



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 7V2E / pdb_00007v2e
EMDB ID : EMD-31643
Title : Active state complex I from Q10-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-08
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

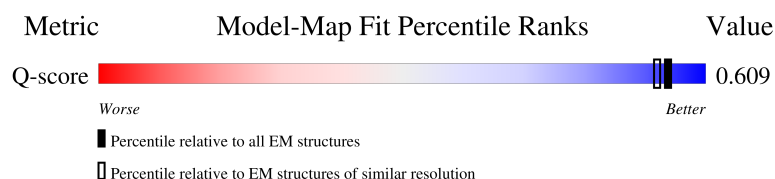
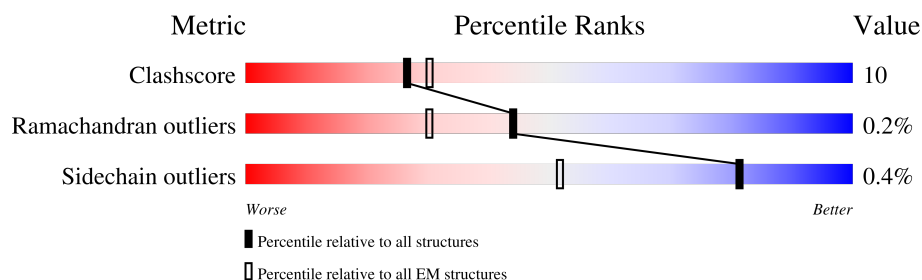
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

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

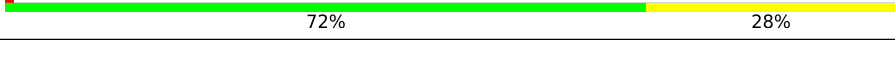
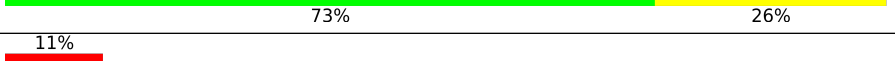
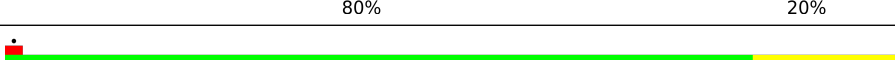
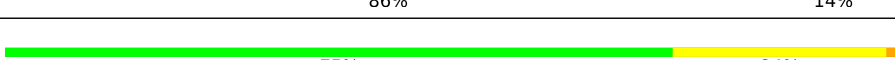
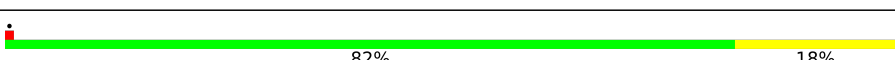
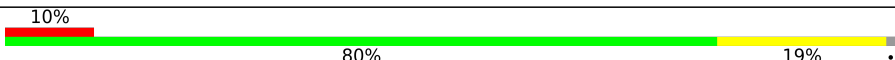
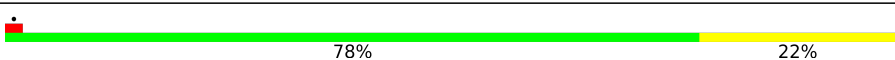
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	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
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-
45	SF4	M	802	-	-	X	-
54	FES	O	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 68244 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
			704	454	104	141	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
			1167	752	200	206	9		

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

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

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

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

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

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

- Molecule 25 is a protein called 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	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			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
			1059	658	202	189	10		

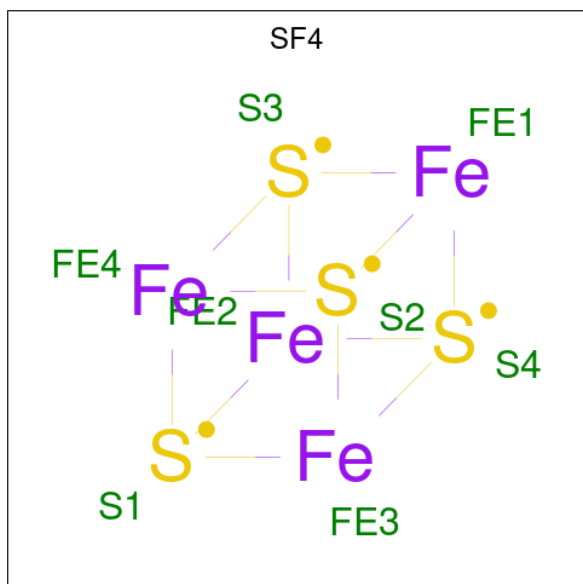
There is a discrepancy between the modelled and reference sequences:

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	

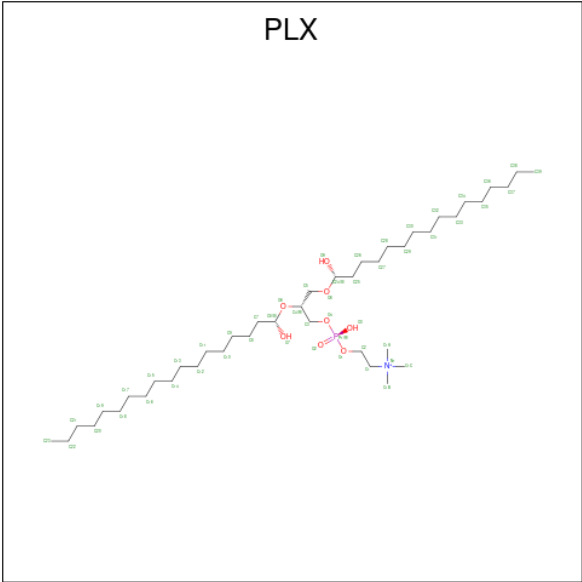
- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).





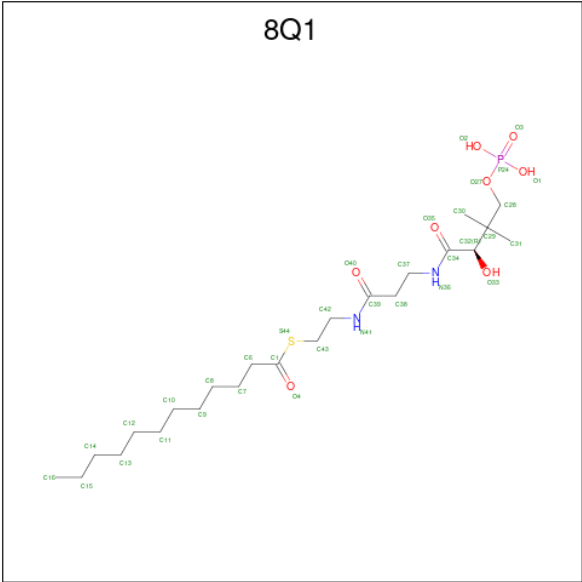
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31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

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



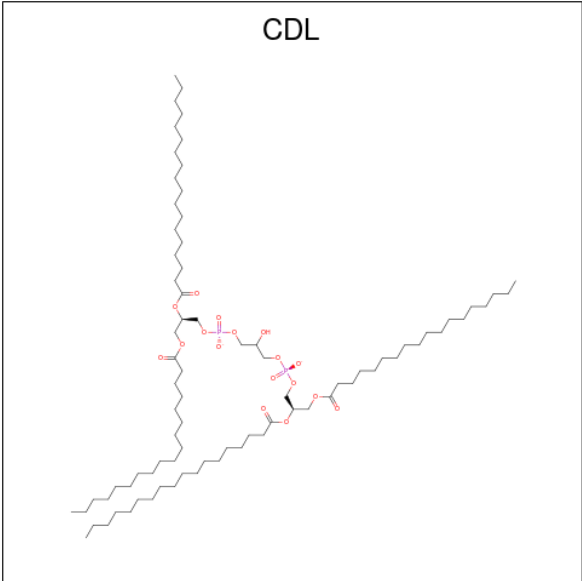
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is 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 CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

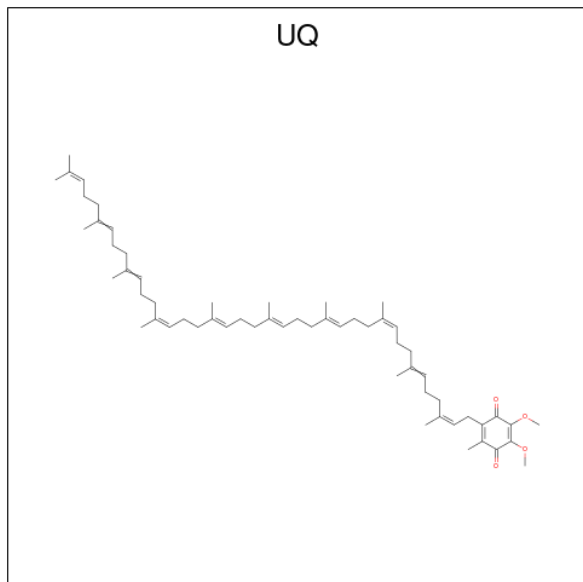
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Mol	Chain	Residues	Atoms				AltConf
51	V	1	Total 94	C 75	O 17	P 2	0
51	V	1	Total 100	C 81	O 17	P 2	0
51	a	1	Total 100	C 81	O 17	P 2	0
51	k	1	Total 100	C 81	O 17	P 2	0
51	l	1	Total 99	C 80	O 17	P 2	0
51	l	1	Total 100	C 81	O 17	P 2	0
51	n	1	Total 55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

- # NDP

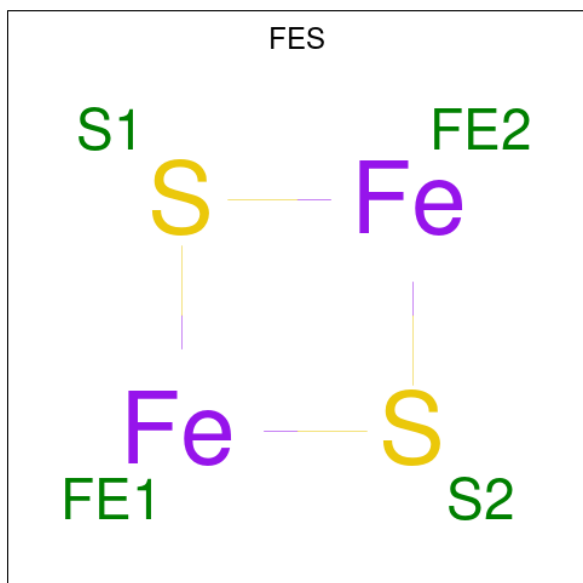
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total 48	C 21	N 7	O 17	P 3	0

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



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

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



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

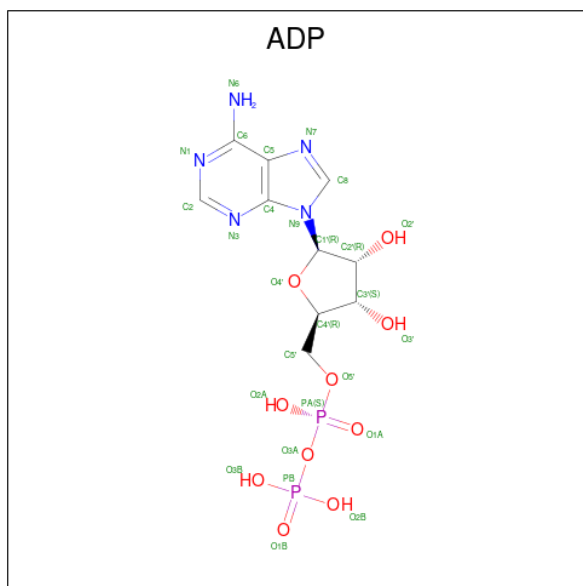
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

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

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

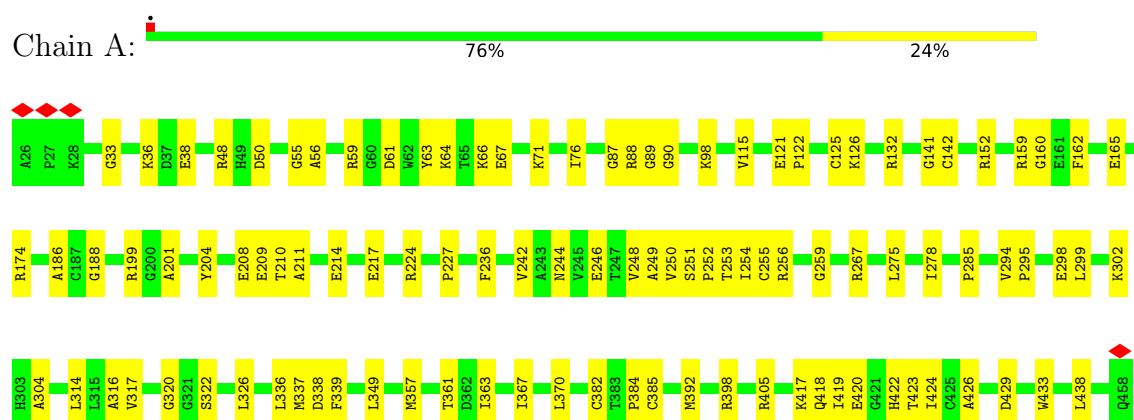


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

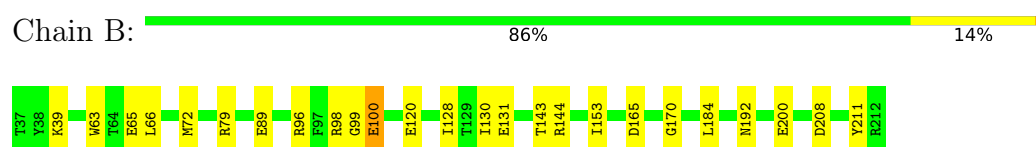
3 Residue-property plots

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

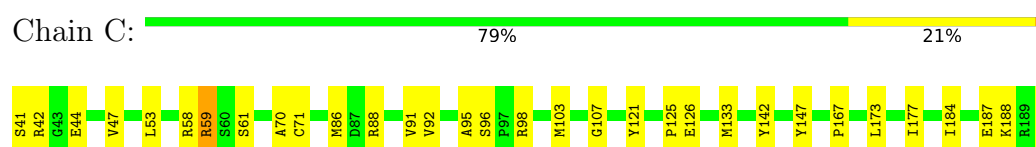
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



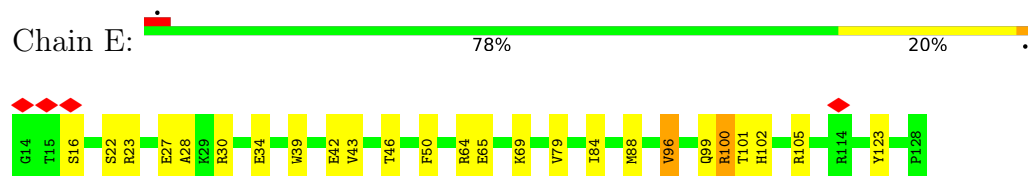
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



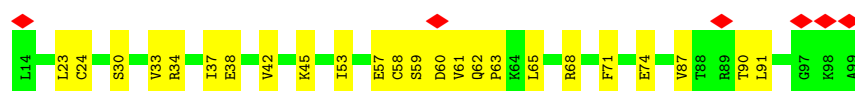
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



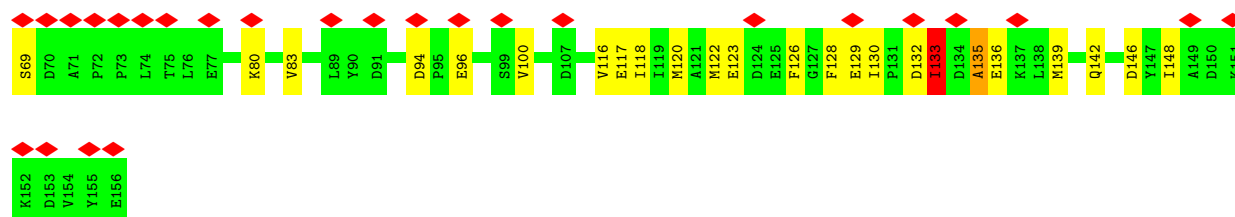
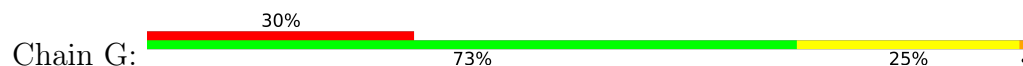
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



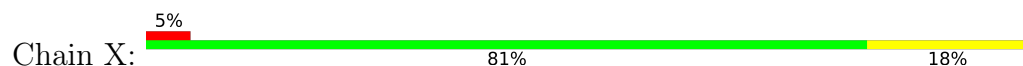
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



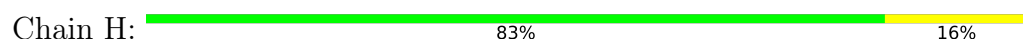
- Molecule 6: Acyl carrier protein, mitochondrial



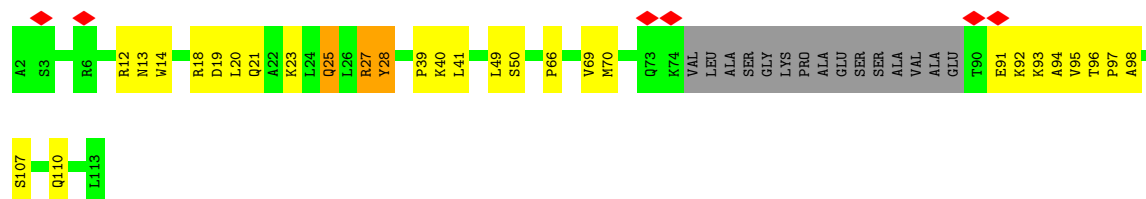
- Molecule 6: Acyl carrier protein, mitochondrial



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

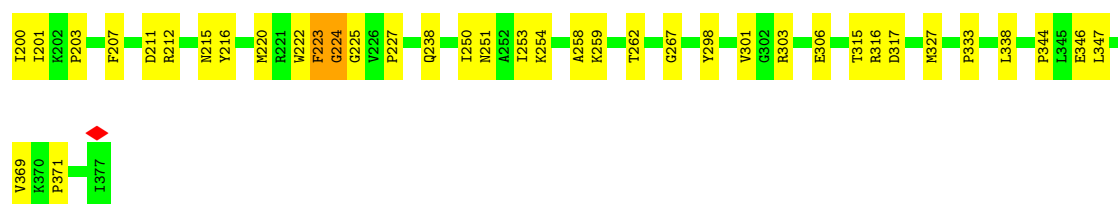


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

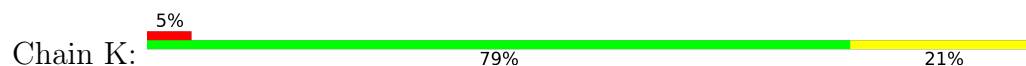


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

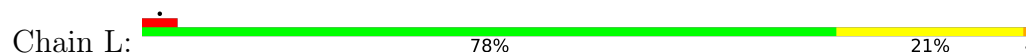




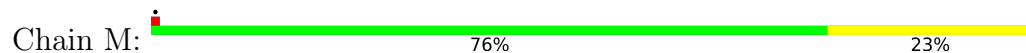
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



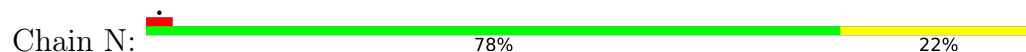
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



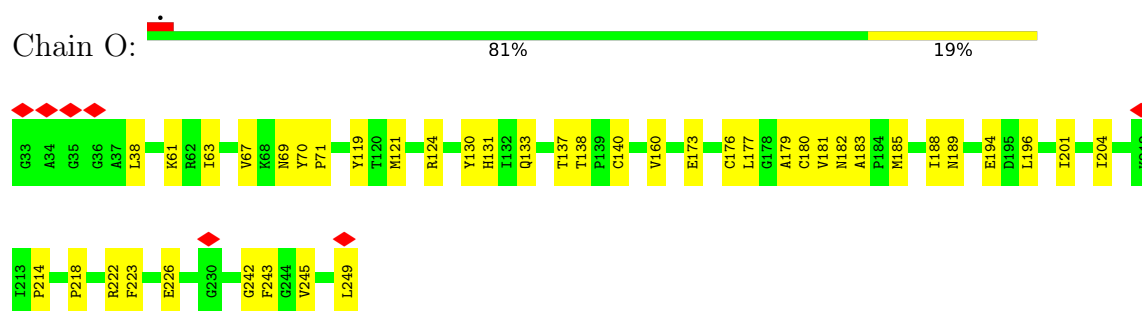
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



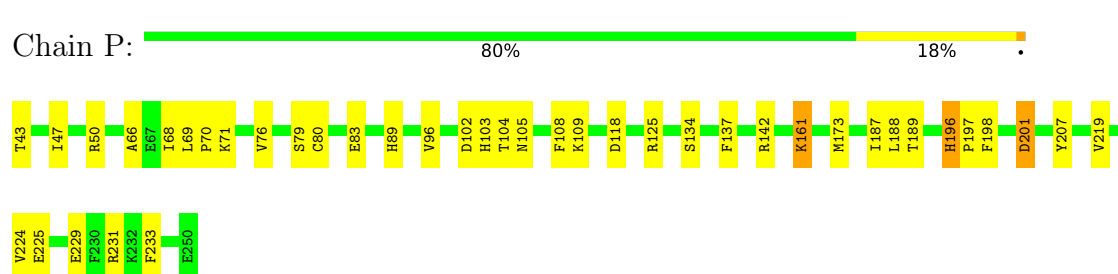
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



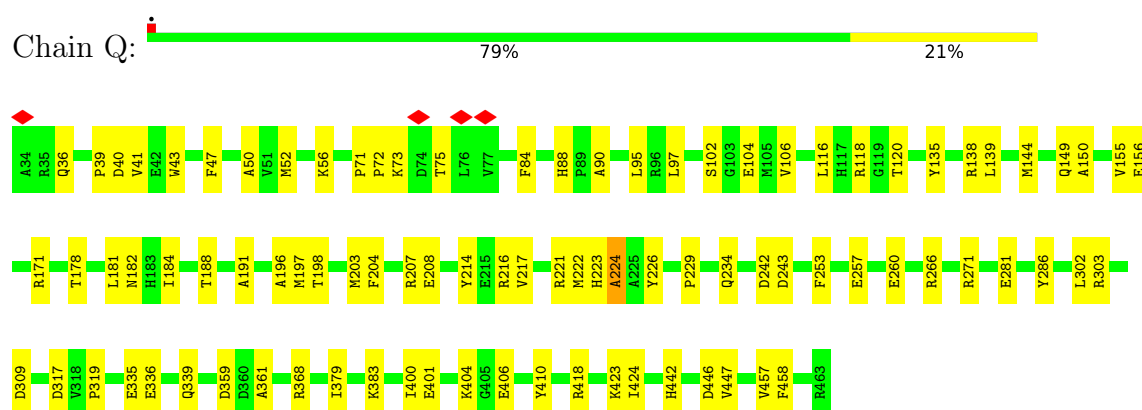
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



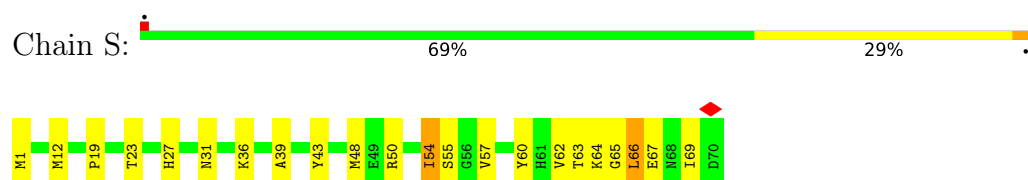
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



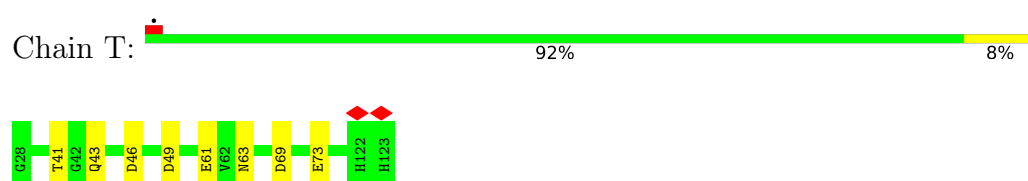
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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

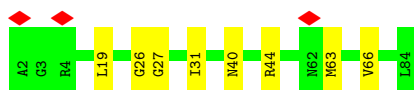


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



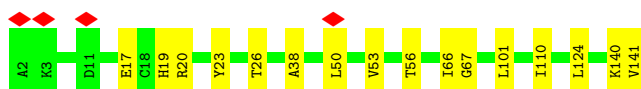
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  90% 10%



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

Chain V:  89% 11%



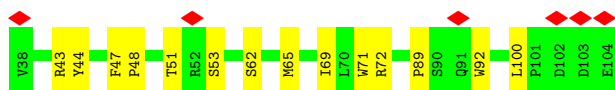
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  82% 18%



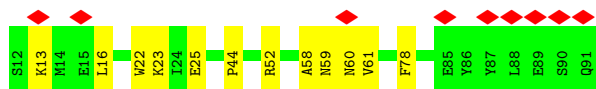
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  9% 79% 21%



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

Chain Z:  11% 85% 15%



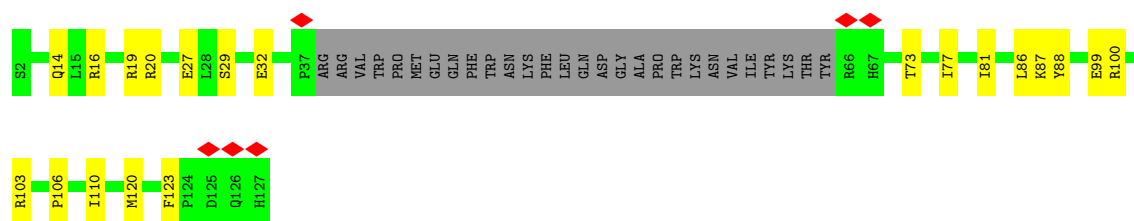
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  83% 17%

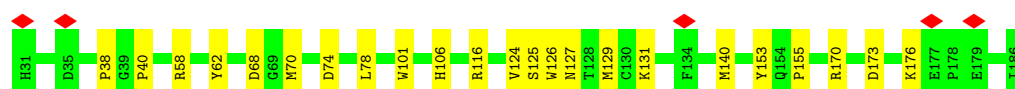
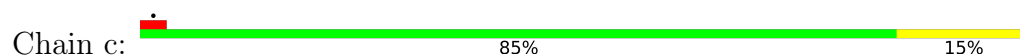


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

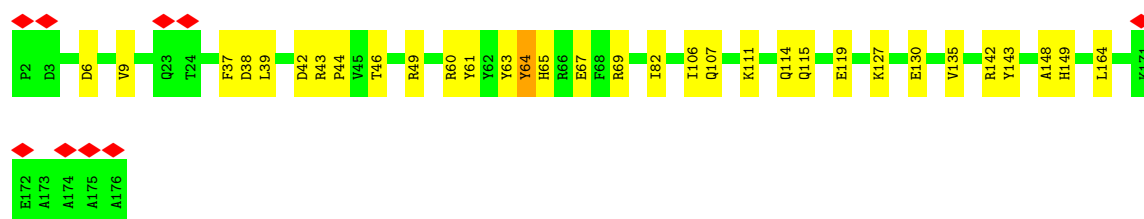
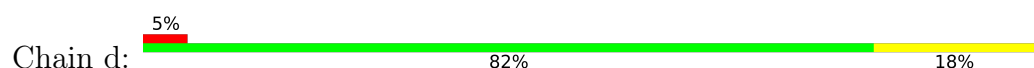
Chain b:  5% 62% 16% 22%



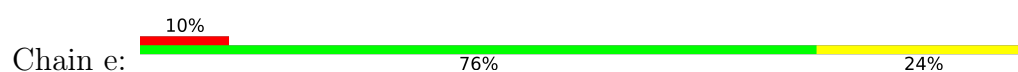
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



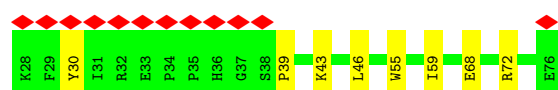
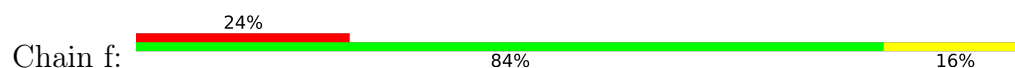
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



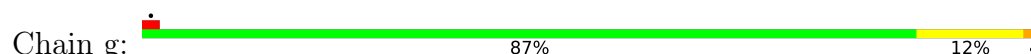
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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



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



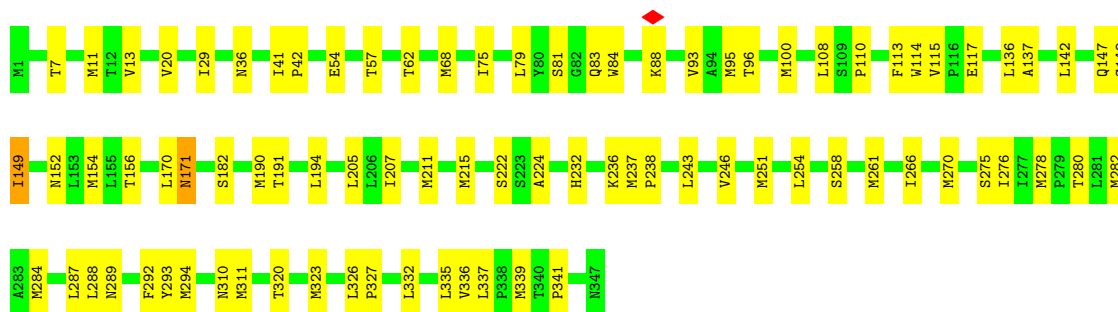
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  87% 12%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  76% 24%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  72% 28%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

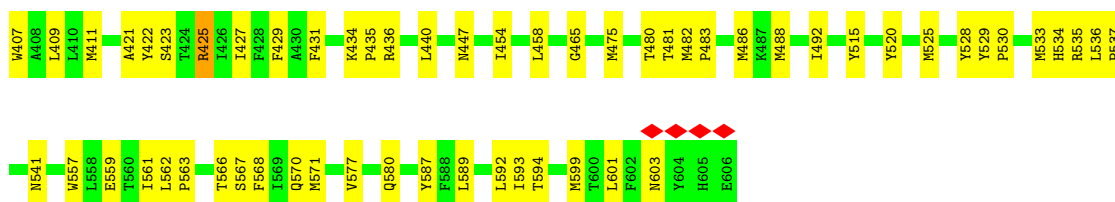
Chain k:  61% 37%



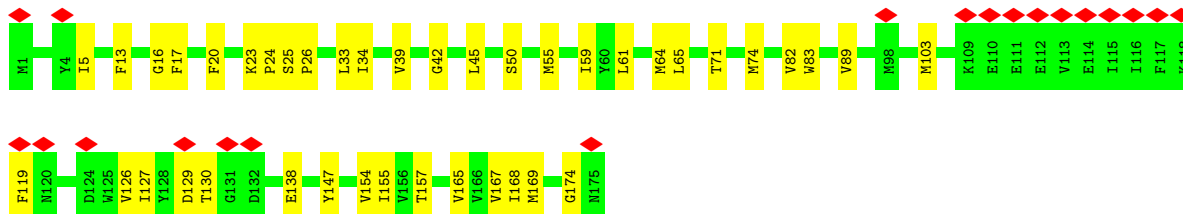
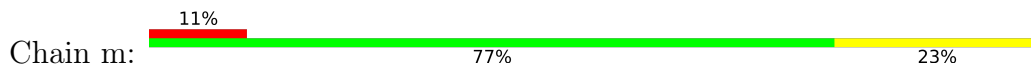
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  73% 26%

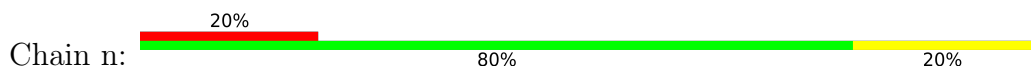




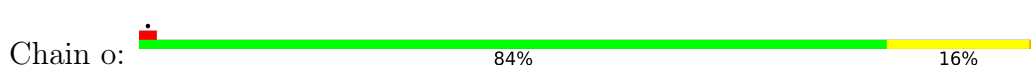
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



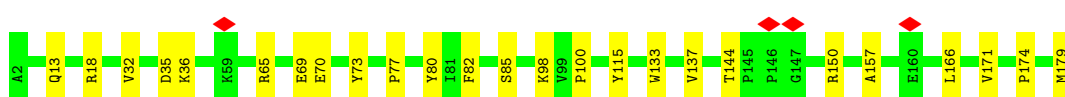
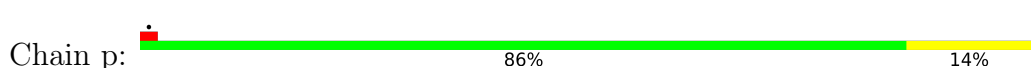
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



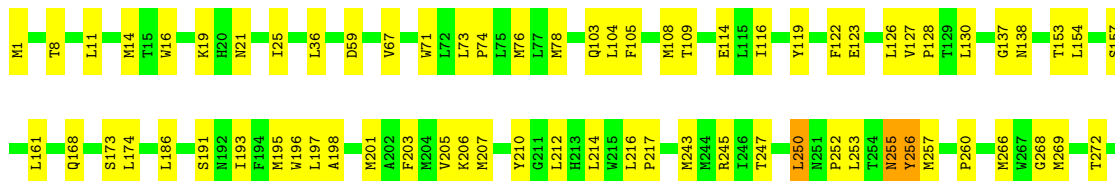
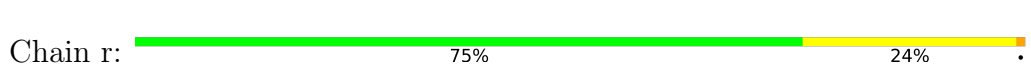
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

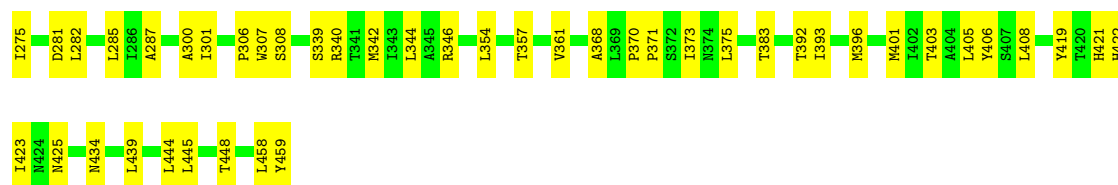


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



• Molecule 40: NADH-ubiquinone oxidoreductase chain 4





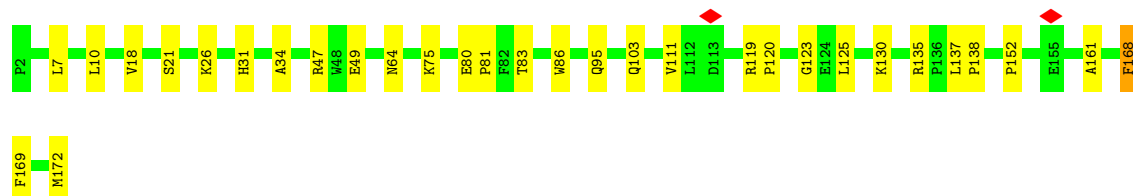
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 75% 25%



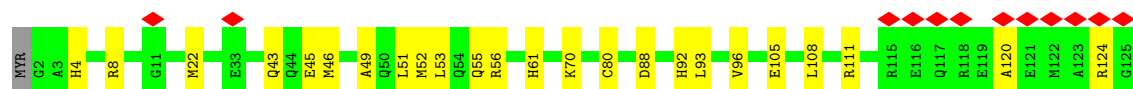
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 82% 18%



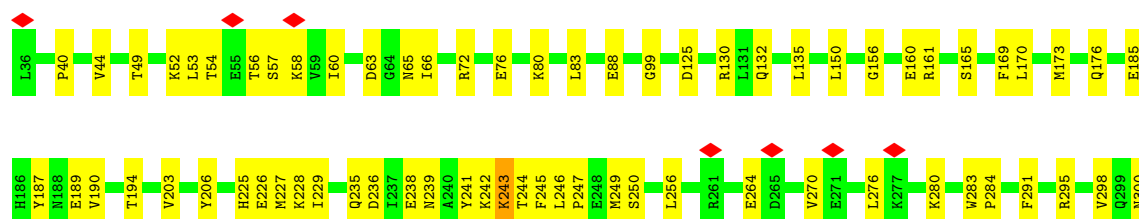
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 10% 80% 19%



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

Chain w: 78% 22%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152604	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	0.205	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0258	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	0/3406	0.41	1/4603 (0.0%)
2	B	0.21	0/1443	0.35	0/1952
3	C	0.22	0/1279	0.39	0/1730
4	E	0.23	0/995	0.41	0/1340
5	F	0.22	0/698	0.46	0/940
6	G	0.22	0/705	0.62	4/956 (0.4%)
6	X	0.18	0/716	0.58	3/968 (0.3%)
7	H	0.18	0/929	0.42	0/1258
8	I	0.28	0/798	0.60	1/1079 (0.1%)
9	J	0.19	0/2828	0.38	0/3834
10	K	0.15	0/377	0.29	0/509
11	L	0.21	0/1039	0.50	3/1403 (0.2%)
12	M	0.26	0/5384	0.58	10/7295 (0.1%)
13	N	0.16	0/1245	0.30	0/1694
14	O	0.19	0/1711	0.48	2/2328 (0.1%)
15	P	0.27	0/1789	0.61	4/2436 (0.2%)
16	Q	0.22	0/3538	0.43	1/4796 (0.0%)
17	S	0.26	0/581	0.64	1/781 (0.1%)
18	T	0.19	0/755	0.37	0/1018
19	U	0.15	0/664	0.30	0/912
20	V	0.17	0/1042	0.41	0/1411
21	W	0.18	0/1198	0.40	0/1617
22	Y	0.14	0/610	0.33	0/836
23	Z	0.12	0/660	0.30	0/892
24	a	0.19	0/1184	0.42	0/1603
25	b	0.19	0/844	0.40	0/1149
26	c	0.20	0/1371	0.42	0/1875
27	d	0.18	0/1494	0.43	2/2015 (0.1%)
28	e	0.15	0/891	0.33	0/1210
29	f	0.19	0/386	0.50	0/523
30	g	0.17	0/1031	0.38	1/1394 (0.1%)
31	h	0.23	0/889	0.59	2/1190 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.25	0/2773	0.52	3/3768 (0.1%)
33	j	0.20	0/938	0.36	0/1281
34	k	0.31	0/759	0.64	3/1029 (0.3%)
35	l	0.21	0/4929	0.43	1/6704 (0.0%)
36	m	0.21	0/1328	0.48	0/1804
37	n	0.14	0/491	0.33	0/663
38	o	0.18	0/1092	0.44	3/1481 (0.2%)
39	p	0.14	0/1590	0.32	0/2155
40	r	0.22	0/3723	0.48	3/5078 (0.1%)
41	s	0.26	0/2581	0.59	4/3529 (0.1%)
42	u	0.19	0/1436	0.48	0/1938
43	v	0.14	0/1083	0.33	0/1448
44	w	0.17	0/2642	0.41	3/3580 (0.1%)
All	All	0.21	0/67845	0.46	55/92005 (0.1%)

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
1	A	0	1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	28	TYR	N-CA-C	8.18	119.98	111.14
41	s	206	GLU	N-CA-C	8.06	120.15	111.36
12	M	74	ASN	N-CA-C	8.04	120.12	111.36
41	s	39	VAL	N-CA-C	7.72	118.52	110.72
31	h	55	GLU	N-CA-C	6.97	118.96	111.36
15	P	109	LYS	N-CA-C	6.90	118.80	111.28
12	M	166	GLY	CA-C-N	6.85	126.66	119.05
12	M	166	GLY	C-N-CA	6.85	126.66	119.05
34	k	51	THR	N-CA-C	-6.83	98.07	109.07
12	M	406	ASN	CA-C-N	6.68	126.47	119.05
12	M	406	ASN	C-N-CA	6.68	126.47	119.05
35	l	68	TRP	N-CA-C	6.45	118.19	111.03
27	d	142	ARG	N-CA-C	6.44	118.09	111.14
6	X	135	ALA	N-CA-C	6.41	118.27	111.28
40	r	421	HIS	N-CA-C	6.41	118.26	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	250	LEU	N-CA-C	6.40	118.25	111.28
11	L	166	TRP	N-CA-C	6.37	118.30	111.36
15	P	196	HIS	CA-C-N	6.35	126.10	119.05
15	P	196	HIS	C-N-CA	6.35	126.10	119.05
40	r	422	HIS	N-CA-C	6.33	118.18	111.28
38	o	127	ILE	N-CA-C	6.07	116.81	110.62
6	X	130	ILE	CA-C-N	5.91	125.86	119.78
6	X	130	ILE	C-N-CA	5.91	125.86	119.78
6	G	132	ASP	CA-C-N	5.87	132.53	121.97
6	G	132	ASP	C-N-CA	5.87	132.53	121.97
14	O	70	TYR	CA-C-N	5.83	125.78	119.78
14	O	70	TYR	C-N-CA	5.83	125.78	119.78
31	h	45	HIS	N-CA-C	5.78	118.72	110.10
12	M	371	VAL	N-CA-C	5.77	116.24	108.17
34	k	53	PHE	N-CA-C	-5.67	99.48	108.73
6	G	135	ALA	N-CA-C	-5.62	106.97	113.88
30	g	3	MET	N-CA-C	5.58	117.36	111.28
15	P	102	ASP	N-CA-C	5.57	120.14	113.23
12	M	173	MET	N-CA-C	5.51	119.10	112.38
1	A	248	VAL	N-CA-C	5.51	116.28	110.72
16	Q	102	SER	N-CA-C	-5.51	98.24	107.99
34	k	50	ASN	N-CA-C	5.43	117.20	111.28
41	s	217	ALA	N-CA-C	5.39	117.20	108.08
17	S	54	ILE	N-CA-C	5.37	116.10	110.62
44	w	244	THR	N-CA-C	5.37	120.07	112.93
32	i	113	PHE	N-CA-C	5.36	117.12	111.28
11	L	170	THR	N-CA-C	5.28	118.82	112.38
38	o	53	ASP	CA-C-N	5.28	124.91	119.05
38	o	53	ASP	C-N-CA	5.28	124.91	119.05
41	s	217	ALA	CB-CA-C	-5.23	110.57	116.63
32	i	115	VAL	N-CA-C	5.22	118.62	112.35
44	w	225	HIS	N-CA-C	5.20	116.94	111.28
11	L	172	VAL	N-CA-C	5.17	115.69	110.05
12	M	612	PRO	CA-C-N	5.14	124.90	119.76
12	M	612	PRO	C-N-CA	5.14	124.90	119.76
6	G	133	ILE	N-CA-CB	5.11	119.67	111.23
12	M	168	LEU	N-CA-C	5.11	116.85	111.28
32	i	115	VAL	CB-CA-C	-5.08	107.35	114.00
44	w	243	LYS	N-CA-C	5.07	116.88	111.36
27	d	143	TYR	N-CA-C	5.02	121.10	114.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	86	0
2	B	1412	0	1363	29	0
3	C	1248	0	1254	30	0
4	E	971	0	975	21	0
5	F	687	0	700	23	0
6	G	693	0	671	17	0
6	X	704	0	695	12	0
7	H	910	0	950	13	0
8	I	780	0	808	27	0
9	J	2751	0	2773	46	0
10	K	366	0	338	9	0
11	L	1016	0	1016	22	0
12	M	5296	0	5328	124	0
13	N	1204	0	1162	20	0
14	O	1671	0	1674	41	0
15	P	1738	0	1693	43	0
16	Q	3459	0	3396	79	0
17	S	566	0	561	20	0
18	T	741	0	702	8	0
19	U	643	0	642	6	0
20	V	1021	0	1025	18	0
21	W	1167	0	1155	22	0
22	Y	584	0	529	11	0
23	Z	641	0	620	10	0
24	a	1151	0	1164	25	0
25	b	819	0	835	19	0
26	c	1315	0	1208	22	0
27	d	1461	0	1429	32	0
28	e	867	0	817	19	0
29	f	378	0	356	8	0
30	g	1000	0	994	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	h	867	0	873	13	0
32	i	2710	0	2874	78	0
33	j	914	0	951	38	0
34	k	748	0	799	39	0
35	l	4800	0	4939	149	0
36	m	1295	0	1263	43	0
37	n	479	0	486	13	0
38	o	1062	0	1072	20	0
39	p	1534	0	1470	24	0
40	r	3631	0	3839	99	0
41	s	2508	0	2607	78	0
42	u	1398	0	1374	30	0
43	v	1059	0	1029	20	0
44	w	2582	0	2531	48	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	3	0
45	M	16	0	0	4	0
46	A	31	0	19	8	0
47	A	44	0	27	7	0
48	B	51	0	82	6	0
48	C	47	0	71	10	0
48	Q	47	0	71	9	0
48	W	41	0	59	11	0
48	b	46	0	69	11	0
48	j	92	0	141	16	0
48	l	91	0	136	21	0
48	r	51	0	82	9	0
49	C	52	0	88	18	0
49	J	52	0	88	2	0
49	a	52	0	88	0	0
49	g	52	0	88	4	0
49	j	52	0	88	3	0
49	r	104	0	176	8	0
50	G	35	0	0	0	0
50	X	35	0	0	4	0
51	I	51	0	46	3	0
51	V	194	0	294	11	0
51	a	100	0	156	11	0
51	k	100	0	156	13	0
51	l	199	0	307	28	0
51	n	55	0	54	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	r	100	0	156	9	0
51	s	89	0	125	8	0
52	J	48	0	26	1	0
53	J	33	0	39	6	0
53	s	38	0	47	5	0
54	M	4	0	0	0	0
54	O	4	0	0	4	0
55	M	1	0	0	0	0
56	T	1	0	0	0	0
57	w	27	0	11	1	0
All	All	68244	0	69022	1372	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 10.

All (1372) 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)
50:X:201:8Q1:C11	39:p:70:GLU:OE1	1.72	1.36
32:i:258:SER:OG	32:i:336:VAL:HG12	1.14	1.28
16:Q:36:GLN:NE2	40:r:137:GLY:O	1.70	1.22
32:i:95:MET:CE	32:i:149:ILE:HD12	1.76	1.14
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.12
41:s:62:ARG:HD3	41:s:68:ILE:HD13	1.29	1.10
11:L:122:SER:OG	15:P:229:GLU:OE2	1.69	1.08
32:i:68:MET:HE1	34:k:37:MET:HE2	1.37	1.06
32:i:95:MET:HE2	32:i:149:ILE:HD12	1.31	1.05
49:C:303:PLX:H361	49:C:303:PLX:C20	1.89	1.03
17:S:31:ASN:ND2	17:S:60:TYR:OH	1.91	1.03
37:n:34:LYS:HZ1	51:n:101:CDL:HB22	1.17	1.03
9:J:135:GLU:OE2	9:J:140:ASP:HB2	1.58	1.03
27:d:107:GLN:HE22	35:l:194:ASN:ND2	1.57	1.03
1:A:50:ASP:O	1:A:59:ARG:NH2	1.92	1.01
16:Q:104:GLU:OE1	41:s:282:TYR:CE1	2.13	1.01
50:X:201:8Q1:C12	39:p:70:GLU:OE1	2.07	1.01
32:i:258:SER:OG	32:i:336:VAL:CG1	2.08	1.01
49:C:303:PLX:H361	49:C:303:PLX:H201	1.44	0.99
40:r:193:ILE:HD11	40:r:256:TYR:OH	1.64	0.98
36:m:26:PRO:HB2	36:m:71:THR:HG21	1.43	0.98
9:J:135:GLU:HG3	9:J:140:ASP:HA	1.45	0.97
53:J:402:UQ:H111	53:J:402:UQ:H153	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:n:34:LYS:NZ	51:n:101:CDL:HB22	1.81	0.96
36:m:26:PRO:HB2	36:m:71:THR:CG2	1.95	0.95
12:M:176:CYS:HG	45:M:802:SF4:FE4	0.84	0.94
33:j:18:VAL:CG1	48:j:202:PEE:H16	1.97	0.94
48:b:201:PEE:H34	51:l:702:CDL:H242	1.48	0.94
12:M:389:THR:H	12:M:514:ASN:HD21	1.15	0.93
27:d:107:GLN:NE2	35:l:194:ASN:HD22	1.67	0.92
36:m:24:PRO:HB3	36:m:89:VAL:HG11	1.50	0.92
48:b:201:PEE:H10	49:r:503:PLX:O2	1.70	0.92
50:X:201:8Q1:O2	39:p:13:GLN:NE2	2.02	0.91
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.52	0.91
35:l:356:ILE:HD11	35:l:425:ARG:NH1	1.85	0.90
32:i:258:SER:HG	32:i:336:VAL:HG12	1.30	0.90
12:M:385:TYR:OH	12:M:527:ASP:OD1	1.90	0.90
6:G:136:GLU:O	6:G:139:MET:HE2	1.72	0.89
12:M:351:LEU:O	12:M:530:TYR:OH	1.90	0.89
48:Q:501:PEE:H37	48:Q:501:PEE:C37	2.02	0.89
12:M:390:THR:HB	12:M:600:GLU:OE1	1.73	0.89
26:c:140:MET:HE1	51:l:703:CDL:H822	1.56	0.88
3:C:190:LEU:HD22	48:C:302:PEE:H13	1.55	0.88
32:i:100:MET:HE1	35:l:599:MET:HE2	1.56	0.87
51:l:703:CDL:H712	51:l:703:CDL:H312	1.56	0.87
41:s:62:ARG:HD3	41:s:68:ILE:CD1	2.04	0.87
51:l:703:CDL:H712	51:l:703:CDL:C31	2.03	0.86
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.56	0.86
35:l:534:HIS:CD2	48:l:704:PEE:H13	2.09	0.86
33:j:18:VAL:HG12	48:j:202:PEE:H16	1.55	0.86
48:Q:501:PEE:H37	48:Q:501:PEE:H60	1.57	0.85
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.09	0.85
27:d:107:GLN:HE22	35:l:194:ASN:HD22	1.16	0.85
24:a:94:GLY:O	27:d:61:TYR:OH	1.95	0.83
1:A:48:ARG:NH2	14:O:226:GLU:OE1	2.11	0.83
5:F:71:PHE:HE1	12:M:334:GLN:HE21	1.25	0.83
32:i:95:MET:HE1	32:i:149:ILE:HD12	1.60	0.82
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.11	0.82
18:T:46:ASP:OD1	18:T:49:ASP:HB2	1.79	0.82
9:J:135:GLU:CG	9:J:140:ASP:HA	2.08	0.82
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.13	0.81
10:K:100:GLN:NE2	14:O:69:ASN:O	2.12	0.81
16:Q:104:GLU:OE1	41:s:282:TYR:CZ	2.33	0.81
44:w:238:GLU:OE2	44:w:242:LYS:HD2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:I:201:CDL:OA9	51:I:201:CDL:H532	1.80	0.81
5:F:71:PHE:HE1	12:M:334:GLN:NE2	1.78	0.81
5:F:71:PHE:CE1	12:M:334:GLN:NE2	2.49	0.81
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.63	0.80
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.63	0.80
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.14	0.79
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.64	0.79
30:g:2:THR:N	30:g:5:SER:HG	1.81	0.79
14:O:140:CYS:SG	14:O:183:ALA:HB1	2.23	0.79
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.65	0.79
33:j:27:LEU:CD2	41:s:60:PRO:HD2	2.12	0.79
15:P:161:LYS:HG2	16:Q:286:TYR:CE2	2.18	0.79
36:m:33:LEU:HD23	36:m:64:MET:HE3	1.65	0.79
6:G:123:GLU:OE2	6:G:129:GLU:OE2	2.00	0.78
40:r:193:ILE:CD1	40:r:256:TYR:OH	2.30	0.78
12:M:389:THR:H	12:M:514:ASN:ND2	1.80	0.78
16:Q:178:THR:HG1	16:Q:214:TYR:HH	1.27	0.78
48:W:201:PEE:C1	48:W:201:PEE:H10	2.13	0.78
38:o:75:ASN:O	38:o:79:ASN:ND2	2.17	0.78
41:s:209:SER:HB3	41:s:213:VAL:HA	1.66	0.78
48:W:201:PEE:C27	51:s:401:CDL:H822	2.14	0.78
48:b:201:PEE:C4	49:r:503:PLX:O2	2.32	0.78
36:m:24:PRO:HB3	36:m:89:VAL:CG1	2.13	0.77
14:O:180:CYS:SG	54:O:301:FES:FE2	1.76	0.77
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.67	0.77
48:C:302:PEE:H36	48:C:302:PEE:H71	1.67	0.77
8:I:40:LYS:HB3	21:W:7:LYS:H	1.50	0.77
48:C:302:PEE:H67	49:C:303:PLX:H212	1.66	0.77
15:P:207:TYR:C	15:P:224:VAL:HG23	2.09	0.76
48:W:201:PEE:H45	51:s:401:CDL:H822	1.65	0.76
16:Q:197:MET:HE2	41:s:32:GLN:HE22	1.49	0.76
16:Q:144:MET:HG2	16:Q:222:MET:O	1.86	0.76
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.18	0.76
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.19	0.76
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.19	0.76
6:G:123:GLU:OE2	6:G:129:GLU:CD	2.28	0.76
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.66	0.76
14:O:180:CYS:HG	54:O:301:FES:FE2	0.98	0.76
20:V:110:ILE:HD11	48:l:701:PEE:H8	1.66	0.76
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.20	0.75
14:O:140:CYS:SG	14:O:183:ALA:CB	2.74	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:53:ILE:O	12:M:380:ASP:OD1	2.04	0.75
32:i:100:MET:CE	35:l:599:MET:HE2	2.16	0.75
41:s:62:ARG:CD	41:s:68:ILE:HD13	2.11	0.75
12:M:389:THR:HG21	12:M:473:MET:SD	2.27	0.75
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.68	0.75
27:d:107:GLN:NE2	35:l:194:ASN:ND2	2.31	0.74
40:r:123:GLU:OE2	40:r:157:SER:OG	2.04	0.74
12:M:337:ASP:O	12:M:542:PRO:HB2	1.88	0.74
1:A:64:LYS:HD3	14:O:249:LEU:HD23	1.70	0.74
30:g:89:ASP:OD2	42:u:161:ALA:HB1	1.88	0.74
12:M:379:THR:HG21	12:M:526:LEU:HD22	1.68	0.74
32:i:95:MET:CE	32:i:149:ILE:CD1	2.63	0.74
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.70	0.74
5:F:53:ILE:C	12:M:380:ASP:OD1	2.31	0.73
20:V:141:VAL:O	24:a:169:TYR:OH	2.04	0.73
51:V:202:CDL:H712	51:V:202:CDL:H512	1.70	0.73
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.69	0.73
6:G:136:GLU:O	6:G:139:MET:CE	2.36	0.73
34:k:79:VAL:HG22	36:m:74:MET:HE1	1.68	0.73
44:w:57:SER:HB3	44:w:150:LEU:HD11	1.71	0.73
5:F:24:CYS:HA	5:F:58:CYS:HB3	1.70	0.72
1:A:246:GLU:OE1	1:A:275:LEU:HD12	1.89	0.72
32:i:215:MET:HE3	32:i:251:MET:HE2	1.71	0.72
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.71	0.72
32:i:254:LEU:CD2	40:r:154:LEU:HD11	2.18	0.72
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.70	0.72
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.72	0.72
9:J:212:ARG:O	9:J:216:TYR:HB2	1.89	0.72
13:N:68:MET:HG3	13:N:69:ASN:H	1.54	0.72
12:M:337:ASP:O	12:M:542:PRO:CB	2.38	0.72
6:X:133:ILE:HD13	39:p:18:ARG:HH22	1.54	0.71
51:s:401:CDL:H332	51:s:401:CDL:H182	1.72	0.71
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.72	0.71
4:E:16:SER:HA	11:L:52:LEU:HD13	1.72	0.71
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.23	0.71
35:l:286:LEU:HD13	35:l:411:MET:SD	2.29	0.71
41:s:15:LEU:HD23	53:s:402:UQ:H272	1.72	0.71
1:A:405:ARG:NH2	8:I:49:LEU:HD11	2.06	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.23	0.71
41:s:222:MET:HA	41:s:225:MET:HE2	1.71	0.71
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:117:ARG:NH2	9:J:158:GLU:OE2	2.24	0.71
7:H:105:GLU:HB3	15:P:89:HIS:CD2	2.26	0.71
41:s:15:LEU:HD23	53:s:402:UQ:C27	2.20	0.71
1:A:66:LYS:HE3	1:A:188:GLY:HA3	1.73	0.70
49:C:303:PLX:O2	49:C:303:PLX:H1A3	1.91	0.70
35:l:481:THR:OG1	43:v:92:HIS:ND1	2.22	0.70
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.23	0.70
33:j:71:LEU:O	36:m:147:TYR:OH	2.08	0.70
46:A:502:FMN:HO3'	46:A:502:FMN:C2	2.05	0.70
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.24	0.70
20:V:140:LYS:O	20:V:140:LYS:HG2	1.90	0.70
32:i:254:LEU:HD21	40:r:154:LEU:HD11	1.72	0.70
6:X:140:CYS:HB2	6:X:143:GLU:HG3	1.72	0.69
2:B:99:GLY:O	2:B:100:GLU:O	2.09	0.69
48:Q:501:PEE:H37	48:Q:501:PEE:H61	1.74	0.69
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.24	0.69
44:w:65:ASN:OD1	44:w:66:ILE:N	2.26	0.69
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.25	0.69
25:b:81:ILE:HG23	48:b:201:PEE:H58	1.74	0.69
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.09	0.69
36:m:23:LYS:N	36:m:24:PRO:HD3	2.08	0.69
2:B:72:MET:HE1	8:I:18:ARG:HH12	1.58	0.69
27:d:38:ASP:OD1	27:d:39:LEU:N	2.26	0.69
37:n:34:LYS:HZ1	51:n:101:CDL:CB2	1.99	0.69
3:C:96:SER:HB2	41:s:209:SER:HB2	1.75	0.68
3:C:167:PRO:HD3	16:Q:223:HIS:CD2	2.27	0.68
9:J:220:MET:HE2	9:J:227:PRO:HD2	1.74	0.68
27:d:111:LYS:HE2	35:l:197:ASP:OD2	1.92	0.68
48:l:701:PEE:O2P	48:l:701:PEE:H7	1.94	0.68
11:L:109:ASN:ND2	11:L:111:LEU:O	2.27	0.68
5:F:24:CYS:CA	5:F:58:CYS:HB3	2.24	0.68
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.74	0.68
49:C:303:PLX:O4	49:C:303:PLX:O7	2.05	0.68
44:w:243:LYS:O	44:w:247:PRO:HG2	1.94	0.68
24:a:137:MET:HE1	37:n:42:SER:HB3	1.76	0.67
40:r:193:ILE:HD11	40:r:256:TYR:HH	1.57	0.67
26:c:140:MET:CE	51:l:703:CDL:H822	2.23	0.67
9:J:87:GLU:HG3	9:J:89:TYR:H	1.60	0.67
12:M:176:CYS:SG	45:M:802:SF4:FE4	1.85	0.67
49:C:303:PLX:H361	49:C:303:PLX:C21	2.25	0.67
24:a:169:TYR:CZ	30:g:3:MET:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:B:303:PEE:H52	41:s:187:ILE:HD12	1.77	0.67
9:J:132:ARG:HH21	52:J:401:NDP:H51A	1.59	0.66
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.77	0.66
36:m:45:LEU:HD23	36:m:50:SER:HA	1.77	0.66
2:B:99:GLY:O	2:B:100:GLU:C	2.36	0.66
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.26	0.66
31:h:18:MET:HE3	34:k:56:ALA:HA	1.76	0.66
40:r:403:THR:HA	40:r:406:TYR:CE2	2.30	0.66
40:r:255:ASN:N	40:r:255:ASN:HD22	1.91	0.66
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.78	0.65
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.78	0.65
48:W:201:PEE:H10	48:W:201:PEE:H3	1.78	0.65
1:A:285:PRO:O	14:O:222:ARG:NH2	2.30	0.65
48:C:302:PEE:H66	48:C:302:PEE:H32	1.79	0.65
53:J:402:UQ:H153	53:J:402:UQ:C11	2.18	0.65
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.28	0.65
1:A:420:GLU:HG3	1:A:429:ASP:OD1	1.96	0.65
11:L:88:GLN:HE21	12:M:136:GLU:C	2.04	0.65
12:M:179:CYS:SG	45:M:802:SF4:FE1	1.88	0.65
23:Z:59:ASN:O	35:l:364:LYS:NZ	2.25	0.65
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.20	0.65
7:H:44:TYR:O	7:H:48:THR:HG22	1.96	0.65
12:M:428:LYS:NZ	12:M:443:ASP:OD2	2.29	0.65
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.78	0.65
32:i:243:LEU:HD23	51:r:504:CDL:H361	1.79	0.65
13:N:96:ASP:HB3	13:N:101:LYS:HG3	1.78	0.65
33:j:18:VAL:HG11	48:j:202:PEE:H16	1.79	0.65
8:I:91:GLU:HB2	8:I:93:LYS:HE3	1.79	0.65
35:l:356:ILE:HD11	35:l:425:ARG:HH11	1.61	0.65
51:l:703:CDL:H312	51:l:703:CDL:C71	2.26	0.65
32:i:7:THR:HG22	32:i:11:MET:HE2	1.79	0.64
51:l:702:CDL:H452	40:r:445:LEU:HB3	1.78	0.64
9:J:192:ARG:NH1	9:J:198:ALA:O	2.31	0.64
48:Q:501:PEE:H60	48:Q:501:PEE:C23	2.28	0.64
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.29	0.64
16:Q:404:LYS:HE2	16:Q:457:VAL:HG23	1.80	0.64
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.78	0.64
48:j:202:PEE:H48	48:j:202:PEE:H1	1.79	0.64
37:n:47:ARG:NH2	37:n:53:GLU:OE2	2.30	0.64
51:n:101:CDL:H581	51:n:101:CDL:H541	1.80	0.64
40:r:19:LYS:NZ	40:r:21:ASN:OD1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:99:GLU:HG2	35:l:61:MET:HG2	1.80	0.64
5:F:65:LEU:HD11	5:F:91:LEU:HD13	1.79	0.64
33:j:79:SER:HA	33:j:87:MET:HE2	1.80	0.64
12:M:257:VAL:O	12:M:598:ASN:OD1	2.15	0.63
35:l:401:MET:HE2	35:l:482:MET:HB3	1.80	0.63
24:a:78:THR:HG21	28:e:96:SER:HA	1.79	0.63
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.81	0.63
34:k:23:ARG:NH1	36:m:89:VAL:CG2	2.62	0.63
40:r:104:LEU:HG	40:r:108:MET:HE2	1.81	0.63
15:P:161:LYS:CD	16:Q:286:TYR:CZ	2.81	0.63
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.79	0.63
41:s:200:LEU:HD13	41:s:282:TYR:CB	2.29	0.63
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.81	0.63
12:M:463:SER:O	12:M:467:LYS:HG3	1.98	0.63
26:c:116:ARG:HG2	48:l:704:PEE:H49	1.81	0.63
28:e:125:LEU:HD23	28:e:129:ARG:HH21	1.63	0.63
44:w:125:ASP:O	44:w:130:ARG:NH2	2.31	0.63
1:A:152:ARG:NH2	10:K:99:PRO:O	2.32	0.62
8:I:40:LYS:CB	21:W:7:LYS:H	2.12	0.62
48:l:704:PEE:H67	40:r:401:MET:HE1	1.81	0.62
4:E:96:VAL:HG12	4:E:96:VAL:O	2.00	0.62
12:M:379:THR:CG2	12:M:526:LEU:HD22	2.28	0.62
5:F:53:ILE:N	12:M:380:ASP:OD1	2.32	0.62
49:C:303:PLX:H372	49:C:303:PLX:H232	1.80	0.62
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.81	0.62
48:j:201:PEE:H40	41:s:302:MET:HE1	1.82	0.62
1:A:87:GLY:HA3	46:A:502:FMN:O2P	1.98	0.62
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.33	0.62
9:J:135:GLU:OE2	9:J:140:ASP:CB	2.42	0.62
32:i:261:MET:HB2	32:i:337:LEU:HD12	1.82	0.62
35:l:180:ILE:HD12	48:l:704:PEE:C47	2.30	0.62
48:r:501:PEE:O1P	48:r:501:PEE:H12	1.99	0.62
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.34	0.61
31:h:31:GLY:HA2	34:k:52:HIS:O	2.00	0.61
32:i:117:GLU:O	34:k:96:LEU:HD13	2.00	0.61
1:A:159:ARG:NH2	14:O:176:CYS:O	2.31	0.61
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.33	0.61
35:l:227:PHE:O	35:l:230:HIS:ND1	2.33	0.61
48:W:201:PEE:H3	48:W:201:PEE:C4	2.30	0.61
32:i:88:LYS:O	32:i:148:SER:CB	2.48	0.61
35:l:70:THR:O	40:r:459:TYR:CE1	2.52	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.32	0.61
48:B:303:PEE:H7	41:s:288:LEU:HD11	1.81	0.61
53:J:402:UQ:O1	53:J:402:UQ:H102	2.01	0.61
35:l:176:ARG:HG2	40:r:401:MET:HA	1.81	0.61
20:V:140:LYS:HD3	20:V:141:VAL:HG23	1.83	0.61
36:m:26:PRO:HB2	36:m:71:THR:HG23	1.82	0.61
16:Q:88:HIS:HD2	16:Q:90:ALA:H	1.47	0.61
35:l:56:HIS:CD2	35:l:57:THR:HG23	2.36	0.61
38:o:45:ARG:HH12	39:p:144:THR:HG21	1.66	0.61
40:r:195:MET:HB2	48:r:501:PEE:O4	2.01	0.61
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.83	0.61
12:M:308:ARG:NH2	12:M:578:PRO:O	2.34	0.61
15:P:207:TYR:O	15:P:224:VAL:HG23	2.00	0.61
36:m:61:LEU:O	41:s:114:TYR:OH	2.18	0.61
8:I:12:ARG:NH2	8:I:21:GLN:OE1	2.34	0.61
12:M:284:GLU:HG2	12:M:284:GLU:O	2.01	0.61
1:A:418:GLN:HE22	12:M:152:ARG:HH21	1.49	0.60
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.41	0.60
15:P:161:LYS:HD3	16:Q:286:TYR:CZ	2.36	0.60
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.83	0.60
35:l:346:ILE:HA	35:l:366:MET:HE1	1.82	0.60
9:J:199:THR:OG1	9:J:258:ALA:O	2.20	0.60
12:M:169:VAL:HG22	12:M:223:ILE:HD11	1.83	0.60
12:M:534:VAL:HG22	12:M:534:VAL:O	2.00	0.60
17:S:63:THR:HG23	42:u:21:SER:HB2	1.83	0.60
1:A:89:GLY:O	47:A:503:NAI:H2N	2.02	0.60
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.82	0.60
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.32	0.60
15:P:105:ASN:O	15:P:137:PHE:CE2	2.53	0.60
26:c:40:PRO:O	26:c:74:ASP:HB2	1.99	0.60
49:g:201:PLX:H232	32:i:332:LEU:HB3	1.83	0.60
51:k:101:CDL:H632	51:k:101:CDL:H802	1.83	0.60
8:I:98:ALA:HB3	15:P:137:PHE:O	2.01	0.60
34:k:20:LEU:HD12	35:l:592:LEU:HD13	1.81	0.60
29:f:68:GLU:HG2	30:g:21:ARG:HE	1.66	0.60
33:j:27:LEU:HD21	41:s:60:PRO:HD2	1.82	0.60
48:j:201:PEE:C24	41:s:302:MET:HE1	2.32	0.60
12:M:472:PRO:O	12:M:510:TRP:NE1	2.27	0.60
49:g:201:PLX:H361	49:g:201:PLX:H311	1.84	0.60
32:i:95:MET:HE1	32:i:149:ILE:CD1	2.30	0.60
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:101:THR:O	4:E:105:ARG:HG3	2.02	0.60
15:P:161:LYS:HD3	16:Q:286:TYR:OH	2.02	0.60
3:C:88:ARG:HA	41:s:37:PRO:HA	1.83	0.59
33:j:18:VAL:HG12	48:j:202:PEE:C12	2.31	0.59
12:M:368:THR:HG21	12:M:522:GLN:OE1	2.02	0.59
26:c:68:ASP:OD1	26:c:70:MET:HG2	2.02	0.59
35:l:387:THR:HG22	35:l:465:GLY:H	1.67	0.59
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.83	0.59
2:B:99:GLY:CA	2:B:170:GLY:O	2.50	0.59
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.37	0.59
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.85	0.59
35:l:359:MET:O	35:l:436:ARG:NH2	2.36	0.59
51:l:702:CDL:H621	51:l:702:CDL:H432	1.85	0.59
40:r:105:PHE:O	40:r:109:THR:OG1	2.20	0.59
1:A:160:GLY:O	1:A:199:ARG:NH2	2.35	0.59
1:A:251:SER:N	1:A:252:PRO:HD2	2.18	0.59
1:A:254:ILE:HG23	1:A:259:GLY:HA2	1.84	0.59
34:k:10:MET:HE3	36:m:103:MET:HG2	1.83	0.59
40:r:73:LEU:HA	40:r:76:MET:HE2	1.85	0.59
1:A:66:LYS:CE	1:A:188:GLY:HA3	2.32	0.59
14:O:140:CYS:SG	14:O:183:ALA:HB2	2.42	0.59
51:a:201:CDL:OB7	48:b:201:PEE:H14	2.03	0.59
9:J:50:SER:OG	15:P:225:GLU:OE2	2.19	0.59
9:J:163:LYS:NZ	9:J:253:ILE:O	2.28	0.59
31:h:53:GLU:OE2	32:i:88:LYS:HE2	2.03	0.59
44:w:245:PHE:O	44:w:249:MET:HG2	2.02	0.59
9:J:178:SER:OG	9:J:317:ASP:OD2	2.20	0.58
33:j:69:ILE:HD11	41:s:144:VAL:HG13	1.84	0.58
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.68	0.58
14:O:38:LEU:O	14:O:124:ARG:NH2	2.36	0.58
26:c:170:ARG:HG2	43:v:53:LEU:HD21	1.84	0.58
35:l:106:TRP:CD1	35:l:447:ASN:HD22	2.21	0.58
51:l:703:CDL:H521	51:l:703:CDL:HB61	1.85	0.58
32:i:278:MET:O	32:i:282:MET:HG3	2.03	0.58
36:m:24:PRO:HG3	36:m:83:TRP:NE1	2.18	0.58
48:b:201:PEE:C21	51:l:702:CDL:H242	2.30	0.58
49:C:303:PLX:H361	49:C:303:PLX:H211	1.85	0.58
16:Q:335:GLU:OE2	16:Q:339:GLN:NE2	2.34	0.58
48:Q:501:PEE:H42	48:Q:501:PEE:H34	1.86	0.58
51:a:201:CDL:H401	27:d:44:PRO:HB3	1.85	0.58
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:355:LYS:HA	12:M:366:LEU:HD11	1.85	0.58
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.85	0.58
1:A:36:LYS:HG3	1:A:38:GLU:HG2	1.86	0.58
3:C:86:MET:HE3	3:C:91:VAL:HG12	1.86	0.58
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.85	0.58
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.85	0.58
11:L:165:SER:OG	11:L:168:LYS:HB2	2.03	0.57
14:O:176:CYS:SG	14:O:180:CYS:SG	3.01	0.57
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.34	0.57
16:Q:144:MET:HE3	16:Q:222:MET:HB2	1.85	0.57
17:S:66:LEU:HD21	42:u:75:LYS:HA	1.86	0.57
32:i:152:ASN:O	32:i:156:THR:OG1	2.11	0.57
44:w:250:SER:O	44:w:280:LYS:NZ	2.33	0.57
16:Q:47:PHE:HD1	16:Q:52:MET:HE1	1.69	0.57
34:k:20:LEU:HD13	35:l:592:LEU:HB2	1.85	0.57
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.69	0.57
32:i:238:PRO:HB2	51:r:504:CDL:HA31	1.86	0.57
40:r:205:VAL:HG22	40:r:212:LEU:HD13	1.86	0.57
48:W:201:PEE:H17	33:j:4:MET:HE3	1.85	0.57
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.40	0.57
35:l:123:LEU:HD13	51:l:702:CDL:H112	1.86	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.86	0.57
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.87	0.57
32:i:190:MET:HE2	32:i:205:LEU:HA	1.87	0.57
38:o:50:GLN:O	38:o:56:ARG:HD3	2.03	0.57
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.86	0.57
6:G:130:ILE:HG22	6:G:135:ALA:HB2	1.86	0.57
14:O:180:CYS:SG	54:O:301:FES:S2	3.03	0.57
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.85	0.57
27:d:164:LEU:HD23	28:e:149:LEU:HD13	1.87	0.57
9:J:212:ARG:O	9:J:216:TYR:CB	2.52	0.56
34:k:17:ALA:O	34:k:21:MET:HG2	2.05	0.56
5:F:42:VAL:HG13	12:M:671:LEU:HG	1.87	0.56
40:r:116:ILE:HG13	42:u:168:PHE:CD1	2.40	0.56
27:d:148:ALA:O	27:d:149:HIS:HB2	2.04	0.56
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.87	0.56
38:o:107:THR:O	38:o:111:LYS:HG3	2.06	0.56
8:I:14:TRP:O	21:W:28:ARG:NH2	2.38	0.56
41:s:87:VAL:HG12	41:s:95:LEU:HD23	1.88	0.56
41:s:293:PHE:O	41:s:297:THR:OG1	2.18	0.56
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:18:ALA:O	41:s:21:THR:OG1	2.17	0.56
43:v:51:LEU:O	43:v:52:MET:HG3	2.06	0.56
1:A:63:TYR:O	1:A:256:ARG:HD3	2.05	0.56
27:d:60:ARG:HH11	27:d:60:ARG:HG3	1.70	0.56
4:E:42:GLU:OE1	4:E:46:THR:OG1	2.23	0.56
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.86	0.56
32:i:88:LYS:O	32:i:148:SER:HB3	2.04	0.56
48:B:303:PEE:H59	41:s:277:TYR:HE2	1.71	0.56
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.86	0.56
40:r:67:VAL:HG12	49:r:503:PLX:H362	1.88	0.56
15:P:50:ARG:NH2	15:P:80:CYS:SG	2.79	0.55
25:b:73:THR:HA	25:b:77:ILE:HD12	1.89	0.55
30:g:89:ASP:OD2	42:u:161:ALA:CB	2.54	0.55
35:l:429:PHE:HE1	39:p:32:VAL:HG21	1.71	0.55
41:s:28:LEU:HD22	41:s:275:ALA:HB2	1.87	0.55
41:s:102:VAL:HG21	41:s:154:LEU:HD11	1.88	0.55
21:W:63:GLU:OE2	42:u:119:ARG:NH2	2.39	0.55
36:m:82:VAL:HG12	36:m:83:TRP:H	1.70	0.55
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.87	0.55
34:k:21:MET:HB3	51:k:101:CDL:HB61	1.89	0.55
38:o:121:LEU:HD23	38:o:123:GLN:HE21	1.71	0.55
40:r:285:LEU:HD13	40:r:342:MET:HE1	1.87	0.55
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.88	0.55
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.88	0.55
35:l:190:LEU:HD21	40:r:307:TRP:CH2	2.41	0.55
44:w:54:THR:HG23	44:w:56:THR:HG22	1.87	0.55
1:A:249:ALA:O	1:A:252:PRO:HD2	2.05	0.55
2:B:99:GLY:HA3	2:B:170:GLY:O	2.07	0.55
12:M:389:THR:N	12:M:514:ASN:HD21	1.95	0.55
33:j:27:LEU:HD22	41:s:60:PRO:HD2	1.86	0.55
38:o:59:VAL:HG22	40:r:423:ILE:CG1	2.37	0.55
3:C:92:VAL:HG21	53:s:402:UQ:H103	1.89	0.55
4:E:99:GLN:O	4:E:100:ARG:C	2.50	0.55
8:I:13:ASN:ND2	8:I:19:ASP:OD1	2.40	0.55
15:P:161:LYS:HG2	16:Q:286:TYR:CZ	2.41	0.55
12:M:374:THR:HG23	12:M:532:PRO:HG2	1.88	0.55
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.88	0.55
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.42	0.55
35:l:257:VAL:HG13	35:l:317:ILE:HD11	1.89	0.55
35:l:520:TYR:HE1	51:l:703:CDL:OB4	1.89	0.55
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:701:PEE:H7	48:l:701:PEE:P	2.47	0.55
7:H:50:GLN:O	7:H:54:GLU:HG3	2.04	0.55
40:r:370:PRO:HG3	40:r:375:LEU:HD13	1.90	0.55
53:J:402:UQ:C11	53:J:402:UQ:C15	2.86	0.54
49:C:303:PLX:O6	49:C:303:PLX:H24	2.08	0.54
12:M:556:THR:HG23	12:M:558:GLN:H	1.72	0.54
18:T:43:GLN:O	18:T:43:GLN:NE2	2.41	0.54
21:W:90:ASN:ND2	21:W:123:GLU:O	2.40	0.54
12:M:213:MET:HB3	12:M:215:MET:HE2	1.88	0.54
51:l:703:CDL:H622	51:l:703:CDL:H571	1.88	0.54
40:r:257:MET:O	40:r:260:PRO:HD2	2.07	0.54
3:C:196:ARG:HG2	9:J:85:ARG:HH12	1.72	0.54
3:C:190:LEU:CD2	48:C:302:PEE:H13	2.34	0.54
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.31	0.54
15:P:161:LYS:HD2	16:Q:286:TYR:CE1	2.42	0.54
29:f:43:LYS:HA	29:f:46:LEU:HD23	1.90	0.54
13:N:4:VAL:O	13:N:8:ARG:HG2	2.07	0.54
35:l:103:PHE:HB2	35:l:341:MET:HE3	1.89	0.54
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.41	0.54
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.42	0.54
49:J:403:PLX:H101	33:j:24:LEU:HD13	1.88	0.54
51:k:101:CDL:H462	51:k:101:CDL:H402	1.89	0.54
12:M:534:VAL:CG2	12:M:555:ILE:HD11	2.38	0.53
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.42	0.53
11:L:86:ASN:O	11:L:86:ASN:ND2	2.41	0.53
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.89	0.53
19:U:66:VAL:O	42:u:130:LYS:HE3	2.07	0.53
48:l:701:PEE:O4	48:l:701:PEE:H2	2.08	0.53
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.90	0.53
12:M:341:ILE:HD11	12:M:555:ILE:HD12	1.89	0.53
49:C:303:PLX:H211	49:C:303:PLX:C37	2.39	0.53
13:N:78:ASP:OD2	13:N:80:SER:OG	2.24	0.53
35:l:70:THR:HG23	35:l:75:GLU:HG2	1.90	0.53
36:m:82:VAL:HG11	51:s:401:CDL:HB31	1.90	0.53
1:A:214:GLU:OE2	11:L:175:LYS:NZ	2.33	0.53
8:I:91:GLU:HG2	8:I:92:LYS:H	1.74	0.53
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.43	0.53
4:E:99:GLN:O	4:E:101:THR:N	2.42	0.53
6:X:155:TYR:OH	25:b:27:GLU:OE2	2.20	0.53
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.90	0.53
43:v:22:MET:HG3	43:v:105:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:72:ARG:HH12	44:w:264:GLU:HA	1.73	0.53
15:P:201:ASP:OD1	15:P:201:ASP:N	2.33	0.53
21:W:91:LEU:HD22	42:u:7:LEU:HD12	1.90	0.53
40:r:346:ARG:O	40:r:419:TYR:HA	2.09	0.53
1:A:422:HIS:O	12:M:76:ARG:HD3	2.08	0.52
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.90	0.52
49:C:303:PLX:H211	49:C:303:PLX:C36	2.39	0.52
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.90	0.52
21:W:88:ARG:NH2	42:u:7:LEU:O	2.41	0.52
35:l:603:ASN:ND2	35:l:603:ASN:O	2.41	0.52
43:v:120:ALA:O	43:v:124:ARG:HG2	2.09	0.52
1:A:66:LYS:CD	1:A:188:GLY:HA3	2.39	0.52
12:M:534:VAL:HG21	12:M:555:ILE:HD11	1.90	0.52
17:S:50:ARG:NH2	42:u:18:VAL:O	2.42	0.52
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.90	0.52
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.91	0.52
34:k:50:ASN:OD1	36:m:127:ILE:HD12	2.08	0.52
1:A:33:GLY:O	1:A:302:LYS:NZ	2.39	0.52
14:O:185:MET:HB3	14:O:194:GLU:HA	1.91	0.52
32:i:75:ILE:HD12	34:k:40:LEU:HD22	1.90	0.52
48:B:303:PEE:H7	41:s:288:LEU:CD1	2.40	0.52
4:E:27:GLU:HA	4:E:30:ARG:HG2	1.91	0.52
4:E:99:GLN:O	4:E:102:HIS:N	2.42	0.52
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.91	0.52
5:F:57:GLU:O	12:M:655:ARG:NH2	2.42	0.52
16:Q:319:PRO:HG2	16:Q:336:GLU:HG3	1.90	0.52
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.91	0.52
12:M:48:THR:OG1	12:M:51:GLN:HG3	2.10	0.52
22:Y:71:TRP:HA	23:Z:78:PHE:HE1	1.74	0.52
33:j:73:LEU:O	41:s:160:TYR:OH	2.28	0.52
40:r:122:PHE:HZ	40:r:206:LYS:HG3	1.73	0.52
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.37	0.52
1:A:208:GLU:HB3	1:A:211:ALA:HB3	1.92	0.52
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.92	0.52
13:N:6:VAL:HG12	13:N:9:ARG:HH12	1.73	0.52
32:i:215:MET:HE3	32:i:251:MET:CE	2.39	0.52
36:m:23:LYS:N	36:m:24:PRO:CD	2.73	0.52
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.91	0.52
3:C:41:SER:OG	3:C:42:ARG:N	2.41	0.52
33:j:70:ALA:HB2	36:m:55:MET:HE2	1.92	0.52
44:w:239:ASN:HD22	44:w:239:ASN:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:168:SER:O	9:J:203:PRO:HD2	2.09	0.52
49:J:403:PLX:H161	33:j:20:ILE:HD11	1.92	0.52
28:e:126:VAL:HG13	28:e:136:LEU:HD11	1.91	0.52
32:i:84:TRP:CH2	34:k:59:MET:HE3	2.45	0.52
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.92	0.52
34:k:2:PRO:HG3	36:m:127:ILE:HD13	1.92	0.52
9:J:127:ILE:HD11	9:J:253:ILE:HD11	1.91	0.52
1:A:236:PHE:O	11:L:166:TRP:HB2	2.10	0.51
1:A:250:VAL:C	1:A:252:PRO:HD2	2.35	0.51
1:A:418:GLN:HE22	12:M:152:ARG:NH2	2.07	0.51
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.74	0.51
32:i:276:ILE:HG21	48:r:501:PEE:H7	1.91	0.51
42:u:103:GLN:N	42:u:103:GLN:OE1	2.42	0.51
44:w:235:GLN:O	44:w:239:ASN:ND2	2.43	0.51
4:E:39:TRP:O	4:E:43:VAL:HG23	2.10	0.51
9:J:108:TRP:CZ3	9:J:110:GLY:HA2	2.44	0.51
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.76	0.51
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.93	0.51
41:s:46:LEU:HD23	41:s:49:ILE:HD12	1.92	0.51
16:Q:36:GLN:HG3	40:r:138:ASN:HA	1.92	0.51
32:i:246:VAL:HG11	51:r:504:CDL:H392	1.92	0.51
7:H:104:VAL:HG23	15:P:71:LYS:HG2	1.92	0.51
22:Y:44:TYR:CD2	23:Z:16:LEU:HD22	2.45	0.51
24:a:169:TYR:CE1	30:g:3:MET:HB2	2.45	0.51
29:f:39:PRO:HD3	44:w:351:TRP:CG	2.46	0.51
44:w:226:GLU:O	44:w:229:ILE:HG13	2.10	0.51
3:C:44:GLU:HA	3:C:47:VAL:HG22	1.93	0.51
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.93	0.51
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.91	0.51
41:s:240:ILE:HG13	41:s:259:PHE:CE1	2.46	0.51
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.32	0.51
17:S:55:SER:HA	17:S:64:LYS:HE2	1.93	0.51
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.30	0.51
48:l:704:PEE:H14	48:l:704:PEE:H7	1.93	0.51
9:J:222:TRP:C	9:J:224:GLY:H	2.19	0.51
9:J:298:TYR:HA	9:J:301:VAL:HG22	1.92	0.51
40:r:126:LEU:HD11	40:r:153:THR:HG21	1.93	0.51
1:A:392:MET:HE2	1:A:419:ILE:HD13	1.93	0.51
16:Q:281:GLU:CD	16:Q:281:GLU:H	2.19	0.51
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.92	0.51
34:k:27:MET:HE1	34:k:75:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:73:THR:OG1	38:o:127:ILE:HG21	2.11	0.51
41:s:128:ALA:HA	41:s:211:PHE:HA	1.93	0.51
41:s:240:ILE:HG13	41:s:259:PHE:HE1	1.76	0.51
1:A:316:ALA:HB1	1:A:326:LEU:HD12	1.93	0.51
25:b:100:ARG:HH22	27:d:119:GLU:HG2	1.75	0.51
25:b:103:ARG:NH1	43:v:49:ALA:O	2.43	0.51
7:H:50:GLN:HE22	8:I:94:ALA:H	1.57	0.51
11:L:84:ARG:NH1	11:L:88:GLN:O	2.41	0.51
11:L:105:GLU:HA	12:M:611:THR:HG21	1.93	0.51
22:Y:51:THR:HG22	22:Y:53:SER:H	1.76	0.51
24:a:139:ILE:O	24:a:143:GLU:HG2	2.10	0.51
51:a:201:CDL:H541	48:b:201:PEE:H15	1.93	0.51
29:f:68:GLU:OE1	29:f:72:ARG:HG3	2.11	0.51
35:l:356:ILE:HD11	35:l:425:ARG:HH12	1.71	0.51
40:r:445:LEU:O	40:r:448:THR:HG22	2.11	0.51
51:r:504:CDL:H782	51:r:504:CDL:H241	1.93	0.51
1:A:66:LYS:HE3	1:A:188:GLY:CA	2.40	0.50
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.45	0.50
7:H:48:THR:HA	7:H:51:ILE:HG12	1.93	0.50
19:U:40:ASN:O	19:U:44:ARG:HG3	2.11	0.50
51:a:201:CDL:H772	51:a:201:CDL:H212	1.93	0.50
32:i:154:MET:HE3	32:i:154:MET:HA	1.93	0.50
6:G:94:ASP:OD1	6:G:96:GLU:HG3	2.11	0.50
14:O:63:ILE:O	14:O:67:VAL:HG23	2.11	0.50
15:P:173:MET:HE1	15:P:189:THR:HG23	1.92	0.50
51:l:702:CDL:H391	40:r:371:PRO:HD2	1.91	0.50
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.93	0.50
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.94	0.50
24:a:130:GLU:HG3	37:n:45:PHE:CG	2.46	0.50
27:d:69:ARG:NH2	37:n:46:LYS:O	2.44	0.50
35:l:520:TYR:CE1	51:l:703:CDL:OB4	2.64	0.50
44:w:256:LEU:HD11	44:w:276:LEU:HD11	1.93	0.50
1:A:392:MET:HE2	1:A:419:ILE:CD1	2.41	0.50
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.43	0.50
12:M:428:LYS:HE2	12:M:465:ILE:HD13	1.92	0.50
12:M:487:THR:OG1	12:M:677:GLN:OE1	2.22	0.50
15:P:118:ASP:OD1	15:P:125:ARG:HG2	2.12	0.50
32:i:326:LEU:N	32:i:327:PRO:CD	2.75	0.50
37:n:30:ARG:NE	51:n:101:CDL:OA4	2.38	0.50
40:r:282:LEU:HD13	40:r:342:MET:HE2	1.94	0.50
13:N:65:THR:O	13:N:73:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.93	0.50
14:O:204:ILE:HG23	14:O:214:PRO:HG3	1.93	0.50
20:V:17:GLU:OE1	20:V:20:ARG:NH1	2.39	0.50
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.46	0.50
40:r:368:ALA:O	40:r:375:LEU:HD12	2.11	0.50
40:r:371:PRO:O	40:r:448:THR:OG1	2.26	0.50
12:M:468:GLU:N	12:M:468:GLU:OE1	2.44	0.50
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.77	0.50
35:l:601:LEU:C	35:l:601:LEU:HD23	2.37	0.50
39:p:35:ASP:OD1	39:p:36:LYS:N	2.43	0.50
8:I:107:SER:OG	16:Q:317:ASP:OD2	2.23	0.50
12:M:406:ASN:O	12:M:410:GLU:HG3	2.11	0.50
30:g:80:ARG:O	30:g:84:MET:HG2	2.11	0.50
1:A:326:LEU:H	1:A:326:LEU:HD23	1.77	0.50
6:G:136:GLU:OE1	6:G:136:GLU:HA	2.11	0.50
9:J:108:TRP:HZ3	9:J:110:GLY:HA2	1.77	0.50
35:l:112:PRO:HG3	39:p:179:MET:HB3	1.94	0.50
35:l:399:VAL:HG12	35:l:409:LEU:HD13	1.93	0.50
51:l:702:CDL:H801	49:r:503:PLX:H181	1.93	0.50
40:r:392:THR:O	40:r:396:MET:HG2	2.12	0.50
41:s:149:ILE:HG21	41:s:185:TRP:HB2	1.92	0.50
21:W:144:THR:CG2	48:W:201:PEE:H3	2.42	0.49
48:W:201:PEE:C1	48:W:201:PEE:C4	2.85	0.49
24:a:176:LYS:H	31:h:45:HIS:CD2	2.29	0.49
34:k:1:MET:HG3	34:k:5:TYR:HD2	1.77	0.49
35:l:84:TYR:CE2	35:l:475:MET:HE1	2.47	0.49
40:r:197:LEU:HB3	48:r:501:PEE:H30	1.94	0.49
44:w:169:PHE:O	44:w:173:MET:HG3	2.12	0.49
6:G:118:ILE:O	6:G:122:MET:HG2	2.12	0.49
21:W:66:GLU:OE2	42:u:123:GLY:N	2.37	0.49
33:j:71:LEU:HB3	33:j:94:LEU:HD21	1.93	0.49
41:s:101:GLY:O	41:s:105:MET:HG2	2.12	0.49
45:C:301:SF4:S2	16:Q:138:ARG:HG2	2.52	0.49
40:r:114:GLU:OE2	42:u:169:PHE:HB3	2.12	0.49
44:w:190:VAL:O	44:w:194:THR:OG1	2.22	0.49
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.95	0.49
51:a:201:CDL:H512	48:b:201:PEE:H52	1.95	0.49
25:b:29:SER:OG	25:b:32:GLU:HG2	2.12	0.49
34:k:25:HIS:CE1	34:k:89:TYR:HE1	2.30	0.49
40:r:354:LEU:O	40:r:357:THR:HG22	2.11	0.49
1:A:67:GLU:O	1:A:71:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.45	0.49
9:J:211:ASP:O	9:J:215:ASN:HB2	2.13	0.49
9:J:262:THR:O	9:J:333:PRO:HD2	2.13	0.49
6:X:133:ILE:CD1	39:p:18:ARG:HH22	2.25	0.49
28:e:97:ILE:O	28:e:101:LEU:HB2	2.13	0.49
30:g:7:ARG:CG	30:g:8:PRO:HD2	2.42	0.49
33:j:94:LEU:HD13	36:m:154:VAL:HG13	1.93	0.49
40:r:214:LEU:O	40:r:217:PRO:HD2	2.12	0.49
44:w:63:ASP:HB3	44:w:241:TYR:CE1	2.48	0.49
3:C:92:VAL:HG21	53:s:402:UQ:C10	2.42	0.49
20:V:124:LEU:HD11	48:r:501:PEE:H64	1.94	0.49
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.93	0.49
12:M:296:GLY:O	12:M:572:HIS:NE2	2.40	0.49
17:S:27:HIS:ND1	17:S:36:LYS:HD3	2.28	0.49
33:j:90:MET:HE3	49:j:203:PLX:H261	1.94	0.49
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.48	0.49
1:A:210:THR:HB	1:A:224:ARG:H	1.76	0.49
1:A:278:ILE:HD11	1:A:299:LEU:HD21	1.95	0.49
19:U:63:MET:O	42:u:130:LYS:NZ	2.38	0.49
48:W:201:PEE:H10	48:W:201:PEE:H2	1.94	0.49
27:d:60:ARG:HG3	27:d:60:ARG:NH1	2.28	0.49
31:h:19:THR:HA	32:i:84:TRP:HB2	1.94	0.49
35:l:530:PRO:O	35:l:534:HIS:HB2	2.13	0.49
51:r:504:CDL:H401	51:r:504:CDL:H221	1.94	0.49
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.95	0.49
4:E:84:ILE:HG22	4:E:88:MET:HE3	1.95	0.49
5:F:61:VAL:HG13	5:F:62:GLN:N	2.28	0.49
13:N:129:THR:HA	18:T:43:GLN:HG2	1.94	0.49
16:Q:410:TYR:HB3	16:Q:423:LYS:HB3	1.95	0.49
36:m:34:ILE:HG13	36:m:64:MET:HG3	1.94	0.49
1:A:338:ASP:OD1	1:A:338:ASP:N	2.46	0.49
6:G:69:SER:N	16:Q:56:LYS:HZ3	2.11	0.49
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.48	0.49
12:M:48:THR:HA	12:M:95:PRO:HA	1.94	0.49
13:N:10:GLY:O	13:N:14:VAL:HG23	2.12	0.49
16:Q:198:THR:OG1	41:s:275:ALA:O	2.21	0.49
22:Y:43:ARG:HD3	22:Y:48:PRO:HA	1.94	0.49
32:i:110:PRO:HG2	35:l:594:THR:HG21	1.94	0.49
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.13	0.48
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.95	0.48
24:a:168:TRP:HB3	30:g:3:MET:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:136:LEU:HD23	32:i:205:LEU:HD21	1.95	0.48
33:j:27:LEU:HD22	41:s:59:GLU:HG3	1.95	0.48
35:l:232:TRP:HH2	35:l:252:MET:HE1	1.78	0.48
40:r:73:LEU:HD22	40:r:103:GLN:OE1	2.13	0.48
42:u:26:LYS:NZ	42:u:95:GLN:O	2.38	0.48
1:A:278:ILE:HG21	1:A:304:ALA:HB2	1.95	0.48
12:M:534:VAL:HG21	12:M:555:ILE:CD1	2.42	0.48
35:l:106:TRP:HD1	35:l:447:ASN:HD22	1.59	0.48
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.94	0.48
40:r:255:ASN:N	40:r:255:ASN:ND2	2.60	0.48
1:A:66:LYS:HD2	1:A:188:GLY:HA3	1.96	0.48
15:P:108:PHE:CD2	15:P:134:SER:HB2	2.47	0.48
16:Q:242:ASP:OD1	21:W:16:TYR:OH	2.21	0.48
23:Z:60:ASN:OD1	23:Z:61:VAL:N	2.46	0.48
49:j:203:PLX:H352	36:m:155:ILE:HG23	1.95	0.48
35:l:293:ILE:HG22	35:l:422:TYR:HB3	1.95	0.48
40:r:272:THR:HA	40:r:275:ILE:HD12	1.94	0.48
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.48	0.48
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.94	0.48
51:l:702:CDL:H352	40:r:361:VAL:HG23	1.94	0.48
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.95	0.48
27:d:65:HIS:CE1	28:e:117:TRP:CD1	3.01	0.48
6:G:123:GLU:HG3	6:G:128:PHE:O	2.13	0.48
30:g:51:ARG:HG3	30:g:51:ARG:HH11	1.77	0.48
31:h:29:ILE:HG21	36:m:138:GLU:HG2	1.96	0.48
7:H:76:GLN:HB2	7:H:79:GLU:OE1	2.14	0.48
9:J:173:ASP:OD1	9:J:176:SER:HB3	2.13	0.48
14:O:185:MET:SD	14:O:185:MET:C	2.96	0.48
6:X:113:LEU:O	6:X:117:GLU:HG3	2.14	0.48
51:a:201:CDL:H541	48:b:201:PEE:C12	2.44	0.48
1:A:98:LYS:NZ	47:A:503:NAI:O3B	2.43	0.48
2:B:72:MET:HE2	16:Q:260:GLU:HG2	1.96	0.48
12:M:358:LEU:HD12	12:M:366:LEU:HD21	1.96	0.48
14:O:179:ALA:HB3	14:O:185:MET:HG2	1.95	0.48
14:O:242:GLY:O	14:O:245:VAL:HG12	2.13	0.48
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.53	0.48
27:d:64:TYR:N	27:d:64:TYR:CD1	2.81	0.48
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.48
34:k:28:SER:HB3	36:m:23:LYS:CG	2.39	0.48
34:k:56:ALA:O	34:k:59:MET:HG3	2.14	0.48
41:s:236:ALA:HB1	41:s:259:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:561:PRO:O	12:M:564:CYS:HB2	2.14	0.48
5:F:71:PHE:CZ	12:M:334:GLN:NE2	2.81	0.48
12:M:372:PHE:CD1	12:M:373:PRO:HD2	2.49	0.48
20:V:38:ALA:HA	51:k:101:CDL:H232	1.96	0.48
24:a:160:MET:SD	24:a:168:TRP:HB2	2.54	0.48
33:j:22:PHE:HA	41:s:60:PRO:HG3	1.95	0.48
13:N:25:ARG:HH21	13:N:66:THR:HG21	1.79	0.47
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.95	0.47
34:k:6:MET:HE3	36:m:119:PHE:CB	2.44	0.47
35:l:488:MET:O	35:l:492:ILE:HG12	2.14	0.47
35:l:515:TYR:OH	39:p:70:GLU:OE2	2.22	0.47
35:l:561:ILE:HG13	35:l:562:LEU:H	1.78	0.47
16:Q:144:MET:HE3	16:Q:222:MET:CB	2.43	0.47
33:j:19:LEU:HD11	48:j:202:PEE:H56	1.96	0.47
35:l:475:MET:HB3	43:v:52:MET:HE1	1.95	0.47
44:w:63:ASP:O	44:w:206:TYR:HA	2.15	0.47
5:F:68:ARG:HA	5:F:74:GLU:HB3	1.95	0.47
32:i:117:GLU:OE1	35:l:587:TYR:CE2	2.67	0.47
33:j:33:LYS:HG2	41:s:61:LEU:HD11	1.96	0.47
51:k:101:CDL:H161	51:k:101:CDL:H191	1.62	0.47
44:w:40:PRO:O	44:w:44:VAL:HG23	2.14	0.47
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.97	0.47
1:A:267:ARG:HH11	1:A:336:LEU:HD12	1.79	0.47
1:A:326:LEU:HD11	1:A:363:ILE:HD11	1.95	0.47
4:E:101:THR:HG23	15:P:219:VAL:O	2.14	0.47
12:M:371:VAL:H	12:M:482:GLN:HE22	1.62	0.47
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.96	0.47
51:a:201:CDL:H111	48:b:201:PEE:H60	1.96	0.47
51:l:702:CDL:H591	51:l:702:CDL:H331	1.97	0.47
44:w:132:GLN:HE22	57:w:401:ADP:HN62	1.63	0.47
49:C:303:PLX:H24	49:C:303:PLX:H81	1.96	0.47
51:l:201:CDL:OB7	13:N:6:VAL:O	2.33	0.47
12:M:483:ARG:HH11	12:M:489:ILE:HD11	1.78	0.47
17:S:65:GLY:C	17:S:67:GLU:N	2.73	0.47
26:c:173:ASP:OD1	26:c:176:LYS:HD3	2.15	0.47
32:i:335:LEU:HD21	51:r:504:CDL:H391	1.95	0.47
51:k:101:CDL:H162	35:l:589:LEU:HD11	1.96	0.47
49:r:502:PLX:H251	49:r:502:PLX:H51	1.41	0.47
48:C:302:PEE:O5	48:C:302:PEE:H52	2.14	0.47
17:S:69:ILE:HG22	17:S:69:ILE:O	2.15	0.47
6:X:82:ARG:HH12	35:l:440:LEU:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.48	0.47
49:g:201:PLX:H102	49:g:201:PLX:H71	1.60	0.47
34:k:16:LEU:HD23	51:k:101:CDL:H841	1.97	0.47
51:n:101:CDL:H541	51:n:101:CDL:C58	2.44	0.47
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.97	0.47
1:A:227:PRO:HD2	12:M:94:MET:SD	2.55	0.47
1:A:357:MET:HB3	1:A:361:THR:HG21	1.95	0.47
3:C:41:SER:HB3	3:C:44:GLU:HG2	1.97	0.47
3:C:126:GLU:HG3	33:j:33:LYS:NZ	2.29	0.47
6:G:83:VAL:HG13	6:G:122:MET:HE1	1.97	0.47
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.95	0.47
7:H:59:VAL:HG22	7:H:68:LEU:HD21	1.96	0.47
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.50	0.47
9:J:49:SER:HB2	15:P:225:GLU:HG2	1.97	0.47
53:J:402:UQ:H221	53:J:402:UQ:H201	1.66	0.47
12:M:58:MET:HE2	12:M:104:THR:HB	1.96	0.47
15:P:161:LYS:CD	16:Q:286:TYR:CE1	2.97	0.47
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.50	0.47
18:T:69:ASP:O	18:T:73:GLU:HG3	2.14	0.47
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.96	0.47
35:l:298:ILE:O	35:l:302:VAL:HG23	2.15	0.47
35:l:571:MET:HB3	35:l:571:MET:HE2	1.83	0.47
43:v:43:GLN:HA	43:v:46:MET:HE2	1.96	0.47
44:w:238:GLU:OE2	44:w:242:LYS:CD	2.56	0.47
2:B:143:THR:O	18:T:41:THR:HG21	2.15	0.47
4:E:30:ARG:O	4:E:34:GLU:HG3	2.15	0.47
22:Y:62:SER:OG	35:l:371:THR:OG1	2.29	0.47
35:l:530:PRO:HA	35:l:534:HIS:ND1	2.30	0.47
40:r:59:ASP:CG	40:r:245:ARG:HH22	2.23	0.47
40:r:201:MET:HE2	48:r:501:PEE:H78	1.97	0.47
1:A:201:ALA:HB1	14:O:121:MET:HB2	1.96	0.47
48:C:302:PEE:H75	48:C:302:PEE:H68	1.53	0.47
12:M:464:GLN:O	12:M:468:GLU:OE1	2.33	0.47
16:Q:271:ARG:NH1	41:s:279:ARG:O	2.43	0.47
35:l:603:ASN:ND2	35:l:603:ASN:C	2.73	0.47
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.43	0.47
13:N:22:GLY:O	13:N:26:VAL:HG12	2.15	0.47
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	1.97	0.47
17:S:23:THR:HG22	17:S:27:HIS:CD2	2.50	0.47
51:l:702:CDL:HA61	51:l:702:CDL:H312	1.60	0.47
51:r:504:CDL:H351	51:r:504:CDL:H381	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:HB2	1:A:242:VAL:HG21	1.97	0.46
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.49	0.46
12:M:158:ARG:NH1	12:M:202:ASN:OD1	2.48	0.46
15:P:207:TYR:C	15:P:224:VAL:CG2	2.86	0.46
29:f:30:TYR:N	44:w:99:GLY:O	2.34	0.46
32:i:95:MET:HE2	32:i:149:ILE:HA	1.95	0.46
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.96	0.46
32:i:232:HIS:HB3	32:i:311:MET:HE1	1.97	0.46
40:r:300:ALA:O	40:r:308:SER:HB3	2.15	0.46
51:s:401:CDL:H141	51:s:401:CDL:H171	1.70	0.46
1:A:122:PRO:HG2	1:A:322:SER:HB3	1.97	0.46
2:B:120:GLU:HB2	2:B:130:ILE:HD12	1.97	0.46
12:M:456:ALA:O	12:M:499:ASN:ND2	2.47	0.46
17:S:31:ASN:ND2	17:S:60:TYR:CZ	2.83	0.46
21:W:12:PRO:CB	21:W:13:PRO:HD2	2.45	0.46
30:g:3:MET:HG2	30:g:4:MET:HG2	1.98	0.46
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.97	0.46
44:w:256:LEU:HD21	44:w:276:LEU:HD21	1.97	0.46
16:Q:104:GLU:OE1	41:s:282:TYR:OH	2.33	0.46
17:S:1:MET:HE3	17:S:1:MET:HB3	1.77	0.46
51:V:202:CDL:H872	51:V:202:CDL:H841	1.77	0.46
51:a:201:CDL:H611	35:l:13:THR:HG22	1.97	0.46
27:d:127:LYS:O	27:d:130:GLU:HG3	2.14	0.46
40:r:203:PHE:O	40:r:207:MET:HG2	2.15	0.46
42:u:83:THR:HA	42:u:86:TRP:CD1	2.50	0.46
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.71	0.46
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.97	0.46
22:Y:69:ILE:HD13	35:l:383:MET:HE2	1.97	0.46
25:b:106:PRO:HG2	25:b:120:MET:SD	2.55	0.46
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.50	0.46
36:m:126:VAL:HG23	36:m:127:ILE:HG23	1.96	0.46
20:V:67:GLY:HA2	51:V:201:CDL:H221	1.97	0.46
35:l:285:THR:HA	35:l:308:SER:HA	1.98	0.46
37:n:42:SER:O	37:n:46:LYS:HB2	2.16	0.46
1:A:418:GLN:NE2	12:M:152:ARG:NH2	2.63	0.46
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.19	0.46
1:A:121:GLU:OE2	1:A:322:SER:N	2.48	0.46
48:Q:501:PEE:H7	35:l:567:SER:HB3	1.98	0.46
17:S:65:GLY:O	17:S:67:GLU:N	2.48	0.46
30:g:2:THR:N	30:g:5:SER:OG	2.46	0.46
30:g:81:GLN:NE2	32:i:341:PRO:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.98	0.46
34:k:54:THR:O	34:k:57:ASN:ND2	2.49	0.46
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.50	0.46
8:I:18:ARG:HD3	16:Q:253:PHE:CE2	2.51	0.46
17:S:57:VAL:HG21	17:S:62:VAL:HG21	1.97	0.46
32:i:84:TRP:HH2	34:k:59:MET:HE3	1.81	0.46
35:l:480:THR:HG21	43:v:88:ASP:HB3	1.98	0.46
40:r:191:SER:HB3	48:r:501:PEE:H3	1.98	0.46
1:A:420:GLU:OE2	1:A:433:TRP:NE1	2.43	0.46
8:I:69:VAL:O	15:P:76:VAL:HB	2.16	0.46
9:J:303:ARG:HB2	9:J:316:ARG:HD3	1.97	0.46
21:W:23:ARG:HD3	21:W:25:LEU:HD12	1.97	0.46
35:l:228:GLY:HA3	48:l:704:PEE:H38	1.98	0.46
51:l:703:CDL:C31	51:l:703:CDL:C71	2.86	0.46
3:C:184:ILE:O	3:C:187:GLU:HG2	2.15	0.46
5:F:59:SER:OG	5:F:60:ASP:N	2.48	0.46
12:M:166:GLY:HA2	12:M:213:MET:SD	2.55	0.46
20:V:53:VAL:HG12	51:k:101:CDL:H341	1.98	0.46
29:f:55:TRP:O	29:f:59:ILE:HG12	2.15	0.46
35:l:356:ILE:CD1	35:l:425:ARG:HH11	2.25	0.46
44:w:49:THR:O	44:w:53:LEU:HD23	2.15	0.46
44:w:80:LYS:HD2	44:w:270:VAL:HG21	1.97	0.46
44:w:185:GLU:O	44:w:189:GLU:HG3	2.15	0.46
1:A:320:GLY:HA3	1:A:349:LEU:O	2.16	0.45
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.56	0.45
19:U:27:GLY:O	19:U:31:ILE:HG12	2.16	0.45
25:b:100:ARG:NH2	27:d:119:GLU:HG2	2.30	0.45
35:l:383:MET:HB3	35:l:386:LEU:HD12	1.98	0.45
41:s:9:LEU:O	41:s:13:ILE:HG12	2.16	0.45
51:s:401:CDL:H362	51:s:401:CDL:H331	1.57	0.45
11:L:67:VAL:HB	11:L:72:ILE:HD11	1.97	0.45
28:e:90:VAL:HG11	40:r:78:MET:HE3	1.98	0.45
37:n:50:ARG:HE	37:n:53:GLU:CD	2.23	0.45
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.31	0.45
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.98	0.45
7:H:67:LYS:HA	7:H:70:GLU:HG2	1.98	0.45
25:b:123:PHE:CZ	43:v:61:HIS:HB2	2.52	0.45
28:e:129:ARG:HA	28:e:134:LEU:HD12	1.97	0.45
48:l:704:PEE:H82	48:l:704:PEE:H74	1.76	0.45
40:r:196:TRP:HB2	40:r:253:LEU:HD23	1.97	0.45
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:90:ASN:HD21	14:O:69:ASN:HD21	1.65	0.45
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.97	0.45
12:M:576:GLY:HA2	12:M:579:MET:HE2	1.98	0.45
14:O:61:LYS:HD3	14:O:61:LYS:HA	1.76	0.45
17:S:27:HIS:CE1	17:S:36:LYS:HD3	2.51	0.45
35:l:312:LEU:HA	35:l:315:VAL:HG22	1.97	0.45
40:r:266:MET:O	40:r:269:MET:HB3	2.16	0.45
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.99	0.45
10:K:100:GLN:HB3	14:O:71:PRO:HA	1.98	0.45
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.97	0.45
35:l:341:MET:HE2	35:l:454:ILE:HG12	1.98	0.45
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.99	0.45
35:l:534:HIS:CG	48:l:704:PEE:H13	2.48	0.45
38:o:4:PRO:HD2	39:p:73:TYR:CE2	2.51	0.45
39:p:100:PRO:HD3	40:r:419:TYR:CE2	2.52	0.45
42:u:47:ARG:HD2	42:u:47:ARG:HA	1.80	0.45
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.98	0.45
8:I:96:THR:HB	8:I:97:PRO:HD2	1.98	0.45
11:L:169:ARG:HD2	12:M:422:TRP:O	2.16	0.45
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.46	0.45
15:P:68:ILE:C	15:P:70:PRO:HD3	2.41	0.45
48:Q:501:PEE:C37	48:Q:501:PEE:C23	2.86	0.45
51:V:202:CDL:H792	51:V:202:CDL:H761	1.62	0.45
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.98	0.45
35:l:137:LEU:N	35:l:196:TRP:O	2.46	0.45
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.98	0.45
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.99	0.45
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.99	0.45
4:E:99:GLN:C	4:E:101:THR:N	2.74	0.45
8:I:14:TRP:CD1	21:W:28:ARG:HH22	2.34	0.45
8:I:27:ARG:H	8:I:27:ARG:HD3	1.81	0.45
26:c:68:ASP:CG	26:c:70:MET:HG2	2.40	0.45
34:k:80:MET:HE1	36:m:174:GLY:HA2	1.98	0.45
2:B:96:ARG:NH1	16:Q:217:VAL:O	2.47	0.45
5:F:30:SER:OG	5:F:63:PRO:HG3	2.17	0.45
5:F:61:VAL:HG13	5:F:62:GLN:H	1.81	0.45
8:I:66:PRO:HB3	15:P:79:SER:HA	1.98	0.45
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.44	0.45
48:Q:501:PEE:H42	48:Q:501:PEE:C21	2.45	0.45
34:k:4:VAL:O	34:k:8:ILE:HG12	2.17	0.45
35:l:288:THR:HG21	35:l:307:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:533:MET:HA	35:l:533:MET:HE2	1.99	0.45
40:r:1:MET:HE3	40:r:1:MET:HB2	1.81	0.45
43:v:4:HIS:CD2	43:v:4:HIS:H	2.34	0.45
44:w:58:LYS:O	44:w:60:ILE:HG13	2.17	0.45
3:C:103:MET:HE1	3:C:121:TYR:HB2	1.99	0.45
49:C:303:PLX:O2	49:C:303:PLX:H11	2.16	0.45
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.47	0.45
16:Q:36:GLN:HG3	40:r:137:GLY:O	2.16	0.45
25:b:87:LYS:HD3	25:b:88:TYR:CZ	2.52	0.45
27:d:106:ILE:HG13	27:d:135:VAL:HG21	1.99	0.45
33:j:67:LEU:HD22	36:m:59:ILE:HD12	1.98	0.45
48:j:202:PEE:H1	48:j:202:PEE:C31	2.41	0.45
36:m:42:GLY:HA2	36:m:45:LEU:HD12	1.99	0.45
38:o:118:GLU:OE1	38:o:120:LYS:HG2	2.17	0.45
39:p:65:ARG:O	39:p:69:GLU:HG3	2.17	0.45
39:p:98:LYS:O	40:r:419:TYR:HE2	2.00	0.45
3:C:167:PRO:HD3	16:Q:223:HIS:HD2	1.78	0.45
5:F:23:LEU:HD23	5:F:23:LEU:H	1.82	0.45
14:O:160:VAL:HG11	14:O:173:GLU:OE2	2.16	0.45
51:V:201:CDL:H512	35:l:580:GLN:HE22	1.81	0.45
6:X:84:LEU:O	6:X:88:LYS:HG3	2.17	0.45
30:g:32:ARG:HB3	32:i:339:MET:HE1	1.98	0.45
32:i:81:SER:O	32:i:83:GLN:N	2.47	0.45
32:i:266:ILE:O	32:i:270:MET:HG3	2.16	0.45
51:k:101:CDL:H581	51:k:101:CDL:H611	1.60	0.45
35:l:271:LYS:O	35:l:275:THR:HG23	2.17	0.45
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.99	0.45
1:A:208:GLU:OE1	46:A:502:FMN:HM83	2.17	0.44
12:M:326:VAL:HG13	12:M:567:ILE:HD13	1.99	0.44
6:X:89:LEU:HD21	23:Z:22:TRP:HD1	1.82	0.44
28:e:111:ASP:OD1	28:e:115:GLN:HG2	2.17	0.44
32:i:294:MET:HE2	40:r:130:LEU:HD21	1.99	0.44
35:l:422:TYR:CD1	35:l:422:TYR:C	2.95	0.44
40:r:419:TYR:CD1	40:r:419:TYR:O	2.70	0.44
44:w:160:GLU:O	44:w:161:ARG:HG3	2.17	0.44
2:B:99:GLY:N	2:B:170:GLY:O	2.50	0.44
14:O:180:CYS:SG	54:O:301:FES:S1	3.15	0.44
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.51	0.44
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.25	0.44
20:V:110:ILE:HG12	48:l:701:PEE:H49	1.98	0.44
25:b:16:ARG:O	25:b:20:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:111:LYS:CE	35:l:197:ASP:OD2	2.63	0.44
51:n:101:CDL:HB31	42:u:172:MET:HE2	1.99	0.44
44:w:49:THR:HG21	44:w:291:PHE:HB3	1.99	0.44
3:C:71:CYS:HB3	45:C:301:SF4:S4	2.52	0.44
9:J:238:GLN:NE2	9:J:267:GLY:O	2.45	0.44
53:J:402:UQ:H111	53:J:402:UQ:C15	2.32	0.44
17:S:39:ALA:HB2	17:S:48:MET:HE2	1.99	0.44
21:W:56:GLU:OE1	21:W:59:ARG:NH2	2.37	0.44
12:M:598:ASN:HB2	12:M:602:ARG:O	2.18	0.44
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.99	0.44
27:d:148:ALA:O	27:d:149:HIS:CB	2.61	0.44
32:i:57:THR:HA	34:k:77:LEU:HD13	1.99	0.44
35:l:137:LEU:HD13	35:l:186:MET:HG2	2.00	0.44
35:l:230:HIS:N	35:l:231:PRO:HD3	2.33	0.44
51:l:703:CDL:H641	51:l:703:CDL:H612	1.67	0.44
36:m:129:ASP:O	36:m:130:THR:OG1	2.31	0.44
38:o:59:VAL:HG22	40:r:423:ILE:CD1	2.48	0.44
38:o:121:LEU:HD23	38:o:123:GLN:NE2	2.32	0.44
3:C:53:LEU:HD22	49:C:303:PLX:H322	1.99	0.44
5:F:87:VAL:HA	5:F:90:THR:HG22	2.00	0.44
9:J:168:SER:OG	9:J:169:HIS:N	2.50	0.44
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.99	0.44
16:Q:120:THR:HG23	16:Q:135:TYR:CD1	2.52	0.44
20:V:140:LYS:HE2	24:a:158:ARG:HD3	1.99	0.44
32:i:117:GLU:OE1	35:l:587:TYR:HE2	2.01	0.44
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.98	0.44
35:l:320:ASN:HD22	35:l:320:ASN:C	2.25	0.44
41:s:24:GLU:OE1	41:s:274:ARG:NH1	2.47	0.44
9:J:251:ASN:ND2	9:J:338:LEU:O	2.42	0.44
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.00	0.44
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.83	0.44
6:X:129:GLU:HB2	39:p:82:PHE:CD2	2.53	0.44
49:j:203:PLX:H161	49:j:203:PLX:H132	1.54	0.44
48:l:704:PEE:H55	40:r:405:LEU:HD13	1.99	0.44
12:M:168:LEU:HD21	12:M:710:CYS:SG	2.58	0.44
48:W:201:PEE:H33	48:W:201:PEE:H41	2.00	0.44
26:c:58:ARG:HD2	38:o:35:GLU:HG3	1.99	0.44
32:i:110:PRO:HG2	35:l:594:THR:CG2	2.47	0.44
35:l:421:ALA:HB2	51:l:703:CDL:H551	1.98	0.44
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.00	0.44
1:A:88:ARG:O	1:A:126:LYS:NZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ILE:CG2	3:C:142:TYR:HB2	2.48	0.44
10:K:98:MET:HE3	10:K:98:MET:HB3	1.86	0.44
12:M:245:THR:HB	12:M:264:SER:HB2	2.00	0.44
26:c:101:TRP:O	26:c:101:TRP:CE3	2.71	0.44
40:r:122:PHE:CZ	40:r:206:LYS:HG3	2.51	0.44
1:A:339:PHE:CE1	1:A:349:LEU:HD23	2.53	0.44
6:G:133:ILE:HD12	6:G:133:ILE:HA	1.93	0.44
22:Y:47:PHE:HZ	35:l:364:LYS:HB3	1.83	0.44
26:c:101:TRP:O	26:c:101:TRP:HE3	2.00	0.44
27:d:6:ASP:HB3	27:d:9:VAL:HG22	2.00	0.44
33:j:4:MET:HE1	36:m:5:ILE:HD13	2.00	0.44
40:r:216:LEU:HD23	40:r:287:ALA:HB1	2.00	0.44
40:r:243:MET:HB3	40:r:301:ILE:HG21	2.00	0.44
9:J:81:ILE:O	9:J:83:PRO:HD3	2.18	0.43
9:J:250:ILE:HG22	9:J:254:LYS:HE2	2.00	0.43
11:L:117:THR:HG21	15:P:229:GLU:HG3	2.00	0.43
14:O:177:LEU:HD13	14:O:185:MET:HE1	2.00	0.43
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.00	0.43
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.53	0.43
35:l:245:ALA:O	35:l:249:SER:HB3	2.18	0.43
35:l:249:SER:OG	35:l:336:LYS:HG3	2.18	0.43
51:l:702:CDL:H812	49:r:503:PLX:H202	1.99	0.43
38:o:59:VAL:HG22	40:r:423:ILE:HD13	2.00	0.43
51:s:401:CDL:H372	51:s:401:CDL:H401	1.59	0.43
15:P:196:HIS:HA	15:P:197:PRO:HD3	1.76	0.43
16:Q:104:GLU:OE1	41:s:282:TYR:HE1	1.90	0.43
19:U:19:LEU:HB3	48:j:201:PEE:H57	2.01	0.43
27:d:107:GLN:HE22	35:l:194:ASN:HD21	1.57	0.43
36:m:65:LEU:HD13	41:s:139:THR:HG21	2.00	0.43
40:r:256:TYR:O	40:r:256:TYR:CD2	2.71	0.43
48:r:501:PEE:H62	48:r:501:PEE:H68	1.62	0.43
11:L:79:ILE:HB	11:L:147:VAL:HG22	1.99	0.43
16:Q:36:GLN:CD	40:r:137:GLY:O	2.52	0.43
51:V:201:CDL:H532	35:l:577:VAL:HG22	1.99	0.43
36:m:165:VAL:O	36:m:168:ILE:HG12	2.19	0.43
44:w:65:ASN:O	44:w:66:ILE:C	2.61	0.43
1:A:66:LYS:HE3	1:A:188:GLY:C	2.44	0.43
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.00	0.43
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.43
51:a:201:CDL:H531	48:b:201:PEE:H56	1.99	0.43
27:d:67:GLU:OE2	28:e:124:ARG:NH2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:20:VAL:HG13	32:i:29:ILE:HG23	2.00	0.43
33:j:17:LEU:HD23	33:j:17:LEU:HA	1.85	0.43
48:l:704:PEE:H7	48:l:704:PEE:C11	2.47	0.43
9:J:201:ILE:HG22	9:J:203:PRO:HD3	2.01	0.43
12:M:382:ARG:HG2	12:M:386:LEU:HD11	2.00	0.43
13:N:85:GLU:HB2	13:N:98:PRO:HB3	2.00	0.43
14:O:131:HIS:HD2	14:O:133:GLN:NE2	2.15	0.43
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.54	0.43
25:b:19:ARG:HA	39:p:171:VAL:HG13	2.00	0.43
40:r:11:LEU:HD23	40:r:14:MET:HE1	2.01	0.43
1:A:122:PRO:HA	14:O:176:CYS:SG	2.59	0.43
1:A:201:ALA:O	14:O:119:TYR:HB3	2.19	0.43
12:M:382:ARG:HG2	12:M:386:LEU:CD1	2.49	0.43
16:Q:41:VAL:HG23	28:e:55:LEU:HD21	2.01	0.43
17:S:54:ILE:HD11	42:u:21:SER:HA	2.00	0.43
18:T:43:GLN:C	18:T:43:GLN:CD	2.86	0.43
51:V:201:CDL:H622	51:V:201:CDL:H592	1.92	0.43
24:a:135:LYS:HD2	37:n:32:ASP:HB2	2.00	0.43
51:a:201:CDL:H171	51:a:201:CDL:H712	2.01	0.43
32:i:270:MET:O	32:i:275:SER:HB3	2.19	0.43
39:p:150:ARG:HD2	39:p:150:ARG:HA	1.85	0.43
1:A:426:ALA:HB3	46:A:502:FMN:HM82	2.01	0.43
51:I:201:CDL:H711	41:s:43:TYR:OH	2.18	0.43
9:J:58:VAL:O	9:J:83:PRO:HD2	2.19	0.43
12:M:163:LYS:HD3	12:M:173:MET:HG3	2.01	0.43
12:M:716:GLU:O	12:M:716:GLU:HG2	2.19	0.43
26:c:127:ASN:O	26:c:131:LYS:HE2	2.19	0.43
27:d:42:ASP:O	27:d:46:THR:HG23	2.18	0.43
32:i:310:ASN:HB2	44:w:309:THR:HG22	2.01	0.43
48:l:701:PEE:H58	48:l:701:PEE:H19	2.01	0.43
42:u:80:GLU:HB2	42:u:81:PRO:HD3	2.00	0.43
43:v:70:LYS:HG2	43:v:80:CYS:SG	2.58	0.43
44:w:242:LYS:HA	44:w:246:LEU:HD12	2.01	0.43
1:A:423:THR:HB	45:A:501:SF4:S4	2.59	0.43
12:M:76:ARG:NH2	12:M:90:ALA:HB2	2.34	0.43
12:M:488:ALA:HB1	12:M:679:LEU:HG	2.01	0.43
17:S:12:MET:HE3	41:s:20:LEU:HB2	2.00	0.43
51:a:201:CDL:H361	51:a:201:CDL:H392	1.40	0.43
28:e:58:ASP:OD2	44:w:326:ARG:NE	2.37	0.43
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.01	0.43
42:u:10:LEU:HD12	42:u:10:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:65:GLU:O	4:E:69:LYS:HG3	2.19	0.43
12:M:329:MET:HG2	12:M:565:PHE:CG	2.54	0.43
20:V:141:VAL:HG13	24:a:157:ARG:HB3	2.00	0.43
51:V:202:CDL:H321	51:V:202:CDL:H352	1.79	0.43
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.54	0.43
35:l:316:THR:HG23	35:l:325:ALA:HB2	1.99	0.43
40:r:266:MET:HE2	40:r:396:MET:HE2	2.01	0.43
41:s:54:LYS:HB3	41:s:54:LYS:HE3	1.81	0.43
41:s:87:VAL:HG23	41:s:88:PRO:HD3	2.01	0.43
1:A:56:ALA:HB1	1:A:61:ASP:OD2	2.19	0.43
5:F:38:GLU:HA	12:M:667:GLN:HE21	1.84	0.43
12:M:339:ALA:HB3	12:M:542:PRO:HG3	2.01	0.43
14:O:243:PHE:CD1	14:O:243:PHE:C	2.95	0.43
35:l:180:ILE:HD12	48:l:704:PEE:H81	2.01	0.43
35:l:227:PHE:N	35:l:284:THR:OG1	2.52	0.43
35:l:251:THR:O	35:l:254:VAL:HG22	2.19	0.43
51:l:703:CDL:CA3	51:l:703:CDL:CA7	2.97	0.43
4:E:23:ARG:HH12	11:L:51:GLN:HB3	1.84	0.42
12:M:299:ARG:HH11	12:M:705:GLN:HG3	1.83	0.42
13:N:55:PHE:CE2	13:N:58:ARG:HG3	2.54	0.42
15:P:161:LYS:CG	16:Q:286:TYR:CZ	3.02	0.42
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.00	0.42
20:V:50:LEU:HA	20:V:53:VAL:HG22	2.01	0.42
22:Y:100:LEU:HB2	43:v:111:ARG:HH12	1.84	0.42
23:Z:58:ALA:O	35:l:434:LYS:NZ	2.43	0.42
32:i:54:GLU:OE1	34:k:95:LEU:HB2	2.18	0.42
32:i:93:VAL:HG22	35:l:603:ASN:OD1	2.19	0.42
34:k:50:ASN:C	34:k:50:ASN:ND2	2.77	0.42
35:l:119:LYS:NZ	51:l:702:CDL:OA3	2.44	0.42
51:n:101:CDL:H551	42:u:169:PHE:HE1	1.84	0.42
40:r:210:TYR:CG	40:r:268:GLY:HA3	2.54	0.42
9:J:223:PHE:O	9:J:225:GLY:N	2.50	0.42
33:j:23:TRP:CZ2	48:j:202:PEE:H55	2.54	0.42
40:r:339:SER:HB3	40:r:344:LEU:HD22	2.00	0.42
8:I:28:TYR:CE2	13:N:55:PHE:HB3	2.54	0.42
23:Z:13:LYS:HA	23:Z:13:LYS:HD2	1.79	0.42
28:e:98:VAL:HG22	40:r:36:LEU:HB2	2.01	0.42
30:g:51:ARG:HG3	30:g:51:ARG:NH1	2.34	0.42
32:i:147:GLN:H	32:i:147:GLN:CD	2.28	0.42
33:j:38:GLU:HB2	33:j:41:PHE:O	2.19	0.42
35:l:27:TYR:O	35:l:115:ASN:ND2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:529:TYR:CZ	35:l:533:MET:HG3	2.54	0.42
35:l:541:ASN:C	35:l:541:ASN:HD22	2.27	0.42
40:r:16:TRP:HB3	51:r:504:CDL:H522	2.01	0.42
1:A:125:CYS:SG	14:O:181:VAL:HG22	2.60	0.42
12:M:43:VAL:HG12	12:M:55:LYS:HD2	2.00	0.42
12:M:275:PRO:HB3	12:M:286:ILE:HG23	2.02	0.42
48:Q:501:PEE:H58	32:i:287:LEU:HB3	2.01	0.42
32:i:96:THR:HG22	32:i:100:MET:HE2	2.01	0.42
41:s:169:GLN:HG2	41:s:174:MET:HG3	2.01	0.42
42:u:83:THR:HA	42:u:86:TRP:NE1	2.34	0.42
1:A:367:ILE:HG13	1:A:438:LEU:HD13	2.01	0.42
3:C:126:GLU:HG3	33:j:33:LYS:HZ3	1.85	0.42
49:C:303:PLX:H22	49:C:303:PLX:H1A2	1.46	0.42
12:M:336:ASN:HD21	12:M:540:ASN:CB	2.32	0.42
33:j:5:LEU:HD21	41:s:3:MET:HG2	2.01	0.42
33:j:73:LEU:N	33:j:74:PRO:HD2	2.34	0.42
35:l:182:PHE:HD1	35:l:186:MET:HE2	1.85	0.42
35:l:483:PRO:HD2	35:l:486:MET:HE2	2.02	0.42
51:l:703:CDL:H312	51:l:703:CDL:H721	2.02	0.42
44:w:52:LYS:HE2	44:w:52:LYS:HB3	1.81	0.42
48:B:303:PEE:H36	48:B:303:PEE:H42	1.33	0.42
6:G:80:LYS:HE2	6:G:100:VAL:HG11	2.00	0.42
12:M:61:PRO:HB2	12:M:77:MET:HG3	2.00	0.42
12:M:647:GLU:HB2	12:M:654:VAL:HG11	2.01	0.42
16:Q:71:PRO:HA	16:Q:72:PRO:HD3	1.93	0.42
51:V:201:CDL:H342	51:V:201:CDL:H371	1.63	0.42
21:W:120:MET:O	21:W:121:MET:HB3	2.19	0.42
24:a:184:LYS:C	24:a:186:THR:H	2.28	0.42
35:l:166:THR:CG2	48:l:704:PEE:H2	2.50	0.42
35:l:407:TRP:CE2	35:l:411:MET:HE2	2.55	0.42
41:s:200:LEU:HD13	41:s:282:TYR:HB2	2.01	0.42
41:s:294:LEU:HB3	41:s:295:PRO:HD3	2.01	0.42
1:A:132:ARG:O	10:K:75:ASN:ND2	2.53	0.42
1:A:250:VAL:O	1:A:251:SER:C	2.62	0.42
1:A:250:VAL:O	1:A:253:THR:N	2.52	0.42
10:K:75:ASN:OD1	10:K:78:HIS:HD2	2.03	0.42
15:P:43:THR:HA	15:P:47:ILE:HD13	2.01	0.42
32:i:280:THR:O	32:i:284:MET:HG2	2.20	0.42
35:l:71:LEU:HG	40:r:307:TRP:CZ2	2.55	0.42
41:s:222:MET:HA	41:s:225:MET:CE	2.45	0.42
12:M:696:MET:HB3	12:M:702:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:73:LYS:O	16:Q:75:THR:N	2.53	0.42
6:X:97:LYS:HE2	6:X:107:ASP:O	2.20	0.42
29:f:68:GLU:HG2	30:g:21:ARG:NE	2.33	0.42
51:k:101:CDL:H192	35:l:593:ILE:HD11	2.02	0.42
51:r:504:CDL:H872	51:r:504:CDL:H841	1.71	0.42
43:v:93:LEU:HA	43:v:96:VAL:HG22	2.01	0.42
4:E:50:PHE:O	4:E:100:ARG:NH1	2.52	0.42
12:M:476:LEU:HB3	12:M:515:ILE:HD13	2.02	0.42
14:O:131:HIS:CD2	14:O:133:GLN:NE2	2.88	0.42
14:O:179:ALA:CB	14:O:185:MET:HG2	2.50	0.42
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.35	0.42
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.55	0.42
26:c:155:PRO:HD3	43:v:4:HIS:NE2	2.35	0.42
31:h:17:TRP:CE3	31:h:18:MET:HB2	2.55	0.42
51:k:101:CDL:H632	51:k:101:CDL:H602	1.78	0.42
35:l:9:LEU:O	35:l:13:THR:HG23	2.20	0.42
51:l:702:CDL:H401	40:r:445:LEU:HD22	2.01	0.42
40:r:408:LEU:HD23	40:r:408:LEU:HA	1.91	0.42
5:F:33:VAL:O	5:F:37:ILE:HG12	2.20	0.42
9:J:171:ASN:HA	9:J:327:MET:HE3	2.01	0.42
20:V:56:THR:HG21	51:k:101:CDL:H361	2.02	0.42
23:Z:52:ARG:HD3	35:l:435:PRO:O	2.20	0.42
27:d:82:ILE:HD12	27:d:82:ILE:HA	1.89	0.42
30:g:12:PRO:HG3	31:h:8:LYS:HD2	2.02	0.42
35:l:557:TRP:O	35:l:561:ILE:HG12	2.20	0.42
39:p:82:PHE:HB2	39:p:85:SER:OG	2.20	0.42
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.02	0.42
41:s:313:SER:O	41:s:313:SER:OG	2.33	0.42
1:A:382:CYS:HB3	1:A:424:ILE:HD12	2.01	0.41
9:J:135:GLU:HG3	9:J:140:ASP:CA	2.33	0.41
12:M:323:LEU:HD23	12:M:323:LEU:HA	1.93	0.41
24:a:78:THR:HB	28:e:96:SER:HB3	2.02	0.41
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.20	0.41
35:l:180:ILE:CD1	48:l:704:PEE:H79	2.50	0.41
38:o:58:GLY:HA2	40:r:425:ASN:ND2	2.35	0.41
40:r:119:TYR:CZ	40:r:161:LEU:HB2	2.55	0.41
3:C:173:LEU:O	3:C:177:ILE:HG12	2.19	0.41
48:C:302:PEE:H12	33:j:26:GLN:NE2	2.35	0.41
8:I:12:ARG:HB3	8:I:20:LEU:HD12	2.02	0.41
12:M:35:PHE:O	12:M:101:ASN:HA	2.20	0.41
12:M:51:GLN:O	12:M:55:LYS:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:144:TYR:CZ	13:N:145:LYS:HD3	2.55	0.41
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.35	0.41
20:V:23:TYR:O	20:V:26:THR:HG22	2.20	0.41
25:b:106:PRO:HG3	43:v:45:GLU:HG2	2.02	0.41
32:i:182:SER:HB2	32:i:293:TYR:OH	2.19	0.41
35:l:136:ASN:HA	35:l:197:ASP:HA	2.01	0.41
35:l:566:THR:O	35:l:570:GLN:HG2	2.19	0.41
40:r:186:LEU:H	40:r:252:PRO:CD	2.32	0.41
44:w:135:LEU:HD23	44:w:135:LEU:HA	1.92	0.41
2:B:128:ILE:O	15:P:231:ARG:NH2	2.53	0.41
9:J:369:VAL:O	9:J:369:VAL:HG12	2.20	0.41
12:M:144:MET:HG3	16:Q:383:LYS:HG3	2.01	0.41
13:N:132:LYS:NZ	13:N:136:GLU:OE2	2.54	0.41
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.02	0.41
24:a:187:PRO:HG3	42:u:47:ARG:HG3	2.02	0.41
30:g:7:ARG:HG2	30:g:8:PRO:HD2	2.02	0.41
33:j:57:LEU:HD21	36:m:169:MET:SD	2.61	0.41
48:j:201:PEE:H30	48:j:201:PEE:H35	1.56	0.41
48:j:201:PEE:H77	48:j:201:PEE:H67	2.02	0.41
35:l:49:VAL:HG12	35:l:53:MET:HE3	2.02	0.41
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.01	0.41
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.02	0.41
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.60	0.41
9:J:207:PHE:HA	9:J:211:ASP:OD2	2.21	0.41
11:L:102:ASP:OD1	11:L:102:ASP:N	2.52	0.41
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.56	0.41
24:a:114:LYS:HB3	27:d:63:TYR:CD1	2.55	0.41
26:c:101:TRP:CE3	26:c:101:TRP:C	2.98	0.41
26:c:126:TRP:O	26:c:127:ASN:HB2	2.20	0.41
33:j:104:TYR:O	33:j:108:GLN:HG2	2.20	0.41
35:l:69:MET:CE	35:l:76:LEU:HD12	2.51	0.41
44:w:226:GLU:O	44:w:228:LYS:N	2.53	0.41
44:w:283:TRP:N	44:w:284:PRO:HD2	2.36	0.41
1:A:217:GLU:OE2	1:A:236:PHE:N	2.47	0.41
2:B:72:MET:HE3	16:Q:257:GLU:HA	2.03	0.41
8:I:13:ASN:ND2	8:I:19:ASP:HA	2.35	0.41
35:l:11:THR:HG21	35:l:47:SER:HB3	2.02	0.41
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.55	0.41
40:r:168:GLN:HB2	40:r:174:LEU:HG	2.03	0.41
44:w:76:GLU:HB3	44:w:80:LYS:HE3	2.01	0.41
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:OE2	16:Q:266:ARG:HB3	2.20	0.41
12:M:372:PHE:CG	12:M:373:PRO:HD2	2.56	0.41
20:V:19:HIS:CD2	20:V:20:ARG:HG3	2.55	0.41
32:i:13:VAL:HG13	32:i:36:ASN:ND2	2.35	0.41
35:l:535:ARG:NH1	38:o:11:LEU:O	2.51	0.41
48:l:701:PEE:H14	48:l:701:PEE:H20	1.76	0.41
40:r:71:TRP:CG	49:r:503:PLX:H341	2.55	0.41
3:C:147:TYR:CZ	15:P:197:PRO:HB3	2.56	0.41
48:C:302:PEE:H31	49:C:303:PLX:H391	2.03	0.41
9:J:119:VAL:HG23	9:J:120:VAL:HG13	2.02	0.41
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.53	0.41
32:i:20:VAL:HG11	32:i:137:ALA:HB1	2.02	0.41
36:m:16:GLY:HA2	51:s:401:CDL:H791	2.02	0.41
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.56	0.41
43:v:52:MET:HB2	43:v:55:GLN:HG3	2.01	0.41
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.01	0.41
2:B:39:LYS:HE2	8:I:110:GLN:O	2.21	0.41
9:J:163:LYS:HG2	9:J:259:LYS:HE2	2.01	0.41
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.56	0.41
29:f:43:LYS:HA	29:f:46:LEU:CD2	2.50	0.41
31:h:12:LEU:HD23	31:h:12:LEU:HA	1.89	0.41
35:l:561:ILE:HG13	35:l:562:LEU:N	2.36	0.41
49:r:502:PLX:H22	49:r:502:PLX:H1C3	1.77	0.41
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.61	0.41
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.81	0.41
2:B:96:ARG:HG3	2:B:208:ASP:OD2	2.21	0.41
3:C:70:ALA:HB2	16:Q:116:LEU:HD11	2.02	0.41
8:I:23:LYS:HD2	16:Q:253:PHE:CG	2.55	0.41
10:K:107:SER:HB3	10:K:110:HIS:ND1	2.36	0.41
11:L:59:LEU:HD12	11:L:59:LEU:HA	1.92	0.41
12:M:77:MET:HE2	12:M:117:MET:HE2	2.03	0.41
12:M:179:CYS:HG	45:M:802:SF4:FE1	1.37	0.41
12:M:354:LEU:HD12	12:M:354:LEU:HA	1.87	0.41
12:M:698:ASP:OD1	12:M:701:SER:OG	2.26	0.41
14:O:185:MET:SD	14:O:185:MET:O	2.79	0.41
16:Q:188:THR:HG21	16:Q:203:MET:HB2	2.03	0.41
17:S:12:MET:HE1	41:s:20:LEU:HD13	2.03	0.41
51:V:201:CDL:H601	51:V:201:CDL:H732	2.02	0.41
48:W:201:PEE:H35	48:W:201:PEE:H42	1.70	0.41
26:c:129:MET:HB3	35:l:528:TYR:CG	2.55	0.41
27:d:37:PHE:CD2	35:l:3:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.50	0.41
34:k:55:LEU:O	34:k:58:MET:HE3	2.21	0.41
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.56	0.41
35:l:568:PHE:HE2	48:l:701:PEE:H50	1.85	0.41
39:p:133:TRP:O	39:p:137:VAL:HG23	2.21	0.41
40:r:8:THR:O	40:r:11:LEU:HB2	2.20	0.41
40:r:186:LEU:H	40:r:252:PRO:HD2	1.84	0.41
43:v:52:MET:O	43:v:56:ARG:HG3	2.21	0.41
44:w:226:GLU:C	44:w:228:LYS:N	2.79	0.41
44:w:226:GLU:C	44:w:228:LYS:H	2.28	0.41
3:C:95:ALA:HB1	41:s:208:VAL:HG13	2.03	0.41
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.01	0.41
12:M:124:HIS:CG	12:M:125:PRO:HD2	2.55	0.41
13:N:85:GLU:H	13:N:85:GLU:CD	2.29	0.41
14:O:188:ILE:O	14:O:189:ASN:C	2.62	0.41
16:Q:52:MET:O	32:i:171:ASN:ND2	2.53	0.41
31:h:18:MET:HE1	34:k:59:MET:HB3	2.02	0.41
35:l:559:GLU:O	35:l:563:PRO:HD2	2.21	0.41
40:r:71:TRP:O	40:r:74:PRO:HD2	2.20	0.41
41:s:139:THR:HA	41:s:142:TYR:CE2	2.56	0.41
1:A:322:SER:HB2	1:A:370:LEU:HD13	2.02	0.40
2:B:131:GLU:OE2	2:B:144:ARG:NE	2.54	0.40
12:M:347:ASP:OD1	12:M:347:ASP:N	2.53	0.40
14:O:137:THR:HG22	14:O:138:THR:H	1.85	0.40
20:V:141:VAL:C	24:a:161:ARG:HH11	2.30	0.40
23:Z:23:LYS:HB3	23:Z:25:GLU:OE1	2.21	0.40
25:b:110:ILE:H	25:b:110:ILE:HD12	1.86	0.40
26:c:125:SER:OG	38:o:7:LYS:O	2.39	0.40
32:i:323:MET:HE3	32:i:323:MET:HB3	1.94	0.40
36:m:24:PRO:CB	36:m:89:VAL:HG11	2.37	0.40
40:r:306:PRO:HB3	40:r:458:LEU:HD12	2.03	0.40
41:s:2:PHE:O	41:s:6:ILE:HG13	2.21	0.40
42:u:31:HIS:NE2	42:u:111:VAL:HG21	2.36	0.40
1:A:314:LEU:HD11	1:A:317:VAL:HG23	2.03	0.40
3:C:133:MET:HE3	3:C:173:LEU:HB2	2.03	0.40
3:C:188:LYS:O	3:C:188:LYS:HG3	2.21	0.40
12:M:677:GLN:HG2	12:M:678:GLN:N	2.37	0.40
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.02	0.40
33:j:62:PHE:O	33:j:66:ASP:HB2	2.21	0.40
33:j:106:TRP:CD2	48:j:201:PEE:H15	2.55	0.40
51:l:703:CDL:H441	51:l:703:CDL:H471	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:13:PHE:HD1	36:m:39:VAL:HG23	1.86	0.40
41:s:52:ALA:CB	53:s:402:UQ:H23	2.51	0.40
1:A:294:VAL:O	1:A:337:MET:HB2	2.21	0.40
3:C:98:ARG:HB3	41:s:216:ALA:HB2	2.03	0.40
16:Q:50:ALA:HB1	34:k:98:CYS:SG	2.61	0.40
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	2.03	0.40
20:V:66:ILE:HD11	20:V:101:LEU:HB2	2.03	0.40
21:W:82:ARG:O	21:W:86:MET:HG3	2.21	0.40
28:e:143:ASP:HB3	28:e:146:LYS:NZ	2.36	0.40
34:k:51:THR:O	34:k:51:THR:OG1	2.37	0.40
35:l:71:LEU:HD13	35:l:71:LEU:HA	1.90	0.40
35:l:241:THR:HG21	35:l:344:GLY:HA3	2.03	0.40
41:s:84:THR:O	41:s:87:VAL:HG22	2.21	0.40
2:B:79:ARG:HH11	8:I:25:GLN:NE2	2.20	0.40
48:C:302:PEE:H31	49:C:303:PLX:C39	2.51	0.40
4:E:27:GLU:O	4:E:30:ARG:HG2	2.21	0.40
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.57	0.40
12:M:306:MET:HB2	12:M:583:ILE:HB	2.04	0.40
21:W:120:MET:HG2	36:m:126:VAL:O	2.21	0.40
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.57	0.40
25:b:32:GLU:HB3	39:p:115:TYR:CD1	2.56	0.40
27:d:115:GLN:HG2	35:l:62:ILE:HG12	2.03	0.40
32:i:320:THR:OG1	44:w:300:ASN:HA	2.22	0.40
32:i:323:MET:O	32:i:323:MET:HG2	2.20	0.40
35:l:73:THR:OG1	38:o:127:ILE:CG2	2.69	0.40
35:l:407:TRP:O	35:l:411:MET:HG2	2.22	0.40
1:A:50:ASP:HB3	1:A:55:GLY:HA3	2.03	0.40
2:B:72:MET:HE1	8:I:18:ARG:NH1	2.30	0.40
7:H:107:PRO:O	7:H:108:PRO:O	2.39	0.40
51:V:201:CDL:H512	51:V:201:CDL:H542	1.88	0.40
28:e:73:SER:C	28:e:75:GLY:H	2.29	0.40
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.02	0.40
48:j:201:PEE:H60	48:j:201:PEE:H55	1.70	0.40
34:k:17:ALA:HB2	51:k:101:CDL:H812	2.04	0.40
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.21	0.40
41:s:200:LEU:HD13	41:s:282:TYR:HB3	2.04	0.40
43:v:108:LEU:HD23	43:v:108:LEU:HA	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	414 (96%)	17 (4%)	0	100	100
2	B	174/176 (99%)	169 (97%)	4 (2%)	1 (1%)	21	51
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	107 (95%)	4 (4%)	2 (2%)	6	23
5	F	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
6	G	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	10	34
6	X	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
7	H	110/112 (98%)	104 (94%)	4 (4%)	2 (2%)	6	23
8	I	93/112 (83%)	84 (90%)	8 (9%)	1 (1%)	11	36
9	J	340/342 (99%)	321 (94%)	16 (5%)	3 (1%)	14	41
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	664 (96%)	24 (4%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
15	P	206/208 (99%)	202 (98%)	4 (2%)	0	100	100
16	Q	427/430 (99%)	413 (97%)	13 (3%)	1 (0%)	43	72
17	S	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	8	28
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	81 (100%)	0	0	100	100
20	V	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
23	Z	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
24	a	136/138 (99%)	131 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	168 (97%)	5 (3%)	0	100	100
28	e	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
32	i	345/347 (99%)	331 (96%)	14 (4%)	0	100	100
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	581 (96%)	23 (4%)	0	100	100
36	m	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	21	51
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	170 (97%)	5 (3%)	1 (1%)	21	51
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
41	s	316/318 (99%)	307 (97%)	8 (2%)	1 (0%)	36	66
42	u	169/171 (99%)	164 (97%)	3 (2%)	2 (1%)	10	34
43	v	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
44	w	318/320 (99%)	301 (95%)	16 (5%)	1 (0%)	36	66
All	All	8174/8313 (98%)	7859 (96%)	297 (4%)	18 (0%)	44	72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100	GLU
7	H	108	PRO
16	Q	224	ALA
42	u	168	PHE
6	G	133	ILE
17	S	66	LEU
4	E	100	ARG
44	w	227	MET
8	I	41	LEU
9	J	38	HIS

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Mol	Chain	Res	Type
9	J	223	PHE
41	s	208	VAL
7	H	77	ILE
9	J	224	GLY
4	E	96	VAL
36	m	25	SER
39	p	174	PRO
42	u	152	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%)	129 (98%)	3 (2%)	44	78
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	75/76 (99%)	75 (100%)	0	100	100
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	79/81 (98%)	79 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	83 (95%)	4 (5%)	24	58
9	J	296/296 (100%)	295 (100%)	1 (0%)	86	95
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%)	576 (99%)	4 (1%)	76	91
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%)	188 (99%)	2 (1%)	65	87
16	Q	370/370 (100%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	122/123 (99%)	122 (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%)	154 (99%)	1 (1%)	78	92
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/108 (100%)	107 (99%)	1 (1%)	70	89
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	309 (99%)	2 (1%)	78	92
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	87
35	l	537/540 (99%)	532 (99%)	5 (1%)	70	89
36	m	130/141 (92%)	130 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	407 (99%)	3 (1%)	76	91
41	s	275/275 (100%)	273 (99%)	2 (1%)	76	91
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	111/111 (100%)	111 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7166/7240 (99%)	7137 (100%)	29 (0%)	81	94

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	58	ARG
3	C	59	ARG
3	C	61	SER
8	I	25	GLN
8	I	27	ARG
8	I	50	SER
8	I	95	VAL
9	J	136	THR
12	M	171	THR
12	M	468	GLU
12	M	688	GLN
12	M	690	THR
15	P	161	LYS
15	P	201	ASP
27	d	64	TYR
30	g	2	THR
32	i	149	ILE
32	i	171	ASN
34	k	50	ASN
35	l	119	LYS
35	l	320	ASN
35	l	423	SER
35	l	425	ARG
35	l	427	ILE
40	r	247	THR
40	r	255	ASN
40	r	256	TYR
41	s	61	LEU
41	s	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	244	ASN
1	A	418	GLN
1	A	451	GLN
1	A	458	GLN
2	B	206	GLN
4	E	72	HIS
4	E	95	ASN
5	F	48	ASN
5	F	81	ASN

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Mol	Chain	Res	Type
7	H	50	GLN
8	I	13	ASN
8	I	29	GLN
9	J	79	GLN
10	K	77	GLN
10	K	78	HIS
11	L	86	ASN
11	L	88	GLN
12	M	278	HIS
12	M	334	GLN
12	M	336	ASN
12	M	459	ASN
12	M	514	ASN
12	M	666	GLN
12	M	678	GLN
13	N	31	ASN
14	O	69	ASN
14	O	131	HIS
15	P	196	HIS
15	P	228	GLN
16	Q	190	HIS
16	Q	285	ASN
17	S	27	HIS
17	S	31	ASN
18	T	43	GLN
19	U	11	ASN
21	W	24	ASN
21	W	76	GLN
22	Y	46	GLN
22	Y	57	GLN
23	Z	21	GLN
26	c	84	GLN
28	e	148	GLN
29	f	73	ASN
30	g	90	HIS
30	g	99	HIS
31	h	34	HIS
31	h	45	HIS
32	i	112	HIS
32	i	186	HIS
32	i	273	ASN
34	k	57	ASN

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Mol	Chain	Res	Type
35	l	135	ASN
35	l	170	GLN
35	l	175	ASN
35	l	194	ASN
35	l	199	GLN
35	l	348	HIS
35	l	534	HIS
35	l	580	GLN
38	o	79	ASN
39	p	51	HIS
40	r	43	ASN
40	r	103	GLN
40	r	175	ASN
40	r	251	ASN
40	r	255	ASN
40	r	293	HIS
40	r	366	ASN
40	r	399	ASN
40	r	415	GLN
40	r	421	HIS
41	s	32	GLN
41	s	230	ASN
41	s	250	HIS
43	v	117	GLN
44	w	149	HIS
44	w	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	2.02	2 (20%)	5,13,15	6.30	3 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.58	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.10	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.88	131.29	119.48
16	Q	118	2MR	CD-NE-CZ	4.59	132.00	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.05	130.20	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
46	FMN	A	502	-	33,33,33	1.43	6 (18%)	48,50,50	1.29	10 (20%)
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	1.02	2 (3%)
49	PLX	g	201	-	51,51,51	1.19	3 (5%)	53,59,59	0.66	1 (1%)
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.88	8 (18%)
52	NDP	J	401	-	51,52,52	2.31	6 (11%)	71,80,80	1.55	16 (22%)
51	CDL	V	201	-	93,93,99	1.13	9 (9%)	99,105,111	0.88	4 (4%)
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.99	2 (3%)
49	PLX	J	403	-	51,51,51	1.20	5 (9%)	53,59,59	0.60	1 (1%)
51	CDL	s	401	-	88,88,99	1.16	8 (9%)	94,100,111	0.95	4 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
48	PEE	Q	501	-	46,46,50	1.22	6 (13%)	49,51,55	1.04	2 (4%)
49	PLX	r	502	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
50	8Q1	X	201	-	32,34,34	2.24	7 (21%)	39,43,43	1.76	12 (30%)
53	UQ	s	402	-	38,38,63	3.63	10 (26%)	48,49,79	2.77	17 (35%)
48	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
50	8Q1	G	201	-	32,34,34	2.21	7 (21%)	39,43,43	1.75	12 (30%)
49	PLX	a	202	-	51,51,51	1.21	5 (9%)	53,59,59	0.60	1 (1%)
45	SF4	M	802	12	0,12,12	-	-	-		
48	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.13	4 (9%)
51	CDL	a	201	-	99,99,99	1.11	9 (9%)	105,111,111	0.87	4 (3%)
51	CDL	k	101	-	99,99,99	1.11	8 (8%)	105,111,111	0.85	4 (3%)
48	PEE	j	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.08	3 (6%)
51	CDL	n	101	-	54,54,99	1.24	4 (7%)	60,66,111	1.24	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
49	PLX	r	503	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
54	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)
49	PLX	C	303	-	51,51,51	0.60	0	53,59,59	0.73	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
45	SF4	M	801	12	0,12,12	-	-	-	-	-
54	FES	M	803	12	0,4,4	-	-	-	-	-
51	CDL	l	703	-	99,99,99	0.92	4 (4%)	105,111,111	1.03	5 (4%)
51	CDL	l	702	-	98,98,99	1.12	8 (8%)	104,110,111	0.90	4 (3%)
51	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.34	6 (10%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
49	PLX	j	203	-	51,51,51	1.21	5 (9%)	53,59,59	0.64	1 (1%)
51	CDL	r	504	-	99,99,99	1.10	8 (8%)	105,111,111	0.90	4 (3%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
53	UQ	J	402	-	33,33,63	3.51	10 (30%)	42,43,79	2.73	14 (33%)
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.71	12 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	V	202	-	-	66/110/110/110	-
46	FMN	A	502	-	-	8/18/18/18	0/3/3/3
48	PEE	r	501	-	-	30/54/54/54	-
49	PLX	g	201	-	-	32/55/55/55	-
48	PEE	C	302	-	-	23/50/50/54	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
52	NDP	J	401	-	-	4/34/77/77	0/5/5/5
51	CDL	V	201	-	-	60/104/104/110	-
49	PLX	J	403	-	-	29/55/55/55	-
48	PEE	j	201	-	-	29/54/54/54	-
51	CDL	s	401	-	-	54/99/99/110	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	Q	501	-	-	21/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	r	502	-	-	35/55/55/55	-
50	8Q1	X	201	-	-	22/41/41/41	-
53	UQ	s	402	-	-	13/33/57/87	0/1/1/1
48	PEE	l	704	-	-	34/54/54/54	-
50	8Q1	G	201	-	-	14/41/41/41	-
49	PLX	a	202	-	-	33/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	l	701	-	-	23/43/43/54	-
51	CDL	a	201	-	-	55/110/110/110	-
51	CDL	k	101	-	-	56/110/110/110	-
48	PEE	j	202	-	-	25/44/44/54	-
51	CDL	n	101	-	-	22/65/65/110	-
48	PEE	b	201	-	-	23/49/49/54	-
49	PLX	r	503	-	-	31/55/55/55	-
54	FES	O	301	14	-	-	0/1/1/1
48	PEE	W	201	-	-	19/44/44/54	-
49	PLX	C	303	-	-	26/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	M	801	12	-	-	0/6/5/5
54	FES	M	803	12	-	-	0/1/1/1
51	CDL	l	703	-	-	70/110/110/110	-
51	CDL	l	702	-	-	58/109/109/110	-
51	CDL	I	201	-	-	28/61/61/110	-
45	SF4	B	302	2	-	-	0/6/5/5
49	PLX	j	203	-	-	25/55/55/55	-
51	CDL	r	504	-	-	63/110/110/110	-
48	PEE	B	303	-	-	30/54/54/54	-
53	UQ	J	402	-	-	12/27/51/87	0/1/1/1
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5

All (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	NDP	P2B-O2B	13.26	1.82	1.59
47	A	503	NAI	C3D-C4D	-10.41	1.26	1.53
53	s	402	UQ	C18-C19	9.97	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	402	UQ	C18-C19	9.93	1.55	1.33
53	s	402	UQ	C13-C14	9.65	1.55	1.33
53	J	402	UQ	C13-C14	9.48	1.54	1.33
53	s	402	UQ	C23-C24	9.43	1.54	1.33
53	J	402	UQ	C8-C9	9.40	1.54	1.33
47	A	503	NAI	O4B-C1B	9.37	1.63	1.42
53	s	402	UQ	C8-C9	9.29	1.54	1.33
57	w	401	ADP	C3'-C4'	-9.02	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.29	1.26	1.45
47	A	503	NAI	C2D-C1D	-7.82	1.28	1.53
57	w	401	ADP	O4'-C4'	7.73	1.62	1.45
50	X	201	8Q1	P24-O27	7.68	1.84	1.60
53	J	402	UQ	C23-C24	7.54	1.55	1.32
50	G	201	8Q1	P24-O27	7.45	1.83	1.60
47	A	503	NAI	C2B-C1B	-7.42	1.30	1.53
53	s	402	UQ	C28-C29	7.38	1.54	1.32
47	A	503	NAI	O4D-C4D	6.82	1.60	1.45
47	A	503	NAI	PA-O3	6.43	1.66	1.59
57	w	401	ADP	PA-O3A	6.40	1.66	1.59
47	A	503	NAI	C2D-C3D	5.89	1.69	1.53
47	A	503	NAI	PN-O3	5.60	1.65	1.59
50	X	201	8Q1	C28-C29	5.49	1.61	1.52
47	A	503	NAI	O4D-C1D	5.45	1.54	1.42
57	w	401	ADP	C6-N6	5.43	1.48	1.34
47	A	503	NAI	C4N-C3N	-5.30	1.40	1.50
47	A	503	NAI	C7N-N7N	5.28	1.48	1.33
50	G	201	8Q1	C28-C29	5.05	1.60	1.52
47	A	503	NAI	C6A-N6A	4.94	1.46	1.34
46	A	502	FMN	C9A-C5A	4.88	1.49	1.41
57	w	401	ADP	O4'-C1'	-4.50	1.31	1.42
52	J	401	NDP	PA-O3	4.41	1.64	1.59
47	A	503	NAI	O2B-C2B	4.31	1.53	1.43
51	I	201	CDL	OA8-CA7	4.28	1.45	1.33
51	l	703	CDL	OB8-CB7	4.26	1.45	1.33
51	n	101	CDL	OA8-CA7	4.25	1.45	1.33
51	I	201	CDL	OB8-CB7	4.24	1.45	1.33
51	l	703	CDL	OA8-CA7	4.24	1.45	1.33
51	n	101	CDL	OB8-CB7	4.21	1.45	1.33
51	n	101	CDL	OB6-CB5	4.15	1.46	1.34
51	l	703	CDL	OA6-CA5	4.13	1.45	1.34
51	I	201	CDL	OA6-CA5	4.10	1.45	1.34
51	n	101	CDL	OA6-CA5	4.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	I	201	CDL	OB6-CB5	4.06	1.45	1.34
51	l	703	CDL	OB6-CB5	4.06	1.45	1.34
50	X	201	8Q1	C1-S44	3.93	1.85	1.76
50	G	201	8Q1	C1-S44	3.88	1.85	1.76
48	l	704	PEE	C18-C19	3.85	1.53	1.31
48	j	202	PEE	C18-C19	3.83	1.53	1.31
48	r	501	PEE	C18-C19	3.83	1.53	1.31
48	C	302	PEE	C18-C19	3.82	1.53	1.31
48	b	201	PEE	C18-C19	3.82	1.53	1.31
48	l	701	PEE	C18-C19	3.80	1.53	1.31
48	B	303	PEE	C18-C19	3.80	1.53	1.31
48	W	201	PEE	C18-C19	3.78	1.53	1.31
48	j	201	PEE	C18-C19	3.77	1.53	1.31
48	Q	501	PEE	C18-C19	3.75	1.53	1.31
52	J	401	NDP	PN-O5D	3.74	1.74	1.59
48	l	701	PEE	C39-C38	3.74	1.52	1.31
48	l	704	PEE	C39-C38	3.74	1.52	1.31
48	b	201	PEE	C39-C38	3.74	1.52	1.31
48	r	501	PEE	C39-C38	3.74	1.52	1.31
48	C	302	PEE	C39-C38	3.71	1.52	1.31
48	j	201	PEE	C39-C38	3.70	1.52	1.31
48	B	303	PEE	C39-C38	3.70	1.52	1.31
48	Q	501	PEE	C39-C38	3.70	1.52	1.31
51	l	702	CDL	OA8-CA7	3.60	1.43	1.33
51	s	401	CDL	OA8-CA7	3.48	1.43	1.33
47	A	503	NAI	C7N-C3N	3.47	1.56	1.48
51	a	201	CDL	OA8-CA7	3.44	1.43	1.33
51	V	202	CDL	OA8-CA7	3.42	1.43	1.33
51	V	201	CDL	OA8-CA7	3.39	1.43	1.33
51	k	101	CDL	OA8-CA7	3.39	1.43	1.33
50	G	201	8Q1	O27-C28	-3.39	1.33	1.43
50	X	201	8Q1	O27-C28	-3.38	1.33	1.43
57	w	401	ADP	C8-N9	-3.36	1.31	1.37
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.49
51	r	504	CDL	OA8-CA7	3.35	1.43	1.33
50	G	201	8Q1	C6-C1	3.31	1.54	1.50
50	G	201	8Q1	C34-N36	3.30	1.41	1.33
52	J	401	NDP	O2B-C2B	-3.27	1.32	1.44
50	X	201	8Q1	C34-N36	3.22	1.41	1.33
46	A	502	FMN	C8-C7	3.20	1.48	1.40
51	V	201	CDL	OA6-CA5	3.17	1.43	1.34
57	w	401	ADP	O2'-C2'	-3.15	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	101	CDL	OA6-CA5	3.12	1.43	1.34
51	a	201	CDL	OB6-CB5	3.09	1.43	1.34
57	w	401	ADP	O3'-C3'	3.05	1.50	1.43
51	l	702	CDL	OB8-CB7	3.05	1.42	1.33
51	s	401	CDL	OA6-CA5	3.02	1.42	1.34
49	g	201	PLX	O6-C4	-3.01	1.40	1.44
51	V	202	CDL	OB6-CB5	3.00	1.42	1.34
49	a	202	PLX	O6-C4	-3.00	1.40	1.44
51	k	101	CDL	OB6-CB5	2.98	1.42	1.34
51	s	401	CDL	OB6-CB5	2.98	1.42	1.34
51	r	504	CDL	OB6-CB5	2.96	1.42	1.34
51	l	702	CDL	OB6-CB5	2.96	1.42	1.34
51	k	101	CDL	OB8-CB7	2.96	1.42	1.33
51	V	202	CDL	OB8-CB7	2.95	1.42	1.33
51	a	201	CDL	OB8-CB7	2.94	1.41	1.33
51	V	202	CDL	OA6-CA5	2.93	1.42	1.34
51	r	504	CDL	OB8-CB7	2.93	1.41	1.33
51	a	201	CDL	OA6-CA5	2.92	1.42	1.34
51	r	504	CDL	OA6-CA5	2.89	1.42	1.34
51	V	201	CDL	OB8-CB7	2.88	1.41	1.33
50	X	201	8Q1	C39-N41	2.88	1.40	1.33
51	V	201	CDL	OB6-CB5	2.85	1.42	1.34
51	l	702	CDL	OA6-CA5	2.84	1.42	1.34
51	s	401	CDL	OB8-CB7	2.81	1.41	1.33
49	j	203	PLX	O6-C4	-2.80	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.78	1.32	1.37
49	r	502	PLX	O6-C4	-2.77	1.41	1.44
53	s	402	UQ	C6-C1	2.77	1.54	1.46
48	B	303	PEE	O2-C2	-2.77	1.40	1.46
48	C	302	PEE	O2-C2	-2.72	1.40	1.46
51	l	702	CDL	OA6-CA4	-2.72	1.40	1.46
46	A	502	FMN	C4-N3	-2.72	1.33	1.38
48	j	202	PEE	O2-C2	-2.69	1.40	1.46
50	G	201	8Q1	C39-N41	2.68	1.39	1.33
51	r	504	CDL	OA6-CA4	-2.68	1.40	1.46
48	j	201	PEE	O2-C2	-2.67	1.40	1.46
49	r	503	PLX	O6-C4	-2.66	1.41	1.44
48	W	201	PEE	O2-C2	-2.64	1.40	1.46
53	J	402	UQ	C6-C1	2.64	1.53	1.46
51	a	201	CDL	OA6-CA4	-2.62	1.40	1.46
48	l	704	PEE	O2-C2	-2.61	1.40	1.46
48	r	501	PEE	O2-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	X	201	8Q1	C6-C1	2.59	1.53	1.50
48	Q	501	PEE	O2-C2	-2.59	1.40	1.46
51	V	202	CDL	OA6-CA4	-2.53	1.40	1.46
51	s	401	CDL	OA6-CA4	-2.52	1.40	1.46
48	l	701	PEE	O2-C2	-2.51	1.40	1.46
48	b	201	PEE	O2-C2	-2.50	1.40	1.46
49	j	203	PLX	C7-C6	2.48	1.55	1.50
51	V	201	CDL	OB6-CB4	-2.47	1.40	1.46
49	J	403	PLX	C7-C6	2.45	1.55	1.50
48	j	202	PEE	O3-C30	2.44	1.40	1.33
48	B	303	PEE	O3-C30	2.43	1.40	1.33
48	C	302	PEE	O3-C30	2.43	1.40	1.33
48	b	201	PEE	O3-C30	2.42	1.40	1.33
49	r	502	PLX	C7-C6	2.42	1.55	1.50
47	A	503	NAI	O3B-C3B	-2.42	1.37	1.43
51	k	101	CDL	OB6-CB4	-2.41	1.40	1.46
48	l	701	PEE	O3-C30	2.41	1.40	1.33
47	A	503	NAI	C6N-C5N	2.40	1.40	1.33
48	r	501	PEE	O3-C30	2.40	1.40	1.33
48	W	201	PEE	O2-C10	2.38	1.41	1.34
47	A	503	NAI	PN-O5D	2.38	1.68	1.59
48	l	704	PEE	O3-C30	2.37	1.40	1.33
57	w	401	ADP	C5-N7	-2.37	1.34	1.39
48	Q	501	PEE	O3-C30	2.35	1.40	1.33
47	A	503	NAI	C5B-C4B	2.35	1.58	1.51
49	a	202	PLX	C7-C6	2.34	1.55	1.50
53	J	402	UQ	C7-C8	2.34	1.54	1.50
49	r	503	PLX	C7-C6	2.34	1.55	1.50
53	s	402	UQ	C7-C8	2.34	1.54	1.50
51	V	202	CDL	OB6-CB4	-2.34	1.41	1.46
51	l	702	CDL	OB6-CB4	-2.33	1.41	1.46
51	k	101	CDL	OA6-CA4	-2.32	1.41	1.46
51	s	401	CDL	OB6-CB4	-2.32	1.41	1.46
48	j	201	PEE	O3-C30	2.32	1.40	1.33
48	W	201	PEE	O3-C30	2.31	1.40	1.33
49	g	201	PLX	C7-C6	2.30	1.55	1.50
48	W	201	PEE	O3-C3	-2.30	1.40	1.45
48	r	501	PEE	O3-C3	-2.29	1.40	1.45
51	V	202	CDL	PB2-OB2	2.27	1.68	1.59
48	b	201	PEE	O2-C10	2.27	1.40	1.34
51	r	504	CDL	OB6-CB4	-2.27	1.41	1.46
48	Q	501	PEE	O3-C3	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	701	PEE	O2-C10	2.25	1.40	1.34
51	V	201	CDL	PB2-OB2	2.25	1.68	1.59
49	J	403	PLX	O6-C4	-2.24	1.41	1.44
48	B	303	PEE	O3-C3	-2.24	1.40	1.45
48	j	201	PEE	O3-C3	-2.24	1.40	1.45
51	s	401	CDL	PB2-OB2	2.24	1.68	1.59
51	a	201	CDL	OB6-CB4	-2.23	1.41	1.46
51	l	702	CDL	PB2-OB5	2.23	1.68	1.59
46	A	502	FMN	C5A-N5	-2.22	1.35	1.39
51	V	202	CDL	PB2-OB5	2.22	1.68	1.59
51	r	504	CDL	PB2-OB2	2.21	1.68	1.59
51	a	201	CDL	PB2-OB5	2.21	1.68	1.59
51	k	101	CDL	PB2-OB5	2.20	1.68	1.59
48	j	202	PEE	O2-C10	2.20	1.40	1.34
48	C	302	PEE	O2-C10	2.20	1.40	1.34
48	Q	501	PEE	O2-C10	2.20	1.40	1.34
51	k	101	CDL	PB2-OB2	2.20	1.68	1.59
51	r	504	CDL	PB2-OB5	2.20	1.68	1.59
48	b	201	PEE	O3-C3	-2.19	1.40	1.45
48	l	704	PEE	O2-C10	2.19	1.40	1.34
51	a	201	CDL	PB2-OB2	2.19	1.68	1.59
48	r	501	PEE	O2-C10	2.19	1.40	1.34
51	l	702	CDL	PB2-OB2	2.18	1.67	1.59
49	a	202	PLX	P1-O4	2.18	1.67	1.59
48	j	201	PEE	O2-C10	2.16	1.40	1.34
51	V	201	CDL	C11-CA5	2.16	1.57	1.50
48	B	303	PEE	O2-C10	2.15	1.40	1.34
51	V	201	CDL	PB2-OB5	2.15	1.67	1.59
48	C	302	PEE	O3-C3	-2.15	1.40	1.45
53	J	402	UQ	O4-C4	-2.15	1.18	1.23
49	J	403	PLX	P1-O4	2.15	1.67	1.59
51	V	201	CDL	OA6-CA4	-2.14	1.41	1.46
49	r	502	PLX	P1-O4	2.14	1.67	1.59
53	J	402	UQ	O3-CM3	-2.13	1.40	1.45
52	J	401	NDP	C5A-C4A	2.13	1.42	1.39
47	A	503	NAI	C5A-N7A	-2.13	1.35	1.39
49	j	203	PLX	P1-O4	2.12	1.67	1.59
53	s	402	UQ	O4-C4	-2.12	1.18	1.23
48	j	202	PEE	O3-C3	-2.12	1.40	1.45
52	J	401	NDP	O5D-C5D	-2.11	1.36	1.44
49	r	503	PLX	P1-O4	2.11	1.67	1.59
48	l	701	PEE	O3-C3	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	s	401	CDL	PB2-OB5	2.08	1.67	1.59
46	A	502	FMN	C2-N3	-2.08	1.34	1.39
53	s	402	UQ	C21-C19	2.07	1.55	1.51
46	A	502	FMN	C4A-N5	2.07	1.35	1.30
53	s	402	UQ	O3-CM3	-2.07	1.40	1.45
49	j	203	PLX	P1-O1	2.06	1.67	1.59
49	g	201	PLX	P1-O4	2.06	1.67	1.59
49	r	503	PLX	P1-O1	2.06	1.67	1.59
48	l	704	PEE	O3-C3	-2.05	1.40	1.45
49	r	502	PLX	P1-O1	2.05	1.67	1.59
49	a	202	PLX	C1-C2	2.04	1.57	1.51
53	J	402	UQ	C21-C19	2.04	1.55	1.51
49	a	202	PLX	P1-O1	2.03	1.67	1.59
53	J	402	UQ	O1-C1	-2.01	1.18	1.23
51	a	201	CDL	C11-CA5	2.01	1.56	1.50
49	J	403	PLX	P1-O1	2.01	1.67	1.59
49	j	203	PLX	C25-C24	2.01	1.54	1.50
49	J	403	PLX	C25-C24	2.01	1.54	1.50

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C7-C8-C9	-7.67	113.62	126.83
53	s	402	UQ	C7-C8-C9	-7.59	113.75	126.83
53	J	402	UQ	C12-C13-C14	-6.59	112.53	127.62
53	J	402	UQ	C17-C18-C19	-6.54	112.64	127.62
53	s	402	UQ	C22-C23-C24	-6.24	113.35	127.62
53	s	402	UQ	C12-C13-C14	-6.04	113.80	127.62
53	s	402	UQ	C17-C18-C19	-5.99	113.92	127.62
47	A	503	NAI	C5A-C4A-N3A	-5.53	119.11	126.72
57	w	401	ADP	C5-C4-N3	-5.47	119.19	126.72
50	G	201	8Q1	C6-C1-S44	4.66	118.95	113.40
57	w	401	ADP	N3-C2-N1	-4.57	121.67	128.58
50	X	201	8Q1	C6-C1-S44	4.55	118.83	113.40
53	J	402	UQ	C22-C23-C24	-4.54	112.50	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.52	121.74	128.58
53	s	402	UQ	C10-C9-C8	-4.43	112.24	123.63
48	r	501	PEE	O2-C10-C11	4.39	120.99	111.48
53	J	402	UQ	C15-C14-C13	-4.35	112.44	123.63
48	j	202	PEE	O2-C10-C11	4.30	120.79	111.48
53	s	402	UQ	C27-C28-C29	-4.30	113.31	127.64
57	w	401	ADP	N3-C4-N9	4.28	134.45	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	P2B-O2B-C2B	-4.26	112.06	123.43
53	s	402	UQ	C25-C24-C23	-4.24	112.75	123.63
51	V	201	CDL	OA6-CA5-C11	4.20	120.57	111.48
53	J	402	UQ	C10-C9-C8	-4.19	112.87	123.63
51	s	401	CDL	OB6-CB5-C51	4.16	120.47	111.48
51	s	401	CDL	OA6-CA5-C11	4.12	120.39	111.48
53	J	402	UQ	C20-C19-C18	-4.07	113.18	123.63
51	l	702	CDL	OB6-CB5-C51	4.05	120.25	111.48
51	l	703	CDL	OB6-CB5-C51	4.04	120.22	111.48
48	l	704	PEE	O2-C10-C11	4.04	120.22	111.48
51	k	101	CDL	OB6-CB5-C51	4.04	120.21	111.48
51	I	201	CDL	OA6-CA5-C11	4.03	120.20	111.48
47	A	503	NAI	N3A-C4A-N9A	4.02	134.01	127.17
51	l	703	CDL	OA6-CA5-C11	4.02	120.18	111.48
51	V	202	CDL	OB6-CB5-C51	4.02	120.17	111.48
51	I	201	CDL	OB6-CB5-C51	4.00	120.14	111.48
48	l	701	PEE	O2-C10-C11	4.00	120.14	111.48
48	b	201	PEE	O2-C10-C11	3.98	120.09	111.48
48	C	302	PEE	O2-C10-C11	3.98	120.09	111.48
51	n	101	CDL	OB6-CB5-C51	3.97	120.06	111.48
51	r	504	CDL	OB6-CB5-C51	3.96	120.05	111.48
51	a	201	CDL	OA6-CA5-C11	3.96	120.04	111.48
51	a	201	CDL	OB6-CB5-C51	3.96	120.04	111.48
50	G	201	8Q1	C43-S44-C1	3.94	113.50	101.84
53	s	402	UQ	C20-C19-C18	-3.91	113.58	123.63
51	r	504	CDL	OA6-CA5-C11	3.91	119.93	111.48
48	j	201	PEE	O2-C10-C11	3.90	119.92	111.48
51	l	702	CDL	OA6-CA5-C11	3.90	119.92	111.48
53	s	402	UQ	C15-C14-C13	-3.89	113.65	123.63
53	s	402	UQ	C21-C19-C18	-3.87	112.49	121.17
51	V	202	CDL	OA6-CA5-C11	3.85	119.81	111.48
50	X	201	8Q1	C43-S44-C1	3.82	113.13	101.84
51	n	101	CDL	OA6-CA5-C11	3.79	119.69	111.48
51	V	201	CDL	OB6-CB5-C51	3.79	119.67	111.48
47	A	503	NAI	C2A-N3A-C4A	3.78	121.06	111.83
53	s	402	UQ	C16-C14-C13	-3.77	112.71	121.17
48	Q	501	PEE	O2-C10-C11	3.77	119.63	111.48
53	s	402	UQ	C11-C9-C8	-3.77	112.71	121.17
48	B	303	PEE	O2-C10-C11	3.75	119.58	111.48
48	W	201	PEE	O2-C10-C11	3.73	119.55	111.48
53	J	402	UQ	C16-C14-C13	-3.72	112.82	121.17
50	X	201	8Q1	O35-C34-N36	-3.71	115.13	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C11-C9-C8	-3.65	112.97	121.17
57	w	401	ADP	C2-N3-C4	3.58	120.58	111.83
51	k	101	CDL	OA6-CA5-C11	3.57	119.20	111.48
52	J	401	NDP	O2B-P2B-O1X	-3.57	96.62	109.33
53	s	402	UQ	C26-C24-C23	-3.55	113.20	121.17
57	w	401	ADP	N9-C8-N7	-3.52	108.94	113.94
47	A	503	NAI	C5A-N7A-C8A	3.34	108.70	103.45
47	A	503	NAI	N9A-C8A-N7A	-3.34	109.20	113.94
53	s	402	UQ	C30-C29-C28	-3.28	112.81	122.66
53	J	402	UQ	C21-C19-C18	-3.28	113.81	121.17
47	A	503	NAI	C4A-C5A-N7A	-3.28	106.83	110.58
57	w	401	ADP	C4-N9-C8	3.21	109.10	105.74
52	J	401	NDP	O3-PA-O1A	-3.20	101.06	110.70
57	w	401	ADP	C5-N7-C8	3.20	108.48	103.45
50	G	201	8Q1	O35-C34-N36	-3.19	116.22	122.98
51	n	101	CDL	OB8-CB7-C71	3.19	121.55	111.83
53	J	402	UQ	C26-C24-C23	-3.16	113.17	122.66
53	s	402	UQ	C31-C29-C28	-3.14	113.23	122.66
48	Q	501	PEE	O3-C30-C31	3.14	121.41	111.83
50	X	201	8Q1	C32-C34-N36	3.12	122.41	116.48
47	A	503	NAI	C4D-O4D-C1D	-3.06	102.71	109.47
53	J	402	UQ	C25-C24-C23	-3.05	113.50	122.66
52	J	401	NDP	PA-O5B-C5B	-3.04	103.95	121.35
57	w	401	ADP	C4-C5-N7	-3.03	107.11	110.58
48	B	303	PEE	O3-C30-C31	2.99	120.96	111.83
50	X	201	8Q1	O2-P24-O27	-2.98	98.90	106.67
51	l	702	CDL	OA8-CA7-C31	2.97	120.90	111.83
48	l	704	PEE	O3-C30-C31	2.97	120.89	111.83
51	l	703	CDL	OB8-CB7-C71	2.91	120.72	111.83
47	A	503	NAI	C3D-C2D-C1D	2.91	106.97	101.46
51	k	101	CDL	OB8-CB7-C71	2.87	120.60	111.83
50	G	201	8Q1	O2-P24-O27	-2.85	99.25	106.67
51	I	201	CDL	OA8-CA7-C31	2.85	120.51	111.83
51	a	201	CDL	OB8-CB7-C71	2.83	120.45	111.83
52	J	401	NDP	PN-O5D-C5D	-2.81	105.23	121.35
51	V	202	CDL	OB8-CB7-C71	2.81	120.41	111.83
51	r	504	CDL	OB8-CB7-C71	2.81	120.41	111.83
51	l	703	CDL	OA8-CA7-C31	2.81	120.40	111.83
51	V	202	CDL	OA8-CA7-C31	2.78	120.31	111.83
51	I	201	CDL	OB8-CB7-C71	2.78	120.31	111.83
51	l	702	CDL	OB8-CB7-C71	2.77	120.28	111.83
51	n	101	CDL	OA8-CA7-C31	2.76	119.53	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	V	201	CDL	OB8-CB7-C71	2.75	120.20	111.83
51	s	401	CDL	OA8-CA7-C31	2.73	120.16	111.83
48	r	501	PEE	O3-C30-C31	2.72	120.14	111.83
48	j	202	PEE	O3-C30-C31	2.71	120.11	111.83
51	k	101	CDL	OA8-CA7-C31	2.71	120.11	111.83
49	g	201	PLX	C1A-N1-C1	2.70	120.63	109.91
50	G	201	8Q1	C32-C34-N36	2.69	121.60	116.48
48	b	201	PEE	O3-C30-C31	2.67	119.97	111.83
52	J	401	NDP	O2N-PN-O3	2.66	114.47	107.27
51	a	201	CDL	OA8-CA7-C31	2.66	119.95	111.83
48	W	201	PEE	O3-C30-C31	2.65	119.93	111.83
51	s	401	CDL	OB8-CB7-C71	2.65	119.91	111.83
51	r	504	CDL	OA8-CA7-C31	2.64	119.89	111.83
48	C	302	PEE	O3-C30-C31	2.64	119.89	111.83
51	I	201	CDL	CB4-OB6-CB5	-2.64	111.48	117.80
47	A	503	NAI	C2D-C3D-C4D	2.62	107.68	102.61
50	G	201	8Q1	C37-C38-C39	2.60	116.72	112.39
50	X	201	8Q1	O40-C39-N41	-2.57	117.99	123.03
46	A	502	FMN	C4A-C10-N1	-2.57	118.29	124.59
48	j	201	PEE	O3-C30-C31	2.56	119.65	111.83
52	J	401	NDP	O4B-C4B-C3B	2.56	110.24	105.15
52	J	401	NDP	O3X-P2B-O2X	2.55	117.37	107.80
52	J	401	NDP	C2A-N1A-C6A	-2.55	114.54	118.73
46	A	502	FMN	C4-C4A-N5	2.54	121.72	118.21
48	l	701	PEE	O3-C30-C31	2.54	119.57	111.83
50	G	201	8Q1	O40-C39-N41	-2.54	118.05	123.03
50	G	201	8Q1	O4-C1-S44	-2.53	119.46	122.68
49	j	203	PLX	C1A-N1-C1	2.53	119.97	109.91
53	J	402	UQ	CM5-C5-C6	-2.52	120.30	124.45
49	r	503	PLX	C1A-N1-C1	2.52	119.93	109.91
47	A	503	NAI	C4A-N9A-C8A	2.52	108.38	105.74
51	I	201	CDL	CA6-CA4-CA3	-2.52	105.92	111.78
52	J	401	NDP	N3A-C4A-N9A	2.49	131.41	127.17
50	X	201	8Q1	O4-C1-C6	-2.49	121.10	123.98
48	j	202	PEE	C2-O2-C10	-2.46	111.90	117.80
51	l	703	CDL	CB4-OB6-CB5	-2.46	111.90	117.80
49	r	502	PLX	C1A-N1-C1	2.46	119.68	109.91
53	J	402	UQ	C7-C6-C5	-2.44	120.72	124.89
49	a	202	PLX	C1A-N1-C1	2.42	119.52	109.91
52	J	401	NDP	O2N-PN-O1N	2.42	123.69	112.44
48	l	701	PEE	C20-C19-C18	-2.41	111.94	126.42
49	J	403	PLX	C1A-N1-C1	2.39	119.41	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	201	8Q1	O1-P24-O2	2.38	116.74	107.80
51	V	201	CDL	OA8-CA7-C31	2.37	119.06	111.83
50	X	201	8Q1	O1-P24-O2	2.35	116.60	107.80
53	s	402	UQ	C7-C6-C5	-2.32	120.91	124.89
52	J	401	NDP	O5D-PN-O1N	-2.32	99.76	108.94
52	J	401	NDP	C5A-C4A-N3A	-2.29	123.56	126.72
46	A	502	FMN	O2-C2-N1	-2.28	118.02	121.80
52	J	401	NDP	C5B-C4B-C3B	-2.26	107.06	115.21
53	s	402	UQ	CM5-C5-C6	-2.25	120.75	124.45
46	A	502	FMN	O4-C4-C4A	-2.21	120.69	126.53
50	G	201	8Q1	C38-C39-N41	2.21	120.37	116.34
47	A	503	NAI	C6N-N1N-C2N	2.21	121.69	119.32
51	n	101	CDL	OB8-CB7-OB9	-2.21	118.11	123.63
50	X	201	8Q1	C38-C39-N41	2.20	120.35	116.34
50	G	201	8Q1	O27-P24-O3	-2.20	100.50	106.44
46	A	502	FMN	C4-N3-C2	-2.19	121.75	125.64
48	l	701	PEE	C2-O2-C10	-2.13	112.71	117.80
50	X	201	8Q1	O27-P24-O3	-2.09	100.80	106.44
46	A	502	FMN	C4A-C4-N3	2.08	118.55	113.25
52	J	401	NDP	O3X-P2B-O2B	-2.08	97.74	105.85
50	X	201	8Q1	C37-C38-C39	2.08	115.86	112.39
46	A	502	FMN	C4'-C3'-C2'	-2.08	110.11	113.57
50	G	201	8Q1	O4-C1-C6	-2.08	121.58	123.98
52	J	401	NDP	C5D-C4D-C3D	-2.07	107.75	115.21
50	X	201	8Q1	O4-C1-S44	-2.06	120.07	122.68
49	C	303	PLX	C6-O6-C4	-2.04	111.12	115.20
49	C	303	PLX	C2-C1-N1	-2.04	109.26	115.82
46	A	502	FMN	C10-N1-C2	2.03	121.25	116.85
46	A	502	FMN	C4A-C10-N10	2.03	119.38	116.48
46	A	502	FMN	C5A-C9A-N10	2.00	119.78	117.97

There are no chirality outliers.

All (1084) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C2'-C1'-N10-C10
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
48	B	303	PEE	O4P-C4-C5-N
48	C	302	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	O4P-C4-C5-N
48	Q	501	PEE	C11-C10-O2-C2
48	Q	501	PEE	O4-C10-O2-C2
48	Q	501	PEE	C1-O3P-P-O2P
48	Q	501	PEE	C1-O3P-P-O1P
48	Q	501	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C19-C20-C21-C22
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	C4-O4P-P-O1P
48	l	701	PEE	C11-C10-O2-C2
48	l	701	PEE	C2-C1-O3P-P
48	l	701	PEE	C1-O3P-P-O2P
48	l	701	PEE	C1-O3P-P-O4P
48	l	701	PEE	C4-O4P-P-O1P
48	l	701	PEE	C39-C40-C41-C42
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
49	C	303	PLX	O7-C6-C7-C8
49	C	303	PLX	C2-O1-P1-O4
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	C1-C2-O1-P1
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	O9-C24-O8-C5
49	a	202	PLX	O7-C6-O6-C4
49	a	202	PLX	C3-O4-P1-O2
49	a	202	PLX	C2-O1-P1-O4
49	a	202	PLX	C2-O1-P1-O2
49	a	202	PLX	C2-O1-P1-O3
49	a	202	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	O7-C6-C7-C8
49	g	201	PLX	O6-C4-C5-O8
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O3
49	g	201	PLX	O9-C24-C25-C26
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	O9-C24-O8-C5
49	j	203	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	C25-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O2
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	C28-O27-P24-O3
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C1-C6-C7-C8
50	X	201	8Q1	O4-C1-S44-C43
50	X	201	8Q1	C6-C1-S44-C43
50	X	201	8Q1	O27-C28-C29-C30
50	X	201	8Q1	O27-C28-C29-C31
50	X	201	8Q1	O27-C28-C29-C32
50	X	201	8Q1	C29-C32-C34-N36
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	O33-C32-C34-N36
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	N41-C42-C43-S44
50	X	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-O27-P24-O2
50	X	201	8Q1	C28-O27-P24-O1
51	I	201	CDL	CA2-OA2-PA1-OA3
51	I	201	CDL	CA2-OA2-PA1-OA5
51	I	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
51	I	201	CDL	CA3-OA5-PA1-OA4
51	I	201	CDL	CA6-CA4-OA6-CA5
51	I	201	CDL	CB2-OB2-PB2-OB4
51	I	201	CDL	CB2-OB2-PB2-OB5
51	I	201	CDL	CB3-OB5-PB2-OB2
51	I	201	CDL	CB3-OB5-PB2-OB4
51	V	201	CDL	CA2-C1-CB2-OB2
51	V	201	CDL	CA2-OA2-PA1-OA3
51	V	201	CDL	CA2-OA2-PA1-OA4
51	V	201	CDL	CA2-OA2-PA1-OA5
51	V	201	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	CB2-OB2-PB2-OB3
51	V	201	CDL	CB2-OB2-PB2-OB5
51	V	201	CDL	CB3-OB5-PB2-OB2
51	V	201	CDL	CB3-OB5-PB2-OB3
51	V	201	CDL	CB3-OB5-PB2-OB4
51	V	202	CDL	CB2-C1-CA2-OA2
51	V	202	CDL	CA2-C1-CB2-OB2
51	V	202	CDL	CA2-OA2-PA1-OA4
51	V	202	CDL	CA2-OA2-PA1-OA5
51	V	202	CDL	CA3-OA5-PA1-OA2
51	V	202	CDL	CA3-OA5-PA1-OA3
51	V	202	CDL	CB2-OB2-PB2-OB3
51	V	202	CDL	CB2-OB2-PB2-OB5
51	a	201	CDL	CA2-C1-CB2-OB2
51	a	201	CDL	CB2-OB2-PB2-OB3
51	a	201	CDL	CB3-OB5-PB2-OB2
51	a	201	CDL	CB3-OB5-PB2-OB3
51	a	201	CDL	CB3-OB5-PB2-OB4
51	k	101	CDL	CA2-OA2-PA1-OA3
51	k	101	CDL	CA3-OA5-PA1-OA2
51	k	101	CDL	CA3-OA5-PA1-OA4
51	k	101	CDL	OA5-CA3-CA4-OA6
51	k	101	CDL	CB3-OB5-PB2-OB2
51	k	101	CDL	CB3-OB5-PB2-OB4
51	k	101	CDL	OB5-CB3-CB4-OB6
51	l	702	CDL	CA2-C1-CB2-OB2
51	l	702	CDL	CA2-OA2-PA1-OA3
51	l	702	CDL	CA2-OA2-PA1-OA5
51	l	702	CDL	CA3-OA5-PA1-OA3
51	l	702	CDL	OA9-CA7-OA8-CA6
51	l	702	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	l	702	CDL	CB2-OB2-PB2-OB3
51	l	702	CDL	CB2-OB2-PB2-OB4
51	l	702	CDL	CB2-OB2-PB2-OB5
51	l	703	CDL	CA2-OA2-PA1-OA4
51	l	703	CDL	CA2-OA2-PA1-OA5
51	l	703	CDL	CA3-OA5-PA1-OA2
51	l	703	CDL	CA3-OA5-PA1-OA3
51	l	703	CDL	CA3-OA5-PA1-OA4
51	l	703	CDL	CB3-OB5-PB2-OB4
51	n	101	CDL	CA2-OA2-PA1-OA3
51	n	101	CDL	CA2-OA2-PA1-OA4
51	n	101	CDL	CA2-OA2-PA1-OA5
51	n	101	CDL	CA3-OA5-PA1-OA3
51	n	101	CDL	CB3-OB5-PB2-OB2
51	n	101	CDL	CB3-OB5-PB2-OB3
51	n	101	CDL	CB3-OB5-PB2-OB4
51	r	504	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB3-OB5-PB2-OB3
51	r	504	CDL	CB3-OB5-PB2-OB4
51	s	401	CDL	CA2-C1-CB2-OB2
51	s	401	CDL	CA2-OA2-PA1-OA3
51	s	401	CDL	CA2-OA2-PA1-OA4
51	s	401	CDL	CA2-OA2-PA1-OA5
53	J	402	UQ	C7-C8-C9-C10
53	J	402	UQ	C17-C18-C19-C20
53	s	402	UQ	C7-C8-C9-C10
53	s	402	UQ	C7-C8-C9-C11
53	s	402	UQ	C18-C19-C21-C22
51	s	401	CDL	OA9-CA7-OA8-CA6
51	l	703	CDL	CA4-CA6-OA8-CA7
51	s	401	CDL	C31-CA7-OA8-CA6
48	Q	501	PEE	O5-C30-O3-C3
48	C	302	PEE	O4-C10-O2-C2
48	l	701	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
51	I	201	CDL	OA7-CA5-OA6-CA4
51	V	201	CDL	OA7-CA5-OA6-CA4
48	Q	501	PEE	C31-C30-O3-C3
51	I	201	CDL	C11-CA5-OA6-CA4
53	J	402	UQ	C12-C11-C9-C10
48	j	202	PEE	C31-C30-O3-C3
48	b	201	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	C17-C18-C19-C20
53	J	402	UQ	C7-C8-C9-C11
53	J	402	UQ	C12-C13-C14-C16
53	s	402	UQ	C17-C18-C19-C21
53	s	402	UQ	C22-C23-C24-C26
48	j	202	PEE	O5-C30-O3-C3
51	I	201	CDL	O1-C1-CA2-OA2
51	I	201	CDL	O1-C1-CB2-OB2
51	V	201	CDL	O1-C1-CA2-OA2
51	V	202	CDL	O1-C1-CA2-OA2
51	a	201	CDL	O1-C1-CA2-OA2
51	k	101	CDL	O1-C1-CB2-OB2
51	l	703	CDL	O1-C1-CA2-OA2
51	s	401	CDL	O1-C1-CA2-OA2
48	j	202	PEE	C11-C10-O2-C2
51	V	202	CDL	C51-CB5-OB6-CB4
51	a	201	CDL	C51-CB5-OB6-CB4
51	r	504	CDL	C51-CB5-OB6-CB4
52	J	401	NDP	O4D-C4D-C5D-O5D
53	J	402	UQ	C13-C14-C16-C17
53	J	402	UQ	C18-C19-C21-C22
51	V	202	CDL	OB7-CB5-OB6-CB4
53	J	402	UQ	C19-C21-C22-C23
48	j	201	PEE	C30-C31-C32-C33
49	g	201	PLX	C9-C10-C11-C12
49	g	201	PLX	C7-C8-C9-C10
48	l	701	PEE	C31-C30-O3-C3
51	l	703	CDL	C71-CB7-OB8-CB6
51	V	202	CDL	C32-C33-C34-C35
51	s	401	CDL	C37-C38-C39-C40
53	J	402	UQ	C22-C23-C24-C26
51	k	101	CDL	C73-C74-C75-C76
48	W	201	PEE	C22-C23-C24-C25
51	V	201	CDL	C62-C63-C64-C65
51	l	703	CDL	C35-C36-C37-C38
48	l	701	PEE	O5-C30-O3-C3
51	l	703	CDL	OB9-CB7-OB8-CB6
51	r	504	CDL	OB7-CB5-OB6-CB4
51	a	201	CDL	CB2-C1-CA2-OA2
48	j	201	PEE	C31-C30-O3-C3
48	l	704	PEE	C31-C30-O3-C3
51	I	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C71-CB7-OB8-CB6
51	l	702	CDL	C71-CB7-OB8-CB6
51	s	401	CDL	C71-CB7-OB8-CB6
51	a	201	CDL	C36-C37-C38-C39
49	g	201	PLX	C2-C1-N1-C1A
51	r	504	CDL	C74-C75-C76-C77
51	l	702	CDL	C55-C56-C57-C58
51	r	504	CDL	C60-C61-C62-C63
51	V	202	CDL	O1-C1-CB2-OB2
51	l	702	CDL	O1-C1-CA2-OA2
51	l	702	CDL	O1-C1-CB2-OB2
51	l	702	CDL	CB5-C51-C52-C53
49	g	201	PLX	C17-C18-C19-C20
51	a	201	CDL	C71-CB7-OB8-CB6
49	r	502	PLX	C7-C8-C9-C10
48	b	201	PEE	C10-C11-C12-C13
48	B	303	PEE	C22-C23-C24-C25
48	W	201	PEE	C11-C12-C13-C14
48	B	303	PEE	C17-C18-C19-C20
51	k	101	CDL	CA7-C31-C32-C33
48	C	302	PEE	C41-C42-C43-C44
51	V	201	CDL	C59-C60-C61-C62
49	j	203	PLX	C13-C14-C15-C16
50	X	201	8Q1	C10-C11-C12-C13
53	s	402	UQ	C27-C28-C29-C31
48	j	202	PEE	O4-C10-O2-C2
51	a	201	CDL	OB7-CB5-OB6-CB4
53	s	402	UQ	C14-C16-C17-C18
48	j	201	PEE	C32-C33-C34-C35
49	g	201	PLX	C2-C1-N1-C1B
51	a	201	CDL	CB5-C51-C52-C53
48	l	704	PEE	O5-C30-O3-C3
51	l	702	CDL	OB9-CB7-OB8-CB6
51	s	401	CDL	OB9-CB7-OB8-CB6
51	k	101	CDL	C11-CA5-OA6-CA4
51	l	702	CDL	CB7-C71-C72-C73
51	n	101	CDL	CB7-C71-C72-C73
48	j	201	PEE	O5-C30-O3-C3
51	I	201	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	OB9-CB7-OB8-CB6
48	Q	501	PEE	C11-C12-C13-C14
51	l	702	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
48	l	701	PEE	C11-C12-C13-C14
49	J	403	PLX	C11-C10-C9-C8
51	k	101	CDL	C40-C41-C42-C43
51	V	201	CDL	O1-C1-CB2-OB2
51	a	201	CDL	O1-C1-CB2-OB2
51	l	702	CDL	CA7-C31-C32-C33
53	s	402	UQ	C22-C23-C24-C25
48	l	704	PEE	C37-C38-C39-C40
46	A	502	FMN	O2'-C2'-C3'-O3'
48	r	501	PEE	C10-C11-C12-C13
51	l	703	CDL	CB5-C51-C52-C53
48	B	303	PEE	C11-C10-O2-C2
48	b	201	PEE	C11-C10-O2-C2
46	A	502	FMN	O2'-C2'-C3'-C4'
49	r	502	PLX	C9-C10-C11-C12
51	V	201	CDL	C34-C35-C36-C37
51	r	504	CDL	C23-C24-C25-C26
48	B	303	PEE	O4-C10-O2-C2
48	b	201	PEE	O4-C10-O2-C2
51	k	101	CDL	OA7-CA5-OA6-CA4
51	V	201	CDL	CB2-C1-CA2-OA2
51	s	401	CDL	CB2-C1-CA2-OA2
48	W	201	PEE	C31-C30-O3-C3
48	b	201	PEE	C31-C30-O3-C3
51	k	101	CDL	C36-C37-C38-C39
51	l	703	CDL	C31-CA7-OA8-CA6
53	J	402	UQ	C20-C19-C21-C22
53	s	402	UQ	C23-C24-C26-C27
49	r	502	PLX	O6-C6-C7-C8
48	r	501	PEE	C11-C10-O2-C2
51	I	201	CDL	C51-CB5-OB6-CB4
51	l	703	CDL	C51-CB5-OB6-CB4
48	r	501	PEE	O4-C10-O2-C2
51	l	703	CDL	OB7-CB5-OB6-CB4
48	W	201	PEE	C17-C18-C19-C20
51	a	201	CDL	OB9-CB7-OB8-CB6
51	k	101	CDL	C16-C17-C18-C19
50	X	201	8Q1	C6-C7-C8-C9
51	s	401	CDL	C33-C34-C35-C36
51	k	101	CDL	C58-C59-C60-C61
51	k	101	CDL	C60-C61-C62-C63
51	s	401	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C2-C1-N1-C1C
48	B	303	PEE	C31-C32-C33-C34
51	V	202	CDL	C59-C60-C61-C62
51	s	401	CDL	C17-C18-C19-C20
48	C	302	PEE	C13-C14-C15-C16
49	C	303	PLX	C14-C15-C16-C17
49	C	303	PLX	C11-C12-C13-C14
49	g	201	PLX	C28-C29-C30-C31
49	j	203	PLX	C14-C15-C16-C17
50	G	201	8Q1	C10-C11-C12-C13
51	V	201	CDL	C55-C56-C57-C58
51	V	202	CDL	C13-C14-C15-C16
51	V	202	CDL	C37-C38-C39-C40
51	k	101	CDL	C55-C56-C57-C58
51	n	101	CDL	CB5-C51-C52-C53
49	a	202	PLX	C14-C15-C16-C17
49	a	202	PLX	C25-C26-C27-C28
49	a	202	PLX	C35-C36-C37-C38
49	j	203	PLX	C16-C17-C18-C19
49	r	502	PLX	C27-C28-C29-C30
51	l	702	CDL	C51-C52-C53-C54
51	l	702	CDL	C56-C57-C58-C59
51	l	702	CDL	C62-C63-C64-C65
51	V	202	CDL	C71-CB7-OB8-CB6
48	B	303	PEE	C13-C14-C15-C16
48	W	201	PEE	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
48	r	501	PEE	C11-C12-C13-C14
49	C	303	PLX	C10-C11-C12-C13
49	J	403	PLX	C14-C15-C16-C17
49	J	403	PLX	C13-C14-C15-C16
49	a	202	PLX	C13-C14-C15-C16
49	r	502	PLX	C34-C35-C36-C37
51	V	202	CDL	C60-C61-C62-C63
51	l	702	CDL	C71-C72-C73-C74
51	l	702	CDL	C74-C75-C76-C77
51	l	703	CDL	C34-C35-C36-C37
51	r	504	CDL	C31-C32-C33-C34
51	I	201	CDL	OB7-CB5-OB6-CB4
49	J	403	PLX	C7-C8-C9-C10
49	g	201	PLX	C13-C14-C15-C16
51	s	401	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
51	s	401	CDL	C52-C53-C54-C55
51	s	401	CDL	C75-C76-C77-C78
48	B	303	PEE	C12-C13-C14-C15
51	V	202	CDL	C56-C57-C58-C59
51	s	401	CDL	C73-C74-C75-C76
51	l	702	CDL	C36-C37-C38-C39
51	l	702	CDL	C75-C76-C77-C78
49	J	403	PLX	O4-C3-C4-C5
48	W	201	PEE	C12-C13-C14-C15
48	l	704	PEE	C21-C22-C23-C24
49	J	403	PLX	C25-C26-C27-C28
51	l	702	CDL	C19-C20-C21-C22
48	l	701	PEE	C10-C11-C12-C13
51	r	504	CDL	CA7-C31-C32-C33
49	g	201	PLX	C32-C33-C34-C35
49	j	203	PLX	C31-C32-C33-C34
51	V	201	CDL	C52-C53-C54-C55
51	a	201	CDL	C35-C36-C37-C38
51	l	703	CDL	C71-C72-C73-C74
48	W	201	PEE	O5-C30-O3-C3
48	b	201	PEE	O5-C30-O3-C3
48	l	704	PEE	C31-C32-C33-C34
51	a	201	CDL	C37-C38-C39-C40
49	j	203	PLX	C34-C35-C36-C37
51	r	504	CDL	C75-C76-C77-C78
49	g	201	PLX	C30-C31-C32-C33
48	B	303	PEE	C42-C43-C44-C45
49	r	503	PLX	C10-C11-C12-C13
49	r	503	PLX	C35-C36-C37-C38
51	V	202	CDL	C33-C34-C35-C36
51	a	201	CDL	C60-C61-C62-C63
51	l	703	CDL	C58-C59-C60-C61
51	l	703	CDL	C59-C60-C61-C62
51	r	504	CDL	C62-C63-C64-C65
48	r	501	PEE	C13-C14-C15-C16
49	r	503	PLX	C25-C26-C27-C28
51	V	201	CDL	C35-C36-C37-C38
51	k	101	CDL	C21-C22-C23-C24
51	s	401	CDL	CB5-C51-C52-C53
48	B	303	PEE	C23-C24-C25-C26
49	r	503	PLX	C12-C13-C14-C15
51	V	202	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C55-C56-C57-C58
51	k	101	CDL	C59-C60-C61-C62
51	l	703	CDL	OA9-CA7-OA8-CA6
51	V	201	CDL	C12-C13-C14-C15
49	r	503	PLX	C13-C14-C15-C16
49	j	203	PLX	C7-C8-C9-C10
51	l	703	CDL	C51-C52-C53-C54
51	l	703	CDL	C54-C55-C56-C57
51	V	201	CDL	CA5-C11-C12-C13
49	g	201	PLX	C33-C34-C35-C36
51	s	401	CDL	C51-C52-C53-C54
51	V	202	CDL	C54-C55-C56-C57
51	k	101	CDL	C71-C72-C73-C74
51	l	702	CDL	C59-C60-C61-C62
48	W	201	PEE	C24-C25-C26-C27
48	j	201	PEE	C22-C23-C24-C25
48	j	201	PEE	C42-C43-C44-C45
48	l	704	PEE	C34-C35-C36-C37
51	V	201	CDL	C37-C38-C39-C40
51	r	504	CDL	C71-C72-C73-C74
51	l	702	CDL	C52-C53-C54-C55
51	V	202	CDL	OB9-CB7-OB8-CB6
49	J	403	PLX	C27-C28-C29-C30
51	a	201	CDL	C22-C23-C24-C25
51	l	703	CDL	C72-C73-C74-C75
49	C	303	PLX	C28-C29-C30-C31
49	j	203	PLX	C29-C30-C31-C32
49	r	502	PLX	C33-C34-C35-C36
51	V	201	CDL	C58-C59-C60-C61
51	l	703	CDL	C80-C81-C82-C83
51	r	504	CDL	C43-C44-C45-C46
48	W	201	PEE	C10-C11-C12-C13
48	C	302	PEE	C42-C43-C44-C45
51	V	201	CDL	C71-C72-C73-C74
51	V	202	CDL	C52-C53-C54-C55
51	a	201	CDL	C52-C53-C54-C55
49	C	303	PLX	C11-C10-C9-C8
49	j	203	PLX	C33-C34-C35-C36
51	k	101	CDL	C75-C76-C77-C78
51	l	702	CDL	C73-C74-C75-C76
51	s	401	CDL	C71-C72-C73-C74
48	b	201	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C9-C10-C11-C12
48	C	302	PEE	C43-C44-C45-C46
48	l	701	PEE	C32-C33-C34-C35
51	a	201	CDL	C73-C74-C75-C76
51	s	401	CDL	C55-C56-C57-C58
48	r	501	PEE	C40-C41-C42-C43
51	s	401	CDL	C36-C37-C38-C39
48	j	201	PEE	C11-C10-O2-C2
51	V	201	CDL	C51-CB5-OB6-CB4
51	l	702	CDL	C11-CA5-OA6-CA4
51	s	401	CDL	CB7-C71-C72-C73
48	Q	501	PEE	C21-C22-C23-C24
51	s	401	CDL	C54-C55-C56-C57
48	j	201	PEE	O4-C10-O2-C2
51	r	504	CDL	C57-C58-C59-C60
48	l	701	PEE	C35-C36-C37-C38
49	J	403	PLX	C29-C30-C31-C32
51	V	202	CDL	C75-C76-C77-C78
51	l	703	CDL	C33-C34-C35-C36
49	a	202	PLX	C10-C11-C12-C13
49	r	502	PLX	C31-C32-C33-C34
47	A	503	NAI	C3D-C4D-C5D-O5D
49	C	303	PLX	C19-C20-C21-C22
49	J	403	PLX	C31-C32-C33-C34
49	J	403	PLX	C33-C34-C35-C36
48	j	201	PEE	C40-C41-C42-C43
49	r	503	PLX	C15-C16-C17-C18
51	V	202	CDL	C76-C77-C78-C79
51	r	504	CDL	C32-C33-C34-C35
51	s	401	CDL	C59-C60-C61-C62
51	r	504	CDL	C41-C42-C43-C44
51	a	201	CDL	C32-C33-C34-C35
51	l	702	CDL	C32-C33-C34-C35
51	s	401	CDL	OA5-CA3-CA4-OA6
48	j	202	PEE	C11-C12-C13-C14
51	r	504	CDL	C83-C84-C85-C86
53	s	402	UQ	C27-C28-C29-C30
49	r	503	PLX	C30-C31-C32-C33
49	r	503	PLX	C28-C29-C30-C31
49	r	503	PLX	C31-C32-C33-C34
51	l	703	CDL	C21-C22-C23-C24
51	n	101	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C35-C36-C37-C38
51	V	202	CDL	OA6-CA4-CA6-OA8
51	l	702	CDL	OA6-CA4-CA6-OA8
51	s	401	CDL	OB6-CB4-CB6-OB8
49	g	201	PLX	C10-C11-C12-C13
48	B	303	PEE	C31-C30-O3-C3
49	C	303	PLX	C13-C14-C15-C16
51	k	101	CDL	C52-C53-C54-C55
51	k	101	CDL	C79-C80-C81-C82
51	s	401	CDL	C35-C36-C37-C38
51	V	201	CDL	C75-C76-C77-C78
51	l	702	CDL	C13-C14-C15-C16
49	a	202	PLX	C16-C17-C18-C19
51	k	101	CDL	C20-C21-C22-C23
51	r	504	CDL	C63-C64-C65-C66
51	l	702	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	C18-C19-C20-C21
51	a	201	CDL	C74-C75-C76-C77
48	l	704	PEE	C44-C45-C46-C47
51	l	703	CDL	C74-C75-C76-C77
51	r	504	CDL	C84-C85-C86-C87
49	j	203	PLX	C12-C13-C14-C15
51	V	202	CDL	C11-CA5-OA6-CA4
51	V	201	CDL	C72-C73-C74-C75
50	X	201	8Q1	O33-C32-C34-O35
51	k	101	CDL	C14-C15-C16-C17
51	l	703	CDL	C17-C18-C19-C20
48	r	501	PEE	C38-C39-C40-C41
48	Q	501	PEE	C35-C36-C37-C38
48	j	202	PEE	C19-C20-C21-C22
48	b	201	PEE	C13-C14-C15-C16
51	a	201	CDL	C62-C63-C64-C65
51	k	101	CDL	OA5-CA3-CA4-CA6
51	k	101	CDL	OB5-CB3-CB4-CB6
51	s	401	CDL	OA5-CA3-CA4-CA6
48	B	303	PEE	C11-C12-C13-C14
49	r	502	PLX	C11-C10-C9-C8
51	l	703	CDL	C38-C39-C40-C41
50	X	201	8Q1	C11-C12-C13-C14
52	J	401	NDP	C3D-C4D-C5D-O5D
49	j	203	PLX	C9-C10-C11-C12
49	C	303	PLX	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C19-C20-C21-C22
51	a	201	CDL	C76-C77-C78-C79
51	a	201	CDL	C11-CA5-OA6-CA4
51	s	401	CDL	C11-CA5-OA6-CA4
48	l	701	PEE	C31-C32-C33-C34
51	V	201	CDL	C32-C33-C34-C35
51	k	101	CDL	C56-C57-C58-C59
51	l	702	CDL	C12-C13-C14-C15
48	l	704	PEE	C30-C31-C32-C33
48	b	201	PEE	C22-C23-C24-C25
49	a	202	PLX	C33-C34-C35-C36
48	j	202	PEE	C22-C23-C24-C25
48	l	701	PEE	C17-C18-C19-C20
48	j	202	PEE	C23-C24-C25-C26
48	j	202	PEE	C10-C11-C12-C13
48	b	201	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8
49	a	202	PLX	C9-C10-C11-C12
51	V	202	CDL	C42-C43-C44-C45
51	s	401	CDL	C14-C15-C16-C17
48	Q	501	PEE	C19-C20-C21-C22
48	W	201	PEE	C19-C20-C21-C22
48	j	202	PEE	C15-C16-C17-C18
48	l	704	PEE	C39-C40-C41-C42
51	k	101	CDL	C41-C42-C43-C44
51	s	401	CDL	O1-C1-CB2-OB2
49	r	502	PLX	C14-C15-C16-C17
49	r	502	PLX	C11-C12-C13-C14
51	l	702	CDL	C37-C38-C39-C40
51	r	504	CDL	C14-C15-C16-C17
51	r	504	CDL	C59-C60-C61-C62
49	J	403	PLX	C28-C29-C30-C31
51	l	703	CDL	C22-C23-C24-C25
48	B	303	PEE	C41-C42-C43-C44
48	l	704	PEE	C32-C33-C34-C35
49	r	503	PLX	C16-C17-C18-C19
51	a	201	CDL	C18-C19-C20-C21
51	r	504	CDL	C54-C55-C56-C57
51	a	201	CDL	CA5-C11-C12-C13
51	V	202	CDL	C84-C85-C86-C87
51	a	201	CDL	C39-C40-C41-C42
51	V	202	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	O5-C30-O3-C3
48	l	704	PEE	C13-C14-C15-C16
49	r	502	PLX	C28-C29-C30-C31
49	r	502	PLX	C30-C31-C32-C33
51	l	702	CDL	C42-C43-C44-C45
48	Q	501	PEE	C23-C24-C25-C26
49	a	202	PLX	C30-C31-C32-C33
51	k	101	CDL	C71-CB7-OB8-CB6
51	k	101	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C35-C36-C37-C38
51	a	201	CDL	C75-C76-C77-C78
48	r	501	PEE	C17-C18-C19-C20
49	j	203	PLX	C27-C28-C29-C30
49	r	503	PLX	C7-C8-C9-C10
51	n	101	CDL	C52-C53-C54-C55
48	j	201	PEE	C38-C39-C40-C41
51	l	703	CDL	C44-C45-C46-C47
48	r	501	PEE	C33-C34-C35-C36
51	l	702	CDL	C17-C18-C19-C20
51	l	703	CDL	C19-C20-C21-C22
51	a	201	CDL	C84-C85-C86-C87
48	B	303	PEE	C14-C15-C16-C17
48	C	302	PEE	C11-C12-C13-C14
49	j	203	PLX	C26-C27-C28-C29
51	V	202	CDL	C73-C74-C75-C76
51	r	504	CDL	C17-C18-C19-C20
51	l	703	CDL	C24-C25-C26-C27
48	B	303	PEE	C21-C22-C23-C24
49	g	201	PLX	C25-C26-C27-C28
51	k	101	CDL	C15-C16-C17-C18
51	l	702	CDL	C80-C81-C82-C83
48	l	701	PEE	O2-C2-C3-O3
51	k	101	CDL	OB6-CB4-CB6-OB8
48	j	202	PEE	C14-C15-C16-C17
49	J	403	PLX	C36-C37-C38-C39
51	r	504	CDL	C64-C65-C66-C67
51	l	703	CDL	CB7-C71-C72-C73
51	V	201	CDL	OB7-CB5-OB6-CB4
50	G	201	8Q1	C30-C29-C32-O33
53	J	402	UQ	C9-C11-C12-C13
51	k	101	CDL	C32-C33-C34-C35
48	j	201	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C14-C15-C16-C17
51	l	703	CDL	C63-C64-C65-C66
48	r	501	PEE	C31-C30-O3-C3
50	X	201	8Q1	C13-C14-C15-C16
51	l	703	CDL	C64-C65-C66-C67
51	s	401	CDL	C40-C41-C42-C43
48	j	201	PEE	C44-C45-C46-C47
51	n	101	CDL	C72-C73-C74-C75
49	J	403	PLX	O9-C24-C25-C26
51	l	703	CDL	C84-C85-C86-C87
48	Q	501	PEE	C34-C35-C36-C37
49	g	201	PLX	C27-C28-C29-C30
49	j	203	PLX	C25-C26-C27-C28
51	V	201	CDL	C64-C65-C66-C67
49	a	202	PLX	C28-C29-C30-C31
51	a	201	CDL	C54-C55-C56-C57
48	l	704	PEE	C33-C34-C35-C36
51	V	202	CDL	C74-C75-C76-C77
51	l	703	CDL	C43-C44-C45-C46
51	a	201	CDL	OA5-CA3-CA4-CA6
51	a	201	CDL	OB5-CB3-CB4-CB6
48	B	303	PEE	C32-C33-C34-C35
51	V	202	CDL	C35-C36-C37-C38
48	W	201	PEE	C21-C22-C23-C24
48	l	701	PEE	C33-C34-C35-C36
51	V	202	CDL	C17-C18-C19-C20
51	V	202	CDL	C82-C83-C84-C85
51	k	101	CDL	OB9-CB7-OB8-CB6
51	l	702	CDL	C15-C16-C17-C18
51	k	101	CDL	CA2-C1-CB2-OB2
49	C	303	PLX	C33-C34-C35-C36
48	j	202	PEE	C1-C2-C3-O3
49	J	403	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
51	V	202	CDL	CA3-CA4-CA6-OA8
51	k	101	CDL	CB3-CB4-CB6-OB8
51	l	702	CDL	CA3-CA4-CA6-OA8
51	s	401	CDL	CB3-CB4-CB6-OB8
49	j	203	PLX	C11-C12-C13-C14
49	r	503	PLX	C27-C28-C29-C30
51	k	101	CDL	C74-C75-C76-C77
51	l	703	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
51	r	504	CDL	C15-C16-C17-C18
51	r	504	CDL	C35-C36-C37-C38
49	g	201	PLX	C12-C13-C14-C15
48	b	201	PEE	O3P-C1-C2-O2
49	J	403	PLX	O4-C3-C4-O6
49	r	502	PLX	O4-C3-C4-O6
51	V	202	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	OA5-CA3-CA4-OA6
51	l	702	CDL	OB5-CB3-CB4-OB6
49	a	202	PLX	C19-C20-C21-C22
49	C	303	PLX	C7-C8-C9-C10
51	a	201	CDL	C71-C72-C73-C74
51	k	101	CDL	C37-C38-C39-C40
51	k	101	CDL	C39-C40-C41-C42
49	r	503	PLX	C32-C33-C34-C35
49	r	502	PLX	C12-C13-C14-C15
50	X	201	8Q1	C9-C10-C11-C12
49	r	502	PLX	O6-C4-C5-O8
51	V	201	CDL	OB6-CB4-CB6-OB8
51	V	202	CDL	OB6-CB4-CB6-OB8
51	n	101	CDL	OA6-CA4-CA6-OA8
51	r	504	CDL	OA6-CA4-CA6-OA8
49	g	201	PLX	C16-C17-C18-C19
48	C	302	PEE	C34-C35-C36-C37
49	r	502	PLX	C13-C14-C15-C16
51	l	703	CDL	C15-C16-C17-C18
49	j	203	PLX	O6-C6-C7-C8
51	a	201	CDL	C20-C21-C22-C23
51	l	703	CDL	C39-C40-C41-C42
48	Q	501	PEE	C10-C11-C12-C13
48	l	704	PEE	C10-C11-C12-C13
49	r	502	PLX	C18-C19-C20-C21
50	G	201	8Q1	C11-C12-C13-C14
51	r	504	CDL	CA5-C11-C12-C13
48	j	201	PEE	C34-C35-C36-C37
48	r	501	PEE	C21-C22-C23-C24
51	V	202	CDL	C39-C40-C41-C42
48	r	501	PEE	C42-C43-C44-C45
51	s	401	CDL	C34-C35-C36-C37
49	j	203	PLX	C36-C37-C38-C39
51	V	202	CDL	C12-C13-C14-C15
51	V	202	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
51	k	101	CDL	C33-C34-C35-C36
49	r	502	PLX	C6-C7-C8-C9
51	r	504	CDL	C19-C20-C21-C22
51	I	201	CDL	CA2-C1-CB2-OB2
51	l	703	CDL	CB2-C1-CA2-OA2
49	r	502	PLX	C10-C11-C12-C13
51	r	504	CDL	C13-C14-C15-C16
48	C	302	PEE	C12-C13-C14-C15
51	V	201	CDL	C43-C44-C45-C46
48	B	303	PEE	O3P-C1-C2-C3
51	k	101	CDL	C84-C85-C86-C87
48	B	303	PEE	C36-C37-C38-C39
48	r	501	PEE	C36-C37-C38-C39
49	J	403	PLX	C10-C11-C12-C13
49	a	202	PLX	C7-C8-C9-C10
49	C	303	PLX	C4-C5-O8-C24
49	J	403	PLX	C24-C25-C26-C27
51	V	202	CDL	OA7-CA5-OA6-CA4
51	a	201	CDL	OA7-CA5-OA6-CA4
51	s	401	CDL	OA7-CA5-OA6-CA4
51	k	101	CDL	C77-C78-C79-C80
51	r	504	CDL	C53-C54-C55-C56
48	r	501	PEE	O5-C30-O3-C3
51	a	201	CDL	C11-C12-C13-C14
48	l	704	PEE	C3-C2-O2-C10
51	V	201	CDL	CA6-CA4-OA6-CA5
48	C	302	PEE	C15-C16-C17-C18
51	V	201	CDL	C44-C45-C46-C47
51	l	703	CDL	C75-C76-C77-C78
51	r	504	CDL	C77-C78-C79-C80
48	j	201	PEE	C21-C22-C23-C24
48	j	201	PEE	O3P-C1-C2-O2
48	l	701	PEE	O3P-C1-C2-O2
49	r	503	PLX	O4-C3-C4-O6
51	V	201	CDL	OB5-CB3-CB4-OB6
51	a	201	CDL	OA5-CA3-CA4-OA6
51	a	201	CDL	OB5-CB3-CB4-OB6
48	W	201	PEE	C34-C35-C36-C37
48	C	302	PEE	C1-C2-C3-O3
48	l	701	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
49	g	201	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
51	n	101	CDL	CA3-CA4-CA6-OA8
51	n	101	CDL	C51-C52-C53-C54
51	k	101	CDL	C64-C65-C66-C67
48	B	303	PEE	C38-C39-C40-C41
48	j	201	PEE	C36-C37-C38-C39
48	B	303	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
48	b	201	PEE	O2-C2-C3-O3
48	j	202	PEE	O2-C2-C3-O3
51	V	202	CDL	C11-C12-C13-C14
48	j	201	PEE	C13-C14-C15-C16
49	r	503	PLX	C11-C10-C9-C8
51	V	202	CDL	C83-C84-C85-C86
51	k	101	CDL	C51-C52-C53-C54
52	J	401	NDP	O4D-C1D-N1N-C6N
51	l	703	CDL	C41-C42-C43-C44
51	s	401	CDL	C16-C17-C18-C19
49	J	403	PLX	N1-C1-C2-O1
51	l	702	CDL	CB2-C1-CA2-OA2
51	k	101	CDL	C62-C63-C64-C65
51	r	504	CDL	C36-C37-C38-C39
51	r	504	CDL	C56-C57-C58-C59
51	V	202	CDL	C64-C65-C66-C67
48	r	501	PEE	C34-C35-C36-C37
51	l	703	CDL	C37-C38-C39-C40
49	C	303	PLX	C15-C16-C17-C18
49	a	202	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
50	G	201	8Q1	C7-C8-C9-C10
51	a	201	CDL	C31-C32-C33-C34
51	r	504	CDL	C72-C71-CB7-OB8
46	A	502	FMN	O4'-C4'-C5'-O5'
48	b	201	PEE	O3P-C1-C2-C3
48	l	701	PEE	O3P-C1-C2-C3
49	r	502	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
51	V	201	CDL	OA5-CA3-CA4-CA6
51	V	201	CDL	OB5-CB3-CB4-CB6
51	V	202	CDL	OA5-CA3-CA4-CA6
51	l	702	CDL	OA5-CA3-CA4-CA6
51	l	703	CDL	C76-C77-C78-C79
50	G	201	8Q1	O27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	k	101	CDL	C11-C12-C13-C14
48	r	501	PEE	C32-C33-C34-C35
49	J	403	PLX	C16-C17-C18-C19
51	k	101	CDL	CA4-CA3-OA5-PA1
48	j	202	PEE	C24-C25-C26-C27
51	V	201	CDL	C54-C55-C56-C57
51	r	504	CDL	C71-CB7-OB8-CB6
49	g	201	PLX	O6-C6-C7-C8
49	j	203	PLX	O8-C24-C25-C26
49	J	403	PLX	C11-C12-C13-C14
51	a	201	CDL	C14-C15-C16-C17
51	s	401	CDL	C18-C19-C20-C21
48	j	202	PEE	C12-C13-C14-C15
51	l	703	CDL	CA7-C31-C32-C33
48	C	302	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
48	l	704	PEE	C22-C23-C24-C25
49	a	202	PLX	C3-C4-C5-O8
51	V	202	CDL	C32-C31-CA7-OA8
51	k	101	CDL	CB5-C51-C52-C53
48	j	201	PEE	C15-C16-C17-C18
48	b	201	PEE	C34-C35-C36-C37
51	r	504	CDL	C12-C13-C14-C15
51	a	201	CDL	C38-C39-C40-C41
51	n	101	CDL	C54-C55-C56-C57
51	r	504	CDL	OB9-CB7-OB8-CB6
51	V	202	CDL	CA7-C31-C32-C33
48	l	704	PEE	C40-C41-C42-C43
51	V	201	CDL	C74-C75-C76-C77
51	l	702	CDL	C54-C55-C56-C57
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C5B-O5B-PA-O3
48	Q	501	PEE	C4-O4P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O4P
48	b	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O2P
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	C2-O1-P1-O4
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C5-C4-O6-C6
49	a	202	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O2
49	j	203	PLX	C2-O1-P1-O3
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	C2-O1-P1-O3
51	I	201	CDL	CA2-OA2-PA1-OA4
51	I	201	CDL	CA3-OA5-PA1-OA3
51	V	201	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB2-OB2-PB2-OB4
51	V	202	CDL	CB3-OB5-PB2-OB2
51	V	202	CDL	CB3-OB5-PB2-OB3
51	V	202	CDL	CB3-OB5-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB4
51	a	201	CDL	CB2-OB2-PB2-OB5
51	k	101	CDL	CB2-OB2-PB2-OB4
51	k	101	CDL	CB2-OB2-PB2-OB5
51	l	702	CDL	CB3-OB5-PB2-OB4
51	l	703	CDL	CB3-OB5-PB2-OB2
51	r	504	CDL	CB2-OB2-PB2-OB3
51	r	504	CDL	CB2-OB2-PB2-OB4
51	r	504	CDL	CB2-OB2-PB2-OB5
51	s	401	CDL	CB3-OB5-PB2-OB3
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
57	w	401	ADP	C5'-O5'-PA-O3A
49	a	202	PLX	C11-C12-C13-C14
51	l	703	CDL	C62-C63-C64-C65
48	B	303	PEE	C39-C40-C41-C42
51	r	504	CDL	C1-CB2-OB2-PB2
49	r	502	PLX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C16-C17-C18-C19
51	a	201	CDL	C57-C58-C59-C60
50	X	201	8Q1	C12-C13-C14-C15
51	l	703	CDL	C11-C12-C13-C14
48	l	704	PEE	C43-C44-C45-C46
51	s	401	CDL	C77-C78-C79-C80
48	b	201	PEE	C14-C15-C16-C17
48	B	303	PEE	C18-C19-C20-C21
48	Q	501	PEE	C16-C17-C18-C19
51	r	504	CDL	CB5-C51-C52-C53
51	I	201	CDL	CB2-C1-CA2-OA2
48	B	303	PEE	O3P-C1-C2-O2
51	V	201	CDL	OA5-CA3-CA4-OA6
49	j	203	PLX	C30-C31-C32-C33
51	a	201	CDL	C64-C65-C66-C67
49	r	502	PLX	C35-C36-C37-C38
51	V	201	CDL	C73-C74-C75-C76
48	l	704	PEE	C14-C15-C16-C17
48	b	201	PEE	C30-C31-C32-C33
51	r	504	CDL	C44-C45-C46-C47
49	J	403	PLX	O6-C4-C5-O8
48	B	303	PEE	C44-C45-C46-C47
48	l	701	PEE	C18-C19-C20-C21
51	V	202	CDL	CB7-C71-C72-C73
51	l	702	CDL	C24-C25-C26-C27
49	r	503	PLX	C11-C12-C13-C14
51	l	702	CDL	C12-C11-CA5-OA6
51	r	504	CDL	CA3-CA4-CA6-OA8
51	a	201	CDL	C12-C13-C14-C15
48	j	202	PEE	C33-C34-C35-C36
49	a	202	PLX	C18-C19-C20-C21
51	l	703	CDL	C32-C33-C34-C35
53	J	402	UQ	C11-C12-C13-C14
51	V	202	CDL	C19-C20-C21-C22
51	s	401	CDL	C83-C84-C85-C86
48	C	302	PEE	C35-C36-C37-C38
48	C	302	PEE	C20-C21-C22-C23
49	g	201	PLX	O8-C24-C25-C26
49	j	203	PLX	C18-C19-C20-C21
48	l	704	PEE	C41-C42-C43-C44
51	V	202	CDL	C36-C37-C38-C39
51	l	703	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
51	V	201	CDL	C38-C39-C40-C41
51	n	101	CDL	C75-C76-C77-C78
48	C	302	PEE	C44-C45-C46-C47
49	C	303	PLX	O4-C3-C4-O6
51	l	703	CDL	OA5-CA3-CA4-OA6
51	n	101	CDL	OA5-CA3-CA4-OA6
48	j	202	PEE	C16-C17-C18-C19
51	r	504	CDL	C39-C40-C41-C42
51	l	703	CDL	C18-C19-C20-C21
51	V	202	CDL	C71-C72-C73-C74
51	n	101	CDL	O1-C1-CB2-OB2
51	r	504	CDL	O1-C1-CA2-OA2
51	r	504	CDL	O1-C1-CB2-OB2
48	Q	501	PEE	C24-C25-C26-C27
51	l	703	CDL	C13-C14-C15-C16
48	b	201	PEE	C18-C19-C20-C21
48	b	201	PEE	C16-C17-C18-C19
48	r	501	PEE	C18-C19-C20-C21
48	l	704	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
51	l	703	CDL	OA6-CA4-CA6-OA8
51	r	504	CDL	C52-C53-C54-C55
51	V	201	CDL	CA4-CA3-OA5-PA1
51	k	101	CDL	C1-CB2-OB2-PB2
51	I	201	CDL	C51-C52-C53-C54
51	V	202	CDL	CB3-CB4-CB6-OB8
49	a	202	PLX	C27-C28-C29-C30
51	a	201	CDL	C56-C57-C58-C59
51	l	703	CDL	CB6-CB4-OB6-CB5
48	C	302	PEE	C32-C33-C34-C35
51	l	703	CDL	C78-C79-C80-C81
48	j	201	PEE	C23-C24-C25-C26
48	j	202	PEE	C13-C14-C15-C16
48	Q	501	PEE	C22-C23-C24-C25
51	l	702	CDL	C82-C83-C84-C85
48	l	704	PEE	O3P-C1-C2-O2
51	n	101	CDL	OB5-CB3-CB4-OB6
51	k	101	CDL	C1-CA2-OA2-PA1
51	a	201	CDL	C21-C22-C23-C24
48	j	201	PEE	O3P-C1-C2-C3
51	l	703	CDL	OA5-CA3-CA4-CA6
48	W	201	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C63-C64-C65-C66
48	C	302	PEE	C16-C17-C18-C19
48	W	201	PEE	C16-C17-C18-C19
48	r	501	PEE	C16-C17-C18-C19
47	A	503	NAI	O4D-C4D-C5D-O5D
47	A	503	NAI	O4D-C1D-N1N-C2N
51	V	201	CDL	C40-C41-C42-C43
51	s	401	CDL	C38-C39-C40-C41
51	r	504	CDL	C42-C43-C44-C45
49	a	202	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
51	n	101	CDL	O1-C1-CA2-OA2
49	a	202	PLX	C24-C25-C26-C27
51	r	504	CDL	C61-C62-C63-C64
48	j	201	PEE	C2-C3-O3-C30
51	l	703	CDL	C42-C43-C44-C45
51	V	201	CDL	CB4-CB3-OB5-PB2
51	l	703	CDL	C61-C62-C63-C64
51	V	201	CDL	C36-C37-C38-C39
51	s	401	CDL	C15-C16-C17-C18
51	V	201	CDL	C80-C81-C82-C83
51	a	201	CDL	C44-C45-C46-C47
47	A	503	NAI	C2D-C1D-N1N-C2N
49	C	303	PLX	C34-C35-C36-C37
51	V	202	CDL	OB5-CB3-CB4-OB6
49	r	503	PLX	C24-C25-C26-C27
53	s	402	UQ	C6-C7-C8-C9
49	J	403	PLX	C30-C31-C32-C33
51	s	401	CDL	C19-C20-C21-C22
48	j	202	PEE	C17-C18-C19-C20
48	r	501	PEE	C37-C38-C39-C40
51	s	401	CDL	C72-C71-CB7-OB8
51	l	702	CDL	C23-C24-C25-C26
51	l	702	CDL	OB5-CB3-CB4-CB6
51	l	703	CDL	OB6-CB4-CB6-OB8
51	l	703	CDL	C12-C11-CA5-OA6
48	B	303	PEE	C16-C17-C18-C19
48	Q	501	PEE	C36-C37-C38-C39
48	l	701	PEE	C38-C39-C40-C41
48	l	704	PEE	C36-C37-C38-C39
51	V	202	CDL	C61-C62-C63-C64
51	l	702	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
51	s	401	CDL	C57-C58-C59-C60
48	l	704	PEE	C24-C25-C26-C27
48	C	302	PEE	C39-C40-C41-C42
48	l	704	PEE	C19-C20-C21-C22
51	V	201	CDL	C53-C54-C55-C56
50	X	201	8Q1	C28-O27-P24-O3
48	Q	501	PEE	C38-C39-C40-C41
48	l	701	PEE	C16-C17-C18-C19
49	g	201	PLX	C11-C10-C9-C8
48	b	201	PEE	C2-C3-O3-C30
48	j	202	PEE	C2-C3-O3-C30
48	r	501	PEE	C24-C25-C26-C27
51	V	201	CDL	C51-C52-C53-C54
48	B	303	PEE	C37-C38-C39-C40
53	s	402	UQ	C12-C13-C14-C16
49	a	202	PLX	C36-C37-C38-C39
48	l	704	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
48	C	302	PEE	C18-C19-C20-C21
51	k	101	CDL	C52-C51-CB5-OB6
49	g	201	PLX	C20-C21-C22-C23
51	l	702	CDL	C77-C78-C79-C80
51	n	101	CDL	C71-C72-C73-C74
48	b	201	PEE	C38-C39-C40-C41
48	l	704	PEE	C16-C17-C18-C19
51	I	201	CDL	C72-C71-CB7-OB8
51	V	202	CDL	OB5-CB3-CB4-CB6
49	g	201	PLX	C14-C15-C16-C17
49	j	203	PLX	C7-C6-O6-C4
51	r	504	CDL	C51-C52-C53-C54
48	r	501	PEE	C14-C15-C16-C17
51	V	202	CDL	C52-C51-CB5-OB6
49	g	201	PLX	C6-C7-C8-C9
48	j	202	PEE	C20-C21-C22-C23
51	s	401	CDL	C12-C11-CA5-OA6
48	j	202	PEE	C18-C19-C20-C21
49	a	202	PLX	C34-C35-C36-C37
51	l	703	CDL	O1-C1-CB2-OB2
51	V	201	CDL	C12-C11-CA5-OA6
51	a	201	CDL	C32-C31-CA7-OA8
51	I	201	CDL	OA5-CA3-CA4-OA6
53	s	402	UQ	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
51	s	401	CDL	C84-C85-C86-C87
49	a	202	PLX	C29-C30-C31-C32
51	V	201	CDL	C14-C15-C16-C17
51	s	401	CDL	C74-C75-C76-C77
51	l	702	CDL	C72-C71-CB7-OB8
51	l	702	CDL	C60-C61-C62-C63
51	s	401	CDL	C56-C57-C58-C59
52	J	401	NDP	O4B-C4B-C5B-O5B
51	r	504	CDL	OA7-CA5-OA6-CA4
51	l	703	CDL	C52-C51-CB5-OB6
51	V	201	CDL	CB3-CB4-CB6-OB8
51	l	703	CDL	CB3-CB4-CB6-OB8
49	a	202	PLX	C12-C13-C14-C15
49	r	503	PLX	C19-C20-C21-C22
51	I	201	CDL	C52-C51-CB5-OB6
51	a	201	CDL	C12-C11-CA5-OA6
51	r	504	CDL	C52-C51-CB5-OB6
50	G	201	8Q1	C12-C13-C14-C15
48	Q	501	PEE	C18-C19-C20-C21
51	r	504	CDL	C12-C11-CA5-OA6
48	l	704	PEE	C42-C43-C44-C45
51	r	504	CDL	C58-C59-C60-C61
51	s	401	CDL	CA7-C31-C32-C33
51	l	703	CDL	CB3-CB4-OB6-CB5
49	j	203	PLX	C10-C11-C12-C13
51	V	201	CDL	C22-C23-C24-C25
51	r	504	CDL	C11-CA5-OA6-CA4
48	b	201	PEE	C24-C25-C26-C27
48	r	501	PEE	C31-C32-C33-C34
48	C	302	PEE	O5-C30-O3-C3
49	r	503	PLX	C18-C19-C20-C21
51	r	504	CDL	C37-C38-C39-C40
51	s	401	CDL	C12-C11-CA5-OA7
51	I	201	CDL	C11-C12-C13-C14
49	a	202	PLX	C15-C16-C17-C18
51	I	201	CDL	C52-C51-CB5-OB7
51	a	201	CDL	C32-C31-CA7-OA9
51	k	101	CDL	C52-C51-CB5-OB7
48	l	704	PEE	C11-C12-C13-C14
51	l	703	CDL	C32-C31-CA7-OA8
49	C	303	PLX	O9-C24-O8-C5
51	r	504	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
51	V	202	CDL	C77-C78-C79-C80
51	l	703	CDL	C72-C71-CB7-OB8
51	I	201	CDL	C72-C71-CB7-OB9
51	l	702	CDL	C72-C71-CB7-OB9
49	g	201	PLX	C11-C12-C13-C14
49	J	403	PLX	C4-C5-O8-C24
49	r	502	PLX	C4-C5-O8-C24
51	V	201	CDL	C12-C11-CA5-OA7
51	V	202	CDL	C52-C51-CB5-OB7
51	l	703	CDL	C52-C51-CB5-OB7
51	r	504	CDL	C78-C79-C80-C81
51	r	504	CDL	CB4-CB3-OB5-PB2
51	a	201	CDL	C12-C11-CA5-OA7
51	r	504	CDL	C52-C51-CB5-OB7
51	V	201	CDL	CA7-C31-C32-C33
51	a	201	CDL	C24-C25-C26-C27
51	l	702	CDL	C16-C17-C18-C19
51	s	401	CDL	C13-C14-C15-C16
48	l	704	PEE	O3P-C1-C2-C3
48	C	302	PEE	C31-C30-O3-C3
49	r	503	PLX	C26-C27-C28-C29
49	r	503	PLX	C29-C30-C31-C32
48	C	302	PEE	O3-C30-C31-C32
51	V	201	CDL	C52-C51-CB5-OB6
48	B	303	PEE	C20-C21-C22-C23
57	w	401	ADP	PB-O3A-PA-O1A
48	B	303	PEE	C15-C16-C17-C18

There are no ring outliers.

37 monomers are involved in 246 short contacts:

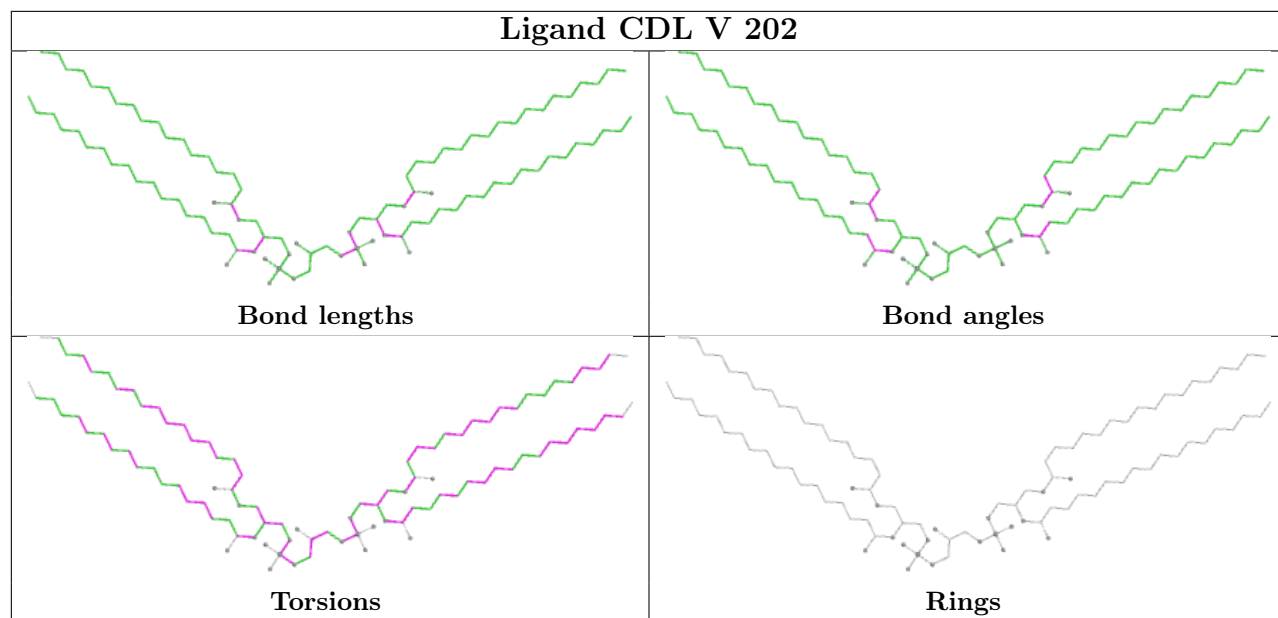
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	V	202	CDL	4	0
46	A	502	FMN	8	0
48	r	501	PEE	9	0
49	g	201	PLX	4	0
48	C	302	PEE	10	0
57	w	401	ADP	1	0
52	J	401	NDP	1	0
51	V	201	CDL	7	0
48	j	201	PEE	8	0
49	J	403	PLX	2	0

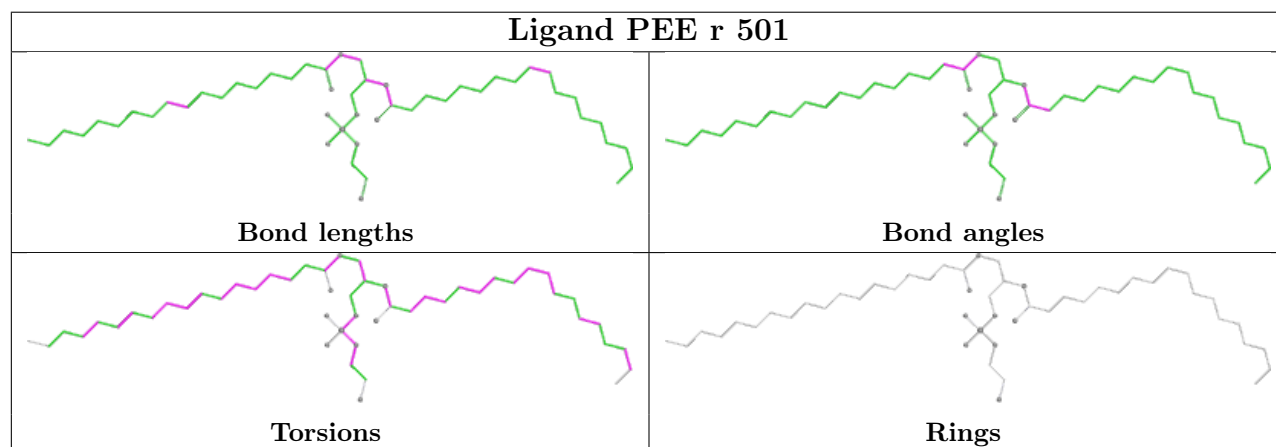
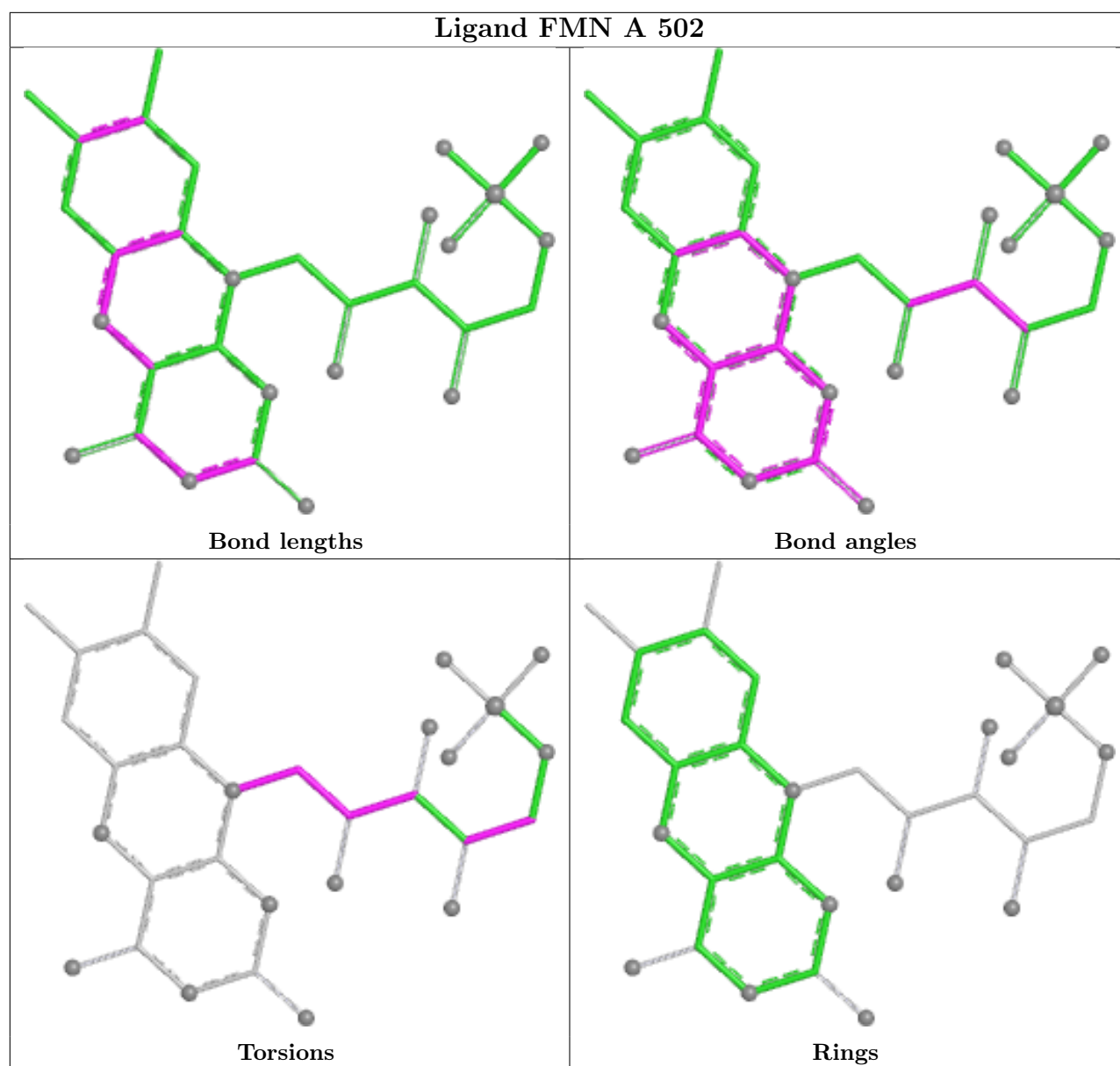
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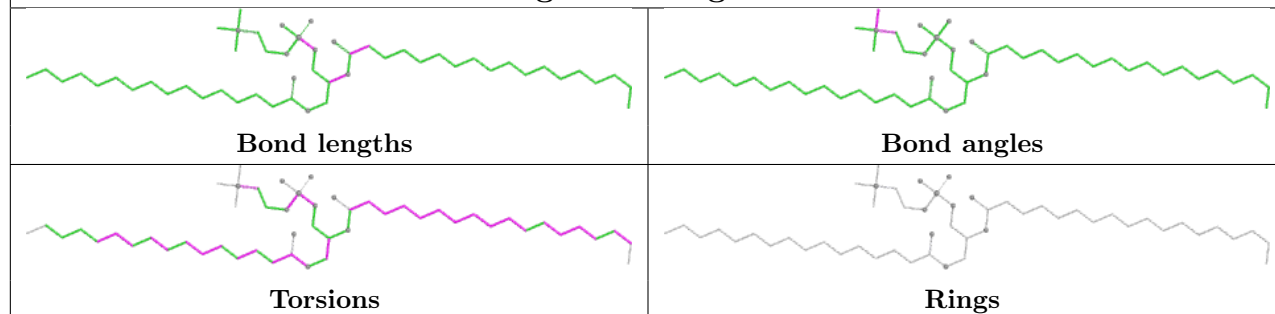
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	s	401	CDL	8	0
45	A	501	SF4	2	0
45	C	301	SF4	3	0
48	Q	501	PEE	9	0
49	r	502	PLX	2	0
50	X	201	8Q1	4	0
53	s	402	UQ	5	0
48	l	704	PEE	13	0
45	M	802	SF4	4	0
48	l	701	PEE	8	0
51	a	201	CDL	11	0
51	k	101	CDL	13	0
48	j	202	PEE	8	0
51	n	101	CDL	8	0
48	b	201	PEE	11	0
49	r	503	PLX	6	0
54	O	301	FES	4	0
48	W	201	PEE	11	0
49	C	303	PLX	18	0
51	l	703	CDL	15	0
51	l	702	CDL	13	0
51	I	201	CDL	3	0
49	j	203	PLX	3	0
51	r	504	CDL	9	0
48	B	303	PEE	6	0
53	J	402	UQ	6	0
47	A	503	NAI	7	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.

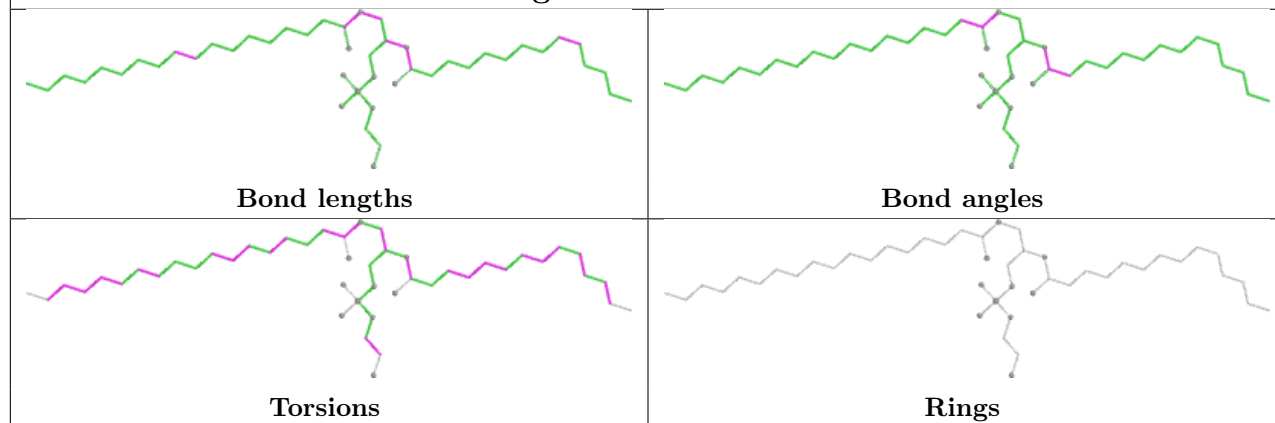




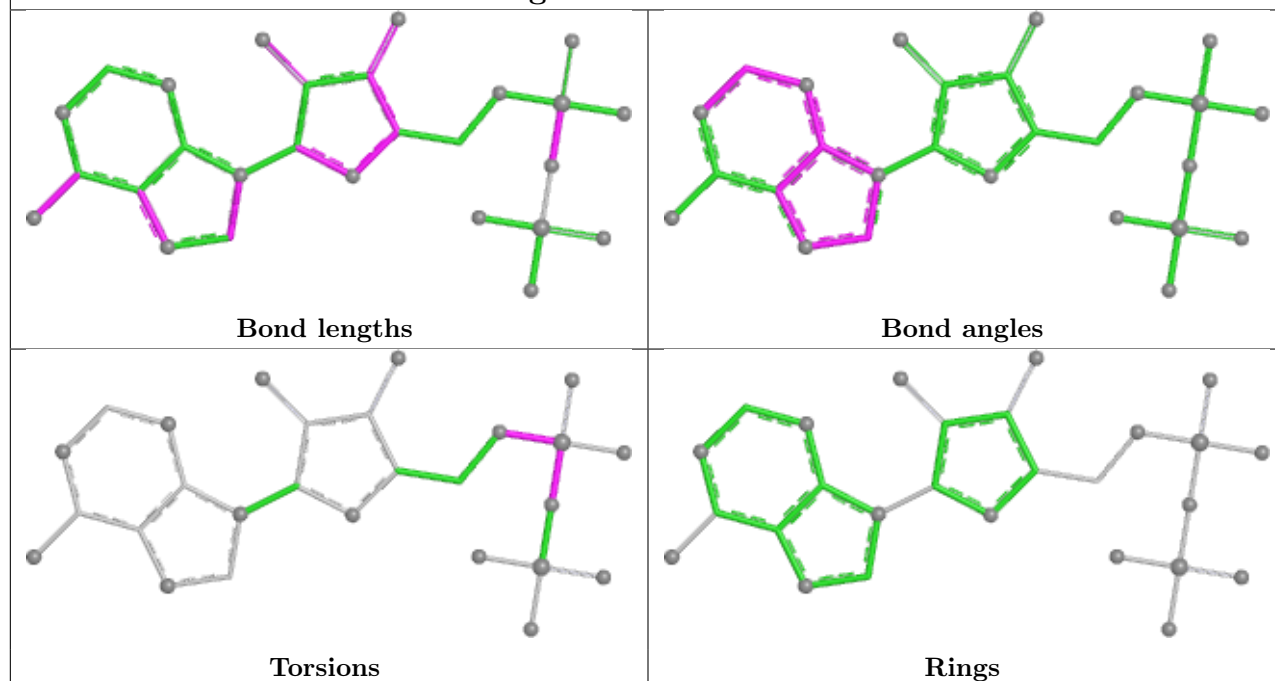
Ligand PLX g 201

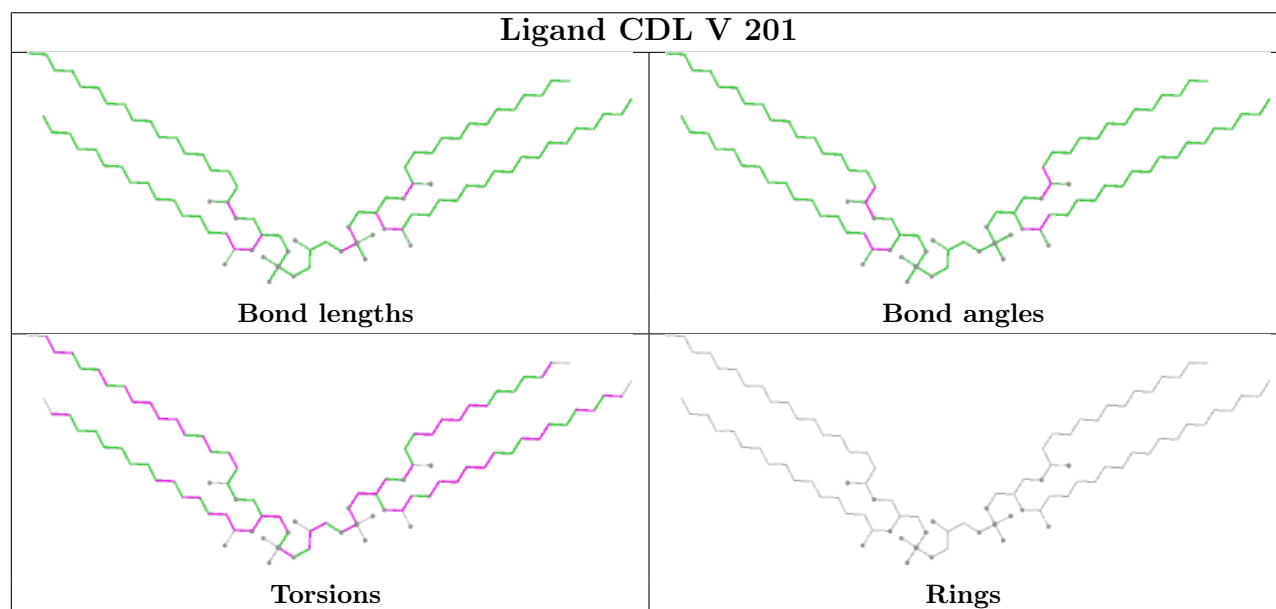
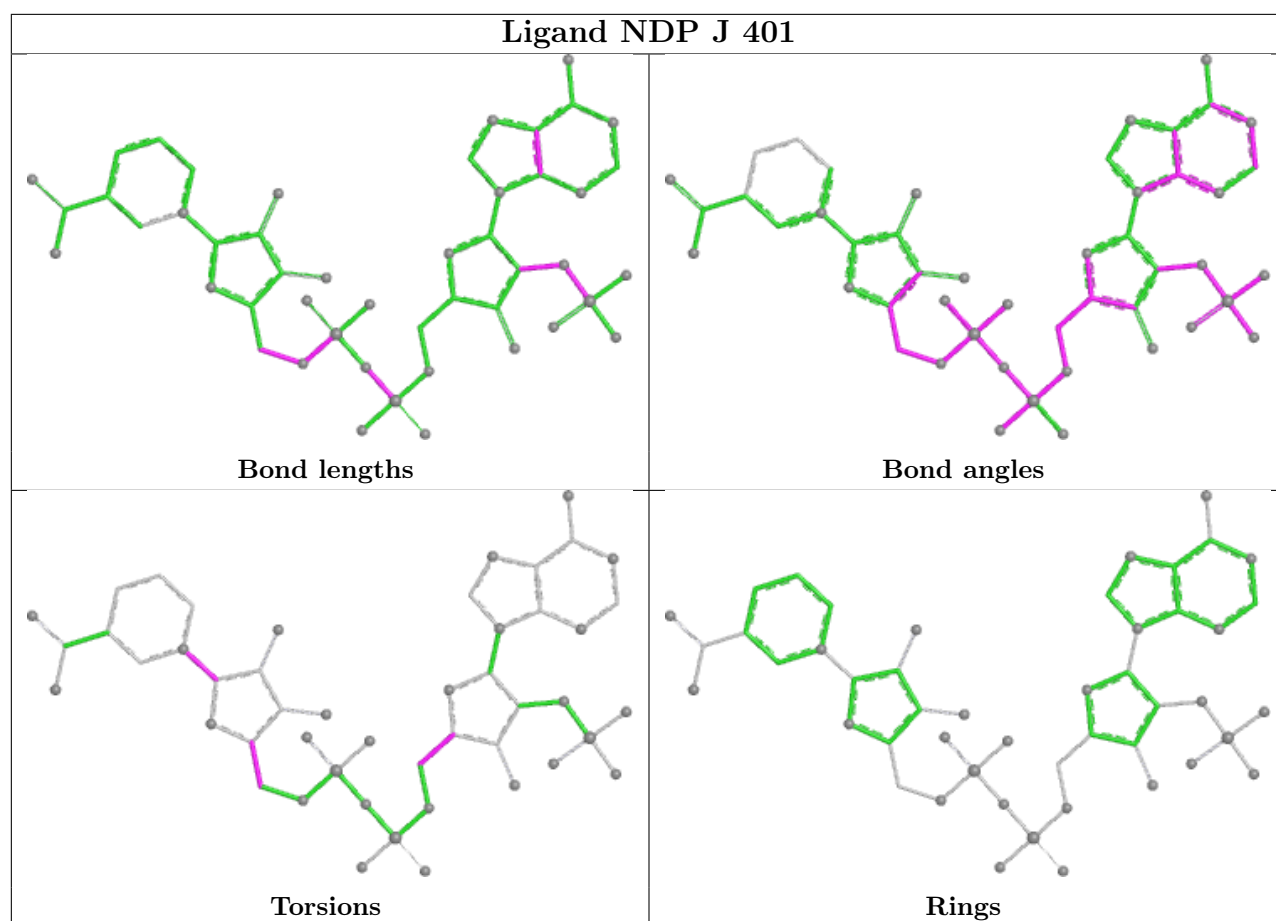


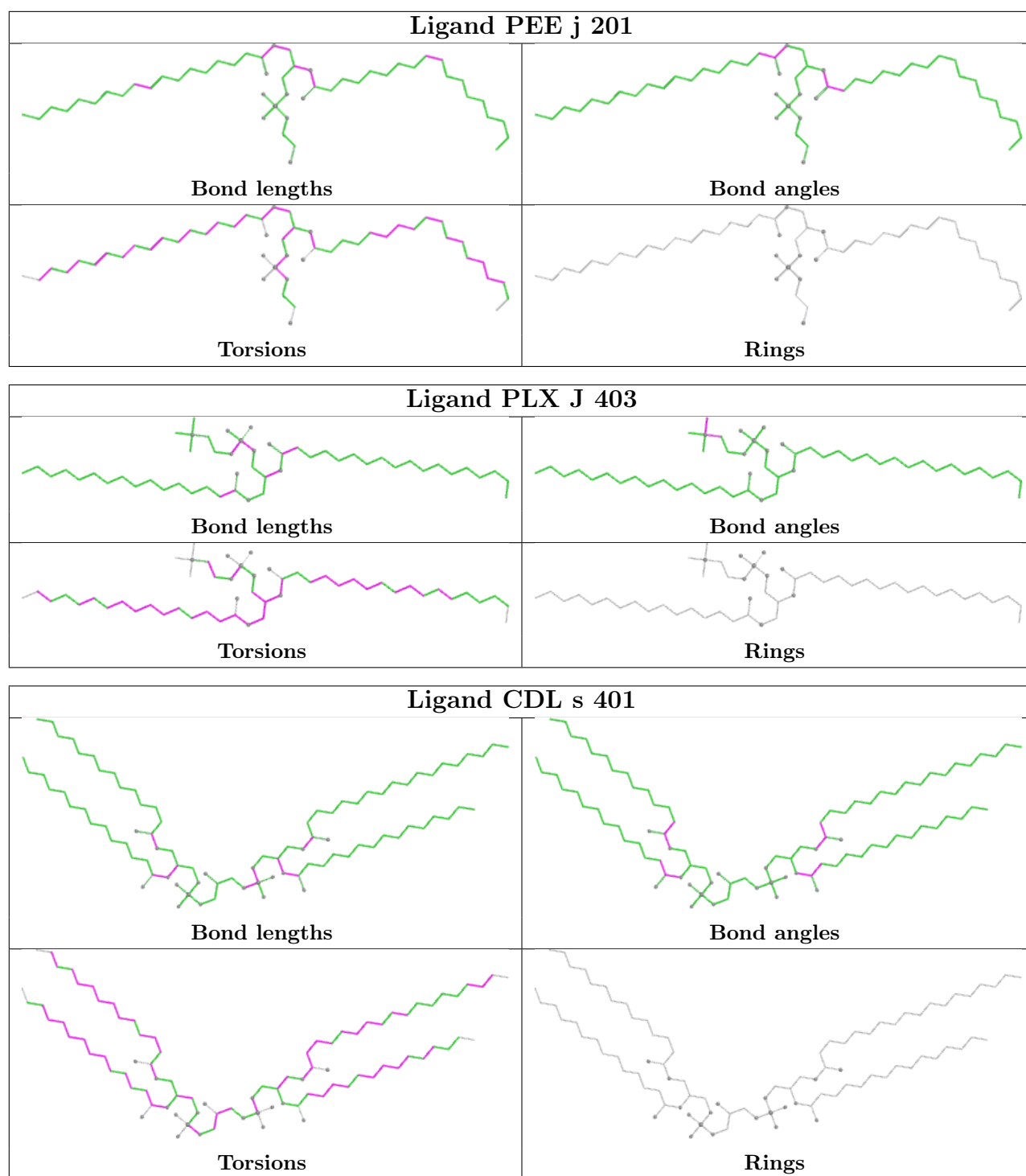
Ligand PEE C 302



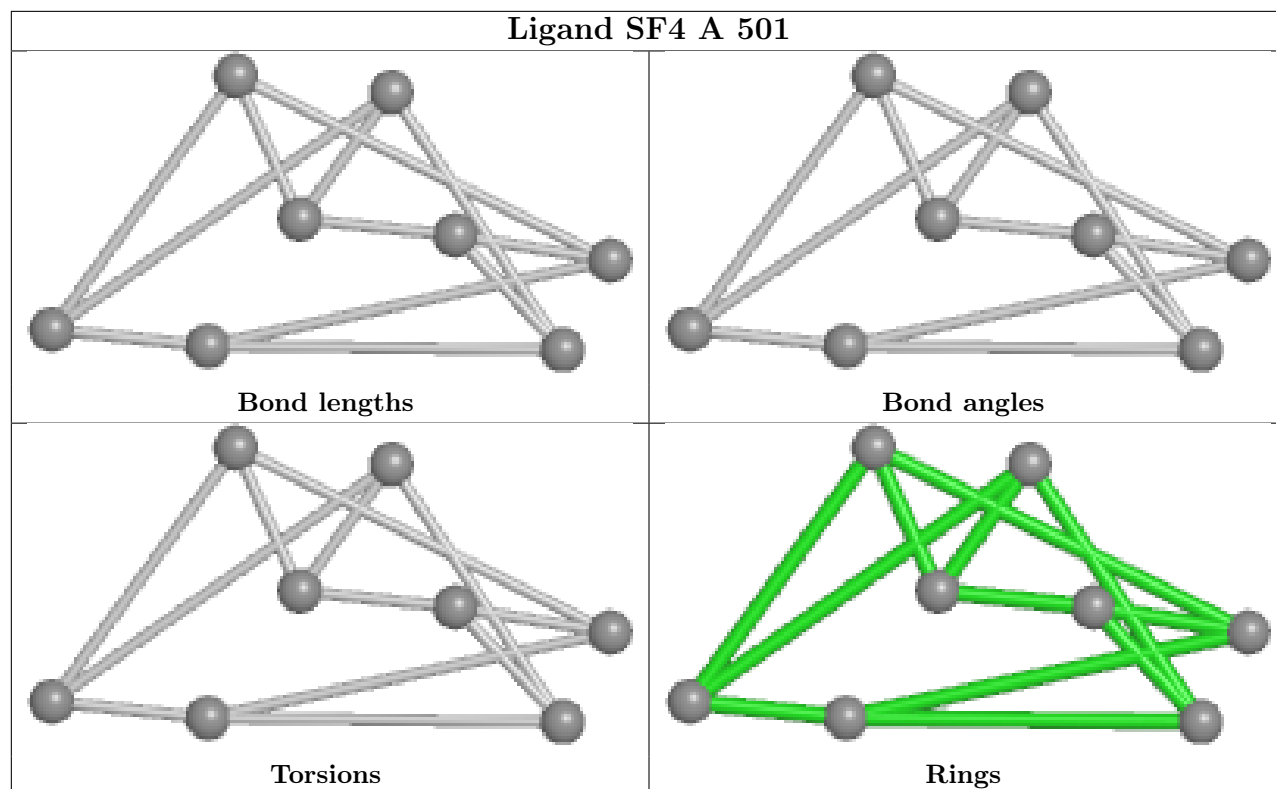
Ligand ADP w 401



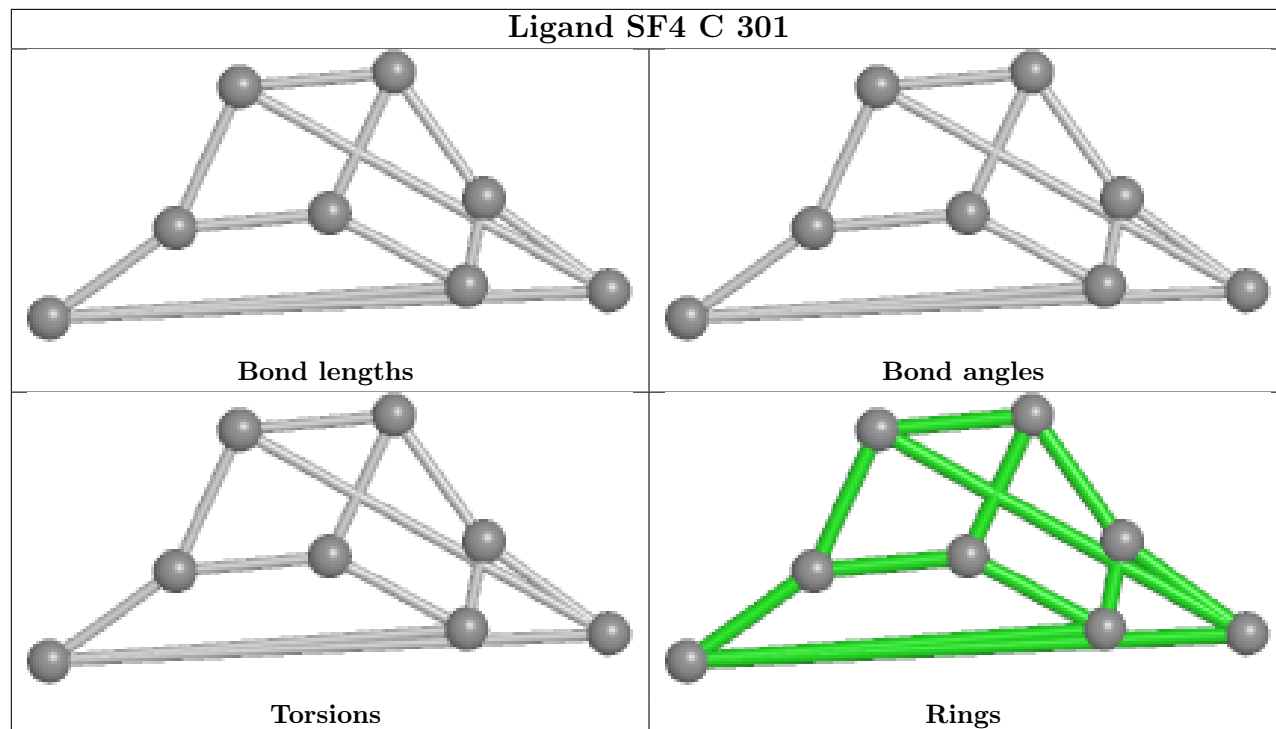


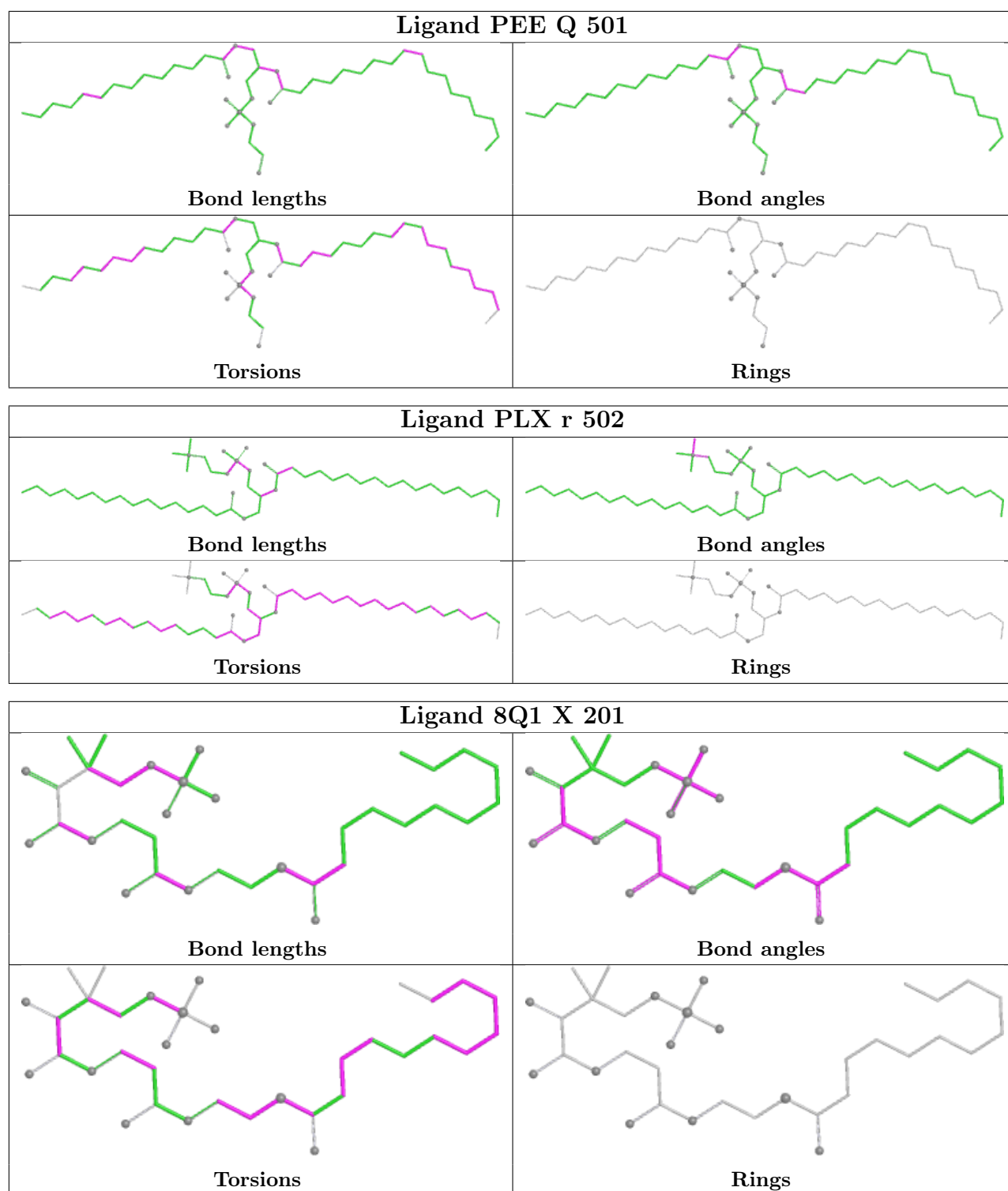


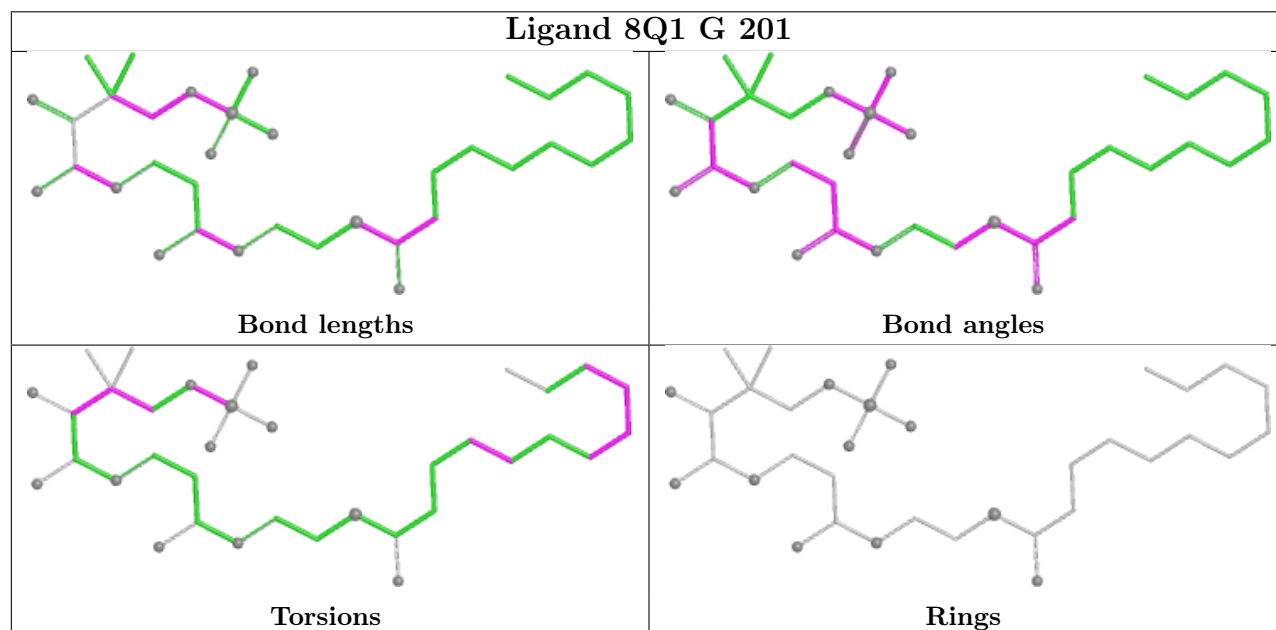
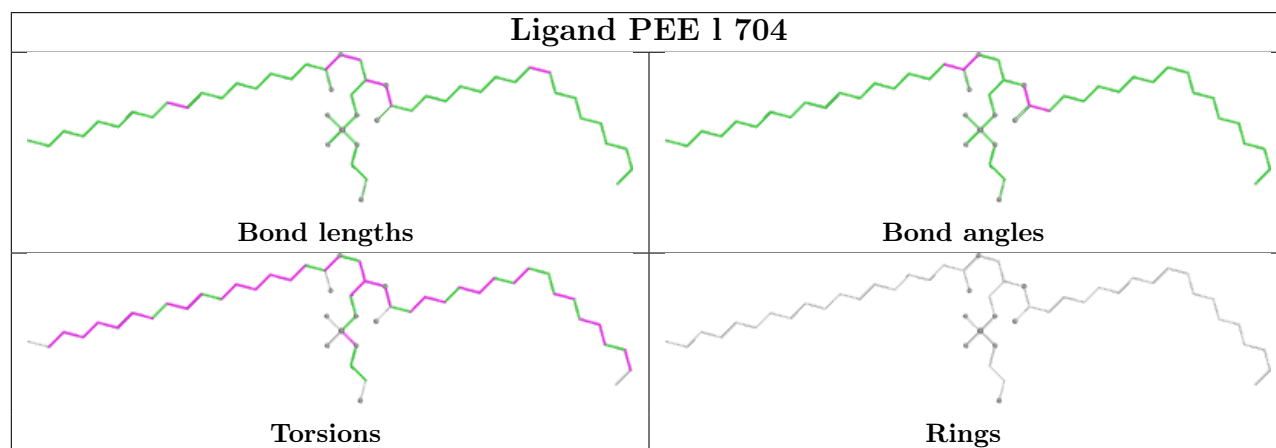
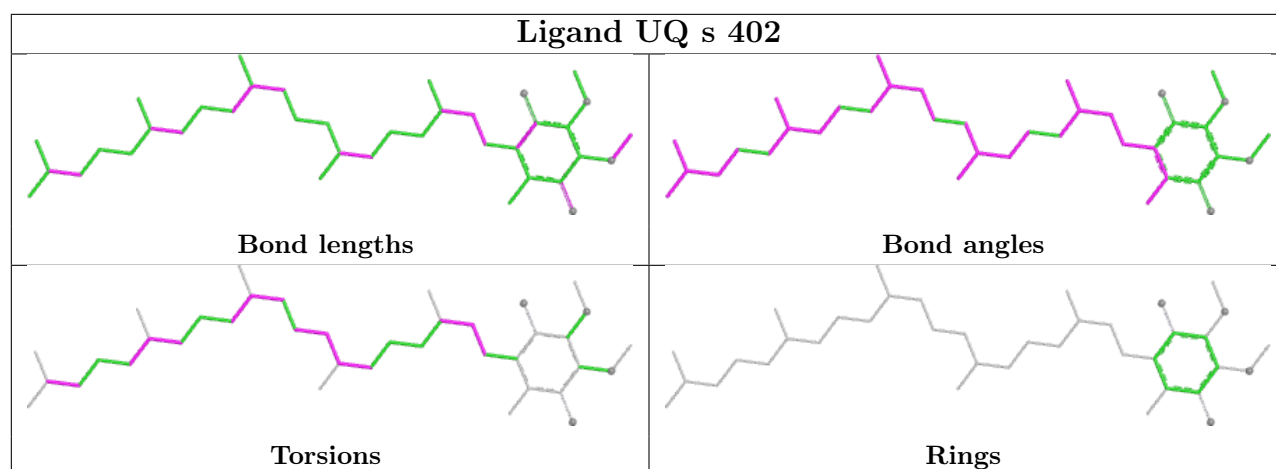
Ligand SF4 A 501

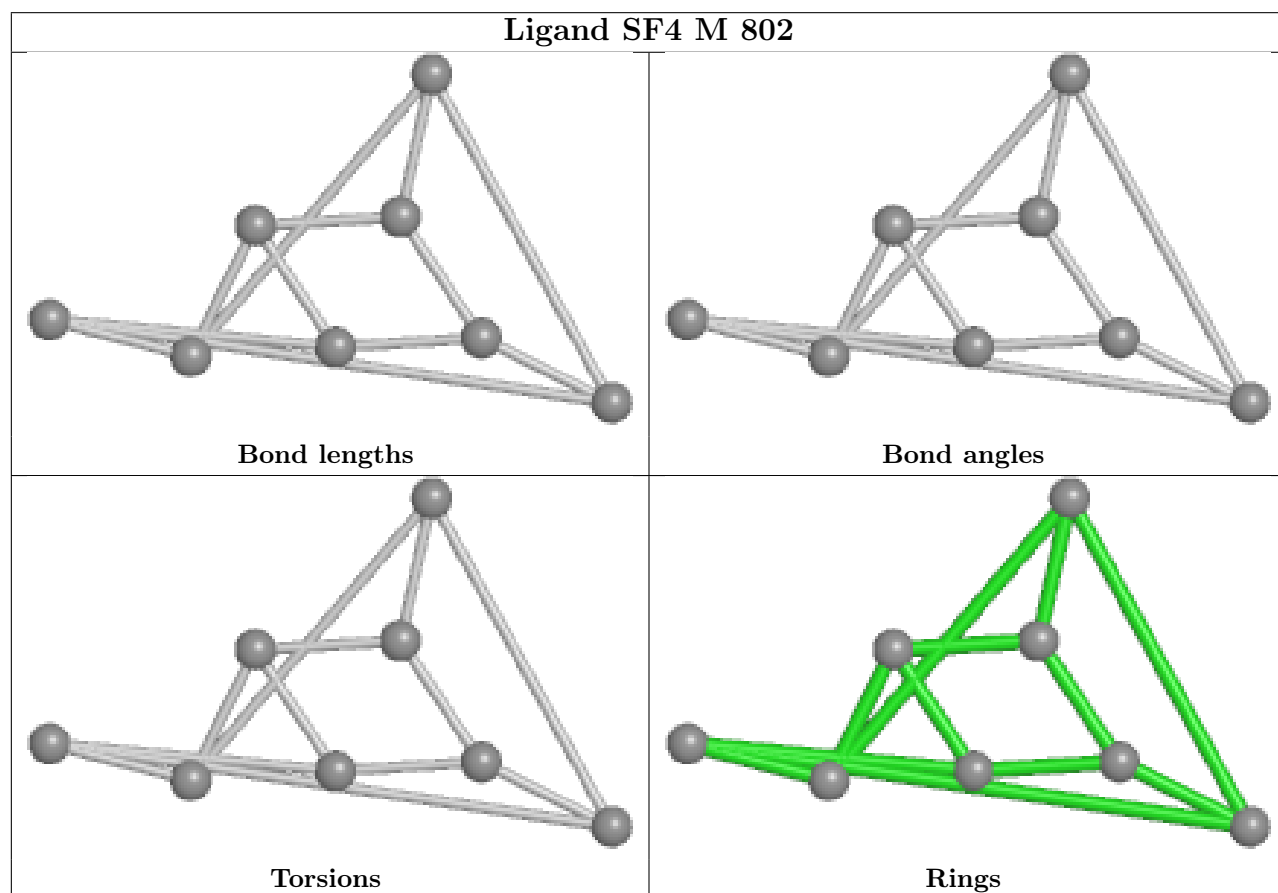
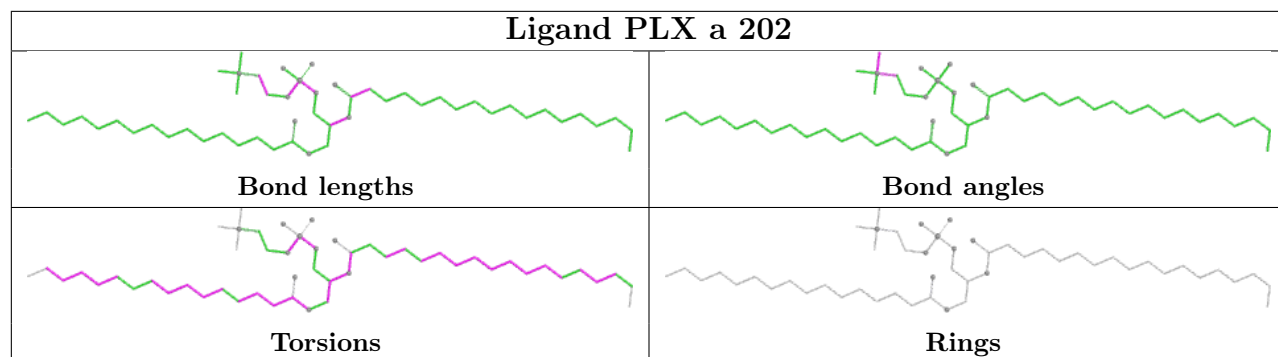


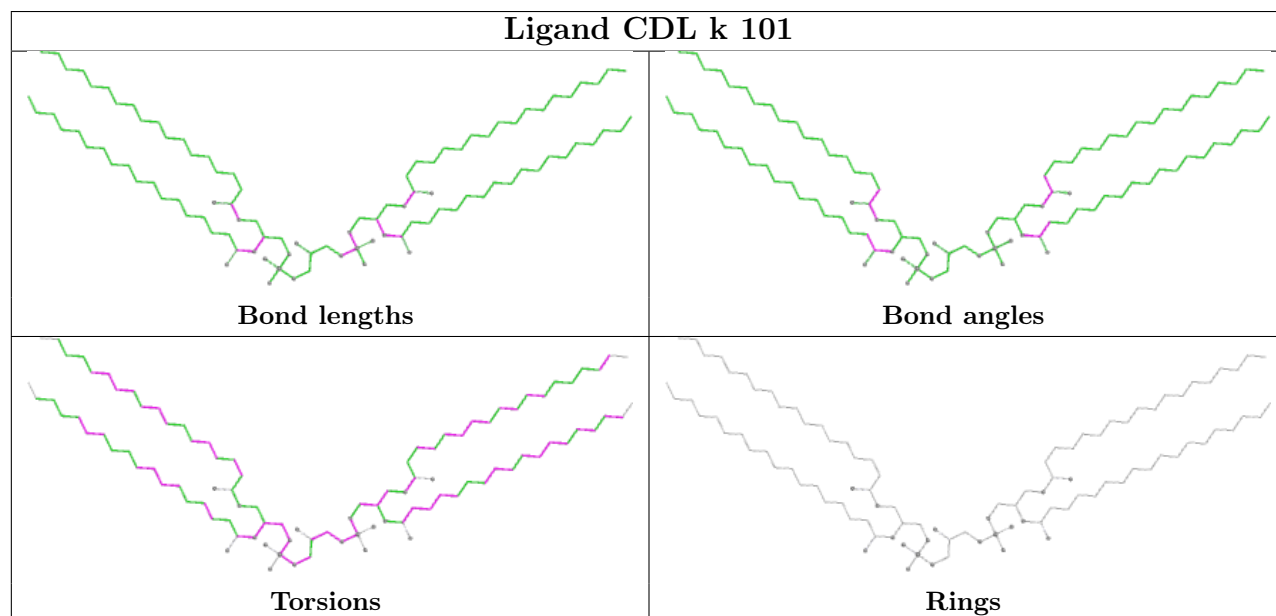
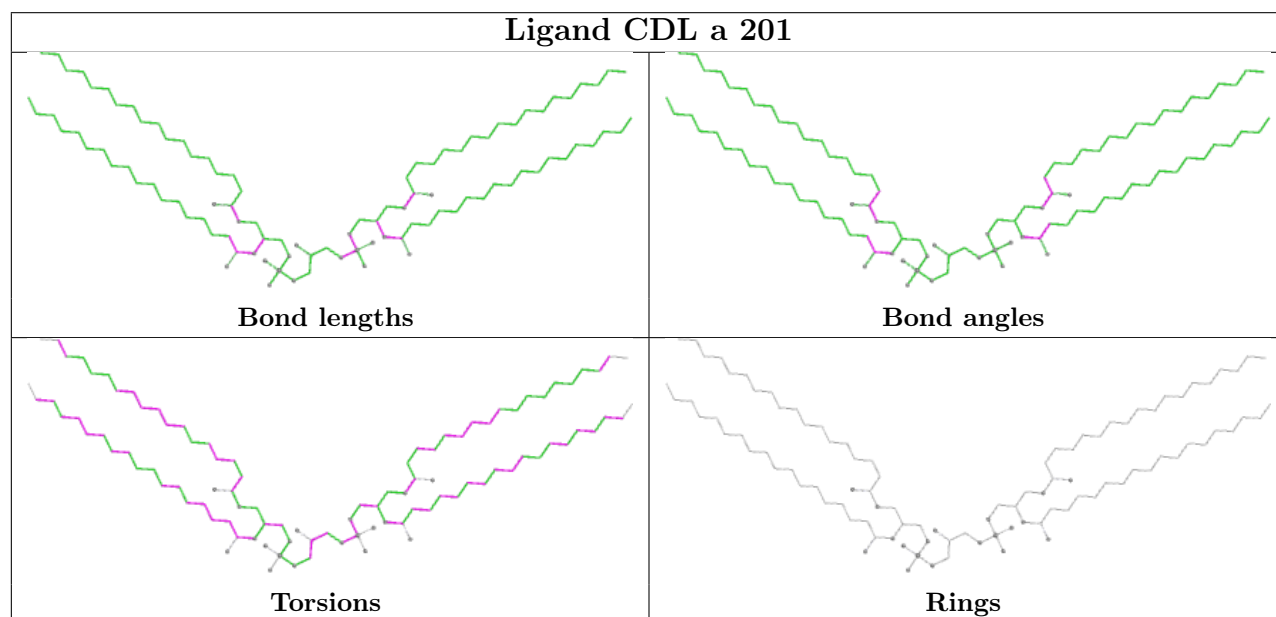
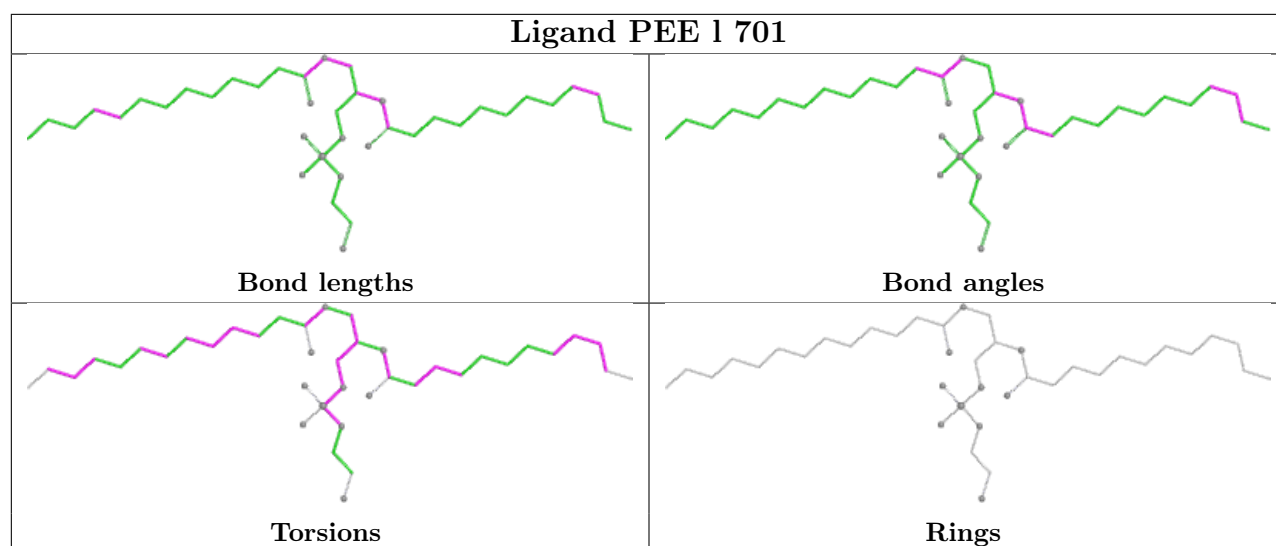
Ligand SF4 C 301

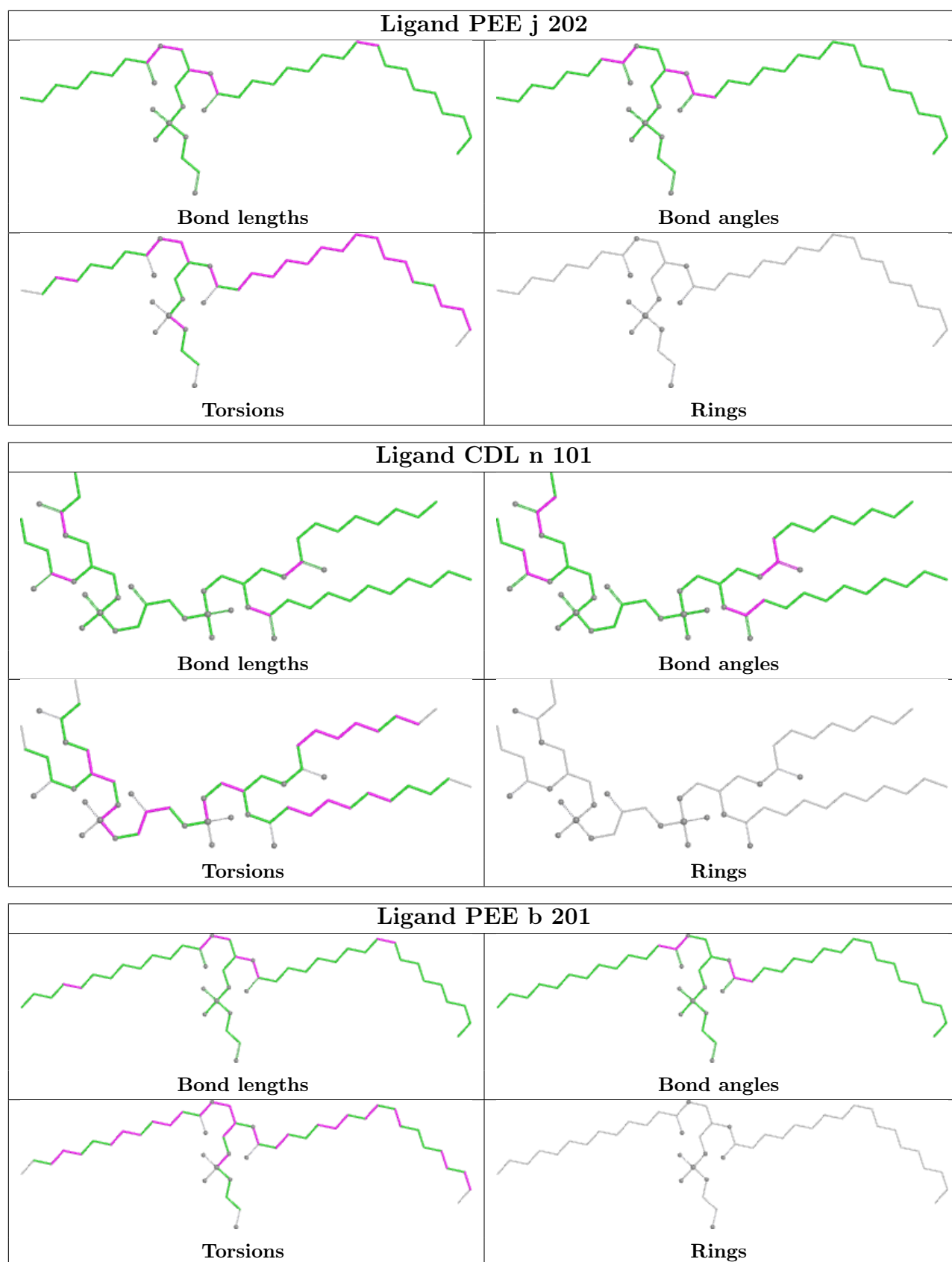


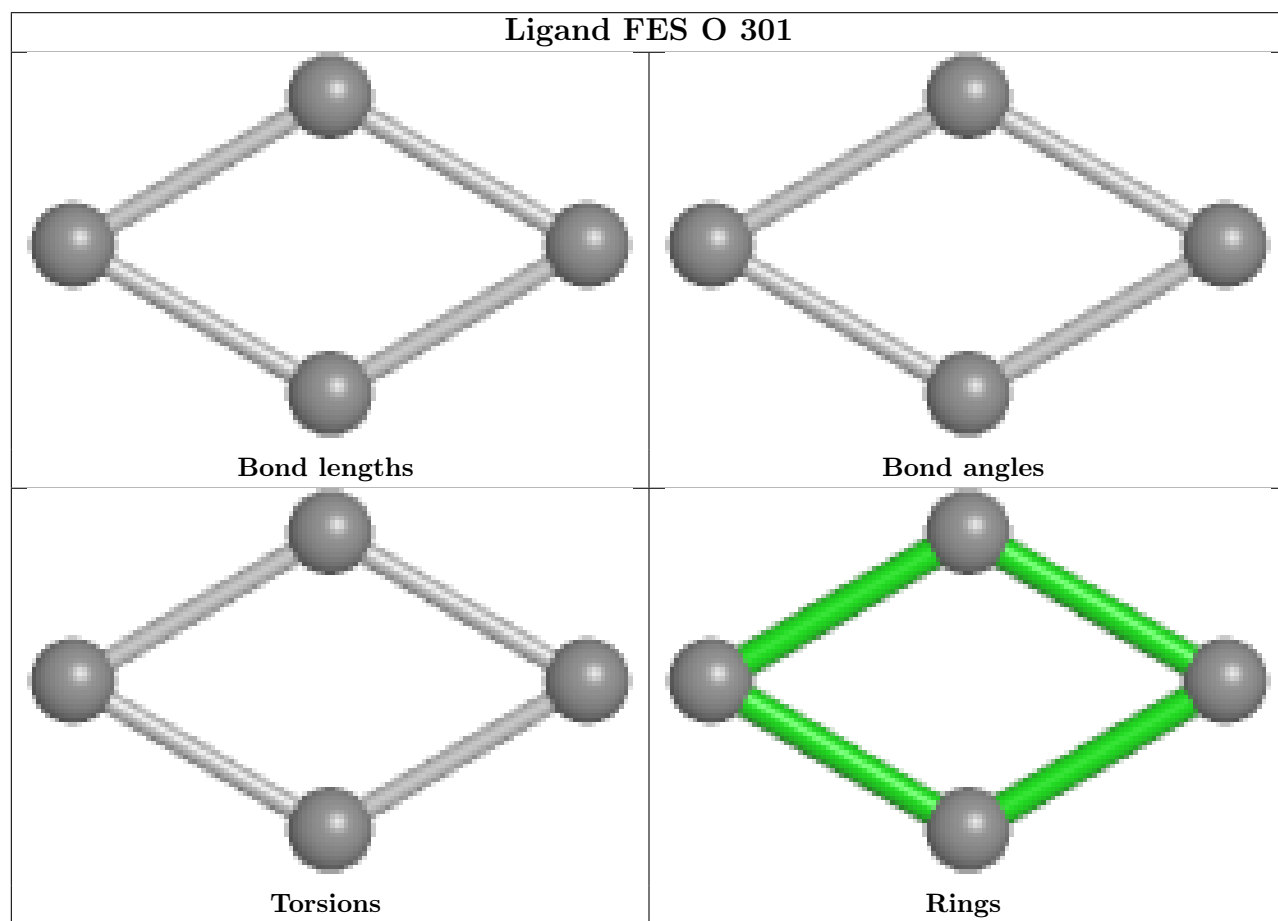
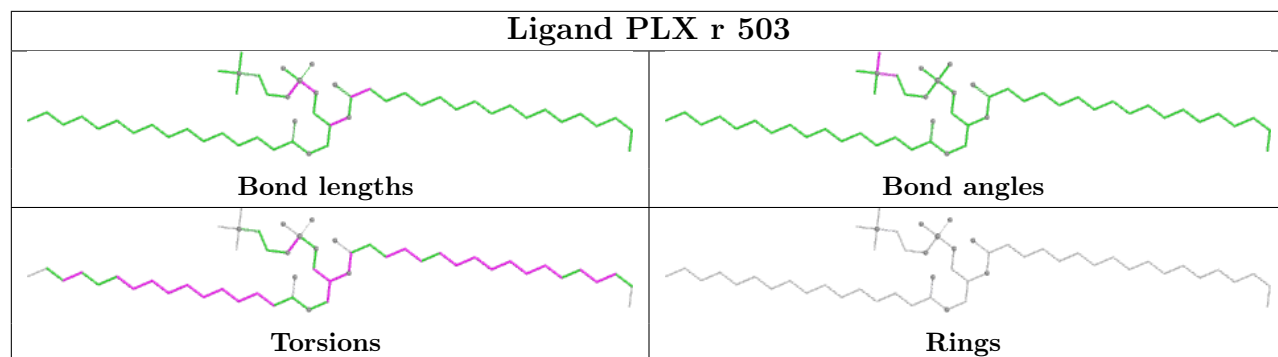


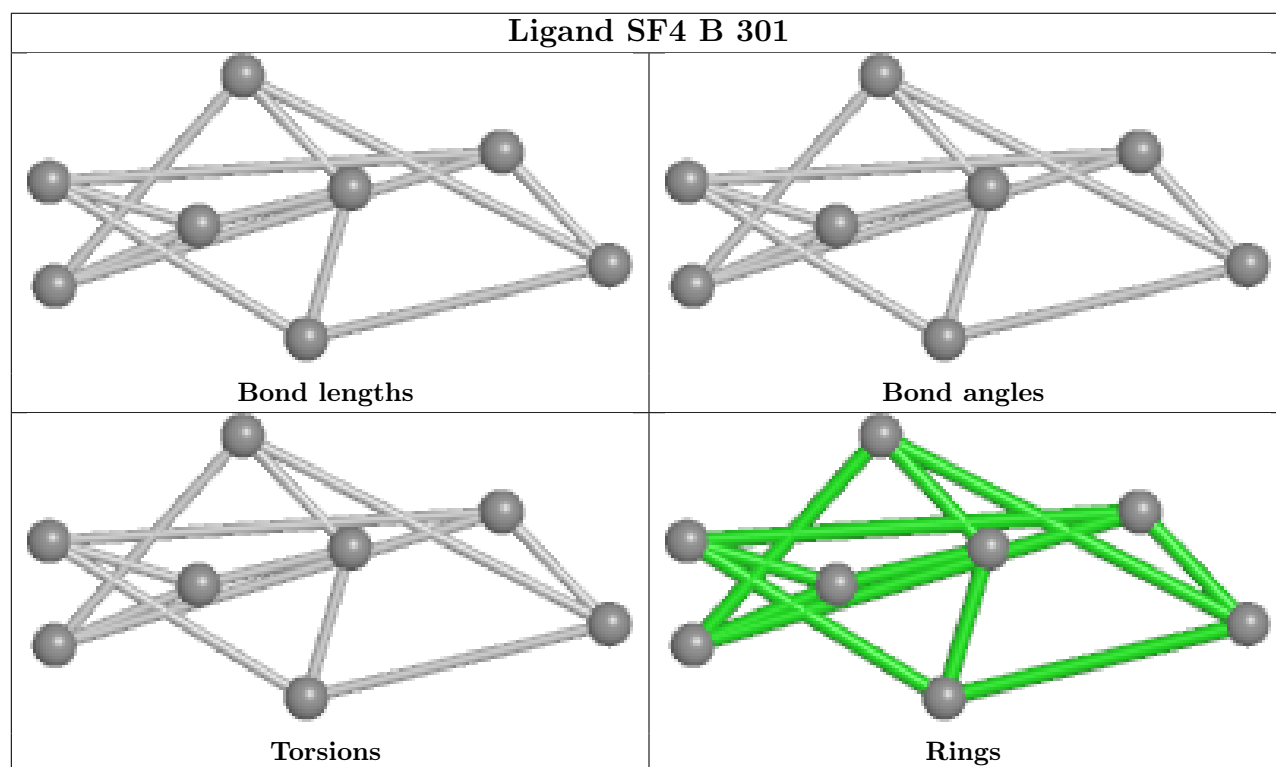
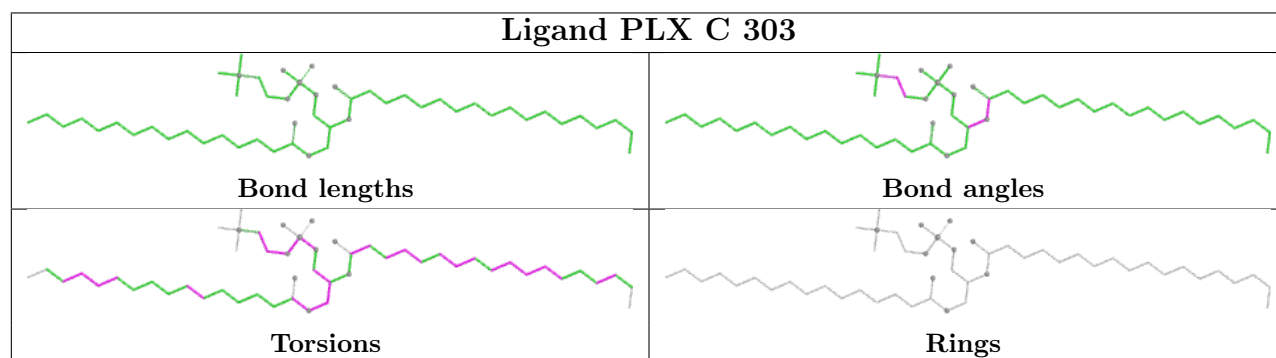
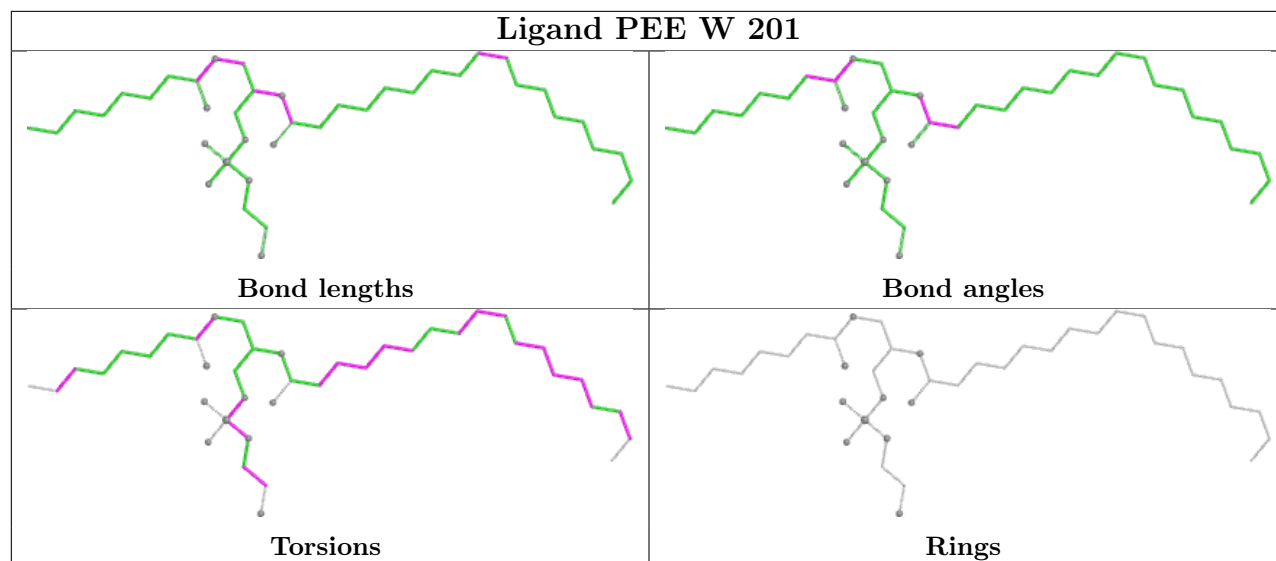


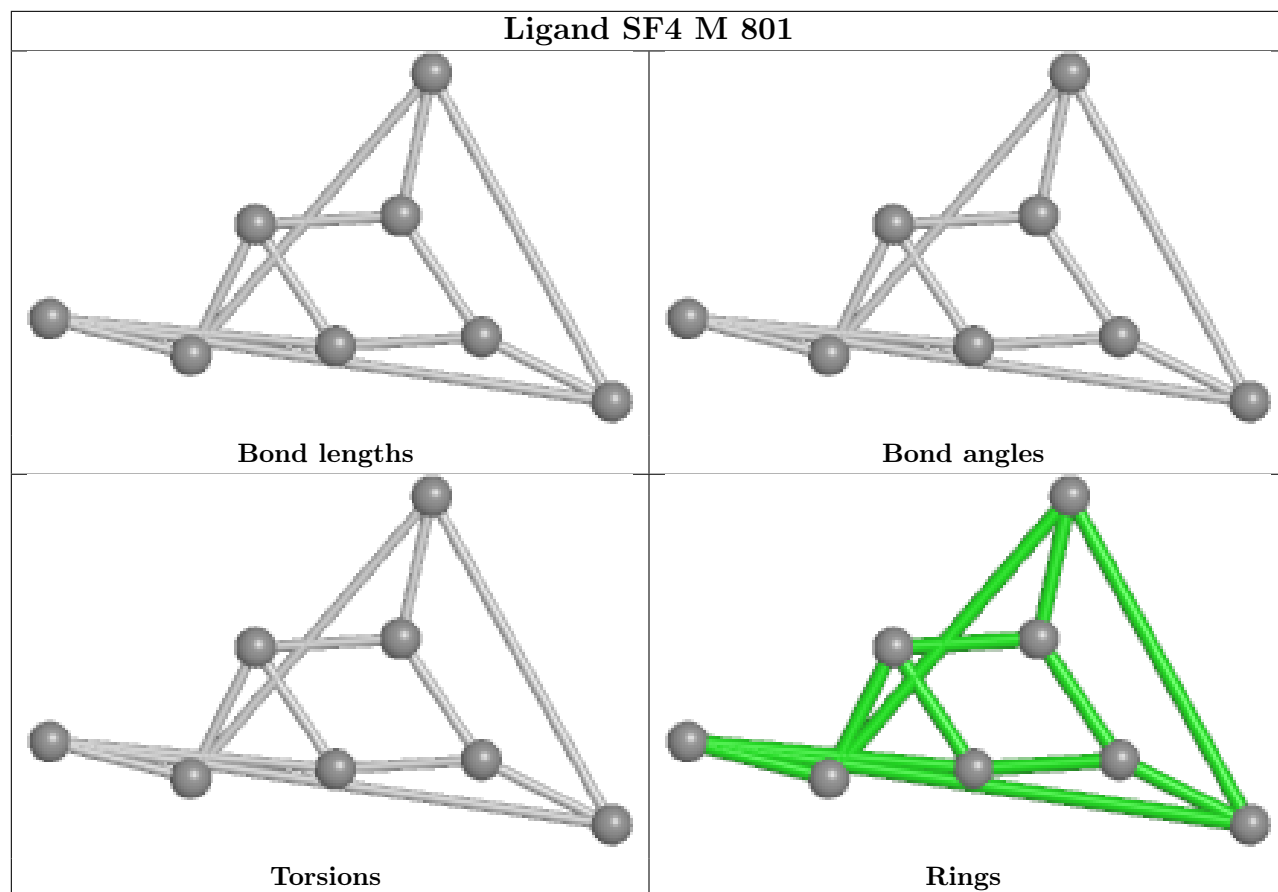


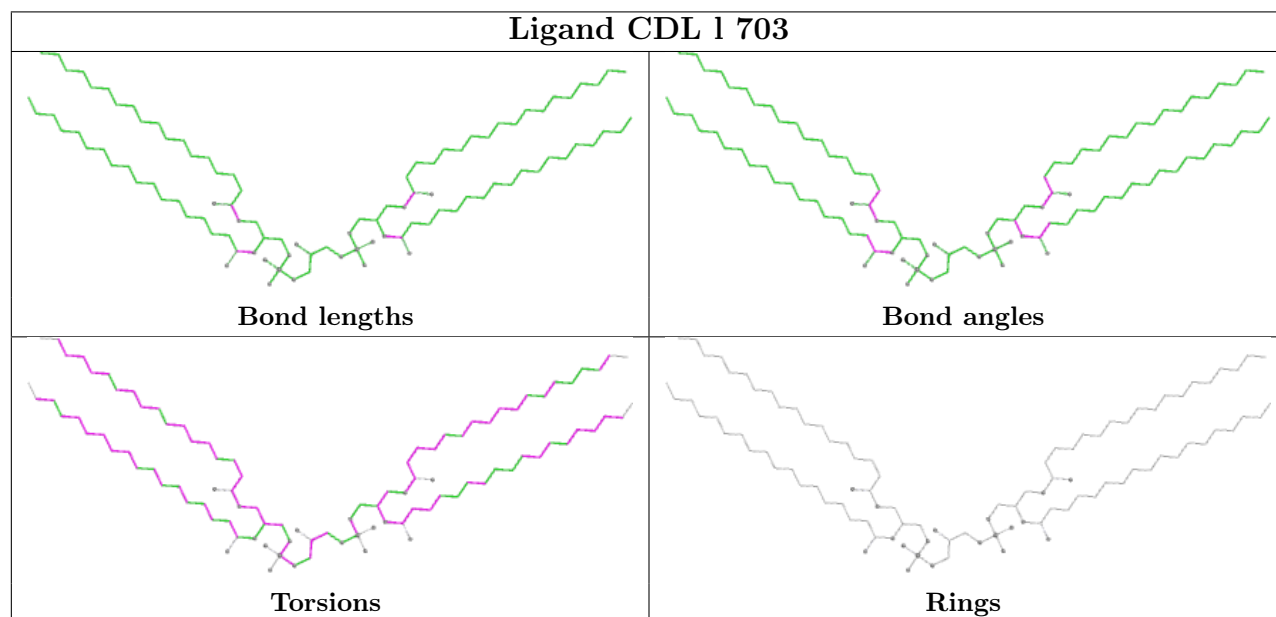
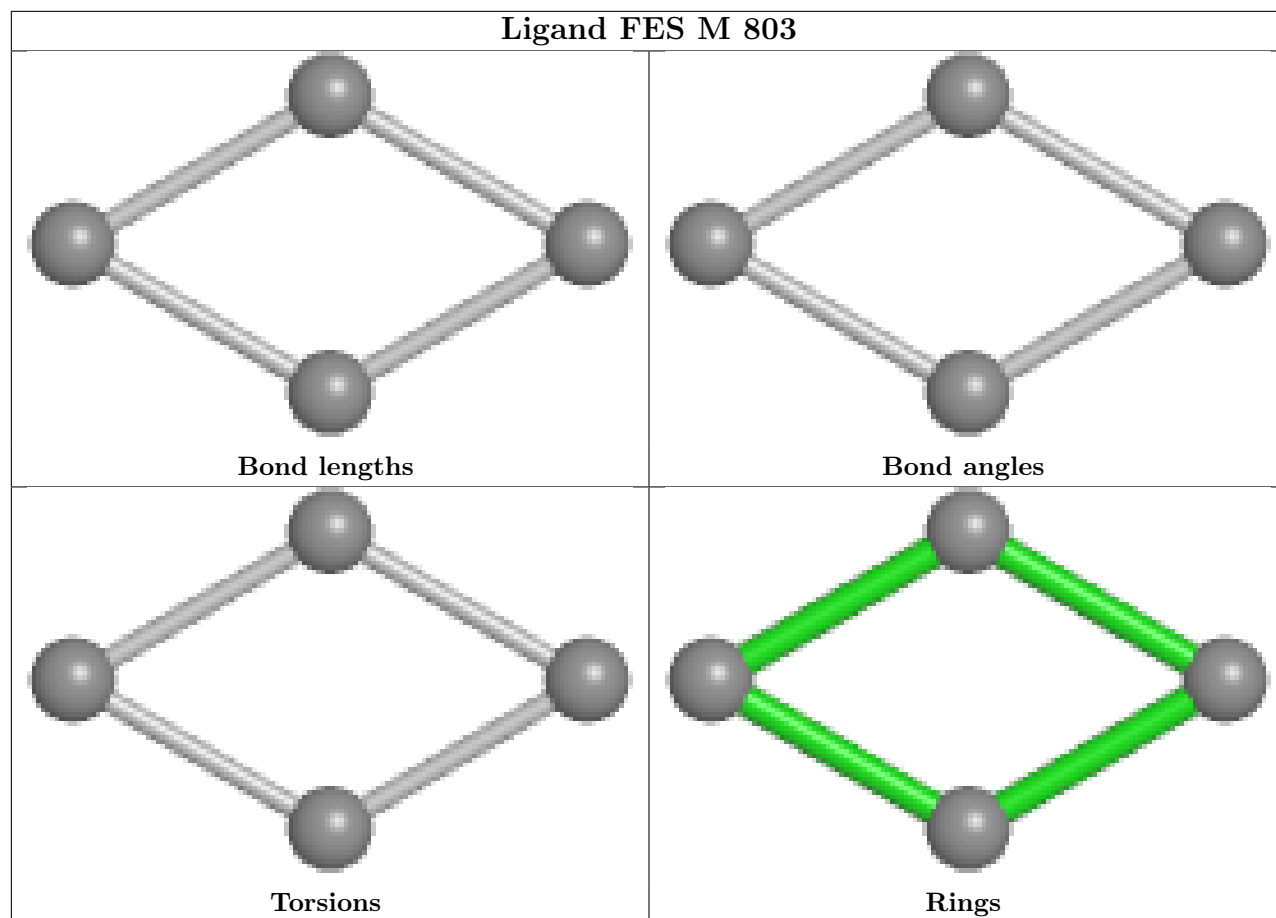


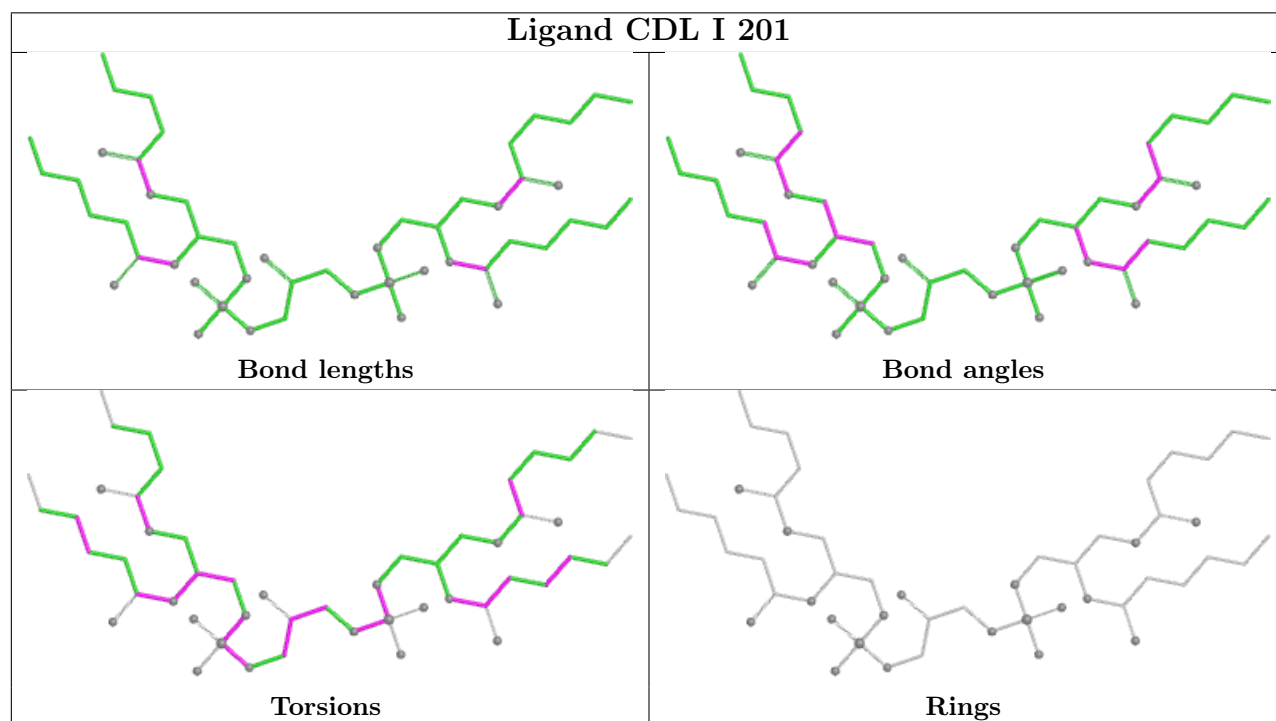
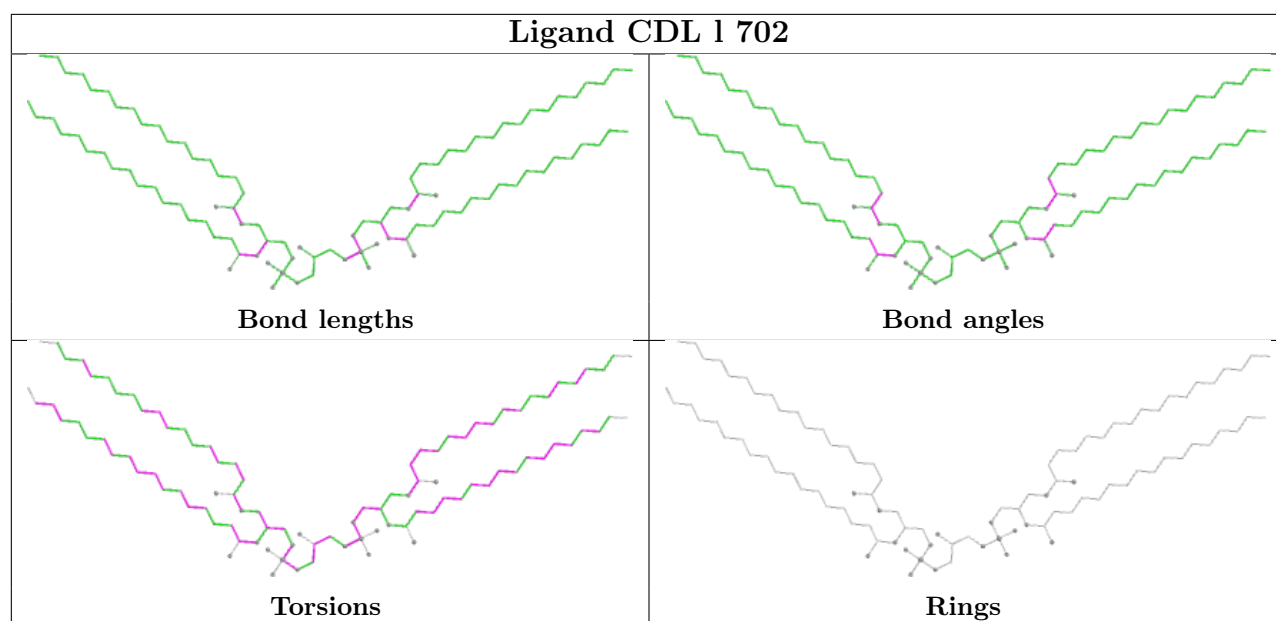


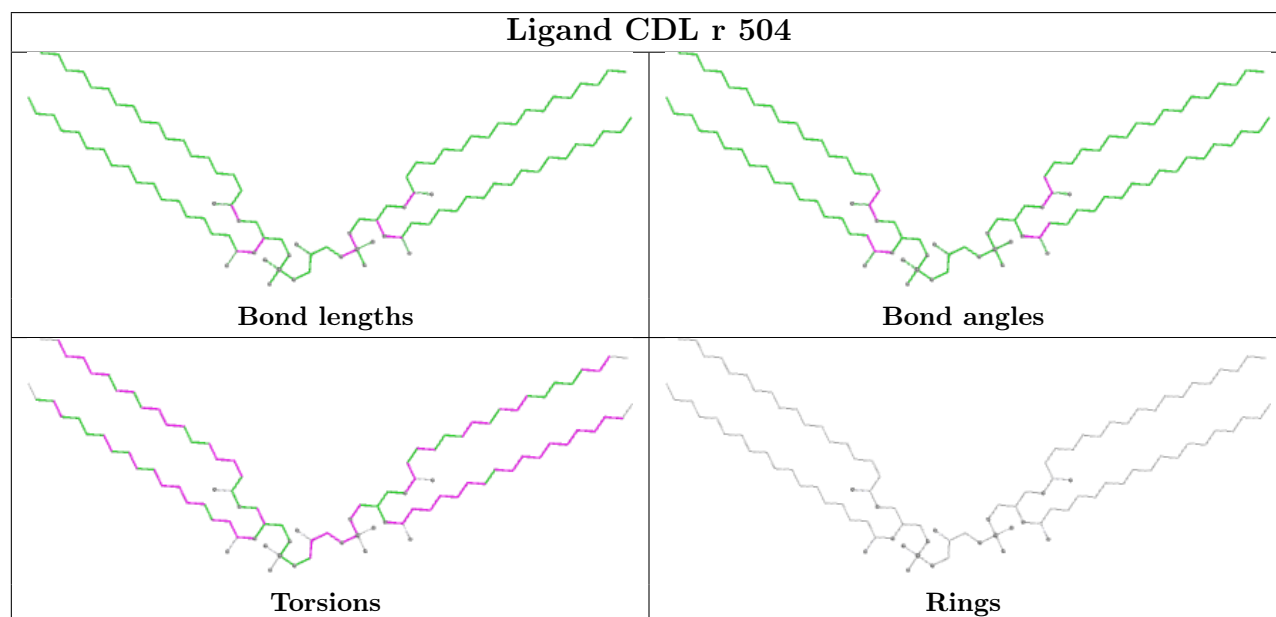
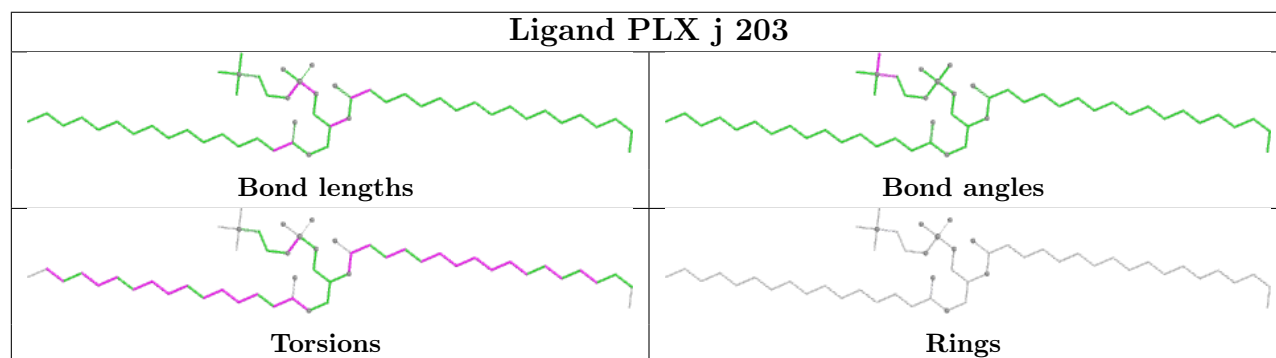
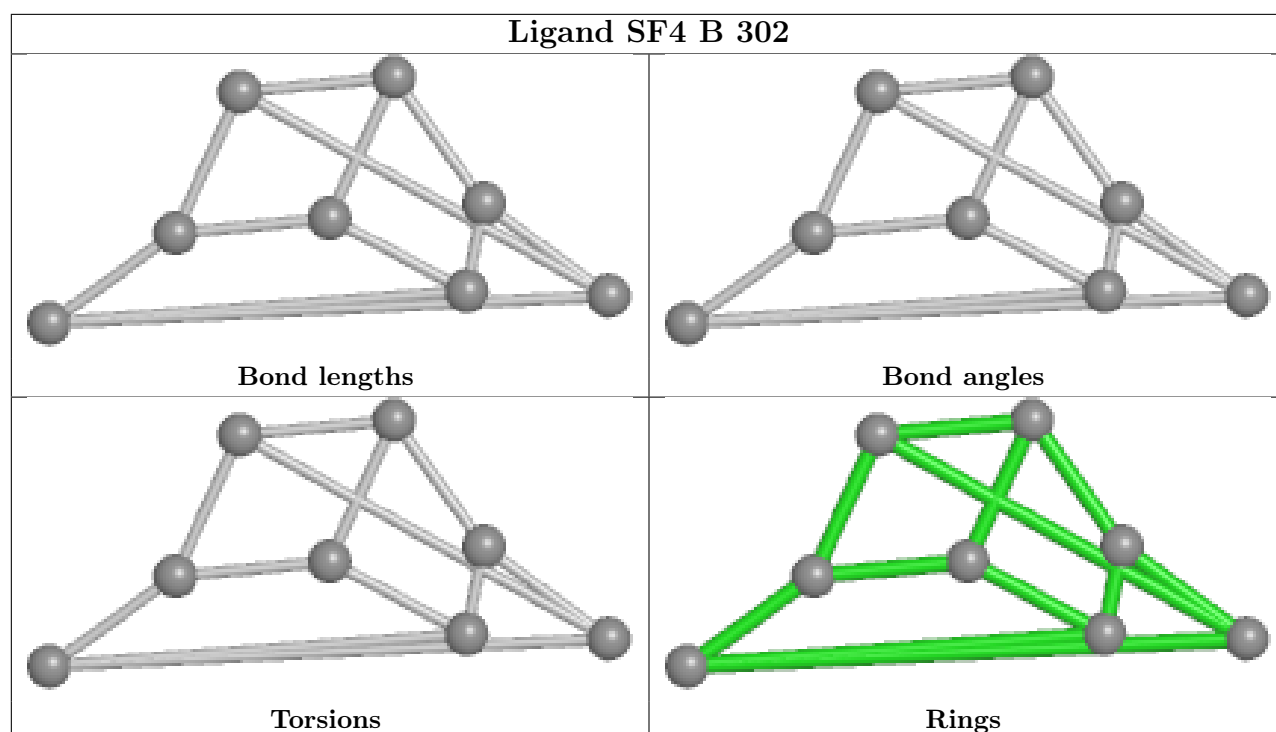


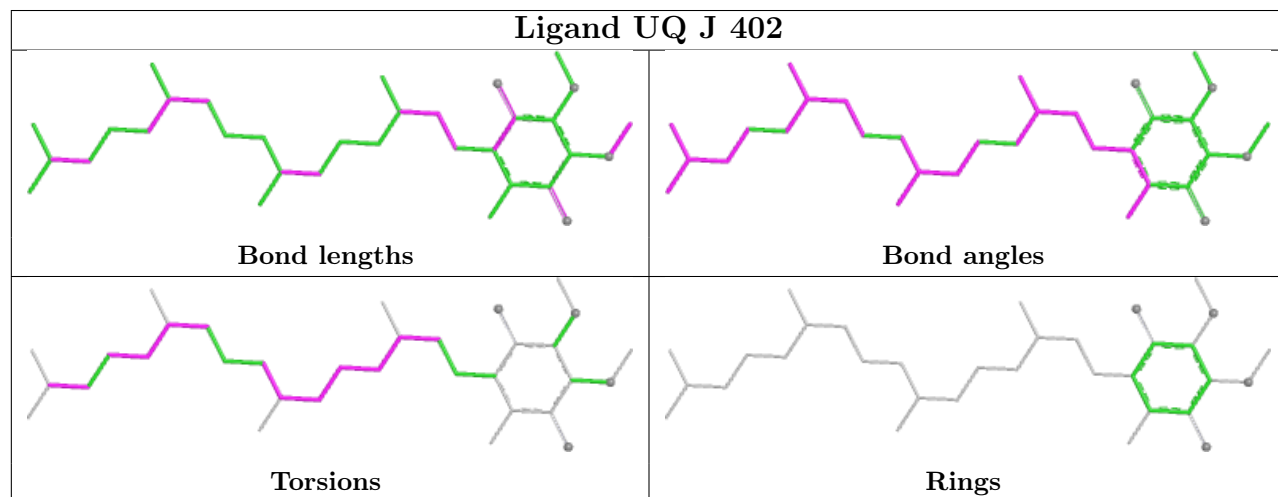
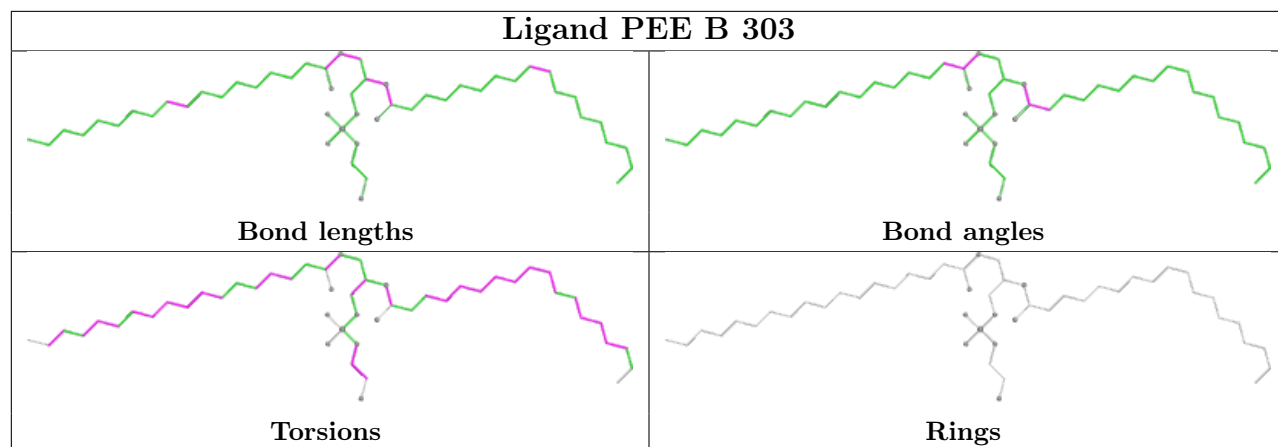


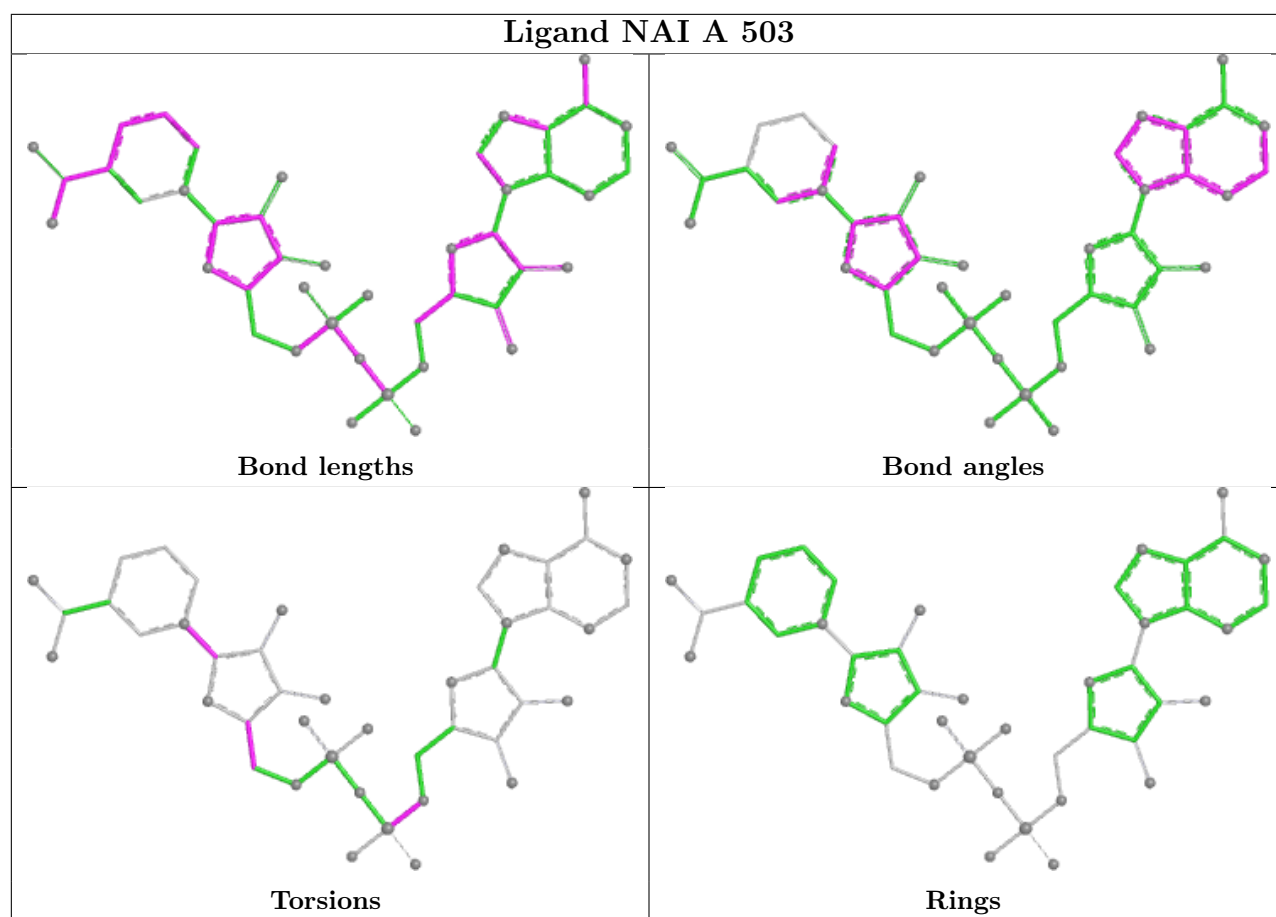












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

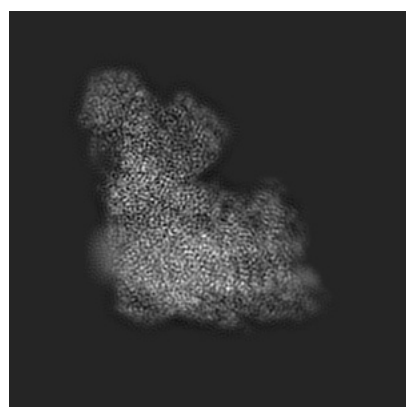
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31643. These allow visual inspection of the internal detail of the map and identification of artifacts.

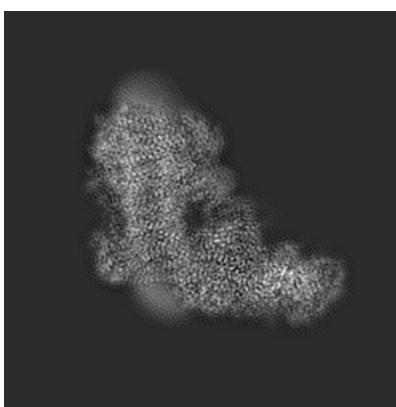
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

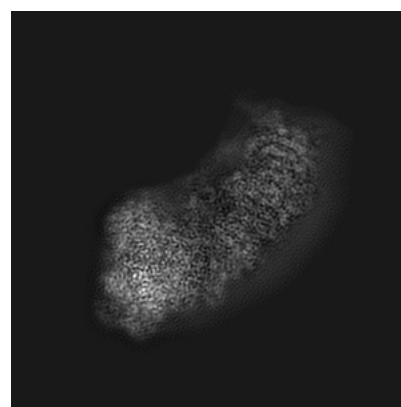
6.1.1 Primary map



X



Y

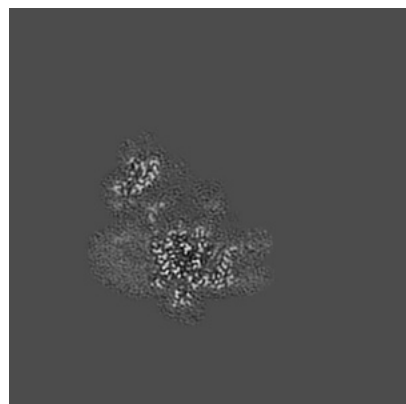


Z

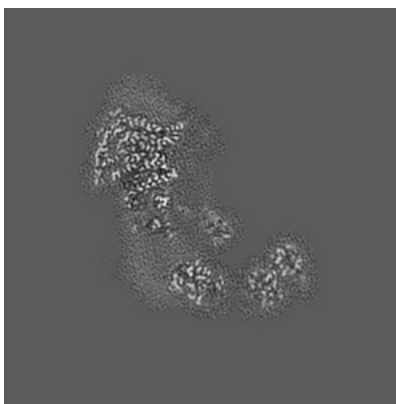
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

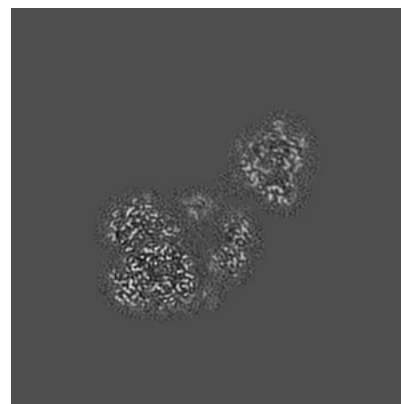
6.2.1 Primary map



X Index: 155



Y Index: 155

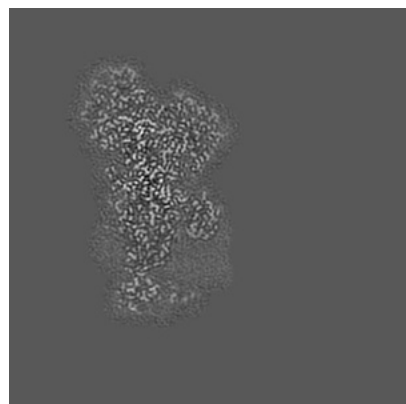


Z Index: 155

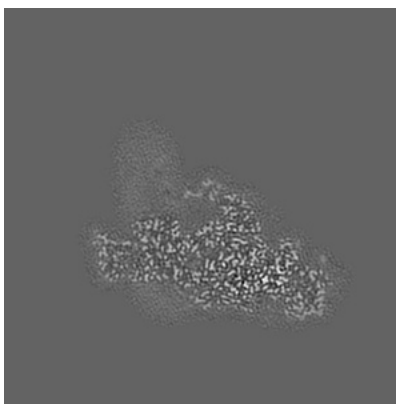
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

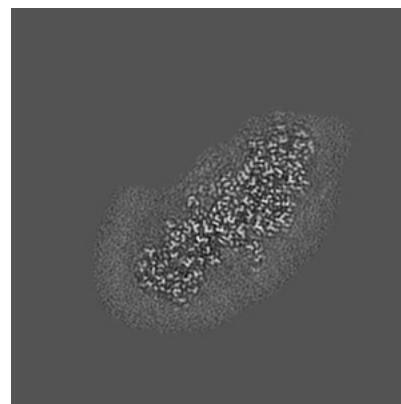
6.3.1 Primary map



X Index: 105



Y Index: 102

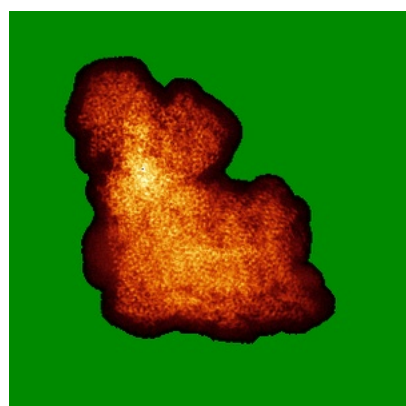


Z Index: 122

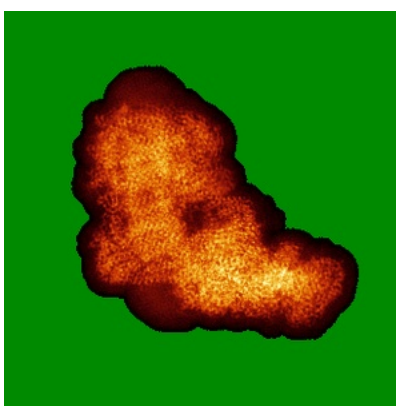
The images above show the largest variance slices of the map in three orthogonal directions.

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

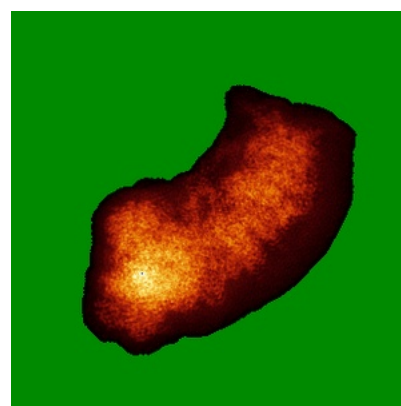
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

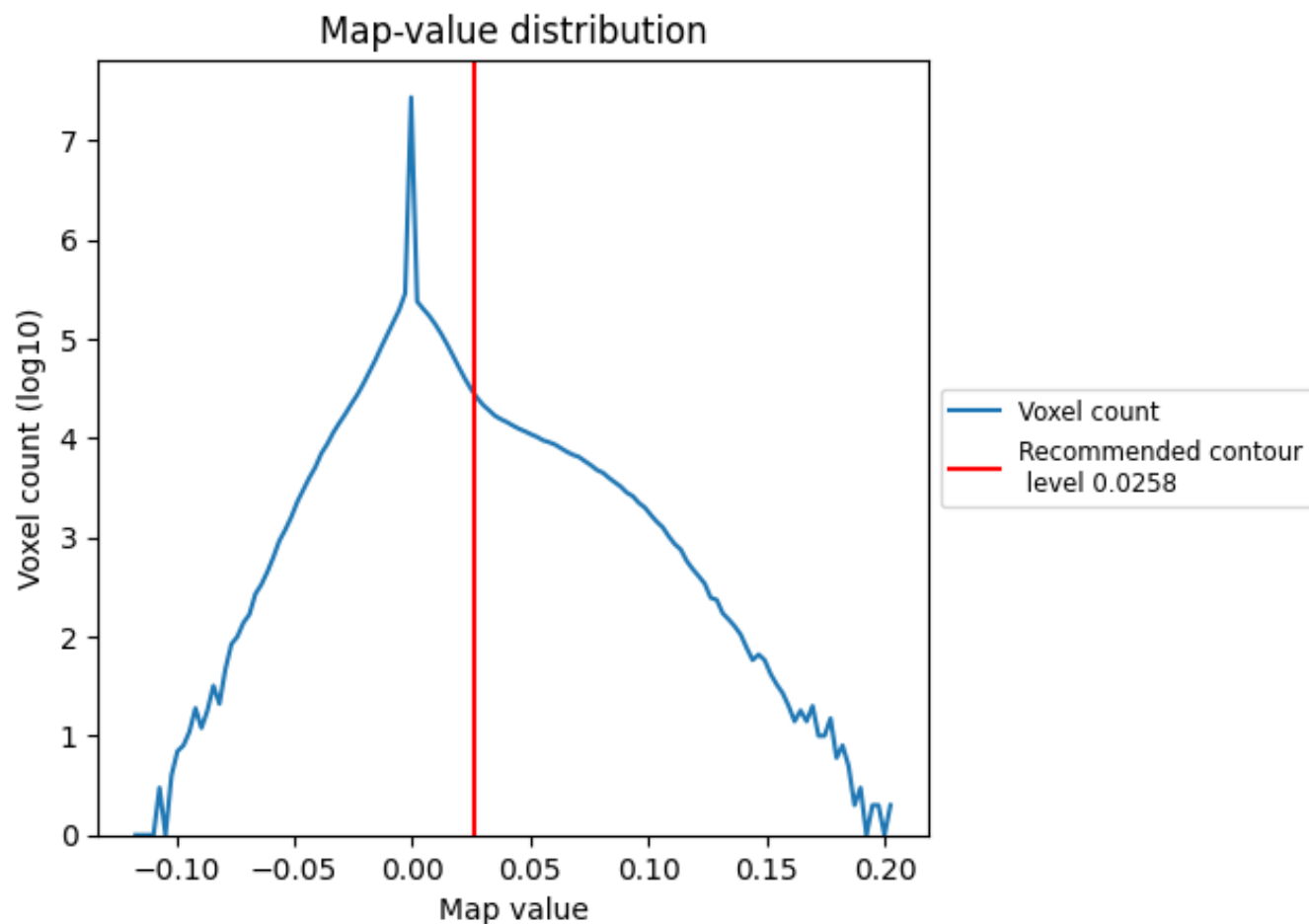
6.6 Mask visualisation

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

7 Map analysis [i](#)

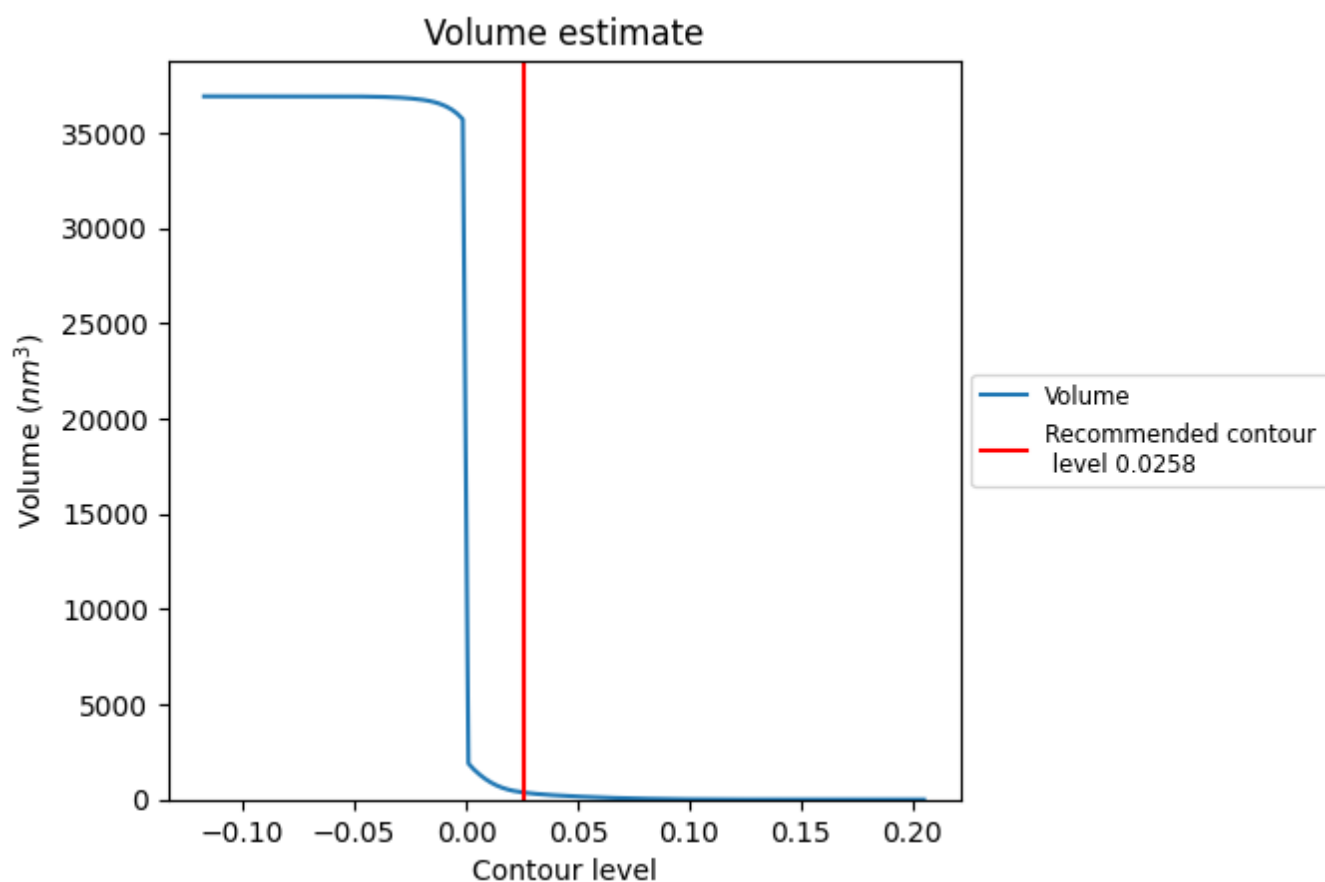
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

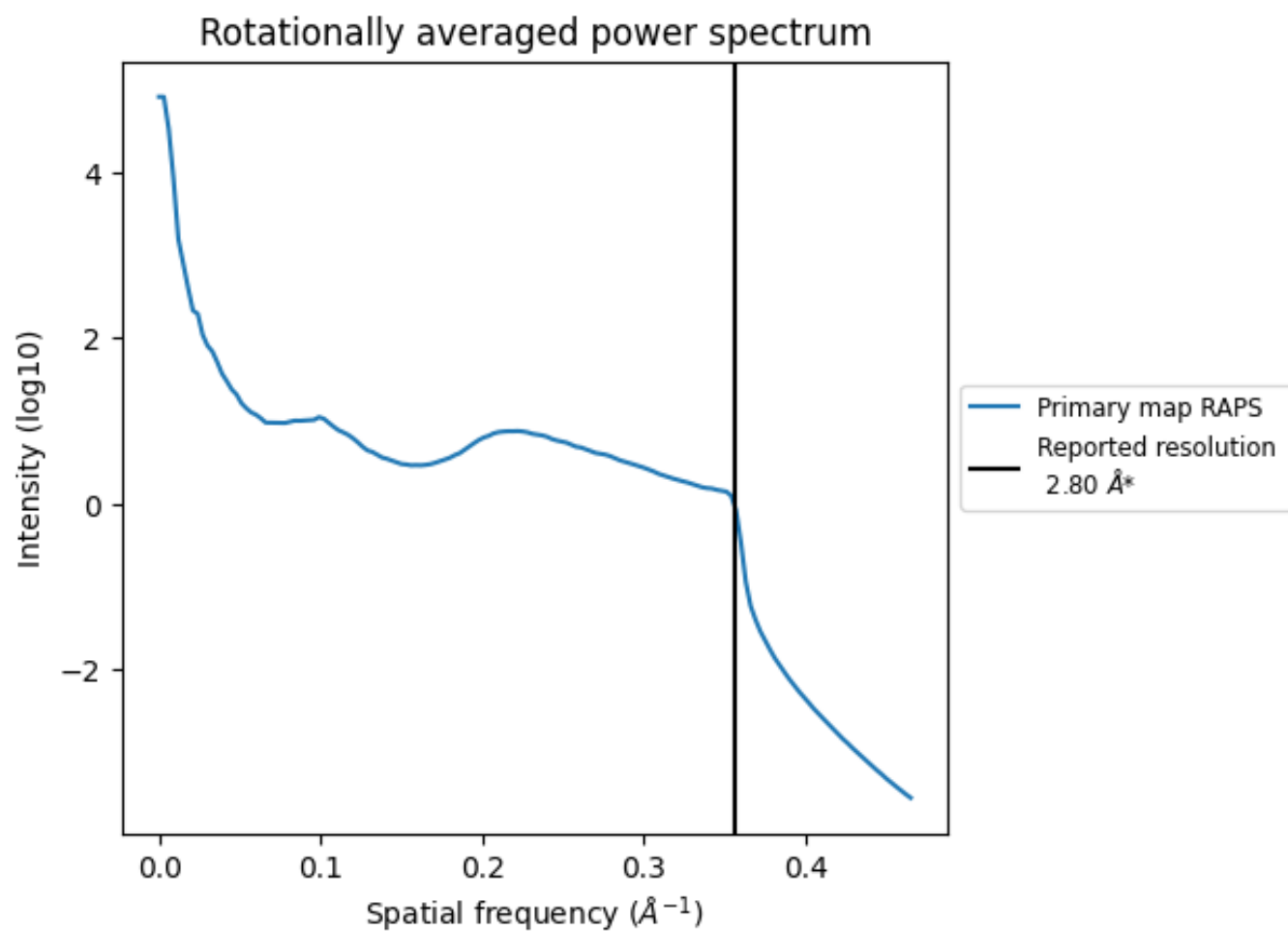
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; 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 0.357 Å⁻¹

8 Fourier-Shell correlation

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

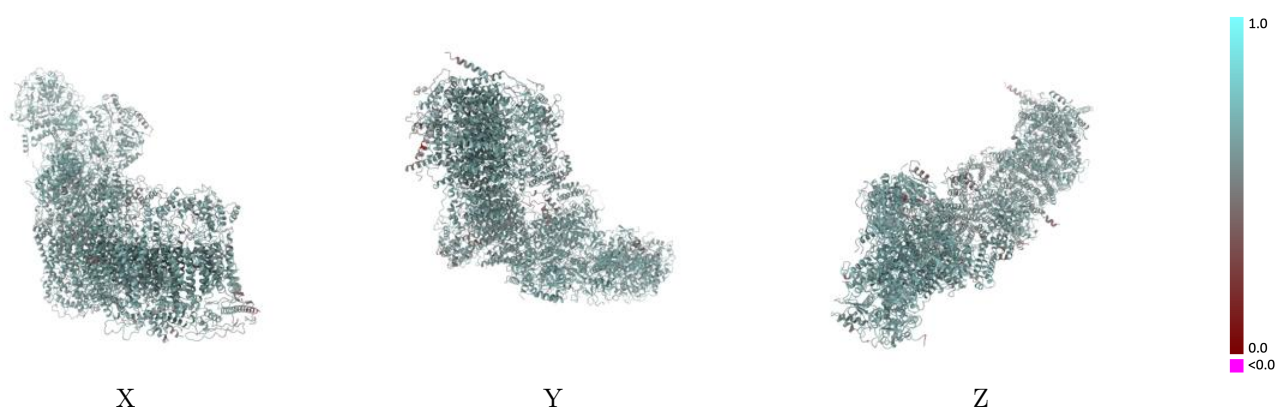
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31643 and PDB model 7V2E. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

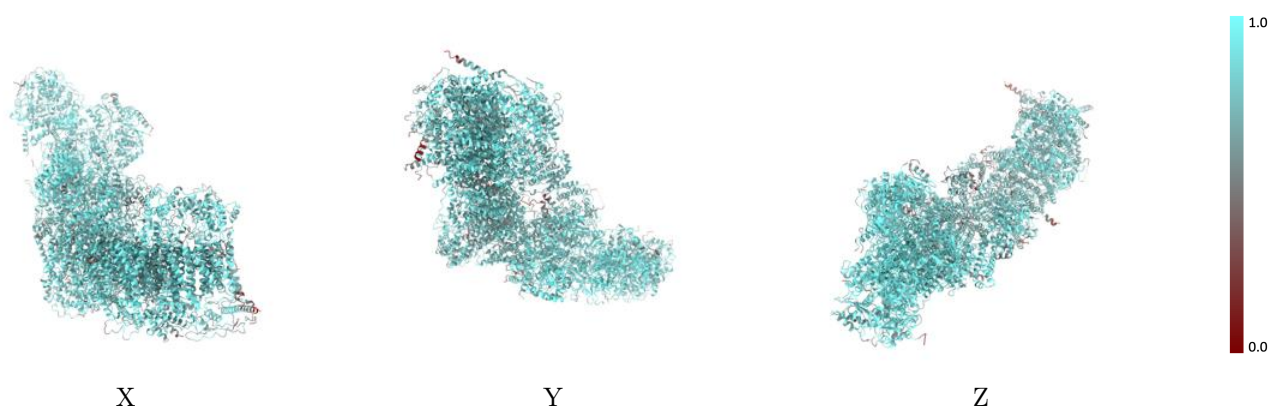
This section was not generated.

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



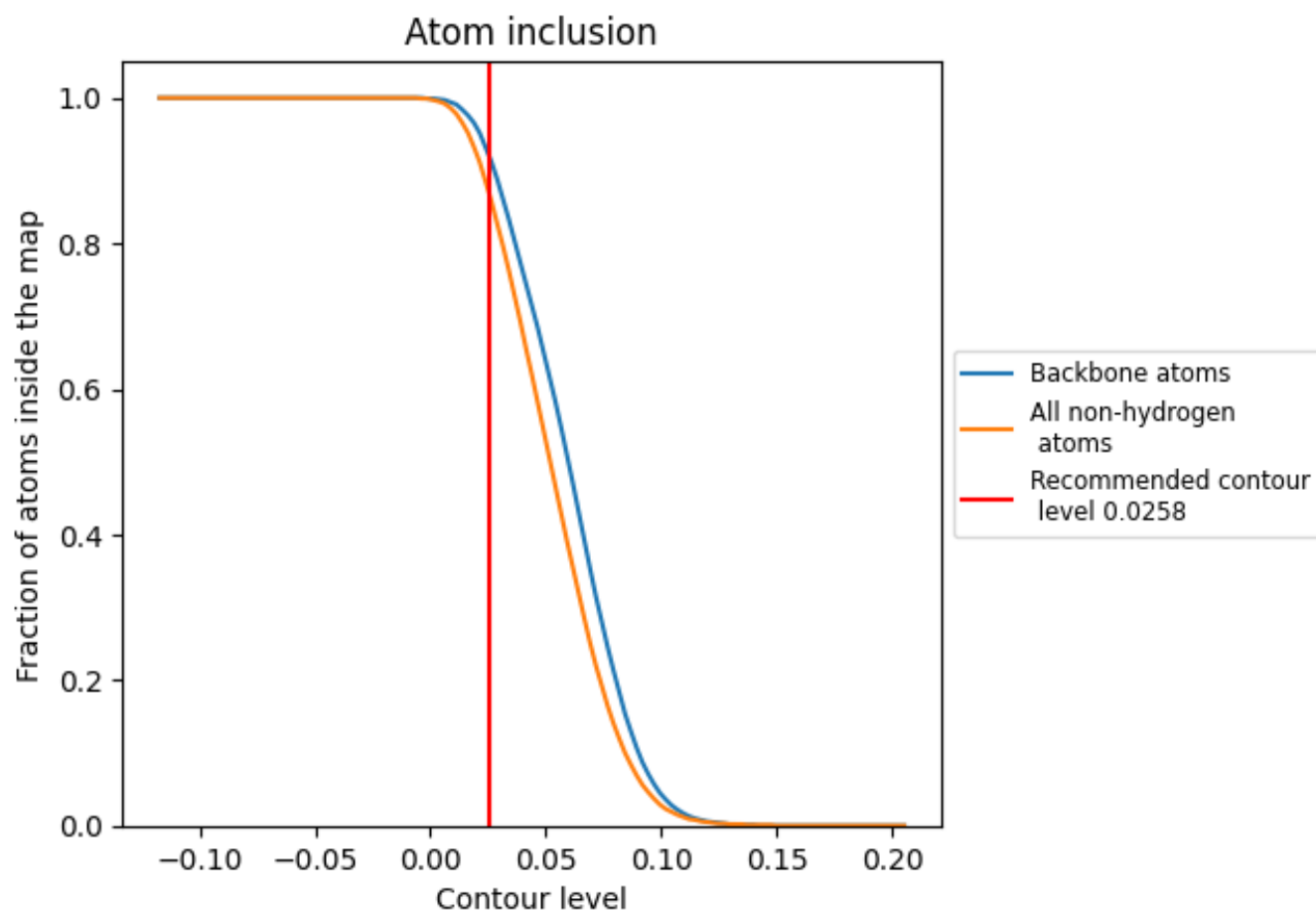
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0258).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.6090
A	 0.8820	 0.6090
B	 0.9500	 0.6500
C	 0.9340	 0.6500
E	 0.8720	 0.6170
F	 0.7770	 0.5480
G	 0.5720	 0.4800
H	 0.8850	 0.6060
I	 0.8170	 0.6040
J	 0.8920	 0.6160
K	 0.8540	 0.6030
L	 0.8970	 0.6350
M	 0.9100	 0.6230
N	 0.8580	 0.6160
O	 0.8380	 0.5910
P	 0.9570	 0.6510
Q	 0.9380	 0.6460
S	 0.9110	 0.6230
T	 0.8950	 0.6220
U	 0.8350	 0.5960
V	 0.7350	 0.5850
W	 0.8620	 0.6040
X	 0.7640	 0.5640
Y	 0.7350	 0.5480
Z	 0.6980	 0.5320
a	 0.8550	 0.6140
b	 0.7770	 0.5700
c	 0.8420	 0.5980
d	 0.8020	 0.5840
e	 0.8040	 0.5870
f	 0.6700	 0.5300
g	 0.8680	 0.6160
h	 0.8480	 0.5850
i	 0.9390	 0.6340
j	 0.8560	 0.6260



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Chain	Atom inclusion	Q-score
k	 0.8550	 0.6140
l	 0.8600	 0.6160
m	 0.8070	 0.5810
n	 0.7050	 0.5550
o	 0.8460	 0.6010
p	 0.8400	 0.5920
r	 0.9020	 0.6280
s	 0.9090	 0.6290
u	 0.8400	 0.5900
v	 0.7100	 0.5310
w	 0.8500	 0.5960