



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:50 AM UTC

PDB ID : 7W1Z / pdb_00007w1z
EMDB ID : EMD-32259
Title : Active state CI from Rotenone-NADH dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-21
Resolution : 2.60 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:

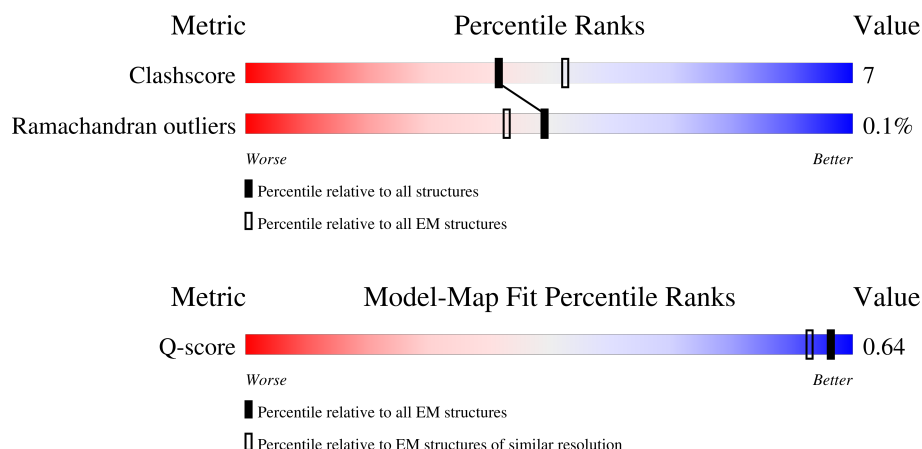
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 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	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	
5	F	86	

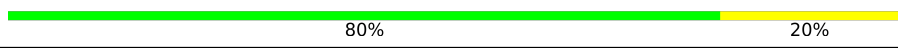
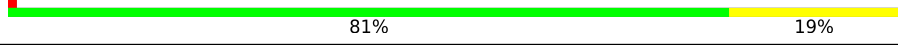
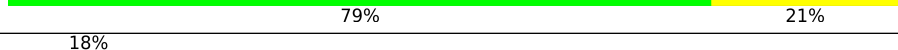
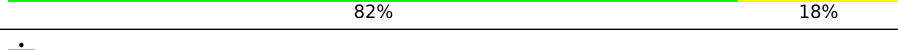
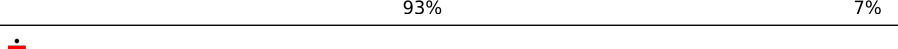
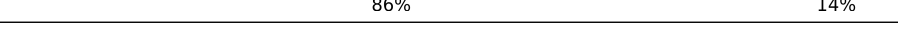
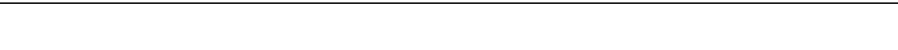
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Mol	Chain	Length	Quality of chain
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	67	
23	Z	80	
24	a	138	
25	b	126	
26	c	156	
27	d	175	
28	e	104	
29	f	49	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68127 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
			684	431	129	122	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5293	3319	923	1012	39		

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

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

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

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

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

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

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			734	449	139	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1161	749	197	206	9		

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

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

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

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

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

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

- Molecule 25 is a protein called Complex I-B17.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1311	851	213	239	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
			1457	914	264	271	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
			377	246	65	66		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4797	3181	743	822	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
			1276	850	187	226	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
			3624	2406	572	608	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
			1036	646	196	185	9		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1645	439	488	10		

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



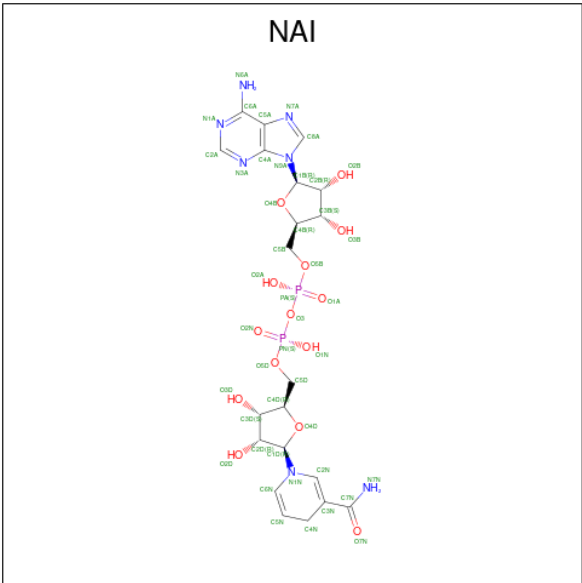
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



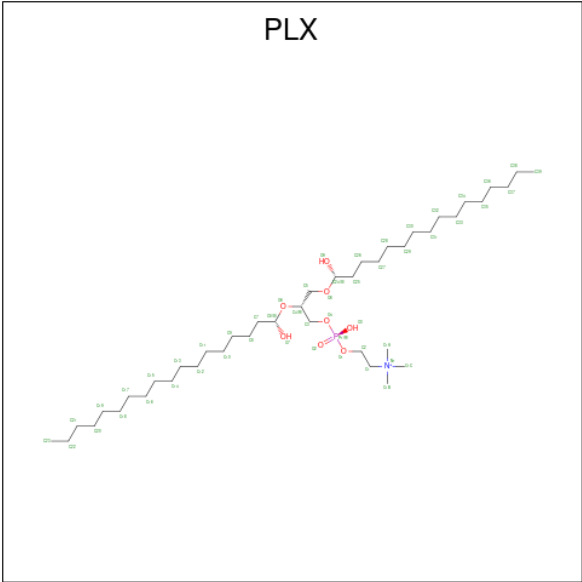
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



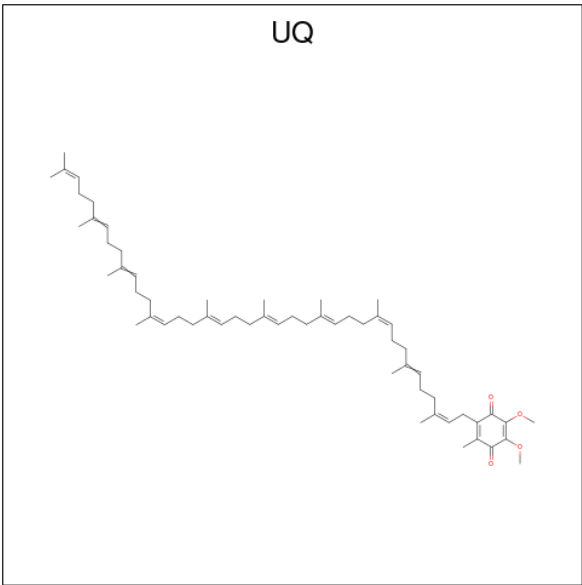
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



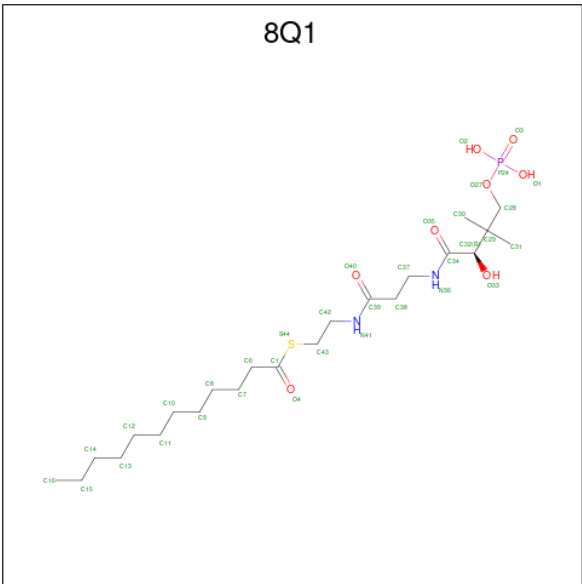
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

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



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

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



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

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

- # NDP

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

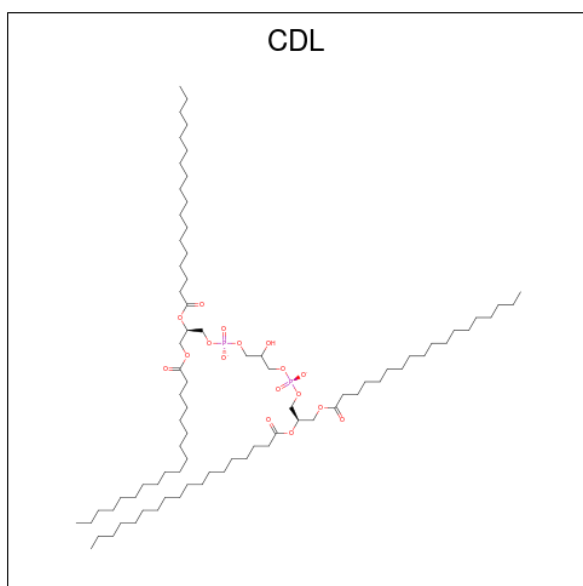
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- Diagram illustrating the structure of a ferredoxin center (FES). The structure shows two iron atoms (Fe1 and Fe2) and two sulfur atoms (S1 and S2) arranged in a square geometry. The bonds between the atoms are represented by lines, with the top and bottom bonds colored yellow and the left and right bonds colored purple.

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



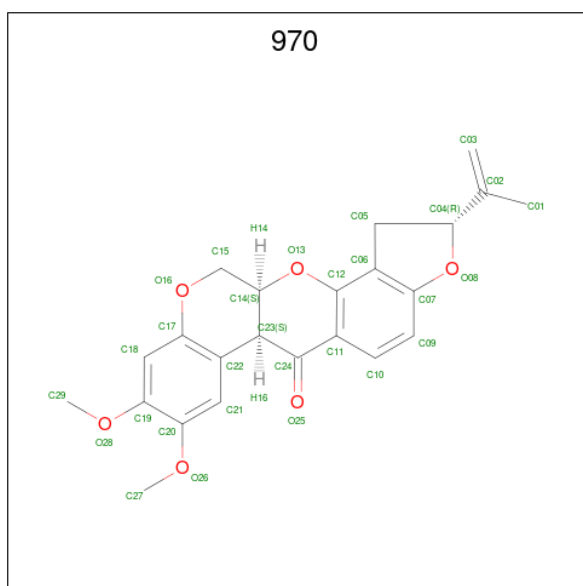
Mol	Chain	Residues	Atoms				AltConf
55	N	1	Total	C	O	P	0
			51	32	17	2	
55	V	1	Total	C	O	P	0
			94	75	17	2	
55	a	1	Total	C	O	P	0
			100	81	17	2	
55	i	1	Total	C	O	P	0
			100	81	17	2	
55	k	1	Total	C	O	P	0
			78	59	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	
55	o	1	Total	C	O	P	0
			100	81	17	2	

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Mol	Chain	Residues	Atoms				AltConf
55	r	1	Total	C	O	P	0
			99	80	17	2	
55	s	1	Total	C	O	P	0
			89	70	17	2	
55	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 56 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆).

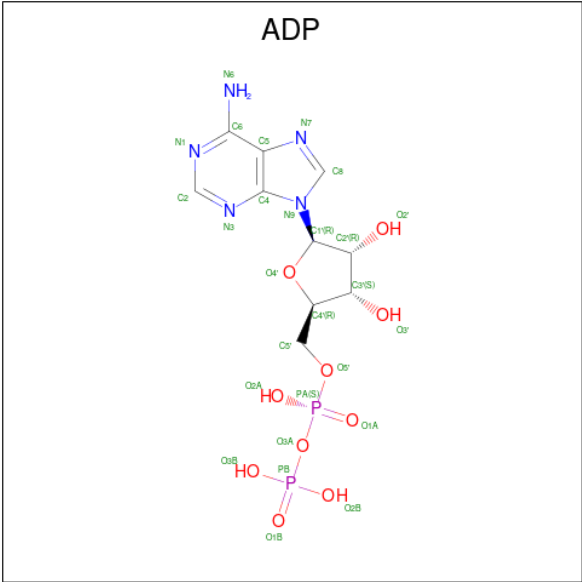


Mol	Chain	Residues	Atoms				AltConf
56	Q	1	Total	C	O		0
			29	23	6		

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

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

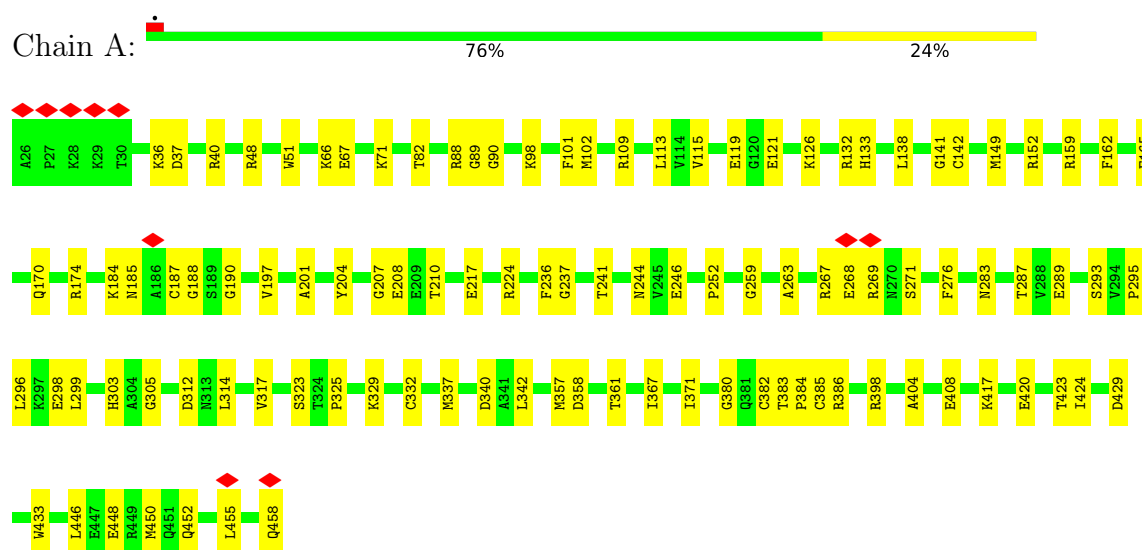


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

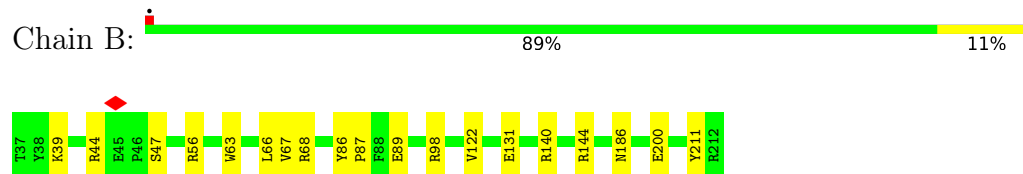
3 Residue-property plots

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

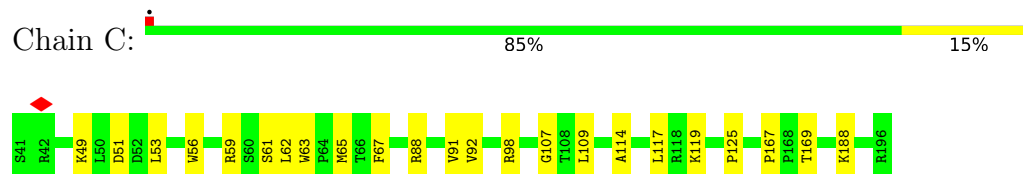
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



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

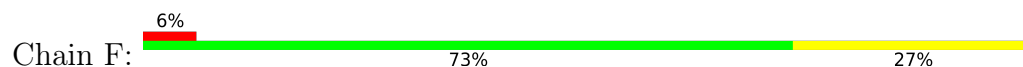


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

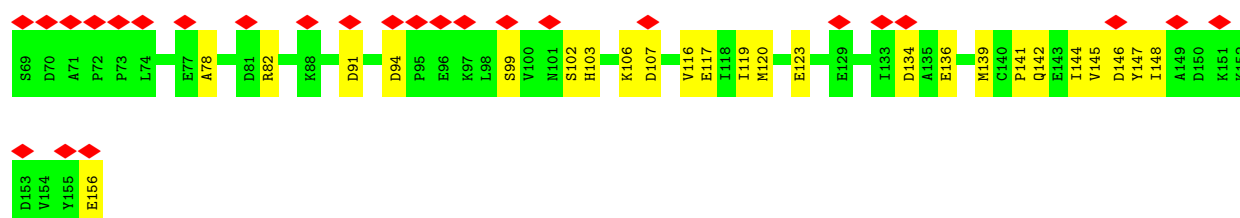
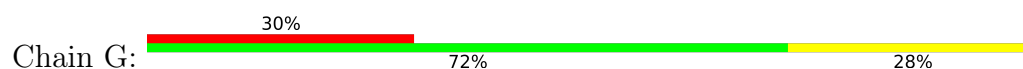




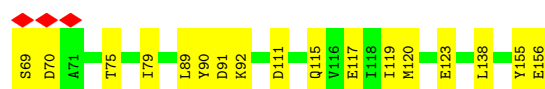
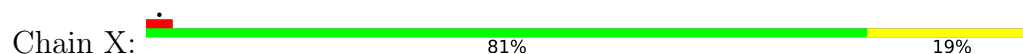
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



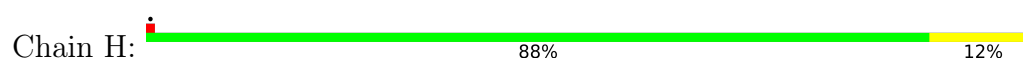
- Molecule 6: Acyl carrier protein



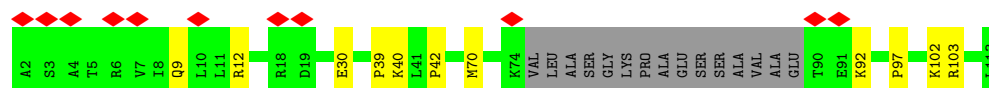
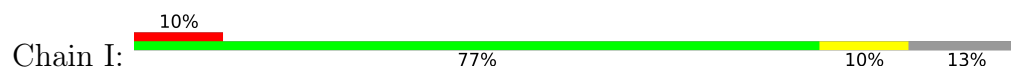
- Molecule 6: Acyl carrier protein



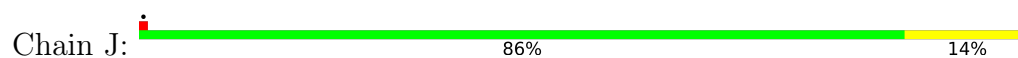
- Molecule 7: Complex I subunit B13

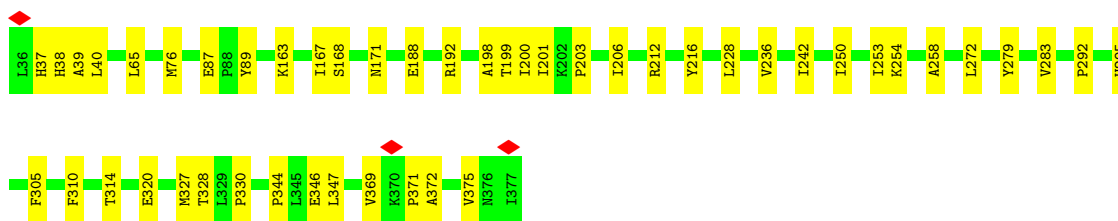


- Molecule 8: Complex I-B14.5a

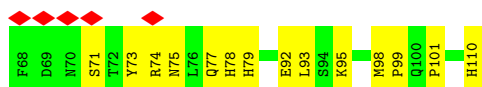


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

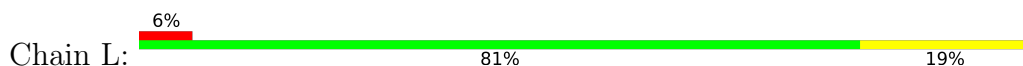




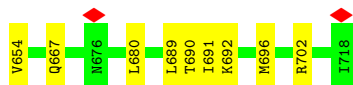
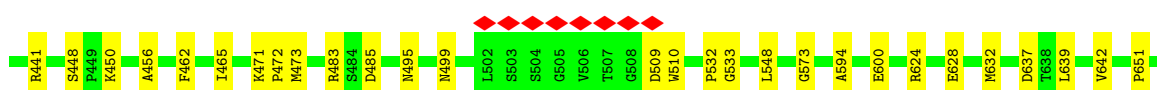
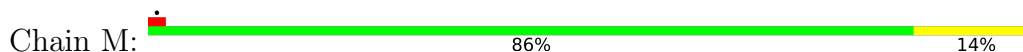
- Molecule 10: Complex I-9kD



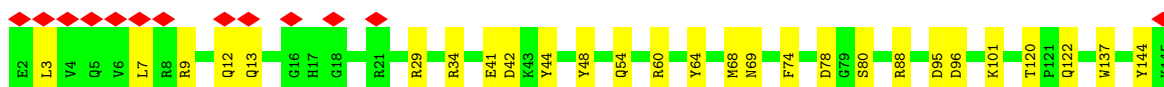
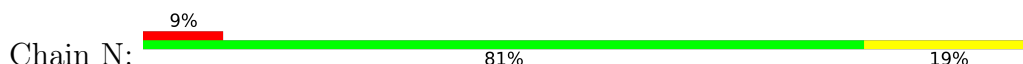
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



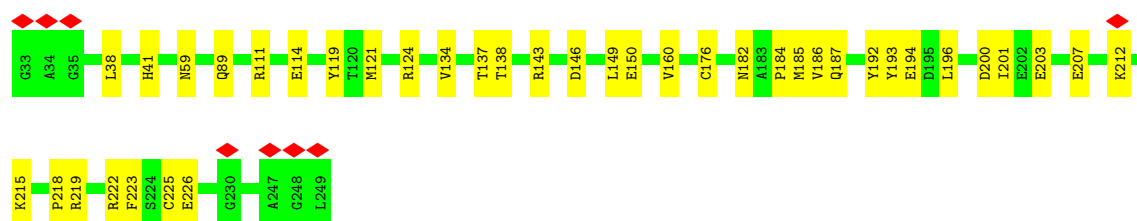
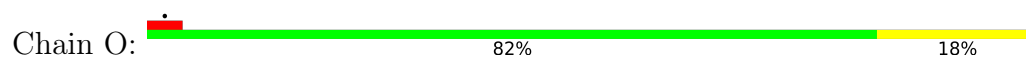
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



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



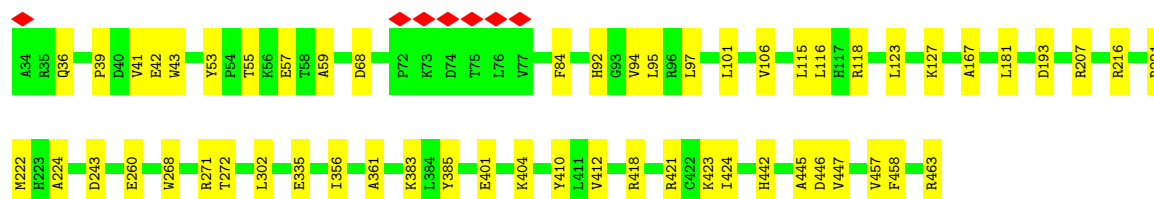
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



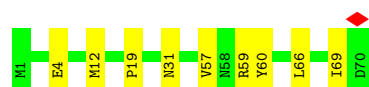
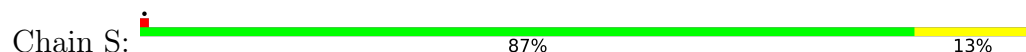
• Molecule 15: Complex I-30kD



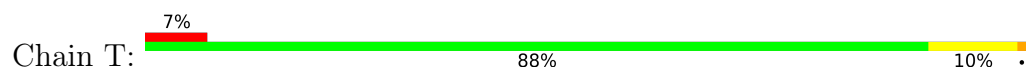
• Molecule 16: Complex I-49kD



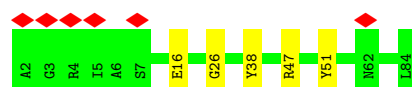
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



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



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

Chain V:  84% 16%

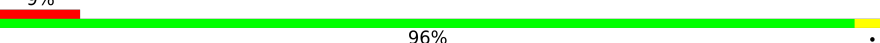


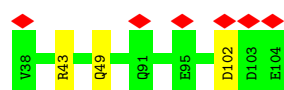
- Molecule 21: Complex I-B16.6

Chain W:  81% 19%



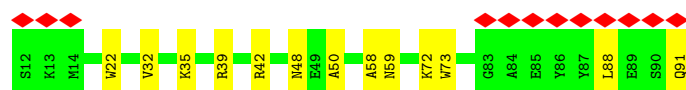
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  96% 9%



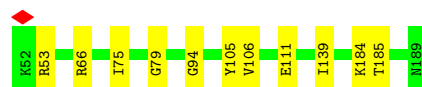
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  84% 16% 15%



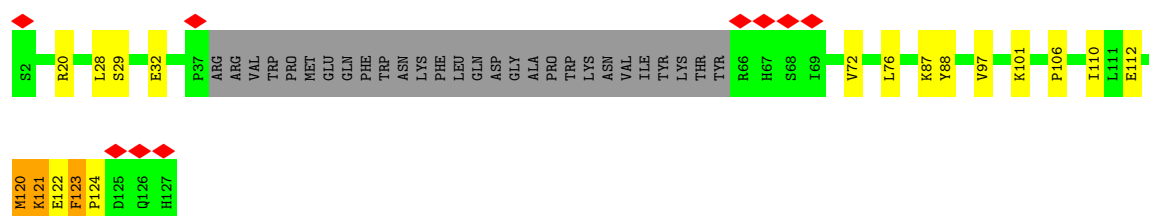
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  92% 8%



- Molecule 25: Complex I-B17

Chain b:  63% 12% 22% 7%



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

Chain c:  85% 15%



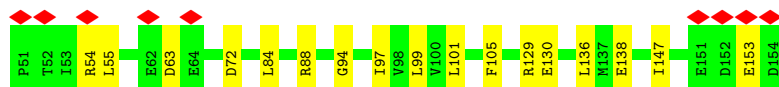
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  5% 85% 15%



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

Chain e:  9% 84% 16%



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

Chain f:  27% 96%



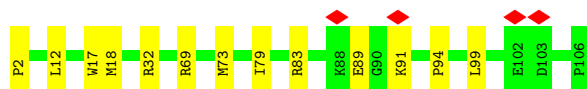
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  88% 12%



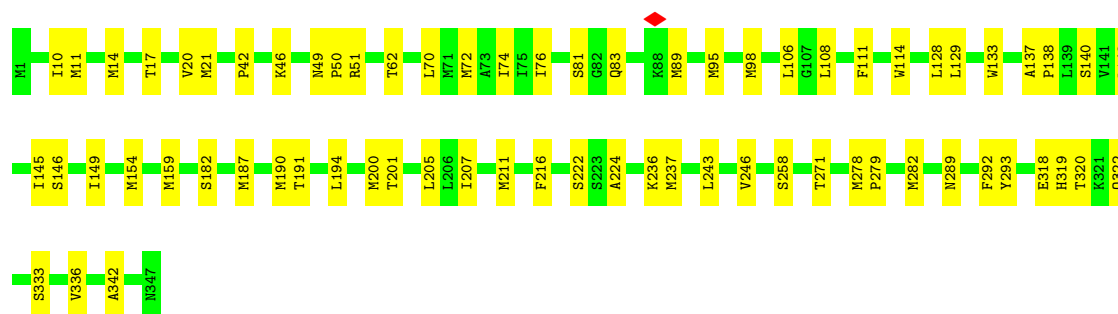
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  88% 12%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  80% 20%



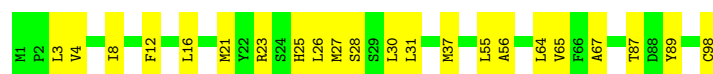
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  81% 19%



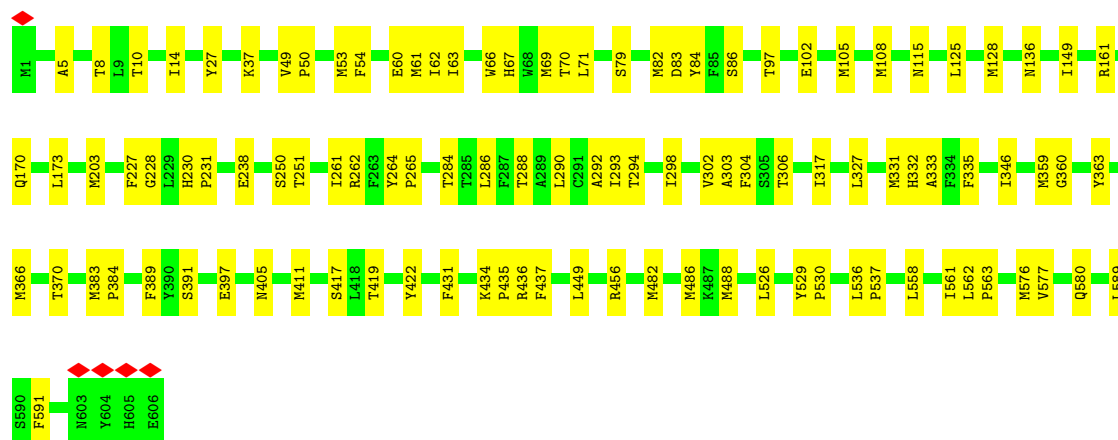
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  78% 22%



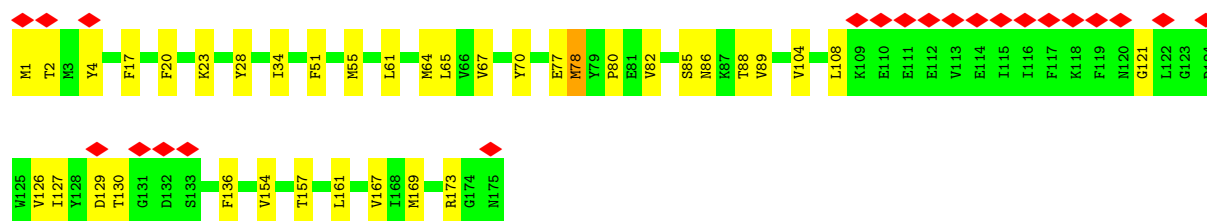
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  83% 17%

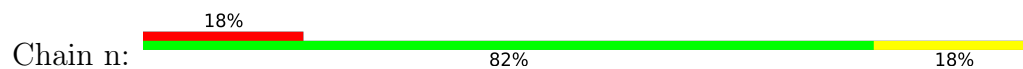


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  13% 79% 21%



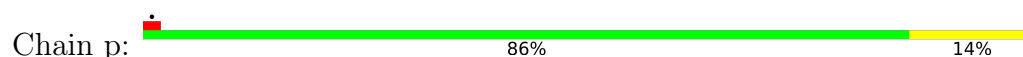
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



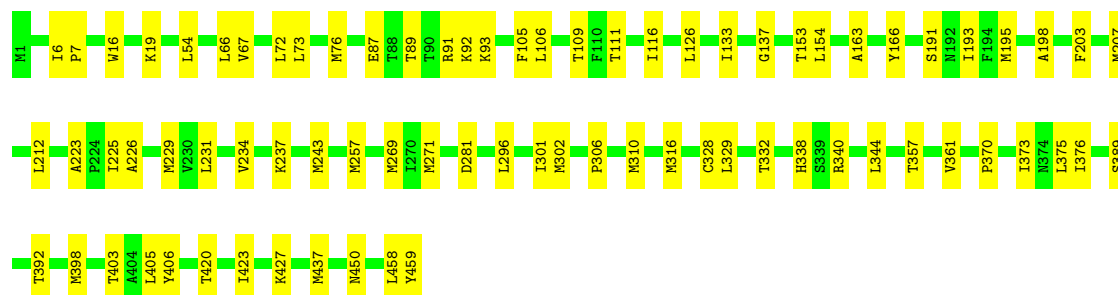
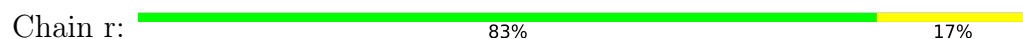
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



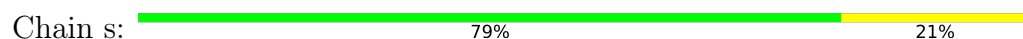
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

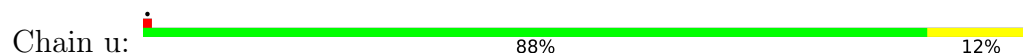


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

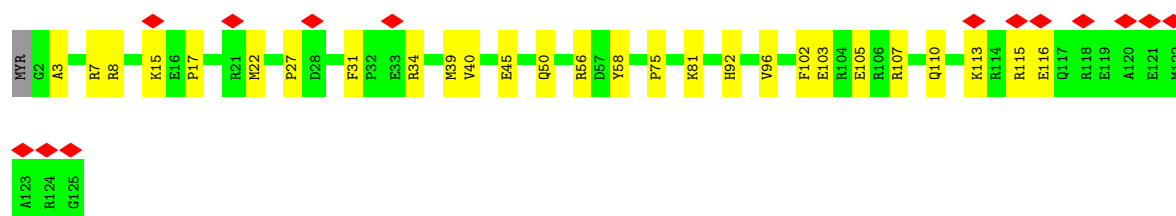
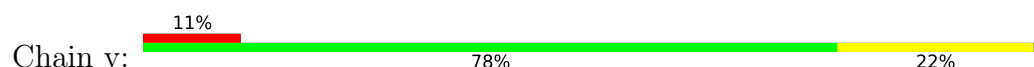




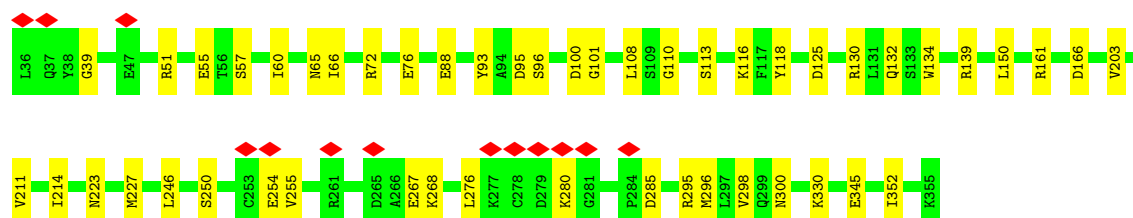
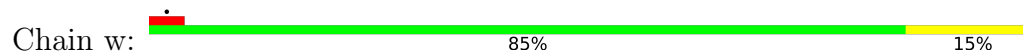
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185329	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	0.245	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0306	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: CDL, PLX, 2MR, FES, PEE, ADP, FMN, SF4, MG, 970, NAI, NDP, 8Q1, UQ, ZN

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	0.16	0/3406	0.35	0/4603
2	B	0.17	0/1443	0.31	0/1952
3	C	0.19	0/1279	0.34	0/1730
4	E	0.17	0/995	0.32	0/1340
5	F	0.14	0/695	0.37	0/936
6	G	0.14	0/705	0.41	0/956
6	X	0.14	0/708	0.28	0/959
7	H	0.15	0/929	0.36	0/1258
8	I	0.16	0/798	0.37	0/1079
9	J	0.15	0/2828	0.33	0/3834
10	K	0.14	0/377	0.34	0/509
11	L	0.15	0/1039	0.30	0/1403
12	M	0.16	0/5381	0.34	0/7291
13	N	0.14	0/1245	0.31	0/1694
14	O	0.15	0/1711	0.33	0/2328
15	P	0.18	0/1789	0.37	0/2436
16	Q	0.18	0/3538	0.34	0/4796
17	S	0.16	0/581	0.34	0/781
18	T	0.26	0/748	0.62	4/1009 (0.4%)
19	U	0.13	0/664	0.30	0/912
20	V	0.24	0/1042	0.45	0/1411
21	W	0.16	0/1192	0.32	0/1610
22	Y	0.14	0/610	0.34	0/836
23	Z	0.12	0/660	0.30	0/892
24	a	0.16	0/1184	0.31	0/1603
25	b	0.17	0/844	0.52	4/1149 (0.3%)
26	c	0.19	0/1367	0.47	2/1870 (0.1%)
27	d	0.17	0/1490	0.34	0/2010
28	e	0.14	0/891	0.34	0/1210
29	f	0.13	0/385	0.27	0/522
30	g	0.15	0/1036	0.30	0/1401
31	h	0.14	0/889	0.31	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.18	0/2773	0.35	0/3768
33	j	0.16	0/938	0.34	0/1281
34	k	0.16	0/759	0.35	0/1029
35	l	0.16	0/4926	0.34	0/6700
36	m	0.21	0/1307	0.44	0/1777
37	n	0.13	0/491	0.28	0/663
38	o	0.14	0/1092	0.29	0/1481
39	p	0.14	0/1590	0.30	0/2155
40	r	0.17	0/3715	0.31	0/5067
41	s	0.20	0/2581	0.39	0/3529
42	u	0.15	0/1436	0.38	0/1938
43	v	0.14	0/1060	0.29	0/1421
44	w	0.14	0/2642	0.32	0/3579
All	All	0.17	0/67759	0.35	10/91898 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	64	GLU	N-CA-C	8.37	120.48	111.36
25	b	120	MET	N-CA-C	7.79	121.31	109.62
18	T	62	VAL	N-CA-C	5.80	121.41	109.34
26	c	44	THR	CA-C-N	5.62	125.29	119.05
26	c	44	THR	C-N-CA	5.62	125.29	119.05
18	T	61	GLU	N-CA-C	5.56	117.02	111.07
18	T	59	GLN	N-CA-C	5.36	117.55	109.41
25	b	123	PHE	CA-C-N	5.11	124.72	119.05
25	b	123	PHE	C-N-CA	5.11	124.72	119.05
25	b	121	LYS	N-CA-C	5.10	119.45	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3292	82	0
2	B	1412	0	1363	19	0
3	C	1248	0	1254	19	0
4	E	971	0	975	9	0
5	F	684	0	698	18	0
6	G	693	0	671	18	0
6	X	696	0	680	12	0
7	H	910	0	950	9	0
8	I	780	0	808	12	0
9	J	2751	0	2773	31	0
10	K	366	0	338	14	0
11	L	1016	0	1016	16	0
12	M	5293	0	5324	67	0
13	N	1204	0	1162	20	0
14	O	1671	0	1673	28	0
15	P	1738	0	1693	20	0
16	Q	3459	0	3396	37	0
17	S	566	0	561	7	0
18	T	734	0	694	8	0
19	U	643	0	642	5	0
20	V	1021	0	1027	17	0
21	W	1161	0	1144	21	0
22	Y	584	0	529	3	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	9	0
25	b	819	0	835	18	0
26	c	1311	0	1204	16	0
27	d	1457	0	1423	24	0
28	e	867	0	817	16	0
29	f	377	0	353	1	0
30	g	1005	0	999	13	0
31	h	867	0	871	11	0
32	i	2710	0	2874	50	0
33	j	914	0	951	20	0
34	k	748	0	799	18	0
35	l	4797	0	4935	75	0
36	m	1276	0	1243	41	0
37	n	479	0	486	9	0
38	o	1062	0	1072	7	0
39	p	1534	0	1470	17	0
40	r	3624	0	3832	56	0
41	s	2508	0	2607	56	0
42	u	1398	0	1374	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1036	0	992	19	0
44	w	2582	0	2537	31	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	7	0
47	A	44	0	27	5	0
48	B	51	0	82	4	0
48	C	47	0	71	2	0
48	Q	47	0	71	3	0
48	W	41	0	59	2	0
48	j	92	0	141	9	0
48	l	96	0	146	7	0
48	r	51	0	82	8	0
49	C	52	0	88	4	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	4	0
49	j	52	0	88	2	0
49	r	104	0	176	6	0
50	C	38	0	47	5	0
50	J	33	0	39	2	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	J	48	0	25	2	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	N	51	0	46	3	0
55	V	94	0	138	6	0
55	a	100	0	156	7	0
55	i	100	0	156	3	0
55	k	78	0	106	6	0
55	l	100	0	156	4	0
55	o	100	0	156	5	0
55	r	99	0	151	8	0
55	s	89	0	125	7	0
55	u	55	0	54	1	0
56	Q	29	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	68127	0	68801	929	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (929) 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)
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.68	1.17
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.17
1:A:244:ASN:HB2	46:A:502:FMN:O2	1.63	0.96
32:i:146:SER:HA	32:i:149:ILE:HD12	1.58	0.84
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.62	0.81
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.64	0.79
36:m:64:MET:HE2	36:m:64:MET:HA	1.62	0.79
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.65	0.78
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.64	0.78
9:J:212:ARG:O	9:J:216:TYR:HB2	1.86	0.76
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.67	0.76
25:b:121:LYS:HB3	43:v:40:VAL:HG13	1.68	0.75
3:C:119:LYS:NZ	33:j:32:GLU:OE1	2.21	0.74
13:N:68:MET:HG3	13:N:69:ASN:H	1.51	0.74
32:i:190:MET:HE2	32:i:205:LEU:HA	1.69	0.73
11:L:109:ASN:ND2	11:L:111:LEU:O	2.21	0.72
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.70	0.72
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.69	0.71
25:b:28:LEU:HD22	25:b:32:GLU:HG2	1.71	0.71
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.23	0.71
8:I:40:LYS:HB3	21:W:7:LYS:H	1.53	0.71
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.73	0.71
13:N:120:THR:HG22	13:N:122:GLN:H	1.56	0.70
20:V:17:GLU:OE2	20:V:20:ARG:NH1	2.23	0.70
28:e:63:ASP:OD2	40:r:338:HIS:NE2	2.24	0.70
12:M:81:GLU:HG3	12:M:108:LYS:HD2	1.73	0.70
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.72	0.70
44:w:125:ASP:O	44:w:130:ARG:NH2	2.25	0.70
35:l:397:GLU:HG2	35:l:482:MET:HE1	1.73	0.70
21:W:81:ARG:HH22	42:u:64:ASN:HD22	1.39	0.70
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.73	0.70
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.75	0.69
2:B:47:SER:O	2:B:56:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.25	0.69
14:O:222:ARG:NH1	14:O:226:GLU:O	2.25	0.69
31:h:18:MET:HE3	34:k:56:ALA:HA	1.75	0.69
14:O:38:LEU:O	14:O:124:ARG:NH2	2.27	0.68
32:i:211:MET:HG2	32:i:333:SER:HB2	1.76	0.68
36:m:55:MET:HA	36:m:55:MET:HE2	1.74	0.68
55:V:201:CDL:H521	35:l:577:VAL:HA	1.75	0.68
1:A:357:MET:HB3	1:A:361:THR:HG21	1.73	0.68
2:B:68:ARG:NH2	21:W:26:PRO:O	2.26	0.68
1:A:152:ARG:NH2	10:K:99:PRO:O	2.27	0.68
5:F:31:GLN:NE2	5:F:35:ASP:OD1	2.26	0.68
11:L:78:ARG:NH1	11:L:148:GLU:OE1	2.27	0.67
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.76	0.67
34:k:37:MET:HE2	34:k:67:ALA:HB2	1.75	0.67
33:j:33:LYS:HG2	41:s:61:LEU:HD21	1.75	0.67
35:l:227:PHE:O	35:l:230:HIS:ND1	2.28	0.67
1:A:185:ASN:OD1	1:A:190:GLY:N	2.25	0.66
27:d:24:THR:HG21	43:v:75:PRO:HD2	1.78	0.66
39:p:57:MET:HE2	39:p:57:MET:HA	1.77	0.66
34:k:25:HIS:NE2	36:m:77:GLU:OE1	2.27	0.66
35:l:170:GLN:NE2	48:l:702:PEE:O1P	2.28	0.66
20:V:81:ARG:NH1	20:V:88:LEU:HD23	2.10	0.66
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.78	0.66
12:M:310:GLU:N	12:M:310:GLU:OE1	2.29	0.66
14:O:215:LYS:O	14:O:219:ARG:NH1	2.28	0.66
27:d:69:ARG:NH2	37:n:46:LYS:O	2.29	0.66
55:s:401:CDL:H552	55:s:401:CDL:H221	1.78	0.66
1:A:296:LEU:HD13	1:A:337:MET:HE2	1.77	0.66
48:r:501:PEE:H79	48:r:501:PEE:H40	1.76	0.66
9:J:212:ARG:O	9:J:216:TYR:CB	2.44	0.65
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.79	0.65
39:p:97:TYR:HB3	39:p:179:MET:HG3	1.76	0.65
31:h:2:PRO:HA	32:i:140:SER:HB2	1.77	0.65
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.29	0.64
28:e:138:GLU:N	28:e:138:GLU:OE2	2.29	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.30	0.64
3:C:53:LEU:HD22	49:C:303:PLX:H322	1.79	0.64
1:A:109:ARG:NH1	1:A:237:GLY:O	2.31	0.64
32:i:10:ILE:O	32:i:14:MET:HG2	1.98	0.64
15:P:173:MET:HE1	15:P:189:THR:HG23	1.79	0.64
1:A:174:ARG:HA	10:K:93:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:HA	14:O:121:MET:HE2	1.80	0.64
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.80	0.64
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.30	0.63
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.80	0.63
44:w:254:GLU:CD	44:w:254:GLU:H	2.07	0.63
2:B:200:GLU:HG3	13:N:88:ARG:HB2	1.79	0.63
12:M:472:PRO:O	12:M:510:TRP:NE1	2.28	0.63
20:V:81:ARG:NH2	20:V:86:ASP:OD2	2.31	0.63
26:c:166:LEU:HD12	26:c:170:ARG:HH21	1.62	0.63
36:m:65:LEU:HD12	41:s:117:LEU:HD11	1.80	0.63
40:r:19:LYS:HE2	40:r:19:LYS:H	1.63	0.63
32:i:278:MET:O	32:i:282:MET:HG3	1.99	0.63
35:l:363:TYR:HA	35:l:370:THR:HG21	1.81	0.63
1:A:159:ARG:NH2	14:O:176:CYS:O	2.32	0.62
44:w:345:GLU:HG3	44:w:352:ILE:HD12	1.80	0.62
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.81	0.62
30:g:47:ASP:OD1	30:g:51:ARG:NH1	2.33	0.62
44:w:250:SER:O	44:w:280:LYS:NZ	2.32	0.62
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.64	0.62
36:m:82:VAL:HG22	36:m:85:SER:HB3	1.82	0.62
32:i:142:LEU:HD22	32:i:154:MET:HE1	1.82	0.62
43:v:113:LYS:HA	43:v:116:GLU:HG2	1.82	0.62
1:A:89:GLY:O	47:A:503:NAI:H2N	2.00	0.61
5:F:61:VAL:O	5:F:62:GLN:NE2	2.32	0.61
55:k:101:CDL:H162	35:l:589:LEU:HD21	1.82	0.61
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.81	0.61
5:F:24:CYS:N	5:F:58:CYS:SG	2.73	0.61
14:O:134:VAL:HG11	14:O:149:LEU:HD13	1.82	0.61
35:l:327:LEU:O	35:l:331:MET:HG2	2.01	0.61
32:i:246:VAL:HG11	55:r:504:CDL:H392	1.83	0.61
44:w:95:ASP:OD1	44:w:95:ASP:N	2.33	0.61
48:W:201:PEE:H45	55:s:401:CDL:H561	1.83	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
27:d:33:LEU:HD13	35:l:49:VAL:HG13	1.83	0.61
27:d:79:GLU:HG2	27:d:80:LYS:HG2	1.83	0.61
33:j:18:VAL:HG23	41:s:222:MET:HE1	1.82	0.61
35:l:293:ILE:HG13	35:l:294:THR:HG23	1.83	0.61
42:u:11:GLU:HA	42:u:14:LYS:HE3	1.82	0.61
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.27	0.60
39:p:50:GLU:HG2	39:p:51:HIS:CD2	2.35	0.60
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:27:PRO:O	43:v:34:ARG:NH1	2.35	0.60
43:v:15:LYS:HZ1	43:v:110:GLN:HB2	1.66	0.60
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.32	0.60
36:m:86:ASN:HD22	36:m:89:VAL:HG23	1.66	0.60
19:U:16:GLU:HG3	48:j:201:PEE:H49	1.83	0.60
25:b:122:GLU:O	25:b:122:GLU:HG3	2.01	0.60
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.02	0.60
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.84	0.60
33:j:16:LEU:O	33:j:20:ILE:HG13	2.02	0.59
27:d:163:MET:HE1	28:e:147:ILE:HG21	1.83	0.59
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.50	0.59
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.85	0.59
1:A:88:ARG:O	1:A:126:LYS:NZ	2.36	0.59
6:G:94:ASP:OD1	6:G:94:ASP:N	2.33	0.59
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.85	0.59
12:M:456:ALA:O	12:M:499:ASN:ND2	2.35	0.59
36:m:55:MET:HE2	36:m:55:MET:CA	2.32	0.59
18:T:47:ASP:O	18:T:52:ARG:NH2	2.35	0.59
1:A:170:GLN:HE21	1:A:197:VAL:HB	1.68	0.59
23:Z:58:ALA:O	35:l:434:LYS:NZ	2.36	0.59
35:l:482:MET:HE2	35:l:486:MET:HG2	1.84	0.59
55:a:201:CDL:H512	48:l:703:PEE:H14	1.85	0.58
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.85	0.58
20:V:46:PRO:HB2	20:V:51:GLU:HG2	1.85	0.58
36:m:61:LEU:O	41:s:114:TYR:OH	2.21	0.58
40:r:226:ALA:HA	40:r:229:MET:HE3	1.84	0.58
1:A:455:LEU:O	1:A:458:GLN:NE2	2.36	0.58
9:J:305:PHE:HD2	9:J:314:THR:HG22	1.68	0.58
12:M:240:ALA:HB2	12:M:271:MET:HE2	1.85	0.58
26:c:116:ARG:HG2	48:l:702:PEE:H49	1.86	0.58
36:m:55:MET:HA	36:m:55:MET:CE	2.33	0.58
12:M:162:ASP:O	18:T:104:LYS:NZ	2.35	0.58
18:T:62:VAL:HG12	18:T:62:VAL:O	2.02	0.58
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.85	0.58
36:m:64:MET:HE2	36:m:64:MET:CA	2.33	0.58
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.37	0.58
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.86	0.58
32:i:49:ASN:O	32:i:51:ARG:N	2.37	0.58
14:O:196:LEU:HD13	14:O:201:ILE:HD13	1.86	0.58
31:h:89:GLU:OE1	31:h:91:LYS:NZ	2.37	0.57
7:H:22:GLU:OE2	7:H:22:GLU:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:29:ARG:NH2	13:N:64:TYR:O	2.36	0.57
1:A:263:ALA:HA	1:A:271:SER:HB3	1.85	0.57
1:A:446:LEU:O	1:A:450:MET:HG3	2.05	0.57
5:F:42:VAL:O	5:F:46:LYS:HG3	2.05	0.57
18:T:51:ARG:O	18:T:54:ARG:HG2	2.04	0.57
35:l:261:ILE:HG13	35:l:317:ILE:HD11	1.86	0.57
1:A:40:ARG:NH1	1:A:289:GLU:O	2.37	0.57
1:A:119:GLU:O	1:A:159:ARG:NH1	2.38	0.57
1:A:448:GLU:O	1:A:452:GLN:HG3	2.05	0.57
34:k:87:THR:HG22	34:k:89:TYR:H	1.69	0.57
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.87	0.57
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.87	0.56
12:M:213:MET:HB3	12:M:215:MET:SD	2.46	0.56
2:B:68:ARG:NH1	16:Q:260:GLU:OE2	2.38	0.56
13:N:144:TYR:HD1	13:N:144:TYR:H	1.54	0.56
20:V:67:GLY:HA2	55:V:201:CDL:H221	1.86	0.56
27:d:160:LYS:NZ	30:g:114:ILE:O	2.33	0.56
2:B:63:TRP:HE1	48:B:303:PEE:H13	1.71	0.56
9:J:206:ILE:HG13	52:J:401:NDP:H42N	1.88	0.56
29:f:60:LYS:O	29:f:64:GLU:HG2	2.06	0.56
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.87	0.56
5:F:42:VAL:HG12	5:F:46:LYS:HE2	1.88	0.56
14:O:111:ARG:NH1	14:O:114:GLU:OE1	2.37	0.56
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.88	0.56
42:u:83:THR:HA	42:u:86:TRP:CD1	2.41	0.56
37:n:47:ARG:NH1	37:n:53:GLU:OE2	2.37	0.56
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.88	0.56
12:M:265:THR:HG22	12:M:270:VAL:HA	1.88	0.56
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.41	0.56
32:i:194:LEU:HD12	32:i:201:THR:HG21	1.87	0.56
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.87	0.55
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.30	0.55
40:r:198:ALA:HB2	48:r:501:PEE:H22	1.88	0.55
28:e:129:ARG:NH1	28:e:136:LEU:O	2.35	0.55
50:J:402:UQ:H101	50:J:402:UQ:H152	1.88	0.55
24:a:106:VAL:O	37:n:50:ARG:NH2	2.38	0.55
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.88	0.55
1:A:102:MET:HE2	1:A:241:THR:OG1	2.05	0.55
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.88	0.55
20:V:95:CYS:HB3	20:V:115:CYS:SG	2.47	0.55
32:i:95:MET:HE2	32:i:149:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.39	0.55
35:l:558:LEU:HD21	55:o:201:CDL:H872	1.87	0.55
6:X:115:GLN:NE2	6:X:138:LEU:O	2.35	0.55
30:g:15:PHE:HB2	49:g:201:PLX:H6	1.88	0.55
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.88	0.55
39:p:35:ASP:OD1	39:p:36:LYS:N	2.39	0.55
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.36	0.55
11:L:154:LYS:HG2	11:L:156:LYS:HZ2	1.72	0.55
17:S:66:LEU:HD13	42:u:75:LYS:HB2	1.88	0.55
26:c:48:ARG:NH2	26:c:63:GLU:OE2	2.38	0.55
35:l:366:MET:O	35:l:370:THR:HG23	2.06	0.55
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.89	0.55
21:W:36:PHE:O	21:W:40:ILE:HG12	2.07	0.54
11:L:84:ARG:NH1	11:L:88:GLN:O	2.39	0.54
15:P:147:THR:HB	15:P:153:ILE:HD11	1.88	0.54
25:b:32:GLU:HG3	39:p:115:TYR:HD1	1.72	0.54
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.89	0.54
36:m:1:MET:SD	36:m:1:MET:N	2.80	0.54
35:l:49:VAL:HG12	35:l:53:MET:HE3	1.90	0.54
32:i:11:MET:HG3	55:i:401:CDL:H562	1.90	0.54
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.89	0.54
40:r:87:GLU:OE2	40:r:91:ARG:HD2	2.07	0.54
3:C:92:VAL:HG11	50:C:304:UQ:H103	1.89	0.54
40:r:73:LEU:HA	40:r:76:MET:HE3	1.90	0.54
1:A:380:GLY:HA2	1:A:386:ARG:HB2	1.90	0.54
5:F:61:VAL:HG22	5:F:62:GLN:HB2	1.89	0.54
3:C:63:TRP:HH2	50:C:304:UQ:H153	1.72	0.53
9:J:168:SER:O	9:J:203:PRO:HD2	2.08	0.53
35:l:286:LEU:HD13	35:l:411:MET:SD	2.48	0.53
6:G:141:PRO:O	6:G:145:VAL:HG23	2.08	0.53
26:c:62:TYR:OH	26:c:74:ASP:O	2.20	0.53
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.90	0.53
12:M:696:MET:HG2	12:M:702:ARG:HA	1.90	0.53
1:A:382:CYS:HB3	1:A:424:ILE:HD12	1.91	0.53
3:C:65:MET:HG2	3:C:67:PHE:HB2	1.91	0.53
12:M:690:THR:OG1	12:M:691:ILE:N	2.42	0.53
38:o:3:PHE:CE2	39:p:70:GLU:HG2	2.43	0.53
3:C:98:ARG:HH11	41:s:61:LEU:HD13	1.74	0.53
6:G:103:HIS:CE1	6:G:139:MET:HB3	2.43	0.53
32:i:271:THR:HG21	40:r:166:TYR:HA	1.89	0.53
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:HG3	2:B:144:ARG:HD2	1.90	0.53
9:J:344:PRO:HG2	9:J:347:LEU:HD13	1.91	0.53
40:r:329:LEU:O	40:r:332:THR:OG1	2.25	0.53
17:S:12:MET:CE	41:s:23:VAL:HG21	2.38	0.53
35:l:228:GLY:HA3	48:l:702:PEE:H38	1.90	0.53
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.73	0.53
32:i:72:MET:HE3	34:k:12:PHE:CG	2.43	0.53
48:Q:502:PEE:H37	48:Q:502:PEE:H60	1.90	0.53
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.90	0.53
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.90	0.53
21:W:74:LEU:O	21:W:78:GLU:HG3	2.09	0.53
41:s:179:TRP:O	41:s:183:MET:HG3	2.08	0.53
1:A:244:ASN:CB	46:A:502:FMN:O2	2.47	0.52
3:C:61:SER:OG	41:s:51:ASP:OD1	2.22	0.52
40:r:310:MET:HE3	40:r:459:TYR:HA	1.90	0.52
20:V:39:TYR:HB3	55:V:201:CDL:H712	1.92	0.52
55:V:201:CDL:H322	35:l:576:MET:HE1	1.91	0.52
25:b:120:MET:O	25:b:120:MET:HG2	2.09	0.52
17:S:19:PRO:HB3	41:s:9:LEU:HD12	1.91	0.52
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.90	0.52
15:P:43:THR:HA	15:P:47:ILE:HD12	1.92	0.52
30:g:2:THR:OG1	30:g:5:SER:HB2	2.09	0.52
1:A:295:PRO:HG2	1:A:298:GLU:HB3	1.92	0.52
49:J:403:PLX:H142	33:j:20:ILE:HG12	1.92	0.52
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.92	0.52
36:m:64:MET:HA	36:m:64:MET:CE	2.27	0.52
3:C:56:TRP:CE2	49:C:303:PLX:H91	2.44	0.52
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.91	0.52
32:i:207:ILE:HG22	32:i:211:MET:HE2	1.92	0.52
44:w:100:ASP:OD1	44:w:100:ASP:N	2.42	0.52
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.75	0.52
18:T:61:GLU:HA	18:T:61:GLU:OE1	2.10	0.52
32:i:159:MET:HB2	32:i:278:MET:HE1	1.91	0.52
6:G:103:HIS:HD2	6:G:106:LYS:HG3	1.74	0.52
31:h:69:ARG:O	31:h:73:MET:HG3	2.10	0.52
40:r:344:LEU:O	40:r:420:THR:HG21	2.10	0.52
7:H:18:GLU:OE1	7:H:18:GLU:N	2.37	0.52
5:F:64:LYS:HD2	5:F:76:ASN:HD22	1.75	0.52
9:J:283:VAL:HG22	9:J:369:VAL:HG11	1.91	0.52
21:W:88:ARG:O	21:W:92:GLU:HG2	2.10	0.52
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.91	0.52
13:N:96:ASP:HB2	13:N:101:LYS:HG3	1.92	0.51
24:a:79:GLY:HA3	55:a:201:CDL:H222	1.92	0.51
25:b:97:VAL:HG13	35:l:61:MET:HE3	1.91	0.51
40:r:66:LEU:HD11	40:r:111:THR:HG23	1.92	0.51
4:E:21:PHE:HE2	4:E:84:ILE:HD11	1.76	0.51
40:r:72:LEU:HD23	40:r:76:MET:HE2	1.92	0.51
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.44	0.51
1:A:184:LYS:HB2	10:K:98:MET:HE3	1.90	0.51
21:W:121:MET:HB2	36:m:130:THR:HG22	1.92	0.51
20:V:14:GLU:OE2	20:V:126:LYS:NZ	2.31	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.43	0.51
12:M:483:ARG:NH1	12:M:485:ASP:OD2	2.43	0.51
44:w:254:GLU:HG3	44:w:276:LEU:HD22	1.91	0.51
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.50	0.51
7:H:76:GLN:O	7:H:78:GLU:N	2.44	0.51
14:O:143:ARG:O	14:O:184:PRO:HG3	2.10	0.51
1:A:98:LYS:NZ	46:A:502:FMN:H5'2	2.25	0.51
33:j:87:MET:HE1	41:s:309:ILE:HD11	1.91	0.51
55:l:701:CDL:H741	55:l:701:CDL:H321	1.93	0.51
55:o:201:CDL:H151	55:o:201:CDL:H362	1.93	0.51
17:S:4:GLU:HG2	41:s:43:TYR:CD1	2.46	0.51
55:s:401:CDL:H311	55:s:401:CDL:H141	1.92	0.51
24:a:94:GLY:O	27:d:61:TYR:OH	2.27	0.51
10:K:78:HIS:CE1	10:K:79:HIS:CE1	2.99	0.51
40:r:212:LEU:HD22	48:r:501:PEE:H46	1.92	0.51
21:W:86:MET:HE1	21:W:125:TYR:CZ	2.46	0.50
5:F:68:ARG:HG3	5:F:74:GLU:HG3	1.93	0.50
12:M:367:CYS:HB3	12:M:533:GLY:O	2.11	0.50
27:d:160:LYS:HA	27:d:163:MET:HE2	1.93	0.50
55:u:201:CDL:H741	55:u:201:CDL:H552	1.94	0.50
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.92	0.50
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.50
41:s:101:GLY:O	41:s:105:MET:HG2	2.11	0.50
6:X:117:GLU:OE1	39:p:45:ARG:NH1	2.43	0.50
22:Y:102:ASP:HA	43:v:115:ARG:HH12	1.76	0.50
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.75	0.50
48:B:303:PEE:H64	41:s:273:ILE:HD11	1.94	0.50
24:a:53:ARG:NH2	25:b:29:SER:O	2.44	0.50
40:r:67:VAL:HG12	49:r:503:PLX:H362	1.93	0.50
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:55:GLU:O	44:w:55:GLU:HG2	2.10	0.50
1:A:283:ASN:ND2	1:A:305:GLY:O	2.42	0.50
15:P:201:ASP:OD1	15:P:201:ASP:N	2.41	0.50
40:r:450:ASN:HB2	49:r:503:PLX:H251	1.93	0.50
5:F:90:THR:O	5:F:94:VAL:HG23	2.11	0.50
12:M:509:ASP:OD1	12:M:509:ASP:N	2.45	0.50
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.93	0.50
26:c:166:LEU:HB2	26:c:170:ARG:HE	1.77	0.50
39:p:134:GLU:H	39:p:134:GLU:CD	2.19	0.50
55:o:201:CDL:H512	55:o:201:CDL:H712	1.92	0.50
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.92	0.50
12:M:667:GLN:N	12:M:667:GLN:OE1	2.44	0.50
30:g:52:ARG:NH1	32:i:318:GLU:OE2	2.45	0.50
37:n:24:GLY:HA2	40:r:6:ILE:HD12	1.93	0.50
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.45	0.49
9:J:375:VAL:HG23	9:J:375:VAL:O	2.10	0.49
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.94	0.49
20:V:123:ALA:O	20:V:127:MET:HG3	2.12	0.49
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.77	0.49
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.37	0.49
16:Q:42:GLU:HG3	28:e:54:ARG:HH21	1.76	0.49
35:l:370:THR:HG22	35:l:431:PHE:CD1	2.48	0.49
36:m:51:PHE:O	36:m:55:MET:HB2	2.12	0.49
40:r:191:SER:HB3	48:r:501:PEE:H2	1.93	0.49
14:O:146:ASP:O	14:O:150:GLU:HG2	2.12	0.49
34:k:4:VAL:O	34:k:8:ILE:HG12	2.12	0.49
35:l:419:THR:HA	35:l:422:TYR:CE2	2.47	0.49
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.44	0.49
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.25	0.49
20:V:95:CYS:CB	20:V:115:CYS:SG	3.01	0.49
21:W:90:ASN:ND2	21:W:123:GLU:O	2.46	0.49
23:Z:35:LYS:O	23:Z:39:ARG:HG3	2.13	0.49
32:i:70:LEU:HG	32:i:98:MET:SD	2.53	0.49
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.45	0.49
26:c:83:GLN:NE2	26:c:97:LEU:O	2.43	0.49
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.94	0.49
17:S:69:ILE:HD11	42:u:20:VAL:HG13	1.94	0.49
30:g:48:ASN:HB3	30:g:55:VAL:HA	1.94	0.49
4:E:23:ARG:HH21	11:L:51:GLN:HB3	1.78	0.49
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.94	0.49
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.94	0.49
34:k:16:LEU:HD23	55:k:101:CDL:H862	1.95	0.49
3:C:109:LEU:HD11	3:C:114:ALA:HA	1.95	0.49
8:I:103:ARG:HH11	8:I:103:ARG:HB3	1.78	0.49
32:i:222:SER:O	32:i:224:ALA:N	2.46	0.49
5:F:88:THR:O	5:F:92:GLU:HG2	2.12	0.49
15:P:127:GLU:OE2	15:P:144:LYS:NZ	2.31	0.49
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.46	0.49
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.95	0.48
39:p:137:VAL:O	39:p:141:GLN:HG2	2.13	0.48
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.94	0.48
21:W:120:MET:HE3	36:m:126:VAL:O	2.13	0.48
35:l:298:ILE:O	35:l:302:VAL:HG23	2.13	0.48
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.47	0.48
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.46	0.48
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	1.95	0.48
41:s:253:GLU:CD	41:s:253:GLU:H	2.21	0.48
43:v:81:LYS:HA	43:v:81:LYS:HD3	1.55	0.48
1:A:296:LEU:HD21	1:A:317:VAL:HG11	1.94	0.48
26:c:85:GLU:OE2	38:o:13:THR:OG1	2.27	0.48
28:e:130:GLU:HG2	28:e:136:LEU:HD11	1.96	0.48
41:s:24:GLU:OE1	41:s:271:LEU:HD22	2.13	0.48
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.95	0.48
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.94	0.48
32:i:17:THR:HG22	32:i:21:MET:HE2	1.95	0.48
13:N:9:ARG:O	13:N:12:GLN:HG3	2.14	0.48
21:W:48:TRP:CZ2	21:W:52:LYS:HE2	2.48	0.48
49:a:202:PLX:H162	28:e:105:PHE:HD1	1.79	0.48
33:j:80:GLN:NE2	41:s:317:GLN:O	2.47	0.48
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.48	0.48
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.94	0.48
16:Q:53:TYR:HE1	48:Q:502:PEE:H2	1.79	0.48
12:M:389:THR:O	12:M:390:THR:OG1	2.27	0.48
12:M:448:SER:OG	12:M:450:LYS:HG2	2.14	0.48
41:s:20:LEU:HD12	41:s:20:LEU:O	2.14	0.48
3:C:51:ASP:OD2	3:C:188:LYS:HA	2.13	0.48
8:I:92:LYS:HD2	8:I:92:LYS:HA	1.58	0.48
10:K:110:HIS:HA	12:M:441:ARG:HD2	1.95	0.48
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.46	0.48
33:j:22:PHE:CE1	41:s:62:ARG:HD3	2.48	0.48
41:s:298:LEU:O	41:s:302:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.49	0.48
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.49	0.48
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.96	0.48
8:I:30:GLU:OE1	8:I:30:GLU:N	2.26	0.48
16:Q:68:ASP:O	32:i:49:ASN:HB2	2.14	0.48
33:j:66:ASP:O	33:j:69:ILE:HG13	2.14	0.48
55:s:401:CDL:H312	55:s:401:CDL:H342	1.49	0.48
42:u:83:THR:HA	42:u:86:TRP:NE1	2.29	0.48
1:A:337:MET:SD	1:A:342:LEU:HD11	2.53	0.47
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.96	0.47
55:N:201:CDL:H511	55:N:201:CDL:H542	1.51	0.47
16:Q:55:THR:O	16:Q:59:ALA:N	2.46	0.47
17:S:57:VAL:HG13	17:S:59:ARG:HB2	1.96	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.48	0.47
55:r:504:CDL:H511	55:r:504:CDL:H541	1.54	0.47
17:S:31:ASN:OD1	17:S:60:TYR:OH	2.24	0.47
26:c:148:GLU:HG2	35:l:405:ASN:HD22	1.79	0.47
27:d:142:ARG:HH21	28:e:138:GLU:HB2	1.79	0.47
32:i:319:HIS:O	32:i:322:GLN:NE2	2.47	0.47
21:W:105:LYS:HD3	42:u:4:ILE:HD11	1.95	0.47
55:a:201:CDL:H342	55:a:201:CDL:H372	1.74	0.47
30:g:85:TYR:CZ	42:u:165:SER:HB2	2.49	0.47
31:h:32:ARG:HH11	31:h:32:ARG:HG2	1.78	0.47
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.48	0.47
55:o:201:CDL:H142	55:o:201:CDL:H111	1.56	0.47
41:s:117:LEU:HD21	41:s:136:VAL:HG23	1.96	0.47
48:C:302:PEE:H58	48:C:302:PEE:H24	1.96	0.47
39:p:55:LYS:HE2	39:p:55:LYS:HB2	1.65	0.47
1:A:210:THR:HB	1:A:224:ARG:H	1.79	0.47
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.96	0.47
15:P:50:ARG:NH2	15:P:80:CYS:SG	2.87	0.47
32:i:278:MET:HB3	32:i:279:PRO:HD3	1.95	0.47
35:l:136:ASN:OD1	35:l:136:ASN:N	2.48	0.47
40:r:87:GLU:O	40:r:92:LYS:NZ	2.44	0.47
41:s:91:MET:HG2	41:s:259:PHE:CE2	2.49	0.47
44:w:285:ASP:OD1	44:w:285:ASP:N	2.47	0.47
1:A:132:ARG:HG3	1:A:133:HIS:CD2	2.50	0.47
3:C:49:LYS:HA	3:C:49:LYS:HD3	1.58	0.47
48:C:302:PEE:H15	9:J:310:PHE:HE1	1.80	0.47
55:l:701:CDL:H642	55:l:701:CDL:H451	1.95	0.47
48:B:303:PEE:H55	48:B:303:PEE:H61	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C:304:UQ:HG212	41:s:225:MET:HG2	1.95	0.47
10:K:74:ARG:O	10:K:77:GLN:NE2	2.47	0.47
14:O:137:THR:HG22	14:O:138:THR:H	1.80	0.47
25:b:106:PRO:HG3	43:v:45:GLU:HG2	1.97	0.47
26:c:127:ASN:O	26:c:131:LYS:HG3	2.15	0.47
32:i:246:VAL:HG21	55:r:504:CDL:H362	1.96	0.47
33:j:57:LEU:HD21	36:m:169:MET:HG2	1.97	0.47
43:v:103:GLU:O	43:v:107:ARG:HG2	2.15	0.47
32:i:187:MET:O	32:i:191:THR:HG23	2.15	0.47
40:r:203:PHE:O	40:r:207:MET:HG2	2.14	0.47
41:s:111:LEU:HG	41:s:111:LEU:O	2.15	0.47
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.97	0.47
8:I:102:LYS:HD2	8:I:102:LYS:HA	1.55	0.47
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.48	0.47
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.14	0.47
55:r:504:CDL:H832	55:r:504:CDL:H861	1.65	0.47
1:A:51:TRP:HE1	10:K:77:GLN:HG2	1.80	0.47
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.97	0.47
30:g:85:TYR:CE2	42:u:165:SER:HB2	2.49	0.47
35:l:8:THR:HB	35:l:82:MET:HE2	1.97	0.47
3:C:59:ARG:NH2	49:C:303:PLX:O3	2.33	0.46
9:J:199:THR:OG1	9:J:258:ALA:O	2.32	0.46
21:W:93:GLU:O	21:W:97:ILE:HG13	2.15	0.46
38:o:75:ASN:O	38:o:79:ASN:ND2	2.47	0.46
40:r:281:ASP:OD1	40:r:340:ARG:HB3	2.15	0.46
6:G:103:HIS:CD2	6:G:106:LYS:HG3	2.50	0.46
6:G:156:GLU:OE1	6:G:156:GLU:N	2.43	0.46
6:X:155:TYR:CD2	6:X:156:GLU:HG3	2.50	0.46
48:j:202:PEE:H31	55:s:401:CDL:H222	1.96	0.46
35:l:66:TRP:CD1	48:l:703:PEE:H16	2.50	0.46
41:s:209:SER:HB3	41:s:213:VAL:HA	1.97	0.46
6:G:91:ASP:N	6:G:91:ASP:OD1	2.49	0.46
13:N:3:LEU:HD23	13:N:7:LEU:HD11	1.98	0.46
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.97	0.46
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.97	0.46
16:Q:94:VAL:HB	16:Q:115:LEU:HB2	1.97	0.46
30:g:36:MET:HE1	49:g:201:PLX:H381	1.98	0.46
27:d:68:PHE:HD1	37:n:44:LEU:HD11	1.80	0.46
35:l:161:ARG:NH2	35:l:238:GLU:OE2	2.45	0.46
40:r:370:PRO:HG3	40:r:375:LEU:HG	1.97	0.46
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:69:MET:HE3	35:l:71:LEU:HD21	1.97	0.46
40:r:237:LYS:HD2	40:r:316:MET:HG2	1.98	0.46
40:r:269:MET:SD	40:r:296:LEU:HD13	2.56	0.46
9:J:163:LYS:NZ	9:J:253:ILE:O	2.39	0.46
14:O:200:ASP:OD2	14:O:219:ARG:HB3	2.16	0.46
28:e:153:GLU:CD	28:e:153:GLU:H	2.24	0.46
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.98	0.46
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.55	0.46
9:J:250:ILE:O	9:J:254:LYS:HG3	2.16	0.46
55:a:201:CDL:H512	55:a:201:CDL:HB4	1.83	0.46
35:l:561:ILE:HG13	35:l:562:LEU:N	2.31	0.46
1:A:185:ASN:C	1:A:187:CYS:H	2.23	0.45
12:M:400:ILE:HG22	12:M:427:LEU:HD11	1.98	0.45
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.51	0.45
16:Q:53:TYR:CE1	48:Q:502:PEE:H2	2.50	0.45
6:X:155:TYR:HA	25:b:20:ARG:HG2	1.98	0.45
41:s:115:SER:O	41:s:119:SER:HB3	2.17	0.45
43:v:15:LYS:NZ	43:v:110:GLN:HB2	2.30	0.45
1:A:420:GLU:HG3	1:A:429:ASP:OD1	2.17	0.45
12:M:144:MET:HE3	12:M:144:MET:HB3	1.75	0.45
31:h:32:ARG:HG2	31:h:32:ARG:NH1	2.32	0.45
40:r:389:SER:O	40:r:392:THR:OG1	2.28	0.45
49:r:502:PLX:H72	49:r:502:PLX:H101	1.72	0.45
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.98	0.45
19:U:26:GLY:HA3	48:j:201:PEE:H38	1.98	0.45
20:V:44:LYS:HE2	20:V:44:LYS:HB2	1.77	0.45
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.51	0.45
49:r:502:PLX:H6	49:r:502:PLX:H51	1.47	0.45
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.51	0.45
44:w:93:TYR:O	44:w:96:SER:OG	2.34	0.45
1:A:37:ASP:OD1	1:A:37:ASP:N	2.50	0.45
19:U:47:ARG:HH11	19:U:47:ARG:HG2	1.81	0.45
27:d:73:ASP:OD1	27:d:75:THR:OG1	2.26	0.45
49:g:201:PLX:H392	32:i:336:VAL:HG22	1.99	0.45
39:p:16:VAL:HG12	39:p:64:LEU:HD13	1.97	0.45
4:E:14:GLY:O	11:L:54:ALA:HA	2.17	0.45
9:J:305:PHE:CD2	9:J:314:THR:HG22	2.49	0.45
13:N:42:ASP:OD2	13:N:44:TYR:HD2	1.99	0.45
35:l:60:GLU:HG2	35:l:83:ASP:HA	1.98	0.45
35:l:63:ILE:O	35:l:79:SER:HA	2.17	0.45
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:29:ARG:HD2	13:N:74:PHE:O	2.17	0.45
14:O:186:VAL:HG12	14:O:193:TYR:HB2	1.99	0.45
18:T:37:LYS:HB2	18:T:62:VAL:HG21	1.98	0.45
1:A:102:MET:HE2	1:A:241:THR:HG1	1.81	0.45
1:A:287:THR:HG22	14:O:225:CYS:HB2	1.99	0.45
1:A:367:ILE:O	1:A:371:ILE:HG12	2.17	0.45
6:G:134:ASP:HB3	6:G:147:TYR:HE2	1.82	0.45
9:J:171:ASN:HA	9:J:327:MET:HE3	1.97	0.45
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.99	0.45
48:j:201:PEE:H67	48:j:201:PEE:H73	1.51	0.45
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.45
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.97	0.45
44:w:72:ARG:O	44:w:76:GLU:HG3	2.16	0.45
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.98	0.45
18:T:29:VAL:HG21	18:T:37:LYS:HE2	1.98	0.45
25:b:87:LYS:NZ	25:b:88:TYR:OH	2.47	0.45
25:b:101:LYS:O	43:v:50:GLN:NE2	2.34	0.45
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.52	0.45
35:l:86:SER:OG	35:l:262:ARG:NH2	2.50	0.45
35:l:561:ILE:HG13	35:l:562:LEU:H	1.81	0.45
41:s:87:VAL:HG22	41:s:88:PRO:HD3	1.98	0.45
2:B:186:ASN:HB3	11:L:112:MET:HE1	1.98	0.45
13:N:41:GLU:HG3	13:N:42:ASP:N	2.32	0.45
35:l:250:SER:HB2	35:l:333:ALA:HA	1.99	0.45
40:r:357:THR:O	40:r:361:VAL:HG23	2.16	0.45
40:r:403:THR:HA	40:r:406:TYR:CE2	2.52	0.45
41:s:200:LEU:HG	41:s:282:TYR:HB3	1.98	0.45
12:M:428:LYS:HE2	12:M:465:ILE:HD13	1.98	0.45
14:O:200:ASP:O	14:O:203:GLU:HG2	2.17	0.45
32:i:106:LEU:HG	32:i:138:PRO:HB2	1.98	0.45
34:k:27:MET:HE1	36:m:70:TYR:HB3	1.98	0.45
35:l:230:HIS:N	35:l:231:PRO:HD3	2.31	0.45
43:v:92:HIS:O	43:v:96:VAL:HG12	2.17	0.45
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.99	0.44
22:Y:43:ARG:HH11	22:Y:49:GLN:HB2	1.81	0.44
28:e:94:GLY:O	28:e:99:LEU:HB2	2.17	0.44
49:g:201:PLX:H332	32:i:342:ALA:HB3	2.00	0.44
35:l:366:MET:HE2	35:l:366:MET:HB3	1.82	0.44
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.34	0.44
21:W:34:SER:O	21:W:38:VAL:HG23	2.17	0.44
24:a:105:TYR:OH	24:a:111:GLU:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:96:ASP:N	26:c:96:ASP:OD1	2.50	0.44
32:i:95:MET:HE1	32:i:145:ILE:HD12	1.99	0.44
33:j:106:TRP:CE3	48:j:201:PEE:H20	2.52	0.44
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.47	0.44
20:V:81:ARG:NH1	20:V:88:LEU:CD2	2.79	0.44
27:d:160:LYS:HE2	28:e:147:ILE:HG23	1.98	0.44
28:e:84:LEU:O	28:e:88:ARG:HG3	2.17	0.44
32:i:81:SER:O	32:i:83:GLN:N	2.44	0.44
41:s:24:GLU:OE2	41:s:274:ARG:NH1	2.48	0.44
41:s:133:LEU:HD13	41:s:133:LEU:HA	1.87	0.44
9:J:295:HIS:NE2	9:J:320:GLU:OE1	2.40	0.44
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.44	0.44
20:V:38:ALA:HA	55:k:101:CDL:H201	1.99	0.44
23:Z:72:LYS:HD3	23:Z:73:TRP:N	2.33	0.44
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.99	0.44
9:J:65:LEU:HA	9:J:242:ILE:HD11	1.98	0.44
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.53	0.44
35:l:128:MET:HE2	35:l:251:THR:O	2.16	0.44
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.53	0.44
1:A:102:MET:HG3	1:A:241:THR:OG1	2.17	0.44
14:O:146:ASP:OD1	14:O:146:ASP:N	2.50	0.44
15:P:173:MET:HE3	15:P:188:LEU:HB2	1.99	0.44
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.99	0.44
24:a:75:ILE:HD13	55:a:201:CDL:H841	1.98	0.44
32:i:200:MET:HA	32:i:200:MET:HE2	1.99	0.44
35:l:488:MET:HE3	35:l:488:MET:HB3	1.90	0.44
36:m:86:ASN:HD21	36:m:88:THR:HB	1.83	0.44
40:r:105:PHE:O	40:r:109:THR:OG1	2.28	0.44
40:r:195:MET:HA	48:r:501:PEE:H16	2.00	0.44
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.98	0.44
50:C:304:UQ:H221	50:C:304:UQ:H262	1.69	0.44
10:K:78:HIS:CE1	10:K:79:HIS:HE1	2.35	0.44
12:M:47:THR:HG23	12:M:51:GLN:HB2	2.00	0.44
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.99	0.44
32:i:258:SER:OG	32:i:336:VAL:HB	2.17	0.44
35:l:417:SER:HB3	55:l:701:CDL:H581	1.99	0.44
40:r:193:ILE:HD13	49:r:502:PLX:H102	1.98	0.44
48:r:501:PEE:H29	48:r:501:PEE:H71	2.00	0.44
42:u:77:HIS:CD2	42:u:115:LEU:HD21	2.52	0.44
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.32	0.44
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:117:GLU:HA	6:G:120:MET:HE3	2.00	0.44
19:U:38:TYR:HB2	41:s:310:MET:O	2.17	0.44
6:X:119:ILE:O	6:X:123:GLU:HG3	2.17	0.44
25:b:121:LYS:O	25:b:121:LYS:HG3	2.17	0.44
35:l:303:ALA:O	35:l:306:THR:HG22	2.17	0.44
3:C:109:LEU:HD13	3:C:117:LEU:HD13	2.00	0.44
31:h:12:LEU:HD12	31:h:12:LEU:HA	1.82	0.44
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.85	0.44
35:l:331:MET:HG3	35:l:391:SER:HB3	1.99	0.44
1:A:358:ASP:O	1:A:361:THR:HG22	2.17	0.43
2:B:63:TRP:O	2:B:67:VAL:HG23	2.18	0.43
4:E:119:LEU:HD11	12:M:628:GLU:HG2	2.00	0.43
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.98	0.43
5:F:91:LEU:HD12	5:F:91:LEU:HA	1.74	0.43
11:L:61:ILE:O	11:L:65:THR:HG23	2.18	0.43
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.99	0.43
36:m:173:ARG:HG3	36:m:173:ARG:NH1	2.33	0.43
44:w:139:ARG:HH12	58:w:401:ADP:N6	2.16	0.43
9:J:201:ILE:HG22	9:J:203:PRO:HD3	2.00	0.43
49:J:403:PLX:H201	33:j:20:ILE:HD11	1.99	0.43
28:e:97:ILE:O	28:e:101:LEU:HB2	2.18	0.43
41:s:152:SER:HA	41:s:155:LEU:HD12	2.00	0.43
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.00	0.43
12:M:428:LYS:HE3	12:M:462:PHE:HE1	1.84	0.43
14:O:207:GLU:HG3	14:O:212:LYS:HB2	2.01	0.43
25:b:110:ILE:HG22	25:b:112:GLU:H	1.82	0.43
49:j:203:PLX:H72	49:j:203:PLX:H4	1.56	0.43
34:k:3:LEU:HD23	36:m:121:GLY:HA2	2.01	0.43
35:l:486:MET:HE3	35:l:486:MET:HB2	1.83	0.43
36:m:34:ILE:HG13	36:m:64:MET:HG3	2.00	0.43
44:w:65:ASN:OD1	44:w:66:ILE:N	2.38	0.43
4:E:16:SER:HA	11:L:52:LEU:HD23	2.00	0.43
13:N:13:GLN:NE2	13:N:34:ARG:HA	2.33	0.43
21:W:98:MET:HE3	31:h:79:ILE:HA	1.98	0.43
55:a:201:CDL:HA31	48:l:703:PEE:H54	2.00	0.43
27:d:120:SER:HB3	43:v:56:ARG:HH22	1.84	0.43
36:m:78:MET:O	36:m:80:PRO:HD3	2.18	0.43
39:p:51:HIS:ND1	39:p:63:LEU:HD21	2.33	0.43
1:A:207:GLY:HA3	46:A:502:FMN:N5	2.34	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.77	0.43
9:J:310:PHE:CG	49:J:403:PLX:H1C2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:69:SER:OG	6:X:70:ASP:N	2.51	0.43
6:X:111:ASP:OD1	6:X:111:ASP:N	2.36	0.43
26:c:40:PRO:O	26:c:74:ASP:HB3	2.18	0.43
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.53	0.43
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.99	0.43
1:A:115:VAL:HG11	1:A:138:LEU:HD11	1.99	0.43
6:G:107:ASP:OD1	6:G:107:ASP:N	2.51	0.43
14:O:149:LEU:HD11	14:O:160:VAL:HG12	2.00	0.43
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.50	0.43
16:Q:271:ARG:NH2	16:Q:445:ALA:HB1	2.33	0.43
35:l:37:LYS:HE3	35:l:37:LYS:HB3	1.69	0.43
40:r:427:LYS:HA	40:r:427:LYS:HD3	1.75	0.43
43:v:3:ALA:O	43:v:7:ARG:HG3	2.19	0.43
44:w:39:GLY:HA2	44:w:296:MET:SD	2.59	0.43
1:A:90:GLY:HA3	47:A:503:NAI:H1D	2.00	0.43
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.49	0.43
2:B:44:ARG:HH11	2:B:44:ARG:HG2	1.83	0.43
3:C:169:THR:HG22	16:Q:221:ARG:HD2	1.99	0.43
8:I:9:GLN:HG2	8:I:12:ARG:HH21	1.83	0.43
13:N:3:LEU:O	13:N:7:LEU:HG	2.19	0.43
5:F:59:SER:O	5:F:61:VAL:N	2.52	0.43
12:M:197:THR:O	14:O:114:GLU:HG2	2.19	0.43
12:M:389:THR:HB	12:M:473:MET:HE3	2.01	0.43
14:O:187:GLN:HG3	14:O:192:TYR:CE1	2.54	0.43
55:V:201:CDL:H402	55:V:201:CDL:H771	2.00	0.43
21:W:127:LEU:HA	31:h:83:ARG:HH22	1.84	0.43
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.54	0.43
32:i:320:THR:HG21	44:w:300:ASN:HA	2.01	0.43
33:j:73:LEU:N	33:j:74:PRO:HD2	2.33	0.43
44:w:211:VAL:O	44:w:214:ILE:HG12	2.19	0.43
12:M:94:MET:HE2	12:M:94:MET:HB2	1.75	0.43
12:M:171:THR:HG23	12:M:173:MET:SD	2.58	0.43
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.43
6:X:89:LEU:HD13	23:Z:48:ASN:HA	2.00	0.43
27:d:110:LEU:HD11	35:l:203:MET:HE2	2.00	0.43
49:j:203:PLX:H1C3	49:j:203:PLX:H22	1.75	0.43
35:l:359:MET:O	35:l:436:ARG:NH2	2.52	0.43
55:l:701:CDL:H351	55:l:701:CDL:H382	1.58	0.43
41:s:62:ARG:HD2	41:s:68:ILE:HD11	2.00	0.43
41:s:145:THR:HG21	41:s:293:PHE:HB3	2.00	0.43
1:A:296:LEU:HD23	1:A:332:CYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.01	0.43
6:G:136:GLU:OE1	6:G:136:GLU:HA	2.18	0.43
55:V:201:CDL:H372	55:V:201:CDL:H341	1.58	0.43
35:l:284:THR:O	35:l:288:THR:OG1	2.34	0.43
36:m:28:TYR:CE2	36:m:82:VAL:HG12	2.54	0.43
40:r:271:MET:HE2	40:r:271:MET:HA	2.01	0.43
44:w:57:SER:HB3	44:w:150:LEU:HD11	2.01	0.43
3:C:88:ARG:HA	41:s:37:PRO:HA	2.00	0.42
21:W:120:MET:O	21:W:121:MET:HB3	2.19	0.42
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	2.01	0.42
26:c:58:ARG:NH1	26:c:61:ASP:OD2	2.50	0.42
40:r:76:MET:HA	40:r:229:MET:HE1	2.02	0.42
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.89	0.42
9:J:228:LEU:O	9:J:292:PRO:HA	2.19	0.42
49:J:403:PLX:H32	49:J:403:PLX:H6	1.54	0.42
32:i:243:LEU:HD23	55:r:504:CDL:H361	2.01	0.42
42:u:80:GLU:HB2	42:u:81:PRO:HD3	2.00	0.42
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.49	0.42
1:A:201:ALA:O	14:O:119:TYR:HB3	2.20	0.42
11:L:154:LYS:HG2	11:L:156:LYS:NZ	2.34	0.42
13:N:3:LEU:HD12	55:N:201:CDL:H122	2.01	0.42
16:Q:101:LEU:HD23	16:Q:106:VAL:HA	2.01	0.42
1:A:36:LYS:H	1:A:36:LYS:HD3	1.85	0.42
1:A:217:GLU:OE2	1:A:236:PHE:N	2.43	0.42
5:F:23:LEU:HD12	5:F:34:ARG:HG2	2.00	0.42
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.53	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.81	0.42
16:Q:55:THR:HG22	16:Q:57:GLU:HG2	2.00	0.42
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.60	0.42
1:A:121:GLU:CD	1:A:323:SER:HG	2.28	0.42
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	2.00	0.42
48:B:303:PEE:H14	48:B:303:PEE:H20	1.84	0.42
9:J:37:HIS:O	9:J:39:ALA:N	2.52	0.42
11:L:76:LYS:HE3	11:L:146:ASP:OD1	2.19	0.42
12:M:456:ALA:HB1	12:M:495:ASN:ND2	2.34	0.42
14:O:185:MET:HE2	14:O:185:MET:HB2	1.77	0.42
27:d:47:LEU:O	27:d:50:GLU:HG2	2.18	0.42
39:p:12:HIS:O	39:p:16:VAL:HG22	2.18	0.42
40:r:133:ILE:HG12	40:r:223:ALA:HB2	2.00	0.42
40:r:302:MET:HE2	40:r:302:MET:HA	2.01	0.42
42:u:85:TYR:HA	42:u:103:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASP:OD1	1:A:340:ASP:N	2.52	0.42
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.01	0.42
15:P:190:ASP:OD1	15:P:191:TYR:N	2.52	0.42
16:Q:383:LYS:HD2	16:Q:383:LYS:HA	1.87	0.42
24:a:184:LYS:O	24:a:185:THR:HG22	2.20	0.42
55:a:201:CDL:H712	55:a:201:CDL:H172	2.02	0.42
41:s:13:ILE:HD13	41:s:13:ILE:HA	1.91	0.42
1:A:268:GLU:HG2	1:A:269:ARG:HE	1.84	0.42
50:C:304:UQ:H152	50:C:304:UQ:H121	1.90	0.42
10:K:95:LYS:HB3	10:K:95:LYS:HE2	1.72	0.42
11:L:99:MET:HE3	11:L:128:PHE:CE1	2.54	0.42
12:M:372:PHE:H	12:M:532:PRO:HB2	1.84	0.42
12:M:639:LEU:O	12:M:642:VAL:HG12	2.19	0.42
15:P:44:ARG:HB2	15:P:44:ARG:CZ	2.49	0.42
22:Y:43:ARG:NH1	22:Y:49:GLN:HB2	2.35	0.42
36:m:104:VAL:O	36:m:108:LEU:HB2	2.20	0.42
40:r:116:ILE:HD13	40:r:116:ILE:HA	1.90	0.42
43:v:31:PHE:CD2	43:v:34:ARG:HD3	2.55	0.42
44:w:51:ARG:HE	44:w:51:ARG:HB3	1.60	0.42
44:w:223:ASN:O	44:w:227:MET:HG3	2.20	0.42
1:A:383:THR:HG21	12:M:120:LEU:HG	2.02	0.42
6:G:144:ILE:O	6:G:148:ILE:HG13	2.19	0.42
7:H:83:GLN:NE2	7:H:83:GLN:HA	2.34	0.42
9:J:40:LEU:HA	9:J:40:LEU:HD23	1.81	0.42
27:d:171:LYS:NZ	28:e:153:GLU:HB2	2.35	0.42
55:k:101:CDL:H191	55:k:101:CDL:H161	1.78	0.42
41:s:106:LEU:HD23	41:s:106:LEU:HA	1.91	0.42
1:A:48:ARG:NH1	10:K:71:SER:HA	2.35	0.42
1:A:82:THR:HG23	1:A:259:GLY:HA3	2.01	0.42
11:L:115:SER:HB2	12:M:267:THR:HB	2.01	0.42
13:N:34:ARG:NH1	13:N:54:GLN:OE1	2.45	0.42
16:Q:410:TYR:HB3	16:Q:423:LYS:HB3	2.02	0.42
20:V:104:ARG:HA	20:V:104:ARG:HD2	1.90	0.42
48:W:201:PEE:H26	48:W:201:PEE:H31	1.88	0.42
25:b:122:GLU:HA	25:b:122:GLU:OE1	2.20	0.42
31:h:94:PRO:HG2	31:h:99:LEU:HD21	2.02	0.42
36:m:169:MET:HE2	36:m:169:MET:HB3	1.90	0.42
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.50	0.42
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.85	0.42
10:K:73:TYR:CZ	10:K:75:ASN:HB3	2.54	0.42
27:d:43:ARG:HB3	27:d:44:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:290:LEU:O	35:l:293:ILE:HG12	2.20	0.42
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.54	0.42
44:w:113:SER:HB3	44:w:116:LYS:HB3	2.02	0.42
1:A:276:PHE:O	1:A:287:THR:HA	2.20	0.41
11:L:101:PHE:HE1	11:L:124:LEU:HD23	1.85	0.41
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.02	0.41
6:X:91:ASP:OD2	23:Z:42:ARG:NH1	2.42	0.41
27:d:36:ILE:HD13	27:d:36:ILE:HA	1.90	0.41
40:r:405:LEU:HA	40:r:405:LEU:HD23	1.83	0.41
41:s:55:LEU:HD23	41:s:55:LEU:HA	1.93	0.41
44:w:267:GLU:HG2	44:w:268:LYS:N	2.35	0.41
1:A:126:LYS:HD2	1:A:246:GLU:OE1	2.20	0.41
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.54	0.41
8:I:9:GLN:HG2	8:I:12:ARG:NH2	2.35	0.41
49:J:403:PLX:H301	49:J:403:PLX:H272	1.60	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.55	0.41
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.43	0.41
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.72	0.41
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.89	0.41
35:l:292:ALA:HB2	35:l:304:PHE:HB3	2.01	0.41
35:l:383:MET:SD	35:l:384:PRO:HD2	2.60	0.41
35:l:526:LEU:HD12	35:l:530:PRO:HG2	2.01	0.41
1:A:66:LYS:HE3	1:A:188:GLY:O	2.20	0.41
1:A:404:ALA:HB3	1:A:450:MET:HE2	2.02	0.41
18:T:49:ASP:OD2	18:T:51:ARG:NH2	2.46	0.41
32:i:14:MET:HB2	55:i:401:CDL:H602	2.01	0.41
33:j:86:THR:O	33:j:90:MET:HG2	2.21	0.41
37:n:9:ARG:HD2	37:n:9:ARG:HA	1.70	0.41
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.84	0.41
38:o:89:LEU:HD23	38:o:89:LEU:HA	1.92	0.41
5:F:61:VAL:HG13	5:F:62:GLN:H	1.84	0.41
12:M:395:GLU:HA	12:M:421:SER:OG	2.20	0.41
19:U:51:TYR:HB3	36:m:136:PHE:HE2	1.85	0.41
6:X:90:TYR:CZ	6:X:92:LYS:HG3	2.56	0.41
27:d:42:ASP:O	27:d:46:THR:HG23	2.20	0.41
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.56	0.41
36:m:129:ASP:O	36:m:130:THR:OG1	2.31	0.41
37:n:54:GLU:HG2	37:n:55:VAL:HG13	2.03	0.41
40:r:89:THR:HG22	40:r:93:LYS:HE3	2.01	0.41
40:r:154:LEU:HD23	40:r:154:LEU:HA	1.96	0.41
44:w:108:LEU:HD21	44:w:330:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:77:MET:HE1	12:M:117:MET:HG2	2.01	0.41
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.55	0.41
12:M:485:ASP:OD1	12:M:680:LEU:HD12	2.20	0.41
12:M:632:MET:H	12:M:632:MET:HG2	1.65	0.41
32:i:46:LYS:NZ	55:i:401:CDL:OB2	2.54	0.41
48:j:201:PEE:H26	41:s:295:PRO:HB3	2.03	0.41
40:r:133:ILE:HD11	40:r:231:LEU:HD11	2.01	0.41
40:r:257:MET:HE3	40:r:257:MET:HB3	1.87	0.41
1:A:113:LEU:HD13	1:A:149:MET:HE1	2.01	0.41
4:E:92:GLU:HG2	4:E:98:LYS:HG3	2.03	0.41
12:M:651:PRO:O	12:M:654:VAL:HG22	2.20	0.41
21:W:81:ARG:NH2	42:u:64:ASN:HD22	2.14	0.41
26:c:82:SER:HA	26:c:112:TYR:HB3	2.02	0.41
32:i:72:MET:O	32:i:76:ILE:HG12	2.20	0.41
33:j:68:GLU:HG2	36:m:161:LEU:HD13	2.03	0.41
34:k:23:ARG:HG3	36:m:23:LYS:HE2	2.01	0.41
35:l:108:MET:HE3	35:l:108:MET:HB3	1.91	0.41
49:r:502:PLX:H111	49:r:502:PLX:H141	1.90	0.41
41:s:72:ILE:HG21	55:s:401:CDL:H151	2.03	0.41
41:s:100:LEU:HD13	41:s:103:LEU:HD12	2.02	0.41
44:w:96:SER:HA	44:w:101:GLY:HA2	2.02	0.41
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.02	0.41
9:J:76:MET:HE2	9:J:76:MET:HB3	1.90	0.41
12:M:89:VAL:HB	12:M:94:MET:HE3	2.01	0.41
55:N:201:CDL:H142	55:N:201:CDL:H111	1.53	0.41
16:Q:41:VAL:HG23	28:e:55:LEU:HD23	2.02	0.41
27:d:80:LYS:HB2	30:g:108:LYS:HZ2	1.85	0.41
30:g:36:MET:HG3	30:g:74:GLY:HA3	2.03	0.41
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.02	0.41
48:r:501:PEE:H52	48:r:501:PEE:H59	1.93	0.41
1:A:48:ARG:HH21	14:O:226:GLU:CD	2.28	0.41
6:G:119:ILE:O	6:G:123:GLU:HG3	2.21	0.41
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.55	0.41
6:X:75:THR:O	6:X:79:ILE:HG13	2.21	0.41
32:i:20:VAL:HG11	32:i:137:ALA:HB1	2.01	0.41
40:r:243:MET:HB3	40:r:301:ILE:HG21	2.03	0.41
48:r:501:PEE:H26	48:r:501:PEE:H32	1.98	0.41
43:v:39:MET:SD	43:v:58:TYR:HA	2.61	0.41
1:A:162:PHE:HB3	1:A:165:GLU:HB2	2.02	0.41
5:F:76:ASN:OD1	5:F:76:ASN:N	2.54	0.41
6:G:78:ALA:O	6:G:82:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:99:SER:O	6:G:102:SER:OG	2.39	0.41
7:H:9:THR:HG21	7:H:14:LEU:HD23	2.03	0.41
12:M:168:LEU:HD22	12:M:292:PHE:CD2	2.56	0.41
12:M:234:LYS:HB3	12:M:235:PRO:HD3	2.02	0.41
16:Q:167:ALA:HB2	16:Q:356:ILE:O	2.21	0.41
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	2.03	0.41
23:Z:59:ASN:OD1	23:Z:59:ASN:N	2.54	0.41
24:a:66:ARG:NH1	28:e:72:ASP:HB2	2.36	0.41
25:b:123:PHE:HA	25:b:124:PRO:HD3	1.90	0.41
32:i:74:ILE:HG13	32:i:98:MET:HE1	2.03	0.41
32:i:182:SER:HB3	32:i:293:TYR:OH	2.20	0.41
33:j:19:LEU:HD21	48:j:202:PEE:H48	2.03	0.41
48:j:202:PEE:O1P	41:s:62:ARG:NH1	2.48	0.41
55:k:101:CDL:OB9	36:m:23:LYS:NZ	2.42	0.41
36:m:126:VAL:HG23	36:m:127:ILE:HG23	2.03	0.41
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.02	0.41
40:r:306:PRO:HA	40:r:458:LEU:HG	2.03	0.41
55:r:504:CDL:H473	55:r:504:CDL:H191	2.02	0.41
41:s:218:GLY:O	41:s:222:MET:HG3	2.21	0.41
1:A:98:LYS:HA	1:A:101:PHE:HD2	1.86	0.41
1:A:424:ILE:HD11	12:M:74:ASN:HA	2.01	0.41
20:V:8:LYS:HB3	20:V:8:LYS:HE3	1.79	0.41
25:b:121:LYS:O	25:b:121:LYS:CG	2.69	0.41
27:d:158:LYS:HG3	30:g:118:PHE:CE2	2.56	0.41
31:h:17:TRP:HE3	34:k:55:LEU:HD13	1.84	0.41
32:i:89:MET:HE3	32:i:98:MET:HE3	2.02	0.41
35:l:10:THR:O	35:l:14:ILE:HG23	2.20	0.41
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.56	0.41
40:r:163:ALA:O	40:r:166:TYR:HB3	2.21	0.41
41:s:267:THR:O	41:s:271:LEU:HG	2.22	0.41
41:s:296:LEU:HA	41:s:296:LEU:HD23	1.87	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.40
12:M:209:TYR:O	14:O:41:HIS:HB3	2.21	0.40
12:M:283:GLU:OE2	12:M:420:LYS:NZ	2.48	0.40
15:P:43:THR:O	15:P:47:ILE:HB	2.21	0.40
33:j:94:LEU:HD13	36:m:154:VAL:HG13	2.03	0.40
35:l:27:TYR:O	35:l:115:ASN:ND2	2.45	0.40
55:o:201:CDL:H811	55:o:201:CDL:H842	1.87	0.40
55:s:401:CDL:H141	55:s:401:CDL:H171	1.77	0.40
4:E:18:LYS:HG3	4:E:19:PRO:HD2	2.03	0.40
5:F:65:LEU:O	5:F:76:ASN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:102:GLY:O	20:V:106:ARG:N	2.54	0.40
32:i:129:LEU:HD23	32:i:133:TRP:HB3	2.02	0.40
34:k:21:MET:HE1	55:k:101:CDL:H561	2.03	0.40
40:r:16:TRP:HA	40:r:93:LYS:HD3	2.03	0.40
40:r:106:LEU:HD13	40:r:234:VAL:HG11	2.02	0.40
55:r:504:CDL:H472	55:r:504:CDL:H412	2.04	0.40
1:A:67:GLU:O	1:A:71:LYS:HG2	2.22	0.40
2:B:211:TYR:CE1	8:I:39:PRO:HG3	2.55	0.40
9:J:87:GLU:HG3	9:J:89:TYR:H	1.85	0.40
50:J:402:UQ:H71	50:J:402:UQ:HM53	1.78	0.40
10:K:73:TYR:HB2	14:O:223:PHE:CD1	2.57	0.40
13:N:78:ASP:OD2	13:N:80:SER:OG	2.27	0.40
33:j:23:TRP:CE2	48:j:202:PEE:H55	2.56	0.40
40:r:126:LEU:HD21	40:r:153:THR:HG21	2.04	0.40
9:J:236:VAL:HG22	9:J:272:LEU:HD23	2.03	0.40
10:K:92:GLU:OE1	10:K:92:GLU:HA	2.21	0.40
12:M:43:VAL:HG21	12:M:96:VAL:HG21	2.04	0.40
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.56	0.40
23:Z:88:LEU:O	23:Z:91:GLN:HG2	2.21	0.40
34:k:64:LEU:O	34:k:67:ALA:HB3	2.22	0.40
35:l:105:MET:HB2	35:l:449:LEU:HD13	2.02	0.40
48:l:702:PEE:H76	40:r:398:MET:HE3	2.04	0.40
36:m:2:THR:C	36:m:4:TYR:H	2.29	0.40
37:n:46:LYS:HB3	37:n:46:LYS:HE2	1.92	0.40
41:s:200:LEU:HD13	41:s:279:ARG:HD3	2.03	0.40
43:v:22:MET:HE1	43:v:102:PHE:HA	2.02	0.40
1:A:98:LYS:HA	1:A:101:PHE:CD2	2.56	0.40
1:A:267:ARG:HG3	1:A:293:SER:OG	2.22	0.40
9:J:279:TYR:O	9:J:283:VAL:HG23	2.21	0.40
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.03	0.40
25:b:72:VAL:HA	25:b:76:LEU:HB2	2.04	0.40
34:k:26:LEU:O	34:k:30:LEU:HG	2.21	0.40
40:r:328:CYS:HB3	40:r:437:MET:HE1	2.04	0.40
55:r:504:CDL:H612	55:r:504:CDL:H641	1.77	0.40
41:s:31:MET:HE1	41:s:272:TRP:CD1	2.56	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	382/433 (88%)	371 (97%)	11 (3%)	0	100	100
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
4	E	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
5	F	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
6	G	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	H	110/112 (98%)	104 (94%)	5 (4%)	1 (1%)	14	30
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	58
10	K	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	20 (3%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	416 (97%)	11 (3%)	0	100	100
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	11	25
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	94/126 (75%)	92 (98%)	2 (2%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	2 (1%)	1 (1%)	21	42
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	330 (96%)	14 (4%)	1 (0%)	36	58
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%)	585 (97%)	19 (3%)	0	100	100
36	m	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	21	42
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	42
40	r	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
41	s	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
42	u	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	21	42
43	v	122/125 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	308 (97%)	10 (3%)	0	100	100
All	All	8126/8314 (98%)	7843 (96%)	275 (3%)	8 (0%)	49	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	77	ILE
9	J	38	HIS
27	d	22	PRO
42	u	152	PRO
36	m	78	MET
32	i	50	PRO
39	p	174	PRO
18	T	62	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.06	1 (10%)	5,13,15	6.06	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.80	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.29	130.75	119.48
16	Q	118	2MR	CD-NE-CZ	4.22	131.30	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.38	130.91	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
49	PLX	C	303	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.06	2 (3%)
48	PEE	j	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.10	3 (6%)
53	FES	M	803	12	0,4,4	-	-	-		
49	PLX	g	201	-	51,51,51	1.19	4 (7%)	53,59,59	0.65	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-		
55	CDL	r	504	-	98,98,99	1.10	8 (8%)	104,110,111	0.88	4 (3%)
56	970	Q	501	-	33,33,33	4.97	16 (48%)	48,50,50	2.54	18 (37%)
55	CDL	k	101	-	77,77,99	1.21	8 (10%)	83,89,111	0.93	4 (4%)
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
51	8Q1	G	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.65	7 (17%)
55	CDL	u	201	-	54,54,99	1.38	8 (14%)	60,66,111	1.11	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	UQ	C	304	-	38,38,63	3.61	10 (26%)	48,49,79	2.82	17 (35%)
55	CDL	i	401	-	99,99,99	1.12	8 (8%)	105,111,111	0.87	4 (3%)
51	8Q1	X	201	6	32,34,34	1.64	5 (15%)	39,43,43	1.58	6 (15%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
55	CDL	l	701	-	99,99,99	1.10	8 (8%)	105,111,111	0.91	5 (4%)
55	CDL	N	201	-	50,50,99	1.43	9 (18%)	56,62,111	1.13	4 (7%)
49	PLX	r	503	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.69	11 (17%)
48	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
53	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
49	PLX	J	403	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	2 (3%)
49	PLX	j	203	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
55	CDL	s	401	-	88,88,99	1.15	8 (9%)	94,100,111	0.89	4 (4%)
48	PEE	l	702	-	49,49,50	1.19	6 (12%)	52,54,55	0.96	2 (3%)
49	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.64	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.96	2 (3%)
49	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.63	1 (1%)
55	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
58	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.89	8 (18%)
55	CDL	V	201	-	93,93,99	1.15	9 (9%)	99,105,111	0.86	4 (4%)
55	CDL	o	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.90	4 (3%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.24	8 (16%)
48	PEE	Q	502	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	3 (6%)
50	UQ	J	402	-	33,33,63	3.52	10 (30%)	42,43,79	2.63	15 (35%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.00	2 (4%)
52	NDP	J	401	-	51,52,52	4.27	25 (49%)	71,80,80	2.31	12 (16%)

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
49	PLX	C	303	-	-	32/55/55/55	-
48	PEE	B	303	-	-	26/54/54/54	-
48	PEE	j	202	-	-	24/44/44/54	-
53	FES	M	803	12	-	-	0/1/1/1
49	PLX	g	201	-	-	33/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5
55	CDL	r	504	-	-	60/109/109/110	-
56	970	Q	501	-	-	4/8/41/41	0/5/5/5
55	CDL	k	101	-	-	50/88/88/110	-
48	PEE	r	501	-	-	31/54/54/54	-
51	8Q1	G	201	-	-	12/41/41/41	-
55	CDL	u	201	-	-	31/65/65/110	-
50	UQ	C	304	-	-	11/33/57/87	0/1/1/1
55	CDL	i	401	-	-	44/110/110/110	-
51	8Q1	X	201	6	-	21/41/41/41	-
55	CDL	l	701	-	-	56/110/110/110	-
45	SF4	M	801	12	-	-	0/6/5/5
55	CDL	N	201	-	-	33/61/61/110	-
49	PLX	r	503	-	-	38/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
48	PEE	l	703	-	-	19/49/49/54	-
53	FES	O	301	14	-	-	0/1/1/1
48	PEE	C	302	-	-	31/50/50/54	-
49	PLX	J	403	-	-	27/55/55/55	-
49	PLX	j	203	-	-	33/55/55/55	-
55	CDL	s	401	-	-	44/99/99/110	-
48	PEE	l	702	-	-	22/53/53/54	-
49	PLX	a	202	-	-	30/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
48	PEE	j	201	-	-	24/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	r	502	-	-	30/55/55/55	-
55	CDL	a	201	-	-	59/110/110/110	-
58	ADP	w	401	-	-	3/16/32/32	0/3/3/3
55	CDL	V	201	-	-	53/104/104/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	o	201	-	-	53/110/110/110	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
48	PEE	Q	502	-	-	27/50/50/54	-
50	UQ	J	402	-	-	9/27/51/87	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
48	PEE	W	201	-	-	19/44/44/54	-
52	NDP	J	401	-	-	4/34/77/77	0/5/5/5

All (269) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Q	501	970	O16-C17	17.52	1.57	1.37
52	J	401	NDP	C3B-C2B	-13.32	1.23	1.53
56	Q	501	970	O25-C24	11.78	1.37	1.22
52	J	401	NDP	O4D-C4D	10.77	1.68	1.45
56	Q	501	970	C23-C24	10.67	1.63	1.52
47	A	503	NAI	C3D-C4D	-10.34	1.26	1.53
50	J	402	UQ	C18-C19	10.06	1.56	1.33
50	C	304	UQ	C18-C19	9.96	1.56	1.33
52	J	401	NDP	C3D-C4D	-9.91	1.27	1.53
50	C	304	UQ	C13-C14	9.59	1.55	1.33
50	J	402	UQ	C13-C14	9.53	1.55	1.33
47	A	503	NAI	O4B-C1B	9.41	1.63	1.42
50	C	304	UQ	C23-C24	9.37	1.54	1.33
50	C	304	UQ	C8-C9	9.25	1.54	1.33
50	J	402	UQ	C8-C9	9.24	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.97	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.29	1.26	1.45
52	J	401	NDP	O4B-C4B	-7.96	1.27	1.45
58	w	401	ADP	O4'-C4'	7.76	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.69	1.29	1.53
50	J	402	UQ	C23-C24	7.51	1.54	1.32
50	C	304	UQ	C28-C29	7.36	1.54	1.32
52	J	401	NDP	C6N-C5N	7.34	1.55	1.33
47	A	503	NAI	C2B-C1B	-7.32	1.30	1.53
52	J	401	NDP	C2N-C3N	7.30	1.55	1.35
56	Q	501	970	C14-C23	-7.15	1.46	1.52
47	A	503	NAI	O4D-C4D	6.88	1.60	1.45
56	Q	501	970	O08-C07	6.54	1.47	1.37
58	w	401	ADP	PA-O3A	6.42	1.66	1.59
52	J	401	NDP	PN-O3	6.28	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	PA-O3	6.21	1.66	1.59
47	A	503	NAI	C2D-C3D	6.00	1.69	1.53
52	J	401	NDP	P2B-O2B	5.72	1.69	1.59
52	J	401	NDP	C6A-N6A	5.68	1.48	1.34
47	A	503	NAI	PN-O3	5.55	1.65	1.59
47	A	503	NAI	O4D-C1D	5.53	1.54	1.42
52	J	401	NDP	PA-O3	5.51	1.65	1.59
47	A	503	NAI	C4N-C3N	-5.38	1.39	1.50
58	w	401	ADP	C6-N6	5.35	1.47	1.34
47	A	503	NAI	C7N-N7N	5.33	1.48	1.33
52	J	401	NDP	C3B-C4B	5.30	1.66	1.53
51	X	201	8Q1	C39-N41	5.26	1.45	1.33
51	G	201	8Q1	C39-N41	5.16	1.45	1.33
56	Q	501	970	O13-C12	5.12	1.45	1.37
56	Q	501	970	C05-C04	-5.06	1.47	1.54
51	X	201	8Q1	C34-N36	5.06	1.45	1.33
47	A	503	NAI	C6A-N6A	5.05	1.47	1.34
51	G	201	8Q1	C34-N36	5.05	1.45	1.33
52	J	401	NDP	O4D-C1D	-5.04	1.30	1.42
56	Q	501	970	C03-C02	4.96	1.53	1.34
52	J	401	NDP	C6N-N1N	4.94	1.49	1.37
52	J	401	NDP	O4B-C1B	4.69	1.52	1.42
52	J	401	NDP	C1B-N9A	-4.66	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.51	1.31	1.42
47	A	503	NAI	O2B-C2B	4.29	1.53	1.43
52	J	401	NDP	O2D-C2D	-4.09	1.32	1.43
48	r	501	PEE	C18-C19	3.86	1.53	1.31
48	l	702	PEE	C18-C19	3.84	1.53	1.31
48	W	201	PEE	C18-C19	3.83	1.53	1.31
48	B	303	PEE	C18-C19	3.82	1.53	1.31
48	j	202	PEE	C18-C19	3.81	1.53	1.31
48	C	302	PEE	C18-C19	3.80	1.53	1.31
48	l	703	PEE	C18-C19	3.80	1.53	1.31
48	Q	502	PEE	C18-C19	3.79	1.53	1.31
52	J	401	NDP	C7N-N7N	3.79	1.44	1.33
48	j	201	PEE	C18-C19	3.79	1.53	1.31
48	r	501	PEE	C39-C38	3.75	1.53	1.31
48	j	201	PEE	C39-C38	3.73	1.52	1.31
48	l	703	PEE	C39-C38	3.72	1.52	1.31
48	B	303	PEE	C39-C38	3.72	1.52	1.31
48	l	702	PEE	C39-C38	3.71	1.52	1.31
48	Q	502	PEE	C39-C38	3.71	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	302	PEE	C39-C38	3.71	1.52	1.31
47	A	503	NAI	C7N-C3N	3.67	1.56	1.48
55	V	201	CDL	OA8-CA7	3.51	1.43	1.33
55	i	401	CDL	OA8-CA7	3.50	1.43	1.33
55	o	201	CDL	OA8-CA7	3.50	1.43	1.33
55	N	201	CDL	OA8-CA7	3.47	1.43	1.33
55	k	101	CDL	OA8-CA7	3.44	1.43	1.33
55	u	201	CDL	OA8-CA7	3.42	1.43	1.33
58	w	401	ADP	C8-N9	-3.42	1.31	1.37
55	s	401	CDL	OA8-CA7	3.41	1.43	1.33
55	a	201	CDL	OA8-CA7	3.41	1.43	1.33
56	Q	501	970	C11-C24	3.41	1.54	1.48
47	A	503	NAI	C4N-C5N	-3.40	1.40	1.49
46	A	502	FMN	C4A-N5	3.40	1.38	1.30
56	Q	501	970	C15-C14	3.33	1.57	1.51
55	r	504	CDL	OA8-CA7	3.31	1.43	1.33
55	l	701	CDL	OA8-CA7	3.31	1.43	1.33
52	J	401	NDP	C8A-N9A	-3.29	1.32	1.37
55	k	101	CDL	OA6-CA5	3.24	1.43	1.34
58	w	401	ADP	O2'-C2'	-3.21	1.35	1.43
52	J	401	NDP	C5A-N7A	-3.15	1.33	1.39
55	V	201	CDL	OA6-CA5	3.12	1.43	1.34
55	a	201	CDL	OB6-CB5	3.11	1.43	1.34
55	i	401	CDL	OB6-CB5	3.04	1.42	1.34
55	l	701	CDL	OB8-CB7	3.04	1.42	1.33
55	N	201	CDL	OB8-CB7	3.04	1.42	1.33
55	V	201	CDL	OB6-CB5	3.03	1.42	1.34
56	Q	501	970	O16-C15	3.03	1.51	1.44
55	k	101	CDL	OB6-CB5	3.01	1.42	1.34
55	r	504	CDL	OB8-CB7	3.01	1.42	1.33
52	J	401	NDP	C7N-C3N	2.99	1.55	1.48
58	w	401	ADP	O3'-C3'	2.99	1.50	1.43
55	N	201	CDL	OB6-CB5	2.99	1.42	1.34
55	a	201	CDL	OB8-CB7	2.98	1.42	1.33
55	i	401	CDL	OB8-CB7	2.97	1.42	1.33
55	s	401	CDL	OB8-CB7	2.97	1.42	1.33
55	k	101	CDL	OB8-CB7	2.97	1.42	1.33
55	s	401	CDL	OA6-CA5	2.96	1.42	1.34
55	u	201	CDL	OB8-CB7	2.95	1.42	1.33
55	l	701	CDL	OB6-CB5	2.94	1.42	1.34
55	V	201	CDL	OB8-CB7	2.94	1.41	1.33
55	u	201	CDL	OB6-CB5	2.94	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	i	401	CDL	OA6-CA5	2.94	1.42	1.34
55	o	201	CDL	OA6-CA5	2.94	1.42	1.34
55	o	201	CDL	OB6-CB5	2.93	1.42	1.34
55	N	201	CDL	OA6-CA5	2.93	1.42	1.34
55	r	504	CDL	OB6-CB5	2.93	1.42	1.34
55	l	701	CDL	OA6-CA5	2.92	1.42	1.34
55	s	401	CDL	OB6-CB5	2.92	1.42	1.34
49	a	202	PLX	O6-C4	-2.91	1.40	1.44
52	J	401	NDP	O3D-C3D	2.89	1.50	1.43
49	r	503	PLX	O6-C4	-2.89	1.40	1.44
55	u	201	CDL	OA6-CA5	2.89	1.42	1.34
55	o	201	CDL	OB8-CB7	2.87	1.41	1.33
49	g	201	PLX	O6-C4	-2.87	1.40	1.44
50	J	402	UQ	C6-C1	2.86	1.54	1.46
55	a	201	CDL	OA6-CA5	2.84	1.42	1.34
55	r	504	CDL	OA6-CA5	2.80	1.42	1.34
49	C	303	PLX	O6-C4	-2.78	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.73	1.32	1.37
55	r	504	CDL	OA6-CA4	-2.73	1.40	1.46
50	C	304	UQ	C6-C1	2.72	1.54	1.46
55	a	201	CDL	OA6-CA4	-2.69	1.40	1.46
56	Q	501	970	C12-C06	2.68	1.43	1.39
48	Q	502	PEE	O2-C2	-2.68	1.40	1.46
49	j	203	PLX	O6-C4	-2.64	1.41	1.44
55	u	201	CDL	OA6-CA4	-2.64	1.40	1.46
48	C	302	PEE	O2-C2	-2.63	1.40	1.46
49	r	502	PLX	O6-C4	-2.63	1.41	1.44
55	l	701	CDL	OA6-CA4	-2.61	1.40	1.46
48	W	201	PEE	O2-C2	-2.61	1.40	1.46
55	o	201	CDL	OA6-CA4	-2.61	1.40	1.46
55	i	401	CDL	OA6-CA4	-2.58	1.40	1.46
48	r	501	PEE	O2-C2	-2.57	1.40	1.46
48	j	201	PEE	O2-C2	-2.57	1.40	1.46
55	s	401	CDL	OA6-CA4	-2.55	1.40	1.46
49	j	203	PLX	C7-C6	2.55	1.56	1.50
48	j	202	PEE	O2-C2	-2.55	1.40	1.46
48	l	702	PEE	O2-C2	-2.54	1.40	1.46
56	Q	501	970	C09-C07	2.54	1.44	1.39
55	N	201	CDL	OA6-CA4	-2.53	1.40	1.46
48	j	201	PEE	O3-C30	2.52	1.40	1.33
46	A	502	FMN	C10-N1	2.52	1.38	1.33
48	B	303	PEE	O2-C2	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	J	403	PLX	C7-C6	2.51	1.56	1.50
48	l	703	PEE	O2-C2	-2.51	1.40	1.46
51	X	201	8Q1	O35-C34	-2.47	1.18	1.23
52	J	401	NDP	O2B-C2B	2.46	1.52	1.44
49	J	403	PLX	O6-C4	-2.44	1.41	1.44
48	j	202	PEE	O3-C30	2.44	1.40	1.33
58	w	401	ADP	C5-N7	-2.44	1.34	1.39
47	A	503	NAI	C6N-C5N	2.43	1.40	1.33
51	G	201	8Q1	C1-S44	2.43	1.82	1.76
48	l	703	PEE	O3-C30	2.43	1.40	1.33
48	W	201	PEE	O3-C30	2.41	1.40	1.33
55	l	701	CDL	OB6-CB4	-2.40	1.40	1.46
48	C	302	PEE	O3-C30	2.40	1.40	1.33
51	G	201	8Q1	O40-C39	-2.39	1.18	1.23
55	s	401	CDL	OB6-CB4	-2.39	1.41	1.46
55	o	201	CDL	OB6-CB4	-2.39	1.41	1.46
47	A	503	NAI	PN-O5D	2.39	1.68	1.59
48	l	702	PEE	O3-C30	2.38	1.40	1.33
55	k	101	CDL	OB6-CB4	-2.38	1.41	1.46
47	A	503	NAI	O3B-C3B	-2.38	1.37	1.43
51	X	201	8Q1	C1-S44	2.37	1.81	1.76
48	B	303	PEE	O3-C30	2.37	1.40	1.33
51	G	201	8Q1	O35-C34	-2.36	1.18	1.23
48	Q	502	PEE	O3-C30	2.36	1.40	1.33
48	l	702	PEE	O2-C10	2.36	1.40	1.34
49	r	502	PLX	C7-C6	2.35	1.55	1.50
49	a	202	PLX	C7-C6	2.35	1.55	1.50
55	N	201	CDL	OB6-CB4	-2.35	1.41	1.46
55	V	201	CDL	OB6-CB4	-2.34	1.41	1.46
48	B	303	PEE	O2-C10	2.34	1.40	1.34
47	A	503	NAI	C5B-C4B	2.34	1.58	1.51
55	a	201	CDL	OB6-CB4	-2.33	1.41	1.46
48	l	703	PEE	O2-C10	2.33	1.40	1.34
49	g	201	PLX	C7-C6	2.32	1.55	1.50
55	u	201	CDL	OB6-CB4	-2.32	1.41	1.46
55	V	201	CDL	OA6-CA4	-2.32	1.41	1.46
51	G	201	8Q1	C6-C1	2.31	1.53	1.50
49	r	503	PLX	C7-C6	2.31	1.55	1.50
48	r	501	PEE	O3-C30	2.31	1.40	1.33
55	u	201	CDL	PB2-OB2	2.30	1.68	1.59
55	r	504	CDL	OB6-CB4	-2.29	1.41	1.46
48	r	501	PEE	O3-C3	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	UQ	C7-C8	2.29	1.54	1.50
51	X	201	8Q1	O40-C39	-2.29	1.18	1.23
55	V	201	CDL	PB2-OB5	2.28	1.68	1.59
55	V	201	CDL	PB2-OB2	2.27	1.68	1.59
55	i	401	CDL	OB6-CB4	-2.27	1.41	1.46
49	C	303	PLX	C7-C6	2.27	1.55	1.50
56	Q	501	970	C04-C02	2.26	1.53	1.50
50	J	402	UQ	C7-C8	2.26	1.54	1.50
55	o	201	CDL	PB2-OB2	2.26	1.68	1.59
48	r	501	PEE	O2-C10	2.25	1.40	1.34
48	j	201	PEE	O2-C10	2.25	1.40	1.34
48	W	201	PEE	O3-C3	-2.25	1.40	1.45
55	i	401	CDL	PB2-OB5	2.25	1.68	1.59
48	B	303	PEE	O3-C3	-2.25	1.40	1.45
52	J	401	NDP	O7N-C7N	-2.25	1.19	1.24
55	l	701	CDL	PB2-OB2	2.24	1.68	1.59
55	a	201	CDL	PB2-OB2	2.24	1.68	1.59
48	C	302	PEE	O3-C3	-2.23	1.40	1.45
48	W	201	PEE	O2-C10	2.23	1.40	1.34
55	i	401	CDL	PB2-OB2	2.23	1.68	1.59
55	o	201	CDL	PB2-OB5	2.23	1.68	1.59
55	a	201	CDL	PB2-OB5	2.22	1.68	1.59
52	J	401	NDP	C2D-C3D	2.22	1.59	1.53
55	r	504	CDL	PB2-OB2	2.21	1.68	1.59
55	l	701	CDL	PB2-OB5	2.20	1.68	1.59
48	C	302	PEE	O2-C10	2.20	1.40	1.34
55	N	201	CDL	PB2-OB2	2.19	1.68	1.59
55	N	201	CDL	PB2-OB5	2.19	1.68	1.59
48	l	702	PEE	O3-C3	-2.19	1.40	1.45
48	j	202	PEE	O2-C10	2.18	1.40	1.34
49	r	502	PLX	P1-O4	2.18	1.67	1.59
49	a	202	PLX	P1-O4	2.18	1.67	1.59
55	k	101	CDL	PB2-OB2	2.18	1.67	1.59
49	C	303	PLX	P1-O4	2.17	1.67	1.59
48	Q	502	PEE	O2-C10	2.17	1.40	1.34
55	s	401	CDL	PB2-OB2	2.17	1.67	1.59
55	r	504	CDL	PB2-OB5	2.17	1.67	1.59
49	j	203	PLX	P1-O4	2.16	1.67	1.59
50	C	304	UQ	O4-C4	-2.16	1.18	1.23
48	Q	502	PEE	O3-C3	-2.16	1.40	1.45
49	g	201	PLX	P1-O4	2.15	1.67	1.59
50	J	402	UQ	O3-CM3	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	u	201	CDL	PB2-OB5	2.13	1.67	1.59
48	l	703	PEE	O3-C3	-2.13	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.13	1.35	1.39
49	r	502	PLX	P1-O1	2.12	1.67	1.59
48	j	202	PEE	O3-C3	-2.12	1.40	1.45
49	j	203	PLX	P1-O1	2.11	1.67	1.59
49	r	503	PLX	P1-O4	2.11	1.67	1.59
49	r	503	PLX	C1-C2	2.11	1.57	1.51
50	J	402	UQ	O4-C4	-2.11	1.18	1.23
55	k	101	CDL	PB2-OB5	2.11	1.67	1.59
50	C	304	UQ	O3-CM3	-2.10	1.40	1.45
52	J	401	NDP	PA-O5B	2.08	1.67	1.59
55	s	401	CDL	PB2-OB5	2.08	1.67	1.59
49	J	403	PLX	P1-O4	2.08	1.67	1.59
49	r	502	PLX	C25-C24	2.08	1.55	1.50
56	Q	501	970	O28-C19	2.07	1.40	1.37
49	J	403	PLX	P1-O1	2.07	1.67	1.59
55	k	101	CDL	OA6-CA4	-2.05	1.41	1.46
49	a	202	PLX	P1-O1	2.05	1.67	1.59
55	V	201	CDL	C11-CA5	2.05	1.56	1.50
50	C	304	UQ	O1-C1	-2.04	1.18	1.23
49	r	503	PLX	P1-O1	2.04	1.67	1.59
55	N	201	CDL	C11-CA5	2.04	1.56	1.50
56	Q	501	970	O26-C20	2.03	1.40	1.37
49	g	201	PLX	P1-O1	2.02	1.67	1.59
50	J	402	UQ	C5-C4	2.02	1.54	1.47
49	C	303	PLX	P1-O1	2.02	1.67	1.59
48	j	201	PEE	O3-C3	-2.01	1.40	1.45
50	J	402	UQ	C21-C19	2.01	1.55	1.51

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C3N-C2N-N1N	-9.39	109.41	123.20
56	Q	501	970	O25-C24-C11	-8.38	109.23	122.18
50	C	304	UQ	C7-C8-C9	-8.05	112.96	126.83
56	Q	501	970	O08-C07-C06	-7.14	108.73	112.99
52	J	401	NDP	C6N-N1N-C2N	-7.07	111.76	119.32
52	J	401	NDP	C1D-N1N-C2N	-6.86	109.84	121.14
50	J	402	UQ	C7-C8-C9	-6.45	115.71	126.83
50	C	304	UQ	C22-C23-C24	-6.36	113.07	127.62
50	C	304	UQ	C17-C18-C19	-6.34	113.10	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	402	UQ	C12-C13-C14	-6.33	113.14	127.62
51	G	201	8Q1	C6-C1-S44	6.08	120.65	113.40
50	C	304	UQ	C12-C13-C14	-5.97	113.95	127.62
50	J	402	UQ	C17-C18-C19	-5.81	114.32	127.62
52	J	401	NDP	C5A-C4A-N3A	-5.62	118.98	126.72
58	w	401	ADP	C5-C4-N3	-5.47	119.18	126.72
51	X	201	8Q1	C6-C1-S44	5.43	119.87	113.40
47	A	503	NAI	C5A-C4A-N3A	-5.39	119.29	126.72
52	J	401	NDP	C1D-N1N-C6N	-5.29	109.59	120.77
56	Q	501	970	C06-C05-C04	5.11	105.93	101.45
50	J	402	UQ	C10-C9-C8	-4.89	111.06	123.63
58	w	401	ADP	N3-C2-N1	-4.61	121.60	128.58
48	j	202	PEE	O2-C10-C11	4.56	121.34	111.48
50	J	402	UQ	C22-C23-C24	-4.52	112.58	127.64
50	C	304	UQ	C27-C28-C29	-4.51	112.59	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.48	121.80	128.58
55	a	201	CDL	OB6-CB5-C51	4.47	121.15	111.48
48	B	303	PEE	O2-C10-C11	4.44	121.08	111.48
56	Q	501	970	C01-C02-C03	-4.39	111.46	121.38
50	C	304	UQ	C10-C9-C8	-4.39	112.36	123.63
58	w	401	ADP	N3-C4-N9	4.33	134.54	127.17
50	C	304	UQ	C25-C24-C23	-4.17	112.92	123.63
51	X	201	8Q1	C37-C38-C39	4.15	119.31	112.39
52	J	401	NDP	N3A-C2A-N1A	-4.09	122.39	128.58
55	i	401	CDL	OA6-CA5-C11	4.09	120.33	111.48
55	l	701	CDL	OA6-CA5-C11	4.07	120.29	111.48
48	l	703	PEE	O2-C10-C11	4.06	120.26	111.48
56	Q	501	970	O25-C24-C23	-4.06	115.37	120.99
48	r	501	PEE	O2-C10-C11	4.04	120.22	111.48
55	r	504	CDL	OA6-CA5-C11	4.01	120.15	111.48
55	u	201	CDL	OB6-CB5-C51	4.00	120.13	111.48
55	o	201	CDL	OB6-CB5-C51	3.98	120.10	111.48
50	C	304	UQ	C20-C19-C18	-3.98	113.41	123.63
48	C	302	PEE	O2-C10-C11	3.95	120.02	111.48
50	J	402	UQ	C15-C14-C13	-3.94	113.50	123.63
55	o	201	CDL	OA6-CA5-C11	3.94	120.00	111.48
55	u	201	CDL	OA6-CA5-C11	3.94	120.00	111.48
55	l	701	CDL	OB6-CB5-C51	3.90	119.92	111.48
48	W	201	PEE	O2-C10-C11	3.89	119.89	111.48
52	J	401	NDP	N3A-C4A-N9A	3.88	133.77	127.17
55	s	401	CDL	OA6-CA5-C11	3.88	119.87	111.48
55	V	201	CDL	OB6-CB5-C51	3.87	119.84	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	N	201	CDL	OA6-CA5-C11	3.86	119.84	111.48
47	A	503	NAI	N3A-C4A-N9A	3.86	133.74	127.17
56	Q	501	970	O08-C07-C09	3.86	131.45	123.85
55	a	201	CDL	OA6-CA5-C11	3.85	119.82	111.48
55	r	504	CDL	OB6-CB5-C51	3.85	119.81	111.48
50	C	304	UQ	C26-C24-C23	-3.84	112.54	121.17
50	J	402	UQ	C21-C19-C18	-3.83	112.56	121.17
50	C	304	UQ	C15-C14-C13	-3.82	113.83	123.63
55	i	401	CDL	OB6-CB5-C51	3.80	119.70	111.48
55	N	201	CDL	OB6-CB5-C51	3.79	119.69	111.48
55	V	201	CDL	OA6-CA5-C11	3.79	119.68	111.48
55	k	101	CDL	OB6-CB5-C51	3.78	119.65	111.48
48	j	201	PEE	O2-C10-C11	3.77	119.64	111.48
55	s	401	CDL	OB6-CB5-C51	3.74	119.58	111.48
48	Q	502	PEE	O2-C10-C11	3.72	119.54	111.48
48	l	702	PEE	O2-C10-C11	3.71	119.51	111.48
50	C	304	UQ	C16-C14-C13	-3.71	112.85	121.17
50	C	304	UQ	C21-C19-C18	-3.70	112.87	121.17
47	A	503	NAI	C2A-N3A-C4A	3.67	120.78	111.83
50	J	402	UQ	C20-C19-C18	-3.61	114.34	123.63
50	C	304	UQ	C11-C9-C8	-3.61	113.06	121.17
50	J	402	UQ	C11-C9-C8	-3.61	113.07	121.17
58	w	401	ADP	C2-N3-C4	3.60	120.63	111.83
52	J	401	NDP	C2A-N3A-C4A	3.60	120.62	111.83
51	G	201	8Q1	O4-C1-C6	-3.54	119.90	123.98
50	J	402	UQ	C16-C14-C13	-3.48	113.37	121.17
58	w	401	ADP	N9-C8-N7	-3.47	109.01	113.94
51	X	201	8Q1	O4-C1-C6	-3.43	120.02	123.98
47	A	503	NAI	C4A-C5A-N7A	-3.35	106.75	110.58
47	A	503	NAI	C5A-N7A-C8A	3.34	108.70	103.45
47	A	503	NAI	N9A-C8A-N7A	-3.30	109.26	113.94
52	J	401	NDP	C4A-C5A-N7A	-3.27	106.84	110.58
50	J	402	UQ	C26-C24-C23	-3.24	112.92	122.66
55	k	101	CDL	OA6-CA5-C11	3.24	118.49	111.48
50	C	304	UQ	C30-C29-C28	-3.24	112.94	122.66
47	A	503	NAI	C4D-O4D-C1D	-3.22	102.35	109.47
50	J	402	UQ	C25-C24-C23	-3.20	113.07	122.66
56	Q	501	970	C09-C07-C06	-3.19	119.82	123.21
50	C	304	UQ	C31-C29-C28	-3.19	113.09	122.66
58	w	401	ADP	C4-N9-C8	3.18	109.08	105.74
46	A	502	FMN	C4-N3-C2	-3.17	120.00	125.64
58	w	401	ADP	C5-N7-C8	3.15	108.40	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Q	501	970	O28-C19-C20	3.14	119.67	115.40
51	G	201	8Q1	C37-C38-C39	3.13	117.61	112.39
48	B	303	PEE	O3-C30-C31	2.99	120.95	111.83
52	J	401	NDP	C5A-N7A-C8A	2.98	108.13	103.45
52	J	401	NDP	N9A-C8A-N7A	-2.97	109.72	113.94
58	w	401	ADP	C4-C5-N7	-2.93	107.23	110.58
48	l	702	PEE	O3-C30-C31	2.92	120.75	111.83
56	Q	501	970	O13-C14-C23	2.91	115.34	112.44
47	A	503	NAI	C3D-C2D-C1D	2.90	106.95	101.46
55	l	701	CDL	OB8-CB7-C71	2.89	120.64	111.83
48	j	201	PEE	O3-C30-C31	2.88	120.61	111.83
55	u	201	CDL	OA8-CA7-C31	2.87	119.87	111.15
55	o	201	CDL	OB8-CB7-C71	2.87	120.58	111.83
56	Q	501	970	C04-C02-C03	-2.83	114.19	120.38
48	r	501	PEE	O3-C30-C31	2.79	120.34	111.83
55	k	101	CDL	OB8-CB7-C71	2.79	120.34	111.83
55	a	201	CDL	OB8-CB7-C71	2.78	120.33	111.83
55	N	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
48	l	703	PEE	O3-C30-C31	2.76	120.25	111.83
48	Q	502	PEE	O3-C30-C31	2.76	120.25	111.83
55	i	401	CDL	OB8-CB7-C71	2.76	120.25	111.83
55	k	101	CDL	OA8-CA7-C31	2.76	120.24	111.83
56	Q	501	970	O26-C20-C19	2.74	119.12	115.40
55	i	401	CDL	OA8-CA7-C31	2.73	120.17	111.83
55	o	201	CDL	OA8-CA7-C31	2.73	120.17	111.83
55	r	504	CDL	OB8-CB7-C71	2.72	120.14	111.83
50	J	402	UQ	C7-C6-C5	-2.69	120.28	124.89
55	N	201	CDL	OA8-CA7-C31	2.68	120.01	111.83
46	A	502	FMN	C4A-C4-N3	2.67	120.06	113.25
55	V	201	CDL	OB8-CB7-C71	2.66	119.94	111.83
55	u	201	CDL	OB8-CB7-C71	2.65	119.92	111.83
48	C	302	PEE	O3-C30-C31	2.65	119.91	111.83
56	Q	501	970	C11-C12-C06	-2.63	119.16	123.22
48	j	202	PEE	O3-C30-C31	2.63	119.86	111.83
55	a	201	CDL	OA8-CA7-C31	2.62	119.83	111.83
46	A	502	FMN	O4-C4-C4A	-2.62	119.63	126.53
55	V	201	CDL	OA8-CA7-C31	2.61	119.80	111.83
55	r	504	CDL	OA8-CA7-C31	2.60	119.75	111.83
48	W	201	PEE	O3-C30-C31	2.58	119.70	111.83
55	s	401	CDL	OB8-CB7-C71	2.56	119.65	111.83
56	Q	501	970	C22-C23-C14	2.56	113.30	109.64
50	J	402	UQ	CM5-C5-C6	-2.54	120.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	G	201	8Q1	O4-C1-S44	-2.54	119.46	122.68
49	a	202	PLX	C1A-N1-C1	2.54	119.99	109.91
47	A	503	NAI	C2D-C3D-C4D	2.53	107.49	102.61
55	s	401	CDL	OA8-CA7-C31	2.52	119.53	111.83
55	l	701	CDL	OA8-CA7-C31	2.49	119.44	111.83
48	Q	502	PEE	C2-O2-C10	-2.46	111.90	117.80
47	A	503	NAI	C4A-N9A-C8A	2.45	108.31	105.74
49	g	201	PLX	C1A-N1-C1	2.45	119.64	109.91
51	X	201	8Q1	C43-S44-C1	2.45	109.07	101.84
46	A	502	FMN	C9A-C5A-N5	-2.43	119.88	122.45
50	J	402	UQ	C10-C9-C11	-2.40	111.06	115.23
49	r	502	PLX	C1A-N1-C1	2.39	119.40	109.91
50	C	304	UQ	CM5-C5-C6	-2.39	120.53	124.45
49	j	203	PLX	C1A-N1-C1	2.38	119.37	109.91
50	C	304	UQ	C7-C6-C5	-2.35	120.86	124.89
49	J	403	PLX	C1A-N1-C1	2.35	119.25	109.91
48	j	202	PEE	C2-O2-C10	-2.28	112.35	117.80
46	A	502	FMN	C5A-C9A-N10	2.27	120.02	117.97
49	C	303	PLX	C1A-N1-C1	2.23	118.78	109.91
51	G	201	8Q1	C43-S44-C1	2.22	108.41	101.84
46	A	502	FMN	C4A-C10-N10	2.22	119.66	116.48
52	J	401	NDP	C4A-N9A-C8A	2.22	108.06	105.74
46	A	502	FMN	C10-C4A-N5	-2.20	120.32	124.81
56	Q	501	970	C15-C14-C23	2.19	112.42	110.65
51	G	201	8Q1	C38-C39-N41	2.17	120.30	116.34
51	G	201	8Q1	C32-C34-N36	2.17	120.61	116.48
55	l	701	CDL	CA4-OA6-CA5	-2.16	112.62	117.80
49	r	503	PLX	C1A-N1-C1	2.11	118.31	109.91
56	Q	501	970	C11-C24-C23	-2.10	113.04	115.89
46	A	502	FMN	C4A-C10-N1	-2.08	119.49	124.59
49	J	403	PLX	C2-C1-N1	-2.05	109.25	115.82
51	X	201	8Q1	O4-C1-S44	-2.02	120.11	122.68
56	Q	501	970	C07-C06-C12	2.02	120.64	118.72
51	X	201	8Q1	C32-C34-N36	2.01	120.30	116.48
56	Q	501	970	O28-C19-C18	-2.01	120.62	124.08
56	Q	501	970	C01-C02-C04	-2.00	112.00	116.45

There are no chirality outliers.

All (1005) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
48	B	303	PEE	C1-O3P-P-O1P
48	B	303	PEE	C1-O3P-P-O4P
48	C	302	PEE	C11-C10-O2-C2
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	C	302	PEE	C4-O4P-P-O3P
48	C	302	PEE	C4-O4P-P-O1P
48	Q	502	PEE	C11-C10-O2-C2
48	Q	502	PEE	C1-O3P-P-O2P
48	Q	502	PEE	C1-O3P-P-O1P
48	Q	502	PEE	C1-O3P-P-O4P
48	W	201	PEE	C1-O3P-P-O2P
48	W	201	PEE	C1-O3P-P-O1P
48	W	201	PEE	C1-O3P-P-O4P
48	W	201	PEE	O4P-C4-C5-N
48	j	201	PEE	C1-O3P-P-O4P
48	j	202	PEE	C11-C10-O2-C2
48	j	202	PEE	C1-O3P-P-O2P
48	j	202	PEE	C4-O4P-P-O2P
48	j	202	PEE	O4P-C4-C5-N
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O4P-C4-C5-N
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O2P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O4-C3-C4-O6
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	C2-O1-P1-O4
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	C2-O1-P1-O3
49	C	303	PLX	N1-C1-C2-O1
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	C3-C4-O6-C6
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C3-O4-P1-O3
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-O8-C5
49	a	202	PLX	O9-C24-C25-C26
49	g	201	PLX	O7-C6-O6-C4
49	g	201	PLX	C3-O4-P1-O1
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C3-O4-P1-O3
49	g	201	PLX	C2-O1-P1-O2
49	j	203	PLX	O7-C6-C7-C8
49	j	203	PLX	C7-C6-O6-C4
49	j	203	PLX	C3-O4-P1-O1
49	j	203	PLX	C3-O4-P1-O2
49	j	203	PLX	O9-C24-O8-C5
49	r	502	PLX	O6-C6-C7-C8
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C3-O4-P1-O2
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O3
50	C	304	UQ	C7-C8-C9-C10
50	C	304	UQ	C7-C8-C9-C11
50	C	304	UQ	C12-C13-C14-C16
50	C	304	UQ	C18-C19-C21-C22
50	C	304	UQ	C22-C23-C24-C26
50	J	402	UQ	C7-C8-C9-C11
51	G	201	8Q1	C1-C6-C7-C8
51	G	201	8Q1	C28-C29-C32-C34
51	G	201	8Q1	C28-C29-C32-O33
51	G	201	8Q1	C30-C29-C32-C34
51	G	201	8Q1	C30-C29-C32-O33
51	G	201	8Q1	C31-C29-C32-C34
51	G	201	8Q1	C31-C29-C32-O33
51	X	201	8Q1	O4-C1-S44-C43
51	X	201	8Q1	C6-C1-S44-C43
51	X	201	8Q1	C28-C29-C32-C34
51	X	201	8Q1	C28-C29-C32-O33
51	X	201	8Q1	C30-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
51	X	201	8Q1	C30-C29-C32-O33
51	X	201	8Q1	C31-C29-C32-C34
51	X	201	8Q1	C31-C29-C32-O33
51	X	201	8Q1	N41-C42-C43-S44
51	X	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-O27-P24-O2
51	X	201	8Q1	C28-O27-P24-O1
55	N	201	CDL	O1-C1-CA2-OA2
55	N	201	CDL	CB2-C1-CA2-OA2
55	N	201	CDL	CA2-OA2-PA1-OA3
55	N	201	CDL	CA2-OA2-PA1-OA4
55	N	201	CDL	CA2-OA2-PA1-OA5
55	N	201	CDL	CB2-OB2-PB2-OB3
55	N	201	CDL	CB2-OB2-PB2-OB4
55	N	201	CDL	CB2-OB2-PB2-OB5
55	N	201	CDL	CB3-OB5-PB2-OB2
55	N	201	CDL	CB3-OB5-PB2-OB3
55	V	201	CDL	OB5-CB3-CB4-OB6
55	V	201	CDL	OB6-CB4-CB6-OB8
55	a	201	CDL	CB2-C1-CA2-OA2
55	a	201	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB2-OB2-PB2-OB5
55	a	201	CDL	OB7-CB5-OB6-CB4
55	a	201	CDL	C51-CB5-OB6-CB4
55	i	401	CDL	CA2-OA2-PA1-OA3
55	i	401	CDL	CA2-OA2-PA1-OA4
55	i	401	CDL	CA2-OA2-PA1-OA5
55	i	401	CDL	CA3-OA5-PA1-OA3
55	i	401	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CB3-OB5-PB2-OB3
55	k	101	CDL	CA2-OA2-PA1-OA3
55	k	101	CDL	CA2-OA2-PA1-OA4
55	k	101	CDL	CA2-OA2-PA1-OA5
55	k	101	CDL	CA3-OA5-PA1-OA3
55	k	101	CDL	CB2-OB2-PB2-OB3
55	k	101	CDL	CB2-OB2-PB2-OB4
55	k	101	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CA2-OA2-PA1-OA4
55	l	701	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CA3-OA5-PA1-OA3
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	CB3-OB5-PB2-OB4
55	o	201	CDL	CA2-OA2-PA1-OA4
55	o	201	CDL	CA2-OA2-PA1-OA5
55	o	201	CDL	CB3-OB5-PB2-OB2
55	o	201	CDL	OB5-CB3-CB4-OB6
55	r	504	CDL	CA3-OA5-PA1-OA2
55	r	504	CDL	CA3-OA5-PA1-OA3
55	r	504	CDL	CB3-OB5-PB2-OB2
55	r	504	CDL	CB3-OB5-PB2-OB3
55	r	504	CDL	CB3-OB5-PB2-OB4
55	r	504	CDL	OB7-CB5-OB6-CB4
55	r	504	CDL	C51-CB5-OB6-CB4
55	s	401	CDL	CA2-OA2-PA1-OA3
55	u	201	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	O1-C1-CB2-OB2
55	u	201	CDL	CB2-OB2-PB2-OB3
55	u	201	CDL	CB2-OB2-PB2-OB5
55	u	201	CDL	CB3-OB5-PB2-OB2
55	u	201	CDL	CB3-OB5-PB2-OB3
55	u	201	CDL	CB3-OB5-PB2-OB4
56	Q	501	970	C03-C02-C04-C05
56	Q	501	970	C03-C02-C04-O08
48	j	201	PEE	O5-C30-O3-C3
48	j	201	PEE	C31-C30-O3-C3
55	i	401	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	OB9-CB7-OB8-CB6
48	C	302	PEE	O4-C10-O2-C2
48	Q	502	PEE	O4-C10-O2-C2
48	j	202	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
55	o	201	CDL	OB7-CB5-OB6-CB4
55	i	401	CDL	C31-CA7-OA8-CA6
55	l	701	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C11-C10-O2-C2
55	o	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
50	C	304	UQ	C23-C24-C26-C27
50	C	304	UQ	C17-C18-C19-C21
50	J	402	UQ	C12-C13-C14-C16
50	J	402	UQ	C17-C18-C19-C21
55	V	201	CDL	OA9-CA7-OA8-CA6
55	l	701	CDL	C75-C76-C77-C78
50	J	402	UQ	C22-C23-C24-C26
55	a	201	CDL	O1-C1-CA2-OA2
55	l	701	CDL	O1-C1-CA2-OA2
55	l	701	CDL	O1-C1-CB2-OB2
55	r	504	CDL	O1-C1-CA2-OA2
55	s	401	CDL	O1-C1-CB2-OB2
55	V	201	CDL	C31-CA7-OA8-CA6
55	V	201	CDL	C11-CA5-OA6-CA4
55	s	401	CDL	C51-CB5-OB6-CB4
50	C	304	UQ	C14-C16-C17-C18
50	J	402	UQ	C14-C16-C17-C18
55	V	201	CDL	C11-C12-C13-C14
55	r	504	CDL	C71-CB7-OB8-CB6
49	r	502	PLX	C9-C10-C11-C12
55	s	401	CDL	CA5-C11-C12-C13
49	r	502	PLX	C11-C12-C13-C14
48	j	201	PEE	C17-C18-C19-C20
49	C	303	PLX	C27-C28-C29-C30
49	r	502	PLX	C7-C8-C9-C10
55	N	201	CDL	C11-C12-C13-C14
55	r	504	CDL	OB9-CB7-OB8-CB6
55	V	201	CDL	OA7-CA5-OA6-CA4
55	s	401	CDL	OB7-CB5-OB6-CB4
55	l	701	CDL	CA2-C1-CB2-OB2
55	s	401	CDL	CA2-C1-CB2-OB2
48	B	303	PEE	C31-C30-O3-C3
48	W	201	PEE	C31-C30-O3-C3
48	l	702	PEE	C31-C30-O3-C3
55	N	201	CDL	C71-CB7-OB8-CB6
55	V	201	CDL	C71-CB7-OB8-CB6
49	C	303	PLX	C25-C26-C27-C28
49	J	403	PLX	C25-C26-C27-C28
49	J	403	PLX	C27-C28-C29-C30
49	j	203	PLX	C13-C14-C15-C16
55	l	701	CDL	C35-C36-C37-C38
50	J	402	UQ	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
55	k	101	CDL	C73-C74-C75-C76
55	a	201	CDL	O1-C1-CB2-OB2
55	o	201	CDL	O1-C1-CA2-OA2
55	u	201	CDL	O1-C1-CA2-OA2
48	B	303	PEE	C34-C35-C36-C37
55	N	201	CDL	CA5-C11-C12-C13
50	C	304	UQ	C27-C28-C29-C31
48	W	201	PEE	O5-C30-O3-C3
48	l	702	PEE	O5-C30-O3-C3
55	l	701	CDL	C51-CB5-OB6-CB4
55	o	201	CDL	OA6-CA4-CA6-OA8
55	o	201	CDL	C11-C12-C13-C14
52	J	401	NDP	C2D-C1D-N1N-C6N
55	l	701	CDL	C17-C18-C19-C20
48	l	703	PEE	C37-C38-C39-C40
55	s	401	CDL	CA7-C31-C32-C33
55	s	401	CDL	C31-C32-C33-C34
48	B	303	PEE	C11-C12-C13-C14
55	r	504	CDL	C51-C52-C53-C54
50	J	402	UQ	C9-C11-C12-C13
55	N	201	CDL	C51-C52-C53-C54
49	g	201	PLX	C2-C1-N1-C1A
55	l	701	CDL	CB5-C51-C52-C53
55	V	201	CDL	OB9-CB7-OB8-CB6
55	N	201	CDL	CA7-C31-C32-C33
55	V	201	CDL	CA7-C31-C32-C33
55	a	201	CDL	CA5-C11-C12-C13
55	l	701	CDL	CA7-C31-C32-C33
55	l	701	CDL	CB7-C71-C72-C73
55	s	401	CDL	CB7-C71-C72-C73
55	N	201	CDL	OB9-CB7-OB8-CB6
55	l	701	CDL	C39-C40-C41-C42
48	Q	502	PEE	C31-C30-O3-C3
48	B	303	PEE	O5-C30-O3-C3
55	r	504	CDL	CB7-C71-C72-C73
55	l	701	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	C34-C35-C36-C37
55	u	201	CDL	C75-C76-C77-C78
48	W	201	PEE	C11-C10-O2-C2
55	V	201	CDL	C51-CB5-OB6-CB4
55	l	701	CDL	C11-CA5-OA6-CA4
48	W	201	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	OA7-CA5-OA6-CA4
55	l	701	CDL	CB2-C1-CA2-OA2
55	o	201	CDL	CB2-C1-CA2-OA2
55	r	504	CDL	CB2-C1-CA2-OA2
55	u	201	CDL	CA2-C1-CB2-OB2
55	s	401	CDL	C31-CA7-OA8-CA6
55	s	401	CDL	C14-C15-C16-C17
55	V	201	CDL	C62-C63-C64-C65
49	g	201	PLX	C2-C1-N1-C1B
55	u	201	CDL	CB5-C51-C52-C53
49	J	403	PLX	O8-C24-C25-C26
48	B	303	PEE	C11-C10-O2-C2
55	N	201	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	O4-C10-O2-C2
55	N	201	CDL	OB7-CB5-OB6-CB4
55	V	201	CDL	OB7-CB5-OB6-CB4
48	W	201	PEE	C17-C18-C19-C20
48	j	201	PEE	C40-C41-C42-C43
48	Q	502	PEE	O5-C30-O3-C3
55	l	701	CDL	C12-C13-C14-C15
48	l	702	PEE	O3P-C1-C2-O2
48	r	501	PEE	C11-C10-O2-C2
55	a	201	CDL	C34-C35-C36-C37
48	C	302	PEE	C31-C30-O3-C3
49	a	202	PLX	C10-C11-C12-C13
49	j	203	PLX	C27-C28-C29-C30
49	r	502	PLX	C28-C29-C30-C31
55	V	201	CDL	C55-C56-C57-C58
55	s	401	CDL	C75-C76-C77-C78
48	Q	502	PEE	C21-C22-C23-C24
48	Q	502	PEE	C11-C12-C13-C14
49	C	303	PLX	C9-C10-C11-C12
49	j	203	PLX	C11-C12-C13-C14
55	l	701	CDL	C15-C16-C17-C18
55	o	201	CDL	C54-C55-C56-C57
55	r	504	CDL	C31-C32-C33-C34
55	r	504	CDL	C55-C56-C57-C58
55	s	401	CDL	C35-C36-C37-C38
55	u	201	CDL	C74-C75-C76-C77
55	o	201	CDL	C60-C61-C62-C63
55	u	201	CDL	C31-CA7-OA8-CA6
49	J	403	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	O7-C6-C7-C8
49	r	503	PLX	O9-C24-C25-C26
49	J	403	PLX	C13-C14-C15-C16
49	a	202	PLX	C7-C8-C9-C10
49	j	203	PLX	C33-C34-C35-C36
49	r	502	PLX	C27-C28-C29-C30
49	r	502	PLX	C33-C34-C35-C36
55	V	201	CDL	C35-C36-C37-C38
55	a	201	CDL	C62-C63-C64-C65
55	k	101	CDL	C11-C12-C13-C14
55	l	701	CDL	C11-C12-C13-C14
55	s	401	CDL	C16-C17-C18-C19
55	u	201	CDL	C55-C56-C57-C58
48	W	201	PEE	C21-C22-C23-C24
48	W	201	PEE	C13-C14-C15-C16
48	j	202	PEE	C11-C12-C13-C14
49	C	303	PLX	C10-C11-C12-C13
49	J	403	PLX	C14-C15-C16-C17
55	V	201	CDL	C31-C32-C33-C34
55	a	201	CDL	C60-C61-C62-C63
48	l	703	PEE	C34-C35-C36-C37
55	o	201	CDL	C37-C38-C39-C40
49	J	403	PLX	C7-C8-C9-C10
55	i	401	CDL	C59-C60-C61-C62
49	a	202	PLX	C33-C34-C35-C36
55	r	504	CDL	C14-C15-C16-C17
55	k	101	CDL	O1-C1-CB2-OB2
55	a	201	CDL	C22-C23-C24-C25
55	o	201	CDL	C83-C84-C85-C86
48	j	202	PEE	C12-C13-C14-C15
48	r	501	PEE	C21-C22-C23-C24
49	J	403	PLX	C33-C34-C35-C36
55	a	201	CDL	C17-C18-C19-C20
49	r	502	PLX	C11-C10-C9-C8
55	s	401	CDL	OA9-CA7-OA8-CA6
55	a	201	CDL	C35-C36-C37-C38
49	g	201	PLX	C14-C15-C16-C17
55	V	201	CDL	C56-C57-C58-C59
55	i	401	CDL	C82-C83-C84-C85
55	l	701	CDL	C40-C41-C42-C43
49	a	202	PLX	C3-C4-C5-O8
49	g	201	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
49	j	203	PLX	C16-C17-C18-C19
49	j	203	PLX	C25-C26-C27-C28
49	r	503	PLX	C25-C26-C27-C28
55	i	401	CDL	C38-C39-C40-C41
55	k	101	CDL	C71-C72-C73-C74
55	o	201	CDL	C14-C15-C16-C17
55	o	201	CDL	C74-C75-C76-C77
49	g	201	PLX	C11-C10-C9-C8
49	g	201	PLX	C27-C28-C29-C30
49	r	502	PLX	C30-C31-C32-C33
55	V	201	CDL	C21-C22-C23-C24
55	V	201	CDL	C71-C72-C73-C74
55	i	401	CDL	C18-C19-C20-C21
55	l	701	CDL	C55-C56-C57-C58
55	s	401	CDL	C59-C60-C61-C62
55	s	401	CDL	C73-C74-C75-C76
49	j	203	PLX	C10-C11-C12-C13
55	o	201	CDL	C59-C60-C61-C62
48	j	201	PEE	C41-C42-C43-C44
48	j	202	PEE	C13-C14-C15-C16
49	C	303	PLX	C17-C18-C19-C20
49	a	202	PLX	C12-C13-C14-C15
55	r	504	CDL	C43-C44-C45-C46
55	s	401	CDL	C32-C33-C34-C35
55	u	201	CDL	C73-C74-C75-C76
55	i	401	CDL	C77-C78-C79-C80
48	B	303	PEE	C35-C36-C37-C38
48	C	302	PEE	C15-C16-C17-C18
48	j	201	PEE	C35-C36-C37-C38
48	W	201	PEE	C12-C13-C14-C15
48	r	501	PEE	C11-C12-C13-C14
49	C	303	PLX	C15-C16-C17-C18
49	J	403	PLX	C31-C32-C33-C34
55	V	201	CDL	C75-C76-C77-C78
55	a	201	CDL	C75-C76-C77-C78
49	a	202	PLX	C9-C10-C11-C12
55	r	504	CDL	C83-C84-C85-C86
55	r	504	CDL	CB5-C51-C52-C53
55	V	201	CDL	C72-C73-C74-C75
55	o	201	CDL	C32-C33-C34-C35
48	C	302	PEE	O5-C30-O3-C3
55	u	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
48	C	302	PEE	C11-C12-C13-C14
48	r	501	PEE	O4-C10-O2-C2
49	j	203	PLX	C14-C15-C16-C17
48	j	202	PEE	C23-C24-C25-C26
49	r	503	PLX	C10-C11-C12-C13
55	k	101	CDL	C81-C82-C83-C84
55	o	201	CDL	C35-C36-C37-C38
55	r	504	CDL	C41-C42-C43-C44
48	j	201	PEE	C12-C13-C14-C15
48	r	501	PEE	C33-C34-C35-C36
49	g	201	PLX	C33-C34-C35-C36
49	r	503	PLX	C34-C35-C36-C37
51	X	201	8Q1	C12-C13-C14-C15
55	i	401	CDL	C71-C72-C73-C74
49	r	503	PLX	C29-C30-C31-C32
55	V	201	CDL	C59-C60-C61-C62
49	g	201	PLX	C32-C33-C34-C35
55	a	201	CDL	C52-C53-C54-C55
55	r	504	CDL	C21-C22-C23-C24
55	r	504	CDL	C32-C33-C34-C35
55	o	201	CDL	C75-C76-C77-C78
48	r	501	PEE	C20-C21-C22-C23
49	C	303	PLX	C11-C12-C13-C14
55	r	504	CDL	C80-C81-C82-C83
49	r	502	PLX	C14-C15-C16-C17
55	a	201	CDL	C73-C74-C75-C76
55	i	401	CDL	C73-C74-C75-C76
55	a	201	CDL	CB5-C51-C52-C53
55	l	701	CDL	C37-C38-C39-C40
49	r	502	PLX	C25-C26-C27-C28
55	u	201	CDL	C71-C72-C73-C74
49	a	202	PLX	C34-C35-C36-C37
55	s	401	CDL	C51-C52-C53-C54
48	l	703	PEE	C13-C14-C15-C16
49	g	201	PLX	C28-C29-C30-C31
55	a	201	CDL	C11-C12-C13-C14
48	B	303	PEE	C13-C14-C15-C16
49	a	202	PLX	C30-C31-C32-C33
55	a	201	CDL	C31-C32-C33-C34
55	r	504	CDL	C17-C18-C19-C20
49	g	201	PLX	C2-C1-N1-C1C
55	N	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C10-C11-C12-C13
55	o	201	CDL	C55-C56-C57-C58
55	N	201	CDL	OA5-CA3-CA4-OA6
55	k	101	CDL	OA5-CA3-CA4-OA6
50	C	304	UQ	C24-C26-C27-C28
49	r	503	PLX	C13-C14-C15-C16
49	r	503	PLX	C7-C8-C9-C10
55	o	201	CDL	C12-C13-C14-C15
49	j	203	PLX	C11-C10-C9-C8
49	r	503	PLX	C32-C33-C34-C35
55	k	101	CDL	C18-C19-C20-C21
55	r	504	CDL	CA5-C11-C12-C13
55	s	401	CDL	C52-C53-C54-C55
48	C	302	PEE	C35-C36-C37-C38
55	i	401	CDL	OB6-CB4-CB6-OB8
55	k	101	CDL	OA6-CA4-CA6-OA8
55	o	201	CDL	OB6-CB4-CB6-OB8
55	s	401	CDL	OB6-CB4-CB6-OB8
48	l	702	PEE	C21-C22-C23-C24
49	g	201	PLX	C13-C14-C15-C16
49	r	503	PLX	C28-C29-C30-C31
49	a	202	PLX	C13-C14-C15-C16
51	X	201	8Q1	C11-C10-C9-C8
55	r	504	CDL	C52-C53-C54-C55
55	V	201	CDL	C17-C18-C19-C20
55	l	701	CDL	C71-C72-C73-C74
55	k	101	CDL	C75-C76-C77-C78
55	k	101	CDL	CB2-C1-CA2-OA2
55	k	101	CDL	C17-C18-C19-C20
55	k	101	CDL	C76-C77-C78-C79
49	a	202	PLX	C19-C20-C21-C22
55	i	401	CDL	C75-C76-C77-C78
55	i	401	CDL	C14-C15-C16-C17
49	J	403	PLX	C12-C13-C14-C15
49	J	403	PLX	C30-C31-C32-C33
55	o	201	CDL	C57-C58-C59-C60
55	o	201	CDL	C82-C83-C84-C85
48	W	201	PEE	C24-C25-C26-C27
55	r	504	CDL	C71-C72-C73-C74
55	u	201	CDL	C72-C73-C74-C75
49	a	202	PLX	C15-C16-C17-C18
48	Q	502	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C19-C20-C21-C22
48	l	703	PEE	C19-C20-C21-C22
48	C	302	PEE	O3P-C1-C2-C3
55	V	201	CDL	OA5-CA3-CA4-CA6
55	V	201	CDL	OB5-CB3-CB4-CB6
55	i	401	CDL	OB5-CB3-CB4-CB6
55	o	201	CDL	OB5-CB3-CB4-CB6
48	j	201	PEE	C13-C14-C15-C16
55	k	101	CDL	C78-C79-C80-C81
55	s	401	CDL	C12-C13-C14-C15
48	B	303	PEE	C10-C11-C12-C13
49	a	202	PLX	C11-C10-C9-C8
55	a	201	CDL	C32-C33-C34-C35
49	j	203	PLX	C19-C20-C21-C22
55	r	504	CDL	C82-C83-C84-C85
55	a	201	CDL	C31-CA7-OA8-CA6
55	a	201	CDL	C71-CB7-OB8-CB6
55	k	101	CDL	C31-CA7-OA8-CA6
48	j	201	PEE	C36-C37-C38-C39
55	l	701	CDL	C61-C62-C63-C64
48	B	303	PEE	C1-C2-C3-O3
48	Q	502	PEE	C1-C2-C3-O3
48	W	201	PEE	C1-C2-C3-O3
55	k	101	CDL	CB3-CB4-CB6-OB8
55	o	201	CDL	CB3-CB4-CB6-OB8
48	C	302	PEE	C19-C20-C21-C22
48	j	202	PEE	C19-C20-C21-C22
48	l	702	PEE	C15-C16-C17-C18
49	r	503	PLX	C16-C17-C18-C19
55	k	101	CDL	C53-C54-C55-C56
55	V	201	CDL	C43-C44-C45-C46
55	a	201	CDL	C39-C40-C41-C42
49	C	303	PLX	C13-C14-C15-C16
49	r	503	PLX	C11-C10-C9-C8
49	J	403	PLX	C28-C29-C30-C31
55	a	201	CDL	C37-C38-C39-C40
55	i	401	CDL	C55-C56-C57-C58
49	g	201	PLX	C11-C12-C13-C14
55	l	701	CDL	C59-C60-C61-C62
51	X	201	8Q1	C6-C7-C8-C9
55	o	201	CDL	C17-C18-C19-C20
49	g	201	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C13-C14-C15-C16
49	r	502	PLX	C12-C13-C14-C15
48	C	302	PEE	C44-C45-C46-C47
55	V	201	CDL	CA6-CA4-OA6-CA5
48	B	303	PEE	C22-C23-C24-C25
51	X	201	8Q1	C10-C11-C12-C13
48	r	501	PEE	C19-C20-C21-C22
48	B	303	PEE	C31-C32-C33-C34
48	j	201	PEE	C31-C32-C33-C34
55	V	201	CDL	C15-C16-C17-C18
55	a	201	CDL	C71-C72-C73-C74
55	l	701	CDL	C79-C80-C81-C82
48	B	303	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
49	g	201	PLX	O4-C3-C4-O6
48	l	702	PEE	C31-C32-C33-C34
55	s	401	CDL	C78-C79-C80-C81
48	j	201	PEE	C42-C43-C44-C45
49	r	503	PLX	C17-C18-C19-C20
49	r	502	PLX	C18-C19-C20-C21
55	V	201	CDL	C52-C53-C54-C55
55	k	101	CDL	C23-C24-C25-C26
55	l	701	CDL	C80-C81-C82-C83
55	r	504	CDL	C11-C12-C13-C14
49	J	403	PLX	C26-C27-C28-C29
49	a	202	PLX	C27-C28-C29-C30
49	j	203	PLX	C30-C31-C32-C33
55	a	201	CDL	OB9-CB7-OB8-CB6
49	r	503	PLX	C14-C15-C16-C17
48	B	303	PEE	O2-C2-C3-O3
55	k	101	CDL	OB6-CB4-CB6-OB8
55	r	504	CDL	OB6-CB4-CB6-OB8
55	k	101	CDL	O1-C1-CA2-OA2
55	V	201	CDL	C57-C58-C59-C60
55	r	504	CDL	C37-C38-C39-C40
55	r	504	CDL	C39-C40-C41-C42
55	a	201	CDL	C57-C58-C59-C60
55	o	201	CDL	C64-C65-C66-C67
49	g	201	PLX	C34-C35-C36-C37
55	a	201	CDL	OA9-CA7-OA8-CA6
49	g	201	PLX	C12-C13-C14-C15
55	k	101	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C17-C18-C19-C20
49	C	303	PLX	O9-C24-C25-C26
48	r	501	PEE	C14-C15-C16-C17
55	i	401	CDL	C16-C17-C18-C19
48	r	501	PEE	C31-C32-C33-C34
55	V	201	CDL	C73-C74-C75-C76
55	s	401	CDL	C71-C72-C73-C74
48	C	302	PEE	C13-C14-C15-C16
55	a	201	CDL	C82-C83-C84-C85
55	o	201	CDL	C1-CB2-OB2-PB2
55	k	101	CDL	OA9-CA7-OA8-CA6
49	C	303	PLX	C19-C20-C21-C22
55	V	201	CDL	C40-C41-C42-C43
55	a	201	CDL	C80-C81-C82-C83
48	r	501	PEE	C41-C42-C43-C44
49	j	203	PLX	C7-C8-C9-C10
51	X	201	8Q1	C13-C14-C15-C16
48	l	702	PEE	O3P-C1-C2-C3
49	C	303	PLX	O4-C3-C4-C5
49	J	403	PLX	O4-C3-C4-C5
55	N	201	CDL	OA5-CA3-CA4-CA6
49	r	503	PLX	C11-C12-C13-C14
55	a	201	CDL	C20-C21-C22-C23
55	l	701	CDL	C64-C65-C66-C67
55	k	101	CDL	CA7-C31-C32-C33
48	B	303	PEE	C38-C39-C40-C41
55	i	401	CDL	C39-C40-C41-C42
55	k	101	CDL	C71-CB7-OB8-CB6
49	C	303	PLX	C34-C35-C36-C37
49	C	303	PLX	C14-C15-C16-C17
48	l	702	PEE	C1-C2-C3-O3
48	l	703	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
51	G	201	8Q1	O33-C32-C34-N36
55	i	401	CDL	CB3-CB4-CB6-OB8
55	k	101	CDL	CA3-CA4-CA6-OA8
55	o	201	CDL	CA3-CA4-CA6-OA8
55	r	504	CDL	CB3-CB4-CB6-OB8
55	s	401	CDL	CA3-CA4-CA6-OA8
55	s	401	CDL	CB3-CB4-CB6-OB8
55	V	201	CDL	C78-C79-C80-C81
48	C	302	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
55	r	504	CDL	C15-C16-C17-C18
48	j	201	PEE	C11-C12-C13-C14
55	r	504	CDL	C60-C61-C62-C63
55	N	201	CDL	CB7-C71-C72-C73
49	a	202	PLX	C25-C26-C27-C28
49	g	201	PLX	C15-C16-C17-C18
50	J	402	UQ	C17-C18-C19-C20
49	j	203	PLX	O4-C3-C4-O6
55	i	401	CDL	OB5-CB3-CB4-OB6
55	a	201	CDL	C76-C77-C78-C79
49	J	403	PLX	C34-C35-C36-C37
55	i	401	CDL	C13-C14-C15-C16
55	o	201	CDL	O1-C1-CB2-OB2
55	i	401	CDL	CB5-C51-C52-C53
51	X	201	8Q1	C7-C8-C9-C10
55	a	201	CDL	C14-C15-C16-C17
55	a	201	CDL	C44-C45-C46-C47
55	o	201	CDL	C32-C31-CA7-OA8
48	l	703	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	C	303	PLX	O6-C4-C5-O8
55	s	401	CDL	OA6-CA4-CA6-OA8
55	o	201	CDL	C84-C85-C86-C87
55	i	401	CDL	C15-C16-C17-C18
49	C	303	PLX	C16-C17-C18-C19
55	V	201	CDL	C54-C55-C56-C57
55	l	701	CDL	C31-C32-C33-C34
48	r	501	PEE	C36-C37-C38-C39
49	a	202	PLX	O8-C24-C25-C26
49	j	203	PLX	O6-C6-C7-C8
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	O8-C24-C25-C26
48	r	501	PEE	C34-C35-C36-C37
49	a	202	PLX	C11-C12-C13-C14
49	j	203	PLX	C12-C13-C14-C15
55	l	701	CDL	C32-C33-C34-C35
55	r	504	CDL	C59-C60-C61-C62
48	j	202	PEE	C24-C25-C26-C27
48	Q	502	PEE	C10-C11-C12-C13
55	s	401	CDL	C40-C41-C42-C43
47	A	503	NAI	PN-O3-PA-O5B
49	r	503	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C11-C10-C9-C8
55	k	101	CDL	C52-C53-C54-C55
48	C	302	PEE	C41-C42-C43-C44
55	r	504	CDL	C62-C63-C64-C65
48	j	202	PEE	C30-C31-C32-C33
48	Q	502	PEE	C24-C25-C26-C27
48	l	703	PEE	C11-C12-C13-C14
55	o	201	CDL	CA2-C1-CB2-OB2
55	l	701	CDL	C31-CA7-OA8-CA6
48	l	702	PEE	C42-C43-C44-C45
48	B	303	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
55	k	101	CDL	OA5-CA3-CA4-CA6
55	o	201	CDL	OA5-CA3-CA4-CA6
55	u	201	CDL	OA5-CA3-CA4-CA6
48	l	702	PEE	C32-C33-C34-C35
55	i	401	CDL	C44-C45-C46-C47
49	j	203	PLX	C18-C19-C20-C21
55	k	101	CDL	C14-C15-C16-C17
55	V	201	CDL	C14-C15-C16-C17
49	r	503	PLX	C19-C20-C21-C22
49	r	503	PLX	C12-C13-C14-C15
49	r	503	PLX	C33-C34-C35-C36
55	r	504	CDL	C73-C74-C75-C76
58	w	401	ADP	PA-O3A-PB-O1B
55	l	701	CDL	C73-C74-C75-C76
48	l	703	PEE	C30-C31-C32-C33
48	j	202	PEE	C31-C32-C33-C34
55	r	504	CDL	C22-C23-C24-C25
48	j	201	PEE	C19-C20-C21-C22
55	s	401	CDL	C55-C56-C57-C58
55	s	401	CDL	C82-C83-C84-C85
55	k	101	CDL	OB9-CB7-OB8-CB6
55	a	201	CDL	C84-C85-C86-C87
48	C	302	PEE	O3P-C1-C2-O2
55	i	401	CDL	OA5-CA3-CA4-OA6
55	o	201	CDL	OA5-CA3-CA4-OA6
48	C	302	PEE	C42-C43-C44-C45
55	i	401	CDL	C32-C33-C34-C35
48	C	302	PEE	C1-C2-C3-O3
48	j	202	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C3-C4-C5-O8
49	r	503	PLX	C3-C4-C5-O8
55	V	201	CDL	CB3-CB4-CB6-OB8
55	N	201	CDL	C52-C53-C54-C55
48	r	501	PEE	C38-C39-C40-C41
48	r	501	PEE	C5-C4-O4P-P
55	i	401	CDL	CA5-C11-C12-C13
48	Q	502	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
55	u	201	CDL	C57-C58-C59-C60
48	C	302	PEE	O2-C2-C3-O3
48	j	202	PEE	O2-C2-C3-O3
48	l	702	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
48	l	703	PEE	C31-C32-C33-C34
49	C	303	PLX	C31-C32-C33-C34
55	i	401	CDL	C35-C36-C37-C38
55	u	201	CDL	C32-C31-CA7-OA8
55	i	401	CDL	C62-C63-C64-C65
49	r	503	PLX	C30-C31-C32-C33
55	o	201	CDL	C16-C17-C18-C19
55	i	401	CDL	CB7-C71-C72-C73
48	l	702	PEE	C24-C25-C26-C27
55	r	504	CDL	C44-C45-C46-C47
55	o	201	CDL	C40-C41-C42-C43
55	r	504	CDL	C12-C13-C14-C15
48	Q	502	PEE	C35-C36-C37-C38
55	a	201	CDL	C36-C37-C38-C39
55	o	201	CDL	C77-C78-C79-C80
48	j	202	PEE	C31-C30-O3-C3
49	g	201	PLX	O9-C24-C25-C26
49	J	403	PLX	C25-C24-O8-C5
49	j	203	PLX	C25-C24-O8-C5
55	l	701	CDL	OA9-CA7-OA8-CA6
49	C	303	PLX	C36-C37-C38-C39
48	C	302	PEE	C38-C39-C40-C41
49	r	503	PLX	O4-C3-C4-C5
50	J	402	UQ	C7-C8-C9-C10
51	G	201	8Q1	O27-C28-C29-C31
51	X	201	8Q1	O27-C28-C29-C31
56	Q	501	970	C01-C02-C04-C05
48	j	201	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C23-C24-C25-C26
48	j	202	PEE	O5-C30-O3-C3
48	B	303	PEE	C30-C31-C32-C33
49	r	503	PLX	C31-C32-C33-C34
52	J	401	NDP	C2B-O2B-P2B-O1X
56	Q	501	970	C01-C02-C04-O08
49	g	201	PLX	O8-C24-C25-C26
49	r	503	PLX	O4-C3-C4-O6
55	V	201	CDL	OA5-CA3-CA4-OA6
55	u	201	CDL	OA5-CA3-CA4-OA6
48	j	201	PEE	C22-C23-C24-C25
49	j	203	PLX	C29-C30-C31-C32
55	l	701	CDL	C16-C17-C18-C19
48	Q	502	PEE	O2-C2-C3-O3
48	W	201	PEE	O2-C2-C3-O3
49	a	202	PLX	O6-C4-C5-O8
49	j	203	PLX	O6-C4-C5-O8
49	r	502	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
55	V	201	CDL	OA6-CA4-CA6-OA8
49	a	202	PLX	C24-C25-C26-C27
49	r	502	PLX	C34-C35-C36-C37
49	J	403	PLX	C3-C4-C5-O8
55	o	201	CDL	C63-C64-C65-C66
55	V	201	CDL	C79-C80-C81-C82
49	r	502	PLX	C31-C32-C33-C34
55	l	701	CDL	C62-C63-C64-C65
55	a	201	CDL	C53-C54-C55-C56
55	a	201	CDL	C15-C16-C17-C18
55	s	401	CDL	C54-C55-C56-C57
47	A	503	NAI	C3D-C4D-C5D-O5D
48	Q	502	PEE	C4-O4P-P-O3P
48	Q	502	PEE	C4-O4P-P-O2P
48	Q	502	PEE	C4-O4P-P-O1P
48	Q	502	PEE	O4P-C4-C5-N
48	j	201	PEE	C1-O3P-P-O1P
48	j	202	PEE	C1-O3P-P-O1P
48	j	202	PEE	C1-O3P-P-O4P
48	j	202	PEE	C4-O4P-P-O3P
48	j	202	PEE	C4-O4P-P-O1P
49	J	403	PLX	C2-O1-P1-O4
49	J	403	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
49	a	202	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O4
49	g	201	PLX	C2-O1-P1-O3
49	j	203	PLX	C3-O4-P1-O3
49	r	502	PLX	C3-O4-P1-O1
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	503	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
55	N	201	CDL	CA3-OA5-PA1-OA3
55	N	201	CDL	CB3-OB5-PB2-OB4
55	V	201	CDL	CA2-OA2-PA1-OA3
55	V	201	CDL	CB3-OB5-PB2-OB2
55	V	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CA3-OA5-PA1-OA2
55	a	201	CDL	CA3-OA5-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	CB2-OB2-PB2-OB4
55	i	401	CDL	CB3-OB5-PB2-OB4
55	k	101	CDL	CA3-OA5-PA1-OA2
55	k	101	CDL	CA3-OA5-PA1-OA4
55	k	101	CDL	CB3-OB5-PB2-OB2
55	k	101	CDL	CB3-OB5-PB2-OB4
55	l	701	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CB3-OB5-PB2-OB3
55	o	201	CDL	CA2-OA2-PA1-OA3
55	r	504	CDL	CA2-OA2-PA1-OA4
55	r	504	CDL	CB2-OB2-PB2-OB3
55	r	504	CDL	CB2-OB2-PB2-OB4
55	r	504	CDL	CB2-OB2-PB2-OB5
55	s	401	CDL	CA2-OA2-PA1-OA5
55	s	401	CDL	CA3-OA5-PA1-OA3
55	u	201	CDL	CA3-OA5-PA1-OA3
48	Q	502	PEE	C2-C1-O3P-P
55	i	401	CDL	C1-CB2-OB2-PB2
55	r	504	CDL	C1-CB2-OB2-PB2
48	l	702	PEE	C30-C31-C32-C33
55	u	201	CDL	C56-C57-C58-C59
55	r	504	CDL	C61-C62-C63-C64
55	N	201	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
55	V	201	CDL	C58-C59-C60-C61
48	r	501	PEE	C30-C31-C32-C33
49	J	403	PLX	O4-C3-C4-O6
55	s	401	CDL	OA5-CA3-CA4-OA6
55	k	101	CDL	C82-C83-C84-C85
55	l	701	CDL	C56-C57-C58-C59
55	r	504	CDL	C54-C55-C56-C57
55	V	201	CDL	C64-C65-C66-C67
55	N	201	CDL	CB5-C51-C52-C53
52	J	401	NDP	O4D-C1D-N1N-C6N
55	l	701	CDL	C78-C79-C80-C81
55	o	201	CDL	OB9-CB7-OB8-CB6
55	u	201	CDL	C1-CB2-OB2-PB2
49	J	403	PLX	C16-C17-C18-C19
55	V	201	CDL	CB7-C71-C72-C73
47	A	503	NAI	C2D-C1D-N1N-C2N
49	r	503	PLX	C24-C25-C26-C27
55	r	504	CDL	C13-C14-C15-C16
49	r	502	PLX	C16-C17-C18-C19
49	r	503	PLX	C27-C28-C29-C30
55	s	401	CDL	C38-C39-C40-C41
55	u	201	CDL	C53-C54-C55-C56
48	j	202	PEE	C18-C19-C20-C21
55	u	201	CDL	C32-C31-CA7-OA9
48	l	703	PEE	C32-C33-C34-C35
55	a	201	CDL	C51-C52-C53-C54
55	k	101	CDL	C12-C13-C14-C15
55	V	201	CDL	C32-C31-CA7-OA8
49	j	203	PLX	O8-C24-C25-C26
49	j	203	PLX	C20-C21-C22-C23
55	o	201	CDL	C71-CB7-OB8-CB6
49	j	203	PLX	C34-C35-C36-C37
55	i	401	CDL	C64-C65-C66-C67
48	C	302	PEE	C17-C18-C19-C20
51	X	201	8Q1	C11-C12-C13-C14
48	C	302	PEE	C30-C31-C32-C33
55	o	201	CDL	C36-C37-C38-C39
49	r	502	PLX	C19-C20-C21-C22
55	a	201	CDL	C59-C60-C61-C62
55	i	401	CDL	C52-C51-CB5-OB6
55	i	401	CDL	C37-C38-C39-C40
48	W	201	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	C38-C39-C40-C41
48	l	702	PEE	C19-C20-C21-C22
55	l	701	CDL	C82-C83-C84-C85
47	A	503	NAI	O4D-C1D-N1N-C2N
49	r	502	PLX	C4-C3-O4-P1
55	u	201	CDL	C54-C55-C56-C57
49	g	201	PLX	C16-C17-C18-C19
55	o	201	CDL	C34-C35-C36-C37
55	a	201	CDL	C56-C57-C58-C59
49	g	201	PLX	C3-C4-C5-O8
49	r	502	PLX	C3-C4-C5-O8
48	j	201	PEE	C23-C24-C25-C26
55	V	201	CDL	C32-C33-C34-C35
49	J	403	PLX	C10-C11-C12-C13
55	s	401	CDL	CB5-C51-C52-C53
48	Q	502	PEE	C18-C19-C20-C21
48	B	303	PEE	C20-C21-C22-C23
55	r	504	CDL	C72-C73-C74-C75
48	l	703	PEE	C18-C19-C20-C21
48	l	703	PEE	C2-C1-O3P-P
48	Q	502	PEE	O3P-C1-C2-C3
55	k	101	CDL	C16-C17-C18-C19
48	W	201	PEE	C16-C17-C18-C19
55	s	401	CDL	C39-C40-C41-C42
49	C	303	PLX	C7-C8-C9-C10
49	j	203	PLX	C9-C10-C11-C12
55	s	401	CDL	C77-C78-C79-C80
55	k	101	CDL	C32-C33-C34-C35
48	r	501	PEE	C13-C14-C15-C16
48	r	501	PEE	C40-C41-C42-C43
48	l	702	PEE	C13-C14-C15-C16
55	r	504	CDL	CB4-CB3-OB5-PB2
55	o	201	CDL	C72-C73-C74-C75
49	r	502	PLX	C36-C37-C38-C39
55	r	504	CDL	C56-C57-C58-C59
52	J	401	NDP	O4D-C4D-C5D-O5D
49	C	303	PLX	O7-C6-C7-C8
48	B	303	PEE	C23-C24-C25-C26
48	l	703	PEE	C21-C22-C23-C24
55	r	504	CDL	C42-C43-C44-C45
48	B	303	PEE	C18-C19-C20-C21
55	V	201	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C64-C65-C66-C67
55	i	401	CDL	C12-C13-C14-C15
46	A	502	FMN	C1'-C2'-C3'-O3'
49	j	203	PLX	O4-C3-C4-C5
55	i	401	CDL	OA5-CA3-CA4-CA6
48	Q	502	PEE	C36-C37-C38-C39
48	l	702	PEE	C2-C1-O3P-P
55	o	201	CDL	C53-C54-C55-C56
55	r	504	CDL	C64-C65-C66-C67
49	a	202	PLX	C16-C17-C18-C19
49	a	202	PLX	C4-C5-O8-C24
48	l	703	PEE	C38-C39-C40-C41
55	s	401	CDL	C15-C16-C17-C18
48	Q	502	PEE	C30-C31-C32-C33
55	N	201	CDL	CB3-CB4-OB6-CB5
55	k	101	CDL	CA6-CA4-OA6-CA5
58	w	401	ADP	PA-O3A-PB-O2B
58	w	401	ADP	PA-O3A-PB-O3B
48	j	201	PEE	C44-C45-C46-C47
48	W	201	PEE	C18-C19-C20-C21
48	l	702	PEE	C18-C19-C20-C21
48	B	303	PEE	C15-C16-C17-C18
55	N	201	CDL	O1-C1-CB2-OB2
48	C	302	PEE	C18-C19-C20-C21
48	C	302	PEE	C16-C17-C18-C19
48	l	703	PEE	C16-C17-C18-C19
55	l	701	CDL	C41-C42-C43-C44
47	A	503	NAI	C2D-C1D-N1N-C6N
51	G	201	8Q1	C11-C10-C9-C8
55	s	401	CDL	C60-C61-C62-C63
55	k	101	CDL	CA2-C1-CB2-OB2
55	V	201	CDL	C51-C52-C53-C54
55	s	401	CDL	C74-C75-C76-C77
49	j	203	PLX	C3-C4-C5-O8
55	V	201	CDL	CA3-CA4-CA6-OA8
55	o	201	CDL	C32-C31-CA7-OA9
48	l	702	PEE	C38-C39-C40-C41
48	r	501	PEE	C16-C17-C18-C19
49	j	203	PLX	C15-C16-C17-C18
55	l	701	CDL	C32-C31-CA7-OA8
55	l	701	CDL	C36-C37-C38-C39
48	l	702	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	C32-C31-CA7-OA8
55	k	101	CDL	C12-C11-CA5-OA6
55	s	401	CDL	OA5-CA3-CA4-CA6
49	r	503	PLX	C2-C1-N1-C1B
55	N	201	CDL	C31-C32-C33-C34
48	B	303	PEE	C16-C17-C18-C19
48	j	202	PEE	C16-C17-C18-C19
46	A	502	FMN	O2'-C2'-C3'-C4'
49	C	303	PLX	C12-C13-C14-C15
55	N	201	CDL	C72-C71-CB7-OB8
55	s	401	CDL	C12-C11-CA5-OA6
55	k	101	CDL	C21-C22-C23-C24
49	r	503	PLX	C2-C1-N1-C1C
55	r	504	CDL	C76-C77-C78-C79
55	a	201	CDL	C43-C44-C45-C46
55	r	504	CDL	C72-C71-CB7-OB8
55	o	201	CDL	C62-C63-C64-C65
48	r	501	PEE	O2-C10-C11-C12
48	j	201	PEE	C39-C40-C41-C42
55	a	201	CDL	CB7-C71-C72-C73
48	C	302	PEE	C20-C21-C22-C23
48	j	201	PEE	O3-C30-C31-C32
49	a	202	PLX	C25-C24-O8-C5
49	r	503	PLX	C2-C1-N1-C1A
49	C	303	PLX	C18-C19-C20-C21
55	u	201	CDL	C52-C51-CB5-OB6
55	r	504	CDL	C53-C54-C55-C56
55	l	701	CDL	C72-C71-CB7-OB8
55	a	201	CDL	C42-C43-C44-C45
51	G	201	8Q1	O27-C28-C29-C30
51	X	201	8Q1	O27-C28-C29-C30
49	j	203	PLX	C17-C18-C19-C20
55	o	201	CDL	C51-C52-C53-C54
55	k	101	CDL	CA3-CA4-OA6-CA5
49	g	201	PLX	C10-C11-C12-C13
55	r	504	CDL	C75-C76-C77-C78
48	l	703	PEE	O2-C10-C11-C12
55	i	401	CDL	C40-C41-C42-C43
55	a	201	CDL	C32-C31-CA7-OA9
48	j	201	PEE	C16-C17-C18-C19
51	G	201	8Q1	C42-C43-S44-C1
55	r	504	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C18-C19-C20-C21
55	V	201	CDL	C44-C45-C46-C47
55	k	101	CDL	C32-C31-CA7-OA8
55	u	201	CDL	C12-C11-CA5-OA6
48	C	302	PEE	C31-C32-C33-C34
48	Q	502	PEE	C16-C17-C18-C19
55	u	201	CDL	C52-C51-CB5-OB7
55	N	201	CDL	C72-C71-CB7-OB9
55	l	701	CDL	C32-C31-CA7-OA9
50	C	304	UQ	C27-C28-C29-C30
55	i	401	CDL	C56-C57-C58-C59
55	o	201	CDL	C81-C82-C83-C84
49	C	303	PLX	O9-C24-O8-C5
49	J	403	PLX	O9-C24-O8-C5
49	g	201	PLX	O9-C24-O8-C5
49	r	503	PLX	C36-C37-C38-C39
48	j	201	PEE	O5-C30-C31-C32
48	C	302	PEE	C32-C33-C34-C35
48	j	202	PEE	C22-C23-C24-C25
55	a	201	CDL	OA7-CA5-OA6-CA4
49	g	201	PLX	O6-C4-C5-O8
55	k	101	CDL	C12-C11-CA5-OA7
55	o	201	CDL	C52-C51-CB5-OB6
55	a	201	CDL	C58-C59-C60-C61
55	V	201	CDL	C33-C34-C35-C36
48	B	303	PEE	C36-C37-C38-C39
55	l	701	CDL	C72-C71-CB7-OB9
55	r	504	CDL	C72-C71-CB7-OB9
55	s	401	CDL	C12-C11-CA5-OA7
48	l	703	PEE	O4-C10-C11-C12
48	r	501	PEE	O4-C10-C11-C12
49	g	201	PLX	C6-C7-C8-C9
48	Q	502	PEE	C38-C39-C40-C41
55	i	401	CDL	C32-C31-CA7-OA8
47	A	503	NAI	O4D-C1D-N1N-C6N
48	C	302	PEE	O3-C30-C31-C32
55	N	201	CDL	C12-C11-CA5-OA6
55	a	201	CDL	C12-C11-CA5-OA6

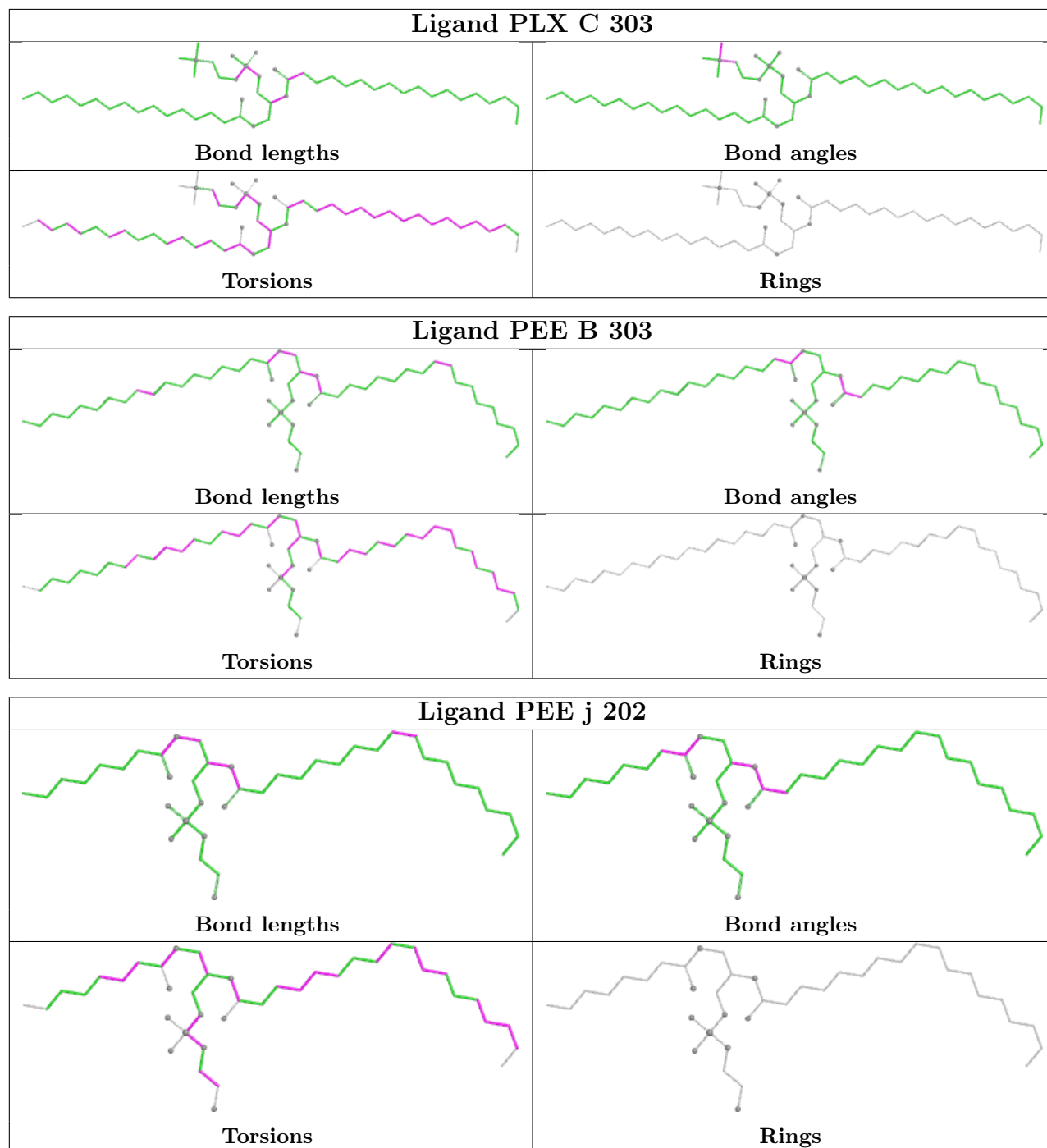
There are no ring outliers.

34 monomers are involved in 130 short contacts:

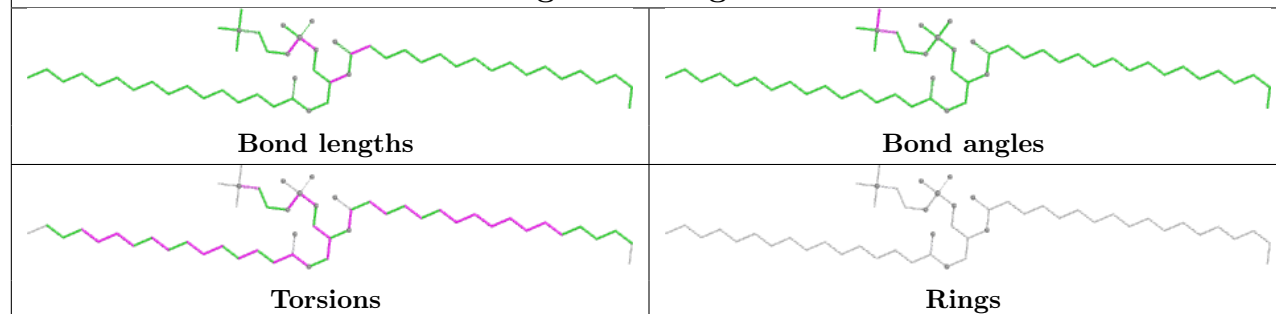
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	C	303	PLX	4	0
48	B	303	PEE	4	0
48	j	202	PEE	4	0
49	g	201	PLX	4	0
45	C	301	SF4	1	0
55	r	504	CDL	8	0
55	k	101	CDL	6	0
48	r	501	PEE	8	0
55	u	201	CDL	1	0
50	C	304	UQ	5	0
55	i	401	CDL	3	0
55	l	701	CDL	4	0
55	N	201	CDL	3	0
49	r	503	PLX	2	0
47	A	503	NAI	5	0
48	l	703	PEE	3	0
48	C	302	PEE	2	0
49	J	403	PLX	5	0
49	j	203	PLX	2	0
55	s	401	CDL	7	0
48	l	702	PEE	4	0
49	a	202	PLX	1	0
45	A	501	SF4	2	0
48	j	201	PEE	5	0
49	r	502	PLX	4	0
55	a	201	CDL	7	0
58	w	401	ADP	3	0
55	V	201	CDL	6	0
55	o	201	CDL	5	0
46	A	502	FMN	7	0
48	Q	502	PEE	3	0
50	J	402	UQ	2	0
48	W	201	PEE	2	0
52	J	401	NDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

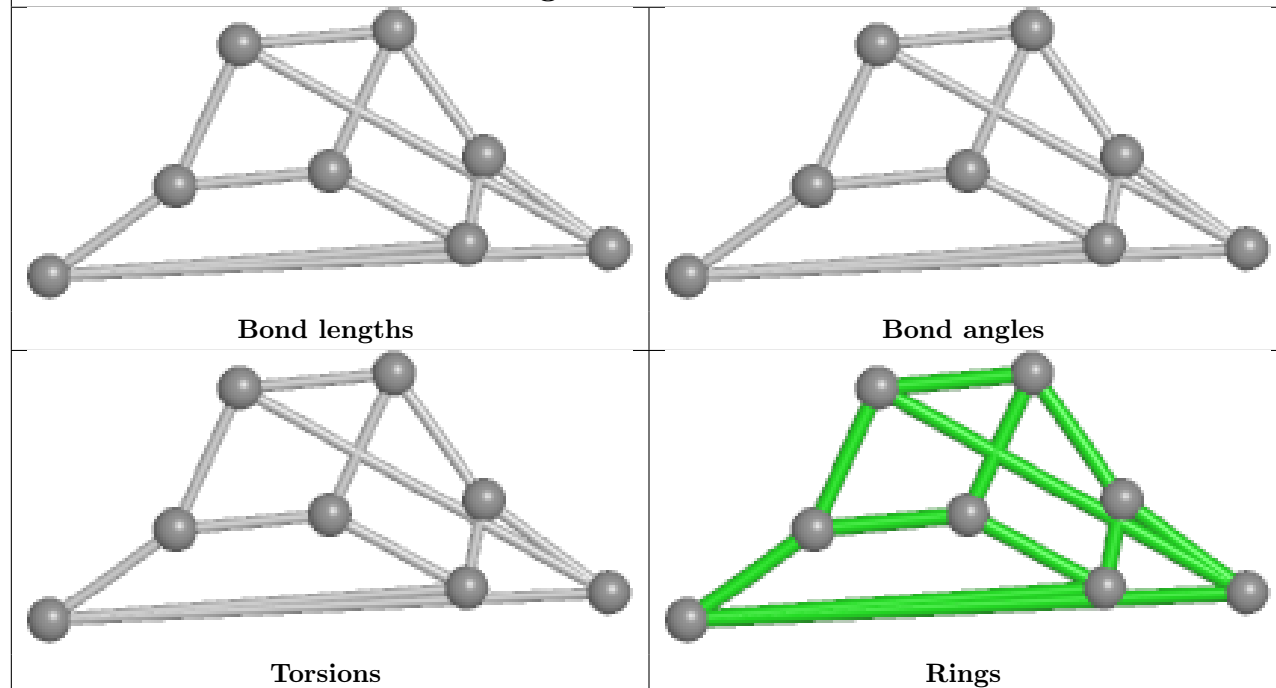
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



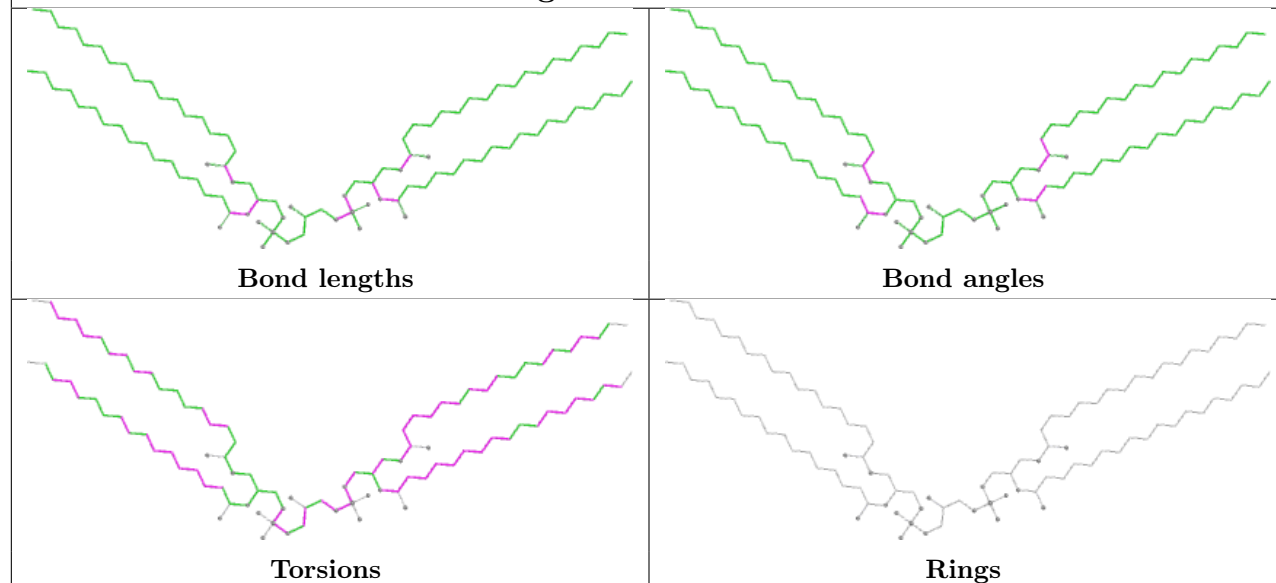
Ligand PLX g 201

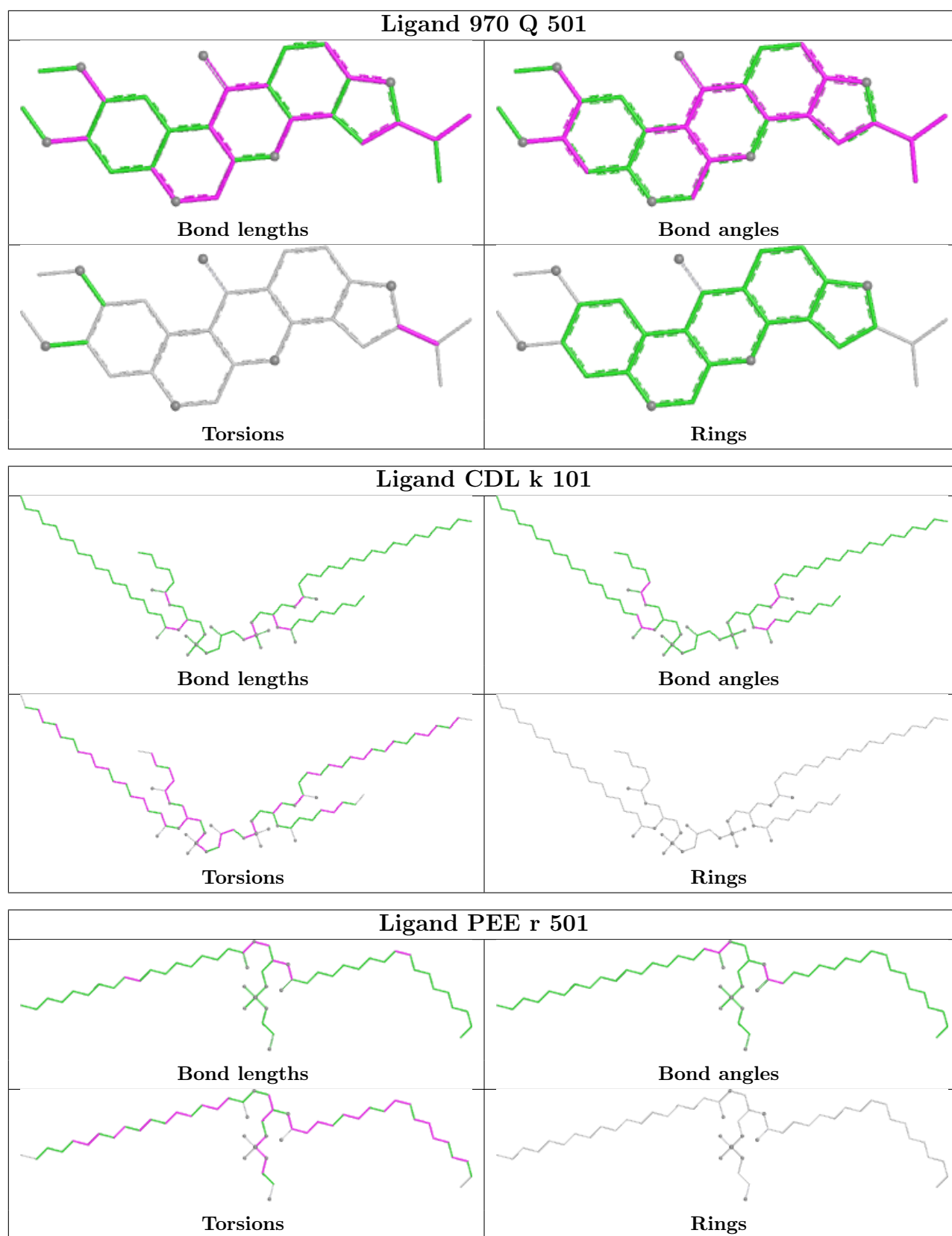


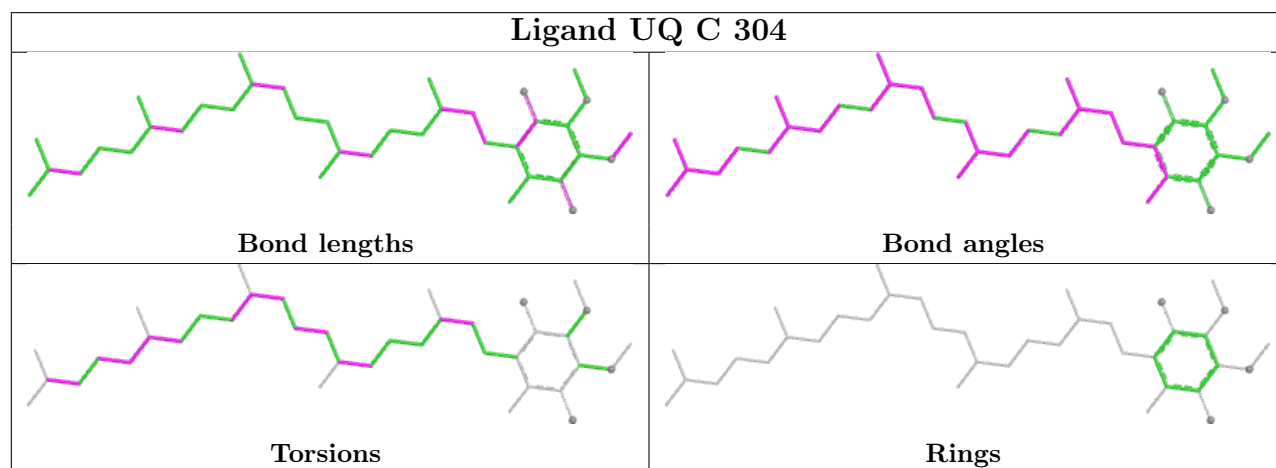
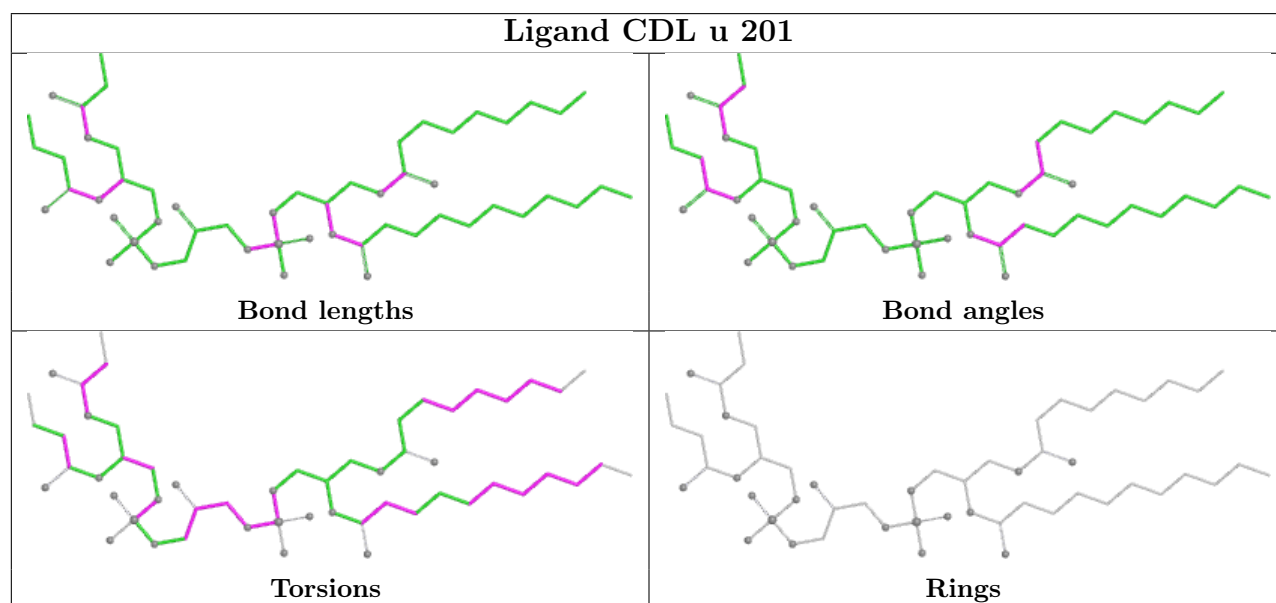
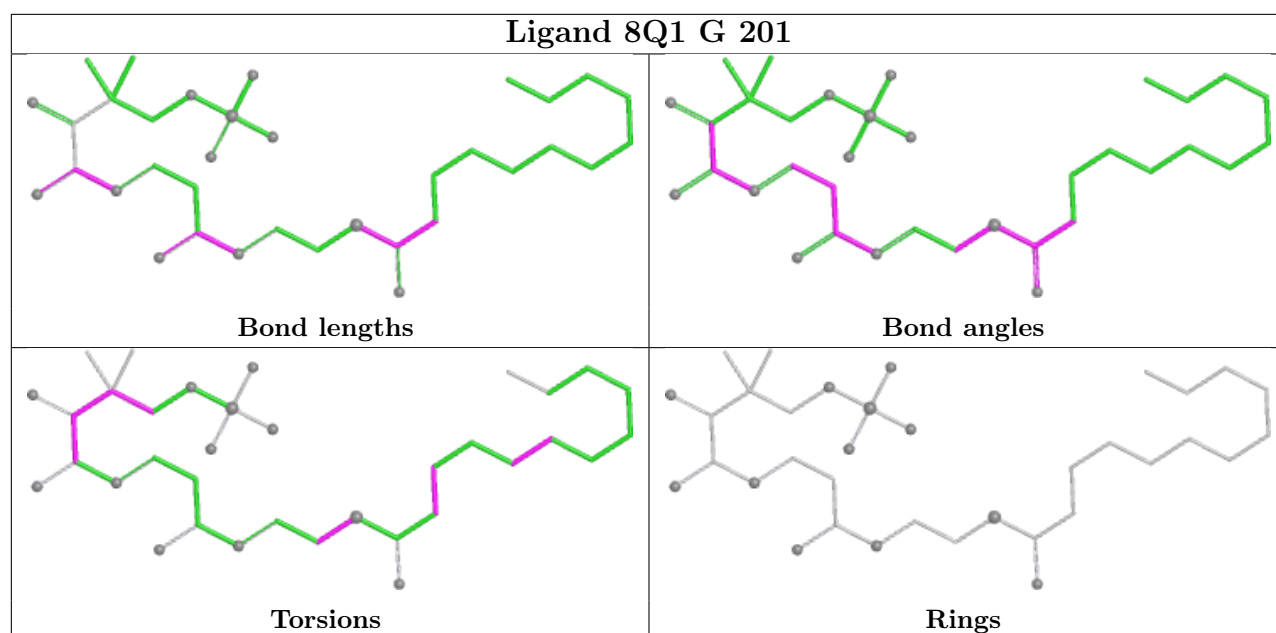
Ligand SF4 C 301

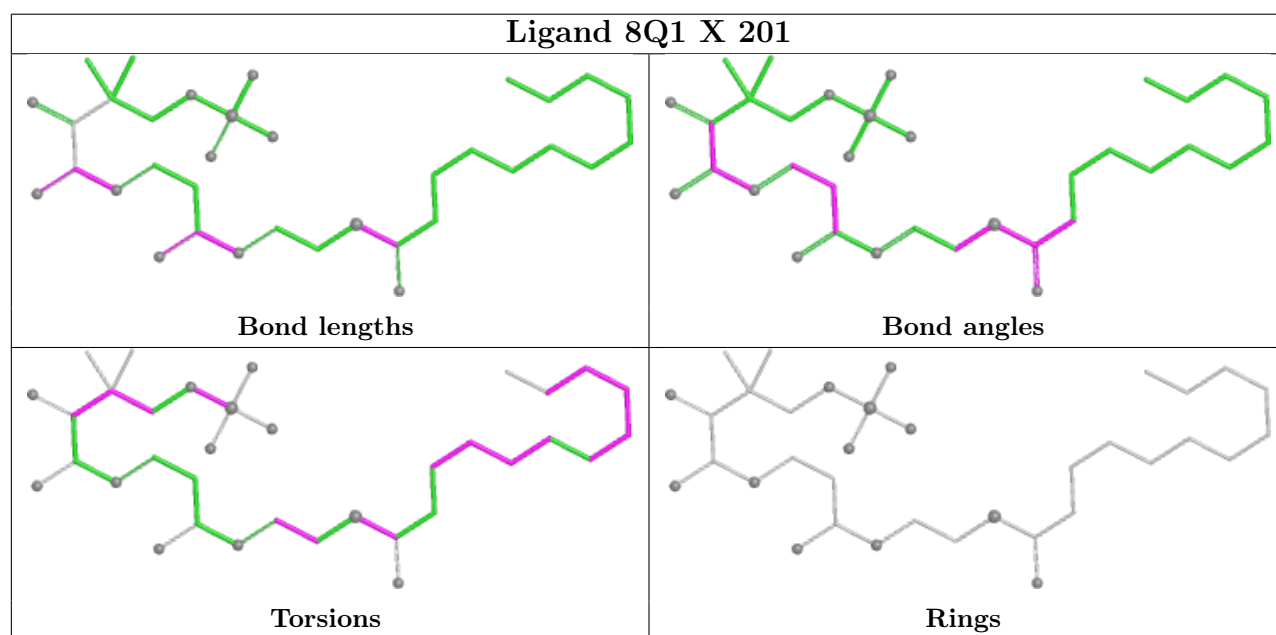
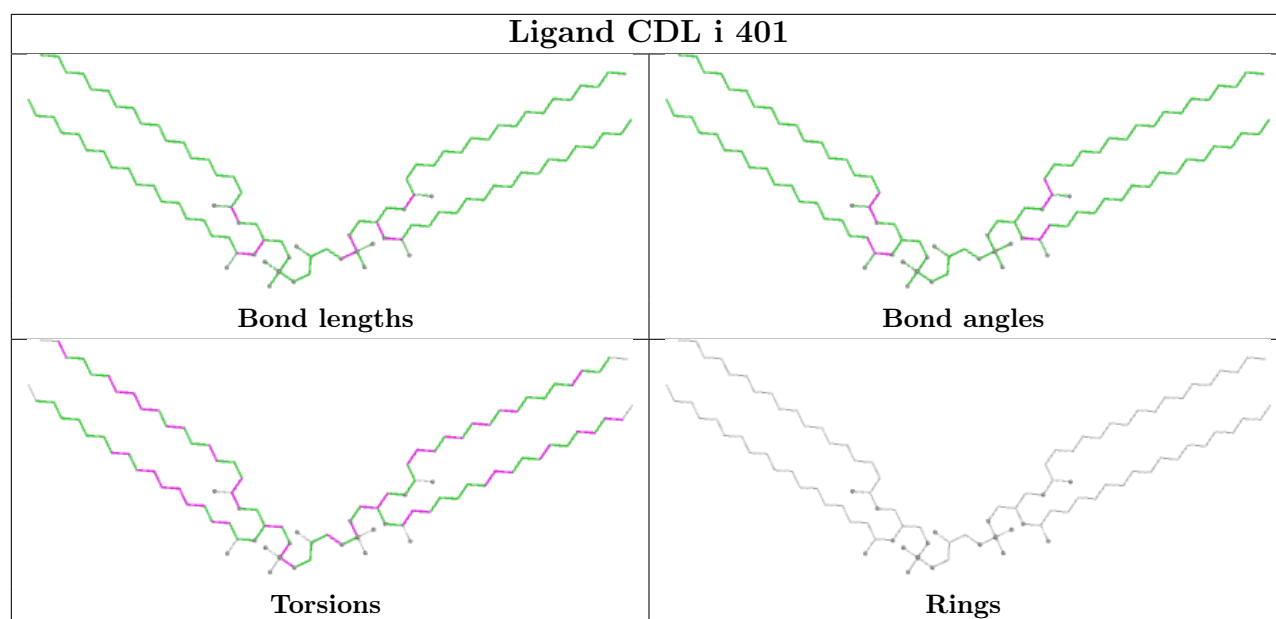


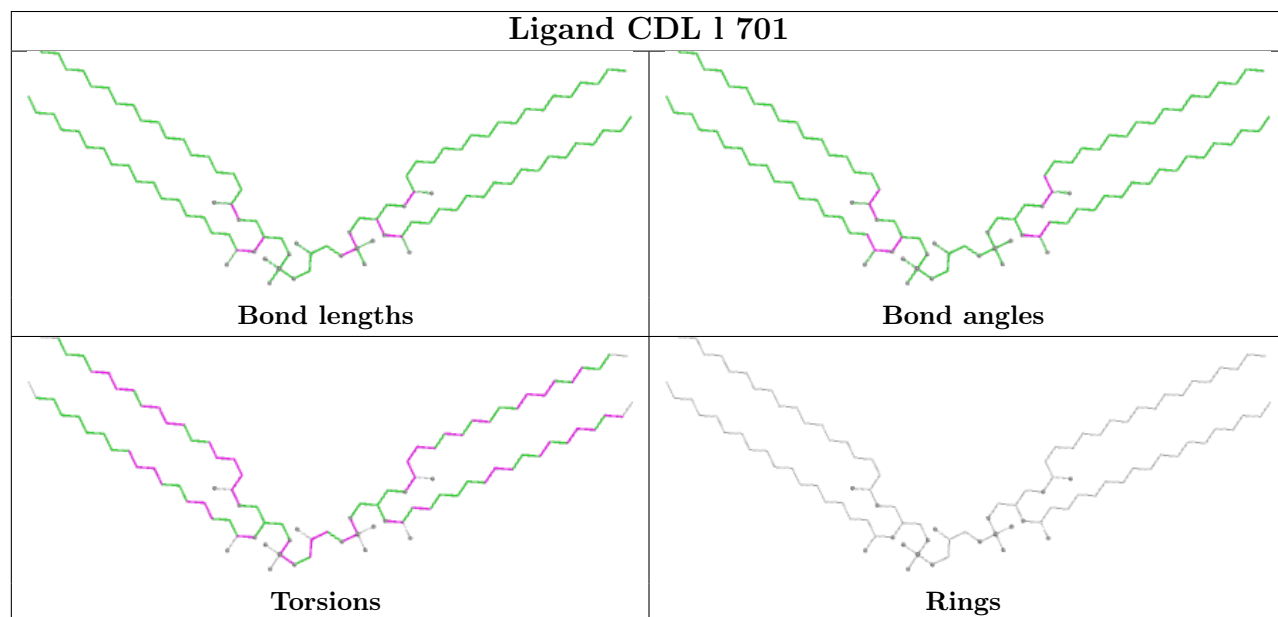
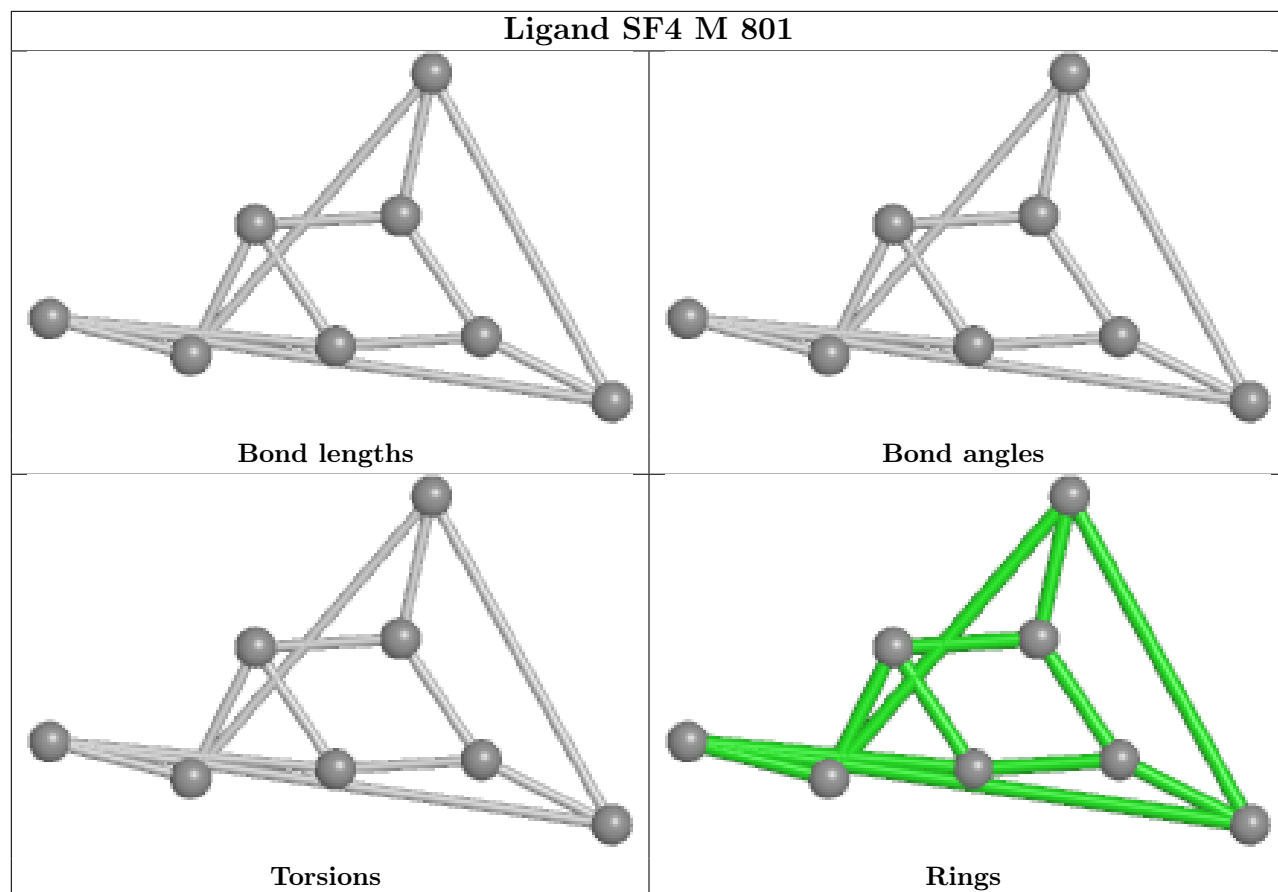
Ligand CDL r 504

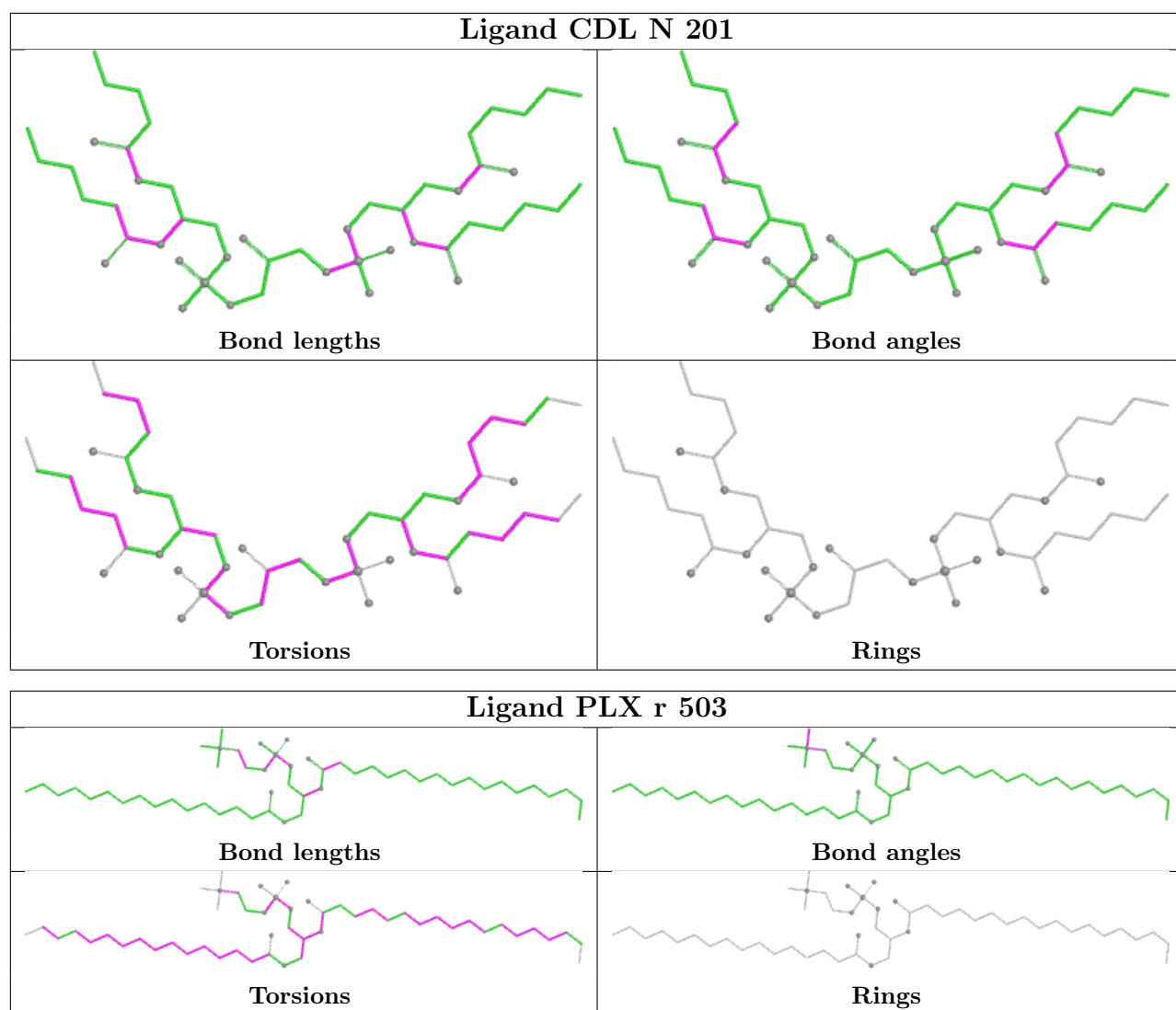




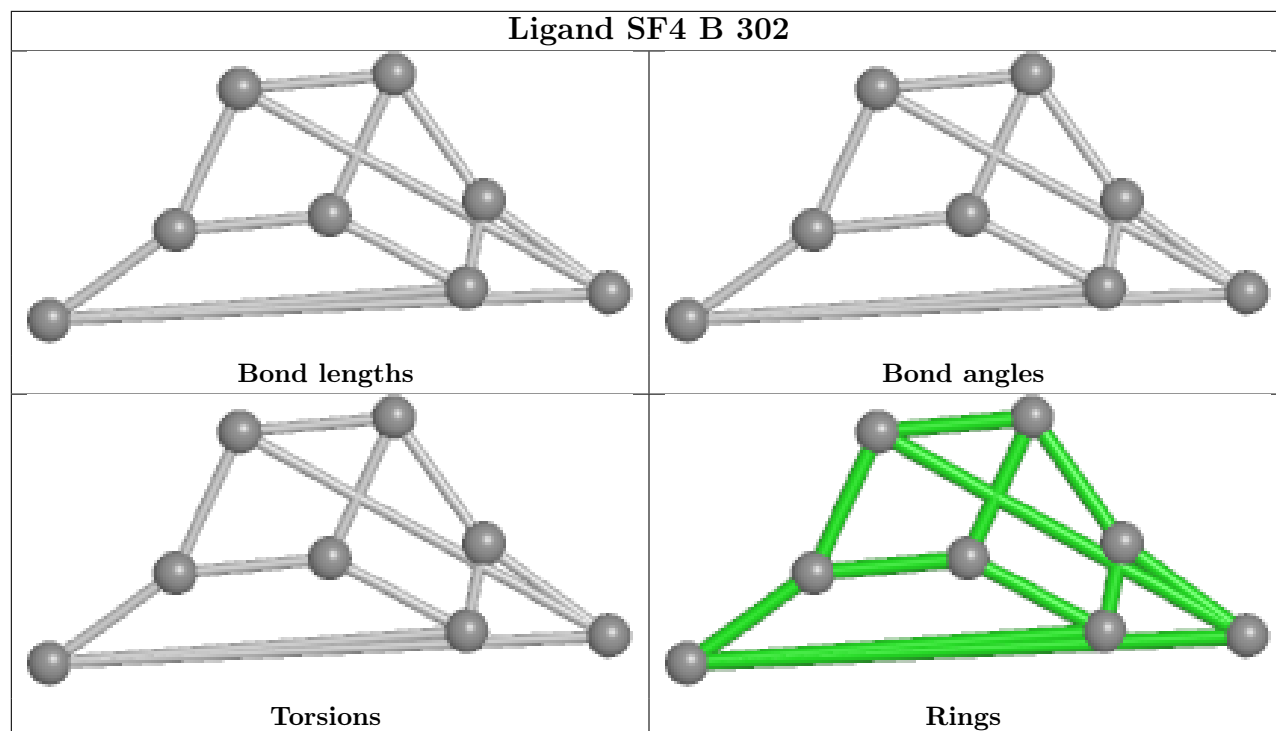




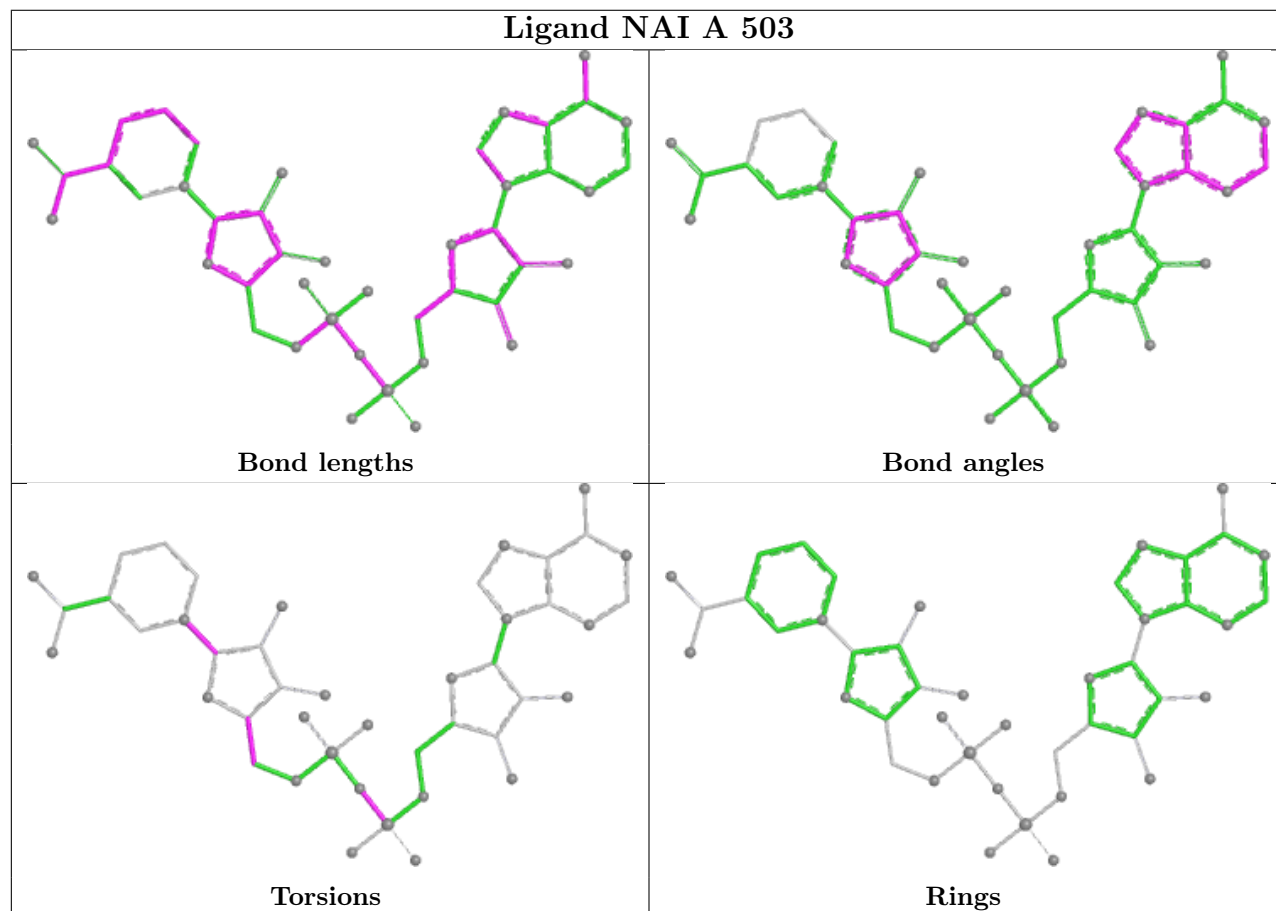


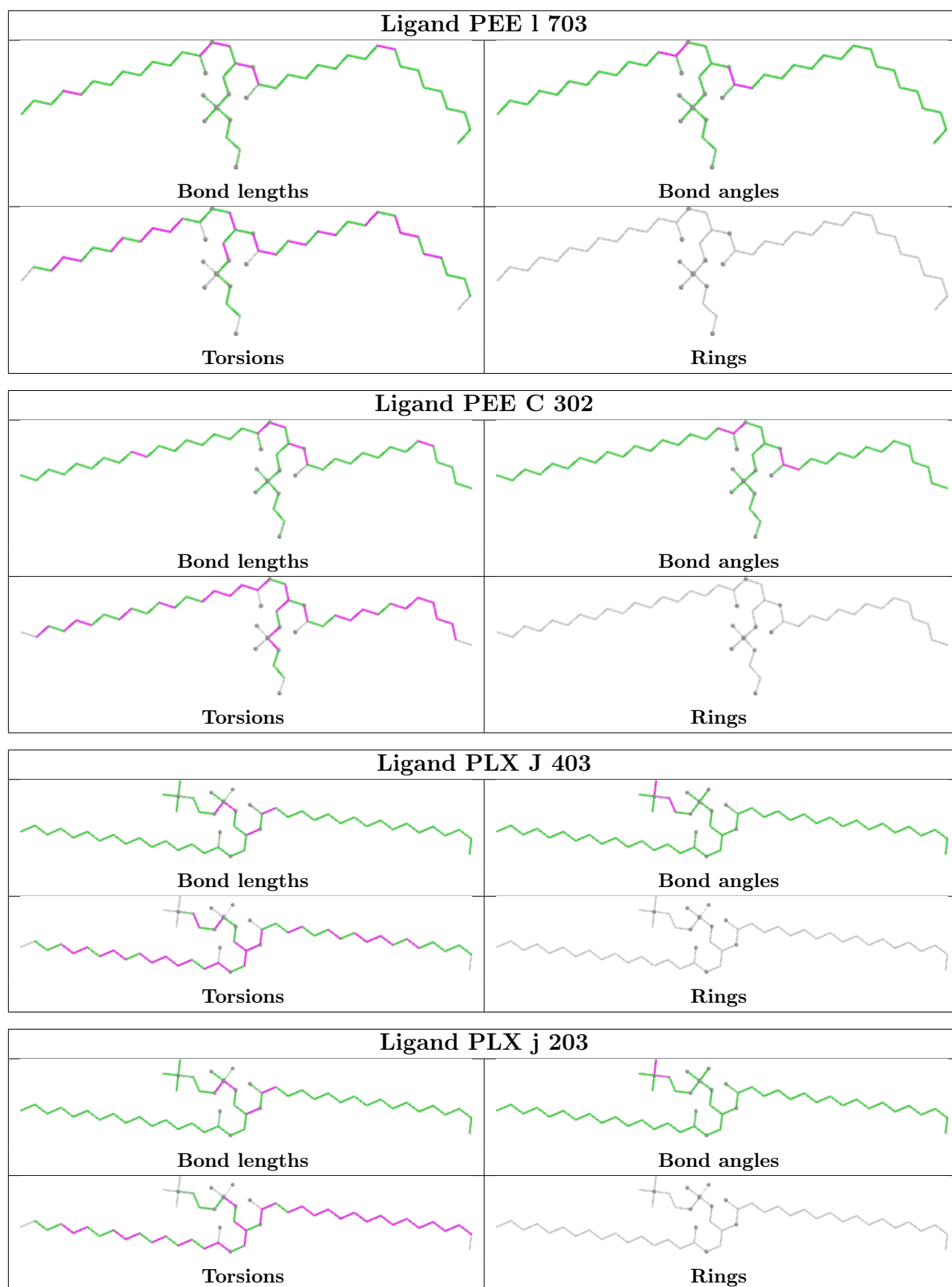


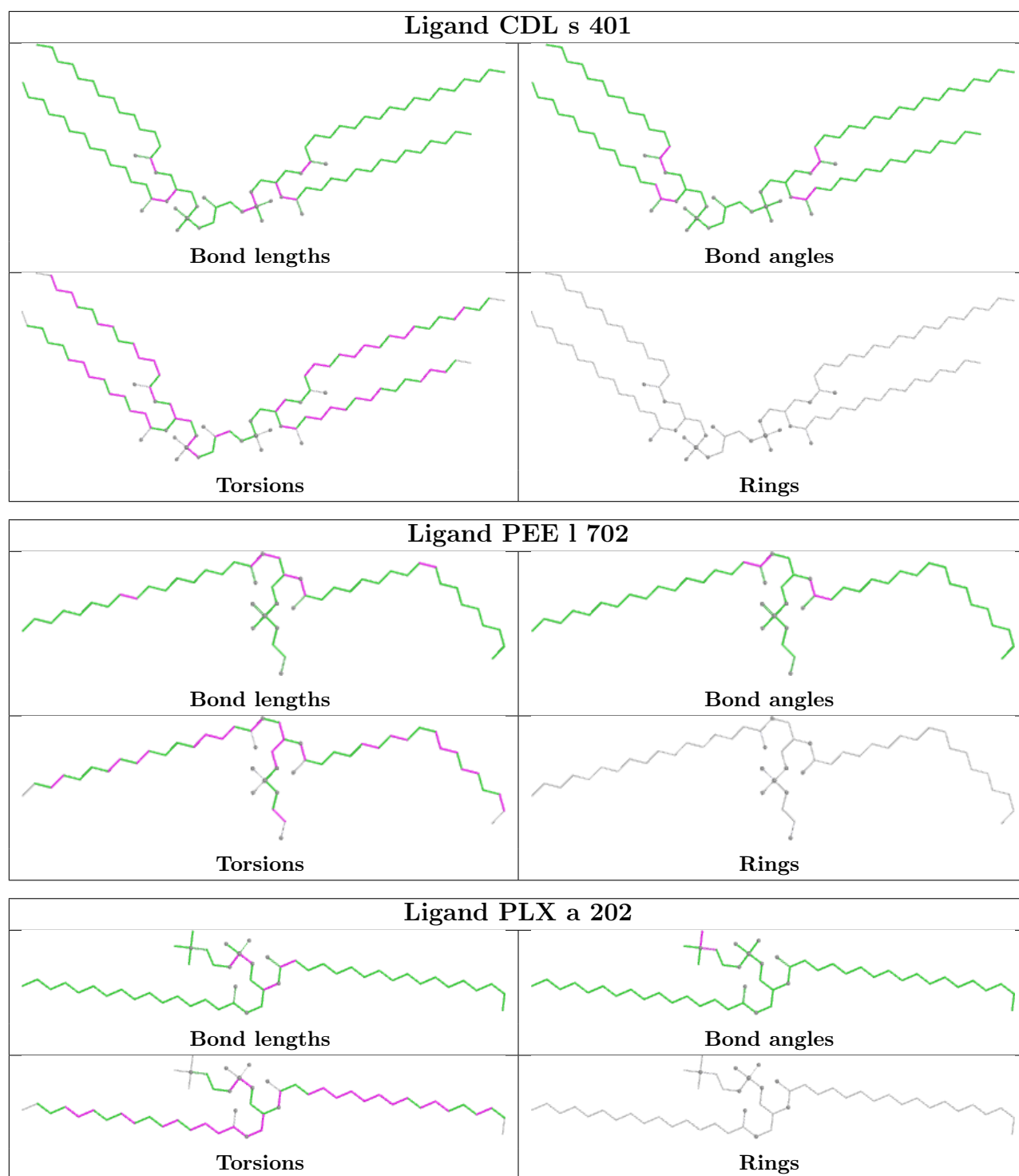
Ligand SF4 B 302

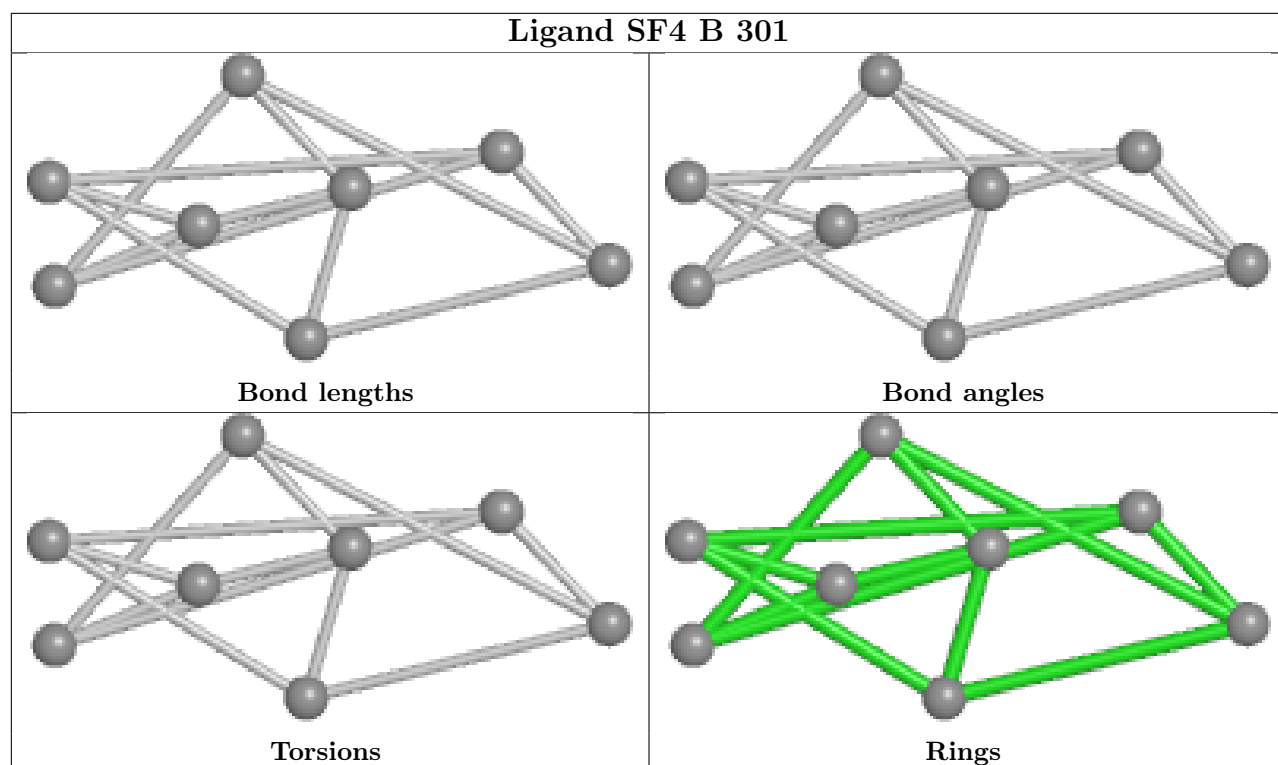
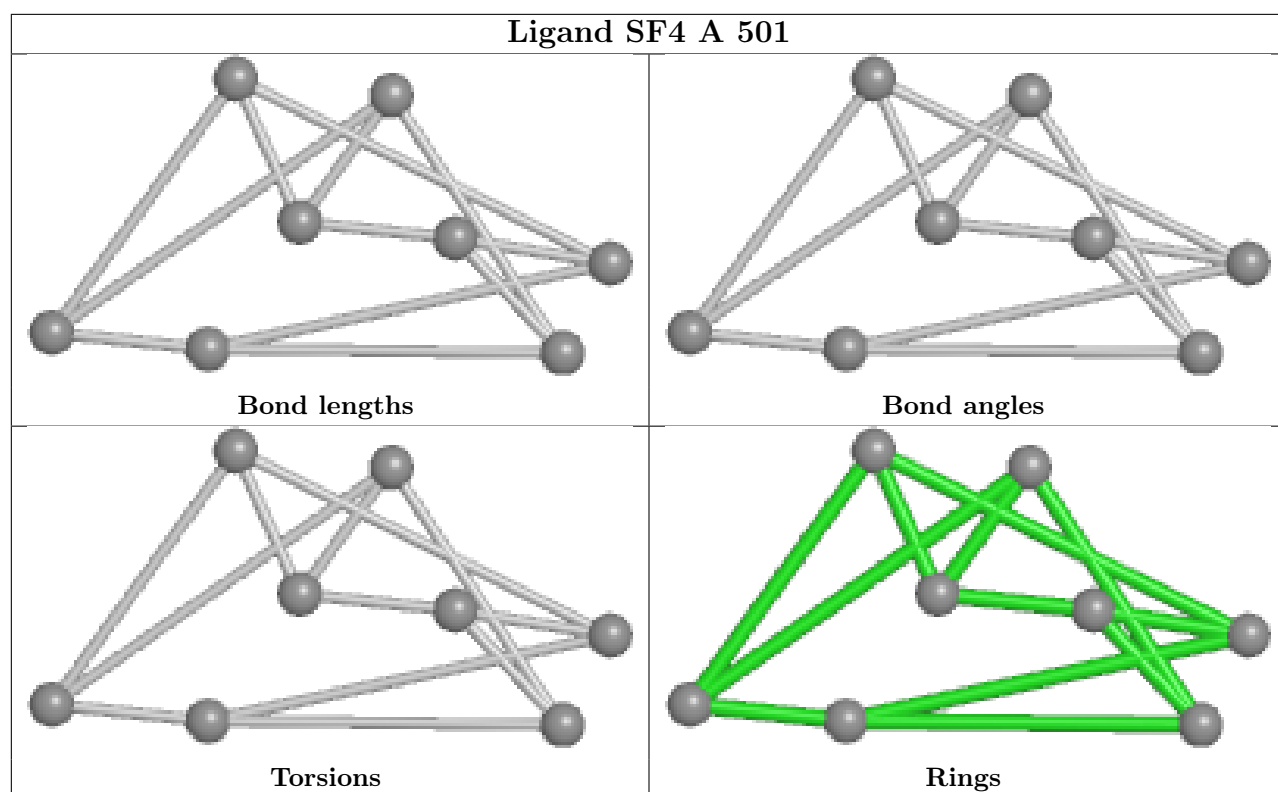


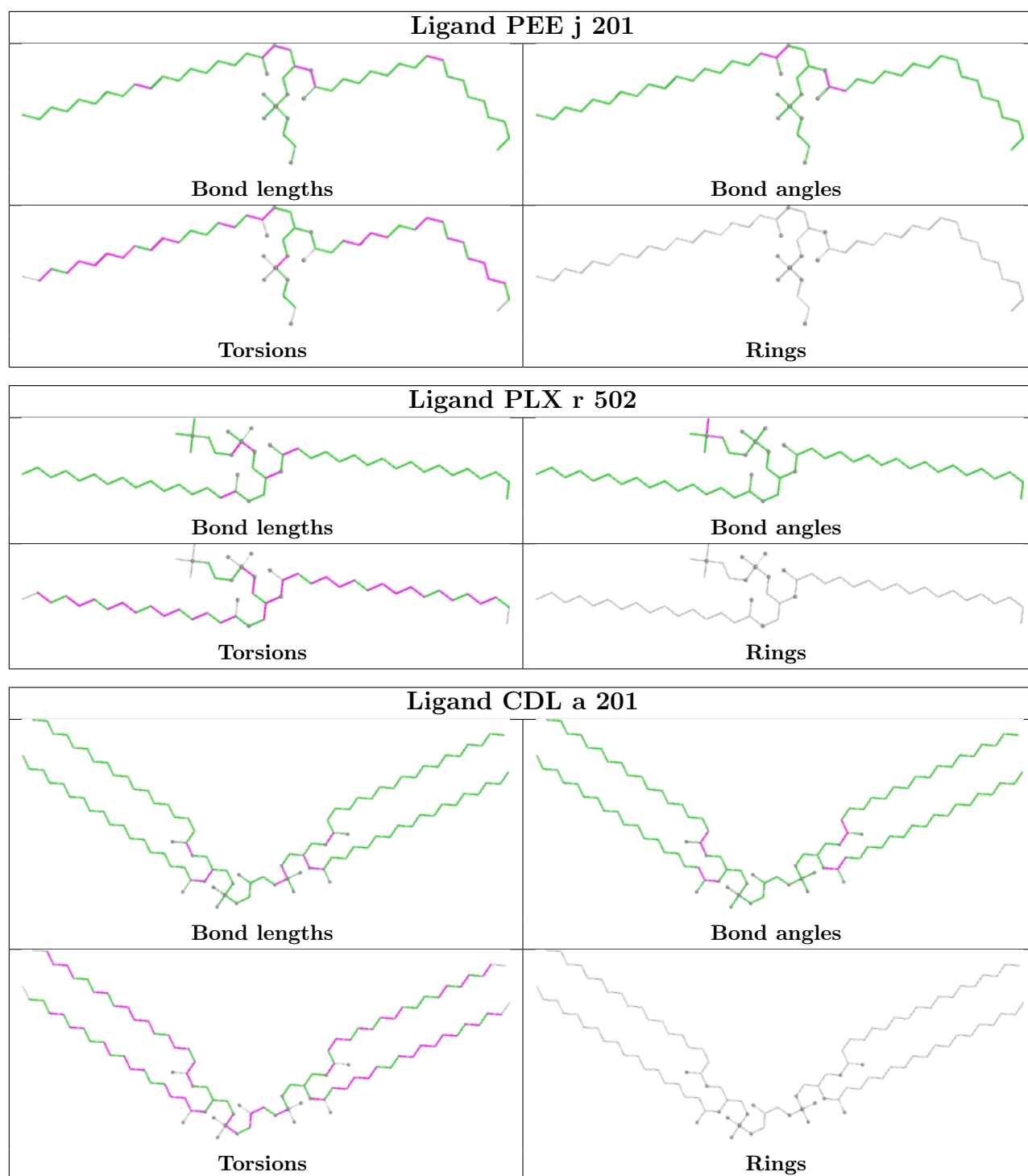
Ligand NAI A 503

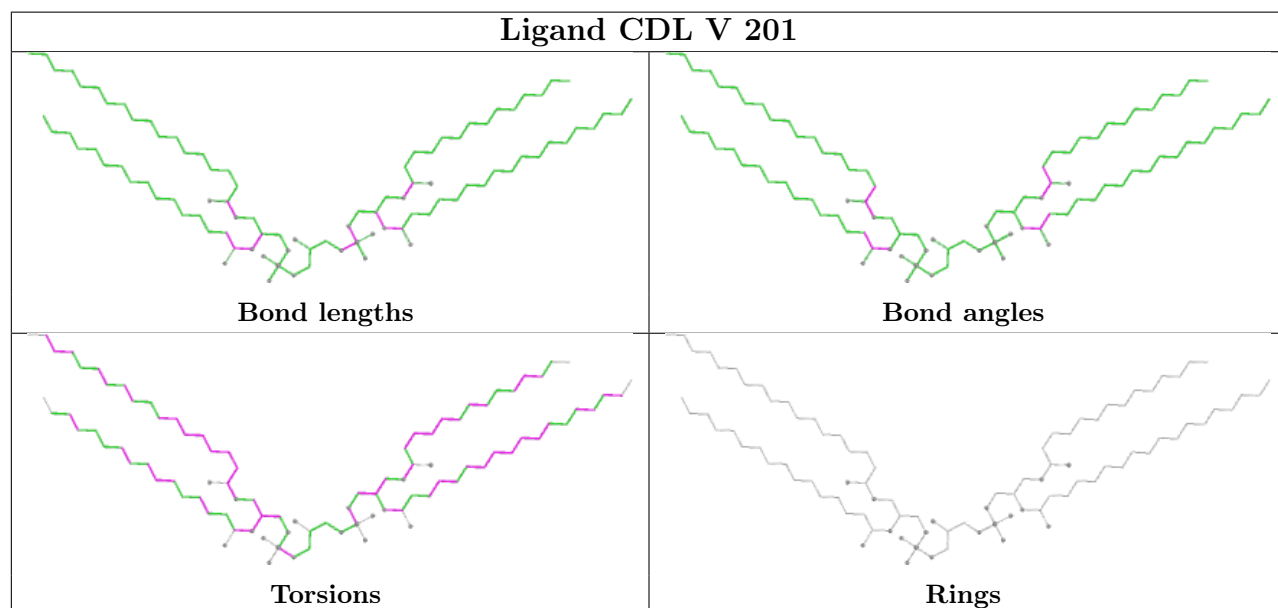
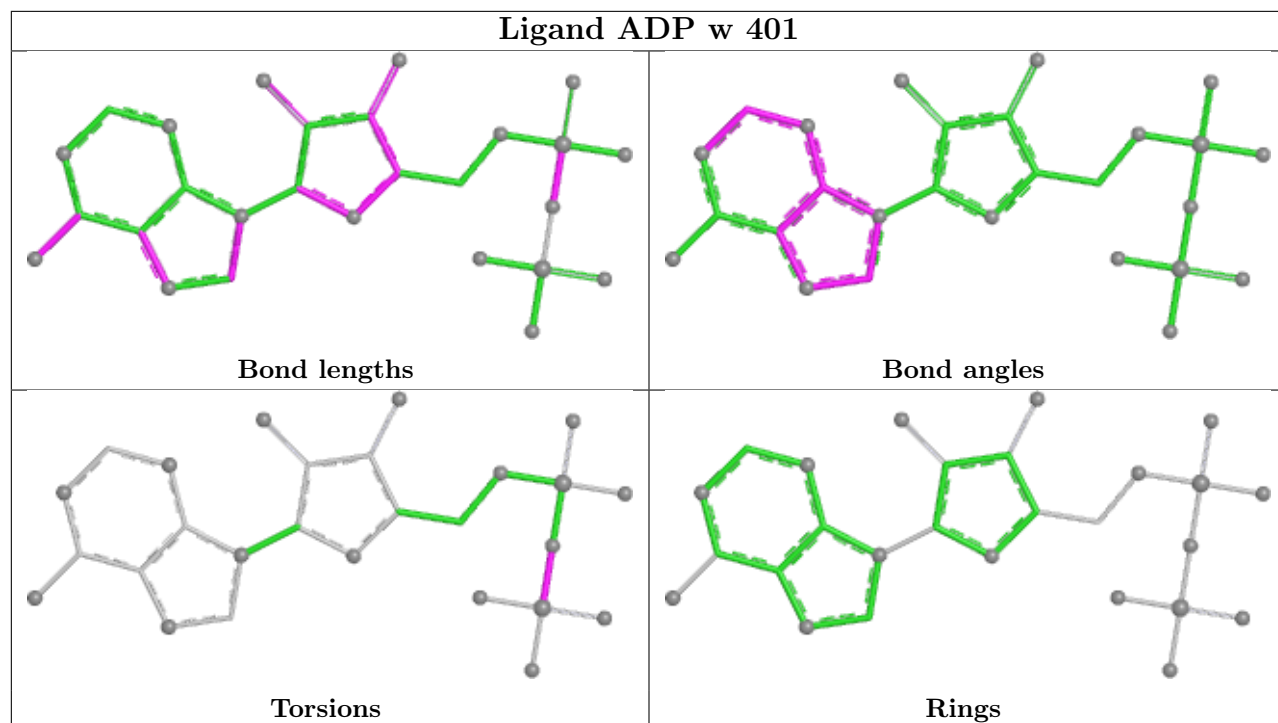


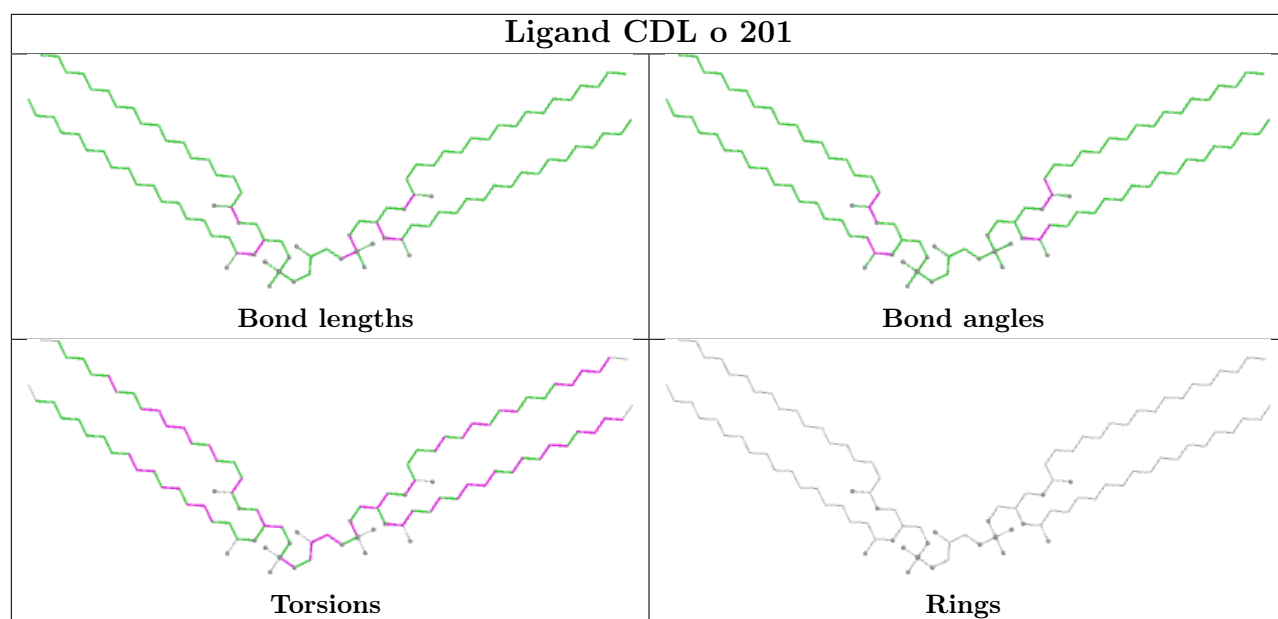


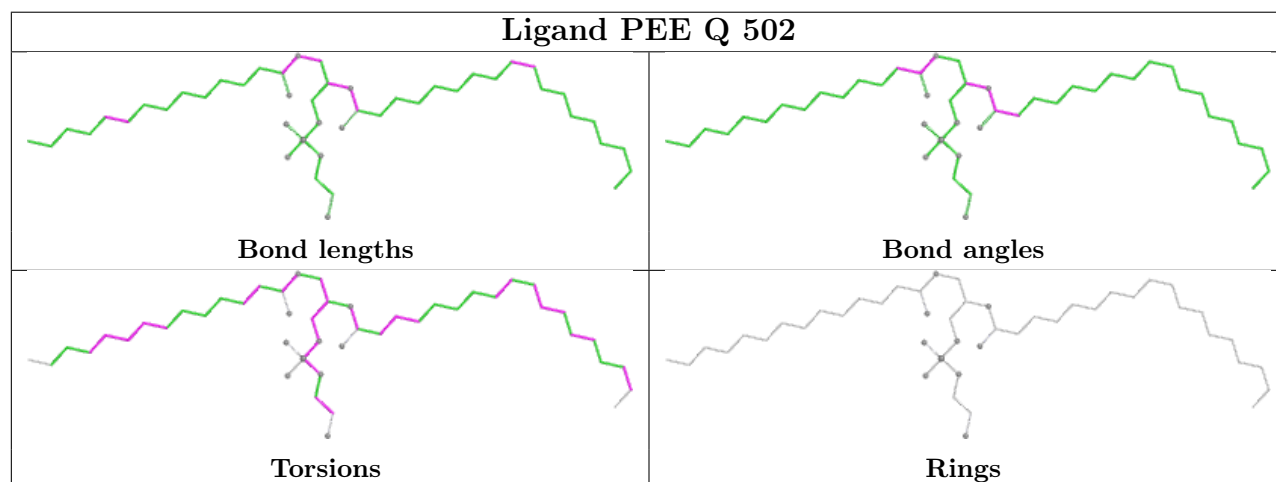
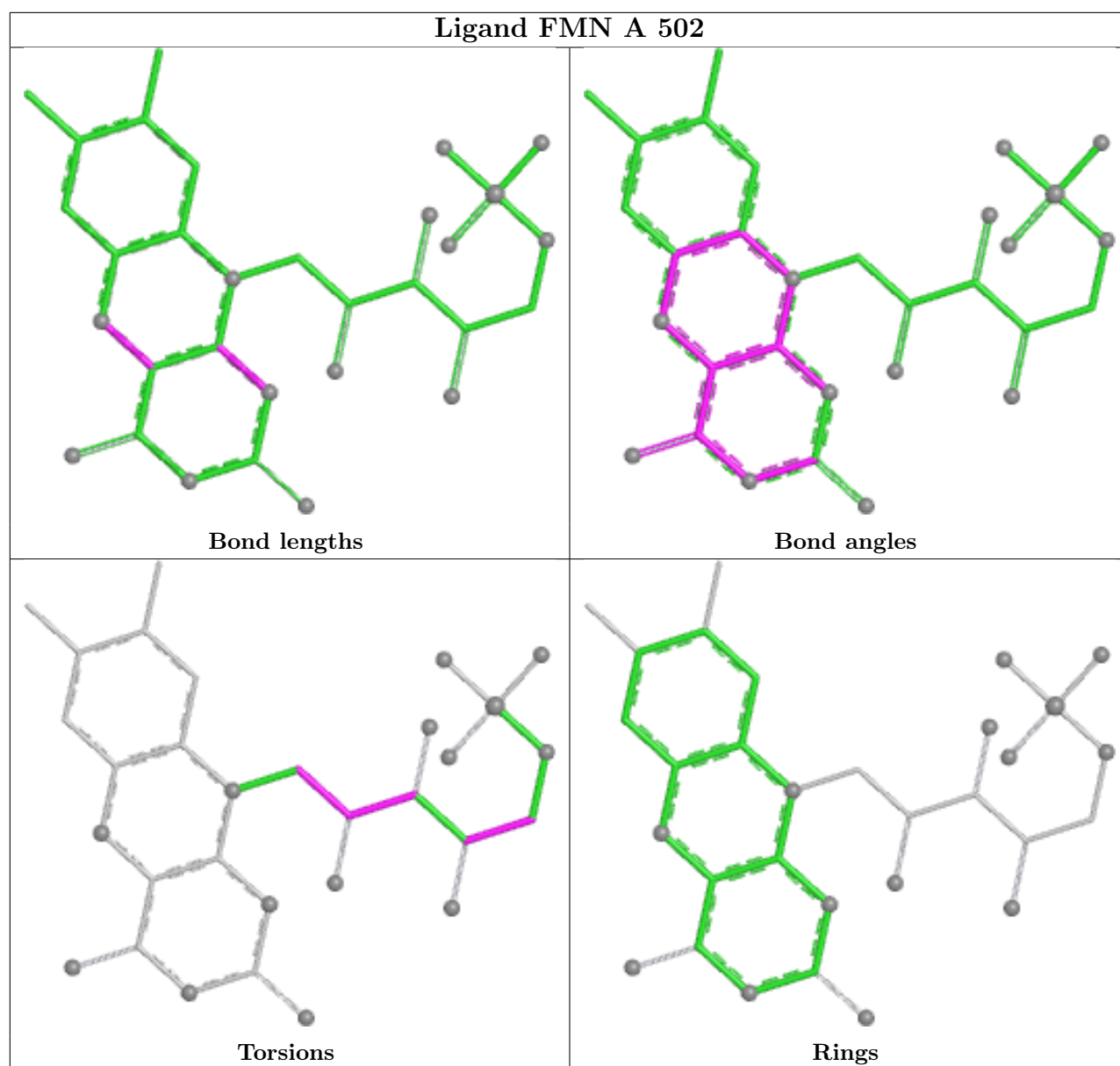


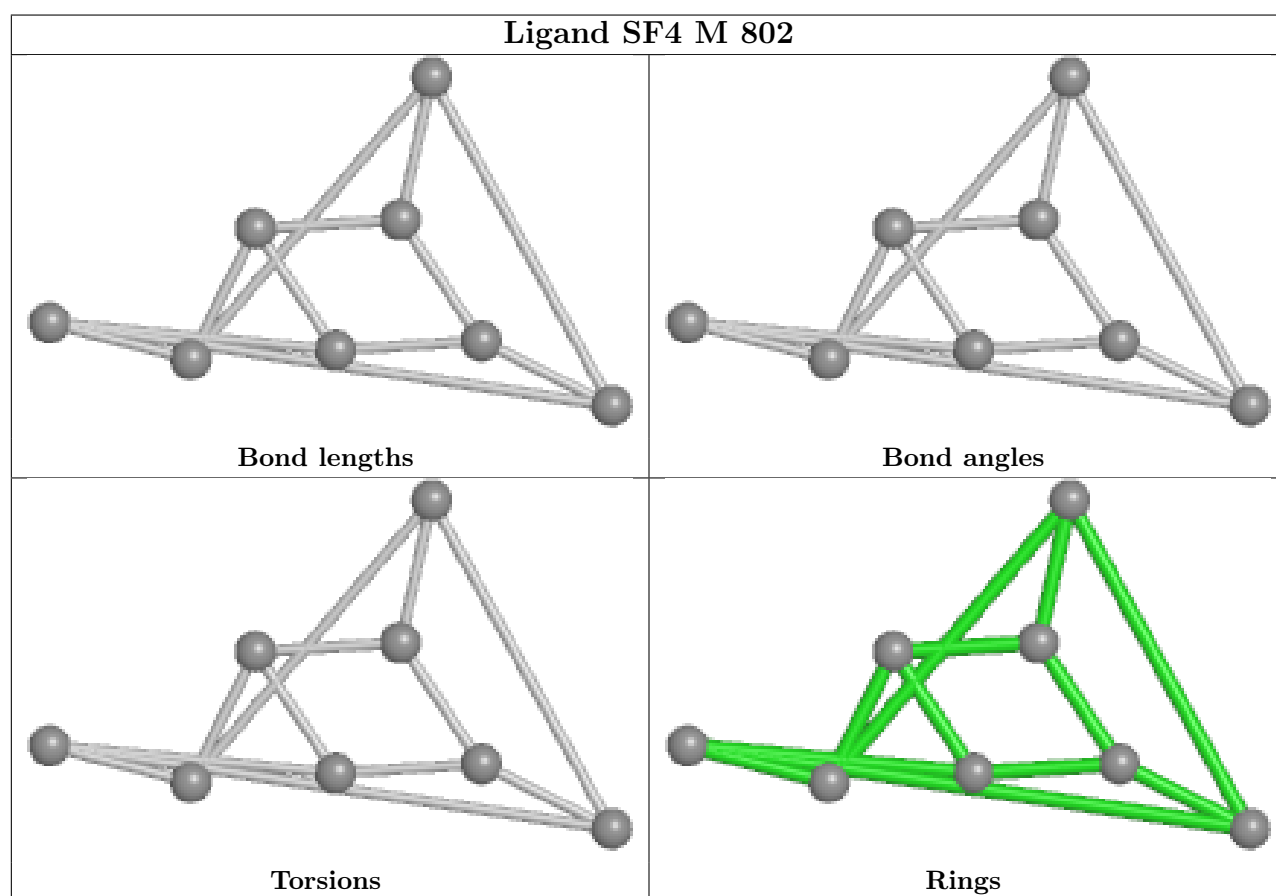
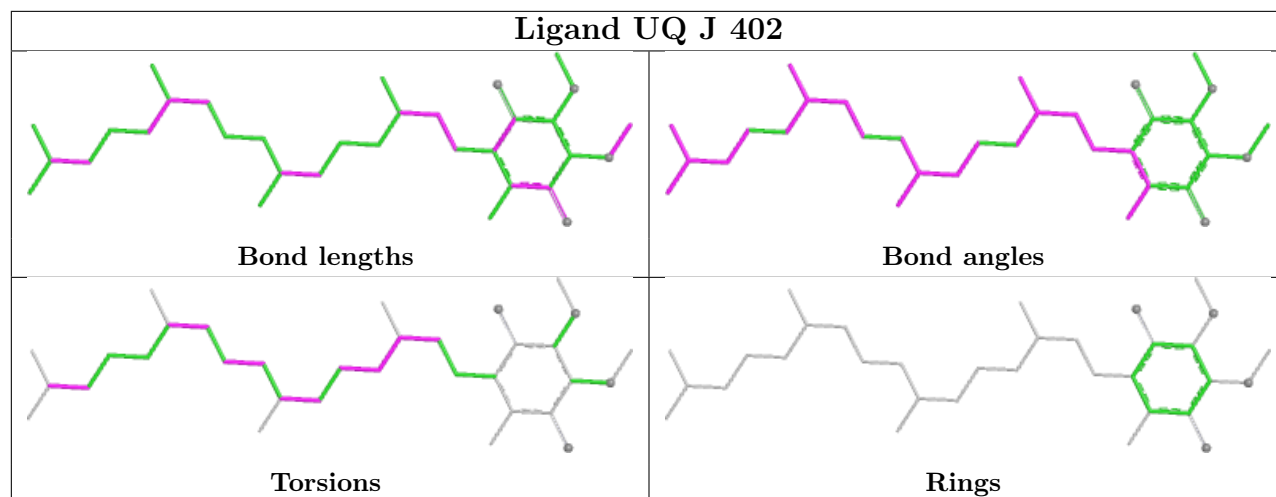


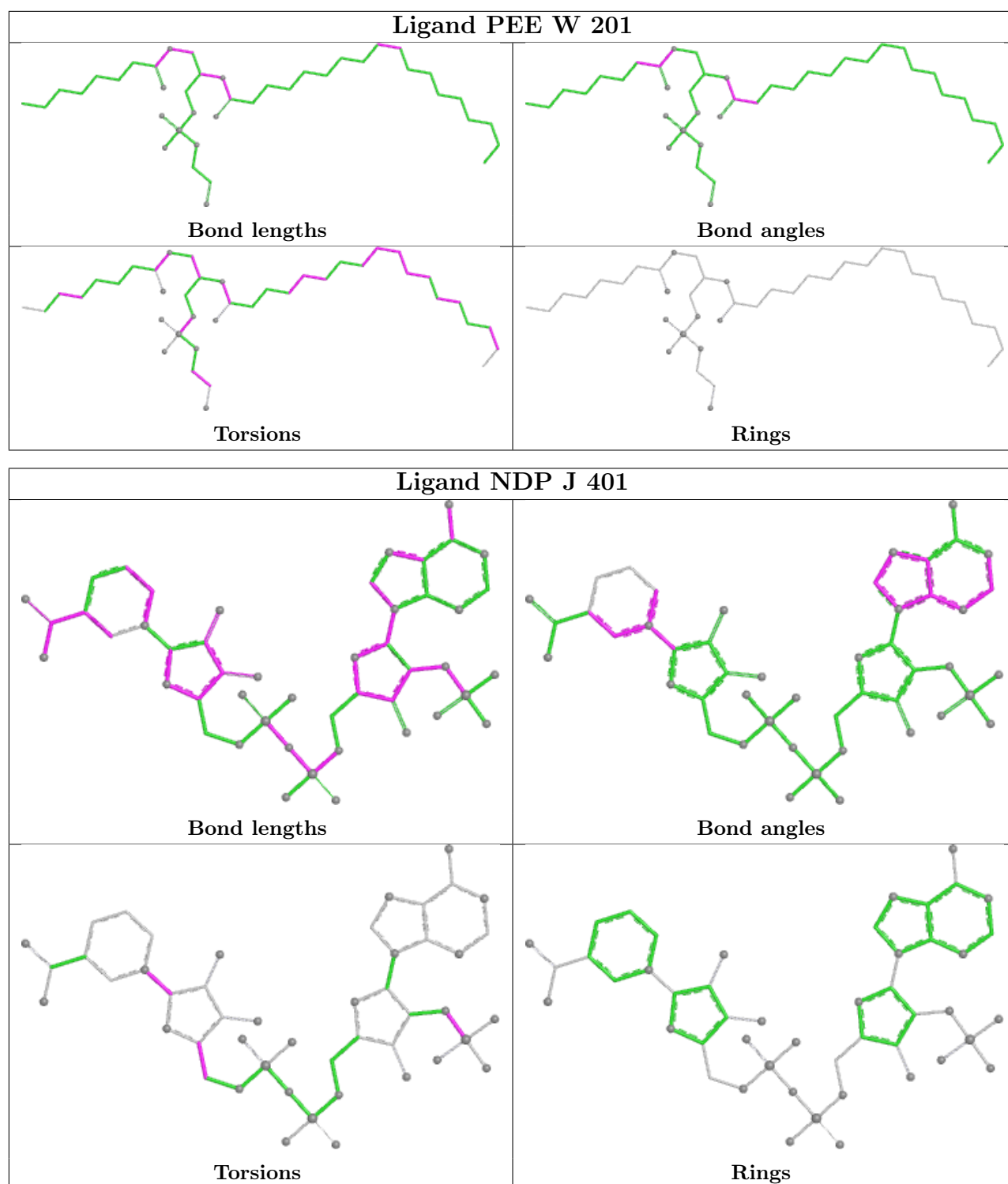












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

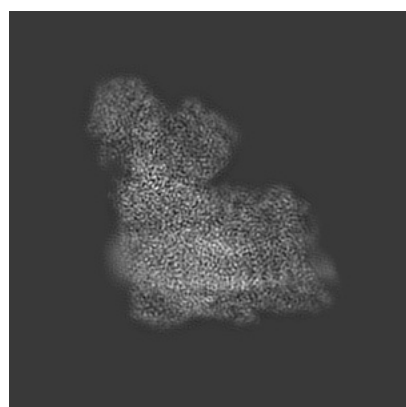
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32259. These allow visual inspection of the internal detail of the map and identification of artifacts.

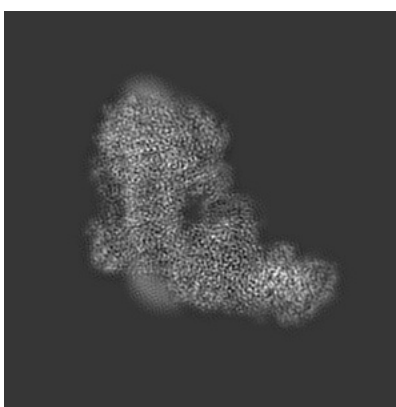
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

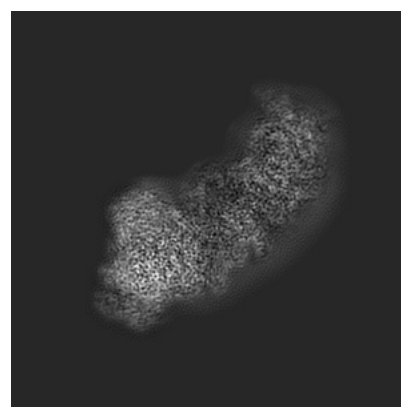
6.1.1 Primary map



X



Y

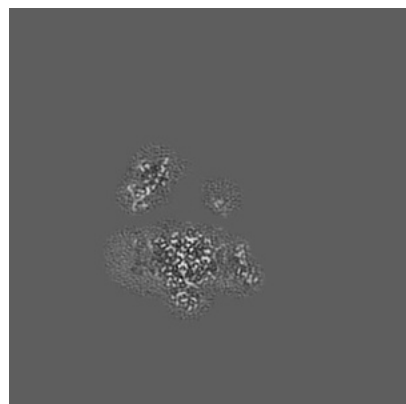


Z

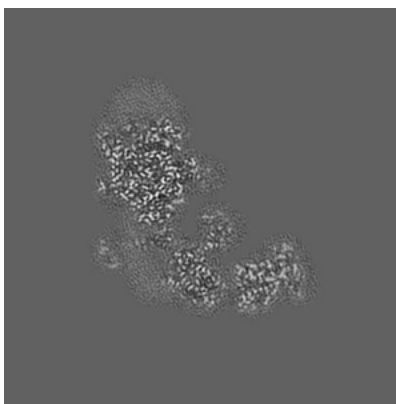
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

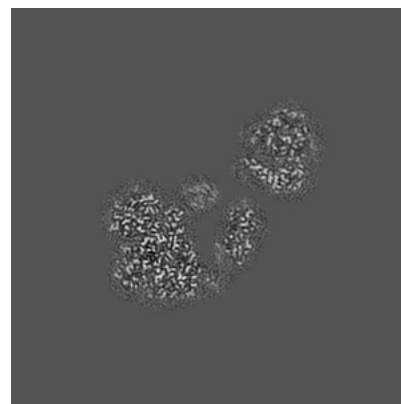
6.2.1 Primary map



X Index: 155



Y Index: 155

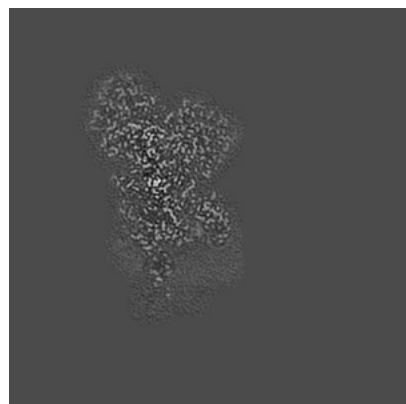


Z Index: 155

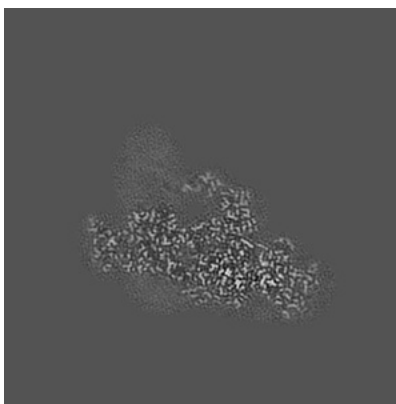
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

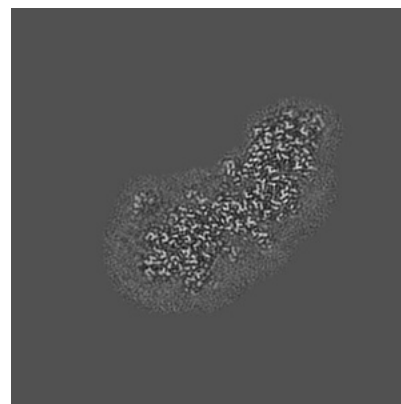
6.3.1 Primary map



X Index: 105



Y Index: 112

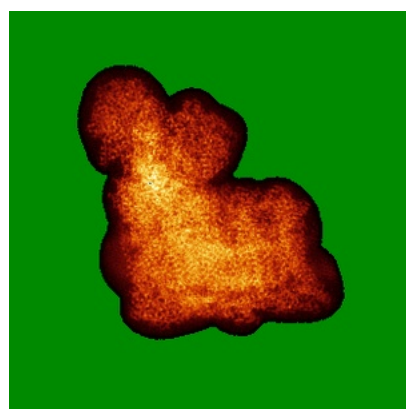


Z Index: 127

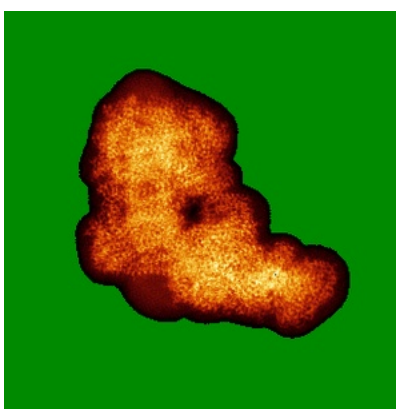
The images above show the largest variance slices of the map in three orthogonal directions.

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

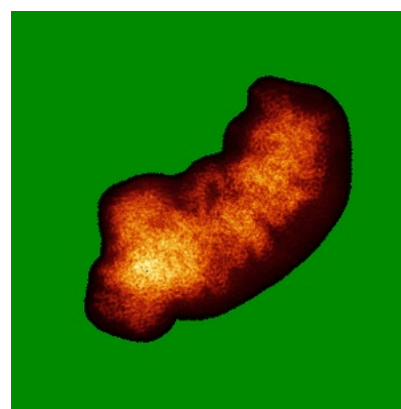
6.4.1 Primary map



X



Y

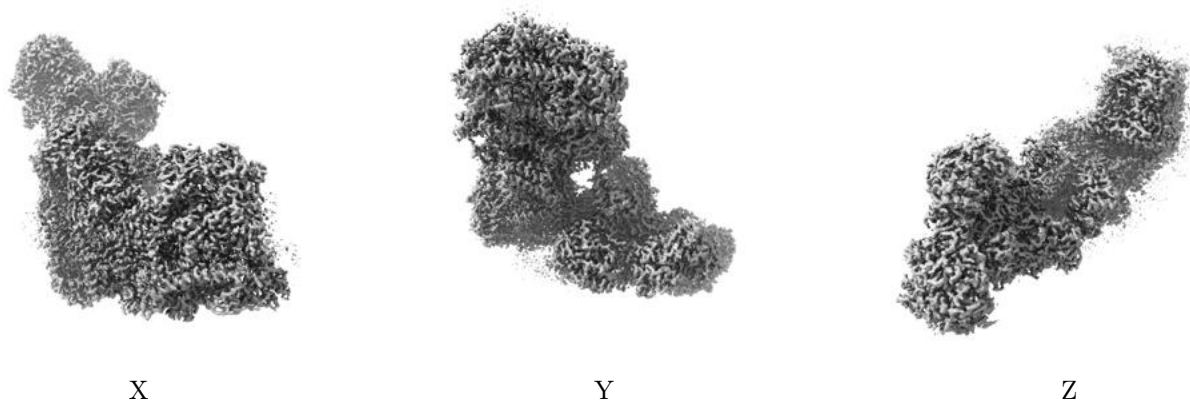


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0306. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

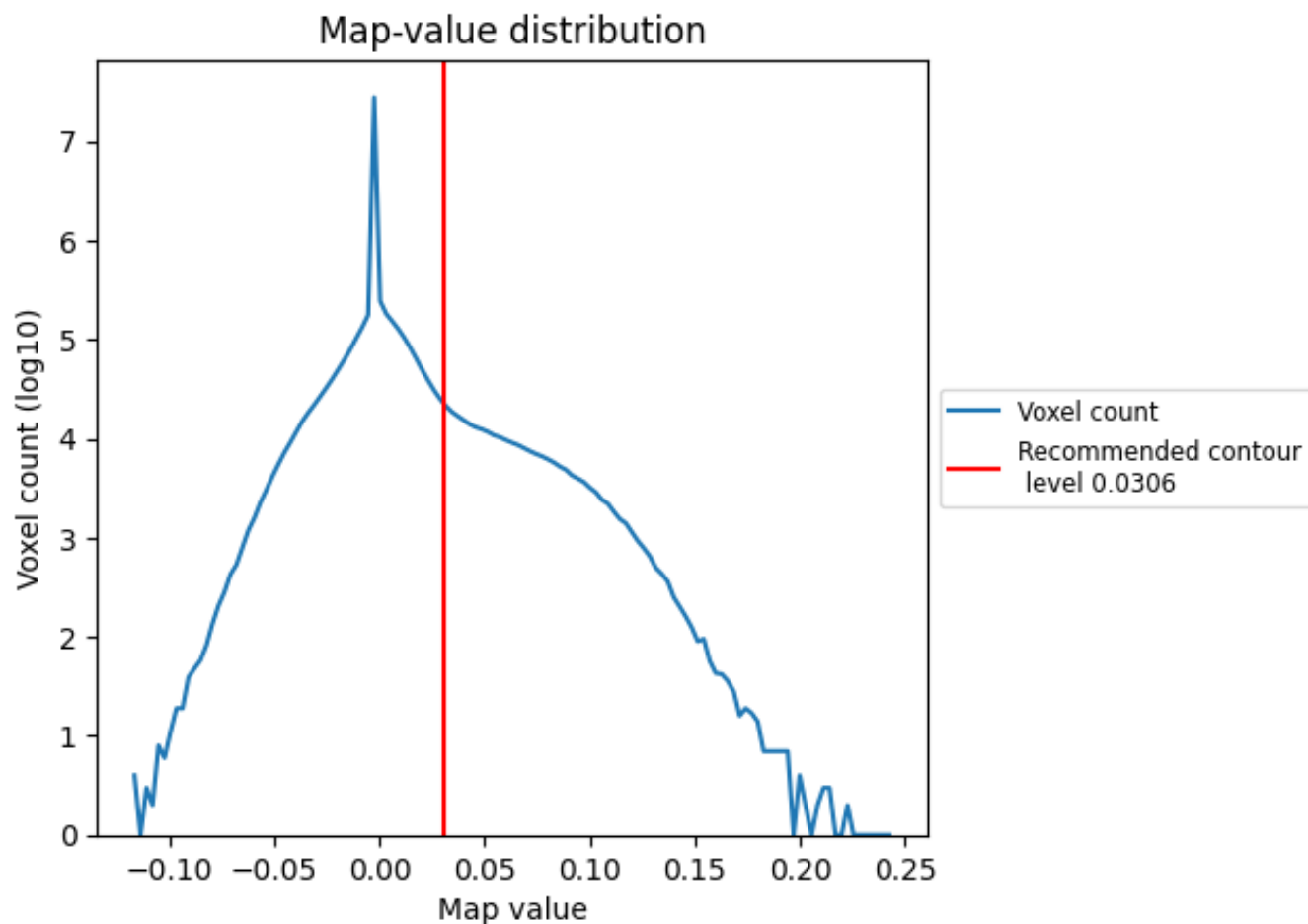
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

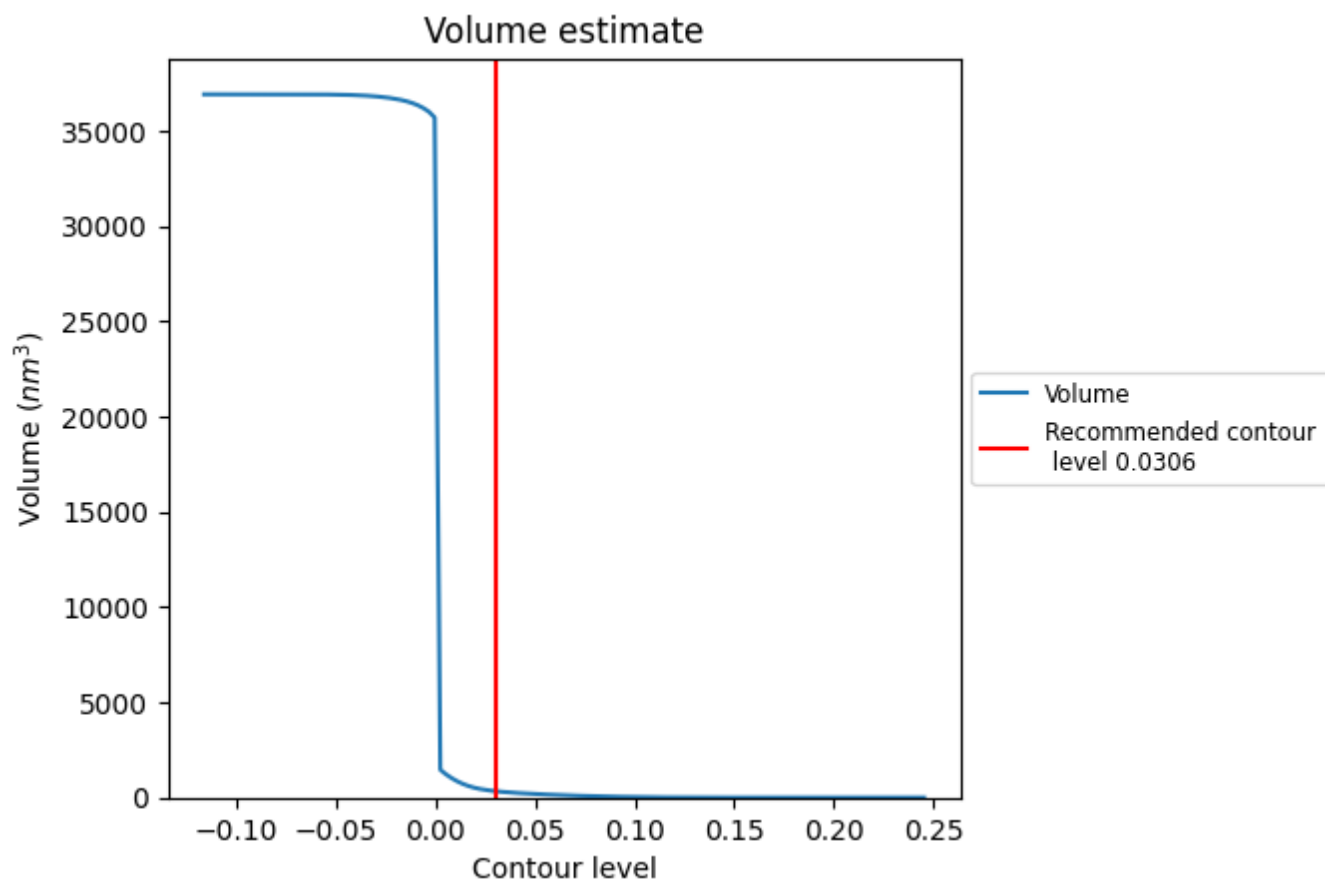
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

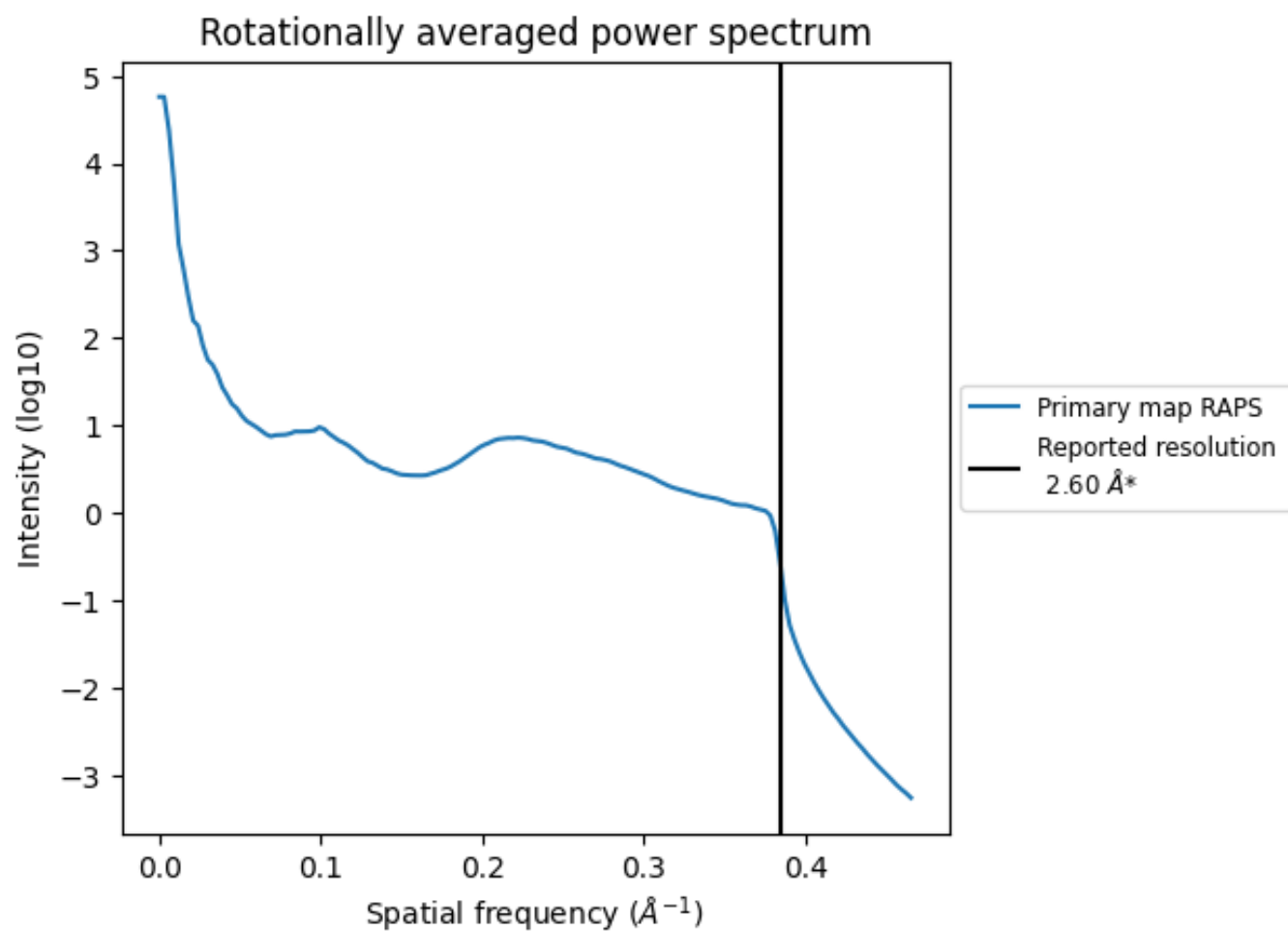
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 328 nm³; this corresponds to an approximate mass of 296 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 0.385 Å⁻¹

8 Fourier-Shell correlation

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

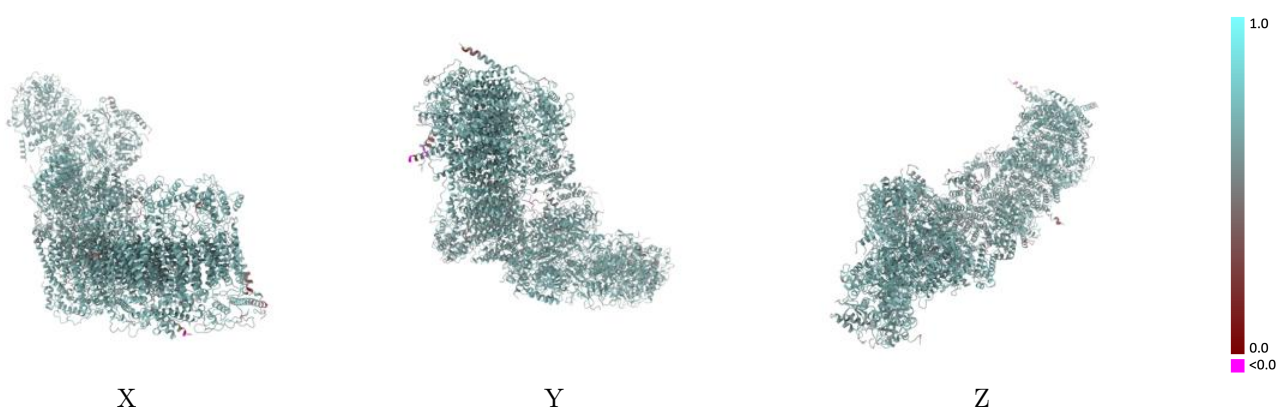
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32259 and PDB model 7W1Z. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)

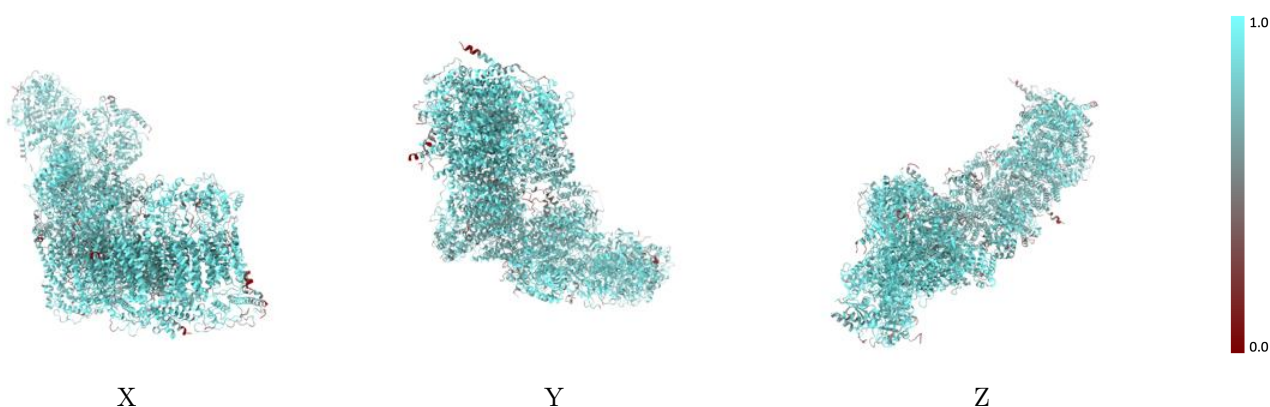
This section was not generated.

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



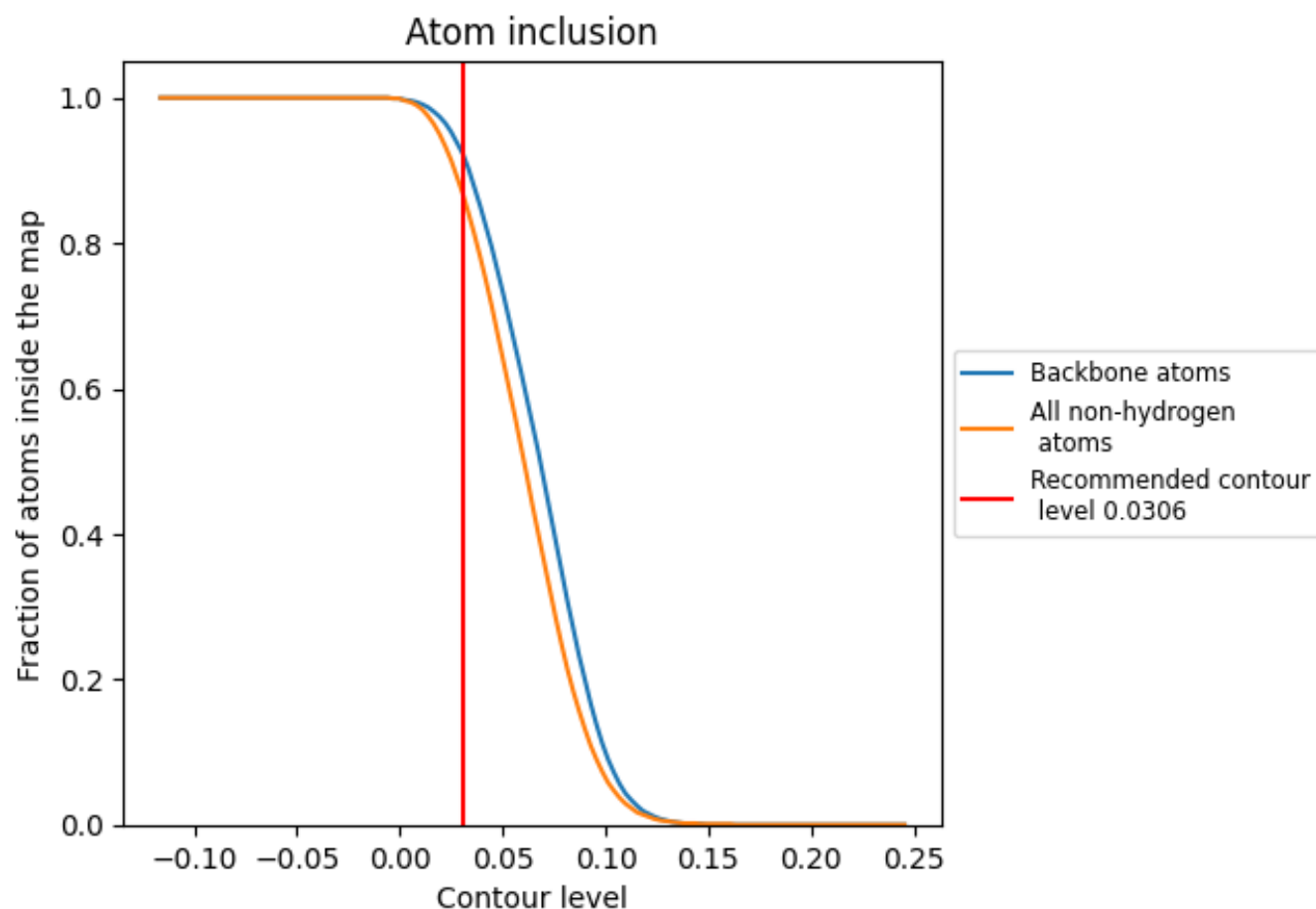
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0306).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.0306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.6400
A	 0.8530	 0.6240
B	 0.9470	 0.6740
C	 0.9200	 0.6660
E	 0.8600	 0.6440
F	 0.7530	 0.5850
G	 0.6030	 0.5210
H	 0.8680	 0.6310
I	 0.7660	 0.6060
J	 0.8860	 0.6470
K	 0.7410	 0.5860
L	 0.8770	 0.6550
M	 0.8940	 0.6460
N	 0.7980	 0.6300
O	 0.8190	 0.6140
P	 0.9460	 0.6750
Q	 0.9370	 0.6690
S	 0.9240	 0.6530
T	 0.8530	 0.6440
U	 0.8440	 0.6320
V	 0.8000	 0.6240
W	 0.8470	 0.6340
X	 0.8180	 0.6230
Y	 0.7610	 0.6100
Z	 0.6980	 0.5690
a	 0.8710	 0.6510
b	 0.8110	 0.6130
c	 0.8660	 0.6360
d	 0.8290	 0.6230
e	 0.8240	 0.6270
f	 0.6970	 0.5750
g	 0.8790	 0.6460
h	 0.8520	 0.6270
i	 0.9350	 0.6640
j	 0.8460	 0.6480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.9190	 0.6630
l	 0.9050	 0.6560
m	 0.8120	 0.6180
n	 0.7050	 0.5800
o	 0.8040	 0.6250
p	 0.8600	 0.6380
r	 0.9340	 0.6630
s	 0.9350	 0.6680
u	 0.8570	 0.6320
v	 0.7730	 0.5980
w	 0.8310	 0.6260