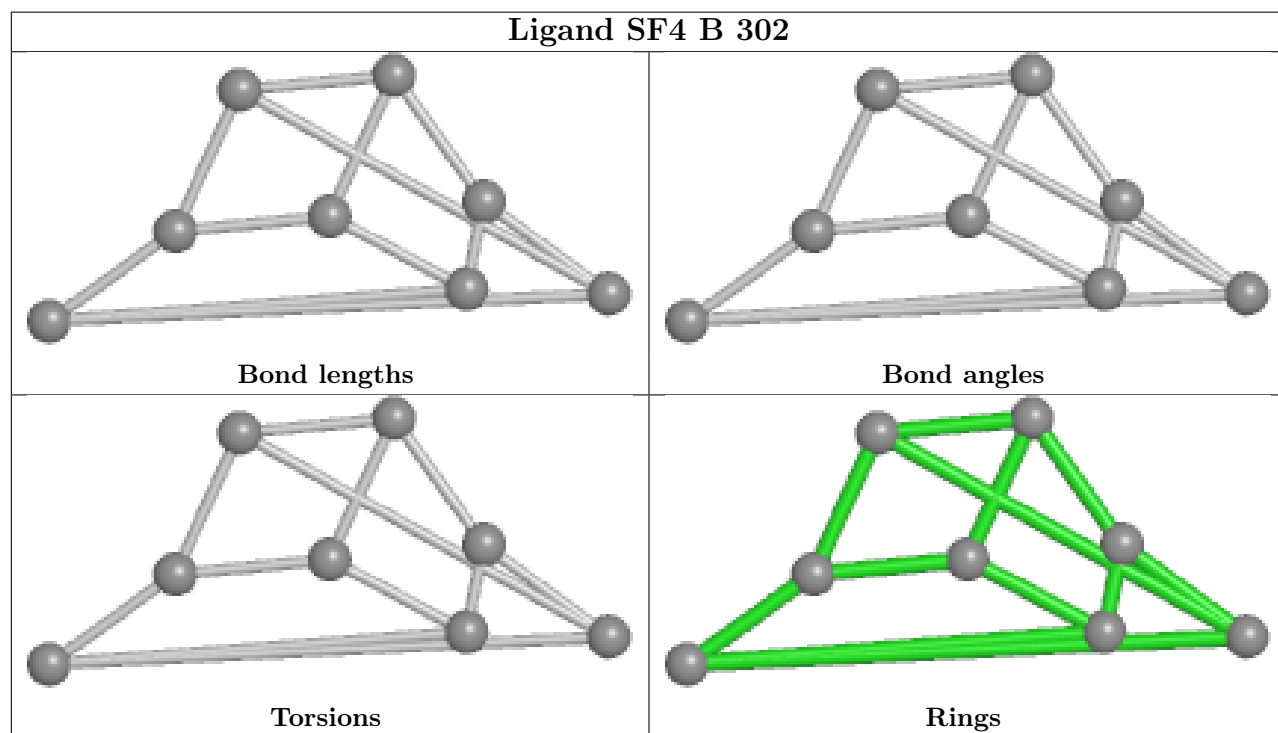
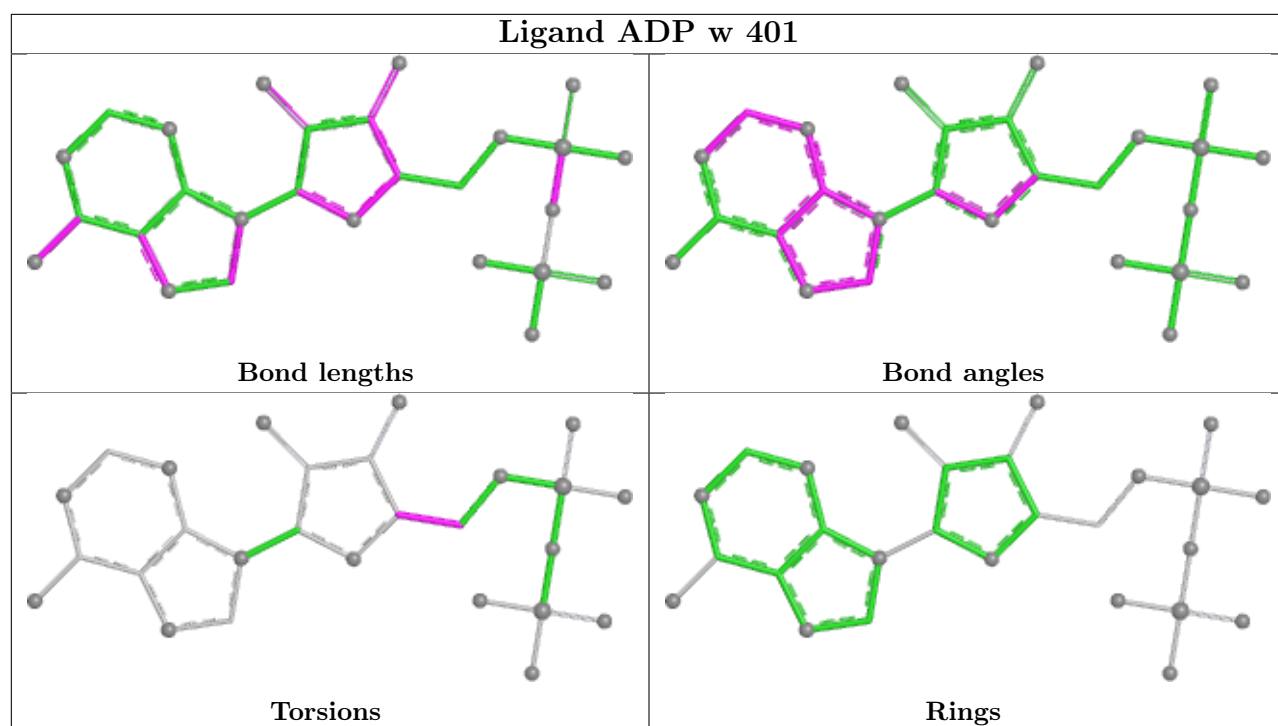
Ligand PEE j 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

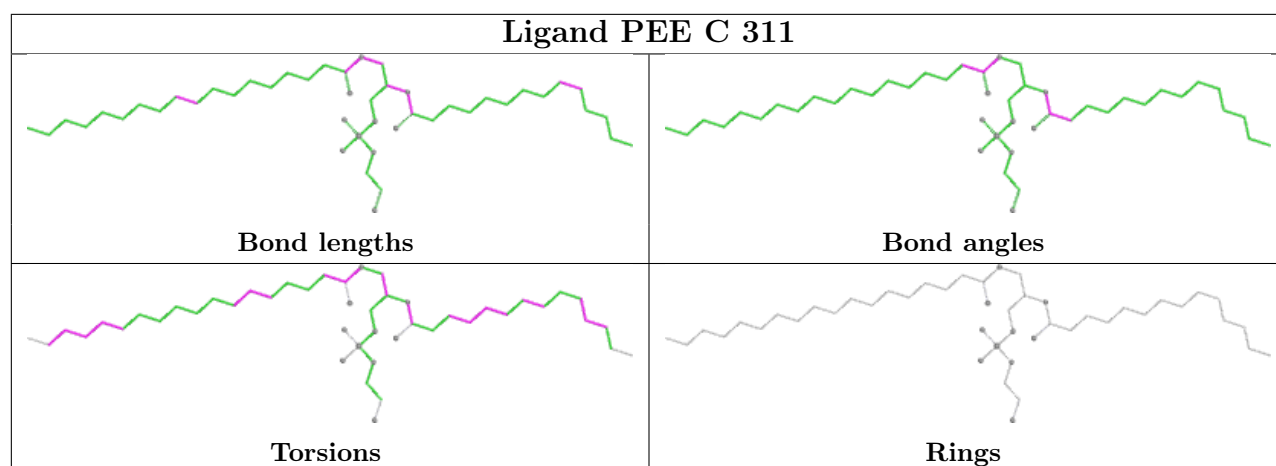
Ligand PLX e 201	
	
Bond lengths	Bond angles
	
Torsions	Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

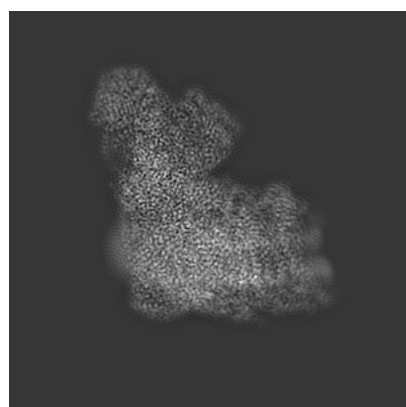
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31645. These allow visual inspection of the internal detail of the map and identification of artifacts.

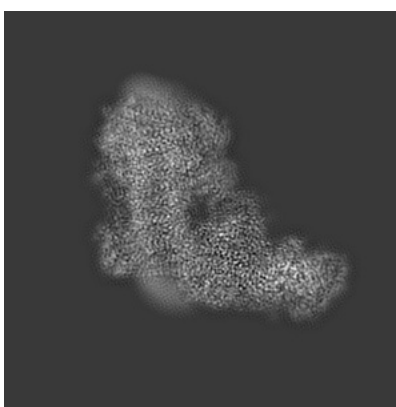
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

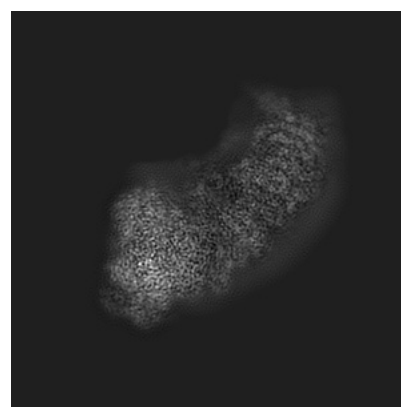
6.1.1 Primary map



X



Y

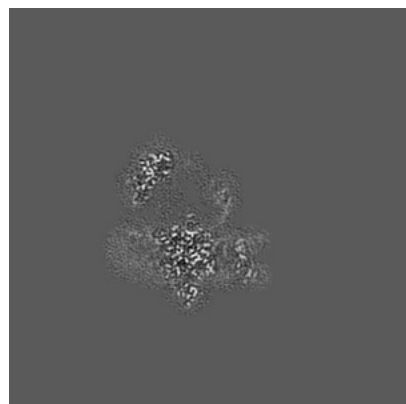


Z

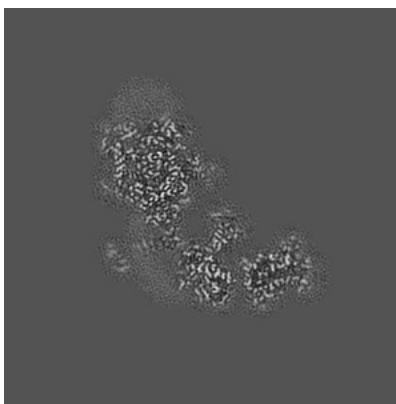
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

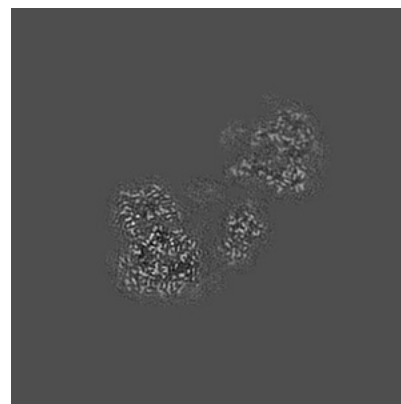
6.2.1 Primary map



X Index: 155



Y Index: 155

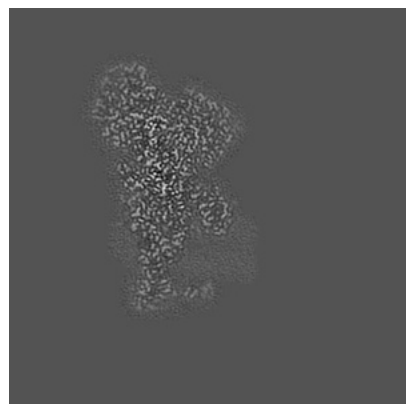


Z Index: 155

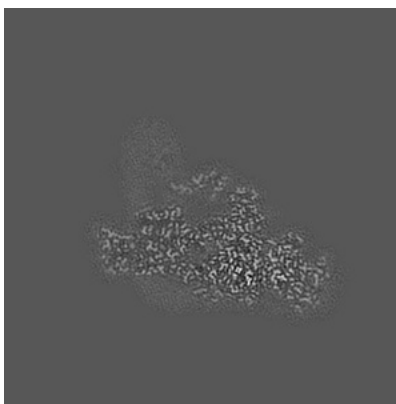
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

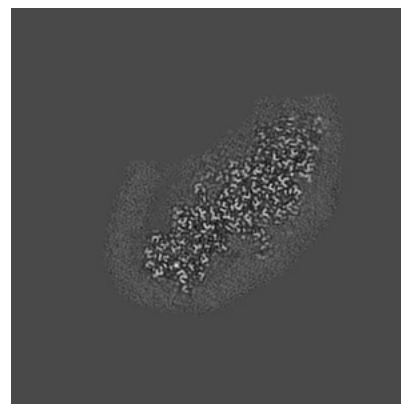
6.3.1 Primary map



X Index: 109



Y Index: 114

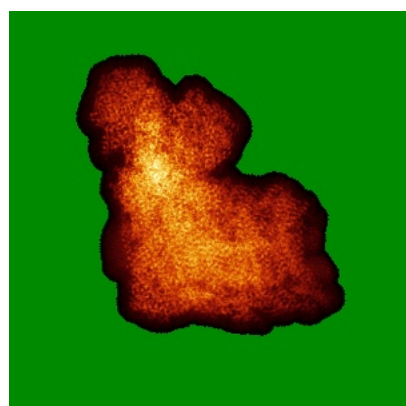


Z Index: 126

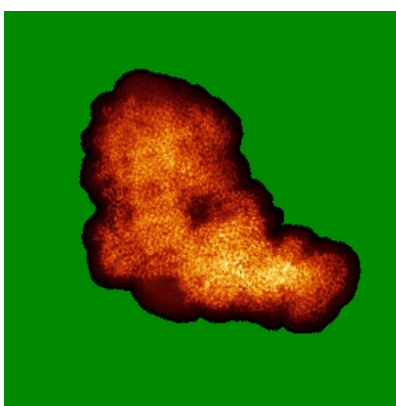
The images above show the largest variance slices of the map in three orthogonal directions.

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

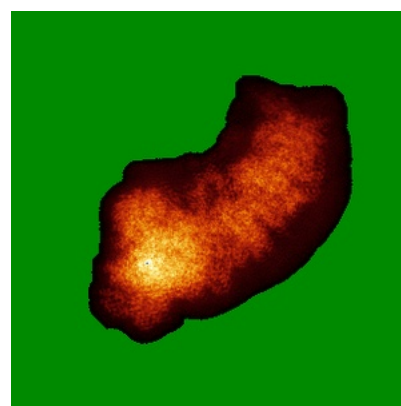
6.4.1 Primary map



X



Y

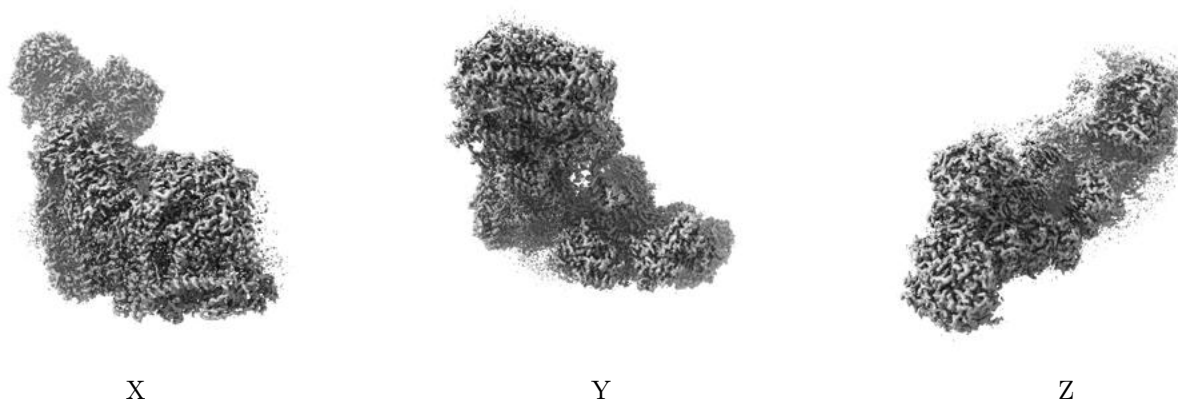


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

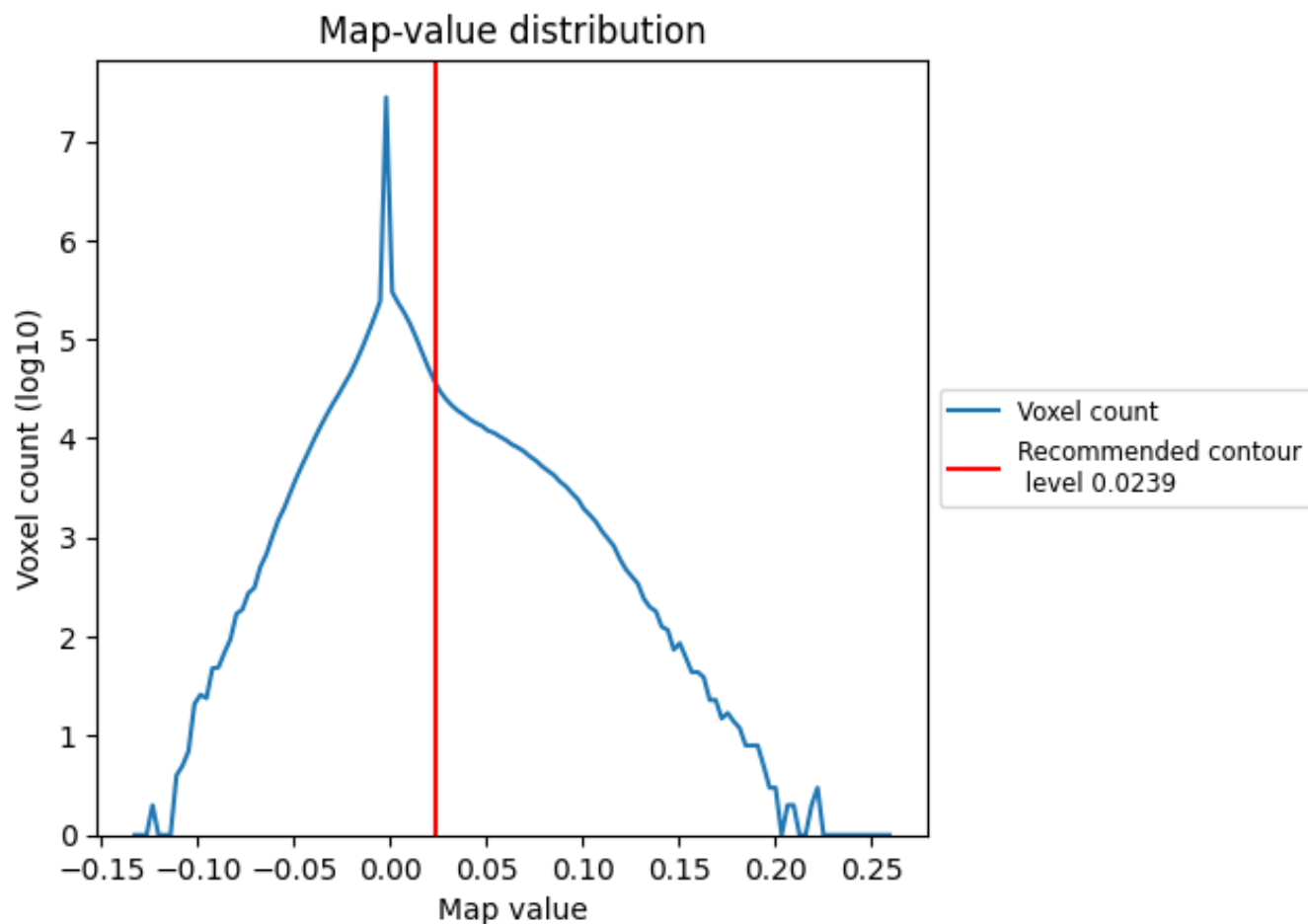
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

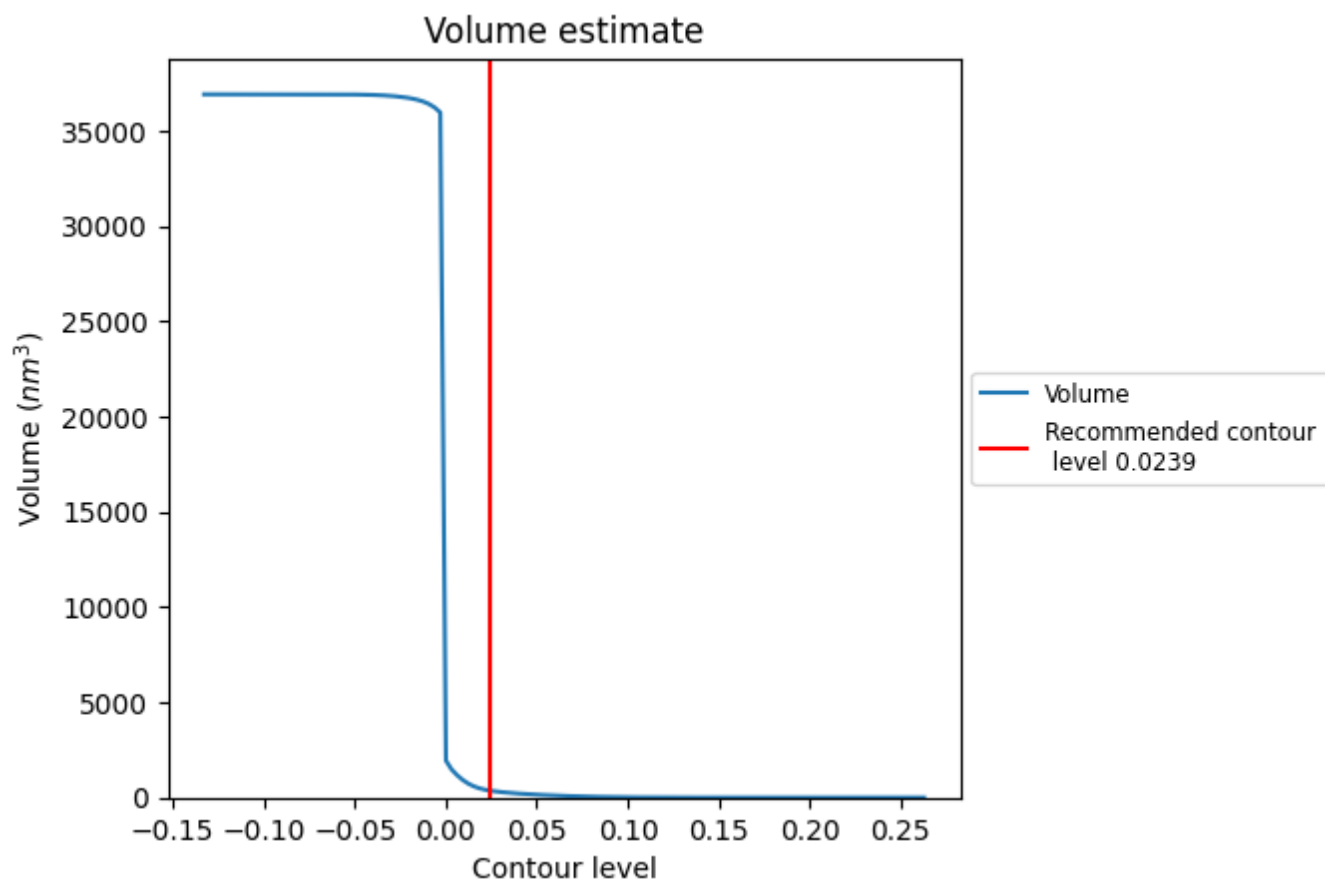
This section contains the results of statistical analysis of the map.

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.

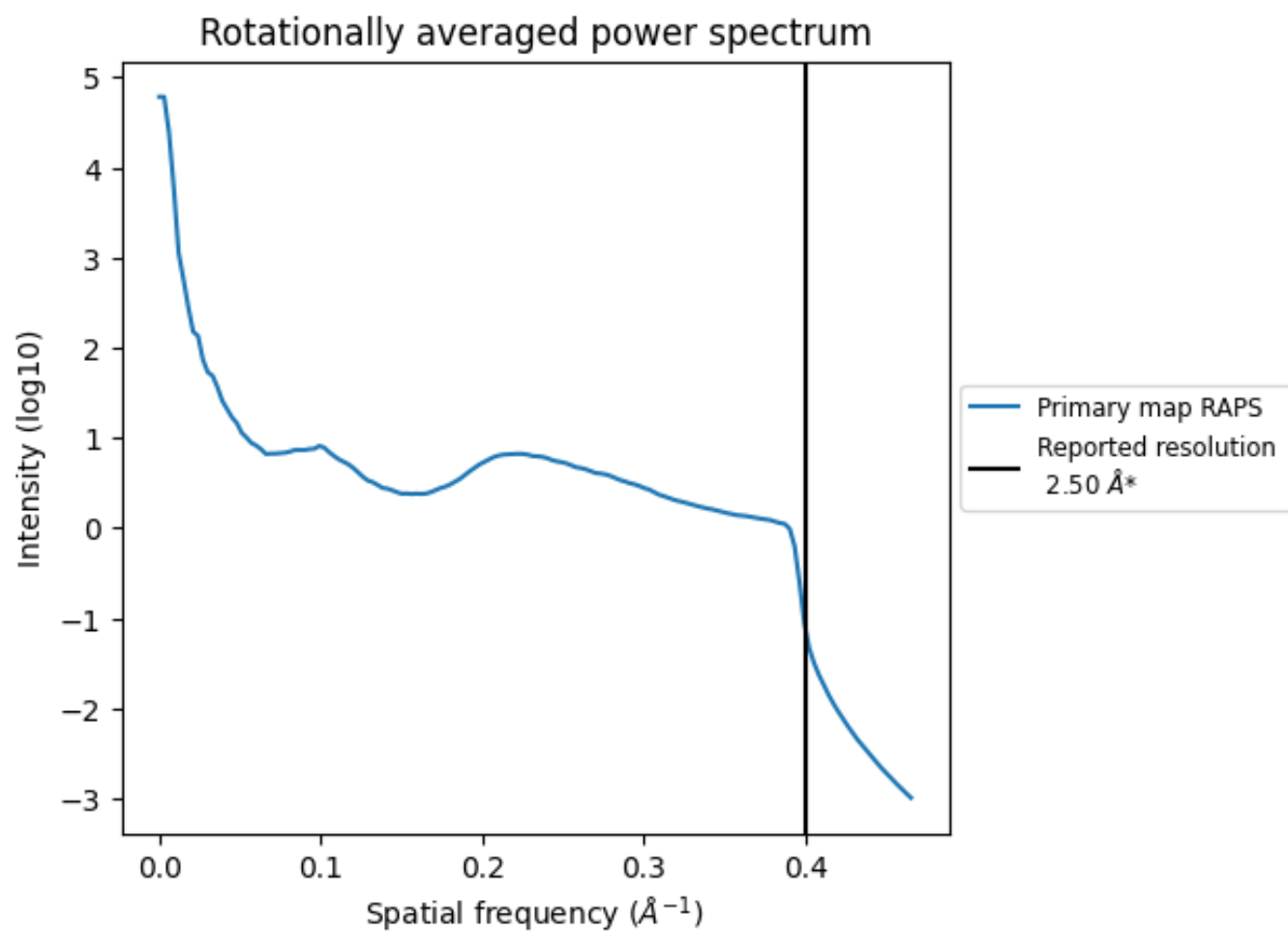
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 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 0.400 Å⁻¹

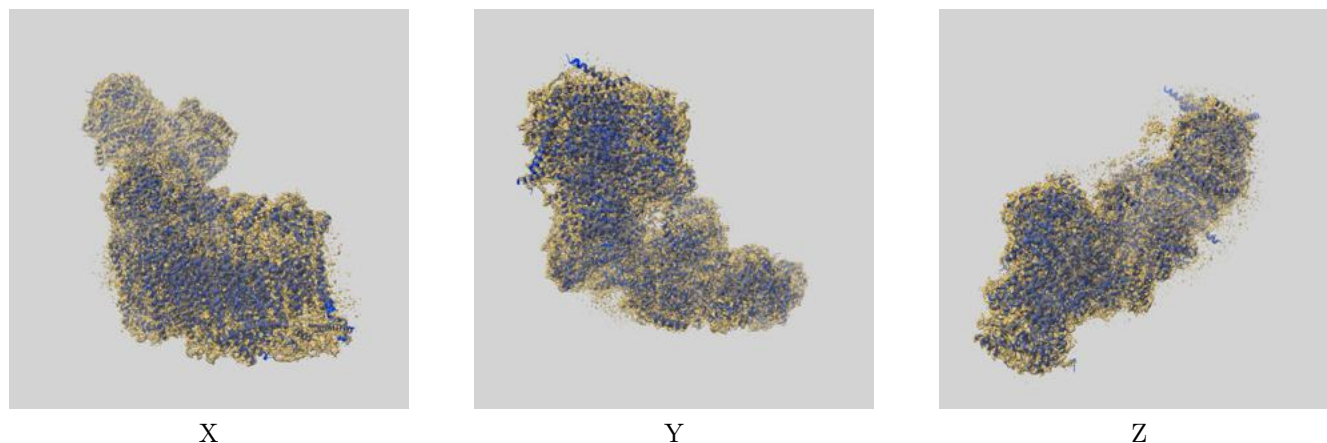
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

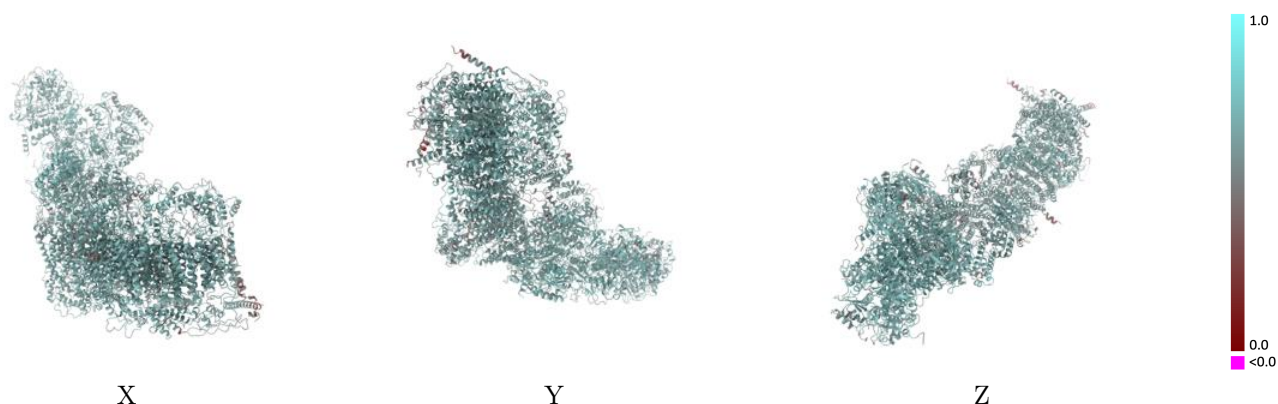
This section contains information regarding the fit between EMDB map EMD-31645 and PDB model 7V2H. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



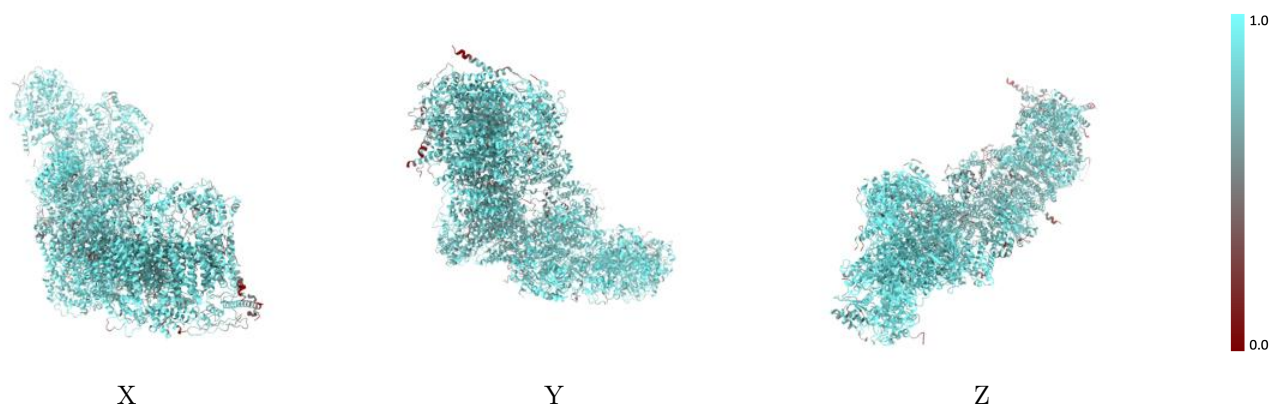
The images above show the 3D surface view of the map at the recommended contour level 0.0239 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



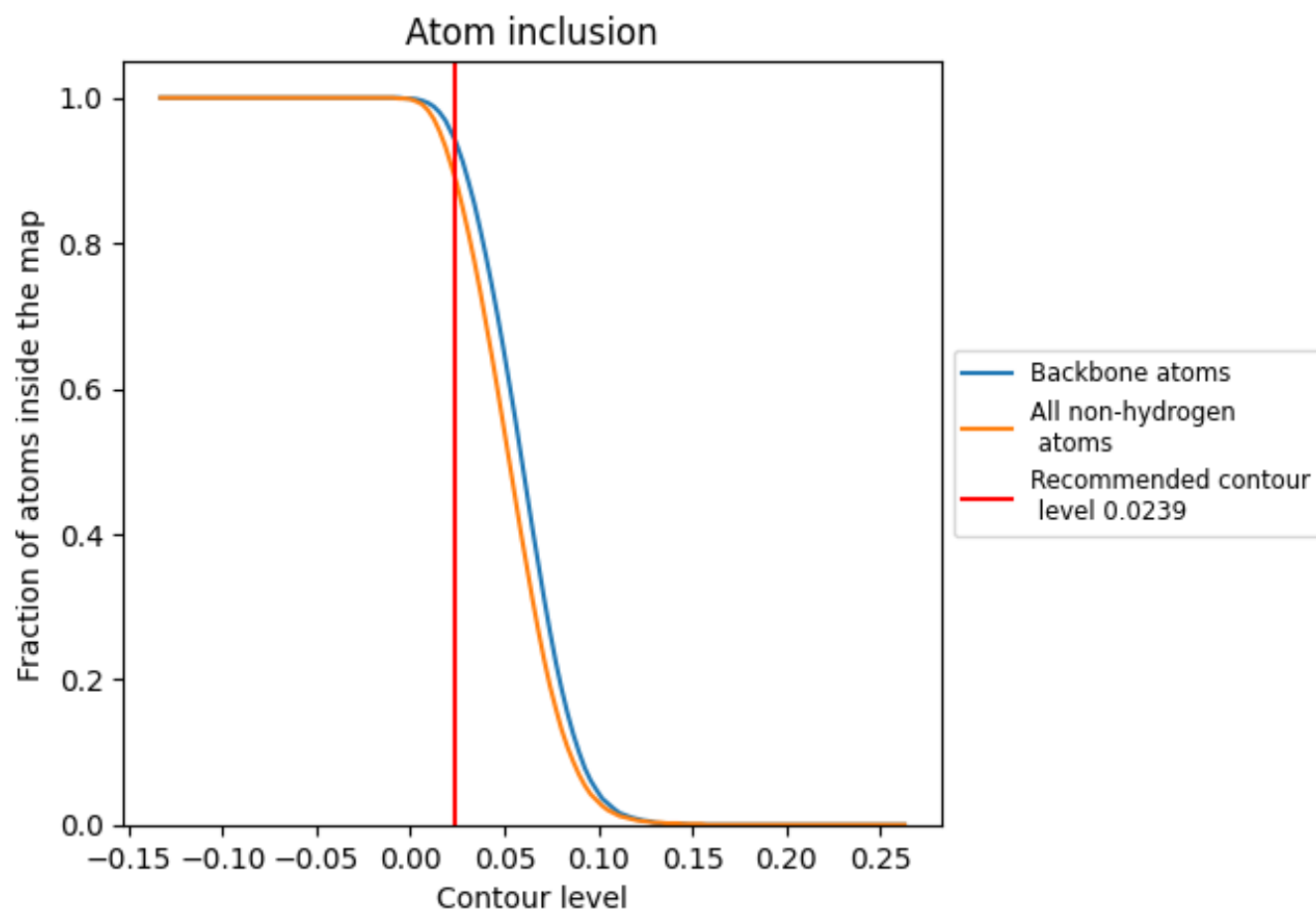
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0239).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.0239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8890	 0.6410
A	 0.9150	 0.6430
B	 0.9680	 0.6870
C	 0.9540	 0.6820
E	 0.9090	 0.6550
F	 0.8370	 0.5950
G	 0.6720	 0.5260
H	 0.9220	 0.6470
I	 0.8200	 0.6210
J	 0.9260	 0.6570
K	 0.8110	 0.5990
L	 0.9100	 0.6670
M	 0.9410	 0.6620
N	 0.8300	 0.6380
O	 0.8560	 0.6180
P	 0.9780	 0.6900
Q	 0.9660	 0.6820
S	 0.9370	 0.6590
T	 0.8640	 0.6490
U	 0.8720	 0.6240
V	 0.7470	 0.6000
W	 0.8900	 0.6360
X	 0.7990	 0.5990
Y	 0.7140	 0.5590
Z	 0.6560	 0.5330
a	 0.8900	 0.6380
b	 0.8000	 0.5910
c	 0.8370	 0.6180
d	 0.8180	 0.6040
e	 0.8220	 0.6060
f	 0.7050	 0.5650
g	 0.9250	 0.6500
h	 0.8910	 0.6280
i	 0.9490	 0.6710
j	 0.8930	 0.6580



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Chain	Atom inclusion	Q-score
k	 0.9000	 0.6550
l	 0.8810	 0.6420
m	 0.8330	 0.6190
n	 0.6950	 0.5680
o	 0.8620	 0.6310
p	 0.8610	 0.6180
r	 0.9590	 0.6670
s	 0.9620	 0.6720
u	 0.9030	 0.6390
v	 0.7100	 0.5470
w	 0.8680	 0.6250