



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:36 AM JST

PDB ID : 7W20 / pdb_00007w20
EMDB ID : EMD-32260
Title : Active state CI from Rotenone-NADH dataset, Subclass 3
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-21
Resolution : 3.00 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

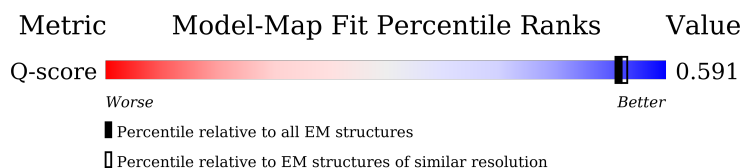
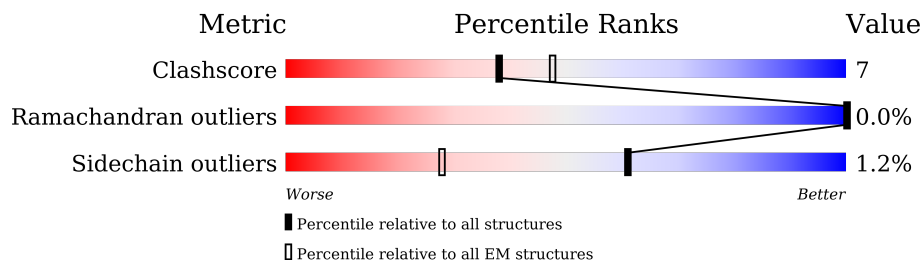
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

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

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

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	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	-
45	SF4	C	301	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68136 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
			967	618	179	165	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
			741	452	140	146	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			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
			1000	651	174	169	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.

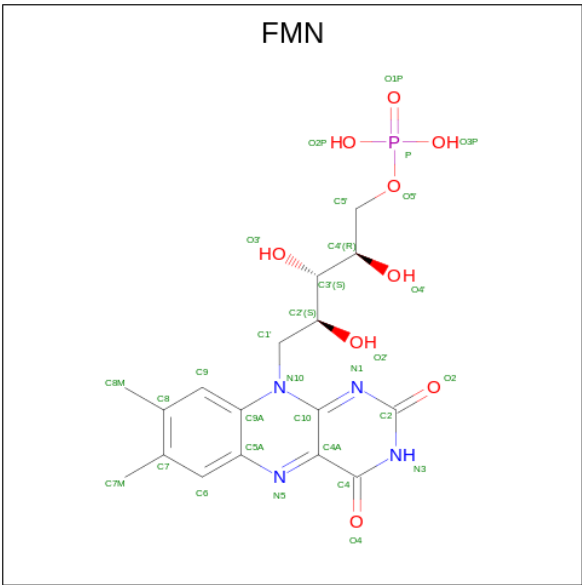
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



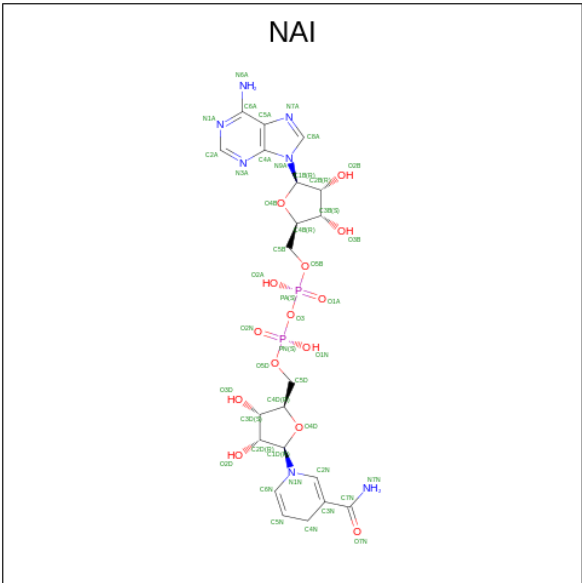
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



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

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



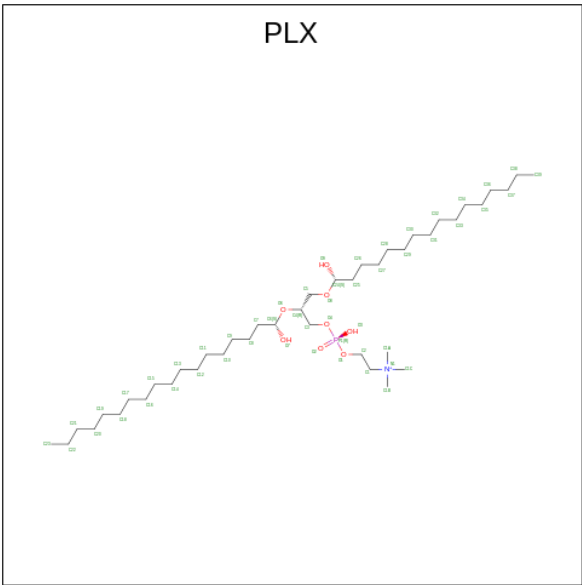
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



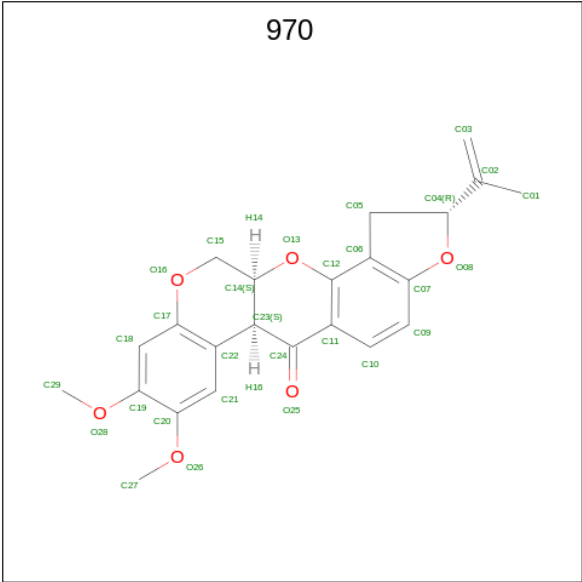
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			50	40	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).



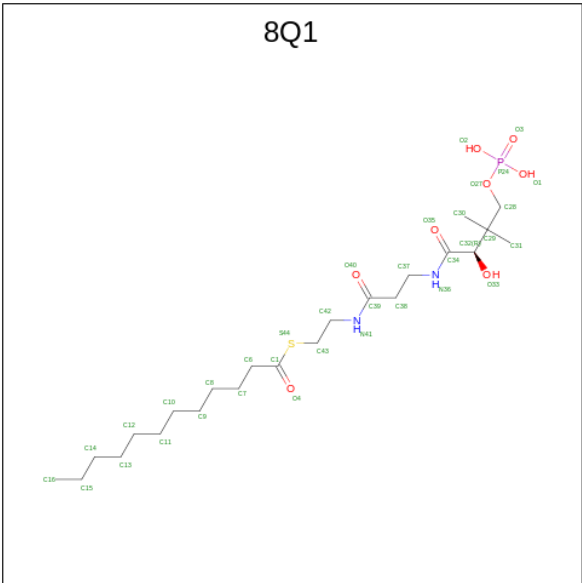
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 50 is (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) (labeled as "Ligand of Interest" by depositor).



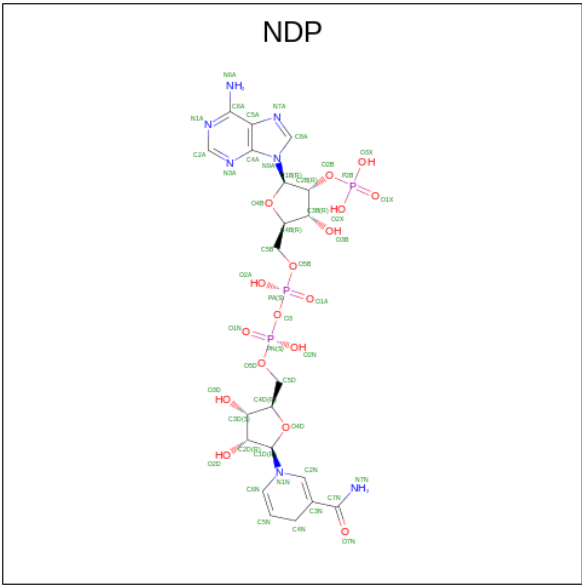
Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			29	23	6	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as
"Ligand of Interest" by depositor).



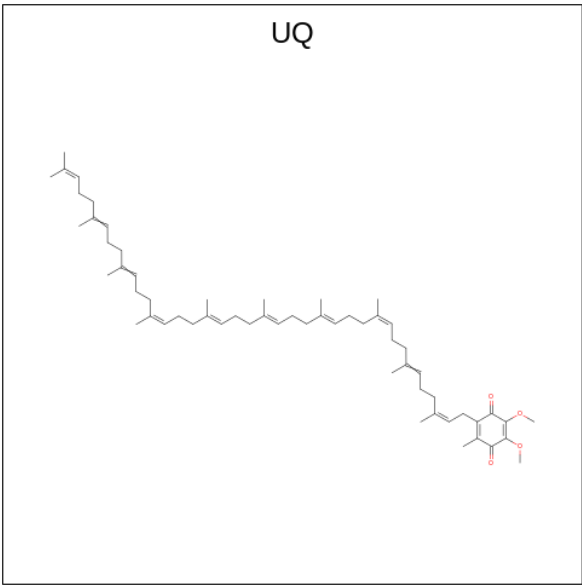
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



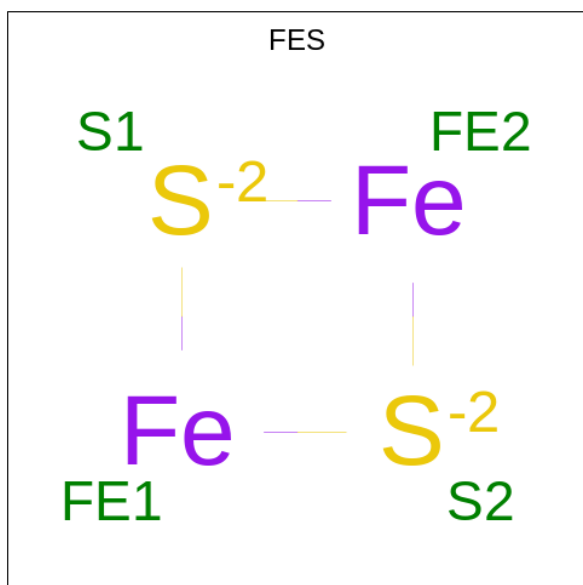
Mol	Chain	Residues	Atoms					AltConf
52	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



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

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

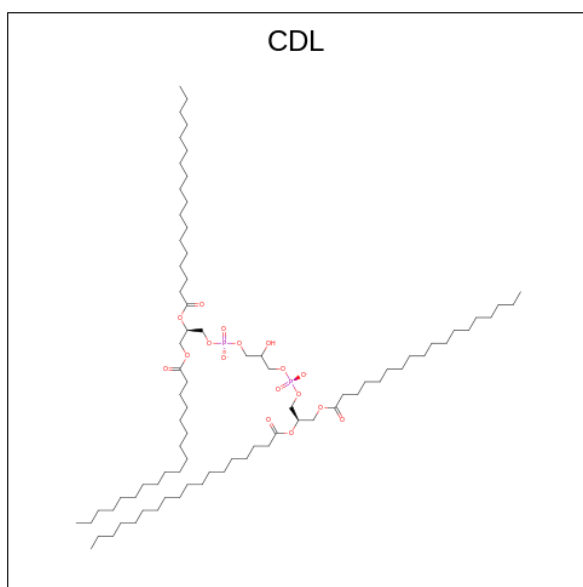


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

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

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

- Molecule 56 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

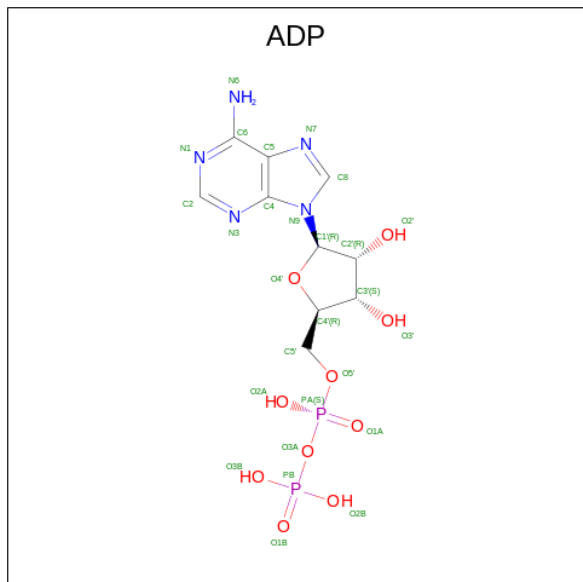


Mol	Chain	Residues	Atoms				AltConf
56	N	1	Total	C	O	P	0
			51	32	17	2	
56	V	1	Total	C	O	P	0
			94	75	17	2	
56	a	1	Total	C	O	P	0
			100	81	17	2	
56	i	1	Total	C	O	P	0
			99	80	17	2	
56	k	1	Total	C	O	P	0
			78	59	17	2	
56	l	1	Total	C	O	P	0
			99	80	17	2	
56	l	1	Total	C	O	P	0
			100	81	17	2	
56	n	1	Total	C	O	P	0
			55	36	17	2	
56	o	1	Total	C	O	P	0
			100	81	17	2	
56	s	1	Total	C	O	P	0
			89	70	17	2	

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

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

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

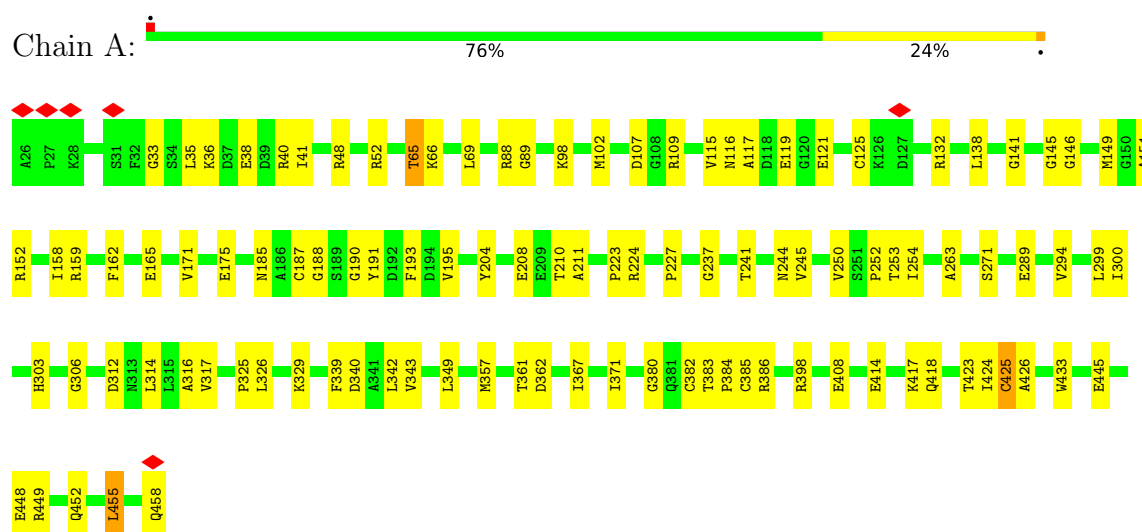


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

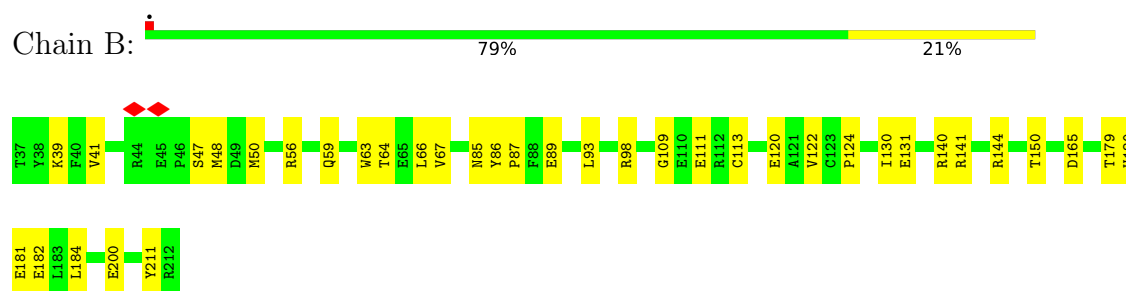
3 Residue-property plots

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.

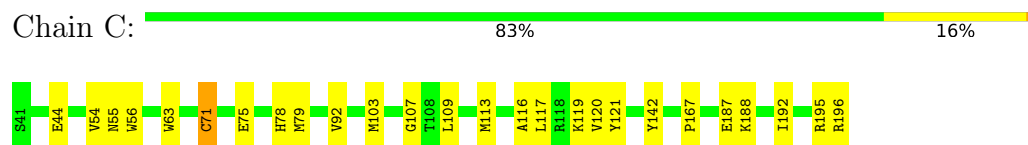
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



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



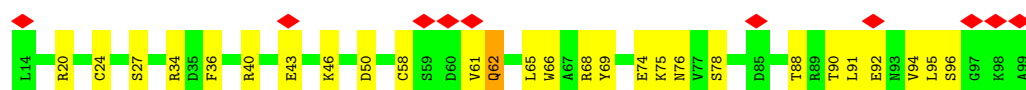
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:  90% 10%



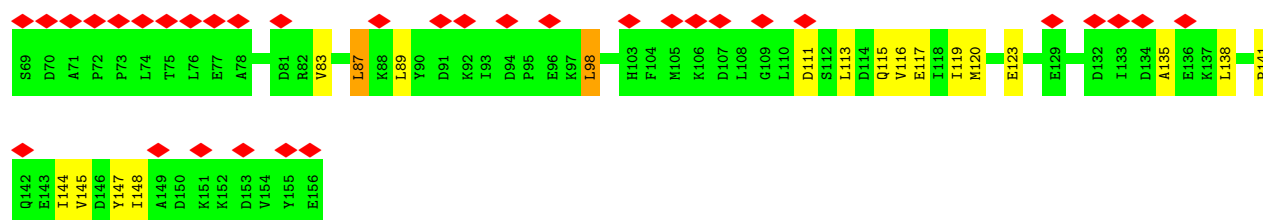
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  12% 69% 30%



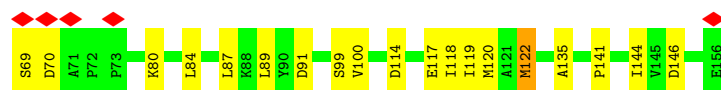
- Molecule 6: Acyl carrier protein

Chain G:  38% 78% 19%



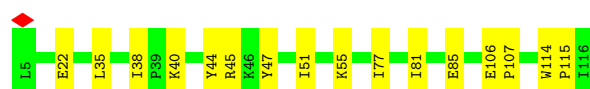
- Molecule 6: Acyl carrier protein

Chain X:  6% 78% 20%



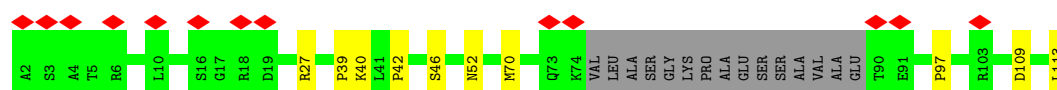
- Molecule 7: Complex I subunit B13

Chain H:  86% 14%



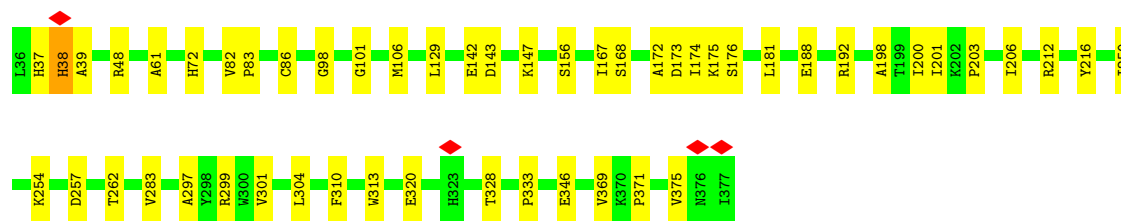
- Molecule 8: Complex I-B14.5a

Chain I:  12% 78% 9% 13%

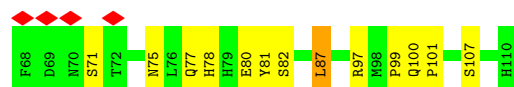


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

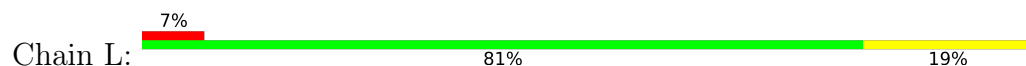
Chain J:  85% 15%



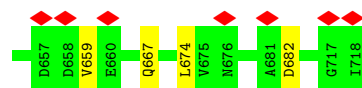
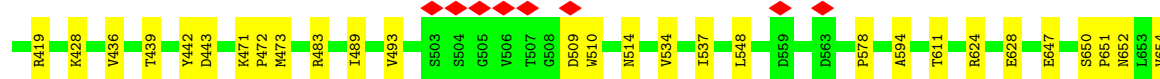
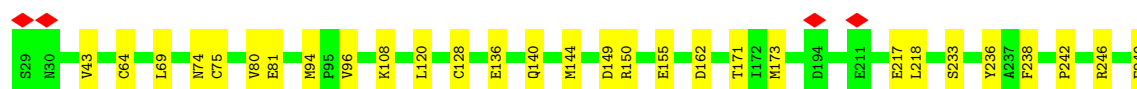
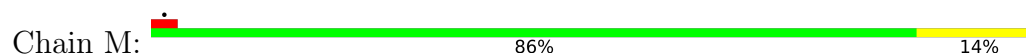
• Molecule 10: Complex I-9kD



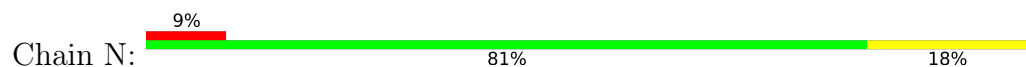
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

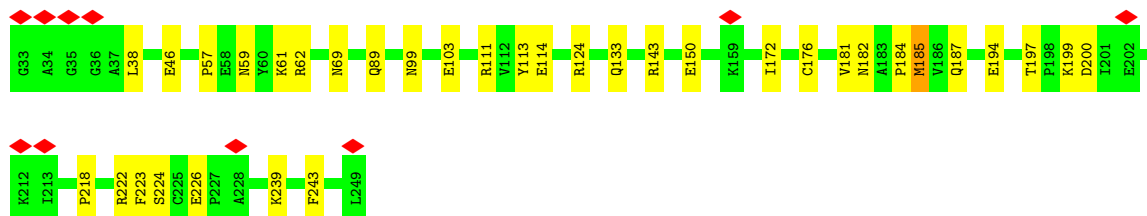
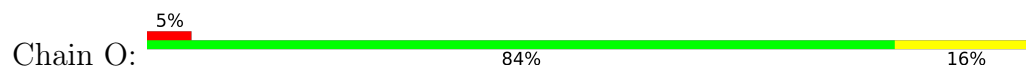


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

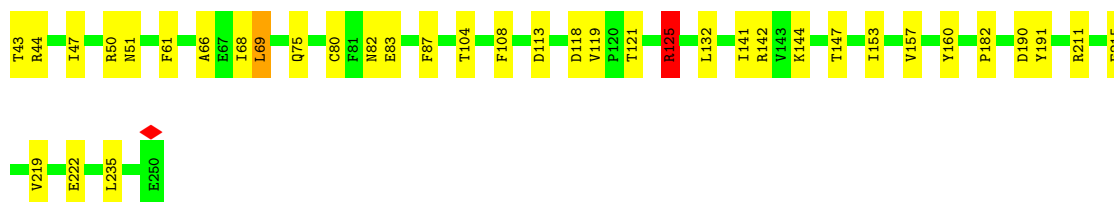
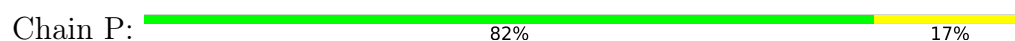




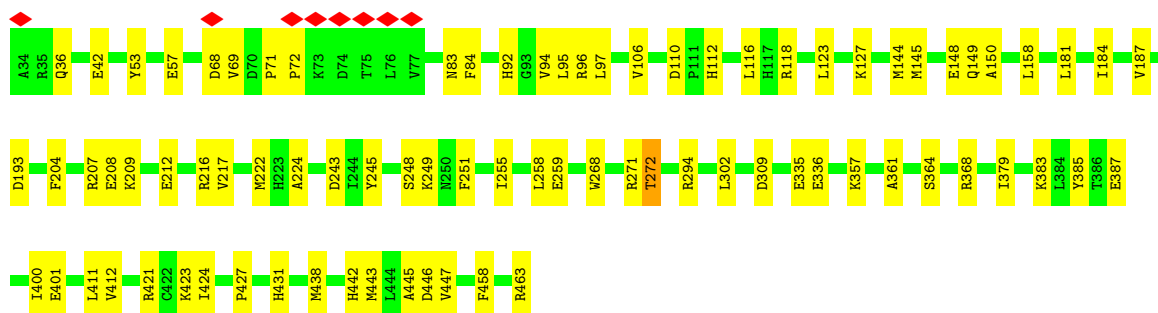
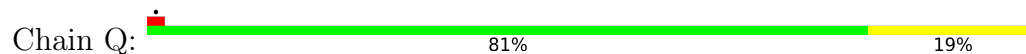
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



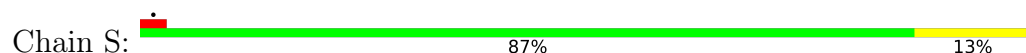
- Molecule 15: Complex I-30kD



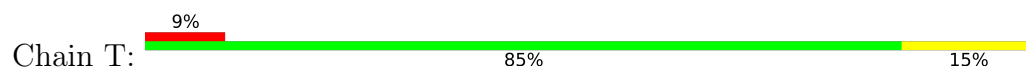
- Molecule 16: Complex I-49kD

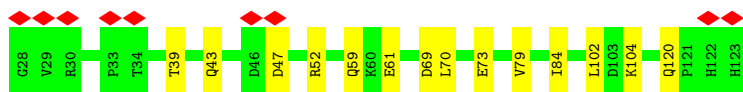


- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

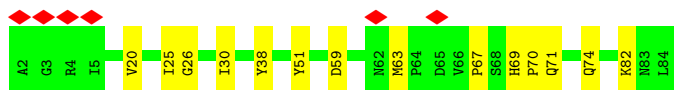
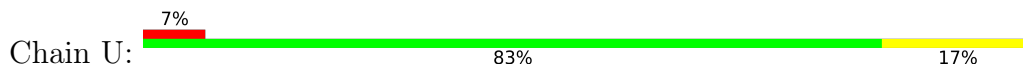


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

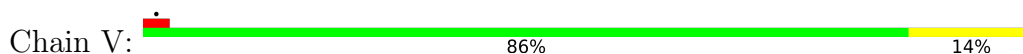




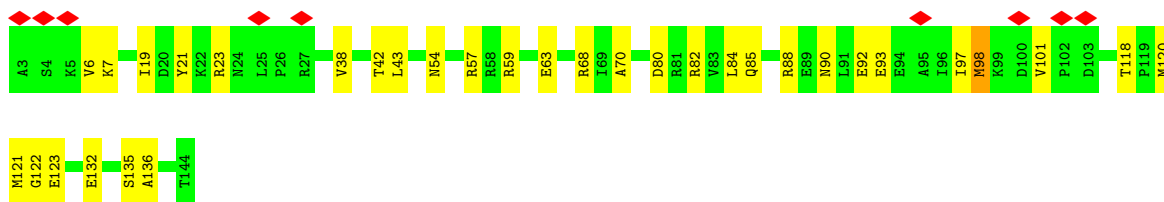
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



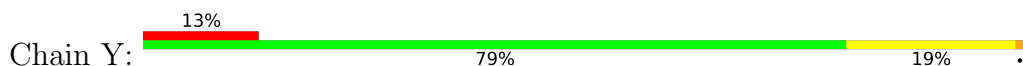
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



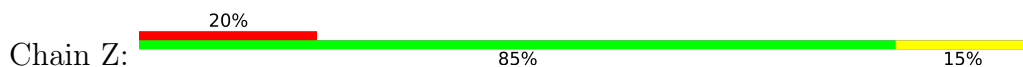
- Molecule 21: Complex I-B16.6



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



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

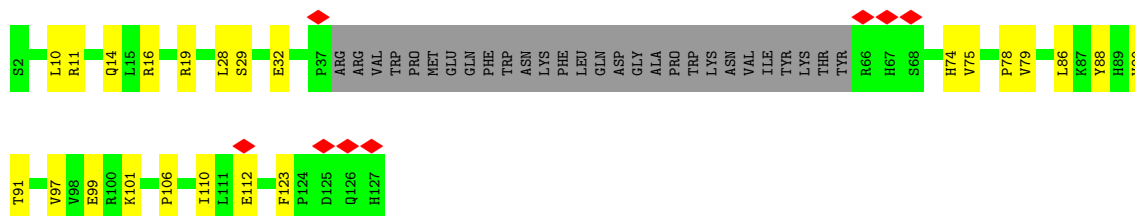


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

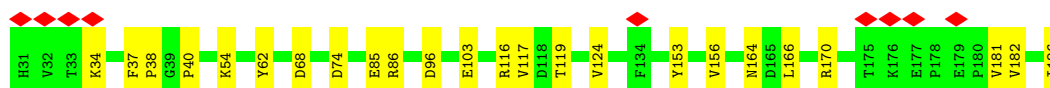
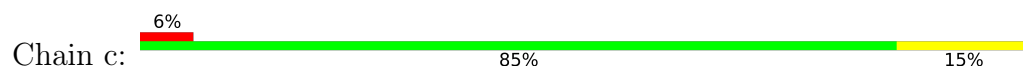




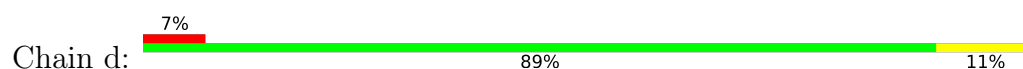
- Molecule 25: Complex I-B17



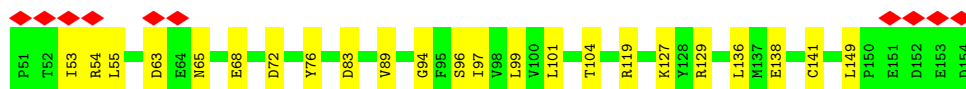
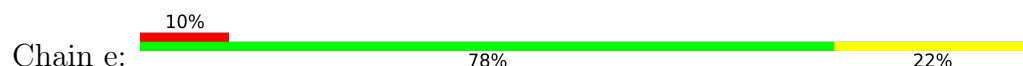
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



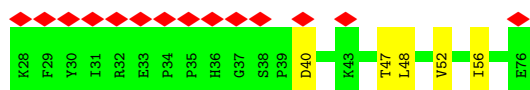
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



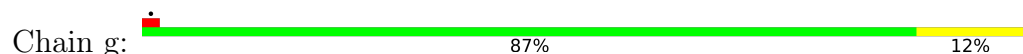
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

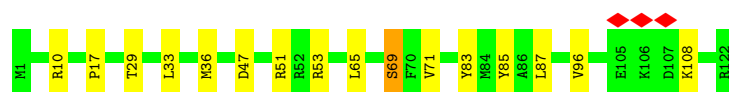


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

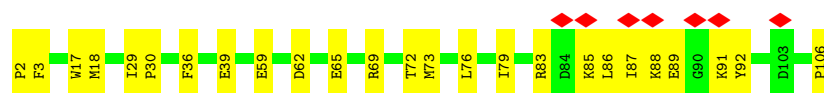
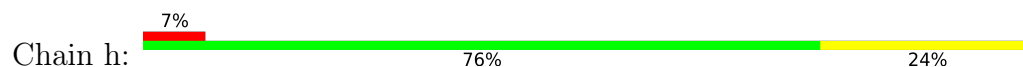


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

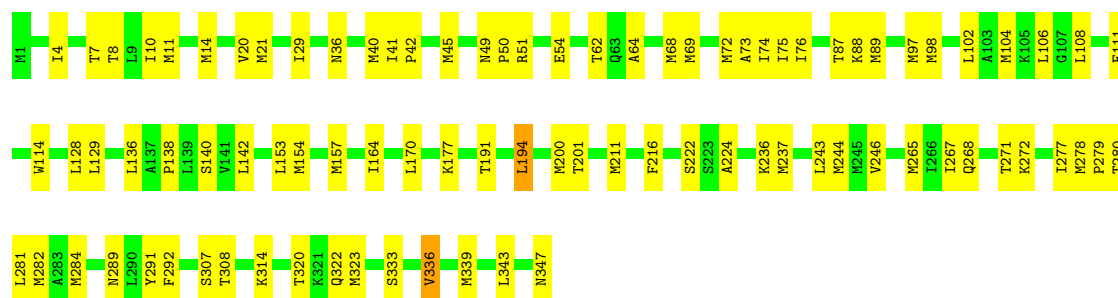




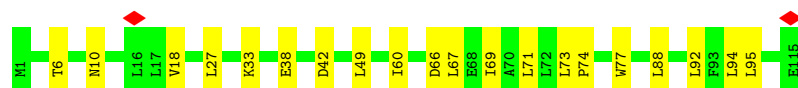
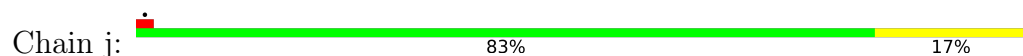
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



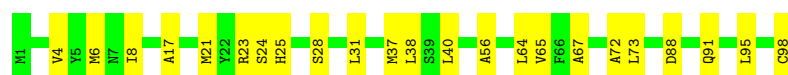
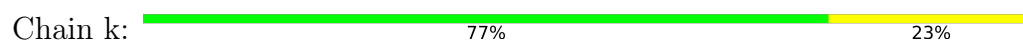
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



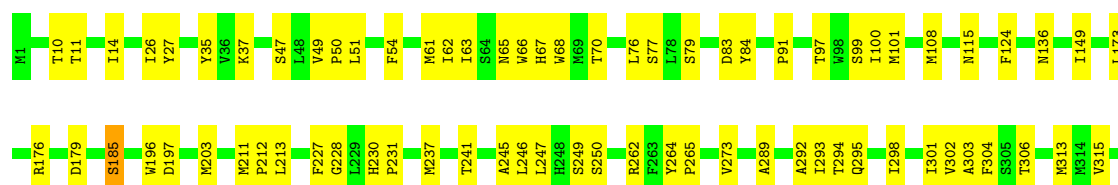
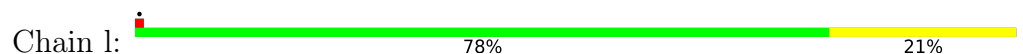
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

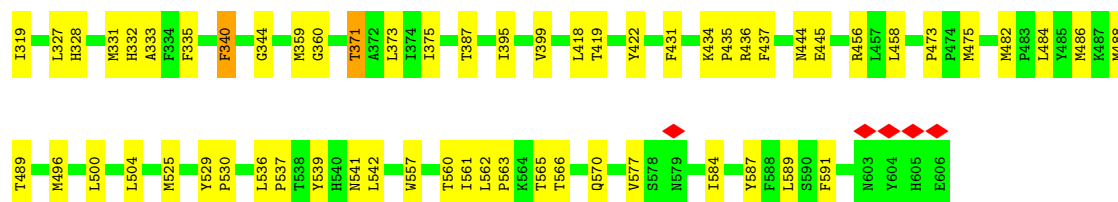


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

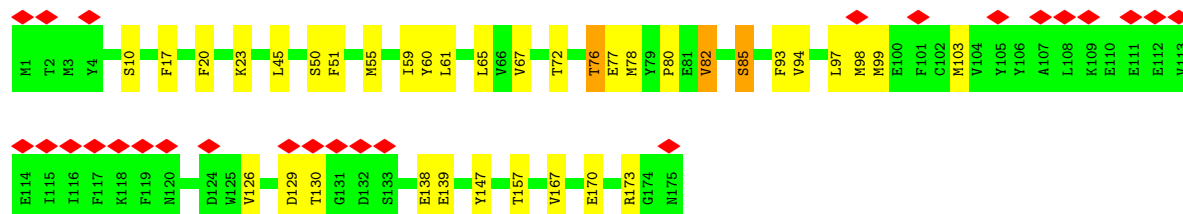
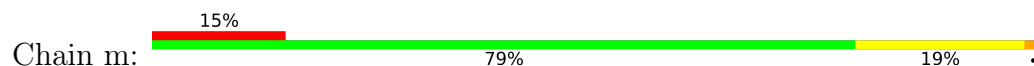


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

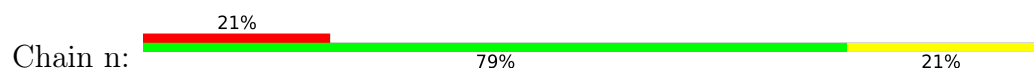




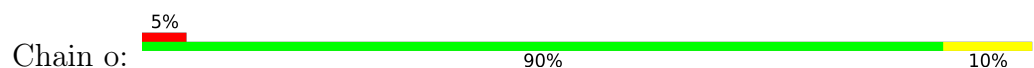
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



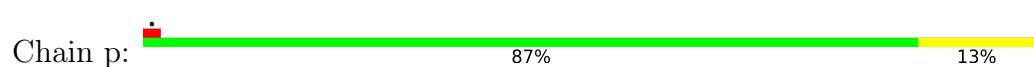
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



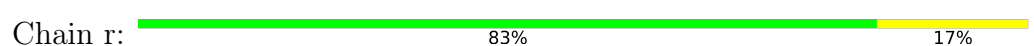
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

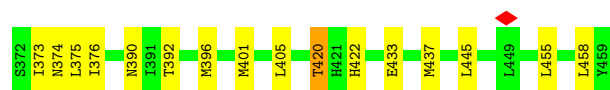


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



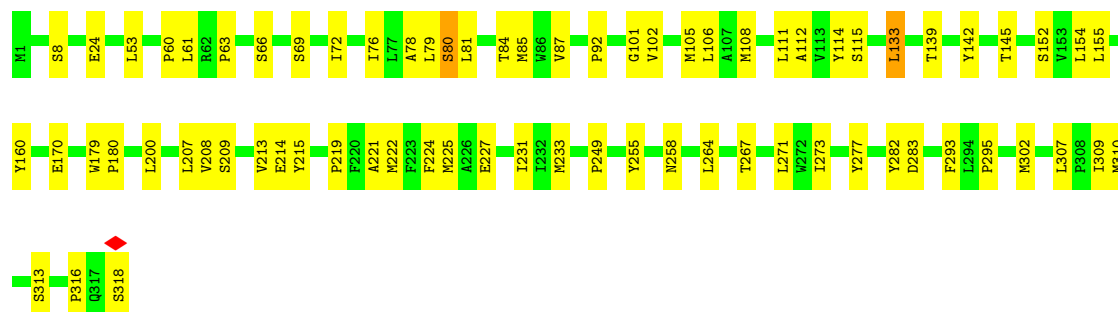
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4





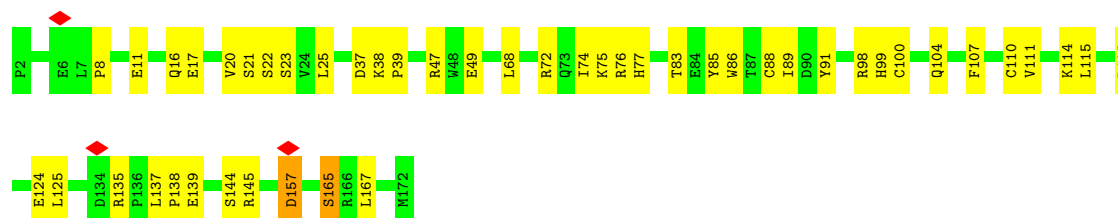
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 77% 22%



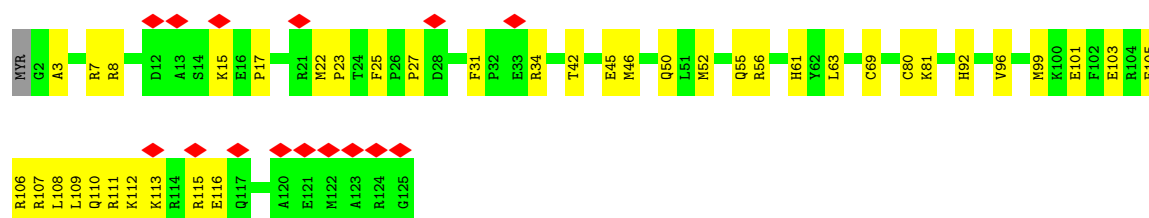
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 73% 26%



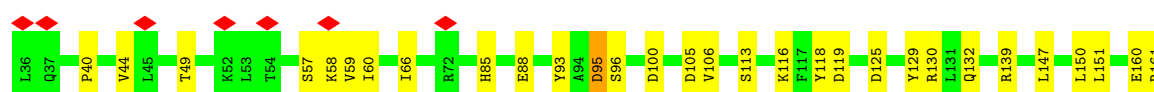
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

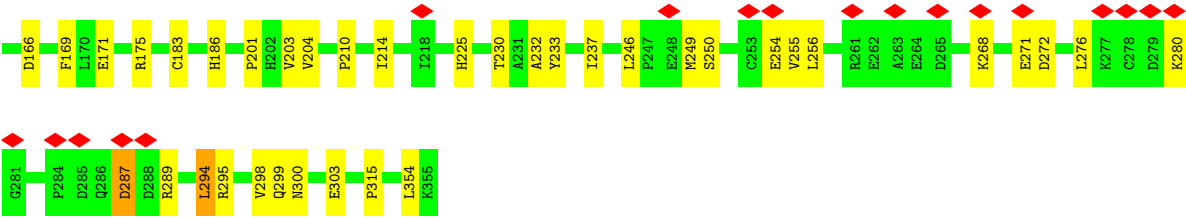
Chain v: 12% 68% 31%



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

Chain w: 8% 79% 20%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76197	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	0.207	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0296	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UQ, 8Q1, ZN, 2MR, NDP, 970, MG, ADP, FES, PEE, NAI, PLX, CDL, SF4, FMN

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	0.13	0/3406	0.33	0/4603
2	B	0.10	0/1443	0.28	0/1952
3	C	0.12	0/1279	0.29	0/1730
4	E	0.12	0/991	0.30	0/1335
5	F	0.14	0/695	0.40	0/936
6	G	0.14	0/705	0.33	0/956
6	X	0.11	0/708	0.35	0/959
7	H	0.12	0/929	0.34	0/1258
8	I	0.12	0/798	0.36	0/1079
9	J	0.11	0/2828	0.31	0/3834
10	K	0.14	0/377	0.36	0/509
11	L	0.09	0/1039	0.26	0/1403
12	M	0.11	0/5381	0.31	0/7291
13	N	0.11	0/1245	0.28	0/1694
14	O	0.12	0/1711	0.32	0/2328
15	P	0.13	0/1789	0.37	1/2436 (0.0%)
16	Q	0.12	0/3538	0.28	0/4796
17	S	0.11	0/581	0.30	0/781
18	T	0.10	0/755	0.30	0/1018
19	U	0.11	0/664	0.31	0/912
20	V	0.11	0/1042	0.27	0/1411
21	W	0.16	0/1192	0.37	0/1610
22	Y	0.11	0/610	0.27	0/836
23	Z	0.11	0/660	0.31	0/892
24	a	0.11	0/1184	0.27	0/1603
25	b	0.12	0/844	0.34	0/1149
26	c	0.11	0/1371	0.34	0/1875
27	d	0.16	0/1494	0.34	1/2015 (0.0%)
28	e	0.12	0/891	0.34	0/1210
29	f	0.13	0/385	0.31	0/522
30	g	0.10	0/1031	0.26	0/1395
31	h	0.10	0/889	0.30	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.13	0/2773	0.33	0/3768
33	j	0.13	0/938	0.31	0/1281
34	k	0.13	0/759	0.35	0/1029
35	l	0.12	0/4926	0.32	1/6700 (0.0%)
36	m	0.14	0/1307	0.36	0/1777
37	n	0.10	0/491	0.24	0/663
38	o	0.11	0/1092	0.25	0/1481
39	p	0.11	0/1590	0.26	0/2155
40	r	0.12	0/3715	0.28	0/5067
41	s	0.14	0/2581	0.33	0/3529
42	u	0.19	0/1436	0.45	0/1938
43	v	0.13	0/1060	0.32	0/1421
44	w	0.10	0/2646	0.28	0/3584
All	All	0.12	0/67769	0.32	3/91911 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	125	ARG	N-CA-C	7.90	120.80	111.71
35	l	26	ILE	N-CA-C	-7.33	106.74	113.71
27	d	22	PRO	CA-N-CD	-5.50	104.30	112.00

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	79	0
2	B	1412	0	1363	30	0
3	C	1248	0	1254	20	0
4	E	967	0	970	9	0
5	F	684	0	698	15	0
6	G	693	0	671	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	696	0	680	12	0
7	H	910	0	950	13	0
8	I	780	0	808	11	0
9	J	2751	0	2773	34	0
10	K	366	0	338	11	0
11	L	1016	0	1016	18	0
12	M	5293	0	5324	61	0
13	N	1204	0	1162	21	0
14	O	1671	0	1673	21	0
15	P	1738	0	1693	28	0
16	Q	3459	0	3396	58	0
17	S	566	0	561	9	0
18	T	741	0	702	8	0
19	U	643	0	642	12	0
20	V	1021	0	1025	13	0
21	W	1161	0	1144	30	0
22	Y	584	0	529	10	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	10	0
25	b	819	0	835	19	0
26	c	1315	0	1208	18	0
27	d	1461	0	1429	15	0
28	e	867	0	817	17	0
29	f	377	0	353	4	0
30	g	1000	0	992	14	0
31	h	867	0	871	21	0
32	i	2710	0	2874	65	0
33	j	914	0	951	23	0
34	k	748	0	799	24	0
35	l	4797	0	4935	89	0
36	m	1276	0	1243	32	0
37	n	479	0	486	10	0
38	o	1062	0	1072	8	0
39	p	1534	0	1470	15	0
40	r	3624	0	3832	54	0
41	s	2508	0	2607	60	0
42	u	1398	0	1374	37	0
43	v	1036	0	992	29	0
44	w	2586	0	2542	44	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	B	51	0	82	6	0
48	C	47	0	71	2	0
48	U	51	0	82	4	0
48	W	41	0	59	0	0
48	i	47	0	71	2	0
48	j	41	0	59	2	0
48	l	96	0	146	7	0
48	r	51	0	82	3	0
49	C	52	0	88	2	0
49	J	52	0	88	3	0
49	a	52	0	88	0	0
49	g	52	0	88	6	0
49	j	52	0	88	3	0
49	r	104	0	176	6	0
50	C	29	0	0	0	0
51	G	35	0	0	0	0
51	X	35	0	0	0	0
52	J	48	0	24	2	0
53	J	33	0	39	2	0
53	s	38	0	47	5	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	N	51	0	46	1	0
56	V	94	0	138	4	0
56	a	100	0	156	5	0
56	i	99	0	151	9	0
56	k	78	0	106	4	0
56	l	199	0	307	16	0
56	n	55	0	54	2	0
56	o	100	0	156	6	0
56	s	89	0	125	8	0
57	T	1	0	0	0	0
58	w	27	0	11	2	0
All	All	68136	0	68804	1006	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 (1006) 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)
1:A:89:GLY:HA2	1:A:244:ASN:ND2	1.53	1.24
42:u:88:CYS:HB3	42:u:100:CYS:SG	1.85	1.16
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.14
52:J:401:NDP:O4D	52:J:401:NDP:C4D	1.69	1.14
42:u:88:CYS:CB	42:u:100:CYS:SG	2.37	1.12
1:A:89:GLY:CA	1:A:244:ASN:HD22	1.63	1.11
1:A:89:GLY:N	1:A:244:ASN:HD22	1.55	1.03
1:A:89:GLY:CA	1:A:244:ASN:ND2	2.23	0.98
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.61	0.82
27:d:80:LYS:H	30:g:108:LYS:HZ3	1.29	0.81
6:X:89:LEU:HD23	23:Z:48:ASN:HA	1.65	0.78
34:k:28:SER:HB3	36:m:23:LYS:HG2	1.65	0.78
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.63	0.78
32:i:236:LYS:HG3	32:i:237:MET:HG3	1.64	0.77
5:F:68:ARG:HG3	5:F:74:GLU:HG2	1.65	0.76
34:k:6:MET:HE3	36:m:103:MET:HE3	1.69	0.74
6:G:87:LEU:HD23	6:G:98:LEU:HD11	1.71	0.73
19:U:59:ASP:HA	19:U:63:MET:HE1	1.69	0.73
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.70	0.73
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.71	0.73
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.71	0.72
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.71	0.71
6:G:144:ILE:O	6:G:148:ILE:HG13	1.91	0.71
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.31	0.70
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.72	0.70
2:B:47:SER:O	2:B:56:ARG:NH2	2.24	0.70
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.74	0.70
44:w:254:GLU:HG3	44:w:276:LEU:HD22	1.74	0.70
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.26	0.69
30:g:10:ARG:NH2	32:i:347:ASN:O	2.25	0.69
41:s:249:PRO:HG2	42:u:99:HIS:CD2	2.28	0.69
1:A:152:ARG:NH2	10:K:99:PRO:O	2.25	0.69
40:r:281:ASP:HB3	40:r:284:SER:HB2	1.74	0.69
41:s:102:VAL:HG21	41:s:154:LEU:HD21	1.74	0.69
34:k:25:HIS:NE2	36:m:77:GLU:OE1	2.26	0.69
15:P:118:ASP:OD1	15:P:125:ARG:HD2	1.93	0.69
21:W:121:MET:HB2	36:m:130:THR:HG23	1.73	0.69
7:H:22:GLU:OE2	7:H:22:GLU:N	2.26	0.69
5:F:27:SER:O	5:F:34:ARG:NH2	2.27	0.68
9:J:174:ILE:HG23	9:J:175:LYS:HG2	1.74	0.68
28:e:63:ASP:OD2	40:r:338:HIS:NE2	2.27	0.68
56:k:101:CDL:H162	35:l:589:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.75	0.68
1:A:159:ARG:NH2	14:O:176:CYS:O	2.27	0.67
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.60	0.67
39:p:97:TYR:HB3	39:p:179:MET:HG3	1.77	0.67
21:W:57:ARG:HB3	41:s:316:PRO:HG3	1.76	0.67
1:A:33:GLY:HA3	1:A:294:VAL:HG23	1.77	0.67
9:J:188:GLU:HG3	9:J:200:ILE:HD13	1.77	0.67
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.77	0.67
37:n:28:ASP:OD2	40:r:3:LYS:NZ	2.28	0.67
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.28	0.67
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.23	0.66
3:C:55:ASN:ND2	3:C:187:GLU:O	2.27	0.66
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.28	0.66
1:A:116:ASN:O	1:A:245:VAL:HG23	1.95	0.66
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.76	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.29	0.66
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.44	0.66
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.29	0.66
35:l:11:THR:HG21	35:l:47:SER:HB3	1.78	0.66
36:m:170:GLU:OE2	36:m:173:ARG:NH2	2.29	0.65
1:A:185:ASN:OD1	1:A:190:GLY:N	2.28	0.65
32:i:41:ILE:HG21	34:k:73:LEU:HD21	1.77	0.65
32:i:278:MET:O	32:i:282:MET:HG3	1.96	0.65
25:b:28:LEU:HD22	25:b:32:GLU:HG2	1.79	0.65
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.29	0.65
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.77	0.65
1:A:89:GLY:HA2	1:A:244:ASN:HD21	1.55	0.65
7:H:38:ILE:O	7:H:45:ARG:NH1	2.30	0.65
11:L:78:ARG:NH1	11:L:148:GLU:OE1	2.30	0.65
26:c:116:ARG:HG2	48:l:703:PEE:H49	1.78	0.65
3:C:71:CYS:HB2	45:C:301:SF4:S4	2.38	0.64
5:F:24:CYS:N	5:F:58:CYS:SG	2.70	0.64
35:l:496:MET:O	35:l:500:LEU:HD12	1.98	0.64
3:C:188:LYS:O	3:C:192:ILE:HD12	1.97	0.64
56:l:701:CDL:H411	40:r:371:PRO:HD2	1.78	0.64
6:G:116:VAL:HG12	6:G:120:MET:HE2	1.78	0.63
13:N:29:ARG:NH2	13:N:64:TYR:O	2.30	0.63
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.80	0.63
56:V:201:CDL:H521	35:l:577:VAL:HA	1.80	0.63
44:w:250:SER:O	44:w:280:LYS:NZ	2.32	0.63
1:A:40:ARG:NH1	1:A:289:GLU:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:107:ARG:HA	43:v:110:GLN:HG2	1.81	0.63
12:M:136:GLU:HG2	12:M:242:PRO:HG3	1.80	0.63
11:L:109:ASN:ND2	11:L:111:LEU:O	2.30	0.62
1:A:227:PRO:HD2	12:M:94:MET:HE1	1.80	0.62
42:u:85:TYR:CZ	42:u:89:ILE:HD11	2.33	0.62
27:d:69:ARG:NH2	37:n:46:LYS:O	2.32	0.62
6:X:117:GLU:OE1	39:p:45:ARG:NH1	2.31	0.62
39:p:62:GLN:O	39:p:66:GLN:HG3	2.00	0.62
16:Q:92:HIS:NE2	16:Q:193:ASP:OD2	2.32	0.62
24:a:53:ARG:NH2	25:b:29:SER:O	2.33	0.62
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.82	0.61
32:i:64:ALA:O	32:i:68:MET:HG2	2.00	0.61
40:r:265:SER:O	40:r:269:MET:HG3	1.99	0.61
35:l:65:ASN:OD1	35:l:66:TRP:N	2.34	0.61
7:H:47:TYR:O	7:H:51:ILE:HG13	2.00	0.61
35:l:473:PRO:HG2	35:l:475:MET:HE2	1.83	0.61
1:A:263:ALA:HA	1:A:271:SER:HB3	1.82	0.61
32:i:4:ILE:O	32:i:8:THR:HG23	2.01	0.61
13:N:120:THR:HG22	13:N:122:GLN:H	1.66	0.60
8:I:27:ARG:NH2	16:Q:212:GLU:OE2	2.34	0.60
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.83	0.60
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.81	0.60
21:W:90:ASN:ND2	21:W:123:GLU:O	2.35	0.60
23:Z:23:LYS:HB3	23:Z:25:GLU:HG2	1.84	0.60
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.84	0.60
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.84	0.60
42:u:107:PHE:O	42:u:111:VAL:HG22	2.02	0.60
1:A:88:ARG:C	1:A:244:ASN:HD22	2.09	0.60
56:l:702:CDL:HA31	56:l:702:CDL:H712	1.82	0.60
1:A:41:ILE:HG13	1:A:253:THR:HG21	1.83	0.60
1:A:109:ARG:NH1	1:A:237:GLY:O	2.35	0.60
32:i:243:LEU:HD23	56:i:402:CDL:H361	1.83	0.60
1:A:299:LEU:HD12	1:A:303:HIS:HD2	1.68	0.59
41:s:79:LEU:HD22	41:s:222:MET:HG2	1.83	0.59
22:Y:62:SER:OG	35:l:371:THR:OG1	2.20	0.59
5:F:62:GLN:OE1	5:F:78:SER:OG	2.20	0.59
12:M:144:MET:HE2	16:Q:383:LYS:HB2	1.85	0.59
5:F:90:THR:O	5:F:94:VAL:HG23	2.03	0.59
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.84	0.59
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.83	0.59
25:b:10:LEU:O	25:b:14:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:O	1:A:159:ARG:NH1	2.36	0.59
3:C:192:ILE:HG21	9:J:86:CYS:HA	1.84	0.59
43:v:81:LYS:HE2	43:v:81:LYS:HA	1.84	0.59
27:d:50:GLU:O	27:d:54:GLN:HG3	2.03	0.59
32:i:87:THR:CG2	32:i:88:LYS:H	2.16	0.59
12:M:472:PRO:O	12:M:510:TRP:NE1	2.31	0.59
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.84	0.59
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.36	0.58
32:i:49:ASN:O	32:i:51:ARG:N	2.36	0.58
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.35	0.58
16:Q:68:ASP:O	32:i:49:ASN:HB2	2.02	0.58
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.37	0.58
1:A:244:ASN:N	46:A:502:FMN:O1P	2.35	0.58
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.85	0.58
43:v:22:MET:HG2	43:v:23:PRO:HA	1.85	0.58
20:V:4:THR:O	20:V:8:LYS:HG3	2.03	0.58
28:e:129:ARG:NH1	28:e:136:LEU:O	2.36	0.58
27:d:115:GLN:HG2	35:l:62:ILE:HG12	1.86	0.58
17:S:51:ASP:OD2	42:u:22:SER:OG	2.20	0.58
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.37	0.58
9:J:299:ARG:NH1	9:J:320:GLU:OE1	2.37	0.58
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.84	0.58
32:i:87:THR:HG22	32:i:88:LYS:H	1.69	0.58
56:l:701:CDL:H452	40:r:445:LEU:HB3	1.86	0.58
42:u:72:ARG:O	42:u:76:ARG:HG3	2.03	0.58
3:C:119:LYS:NZ	33:j:42:ASP:OD1	2.34	0.58
44:w:230:THR:HG22	44:w:232:ALA:H	1.67	0.58
35:l:228:GLY:HA3	48:l:703:PEE:H37	1.86	0.58
1:A:89:GLY:O	47:A:503:NAI:H2N	2.04	0.57
1:A:357:MET:HB3	1:A:361:THR:HG21	1.86	0.57
9:J:192:ARG:NH1	9:J:198:ALA:O	2.37	0.57
44:w:125:ASP:O	44:w:130:ARG:NH2	2.37	0.57
56:l:702:CDL:H721	56:l:702:CDL:H321	1.86	0.57
32:i:68:MET:HA	32:i:68:MET:HE3	1.86	0.57
41:s:307:LEU:HA	41:s:310:MET:HE3	1.86	0.57
21:W:80:ASP:OD2	42:u:47:ARG:NE	2.26	0.57
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.40	0.57
40:r:433:GLU:O	40:r:437:MET:HG2	2.04	0.57
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.69	0.57
13:N:68:MET:HG3	13:N:69:ASN:H	1.69	0.57
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:36:MET:HE1	49:g:201:PLX:H393	1.85	0.57
16:Q:42:GLU:OE1	28:e:54:ARG:NH1	2.38	0.57
24:a:74:TYR:O	28:e:96:SER:OG	2.22	0.57
1:A:36:LYS:H	1:A:36:LYS:HD3	1.68	0.56
7:H:81:ILE:O	7:H:85:GLU:HG3	2.05	0.56
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.37	0.56
35:l:250:SER:HB2	35:l:333:ALA:HA	1.85	0.56
5:F:46:LYS:HE2	12:M:674:LEU:HD11	1.86	0.56
9:J:173:ASP:HB3	9:J:176:SER:HB2	1.87	0.56
43:v:103:GLU:OE2	43:v:106:ARG:NH2	2.38	0.56
15:P:125:ARG:O	15:P:125:ARG:HG3	2.04	0.56
42:u:85:TYR:CE1	42:u:104:GLN:HB2	2.40	0.56
1:A:448:GLU:O	1:A:452:GLN:HG2	2.05	0.56
4:E:64:ARG:NH2	6:G:117:GLU:OE2	2.37	0.56
15:P:50:ARG:NH1	15:P:80:CYS:SG	2.78	0.56
41:s:249:PRO:HG2	42:u:99:HIS:NE2	2.19	0.56
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.36	0.56
23:Z:30:GLU:O	23:Z:34:GLU:HG3	2.06	0.56
26:c:164:ASN:HA	26:c:181:VAL:HG22	1.88	0.56
35:l:561:ILE:HG13	35:l:562:LEU:H	1.70	0.56
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.86	0.56
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.87	0.56
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.87	0.56
6:G:141:PRO:O	6:G:145:VAL:HG23	2.06	0.55
12:M:308:ARG:NH2	12:M:578:PRO:O	2.39	0.55
22:Y:54:GLN:NE2	35:l:445:GLU:OE2	2.39	0.55
32:i:246:VAL:HG21	56:i:402:CDL:H362	1.87	0.55
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.88	0.55
28:e:65:ASN:HB3	28:e:68:GLU:HG2	1.88	0.55
33:j:18:VAL:HG22	41:s:222:MET:HE1	1.87	0.55
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.38	0.55
32:i:211:MET:HG3	32:i:333:SER:HB2	1.88	0.55
35:l:136:ASN:HA	35:l:197:ASP:HA	1.86	0.55
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.88	0.55
9:J:143:ASP:OD1	9:J:147:LYS:NZ	2.39	0.55
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.88	0.55
26:c:186:ILE:HG21	43:v:101:GLU:HG2	1.88	0.55
34:k:4:VAL:O	34:k:8:ILE:HG12	2.07	0.55
44:w:147:LEU:HD13	44:w:294:LEU:HD11	1.89	0.55
12:M:81:GLU:HG3	12:M:108:LYS:HD2	1.87	0.55
24:a:79:GLY:HA3	56:a:201:CDL:H222	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:268:GLN:O	32:i:271:THR:OG1	2.23	0.55
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.22	0.55
9:J:61:ALA:HB3	9:J:82:VAL:HG13	1.89	0.55
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.79	0.55
31:h:89:GLU:OE1	31:h:91:LYS:NZ	2.39	0.55
41:s:213:VAL:HG13	41:s:214:GLU:HG2	1.88	0.55
1:A:89:GLY:N	1:A:244:ASN:ND2	2.40	0.55
29:f:40:ASP:OD1	29:f:40:ASP:N	2.35	0.55
31:h:29:ILE:HG21	36:m:138:GLU:HG3	1.89	0.55
35:l:542:LEU:O	40:r:278:ARG:NH1	2.40	0.55
44:w:204:VAL:HG21	44:w:249:MET:HG2	1.89	0.55
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.89	0.55
43:v:27:PRO:O	43:v:34:ARG:NH1	2.40	0.55
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.88	0.54
15:P:211:ARG:NE	15:P:222:GLU:OE1	2.40	0.54
40:r:118:PHE:O	40:r:122:PHE:HB3	2.07	0.54
9:J:206:ILE:HG13	52:J:401:NDP:H42N	1.90	0.54
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.89	0.54
21:W:93:GLU:O	21:W:97:ILE:HG13	2.08	0.54
30:g:33:LEU:HD22	30:g:71:VAL:HG13	1.89	0.54
1:A:102:MET:HG3	1:A:241:THR:OG1	2.08	0.54
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.73	0.54
12:M:428:LYS:NZ	12:M:443:ASP:OD2	2.31	0.54
41:s:76:ILE:O	41:s:80:SER:OG	2.23	0.54
48:U:101:PEE:H26	41:s:295:PRO:HB3	1.89	0.54
32:i:20:VAL:HG13	32:i:29:ILE:HG23	1.90	0.54
56:l:702:CDL:H371	56:l:702:CDL:H601	1.89	0.54
20:V:140:LYS:HG3	20:V:141:VAL:HG13	1.90	0.54
30:g:47:ASP:O	30:g:51:ARG:HG2	2.08	0.54
35:l:100:ILE:HG21	35:l:246:LEU:HB2	1.90	0.54
35:l:359:MET:O	35:l:436:ARG:NH2	2.41	0.54
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.89	0.54
8:I:40:LYS:HB3	21:W:7:LYS:H	1.73	0.53
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.89	0.53
36:m:45:LEU:HD12	36:m:50:SER:HA	1.90	0.53
1:A:145:GLY:O	1:A:149:MET:HG3	2.07	0.53
8:I:46:SER:O	8:I:52:ASN:ND2	2.39	0.53
32:i:265:MET:HE1	42:u:167:LEU:HD11	1.90	0.53
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.90	0.53
36:m:129:ASP:O	36:m:130:THR:OG1	2.22	0.53
41:s:221:ALA:O	41:s:225:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:91:TYR:CD1	42:u:91:TYR:C	2.85	0.53
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.40	0.53
6:G:113:LEU:O	6:G:117:GLU:HG3	2.09	0.53
18:T:69:ASP:O	18:T:73:GLU:HG3	2.08	0.53
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.91	0.53
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.25	0.53
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.88	0.53
35:l:97:THR:HG22	35:l:101:MET:HE3	1.91	0.53
56:l:701:CDL:H522	56:l:701:CDL:HA62	1.91	0.53
35:l:419:THR:HA	35:l:422:TYR:CE2	2.43	0.53
4:E:19:PRO:HB3	11:L:53:ILE:HD13	1.91	0.53
12:M:299:ARG:HH21	12:M:300:GLN:HE21	1.57	0.53
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.90	0.53
41:s:112:ALA:O	41:s:115:SER:OG	2.22	0.53
3:C:167:PRO:HG3	16:Q:222:MET:HE2	1.90	0.53
21:W:120:MET:HE3	36:m:126:VAL:HB	1.90	0.53
25:b:106:PRO:HG3	43:v:45:GLU:HG2	1.90	0.53
2:B:63:TRP:HE1	48:B:303:PEE:H13	1.74	0.53
12:M:647:GLU:HB2	12:M:654:VAL:HG11	1.90	0.53
4:E:25:MET:HE2	4:E:25:MET:HA	1.91	0.53
3:C:78:HIS:HD1	16:Q:208:GLU:HG2	1.73	0.52
8:I:27:ARG:HD2	16:Q:209:LYS:HD3	1.91	0.52
56:l:701:CDL:H352	40:r:361:VAL:HG13	1.90	0.52
3:C:44:GLU:OE1	3:C:195:ARG:NH1	2.43	0.52
9:J:142:GLU:HG2	9:J:147:LYS:HZ2	1.74	0.52
41:s:215:TYR:HD2	41:s:219:PRO:HB2	1.74	0.52
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.10	0.52
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.92	0.52
31:h:39:GLU:OE2	42:u:144:SER:OG	2.25	0.52
39:p:98:LYS:HG2	39:p:178:PRO:HG3	1.92	0.52
40:r:310:MET:HB3	40:r:455:LEU:HD22	1.91	0.52
43:v:69:CYS:SG	43:v:80:CYS:HB3	2.49	0.52
33:j:27:LEU:HD21	41:s:60:PRO:HD2	1.90	0.52
35:l:136:ASN:OD1	35:l:136:ASN:N	2.43	0.52
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.44	0.52
37:n:54:GLU:HG2	37:n:55:VAL:HG22	1.90	0.52
44:w:49:THR:HG21	44:w:151:LEU:HD22	1.92	0.52
44:w:171:GLU:HB3	44:w:175:ARG:HH21	1.74	0.52
17:S:63:THR:HG23	42:u:21:SER:HB2	1.92	0.52
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.91	0.52
41:s:152:SER:HA	41:s:155:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.90	0.52
14:O:222:ARG:NH1	14:O:226:GLU:O	2.36	0.52
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.21	0.52
21:W:120:MET:O	21:W:121:MET:HB3	2.08	0.52
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.91	0.52
11:L:154:LYS:O	11:L:156:LYS:NZ	2.43	0.52
31:h:2:PRO:HA	32:i:140:SER:HB2	1.92	0.52
35:l:331:MET:HG3	35:l:387:THR:OG1	2.10	0.52
40:r:370:PRO:HG3	40:r:375:LEU:HG	1.92	0.52
11:L:87:MET:HE2	12:M:274:LEU:HD21	1.91	0.51
11:L:105:GLU:HA	12:M:611:THR:HG21	1.92	0.51
1:A:171:VAL:O	1:A:175:GLU:HG2	2.10	0.51
12:M:311:LYS:HG3	12:M:313:LEU:HG	1.91	0.51
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.91	0.51
32:i:194:LEU:HD12	32:i:201:THR:HG21	1.92	0.51
38:o:56:ARG:NH2	40:r:422:HIS:O	2.43	0.51
48:C:302:PEE:H65	41:s:53:LEU:HD21	1.93	0.51
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.43	0.51
20:V:95:CYS:HA	20:V:115:CYS:HA	1.93	0.51
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.92	0.51
12:M:338:VAL:O	12:M:363:SER:OG	2.24	0.51
19:U:69:HIS:CE1	19:U:71:GLN:HG3	2.45	0.51
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.42	0.51
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.35	0.51
36:m:94:VAL:O	36:m:98:MET:HG2	2.11	0.51
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.92	0.51
20:V:67:GLY:HA2	56:V:201:CDL:H221	1.91	0.51
7:H:22:GLU:H	7:H:22:GLU:CD	2.18	0.51
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.93	0.51
19:U:26:GLY:O	19:U:30:ILE:HG13	2.11	0.50
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.92	0.50
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.33	0.50
11:L:158:LYS:NZ	12:M:69:LEU:O	2.40	0.50
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.93	0.50
34:k:37:MET:HA	34:k:37:MET:HE3	1.92	0.50
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.92	0.50
14:O:133:GLN:OE1	14:O:187:GLN:NE2	2.44	0.50
1:A:185:ASN:ND2	1:A:187:CYS:O	2.44	0.50
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.50
21:W:63:GLU:OE1	42:u:119:ARG:NH2	2.43	0.50
35:l:76:LEU:HD21	35:l:196:TRP:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:489:ILE:O	12:M:493:VAL:HG23	2.12	0.50
39:p:68:GLU:OE1	39:p:68:GLU:HA	2.11	0.50
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.11	0.50
32:i:36:ASN:O	32:i:40:MET:HB2	2.12	0.50
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.44	0.50
42:u:20:VAL:HG23	42:u:25:LEU:HG	1.93	0.50
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.93	0.50
22:Y:40:ILE:HD11	35:l:444:ASN:HB2	1.94	0.50
31:h:72:THR:O	31:h:76:LEU:HD23	2.12	0.50
40:r:344:LEU:O	40:r:420:THR:HG21	2.12	0.50
44:w:256:LEU:HD11	44:w:276:LEU:HD11	1.93	0.50
1:A:445:GLU:OE2	1:A:445:GLU:N	2.44	0.50
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.94	0.50
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.93	0.50
44:w:85:HIS:NE2	44:w:160:GLU:OE2	2.34	0.50
1:A:314:LEU:HD11	1:A:317:VAL:HG23	1.94	0.49
1:A:424:ILE:HD11	12:M:74:ASN:HA	1.94	0.49
9:J:48:ARG:NH2	9:J:98:GLY:O	2.45	0.49
35:l:298:ILE:O	35:l:302:VAL:HG23	2.11	0.49
38:o:65:LEU:HD11	40:r:343:ILE:HD11	1.94	0.49
44:w:256:LEU:HD21	44:w:276:LEU:HD21	1.94	0.49
2:B:39:LYS:HD2	16:Q:335:GLU:HG2	1.94	0.49
32:i:291:TYR:OH	48:i:401:PEE:O1P	2.25	0.49
10:K:77:GLN:OE1	10:K:77:GLN:N	2.45	0.49
11:L:84:ARG:NH1	11:L:88:GLN:O	2.46	0.49
25:b:86:LEU:O	25:b:91:THR:HG23	2.12	0.49
40:r:282:LEU:HD21	40:r:359:TRP:HH2	1.78	0.49
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.94	0.49
41:s:101:GLY:O	41:s:105:MET:HG2	2.12	0.49
41:s:200:LEU:HG	41:s:282:TYR:HB3	1.95	0.49
1:A:141:GLY:HA2	1:A:252:PRO:HD3	1.95	0.49
2:B:124:PRO:O	16:Q:127:LYS:NZ	2.31	0.49
40:r:212:LEU:HD21	49:r:502:PLX:H212	1.93	0.49
44:w:204:VAL:HB	44:w:255:VAL:HG22	1.94	0.49
1:A:98:LYS:NZ	46:A:502:FMN:H5'2	2.28	0.49
12:M:162:ASP:O	18:T:104:LYS:NZ	2.42	0.49
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.48	0.49
1:A:107:ASP:OD1	1:A:107:ASP:N	2.44	0.49
15:P:113:ASP:OD1	16:Q:423:LYS:NZ	2.43	0.49
16:Q:36:GLN:NE2	40:r:137:GLY:O	2.46	0.49
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:54:ASN:ND2	41:s:313:SER:O	2.45	0.49
21:W:82:ARG:NH1	31:h:106:PRO:O	2.45	0.49
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.94	0.49
35:l:245:ALA:O	35:l:249:SER:OG	2.28	0.49
12:M:650:SER:OG	12:M:652:ASN:OD1	2.30	0.49
14:O:57:PRO:O	14:O:61:LYS:HG3	2.13	0.49
16:Q:259:GLU:OE1	21:W:23:ARG:NH1	2.37	0.49
12:M:43:VAL:HG21	12:M:96:VAL:HG21	1.94	0.49
17:S:66:LEU:HD13	42:u:75:LYS:HB2	1.93	0.49
36:m:82:VAL:H	36:m:85:SER:HB3	1.77	0.49
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.48	0.49
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.31	0.49
1:A:185:ASN:O	1:A:187:CYS:N	2.46	0.48
9:J:375:VAL:HG23	9:J:375:VAL:O	2.12	0.48
33:j:69:ILE:O	33:j:73:LEU:HG	2.13	0.48
37:n:18:PRO:O	37:n:21:PHE:HB3	2.13	0.48
42:u:77:HIS:CD2	42:u:115:LEU:HD21	2.48	0.48
1:A:250:VAL:O	1:A:254:ILE:HG13	2.13	0.48
1:A:455:LEU:O	1:A:458:GLN:NE2	2.45	0.48
2:B:181:GLU:OE2	9:J:101:GLY:N	2.43	0.48
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.46	0.48
41:s:69:SER:OG	56:s:401:CDL:OB4	2.25	0.48
41:s:227:GLU:O	41:s:231:ILE:HG12	2.14	0.48
42:u:83:THR:HA	42:u:86:TRP:CD1	2.48	0.48
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.96	0.48
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.96	0.48
32:i:236:LYS:NZ	32:i:314:LYS:O	2.40	0.48
36:m:78:MET:O	36:m:80:PRO:HD3	2.13	0.48
37:n:56:THR:HG1	37:n:57:TRP:CD1	2.32	0.48
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.48	0.48
1:A:88:ARG:C	1:A:244:ASN:ND2	2.71	0.48
56:i:402:CDL:H231	56:i:402:CDL:H332	1.94	0.48
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.78	0.48
16:Q:438:MET:HE2	16:Q:438:MET:HB3	1.80	0.48
18:T:79:VAL:HG21	18:T:84:ILE:HD13	1.96	0.48
21:W:121:MET:HE2	36:m:130:THR:HG23	1.95	0.48
6:X:114:ASP:O	6:X:118:ILE:HG13	2.13	0.48
23:Z:49:GLU:OE1	39:p:34:ARG:HB3	2.13	0.48
30:g:51:ARG:HB2	30:g:53:ARG:HG3	1.95	0.48
43:v:52:MET:HB2	43:v:55:GLN:HG3	1.93	0.48
6:G:111:ASP:OD1	6:G:111:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:18:MET:HE2	34:k:56:ALA:HA	1.94	0.48
1:A:36:LYS:HG2	1:A:38:GLU:HG2	1.95	0.48
9:J:313:TRP:CD1	53:J:402:UQ:H72	2.49	0.48
21:W:84:LEU:HD13	42:u:8:PRO:HG2	1.95	0.48
25:b:101:LYS:O	43:v:50:GLN:NE2	2.35	0.48
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.79	0.48
48:j:201:PEE:H13	41:s:72:ILE:HD13	1.95	0.48
40:r:329:LEU:O	40:r:332:THR:OG1	2.31	0.48
53:s:402:UQ:H221	53:s:402:UQ:H262	1.65	0.48
5:F:36:PHE:CD1	5:F:40:ARG:HB2	2.48	0.48
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.96	0.48
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.49	0.48
56:l:701:CDL:H822	56:l:701:CDL:H631	1.96	0.48
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.96	0.48
43:v:92:HIS:O	43:v:96:VAL:HG13	2.14	0.48
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.49	0.48
13:N:14:VAL:HA	13:N:23:TYR:CD1	2.49	0.48
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.95	0.48
38:o:91:ALA:O	38:o:95:ILE:HB	2.13	0.48
12:M:419:ARG:NH1	12:M:439:THR:O	2.47	0.48
12:M:651:PRO:O	12:M:654:VAL:HG22	2.14	0.48
56:V:201:CDL:H322	56:V:201:CDL:H352	1.64	0.48
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.96	0.48
32:i:322:GLN:HG2	32:i:323:MET:N	2.29	0.48
33:j:66:ASP:O	33:j:69:ILE:HG13	2.13	0.48
34:k:17:ALA:HB2	56:k:101:CDL:H812	1.95	0.48
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.49	0.48
38:o:102:TYR:HB2	40:r:263:MET:HG3	1.96	0.48
38:o:118:GLU:HG3	38:o:120:LYS:HG2	1.96	0.48
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.47	0.47
26:c:96:ASP:OD1	26:c:96:ASP:N	2.47	0.47
27:d:6:ASP:OD2	28:e:127:LYS:NZ	2.31	0.47
34:k:23:ARG:NE	56:k:101:CDL:OB4	2.46	0.47
41:s:145:THR:HG21	41:s:293:PHE:HB3	1.95	0.47
41:s:170:GLU:OE2	42:u:98:ARG:NH1	2.47	0.47
1:A:312:ASP:HA	1:A:329:LYS:HE3	1.96	0.47
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.49	0.47
10:K:80:GLU:HG3	10:K:80:GLU:O	2.14	0.47
18:T:47:ASP:O	18:T:52:ARG:NH1	2.47	0.47
2:B:109:GLY:HA3	18:T:70:LEU:HD23	1.96	0.47
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.96	0.47
9:J:129:LEU:HD23	9:J:167:ILE:HG13	1.95	0.47
26:c:166:LEU:HD12	26:c:170:ARG:HH21	1.79	0.47
27:d:80:LYS:N	30:g:108:LYS:HZ3	2.06	0.47
33:j:33:LYS:HD3	41:s:61:LEU:HD21	1.95	0.47
2:B:113:CYS:O	2:B:141:ARG:NH1	2.46	0.47
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.50	0.47
26:c:156:VAL:HG12	43:v:99:MET:HG3	1.96	0.47
56:i:402:CDL:H872	56:n:101:CDL:H771	1.97	0.47
36:m:65:LEU:N	41:s:114:TYR:OH	2.48	0.47
42:u:16:GLN:HB3	42:u:68:LEU:HD11	1.96	0.47
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.95	0.47
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.50	0.47
56:l:701:CDL:H242	48:l:704:PEE:H34	1.95	0.47
37:n:19:VAL:HA	37:n:22:VAL:HG22	1.96	0.47
2:B:111:GLU:O	2:B:141:ARG:NH1	2.48	0.47
13:N:144:TYR:HD1	13:N:144:TYR:H	1.61	0.47
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	1.95	0.47
19:U:20:VAL:HA	48:U:101:PEE:H64	1.96	0.47
44:w:105:ASP:OD1	44:w:106:VAL:N	2.48	0.47
2:B:41:VAL:HG12	8:I:113:LEU:HD12	1.95	0.47
2:B:50:MET:HE3	2:B:50:MET:O	2.15	0.47
2:B:179:THR:OG1	2:B:182:GLU:OE2	2.33	0.47
9:J:304:LEU:HD21	49:J:403:PLX:H312	1.97	0.47
12:M:265:THR:HG22	12:M:270:VAL:HA	1.97	0.47
20:V:39:TYR:HB3	56:V:201:CDL:H712	1.97	0.47
6:X:122:MET:HG3	6:X:144:ILE:HG21	1.96	0.47
56:a:201:CDL:H312	48:l:704:PEE:H59	1.96	0.47
28:e:53:ILE:O	44:w:315:PRO:HB3	2.14	0.47
32:i:68:MET:HE1	34:k:37:MET:SD	2.55	0.47
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.49	0.47
37:n:24:GLY:HA2	40:r:6:ILE:HD12	1.95	0.47
41:s:209:SER:HB3	41:s:213:VAL:HA	1.97	0.47
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.97	0.47
1:A:210:THR:HB	1:A:224:ARG:H	1.79	0.47
12:M:249:GLU:HG3	12:M:262:VAL:HG22	1.96	0.47
22:Y:61:PHE:CD2	35:l:458:LEU:HD23	2.50	0.47
24:a:106:VAL:O	37:n:50:ARG:NH2	2.47	0.47
32:i:74:ILE:HG13	32:i:98:MET:HE1	1.96	0.47
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.97	0.47
41:s:207:LEU:O	41:s:209:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:CYS:SG	1:A:426:ALA:N	2.88	0.47
2:B:59:GLN:OE1	2:B:64:THR:OG1	2.33	0.47
33:j:10:ASN:ND2	41:s:84:THR:OG1	2.45	0.47
48:r:501:PEE:H29	48:r:501:PEE:H71	1.97	0.47
43:v:42:THR:O	43:v:46:MET:HG3	2.14	0.47
12:M:249:GLU:HG2	12:M:276:ARG:HD3	1.95	0.47
21:W:38:VAL:O	21:W:42:THR:HG22	2.15	0.47
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.97	0.47
35:l:227:PHE:O	35:l:230:HIS:ND1	2.46	0.47
42:u:139:GLU:OE2	42:u:139:GLU:N	2.45	0.47
26:c:68:ASP:OD1	26:c:68:ASP:N	2.48	0.46
34:k:25:HIS:ND1	34:k:88:ASP:OD1	2.31	0.46
39:p:12:HIS:O	39:p:16:VAL:HG23	2.14	0.46
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.46
32:i:87:THR:HG22	32:i:88:LYS:N	2.30	0.46
56:l:701:CDL:H572	56:l:701:CDL:H861	1.97	0.46
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.97	0.46
11:L:78:ARG:O	11:L:99:MET:HA	2.15	0.46
21:W:121:MET:O	21:W:121:MET:HG3	2.16	0.46
6:X:87:LEU:HD12	6:X:141:PRO:HG3	1.97	0.46
41:s:78:ALA:HB2	41:s:115:SER:HB2	1.96	0.46
20:V:14:GLU:OE2	20:V:126:LYS:NZ	2.46	0.46
49:g:201:PLX:H122	49:g:201:PLX:H91	1.60	0.46
35:l:37:LYS:HB3	35:l:37:LYS:HE3	1.76	0.46
16:Q:144:MET:O	16:Q:148:GLU:HG3	2.15	0.46
21:W:88:ARG:NH1	21:W:92:GLU:OE1	2.48	0.46
27:d:140:GLN:O	27:d:144:SER:HB2	2.16	0.46
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.50	0.46
40:r:357:THR:O	40:r:361:VAL:HG23	2.15	0.46
40:r:396:MET:H	40:r:396:MET:HG2	1.54	0.46
43:v:3:ALA:O	43:v:7:ARG:HG3	2.15	0.46
7:H:40:LYS:HA	7:H:45:ARG:HD3	1.97	0.46
9:J:212:ARG:O	9:J:216:TYR:CB	2.64	0.46
17:S:13:ALA:HB2	41:s:264:LEU:HD11	1.98	0.46
6:X:80:LYS:HE3	6:X:84:LEU:HD12	1.97	0.46
35:l:373:LEU:HD22	35:l:431:PHE:CE2	2.50	0.46
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.47	0.46
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.97	0.46
33:j:73:LEU:O	41:s:160:TYR:OH	2.24	0.46
35:l:10:THR:O	35:l:14:ILE:HG23	2.16	0.46
56:l:701:CDL:H641	49:r:503:PLX:H102	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:93:TYR:O	44:w:96:SER:OG	2.33	0.46
31:h:106:PRO:HG2	42:u:17:GLU:HB3	1.97	0.46
48:l:703:PEE:H62	40:r:401:MET:HE1	1.98	0.46
56:o:201:CDL:H512	56:o:201:CDL:H712	1.97	0.46
56:o:201:CDL:OB7	56:o:201:CDL:O1	2.29	0.46
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.76	0.46
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.80	0.46
7:H:40:LYS:HB2	7:H:40:LYS:HE2	1.69	0.46
10:K:78:HIS:HA	10:K:81:TYR:CD2	2.51	0.46
14:O:197:THR:H	14:O:200:ASP:HB2	1.81	0.46
56:a:201:CDL:HB4	56:a:201:CDL:H512	1.76	0.46
31:h:85:LYS:HE3	31:h:86:LEU:HD22	1.98	0.46
40:r:262:LEU:O	40:r:266:MET:HG3	2.16	0.46
44:w:287:ASP:OD1	44:w:289:ARG:HG2	2.16	0.46
3:C:54:VAL:HG21	48:C:302:PEE:H55	1.98	0.46
32:i:45:MET:HB3	32:i:45:MET:HE2	1.77	0.46
48:j:201:PEE:H26	56:s:401:CDL:H162	1.98	0.46
56:l:701:CDL:H202	56:l:701:CDL:H231	1.86	0.46
14:O:46:GLU:OE1	14:O:46:GLU:N	2.47	0.45
14:O:224:SER:HB2	14:O:226:GLU:HG2	1.98	0.45
15:P:43:THR:HA	15:P:47:ILE:HD12	1.98	0.45
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.98	0.45
56:i:402:CDL:H351	56:i:402:CDL:H381	1.82	0.45
37:n:54:GLU:OE1	37:n:54:GLU:N	2.45	0.45
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.97	0.45
2:B:63:TRP:O	2:B:67:VAL:HG23	2.17	0.45
9:J:250:ILE:O	9:J:254:LYS:HG3	2.16	0.45
10:K:75:ASN:O	10:K:78:HIS:NE2	2.49	0.45
20:V:22:ALA:O	20:V:26:THR:OG1	2.30	0.45
22:Y:100:LEU:HB2	43:v:111:ARG:NH1	2.31	0.45
41:s:85:MET:SD	41:s:108:MET:HB2	2.56	0.45
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.97	0.45
20:V:44:LYS:HE2	20:V:44:LYS:HB2	1.76	0.45
26:c:85:GLU:OE2	26:c:119:THR:OG1	2.34	0.45
27:d:142:ARG:HD2	28:e:138:GLU:O	2.17	0.45
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.99	0.45
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.51	0.45
35:l:561:ILE:HG13	35:l:562:LEU:N	2.31	0.45
1:A:36:LYS:H	1:A:36:LYS:CD	2.29	0.45
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.50	0.45
9:J:212:ARG:O	9:J:216:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:86:LEU:HA	25:b:90:VAL:HB	1.99	0.45
30:g:85:TYR:CE2	42:u:165:SER:HB2	2.51	0.45
49:g:201:PLX:H102	49:g:201:PLX:H72	1.56	0.45
32:i:7:THR:O	32:i:11:MET:HG3	2.17	0.45
35:l:395:ILE:O	35:l:399:VAL:HG23	2.17	0.45
40:r:220:HIS:CE1	40:r:231:LEU:HB3	2.52	0.45
1:A:316:ALA:HB1	1:A:326:LEU:HD12	1.99	0.45
1:A:325:PRO:HG3	1:A:433:TRP:HB3	1.98	0.45
3:C:92:VAL:HG21	53:s:402:UQ:H103	1.98	0.45
9:J:168:SER:O	9:J:203:PRO:HD2	2.17	0.45
49:J:403:PLX:H272	49:J:403:PLX:H301	1.43	0.45
11:L:131:LYS:NZ	11:L:149:GLU:OE1	2.49	0.45
12:M:217:GLU:H	12:M:217:GLU:CD	2.25	0.45
28:e:72:ASP:OD1	28:e:72:ASP:N	2.44	0.45
56:l:701:CDL:H372	56:l:701:CDL:H342	1.70	0.45
43:v:106:ARG:HA	43:v:109:LEU:HD12	1.99	0.45
44:w:300:ASN:ND2	44:w:303:GLU:HB2	2.32	0.45
2:B:85:ASN:HB2	13:N:58:ARG:HH21	1.81	0.45
12:M:250:SER:OG	12:M:251:ILE:N	2.47	0.45
34:k:4:VAL:HG23	36:m:10:SER:HB3	1.99	0.45
43:v:103:GLU:OE2	43:v:107:ARG:NH2	2.49	0.45
1:A:340:ASP:OD1	1:A:340:ASP:N	2.50	0.45
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.57	0.45
6:G:119:ILE:O	6:G:123:GLU:HG3	2.17	0.45
6:G:138:LEU:HD21	6:G:147:TYR:CD2	2.52	0.45
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.99	0.45
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.99	0.45
14:O:199:LYS:HB2	14:O:199:LYS:HE3	1.75	0.45
15:P:118:ASP:OD1	15:P:125:ARG:CD	2.65	0.45
32:i:54:GLU:OE2	34:k:95:LEU:HB2	2.17	0.45
33:j:92:LEU:HD13	41:s:302:MET:HG2	1.99	0.45
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.45
40:r:12:LEU:HD22	40:r:97:THR:HG23	1.98	0.45
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.99	0.45
4:E:101:THR:OG1	15:P:219:VAL:O	2.25	0.45
5:F:92:GLU:O	5:F:96:SER:OG	2.20	0.45
15:P:44:ARG:NH1	15:P:44:ARG:HB2	2.32	0.45
27:d:101:GLU:OE1	28:e:119:ARG:NE	2.43	0.45
39:p:97:TYR:HB2	39:p:178:PRO:HG2	1.98	0.45
41:s:84:THR:O	41:s:87:VAL:HG22	2.17	0.45
41:s:267:THR:O	41:s:271:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.98	0.45
6:G:83:VAL:O	6:G:87:LEU:HD13	2.17	0.45
9:J:173:ASP:OD1	9:J:174:ILE:N	2.49	0.45
15:P:87:PHE:CE2	15:P:144:LYS:HE3	2.52	0.45
48:U:101:PEE:H64	48:U:101:PEE:H58	1.83	0.45
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.99	0.45
32:i:271:THR:HG21	40:r:165:VAL:HG23	1.99	0.45
44:w:40:PRO:O	44:w:44:VAL:HG13	2.17	0.45
15:P:118:ASP:OD1	15:P:125:ARG:HG3	2.17	0.44
16:Q:144:MET:HE3	16:Q:222:MET:O	2.17	0.44
56:a:201:CDL:HA31	48:l:704:PEE:H54	1.99	0.44
28:e:68:GLU:HA	28:e:68:GLU:OE1	2.17	0.44
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.52	0.44
35:l:99:SER:HA	35:l:456:ARG:HH21	1.81	0.44
27:d:90:MET:SD	40:r:48:ASN:HB3	2.57	0.44
38:o:116:ILE:HG13	38:o:121:LEU:HD12	1.99	0.44
48:r:501:PEE:H76	49:r:502:PLX:H393	1.98	0.44
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.74	0.44
8:I:109:ASP:OD2	21:W:21:TYR:OH	2.36	0.44
16:Q:110:ASP:OD2	16:Q:112:HIS:NE2	2.51	0.44
21:W:120:MET:SD	31:h:69:ARG:HG2	2.58	0.44
23:Z:25:GLU:HA	23:Z:30:GLU:OE2	2.17	0.44
28:e:97:ILE:O	28:e:101:LEU:HB2	2.17	0.44
30:g:10:ARG:NH1	49:g:201:PLX:O3	2.50	0.44
36:m:61:LEU:O	41:s:114:TYR:OH	2.32	0.44
56:o:201:CDL:H111	56:o:201:CDL:H142	1.71	0.44
40:r:392:THR:O	40:r:396:MET:HG2	2.17	0.44
49:r:502:PLX:H51	49:r:502:PLX:H6	1.54	0.44
43:v:112:LYS:O	43:v:116:GLU:HG3	2.17	0.44
5:F:69:TYR:OH	5:F:75:LYS:NZ	2.50	0.44
7:H:51:ILE:HG22	7:H:55:LYS:HE2	1.99	0.44
25:b:110:ILE:HG22	25:b:112:GLU:H	1.82	0.44
32:i:277:ILE:O	32:i:281:LEU:HG	2.17	0.44
32:i:339:MET:HE3	32:i:339:MET:HB3	1.77	0.44
34:k:64:LEU:O	34:k:67:ALA:HB3	2.18	0.44
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.53	0.44
41:s:85:MET:HE3	41:s:85:MET:HB3	1.90	0.44
5:F:91:LEU:O	5:F:95:LEU:HD12	2.18	0.44
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.99	0.44
25:b:97:VAL:HG22	35:l:63:ILE:HG23	2.00	0.44
27:d:42:ASP:O	27:d:46:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s:402:UQ:H102	53:s:402:UQ:H122	1.84	0.44
43:v:46:MET:HE3	43:v:56:ARG:HB3	2.00	0.44
1:A:380:GLY:HA2	1:A:386:ARG:HB2	2.00	0.44
9:J:83:PRO:HA	9:J:106:MET:O	2.17	0.44
12:M:509:ASP:OD1	12:M:509:ASP:N	2.45	0.44
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.99	0.44
15:P:108:PHE:O	15:P:160:TYR:OH	2.35	0.44
16:Q:69:VAL:HG22	32:i:49:ASN:HB3	1.99	0.44
16:Q:187:VAL:HG11	16:Q:258:LEU:HD21	1.99	0.44
36:m:51:PHE:HB3	36:m:139:GLU:OE1	2.17	0.44
40:r:19:LYS:HB2	40:r:22:MET:HB2	2.00	0.44
1:A:65:THR:O	1:A:69:LEU:HG	2.18	0.44
5:F:88:THR:HA	5:F:91:LEU:HD12	2.00	0.44
9:J:262:THR:O	9:J:333:PRO:HD2	2.18	0.44
32:i:200:MET:HE1	32:i:343:LEU:HD13	1.99	0.44
32:i:307:SER:OG	32:i:308:THR:N	2.51	0.44
35:l:560:THR:O	35:l:565:THR:OG1	2.28	0.44
40:r:130:LEU:HD22	40:r:150:LEU:HD13	2.00	0.44
1:A:185:ASN:C	1:A:187:CYS:H	2.25	0.44
12:M:667:GLN:N	12:M:667:GLN:OE1	2.51	0.44
15:P:190:ASP:OD1	15:P:191:TYR:N	2.50	0.44
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.99	0.44
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.48	0.44
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.53	0.44
3:C:103:MET:HE1	3:C:121:TYR:HB2	2.00	0.44
6:G:87:LEU:HD21	6:G:141:PRO:HG3	1.99	0.44
9:J:257:ASP:OD1	9:J:257:ASP:C	2.60	0.44
56:N:201:CDL:H511	56:N:201:CDL:H542	1.74	0.44
56:i:402:CDL:H861	56:i:402:CDL:H832	1.77	0.44
3:C:56:TRP:CE2	49:C:303:PLX:H91	2.52	0.43
25:b:11:ARG:HB2	39:p:156:PRO:HB3	1.99	0.43
26:c:117:VAL:HG21	35:l:539:TYR:HA	2.00	0.43
32:i:75:ILE:HD12	34:k:40:LEU:HD22	2.00	0.43
33:j:73:LEU:HD12	36:m:55:MET:SD	2.58	0.43
56:s:401:CDL:H312	56:s:401:CDL:H342	1.54	0.43
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.99	0.43
12:M:311:LYS:HD2	13:N:143:PRO:HG3	1.99	0.43
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.00	0.43
32:i:154:MET:HE3	32:i:157:MET:HE3	2.01	0.43
33:j:67:LEU:HD22	36:m:59:ILE:HD12	2.00	0.43
36:m:93:PHE:CE2	36:m:97:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:11:GLU:N	42:u:11:GLU:OE2	2.50	0.43
10:K:100:GLN:NE2	14:O:69:ASN:O	2.51	0.43
6:X:99:SER:OG	6:X:100:VAL:N	2.51	0.43
35:l:500:LEU:O	35:l:504:LEU:HD12	2.18	0.43
40:r:89:THR:HG22	40:r:93:LYS:HE3	2.00	0.43
44:w:249:MET:HE2	44:w:249:MET:HB2	1.77	0.43
28:e:76:TYR:HB2	28:e:83:ASP:OD2	2.18	0.43
32:i:69:MET:SD	32:i:104:MET:HE1	2.59	0.43
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.54	0.43
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.87	0.43
35:l:237:MET:HE3	35:l:303:ALA:HB2	1.98	0.43
35:l:303:ALA:O	35:l:306:THR:HG22	2.17	0.43
44:w:57:SER:HB3	44:w:150:LEU:HD11	2.01	0.43
16:Q:443:MET:HE1	41:s:283:ASP:HB3	1.98	0.43
6:X:146:ASP:HB3	25:b:16:ARG:NH1	2.33	0.43
22:Y:65:MET:SD	35:l:375:ILE:HG12	2.58	0.43
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.53	0.43
32:i:73:ALA:HB2	32:i:97:MET:HB3	2.00	0.43
32:i:89:MET:HE1	32:i:98:MET:HE2	2.00	0.43
32:i:222:SER:O	32:i:224:ALA:N	2.51	0.43
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.99	0.43
33:j:73:LEU:N	33:j:74:PRO:HD2	2.34	0.43
43:v:31:PHE:CG	43:v:34:ARG:HD3	2.54	0.43
44:w:95:ASP:OD1	44:w:95:ASP:N	2.48	0.43
4:E:24:ASP:OD1	4:E:24:ASP:N	2.52	0.43
9:J:297:ALA:O	9:J:301:VAL:HG23	2.19	0.43
31:h:59:GLU:OE2	42:u:145:ARG:NH2	2.48	0.43
32:i:128:LEU:HD12	32:i:216:PHE:HB3	2.01	0.43
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.01	0.43
40:r:306:PRO:O	40:r:310:MET:HG3	2.17	0.43
43:v:15:LYS:HG2	43:v:113:LYS:HE2	2.00	0.43
1:A:52:ARG:NH2	10:K:77:GLN:HE21	2.16	0.43
1:A:151:ALA:O	1:A:191:TYR:OH	2.24	0.43
7:H:44:TYR:HB2	15:P:68:ILE:HG23	2.01	0.43
9:J:38:HIS:CE1	13:N:132:LYS:HD2	2.54	0.43
14:O:133:GLN:HG2	14:O:172:ILE:HD11	2.01	0.43
17:S:59:ARG:HB2	17:S:62:VAL:HG23	2.00	0.43
19:U:30:ILE:HG12	33:j:92:LEU:HD12	2.00	0.43
56:a:201:CDL:H441	56:a:201:CDL:H411	1.79	0.43
35:l:584:ILE:HG22	35:l:587:TYR:OH	2.18	0.43
56:s:401:CDL:H332	56:s:401:CDL:H182	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB3	1:A:158:ILE:HA	2.01	0.43
22:Y:56:ILE:HG13	22:Y:57:GLN:N	2.32	0.43
56:i:402:CDL:H641	56:i:402:CDL:H612	1.84	0.43
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.00	0.43
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.54	0.43
16:Q:71:PRO:HA	16:Q:72:PRO:HD3	1.94	0.43
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	2.01	0.43
19:U:70:PRO:HB3	42:u:124:GLU:O	2.19	0.43
23:Z:76:ALA:O	23:Z:80:VAL:HG12	2.19	0.43
40:r:318:ALA:HB1	40:r:374:ASN:CG	2.44	0.43
9:J:310:PHE:CG	49:J:403:PLX:H1C2	2.53	0.43
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	2.00	0.43
6:X:91:ASP:HB2	23:Z:44:PRO:HA	2.01	0.43
34:k:38:LEU:HB2	36:m:60:TYR:CZ	2.54	0.43
35:l:484:LEU:O	35:l:488:MET:HG2	2.19	0.43
40:r:87:GLU:O	40:r:92:LYS:HE3	2.19	0.43
44:w:58:LYS:O	44:w:60:ILE:HG13	2.19	0.43
3:C:63:TRP:CD1	3:C:92:VAL:HG22	2.54	0.42
12:M:534:VAL:HG22	12:M:537:ILE:HB	2.01	0.42
16:Q:245:TYR:O	16:Q:249:LYS:HG2	2.18	0.42
19:U:20:VAL:HG13	48:U:101:PEE:H67	2.01	0.42
20:V:125:VAL:O	20:V:129:GLN:HG3	2.19	0.42
33:j:71:LEU:O	36:m:147:TYR:OH	2.35	0.42
35:l:211:MET:HE1	40:r:390:ASN:ND2	2.34	0.42
35:l:557:TRP:CD2	56:o:201:CDL:H782	2.54	0.42
41:s:215:TYR:CD2	41:s:219:PRO:HB2	2.53	0.42
44:w:129:TYR:CG	44:w:183:CYS:HB3	2.53	0.42
1:A:48:ARG:NH1	10:K:71:SER:HA	2.33	0.42
1:A:115:VAL:HG11	1:A:138:LEU:HD11	2.01	0.42
13:N:127:TYR:OH	18:T:61:GLU:O	2.24	0.42
21:W:98:MET:HE1	31:h:79:ILE:HA	2.00	0.42
21:W:132:GLU:H	21:W:132:GLU:HG2	1.68	0.42
25:b:123:PHE:CZ	43:v:61:HIS:HB2	2.54	0.42
26:c:62:TYR:OH	26:c:74:ASP:O	2.25	0.42
32:i:177:LYS:NZ	34:k:98:CYS:O	2.37	0.42
39:p:159:LYS:HB2	39:p:162:ASP:OD2	2.20	0.42
40:r:455:LEU:HD23	40:r:455:LEU:HA	1.93	0.42
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.93	0.42
4:E:14:GLY:O	11:L:54:ALA:HA	2.20	0.42
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.54	0.42
14:O:143:ARG:O	14:O:184:PRO:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.00	0.42
41:s:69:SER:HA	56:s:401:CDL:H142	2.01	0.42
42:u:157:ASP:OD1	42:u:157:ASP:N	2.52	0.42
1:A:382:CYS:HB3	1:A:424:ILE:HD12	2.01	0.42
16:Q:427:PRO:HB2	16:Q:431:HIS:CE1	2.54	0.42
22:Y:74:TRP:HD1	22:Y:75:HIS:ND1	2.17	0.42
25:b:32:GLU:HG3	39:p:115:TYR:HA	2.01	0.42
41:s:105:MET:HE3	41:s:105:MET:HB3	1.95	0.42
14:O:99:ASN:OD1	14:O:113:TYR:OH	2.34	0.42
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.19	0.42
20:V:25:SER:OG	20:V:67:GLY:O	2.31	0.42
20:V:73:THR:OG1	20:V:93:GLY:HA2	2.20	0.42
6:X:119:ILE:HG21	6:X:135:ALA:HB1	2.01	0.42
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.01	0.42
26:c:37:PHE:HD1	26:c:38:PRO:HD2	1.84	0.42
35:l:185:SER:OG	35:l:212:PRO:O	2.37	0.42
35:l:230:HIS:N	35:l:231:PRO:HD3	2.35	0.42
39:p:35:ASP:OD1	39:p:36:LYS:N	2.53	0.42
40:r:271:MET:HE2	40:r:271:MET:HA	2.02	0.42
43:v:111:ARG:NH1	43:v:115:ARG:HH21	2.17	0.42
44:w:66:ILE:HD11	44:w:169:PHE:CE1	2.54	0.42
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.99	0.42
13:N:3:LEU:O	13:N:7:LEU:HG	2.20	0.42
14:O:185:MET:HB2	14:O:185:MET:HE2	1.78	0.42
15:P:235:LEU:HB3	16:Q:387:GLU:HG3	2.02	0.42
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.90	0.42
30:g:65:LEU:O	30:g:69:SER:OG	2.34	0.42
49:j:202:PLX:H1C3	49:j:202:PLX:H22	1.70	0.42
49:r:502:PLX:H101	49:r:502:PLX:H72	1.60	0.42
42:u:110:CYS:O	42:u:114:LYS:HB2	2.20	0.42
12:M:382:ARG:HA	12:M:385:TYR:CE2	2.55	0.42
23:Z:24:ILE:HB	23:Z:29:LEU:HB2	2.02	0.42
32:i:153:LEU:HG	32:i:157:MET:HE2	2.01	0.42
35:l:313:MET:HG3	35:l:328:HIS:HD2	1.84	0.42
44:w:100:ASP:OD1	44:w:100:ASP:N	2.45	0.42
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.29	0.42
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.54	0.42
28:e:94:GLY:O	28:e:99:LEU:HB2	2.19	0.42
31:h:83:ARG:HD3	31:h:87:ILE:HD12	2.02	0.42
32:i:72:MET:HE2	32:i:76:ILE:HG12	2.02	0.42
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:i:402:CDL:H541	56:i:402:CDL:H511	1.65	0.42
35:l:293:ILE:HG13	35:l:294:THR:HG23	2.02	0.42
43:v:15:LYS:HB3	43:v:15:LYS:HE3	1.66	0.42
7:H:35:LEU:HD23	7:H:38:ILE:HD12	2.01	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.42
15:P:51:ASN:HB3	15:P:82:ASN:HD21	1.83	0.42
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.01	0.42
25:b:75:VAL:C	25:b:78:PRO:HD2	2.45	0.42
49:g:201:PLX:H351	32:i:336:VAL:HG13	2.02	0.42
31:h:65:GLU:O	31:h:69:ARG:HD2	2.19	0.42
35:l:108:MET:HE3	35:l:108:MET:HB3	1.86	0.42
35:l:289:ALA:O	35:l:293:ILE:HG23	2.20	0.42
53:J:402:UQ:H101	53:J:402:UQ:H121	1.72	0.42
31:h:2:PRO:HB2	31:h:3:PHE:H	1.66	0.42
31:h:69:ARG:O	31:h:73:MET:HG3	2.20	0.42
33:j:88:LEU:HD13	41:s:309:ILE:HD12	2.02	0.42
49:j:202:PLX:H4	49:j:202:PLX:H72	1.72	0.42
56:l:702:CDL:H781	56:l:702:CDL:H751	1.83	0.42
6:G:147:TYR:CD1	6:G:147:TYR:C	2.98	0.41
8:I:70:MET:O	8:I:70:MET:SD	2.78	0.41
10:K:87:LEU:HB3	14:O:62:ARG:HD3	2.01	0.41
16:Q:53:TYR:HE1	48:i:401:PEE:H2	1.85	0.41
19:U:38:TYR:HB2	41:s:310:MET:O	2.20	0.41
19:U:67:PRO:HG3	19:U:74:GLN:C	2.45	0.41
25:b:75:VAL:O	25:b:79:VAL:HG12	2.20	0.41
49:g:201:PLX:H361	49:g:201:PLX:H311	2.02	0.41
32:i:10:ILE:O	32:i:14:MET:HG3	2.20	0.41
56:i:402:CDL:H441	40:r:101:LEU:HD13	2.00	0.41
35:l:51:LEU:HD22	35:l:91:PRO:HG3	2.02	0.41
35:l:245:ALA:HB2	35:l:340:PHE:HB3	2.02	0.41
40:r:186:LEU:HD23	40:r:186:LEU:HA	1.90	0.41
41:s:233:MET:HE3	41:s:233:MET:HB3	1.81	0.41
2:B:63:TRP:NE1	48:B:303:PEE:H13	2.35	0.41
4:E:93:THR:HG23	4:E:103:ILE:HD11	2.02	0.41
5:F:65:LEU:O	5:F:76:ASN:HA	2.20	0.41
24:a:66:ARG:HH12	28:e:72:ASP:HB2	1.85	0.41
33:j:49:LEU:C	36:m:76:THR:HG21	2.45	0.41
35:l:176:ARG:HA	35:l:179:ASP:HB2	2.02	0.41
35:l:504:LEU:HD13	56:l:702:CDL:H522	2.02	0.41
56:o:201:CDL:H392	56:o:201:CDL:H361	1.75	0.41
56:o:201:CDL:H761	56:o:201:CDL:H792	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:139:THR:HA	41:s:142:TYR:CE2	2.55	0.41
11:L:115:SER:HB2	12:M:267:THR:HB	2.01	0.41
26:c:86:ARG:NH2	26:c:103:GLU:OE2	2.48	0.41
31:h:88:LYS:HE2	31:h:88:LYS:HB2	1.91	0.41
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.55	0.41
35:l:486:MET:O	35:l:489:THR:HG22	2.21	0.41
1:A:66:LYS:HE3	1:A:188:GLY:O	2.20	0.41
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.60	0.41
3:C:113:MET:O	3:C:113:MET:HG3	2.19	0.41
17:S:34:LYS:HB2	42:u:91:TYR:HA	2.02	0.41
25:b:19:ARG:HA	39:p:171:VAL:HG13	2.02	0.41
26:c:40:PRO:O	26:c:74:ASP:HB3	2.20	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.55	0.41
56:s:401:CDL:H141	56:s:401:CDL:H171	1.56	0.41
3:C:75:GLU:HG3	3:C:167:PRO:HB2	2.03	0.41
16:Q:271:ARG:NH2	16:Q:445:ALA:HB1	2.35	0.41
56:l:702:CDL:H351	56:l:702:CDL:H382	1.65	0.41
41:s:81:LEU:HD21	41:s:111:LEU:HD23	2.02	0.41
56:s:401:CDL:H771	56:s:401:CDL:H801	1.88	0.41
1:A:300:ILE:HG22	1:A:306:GLY:HA2	2.03	0.41
3:C:116:ALA:O	3:C:120:VAL:HG13	2.19	0.41
12:M:436:VAL:O	12:M:442:TYR:OH	2.35	0.41
16:Q:222:MET:HE3	16:Q:222:MET:HB3	1.77	0.41
17:S:59:ARG:HB3	17:S:61:HIS:CE1	2.55	0.41
32:i:320:THR:HG21	44:w:300:ASN:HA	2.02	0.41
35:l:292:ALA:HB2	35:l:304:PHE:HB3	2.03	0.41
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.56	0.41
1:A:195:VAL:O	10:K:97:ARG:NH1	2.47	0.41
1:A:414:GLU:O	1:A:418:GLN:HG3	2.21	0.41
2:B:48:MET:HA	2:B:48:MET:HE2	2.01	0.41
6:G:89:LEU:HD23	6:G:89:LEU:HA	1.85	0.41
15:P:157:VAL:HG21	15:P:182:PRO:HD3	2.02	0.41
6:X:120:MET:HE3	6:X:120:MET:HB3	1.84	0.41
26:c:34:LYS:HD2	26:c:37:PHE:HD2	1.86	0.41
27:d:70:ARG:HD2	27:d:70:ARG:HA	1.70	0.41
30:g:17:PRO:HG2	30:g:83:TYR:OH	2.20	0.41
32:i:280:THR:O	32:i:284:MET:HG2	2.20	0.41
35:l:293:ILE:HD13	35:l:418:LEU:HD22	2.03	0.41
35:l:319:ILE:HD13	35:l:399:VAL:HG22	2.02	0.41
35:l:327:LEU:HG	35:l:331:MET:HE2	2.02	0.41
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.56	0.41
1:A:362:ASP:CG	1:A:449:ARG:HH12	2.29	0.41
2:B:93:LEU:HB3	13:N:93:MET:HE3	2.03	0.41
2:B:120:GLU:HB2	2:B:130:ILE:HD12	2.03	0.41
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.55	0.41
12:M:413:LEU:HD13	12:M:413:LEU:HA	1.93	0.41
16:Q:446:ASP:OD1	16:Q:446:ASP:N	2.53	0.41
33:j:60:ILE:HG23	34:k:72:ALA:HB1	2.03	0.41
44:w:119:ASP:OD1	44:w:225:HIS:ND1	2.53	0.41
44:w:268:LYS:O	44:w:271:GLU:HG2	2.21	0.41
44:w:354:LEU:HA	44:w:354:LEU:HD23	1.79	0.41
1:A:342:LEU:HD13	1:A:349:LEU:HA	2.02	0.41
1:A:367:ILE:O	1:A:371:ILE:HG12	2.21	0.41
1:A:383:THR:HG21	12:M:120:LEU:HG	2.03	0.41
48:B:303:PEE:H64	41:s:273:ILE:HD11	2.03	0.41
4:E:14:GLY:C	4:E:16:SER:H	2.29	0.41
9:J:106:MET:HE2	9:J:106:MET:HB3	1.93	0.41
15:P:147:THR:HB	15:P:153:ILE:HD11	2.01	0.41
16:Q:248:SER:HB2	21:W:19:ILE:HD13	2.02	0.41
18:T:102:LEU:O	18:T:120:GLN:NE2	2.45	0.41
26:c:54:LYS:NZ	26:c:74:ASP:OD2	2.53	0.41
27:d:163:MET:HE2	28:e:149:LEU:HD11	2.03	0.41
34:k:23:ARG:HG3	36:m:23:LYS:HE2	2.02	0.41
35:l:566:THR:O	35:l:570:GLN:HG2	2.21	0.41
36:m:99:MET:HE3	36:m:99:MET:HB2	1.82	0.41
56:n:101:CDL:H741	56:n:101:CDL:H711	1.75	0.41
40:r:116:ILE:HD13	40:r:116:ILE:HA	1.94	0.41
49:r:502:PLX:H111	49:r:502:PLX:H141	1.75	0.41
43:v:25:PHE:CG	43:v:108:LEU:HD23	2.56	0.41
44:w:210:PRO:O	44:w:214:ILE:HG12	2.21	0.41
2:B:98:ARG:NH2	16:Q:224:ALA:O	2.53	0.41
3:C:79:MET:HE2	3:C:79:MET:HB3	1.78	0.41
13:N:78:ASP:OD1	13:N:78:ASP:N	2.54	0.41
15:P:118:ASP:OD1	15:P:125:ARG:CG	2.69	0.41
20:V:141:VAL:HG21	32:i:272:LYS:HB3	2.03	0.41
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.33	0.41
29:f:48:LEU:O	29:f:52:VAL:HG23	2.20	0.41
32:i:76:ILE:HG13	32:i:97:MET:HE1	2.02	0.41
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.03	0.41
32:i:164:ILE:HD13	32:i:164:ILE:HA	1.88	0.41
33:j:67:LEU:HD12	34:k:65:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:77:TRP:HD1	41:s:318:SER:C	2.29	0.41
35:l:557:TRP:O	35:l:561:ILE:HG12	2.21	0.41
40:r:218:LYS:O	40:r:222:GLU:HG2	2.20	0.41
48:B:303:PEE:H38	19:U:25:ILE:HD11	2.04	0.40
11:L:84:ARG:HD3	11:L:91:VAL:HG12	2.03	0.40
14:O:239:LYS:HD3	14:O:243:PHE:CG	2.56	0.40
19:U:82:LYS:HA	21:W:59:ARG:HD3	2.02	0.40
21:W:120:MET:HG2	21:W:122:GLY:H	1.87	0.40
21:W:135:SER:OG	21:W:136:ALA:N	2.54	0.40
31:h:17:TRP:CD1	31:h:17:TRP:H	2.39	0.40
32:i:21:MET:HE3	32:i:136:LEU:HB3	2.03	0.40
35:l:67:HIS:NE2	35:l:70:THR:OG1	2.46	0.40
35:l:68:TRP:H	35:l:77:SER:HA	1.86	0.40
40:r:200:ILE:HD13	40:r:200:ILE:HA	1.98	0.40
56:s:401:CDL:HB61	56:s:401:CDL:H321	2.03	0.40
44:w:59:VAL:HG12	44:w:201:PRO:HB3	2.02	0.40
1:A:423:THR:OG1	1:A:425:CYS:O	2.32	0.40
5:F:43:GLU:OE1	5:F:43:GLU:N	2.54	0.40
31:h:86:LEU:HB3	31:h:92:TYR:HB2	2.03	0.40
40:r:16:TRP:HA	40:r:93:LYS:HD3	2.03	0.40
53:s:402:UQ:H152	53:s:402:UQ:H121	1.82	0.40
1:A:339:PHE:O	1:A:343:VAL:HG23	2.20	0.40
6:G:115:GLN:NE2	6:G:135:ALA:O	2.45	0.40
9:J:37:HIS:O	9:J:39:ALA:N	2.54	0.40
9:J:283:VAL:HG22	9:J:369:VAL:HG11	2.03	0.40
12:M:173:MET:HA	12:M:173:MET:HE2	2.03	0.40
16:Q:184:ILE:HG21	16:Q:207:ARG:HG3	2.03	0.40
21:W:57:ARG:HB3	41:s:316:PRO:CG	2.48	0.40
6:X:69:SER:OG	6:X:70:ASP:N	2.54	0.40
35:l:27:TYR:O	35:l:115:ASN:ND2	2.45	0.40
35:l:124:PHE:CZ	35:l:247:LEU:HG	2.57	0.40
38:o:37:LEU:O	38:o:41:SER:OG	2.31	0.40
40:r:104:LEU:HG	40:r:108:MET:HE2	2.03	0.40
41:s:106:LEU:HD23	41:s:106:LEU:HA	1.96	0.40
53:s:402:UQ:H202	53:s:402:UQ:H172	1.89	0.40
44:w:233:TYR:O	44:w:237:ILE:HG13	2.21	0.40
3:C:192:ILE:O	3:C:196:ARG:HG3	2.22	0.40
9:J:167:ILE:HD13	9:J:201:ILE:HB	2.03	0.40
12:M:233:SER:HB3	12:M:236:TYR:HB3	2.04	0.40
13:N:21:ARG:CZ	13:N:21:ARG:HB2	2.51	0.40
17:S:66:LEU:HD11	42:u:74:ILE:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:69:ILE:HD11	42:u:20:VAL:HG13	2.03	0.40
19:U:51:TYR:O	21:W:68:ARG:NH1	2.47	0.40
29:f:52:VAL:HG12	29:f:56:ILE:HD12	2.03	0.40
31:h:36:PHE:CD1	31:h:62:ASP:HB3	2.56	0.40
34:k:21:MET:SD	56:k:101:CDL:H712	2.62	0.40
35:l:68:TRP:CD2	48:l:704:PEE:H42	2.56	0.40
48:r:501:PEE:H68	48:r:501:PEE:H62	1.89	0.40
44:w:66:ILE:HD11	44:w:169:PHE:HE1	1.87	0.40
48:B:303:PEE:H55	48:B:303:PEE:H61	1.69	0.40
11:L:81:VAL:HG21	11:L:150:ARG:HG3	2.03	0.40
13:N:42:ASP:HB2	13:N:48:TYR:CE1	2.48	0.40
14:O:239:LYS:HD3	14:O:243:PHE:CD2	2.57	0.40
20:V:34:LEU:HD12	20:V:34:LEU:HA	1.87	0.40
22:Y:102:ASP:HA	43:v:115:ARG:HH22	1.86	0.40
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.86	0.40
32:i:244:MET:HE2	32:i:244:MET:HB2	1.87	0.40
33:j:71:LEU:HD13	33:j:94:LEU:HD21	2.03	0.40
49:j:202:PLX:H372	49:j:202:PLX:H342	1.92	0.40
34:k:91:GLN:H	34:k:91:GLN:HG3	1.59	0.40
43:v:55:GLN:OE1	43:v:63:LEU:HD21	2.22	0.40
44:w:295:ARG:O	44:w:299:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/433 (100%)	422 (98%)	9 (2%)	0	100	100
2	B	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	80 (93%)	6 (7%)	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	48
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	36	70
10	K	41/43 (95%)	41 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	672 (98%)	16 (2%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	202 (94%)	13 (6%)	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%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
24	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
25	b	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
28	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
29	f	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
30	g	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
31	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
32	i	345/347 (99%)	331 (96%)	13 (4%)	1 (0%)	36	70
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	604/606 (100%)	579 (96%)	25 (4%)	0	100	100
36	m	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
39	p	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
40	r	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
41	s	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	36	70
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8175/8314 (98%)	7910 (97%)	261 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	38	HIS
7	H	77	ILE
32	i	50	PRO
41	s	208	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	341 (99%)	5 (1%)	59	80
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	80
4	E	105/107 (98%)	104 (99%)	1 (1%)	68	84
5	F	74/76 (97%)	71 (96%)	3 (4%)	27	61
6	G	76/81 (94%)	74 (97%)	2 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X	77/81 (95%)	76 (99%)	1 (1%)	61	81
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	294 (99%)	2 (1%)	76	86
10	K	42/42 (100%)	39 (93%)	3 (7%)	13	43
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	579/580 (100%)	574 (99%)	5 (1%)	70	85
13	N	130/130 (100%)	129 (99%)	1 (1%)	73	86
14	O	183/183 (100%)	179 (98%)	4 (2%)	45	74
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	83
16	Q	370/370 (100%)	366 (99%)	4 (1%)	65	83
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	77 (98%)	2 (2%)	42	72
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	100 (99%)	1 (1%)	68	84
21	W	121/123 (98%)	117 (97%)	4 (3%)	33	67
22	Y	62/62 (100%)	60 (97%)	2 (3%)	34	67
23	Z	62/62 (100%)	62 (100%)	0	100	100
24	a	121/121 (100%)	120 (99%)	1 (1%)	73	86
25	b	90/119 (76%)	90 (100%)	0	100	100
26	c	141/141 (100%)	140 (99%)	1 (1%)	76	86
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	76
28	e	96/96 (100%)	93 (97%)	3 (3%)	35	68
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	106/109 (97%)	104 (98%)	2 (2%)	50	76
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	309 (99%)	2 (1%)	78	88
33	j	100/100 (100%)	100 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	82
35	l	536/540 (99%)	529 (99%)	7 (1%)	61	81
36	m	127/141 (90%)	124 (98%)	3 (2%)	43	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	85
39	p	159/159 (100%)	157 (99%)	2 (1%)	61	81
40	r	409/410 (100%)	403 (98%)	6 (2%)	57	80
41	s	275/275 (100%)	270 (98%)	5 (2%)	51	77
42	u	153/153 (100%)	149 (97%)	4 (3%)	40	72
43	v	106/111 (96%)	106 (100%)	0	100	100
44	w	282/283 (100%)	278 (99%)	4 (1%)	59	80
All	All	7147/7241 (99%)	7058 (99%)	89 (1%)	61	82

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	65	THR
1	A	125	CYS
1	A	425	CYS
1	A	455	LEU
3	C	71	CYS
3	C	142	TYR
4	E	89	GLU
5	F	50	ASP
5	F	61	VAL
5	F	62	GLN
6	G	87	LEU
6	G	98	LEU
9	J	156	SER
9	J	328	THR
10	K	82	SER
10	K	87	LEU
10	K	107	SER
12	M	80	VAL
12	M	150	ARG
12	M	171	THR
12	M	352	VAL
12	M	659	VAL
13	N	120	THR
14	O	103	GLU
14	O	150	GLU

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Mol	Chain	Res	Type
14	O	181	VAL
14	O	185	MET
15	P	69	LEU
15	P	125	ARG
16	Q	57	GLU
16	Q	145	MET
16	Q	217	VAL
16	Q	272	THR
18	T	39	THR
18	T	43	GLN
20	V	79	GLN
21	W	85	GLN
21	W	98	MET
21	W	101	VAL
21	W	118	THR
6	X	122	MET
22	Y	77	SER
22	Y	99	ILE
24	a	130	GLU
26	c	182	VAL
27	d	9	VAL
27	d	120	SER
27	d	144	SER
28	e	55	LEU
28	e	104	THR
28	e	141	CYS
30	g	29	THR
30	g	69	SER
32	i	194	LEU
32	i	336	VAL
34	k	24	SER
35	l	79	SER
35	l	185	SER
35	l	315	VAL
35	l	340	PHE
35	l	371	THR
35	l	482	MET
35	l	541	ASN
36	m	76	THR
36	m	82	VAL
36	m	85	SER
38	o	29	THR

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Mol	Chain	Res	Type
39	p	110	SER
39	p	117	ASP
40	r	60	SER
40	r	66	LEU
40	r	107	ILE
40	r	116	ILE
40	r	247	THR
40	r	420	THR
41	s	8	SER
41	s	80	SER
41	s	133	LEU
41	s	224	PHE
41	s	258	ASN
42	u	23	SER
42	u	37	ASP
42	u	157	ASP
42	u	165	SER
44	w	95	ASP
44	w	272	ASP
44	w	287	ASP
44	w	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	283	ASN
1	A	393	ASN
1	A	452	GLN
3	C	111	ASN
4	E	26	ASN
4	E	45	ASN
5	F	48	ASN
6	G	142	GLN
7	H	71	GLN
7	H	110	ASN
9	J	122	HIS
10	K	106	GLN
11	L	71	HIS
12	M	425	ASN
12	M	464	GLN
12	M	498	GLN

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Mol	Chain	Res	Type
12	M	540	ASN
12	M	569	GLN
12	M	669	ASN
12	M	688	GLN
13	N	135	GLN
14	O	131	HIS
14	O	144	ASN
14	O	187	GLN
15	P	55	HIS
15	P	77	GLN
15	P	196	HIS
15	P	228	GLN
16	Q	285	ASN
18	T	117	GLN
18	T	123	HIS
20	V	7	HIS
20	V	79	GLN
22	Y	46	GLN
24	a	170	GLN
26	c	183	HIS
27	d	28	ASN
27	d	124	ASN
30	g	90	HIS
31	h	7	GLN
31	h	34	HIS
32	i	2	ASN
32	i	63	GLN
32	i	77	ASN
32	i	204	ASN
34	k	92	ASN
35	l	56	HIS
35	l	109	HIS
35	l	270	ASN
35	l	296	ASN
35	l	309	GLN
35	l	348	HIS
35	l	444	ASN
35	l	446	ASN
35	l	447	ASN
35	l	470	ASN
35	l	534	HIS
36	m	86	ASN

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Mol	Chain	Res	Type
37	n	52	ASN
38	o	50	GLN
38	o	52	ASN
40	r	43	ASN
40	r	48	ASN
40	r	192	ASN
40	r	220	HIS
40	r	366	ASN
40	r	390	ASN
41	s	258	ASN
42	u	151	ASN
43	v	47	ASN
44	w	132	GLN
44	w	299	GLN
44	w	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	5.89	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.76	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	12.05	130.53	119.48
16	Q	118	2MR	CD-NE-CZ	4.10	131.09	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.17	130.87	123.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
53	UQ	J	402	-	33,33,63	3.45	9 (27%)	40,43,79	2.73	13 (32%)
49	PLX	r	503	-	51,51,51	1.15	4 (7%)	55,59,59	0.54	1 (1%)
48	PEE	U	101	-	50,50,50	1.16	5 (10%)	53,55,55	0.92	2 (3%)
48	PEE	B	303	-	50,50,50	1.17	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
49	PLX	j	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.59	1 (1%)
56	CDL	o	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.87	4 (3%)
52	NDP	J	401	-	49,52,52	4.39	23 (46%)	66,80,80	2.24	13 (19%)
58	ADP	w	401	-	27,29,29	2.96	8 (29%)	42,45,45	2.00	9 (21%)
56	CDL	a	201	-	99,99,99	1.09	8 (8%)	105,111,111	0.85	4 (3%)
56	CDL	l	702	-	99,99,99	1.09	8 (8%)	105,111,111	0.90	5 (4%)
49	PLX	g	201	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
47	NAI	A	503	-	45,48,48	3.91	19 (42%)	60,73,73	1.78	12 (20%)
48	PEE	C	302	-	46,46,50	1.20	6 (13%)	49,51,55	0.98	2 (4%)
48	PEE	j	201	-	40,40,50	1.15	5 (12%)	43,45,55	1.02	2 (4%)
49	PLX	J	403	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
50	970	C	304	-	33,33,33	4.89	16 (48%)	48,50,50	2.49	17 (35%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
56	CDL	k	101	-	77,77,99	1.20	7 (9%)	83,89,111	0.94	4 (4%)
48	PEE	l	704	-	45,45,50	1.22	6 (13%)	48,50,55	1.00	2 (4%)
48	PEE	i	401	-	46,46,50	1.21	6 (13%)	49,51,55	0.98	2 (4%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
54	FES	O	301	14	0,4,4	-	-	-	-	-
49	PLX	C	303	-	51,51,51	1.16	4 (7%)	55,59,59	0.59	1 (1%)
54	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	W	201	-	40,40,50	1.15	5 (12%)	43,45,55	0.99	2 (4%)
48	PEE	l	703	-	49,49,50	1.18	6 (12%)	52,54,55	0.94	2 (3%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.23	8 (16%)
51	8Q1	X	201	6	31,34,34	1.71	6 (19%)	40,43,43	1.57	6 (15%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
56	CDL	s	401	-	88,88,99	1.14	8 (9%)	94,100,111	0.91	4 (4%)
56	CDL	n	101	-	54,54,99	1.37	9 (16%)	60,66,111	1.14	4 (6%)
51	8Q1	G	201	-	31,34,34	1.69	6 (19%)	40,43,43	1.58	5 (12%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.60	1 (1%)
49	PLX	r	502	-	51,51,51	1.15	5 (9%)	55,59,59	0.60	1 (1%)
56	CDL	N	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.12	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	CDL	l	701	-	98,98,99	1.09	8 (8%)	104,110,111	0.88	4 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
53	UQ	s	402	-	38,38,63	3.54	9 (23%)	46,49,79	2.86	16 (34%)
56	CDL	V	201	-	93,93,99	1.12	8 (8%)	99,105,111	0.87	4 (4%)
48	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.97	2 (3%)
56	CDL	i	402	-	98,98,99	1.09	8 (8%)	104,110,111	0.85	4 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	UQ	J	402	-	-	9/27/51/87	0/1/1/1
49	PLX	r	503	-	-	35/55/55/55	-
48	PEE	U	101	-	-	23/54/54/54	-
48	PEE	B	303	-	-	25/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	j	202	-	-	32/55/55/55	-
56	CDL	o	201	-	-	56/110/110/110	-
52	NDP	J	401	-	-	11/34/77/77	0/4/5/5
58	ADP	w	401	-	-	4/16/32/32	0/3/3/3
56	CDL	a	201	-	-	56/110/110/110	-
56	CDL	l	702	-	-	53/110/110/110	-
49	PLX	g	201	-	-	33/55/55/55	-
48	PEE	C	302	-	-	30/50/50/54	-
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
48	PEE	j	201	-	-	20/44/44/54	-
49	PLX	J	403	-	-	25/55/55/55	-
50	970	C	304	-	-	4/8/41/41	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
56	CDL	k	101	-	-	52/88/88/110	-
48	PEE	l	704	-	-	20/49/49/54	-
48	PEE	i	401	-	-	27/50/50/54	-
45	SF4	C	301	3	-	-	0/6/5/5
54	FES	O	301	14	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PLX	C	303	-	-	28/55/55/55	-
54	FES	M	803	12	-	-	0/1/1/1
48	PEE	W	201	-	-	24/44/44/54	-
48	PEE	l	703	-	-	25/53/53/54	-
46	FMN	A	502	-	-	4/18/18/18	0/3/3/3
51	8Q1	X	201	6	-	25/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
56	CDL	s	401	-	-	53/99/99/110	-
56	CDL	n	101	-	-	30/65/65/110	-
51	8Q1	G	201	-	-	10/41/41/41	-
49	PLX	a	202	-	-	29/55/55/55	-
49	PLX	r	502	-	-	29/55/55/55	-
56	CDL	N	201	-	-	32/61/61/110	-
56	CDL	l	701	-	-	54/109/109/110	-
45	SF4	B	302	2	-	-	0/6/5/5
53	UQ	s	402	-	-	11/33/57/87	0/1/1/1
45	SF4	A	501	1	-	-	0/6/5/5
56	CDL	V	201	-	-	55/104/104/110	-
48	PEE	r	501	-	-	32/54/54/54	-
56	CDL	i	402	-	-	58/109/109/110	-

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	304	970	O16-C17	17.90	1.57	1.37
52	J	401	NDP	C3B-C2B	-12.70	1.24	1.52
52	J	401	NDP	C6N-C5N	12.49	1.55	1.33
50	C	304	970	O25-C24	11.10	1.37	1.22
52	J	401	NDP	O4D-C4D	10.75	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.23	1.26	1.53
50	C	304	970	C23-C24	9.92	1.63	1.52
52	J	401	NDP	C3D-C4D	-9.85	1.27	1.53
53	s	402	UQ	C18-C19	9.63	1.56	1.33
53	J	402	UQ	C18-C19	9.63	1.56	1.33
53	J	402	UQ	C13-C14	9.34	1.55	1.33
53	s	402	UQ	C13-C14	9.24	1.55	1.33
47	A	503	NAI	O4B-C1B	9.17	1.63	1.42
53	s	402	UQ	C23-C24	9.06	1.54	1.33
53	s	402	UQ	C8-C9	8.97	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	402	UQ	C8-C9	8.89	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.85	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.20	1.26	1.45
52	J	401	NDP	O4B-C4B	-7.98	1.27	1.45
53	J	402	UQ	C23-C24	7.82	1.54	1.32
58	w	401	ADP	O4'-C4'	7.76	1.62	1.45
53	s	402	UQ	C28-C29	7.70	1.54	1.32
47	A	503	NAI	C2D-C1D	-7.52	1.29	1.53
52	J	401	NDP	C2N-C3N	7.35	1.55	1.34
47	A	503	NAI	C2B-C1B	-7.24	1.30	1.53
47	A	503	NAI	O4D-C4D	6.95	1.60	1.45
50	C	304	970	C14-C23	-6.83	1.46	1.52
50	C	304	970	O08-C07	6.37	1.47	1.37
47	A	503	NAI	C2D-C3D	5.96	1.69	1.53
52	J	401	NDP	C6A-N6A	5.95	1.49	1.34
52	J	401	NDP	P2B-O2B	5.76	1.70	1.59
47	A	503	NAI	C7N-N7N	5.75	1.48	1.33
58	w	401	ADP	C6-N6	5.55	1.48	1.34
51	X	201	8Q1	C34-N36	5.52	1.45	1.33
52	J	401	NDP	C3B-C4B	5.49	1.67	1.53
47	A	503	NAI	O4D-C1D	5.47	1.55	1.42
51	G	201	8Q1	C34-N36	5.43	1.45	1.33
51	X	201	8Q1	C39-N41	5.37	1.45	1.33
50	C	304	970	O13-C12	5.36	1.45	1.37
51	G	201	8Q1	C39-N41	5.29	1.45	1.33
47	A	503	NAI	C6A-N6A	5.24	1.47	1.34
47	A	503	NAI	C4N-C3N	-5.07	1.40	1.49
50	C	304	970	C05-C04	-4.90	1.47	1.54
52	J	401	NDP	O4D-C1D	-4.88	1.30	1.42
52	J	401	NDP	C6N-N1N	4.84	1.49	1.37
50	C	304	970	C03-C02	4.72	1.53	1.34
47	A	503	NAI	O2B-C2B	4.56	1.53	1.43
52	J	401	NDP	O4B-C1B	4.50	1.52	1.42
52	J	401	NDP	C1B-N9A	-4.45	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.41	1.31	1.42
52	J	401	NDP	C7N-N7N	4.18	1.44	1.33
52	J	401	NDP	O2D-C2D	-4.17	1.33	1.43
47	A	503	NAI	C6N-C5N	3.96	1.40	1.33
46	A	502	FMN	C4A-N5	3.85	1.38	1.30
48	B	303	PEE	C18-C19	3.74	1.53	1.31
48	W	201	PEE	C18-C19	3.73	1.53	1.31
48	r	501	PEE	C18-C19	3.73	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	j	201	PEE	C18-C19	3.73	1.53	1.31
48	l	704	PEE	C18-C19	3.72	1.53	1.31
48	C	302	PEE	C18-C19	3.72	1.53	1.31
48	i	401	PEE	C18-C19	3.72	1.53	1.31
48	U	101	PEE	C18-C19	3.72	1.53	1.31
48	l	703	PEE	C18-C19	3.72	1.53	1.31
48	l	703	PEE	C39-C38	3.66	1.53	1.31
48	U	101	PEE	C39-C38	3.66	1.53	1.31
48	r	501	PEE	C39-C38	3.65	1.52	1.31
48	B	303	PEE	C39-C38	3.65	1.52	1.31
48	i	401	PEE	C39-C38	3.64	1.52	1.31
48	C	302	PEE	C39-C38	3.64	1.52	1.31
48	l	704	PEE	C39-C38	3.64	1.52	1.31
47	A	503	NAI	C7N-C3N	3.62	1.56	1.48
56	n	101	CDL	OA8-CA7	3.49	1.43	1.33
56	o	201	CDL	OA8-CA7	3.47	1.43	1.33
56	k	101	CDL	OA8-CA7	3.47	1.43	1.33
56	l	702	CDL	OA8-CA7	3.46	1.43	1.33
56	V	201	CDL	OA8-CA7	3.46	1.43	1.33
56	N	201	CDL	OA8-CA7	3.46	1.43	1.33
56	l	701	CDL	OA8-CA7	3.45	1.43	1.33
50	C	304	970	C15-C14	3.43	1.57	1.51
56	s	401	CDL	OA8-CA7	3.42	1.43	1.33
56	i	402	CDL	OA8-CA7	3.41	1.43	1.33
56	a	201	CDL	OA8-CA7	3.39	1.43	1.33
58	w	401	ADP	O2'-C2'	-3.34	1.35	1.43
50	C	304	970	C11-C24	3.29	1.54	1.48
56	k	101	CDL	OA6-CA5	3.27	1.43	1.34
47	A	503	NAI	C4N-C5N	-3.26	1.40	1.48
58	w	401	ADP	C8-N9	-3.18	1.31	1.37
50	C	304	970	O16-C15	3.15	1.52	1.44
58	w	401	ADP	O3'-C3'	3.13	1.50	1.43
52	J	401	NDP	O3D-C3D	3.11	1.50	1.43
56	V	201	CDL	OA6-CA5	3.09	1.43	1.34
56	l	702	CDL	OB8-CB7	3.09	1.42	1.33
56	l	702	CDL	OB6-CB5	3.06	1.42	1.34
56	k	101	CDL	OB8-CB7	3.04	1.42	1.33
56	k	101	CDL	OB6-CB5	3.03	1.42	1.34
56	N	201	CDL	OB6-CB5	3.03	1.42	1.34
56	o	201	CDL	OB8-CB7	3.02	1.42	1.33
56	a	201	CDL	OB6-CB5	3.02	1.42	1.34
56	i	402	CDL	OB8-CB7	3.02	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	V	201	CDL	OB6-CB5	3.02	1.42	1.34
56	s	401	CDL	OB6-CB5	3.02	1.42	1.34
52	J	401	NDP	C7N-C3N	3.02	1.55	1.48
56	N	201	CDL	OB8-CB7	3.02	1.42	1.33
56	o	201	CDL	OB6-CB5	3.02	1.42	1.34
56	l	701	CDL	OB8-CB7	3.01	1.42	1.33
56	l	701	CDL	OB6-CB5	3.00	1.42	1.34
56	n	101	CDL	OB6-CB5	3.00	1.42	1.34
56	i	402	CDL	OB6-CB5	3.00	1.42	1.34
56	n	101	CDL	OB8-CB7	3.00	1.42	1.33
56	V	201	CDL	OB8-CB7	2.99	1.42	1.33
52	J	401	NDP	C8A-N9A	-2.99	1.32	1.37
56	a	201	CDL	OB8-CB7	2.98	1.42	1.33
56	n	101	CDL	OA6-CA5	2.98	1.42	1.34
56	N	201	CDL	OA6-CA5	2.96	1.42	1.34
56	s	401	CDL	OA6-CA5	2.95	1.42	1.34
56	o	201	CDL	OA6-CA5	2.95	1.42	1.34
56	s	401	CDL	OB8-CB7	2.95	1.41	1.33
56	a	201	CDL	OA6-CA5	2.94	1.42	1.34
56	i	402	CDL	OA6-CA5	2.94	1.42	1.34
56	l	702	CDL	OA6-CA5	2.92	1.42	1.34
52	J	401	NDP	C5A-N7A	-2.88	1.33	1.39
56	l	701	CDL	OA6-CA5	2.88	1.42	1.34
50	C	304	970	C12-C06	2.87	1.44	1.39
53	J	402	UQ	C6-C1	2.78	1.54	1.46
49	r	503	PLX	O6-C4	-2.71	1.41	1.44
53	s	402	UQ	C6-C1	2.70	1.54	1.46
49	g	201	PLX	O6-C4	-2.68	1.41	1.44
49	C	303	PLX	O6-C4	-2.68	1.41	1.44
49	a	202	PLX	O6-C4	-2.67	1.41	1.44
49	j	202	PLX	O6-C4	-2.59	1.41	1.44
49	r	502	PLX	O6-C4	-2.58	1.41	1.44
50	C	304	970	C09-C07	2.57	1.45	1.39
47	A	503	NAI	C8A-N9A	-2.54	1.33	1.37
46	A	502	FMN	C10-N1	2.53	1.38	1.33
48	j	201	PEE	O3-C30	2.51	1.40	1.33
48	l	703	PEE	O3-C30	2.50	1.40	1.33
48	U	101	PEE	O3-C30	2.49	1.40	1.33
48	l	704	PEE	O3-C30	2.47	1.40	1.33
53	s	402	UQ	C7-C8	2.46	1.54	1.50
48	B	303	PEE	O3-C30	2.45	1.40	1.33
47	A	503	NAI	O3B-C3B	-2.45	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	O3-C30	2.45	1.40	1.33
49	J	403	PLX	O6-C4	-2.44	1.41	1.44
52	J	401	NDP	O2B-C2B	2.44	1.53	1.44
56	a	201	CDL	OA6-CA4	-2.44	1.40	1.46
47	A	503	NAI	PN-O5D	2.44	1.69	1.59
48	i	401	PEE	O2-C2	-2.43	1.40	1.46
56	l	701	CDL	OA6-CA4	-2.43	1.40	1.46
56	l	702	CDL	OA6-CA4	-2.43	1.40	1.46
56	i	402	CDL	OA6-CA4	-2.42	1.40	1.46
48	C	302	PEE	O3-C30	2.42	1.40	1.33
48	C	302	PEE	O2-C2	-2.42	1.40	1.46
48	r	501	PEE	O3-C30	2.42	1.40	1.33
48	W	201	PEE	O2-C2	-2.40	1.40	1.46
48	i	401	PEE	O3-C30	2.40	1.40	1.33
48	B	303	PEE	O2-C10	2.40	1.41	1.34
49	a	202	PLX	C7-C6	2.40	1.55	1.50
48	U	101	PEE	O2-C2	-2.40	1.40	1.46
49	J	403	PLX	C7-C6	2.40	1.55	1.50
48	r	501	PEE	O2-C2	-2.39	1.40	1.46
53	J	402	UQ	C7-C8	2.39	1.54	1.50
48	l	703	PEE	O2-C2	-2.38	1.40	1.46
56	s	401	CDL	OA6-CA4	-2.38	1.40	1.46
49	j	202	PLX	C7-C6	2.38	1.55	1.50
51	X	201	8Q1	C1-S44	2.38	1.81	1.76
49	r	502	PLX	C7-C6	2.37	1.55	1.50
51	G	201	8Q1	C1-S44	2.37	1.81	1.76
56	N	201	CDL	OA6-CA4	-2.36	1.40	1.46
56	n	101	CDL	OA6-CA4	-2.35	1.40	1.46
48	l	704	PEE	O2-C2	-2.35	1.40	1.46
49	C	303	PLX	C7-C6	2.35	1.55	1.50
48	j	201	PEE	O2-C2	-2.35	1.40	1.46
56	o	201	CDL	OA6-CA4	-2.34	1.40	1.46
49	g	201	PLX	C7-C6	2.34	1.55	1.50
48	l	703	PEE	O2-C10	2.33	1.40	1.34
48	B	303	PEE	O2-C2	-2.32	1.40	1.46
48	l	704	PEE	O2-C10	2.31	1.40	1.34
52	J	401	NDP	C2D-C3D	2.31	1.59	1.53
51	X	201	8Q1	O35-C34	-2.30	1.18	1.23
58	w	401	ADP	C5-N7	-2.30	1.34	1.39
48	W	201	PEE	O2-C10	2.30	1.40	1.34
48	U	101	PEE	O2-C10	2.29	1.40	1.34
47	A	503	NAI	C5B-C4B	2.29	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	r	503	PLX	C7-C6	2.28	1.55	1.50
48	C	302	PEE	O2-C10	2.28	1.40	1.34
48	i	401	PEE	O2-C10	2.27	1.40	1.34
48	r	501	PEE	O2-C10	2.26	1.40	1.34
48	j	201	PEE	O2-C10	2.26	1.40	1.34
56	V	201	CDL	PB2-OB2	2.25	1.68	1.59
51	X	201	8Q1	C6-C1	2.25	1.53	1.50
56	l	701	CDL	PB2-OB2	2.23	1.68	1.59
56	n	101	CDL	PB2-OB2	2.22	1.68	1.59
51	G	201	8Q1	O40-C39	-2.22	1.18	1.23
56	i	402	CDL	PB2-OB2	2.22	1.68	1.59
56	o	201	CDL	PB2-OB2	2.22	1.68	1.59
56	l	702	CDL	PB2-OB2	2.22	1.68	1.59
56	a	201	CDL	PB2-OB2	2.22	1.68	1.59
56	s	401	CDL	PB2-OB2	2.22	1.68	1.59
51	X	201	8Q1	O40-C39	-2.21	1.18	1.23
56	V	201	CDL	PB2-OB5	2.21	1.68	1.59
51	G	201	8Q1	O35-C34	-2.21	1.19	1.23
56	o	201	CDL	PB2-OB5	2.20	1.68	1.59
51	G	201	8Q1	C6-C1	2.20	1.53	1.50
56	l	701	CDL	PB2-OB5	2.20	1.68	1.59
56	n	101	CDL	PB2-OB5	2.19	1.68	1.59
56	N	201	CDL	PB2-OB2	2.19	1.68	1.59
56	k	101	CDL	PB2-OB2	2.18	1.68	1.59
56	a	201	CDL	PB2-OB5	2.18	1.68	1.59
56	l	702	CDL	PB2-OB5	2.18	1.68	1.59
53	J	402	UQ	O4-C4	-2.18	1.18	1.23
56	N	201	CDL	OB6-CB4	-2.17	1.41	1.46
50	C	304	970	C04-C02	2.17	1.53	1.50
49	r	502	PLX	P1-O4	2.17	1.68	1.59
56	i	402	CDL	PB2-OB5	2.17	1.68	1.59
49	J	403	PLX	P1-O4	2.17	1.68	1.59
56	s	401	CDL	PB2-OB5	2.17	1.68	1.59
56	l	702	CDL	OB6-CB4	-2.16	1.41	1.46
56	k	101	CDL	PB2-OB5	2.16	1.68	1.59
49	C	303	PLX	P1-O4	2.16	1.68	1.59
53	s	402	UQ	O4-C4	-2.15	1.18	1.23
56	a	201	CDL	OB6-CB4	-2.15	1.41	1.46
56	n	101	CDL	OB6-CB4	-2.15	1.41	1.46
56	l	701	CDL	OB6-CB4	-2.15	1.41	1.46
56	o	201	CDL	OB6-CB4	-2.15	1.41	1.46
49	j	202	PLX	P1-O4	2.15	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	k	101	CDL	OB6-CB4	-2.15	1.41	1.46
50	C	304	970	O28-C19	2.14	1.40	1.37
56	V	201	CDL	OB6-CB4	-2.14	1.41	1.46
49	g	201	PLX	P1-O4	2.14	1.68	1.59
49	a	202	PLX	P1-O4	2.14	1.68	1.59
56	i	402	CDL	OB6-CB4	-2.14	1.41	1.46
56	s	401	CDL	OB6-CB4	-2.13	1.41	1.46
52	J	401	NDP	PA-O5B	2.13	1.67	1.59
56	N	201	CDL	PB2-OB5	2.13	1.67	1.59
56	V	201	CDL	OA6-CA4	-2.12	1.41	1.46
52	J	401	NDP	O7N-C7N	-2.12	1.19	1.24
49	r	503	PLX	P1-O4	2.10	1.67	1.59
48	i	401	PEE	O3-C3	-2.09	1.40	1.45
48	l	703	PEE	O3-C3	-2.08	1.40	1.45
48	l	704	PEE	O3-C3	-2.08	1.40	1.45
49	r	502	PLX	P1-O1	2.08	1.67	1.59
48	C	302	PEE	O3-C3	-2.08	1.40	1.45
48	j	201	PEE	O3-C3	-2.07	1.40	1.45
50	C	304	970	O26-C20	2.07	1.40	1.37
48	W	201	PEE	O3-C3	-2.07	1.40	1.45
48	B	303	PEE	O3-C3	-2.07	1.40	1.45
49	J	403	PLX	P1-O1	2.05	1.67	1.59
49	C	303	PLX	P1-O1	2.04	1.67	1.59
49	g	201	PLX	P1-O1	2.04	1.67	1.59
53	J	402	UQ	O3-CM3	-2.03	1.40	1.45
49	r	503	PLX	P1-O1	2.03	1.67	1.59
49	j	202	PLX	P1-O1	2.03	1.67	1.59
48	r	501	PEE	O3-C3	-2.02	1.40	1.45
53	s	402	UQ	O1-C1	-2.02	1.19	1.23
56	n	101	CDL	C11-CA5	2.01	1.56	1.50
53	J	402	UQ	C21-C19	2.01	1.55	1.51
49	a	202	PLX	P1-O1	2.00	1.67	1.59
49	r	502	PLX	C25-C24	2.00	1.55	1.50

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C3N-C2N-N1N	-9.04	110.20	123.10
53	s	402	UQ	C7-C8-C9	-8.25	113.05	126.79
50	C	304	970	O25-C24-C11	-7.75	109.56	121.98
53	J	402	UQ	C7-C8-C9	-7.73	113.93	126.79
50	C	304	970	O08-C07-C06	-6.75	108.88	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	C1D-N1N-C2N	-6.63	110.07	121.11
53	s	402	UQ	C22-C23-C24	-6.13	112.89	127.66
51	G	201	8Q1	C6-C1-S44	5.98	120.42	113.46
53	s	402	UQ	C12-C13-C14	-5.93	113.38	127.66
52	J	401	NDP	C5A-C4A-N3A	-5.93	119.02	126.75
53	J	402	UQ	C17-C18-C19	-5.89	113.49	127.66
47	A	503	NAI	C5A-C4A-N3A	-5.80	119.18	126.75
53	s	402	UQ	C17-C18-C19	-5.80	113.70	127.66
53	J	402	UQ	C12-C13-C14	-5.78	113.75	127.66
58	w	401	ADP	C5-C4-N3	-5.74	119.26	126.75
51	X	201	8Q1	C6-C1-S44	5.70	120.09	113.46
50	C	304	970	C06-C05-C04	5.30	106.20	101.45
52	J	401	NDP	C1D-N1N-C6N	-5.15	109.73	120.83
53	J	402	UQ	C10-C9-C8	-4.69	111.65	123.68
58	w	401	ADP	N3-C2-N1	-4.46	121.63	128.60
58	w	401	ADP	N3-C4-N9	4.44	134.40	127.08
53	J	402	UQ	C22-C23-C24	-4.41	112.68	127.75
47	A	503	NAI	N3A-C2A-N1A	-4.33	121.83	128.60
53	s	402	UQ	C10-C9-C8	-4.29	112.66	123.68
53	s	402	UQ	C25-C24-C23	-4.27	112.72	123.68
53	s	402	UQ	C27-C28-C29	-4.25	113.23	127.75
53	J	402	UQ	C11-C9-C8	-4.22	112.58	121.12
50	C	304	970	C01-C02-C03	-4.21	111.26	121.38
52	J	401	NDP	N3A-C4A-N9A	4.16	133.94	127.08
53	s	402	UQ	C26-C24-C23	-4.15	112.71	121.12
53	J	402	UQ	C21-C19-C18	-4.13	112.76	121.12
56	l	702	CDL	OA6-CA5-C11	4.13	120.40	111.50
48	B	303	PEE	O2-C10-C11	4.12	120.39	111.50
56	n	101	CDL	OB6-CB5-C51	4.12	120.38	111.50
48	j	201	PEE	O2-C10-C11	4.12	120.38	111.50
56	a	201	CDL	OB6-CB5-C51	4.10	120.35	111.50
53	s	402	UQ	C11-C9-C8	-4.06	112.89	121.12
47	A	503	NAI	N3A-C4A-N9A	4.06	133.77	127.08
48	l	704	PEE	O2-C10-C11	4.04	120.22	111.50
51	X	201	8Q1	C37-C38-C39	4.04	119.09	112.36
56	n	101	CDL	OA6-CA5-C11	4.04	120.20	111.50
48	r	501	PEE	O2-C10-C11	4.03	120.19	111.50
56	s	401	CDL	OB6-CB5-C51	4.03	120.18	111.50
56	V	201	CDL	OB6-CB5-C51	4.01	120.15	111.50
52	J	401	NDP	N3A-C2A-N1A	-4.01	122.34	128.60
56	o	201	CDL	OB6-CB5-C51	4.00	120.11	111.50
53	s	402	UQ	C21-C19-C18	-3.99	113.05	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	l	702	CDL	OB6-CB5-C51	3.97	120.06	111.50
56	s	401	CDL	OA6-CA5-C11	3.95	120.02	111.50
48	C	302	PEE	O2-C10-C11	3.95	120.02	111.50
56	o	201	CDL	OA6-CA5-C11	3.95	120.01	111.50
53	J	402	UQ	C20-C19-C18	-3.93	113.61	123.68
56	N	201	CDL	OA6-CA5-C11	3.92	119.95	111.50
48	W	201	PEE	O2-C10-C11	3.91	119.93	111.50
56	k	101	CDL	OB6-CB5-C51	3.91	119.92	111.50
56	l	701	CDL	OA6-CA5-C11	3.90	119.90	111.50
56	l	701	CDL	OB6-CB5-C51	3.89	119.88	111.50
56	N	201	CDL	OB6-CB5-C51	3.88	119.87	111.50
53	s	402	UQ	C20-C19-C18	-3.88	113.72	123.68
47	A	503	NAI	C2A-N3A-C4A	3.87	120.90	111.75
56	i	402	CDL	OA6-CA5-C11	3.87	119.83	111.50
56	i	402	CDL	OB6-CB5-C51	3.87	119.83	111.50
53	s	402	UQ	C16-C14-C13	-3.86	113.31	121.12
56	a	201	CDL	OA6-CA5-C11	3.85	119.81	111.50
53	s	402	UQ	C15-C14-C13	-3.85	113.81	123.68
48	i	401	PEE	O2-C10-C11	3.82	119.73	111.50
56	V	201	CDL	OA6-CA5-C11	3.81	119.72	111.50
53	J	402	UQ	C15-C14-C13	-3.81	113.91	123.68
48	l	703	PEE	O2-C10-C11	3.80	119.69	111.50
52	J	401	NDP	C2A-N3A-C4A	3.74	120.59	111.75
58	w	401	ADP	C2-N3-C4	3.73	120.56	111.75
47	A	503	NAI	C5A-N7A-C8A	3.70	108.77	103.51
50	C	304	970	O25-C24-C23	-3.64	115.77	121.00
58	w	401	ADP	N9-C8-N7	-3.62	108.96	113.91
50	C	304	970	O08-C07-C09	3.62	131.24	123.89
48	U	101	PEE	O2-C10-C11	3.58	119.22	111.50
50	C	304	970	O13-C14-C23	3.58	116.02	112.40
58	w	401	ADP	C5-N7-C8	3.50	108.48	103.51
51	G	201	8Q1	O4-C1-C6	-3.47	119.89	123.99
53	J	402	UQ	C16-C14-C13	-3.44	114.16	121.12
56	k	101	CDL	OA6-CA5-C11	3.42	118.87	111.50
53	s	402	UQ	C30-C29-C28	-3.40	112.81	122.65
53	J	402	UQ	C25-C24-C23	-3.38	112.88	122.65
47	A	503	NAI	N9A-C8A-N7A	-3.38	109.30	113.91
53	J	402	UQ	C26-C24-C23	-3.37	112.90	122.65
51	X	201	8Q1	O4-C1-C6	-3.33	120.06	123.99
52	J	401	NDP	C5A-N7A-C8A	3.30	108.20	103.51
47	A	503	NAI	C3D-C2D-C1D	3.28	107.65	101.43
47	A	503	NAI	C4A-C5A-N7A	-3.27	106.64	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	401	NDP	N9A-C8A-N7A	-3.24	109.49	113.91
56	n	101	CDL	OA8-CA7-C31	3.23	119.85	111.38
50	C	304	970	O26-C20-C19	3.12	119.75	115.41
50	C	304	970	C09-C07-C06	-3.10	119.88	123.20
53	s	402	UQ	C31-C29-C28	-3.07	113.78	122.65
58	w	401	ADP	C4-N9-C8	3.07	109.05	105.73
46	A	502	FMN	C4-N3-C2	-3.06	120.00	125.64
52	J	401	NDP	C4A-C5A-N7A	-3.02	106.94	110.62
50	C	304	970	O28-C19-C20	2.96	119.53	115.41
50	C	304	970	C04-C02-C03	-2.93	113.70	120.31
51	G	201	8Q1	C37-C38-C39	2.86	117.13	112.36
50	C	304	970	C22-C23-C14	2.85	113.54	109.56
58	w	401	ADP	C4-C5-N7	-2.83	107.17	110.62
48	B	303	PEE	O3-C30-C31	2.80	120.71	111.91
47	A	503	NAI	C2D-C3D-C4D	2.79	108.06	102.64
56	l	702	CDL	OA8-CA7-C31	2.76	120.57	111.91
52	J	401	NDP	C2B-C3B-C4B	2.76	107.98	101.99
56	k	101	CDL	OA8-CA7-C31	2.75	120.53	111.91
56	l	702	CDL	OB8-CB7-C71	2.73	120.48	111.91
56	n	101	CDL	OB8-CB7-C71	2.71	120.41	111.91
46	A	502	FMN	C4A-C4-N3	2.71	120.06	113.19
48	l	703	PEE	O3-C30-C31	2.69	120.36	111.91
48	U	101	PEE	O3-C30-C31	2.68	120.32	111.91
56	V	201	CDL	OB8-CB7-C71	2.67	120.29	111.91
48	r	501	PEE	O3-C30-C31	2.66	120.25	111.91
56	N	201	CDL	OB8-CB7-C71	2.65	120.23	111.91
56	l	701	CDL	OB8-CB7-C71	2.64	120.20	111.91
58	w	401	ADP	PA-O3A-PB	-2.64	123.76	132.83
56	l	701	CDL	OA8-CA7-C31	2.64	120.20	111.91
56	N	201	CDL	OA8-CA7-C31	2.64	120.18	111.91
56	o	201	CDL	OA8-CA7-C31	2.62	120.12	111.91
50	C	304	970	C11-C12-C06	-2.61	118.94	123.16
56	o	201	CDL	OB8-CB7-C71	2.60	120.07	111.91
56	a	201	CDL	OB8-CB7-C71	2.60	120.05	111.91
48	i	401	PEE	O3-C30-C31	2.60	120.05	111.91
52	J	401	NDP	PN-O3-PA	-2.59	123.93	132.83
56	i	402	CDL	OB8-CB7-C71	2.58	120.00	111.91
48	W	201	PEE	O3-C30-C31	2.57	119.97	111.91
47	A	503	NAI	C4D-O4D-C1D	-2.56	103.81	109.47
56	k	101	CDL	OB8-CB7-C71	2.56	119.95	111.91
56	s	401	CDL	OA8-CA7-C31	2.55	119.91	111.91
56	i	402	CDL	OA8-CA7-C31	2.55	119.90	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	CDL	OB8-CB7-C71	2.54	119.89	111.91
48	j	201	PEE	O3-C30-C31	2.54	119.86	111.91
53	J	402	UQ	CM5-C5-C6	-2.52	120.28	124.40
47	A	503	NAI	PN-O3-PA	-2.52	124.17	132.83
46	A	502	FMN	O4-C4-C4A	-2.52	119.92	126.60
48	l	704	PEE	O3-C30-C31	2.52	119.80	111.91
56	a	201	CDL	OA8-CA7-C31	2.50	119.75	111.91
48	C	302	PEE	O3-C30-C31	2.50	119.74	111.91
56	V	201	CDL	OA8-CA7-C31	2.49	119.72	111.91
53	s	402	UQ	CM5-C5-C6	-2.47	120.37	124.40
49	g	201	PLX	C1A-N1-C1	2.43	119.87	109.92
49	r	502	PLX	C1A-N1-C1	2.42	119.81	109.92
52	J	401	NDP	C4A-N9A-C8A	2.39	108.32	105.73
49	a	202	PLX	C1A-N1-C1	2.37	119.62	109.92
49	J	403	PLX	C1A-N1-C1	2.33	119.46	109.92
46	A	502	FMN	C4A-C10-N10	2.33	119.88	116.48
47	A	503	NAI	C4A-N9A-C8A	2.32	108.25	105.73
49	j	202	PLX	C1A-N1-C1	2.32	119.40	109.92
46	A	502	FMN	C4A-C10-N1	-2.31	119.37	124.73
51	G	201	8Q1	C38-C39-N41	2.30	120.29	116.42
51	X	201	8Q1	C32-C34-N36	2.30	121.15	116.58
51	X	201	8Q1	C43-S44-C1	2.28	108.98	101.87
51	G	201	8Q1	O4-C1-S44	-2.25	119.69	122.61
49	C	303	PLX	C1A-N1-C1	2.24	119.10	109.92
46	A	502	FMN	C9A-C5A-N5	-2.21	120.03	122.43
46	A	502	FMN	C10-C4A-N5	-2.18	120.23	124.86
49	r	503	PLX	C1A-N1-C1	2.17	118.81	109.92
50	C	304	970	C05-C04-C02	-2.16	112.46	115.62
51	X	201	8Q1	O4-C1-S44	-2.13	119.85	122.61
56	l	702	CDL	CA4-OA6-CA5	-2.12	112.56	117.79
50	C	304	970	C15-C14-C23	2.12	112.33	110.62
50	C	304	970	O26-C20-C21	-2.09	120.52	124.12
46	A	502	FMN	C5A-C9A-N10	2.09	120.11	117.95
50	C	304	970	C07-C06-C12	2.06	120.76	118.74

There are no chirality outliers.

All (1020) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
47	A	503	NAI	C5B-O5B-PA-O1A
48	B	303	PEE	C1-O3P-P-O1P
48	B	303	PEE	O4P-C4-C5-N
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	U	101	PEE	C4-O4P-P-O3P
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	i	401	PEE	C11-C10-O2-C2
48	i	401	PEE	C4-O4P-P-O3P
48	i	401	PEE	C4-O4P-P-O2P
48	i	401	PEE	C4-O4P-P-O1P
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	O4P-C4-C5-N
48	l	703	PEE	O3P-C1-C2-O2
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O2P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O6-C4-C5-O8
49	C	303	PLX	N1-C1-C2-O1
49	J	403	PLX	O7-C6-O6-C4
49	J	403	PLX	N1-C1-C2-O1
49	a	202	PLX	O7-C6-O6-C4
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-C7-C8
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	g	201	PLX	C2-O1-P1-O3
49	j	202	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C7-C6-O6-C4
49	j	202	PLX	C3-O4-P1-O2
49	j	202	PLX	C3-O4-P1-O3
49	j	202	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	C3-C4-O6-C6
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	O9-C24-C25-C26
50	C	304	970	C03-C02-C04-C05
50	C	304	970	C03-C02-C04-O08
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	G	201	8Q1	C42-C43-S44-C1
51	G	201	8Q1	C28-O27-P24-O3
51	X	201	8Q1	C28-C29-C32-C34
51	X	201	8Q1	C28-C29-C32-O33
51	X	201	8Q1	C30-C29-C32-C34
51	X	201	8Q1	C30-C29-C32-O33
51	X	201	8Q1	C31-C29-C32-C34
51	X	201	8Q1	C29-C32-C34-N36
51	X	201	8Q1	C29-C32-C34-O35
51	X	201	8Q1	O33-C32-C34-N36
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
52	J	401	NDP	C5B-O5B-PA-O1A
52	J	401	NDP	C5B-O5B-PA-O3
53	J	402	UQ	C7-C8-C9-C10
53	J	402	UQ	C7-C8-C9-C11
53	s	402	UQ	C7-C8-C9-C10
53	s	402	UQ	C7-C8-C9-C11
53	s	402	UQ	C18-C19-C21-C22
53	s	402	UQ	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
53	s	402	UQ	C27-C28-C29-C30
56	N	201	CDL	O1-C1-CA2-OA2
56	N	201	CDL	CB2-C1-CA2-OA2
56	N	201	CDL	CA2-OA2-PA1-OA3
56	N	201	CDL	CA2-OA2-PA1-OA4
56	N	201	CDL	CA3-OA5-PA1-OA3
56	N	201	CDL	CB2-OB2-PB2-OB3
56	N	201	CDL	CB2-OB2-PB2-OB4
56	N	201	CDL	CB2-OB2-PB2-OB5
56	V	201	CDL	CB3-OB5-PB2-OB3
56	V	201	CDL	CB3-OB5-PB2-OB4
56	a	201	CDL	CA2-C1-CB2-OB2
56	a	201	CDL	CA2-OA2-PA1-OA3
56	a	201	CDL	CA3-OA5-PA1-OA2
56	a	201	CDL	CA3-OA5-PA1-OA3
56	a	201	CDL	CA3-OA5-PA1-OA4
56	a	201	CDL	CB2-OB2-PB2-OB3
56	a	201	CDL	OB7-CB5-OB6-CB4
56	a	201	CDL	C51-CB5-OB6-CB4
56	i	402	CDL	CA2-OA2-PA1-OA3
56	i	402	CDL	CA3-OA5-PA1-OA2
56	i	402	CDL	CA3-OA5-PA1-OA3
56	i	402	CDL	CB3-OB5-PB2-OB3
56	i	402	CDL	C51-CB5-OB6-CB4
56	k	101	CDL	CB2-C1-CA2-OA2
56	k	101	CDL	CA2-OA2-PA1-OA3
56	k	101	CDL	CA2-OA2-PA1-OA4
56	k	101	CDL	CA2-OA2-PA1-OA5
56	k	101	CDL	CA3-OA5-PA1-OA3
56	k	101	CDL	OA5-CA3-CA4-OA6
56	k	101	CDL	CB2-OB2-PB2-OB3
56	k	101	CDL	CB3-OB5-PB2-OB3
56	k	101	CDL	CB3-OB5-PB2-OB4
56	l	701	CDL	O1-C1-CA2-OA2
56	l	701	CDL	CB2-OB2-PB2-OB4
56	l	701	CDL	CB3-OB5-PB2-OB3
56	l	702	CDL	O1-C1-CB2-OB2
56	l	702	CDL	CA2-OA2-PA1-OA5
56	l	702	CDL	CA3-OA5-PA1-OA3
56	l	702	CDL	CA3-OA5-PA1-OA4
56	n	101	CDL	CA2-OA2-PA1-OA3
56	n	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
56	n	101	CDL	CA3-OA5-PA1-OA4
56	n	101	CDL	CB3-OB5-PB2-OB3
56	n	101	CDL	CB3-OB5-PB2-OB4
56	o	201	CDL	CA2-OA2-PA1-OA3
56	o	201	CDL	CA2-OA2-PA1-OA4
56	o	201	CDL	CA3-OA5-PA1-OA3
56	o	201	CDL	CB3-OB5-PB2-OB2
56	o	201	CDL	CB3-OB5-PB2-OB3
56	o	201	CDL	CB3-OB5-PB2-OB4
56	s	401	CDL	CA2-OA2-PA1-OA3
56	s	401	CDL	CB3-OB5-PB2-OB4
56	l	701	CDL	OA9-CA7-OA8-CA6
56	l	701	CDL	C31-CA7-OA8-CA6
48	U	101	PEE	O5-C30-O3-C3
56	l	702	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	O4-C10-O2-C2
48	l	703	PEE	O4-C10-O2-C2
56	i	402	CDL	OB7-CB5-OB6-CB4
48	U	101	PEE	C31-C30-O3-C3
56	i	402	CDL	C71-CB7-OB8-CB6
56	l	702	CDL	C71-CB7-OB8-CB6
48	C	302	PEE	C11-C10-O2-C2
53	J	402	UQ	C22-C23-C24-C26
48	B	303	PEE	C17-C18-C19-C20
48	U	101	PEE	C17-C18-C19-C20
48	l	704	PEE	C37-C38-C39-C40
49	g	201	PLX	C7-C8-C9-C10
48	C	302	PEE	O4-C10-O2-C2
48	i	401	PEE	O4-C10-O2-C2
53	J	402	UQ	C12-C13-C14-C16
53	J	402	UQ	C17-C18-C19-C21
53	s	402	UQ	C17-C18-C19-C21
56	i	402	CDL	OB9-CB7-OB8-CB6
49	r	502	PLX	C11-C12-C13-C14
56	a	201	CDL	O1-C1-CA2-OA2
56	i	402	CDL	O1-C1-CA2-OA2
56	l	701	CDL	O1-C1-CB2-OB2
56	l	702	CDL	O1-C1-CA2-OA2
56	o	201	CDL	O1-C1-CB2-OB2
56	s	401	CDL	O1-C1-CB2-OB2
49	J	403	PLX	C27-C28-C29-C30
48	l	703	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
48	l	704	PEE	C11-C10-O2-C2
56	V	201	CDL	C11-CA5-OA6-CA4
56	l	702	CDL	C51-CB5-OB6-CB4
56	o	201	CDL	C51-CB5-OB6-CB4
56	s	401	CDL	C51-CB5-OB6-CB4
56	V	201	CDL	C11-C12-C13-C14
49	C	303	PLX	C25-C26-C27-C28
49	C	303	PLX	C27-C28-C29-C30
49	J	403	PLX	C25-C26-C27-C28
56	n	101	CDL	C71-C72-C73-C74
49	r	502	PLX	C9-C10-C11-C12
49	r	502	PLX	C7-C8-C9-C10
56	l	702	CDL	C75-C76-C77-C78
49	g	201	PLX	C9-C10-C11-C12
52	J	401	NDP	O4B-C4B-C5B-O5B
56	V	201	CDL	OA7-CA5-OA6-CA4
56	k	101	CDL	C73-C74-C75-C76
53	J	402	UQ	C12-C11-C9-C8
56	o	201	CDL	C11-C12-C13-C14
53	s	402	UQ	C9-C11-C12-C13
53	s	402	UQ	C14-C16-C17-C18
56	l	701	CDL	C55-C56-C57-C58
56	V	201	CDL	C31-CA7-OA8-CA6
56	V	201	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C13-C14-C15-C16
56	a	201	CDL	CB2-C1-CA2-OA2
56	l	701	CDL	CB2-C1-CA2-OA2
56	l	701	CDL	CA2-C1-CB2-OB2
56	l	702	CDL	CA2-C1-CB2-OB2
56	o	201	CDL	CA2-C1-CB2-OB2
56	s	401	CDL	CA2-C1-CB2-OB2
48	l	704	PEE	O4-C10-O2-C2
56	l	702	CDL	OB7-CB5-OB6-CB4
56	o	201	CDL	OB7-CB5-OB6-CB4
56	s	401	CDL	OB7-CB5-OB6-CB4
56	s	401	CDL	C31-C32-C33-C34
49	g	201	PLX	C2-C1-N1-C1B
49	g	201	PLX	C2-C1-N1-C1A
48	i	401	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C30-O3-C3
56	a	201	CDL	C71-CB7-OB8-CB6
56	k	101	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
56	V	201	CDL	C32-C33-C34-C35
56	s	401	CDL	C14-C15-C16-C17
56	V	201	CDL	OB5-CB3-CB4-OB6
48	B	303	PEE	C34-C35-C36-C37
56	k	101	CDL	O1-C1-CA2-OA2
56	o	201	CDL	O1-C1-CA2-OA2
56	V	201	CDL	OB6-CB4-CB6-OB8
56	s	401	CDL	OB6-CB4-CB6-OB8
56	l	702	CDL	C12-C13-C14-C15
48	l	703	PEE	O5-C30-O3-C3
56	a	201	CDL	CA5-C11-C12-C13
56	k	101	CDL	CA7-C31-C32-C33
56	s	401	CDL	CA7-C31-C32-C33
56	a	201	CDL	OB9-CB7-OB8-CB6
48	l	704	PEE	C34-C35-C36-C37
56	i	402	CDL	CA5-C11-C12-C13
56	l	702	CDL	CB5-C51-C52-C53
56	l	702	CDL	C35-C36-C37-C38
56	N	201	CDL	CA7-C31-C32-C33
56	i	402	CDL	CB7-C71-C72-C73
56	l	701	CDL	CB5-C51-C52-C53
56	l	701	CDL	CB7-C71-C72-C73
56	n	101	CDL	CB7-C71-C72-C73
56	o	201	CDL	CB7-C71-C72-C73
52	J	401	NDP	O4D-C4D-C5D-O5D
52	J	401	NDP	C3D-C4D-C5D-O5D
48	l	704	PEE	C21-C22-C23-C24
56	l	701	CDL	C58-C59-C60-C61
56	k	101	CDL	OB9-CB7-OB8-CB6
48	i	401	PEE	O5-C30-O3-C3
48	B	303	PEE	C11-C12-C13-C14
56	a	201	CDL	CB7-C71-C72-C73
56	a	201	CDL	O1-C1-CB2-OB2
56	l	701	CDL	C34-C35-C36-C37
56	s	401	CDL	C36-C37-C38-C39
56	V	201	CDL	OA9-CA7-OA8-CA6
56	V	201	CDL	OB9-CB7-OB8-CB6
56	n	101	CDL	C75-C76-C77-C78
48	W	201	PEE	C17-C18-C19-C20
56	i	402	CDL	C51-C52-C53-C54
48	C	302	PEE	C4-O4P-P-O3P
48	U	101	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C4-O4P-P-O3P
48	i	401	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
49	C	303	PLX	C3-O4-P1-O1
49	a	202	PLX	C3-O4-P1-O1
49	g	201	PLX	C2-O1-P1-O4
49	j	202	PLX	C3-O4-P1-O1
49	r	503	PLX	C2-O1-P1-O4
56	N	201	CDL	CA2-OA2-PA1-OA5
56	V	201	CDL	CB3-OB5-PB2-OB2
56	a	201	CDL	CB2-OB2-PB2-OB5
56	i	402	CDL	CB2-OB2-PB2-OB5
56	i	402	CDL	CB3-OB5-PB2-OB2
56	k	101	CDL	CA3-OA5-PA1-OA2
56	k	101	CDL	CB2-OB2-PB2-OB5
56	k	101	CDL	CB3-OB5-PB2-OB2
56	l	701	CDL	CB2-OB2-PB2-OB5
56	l	702	CDL	CA3-OA5-PA1-OA2
56	n	101	CDL	CA2-OA2-PA1-OA5
56	n	101	CDL	CA3-OA5-PA1-OA2
56	n	101	CDL	CB3-OB5-PB2-OB2
56	o	201	CDL	CA2-OA2-PA1-OA5
56	s	401	CDL	CB3-OB5-PB2-OB2
56	s	401	CDL	CB5-C51-C52-C53
52	J	401	NDP	C2D-C1D-N1N-C6N
48	B	303	PEE	C31-C30-O3-C3
56	N	201	CDL	C51-C52-C53-C54
56	s	401	CDL	CB7-C71-C72-C73
56	i	402	CDL	CB2-C1-CA2-OA2
56	l	702	CDL	CB2-C1-CA2-OA2
56	o	201	CDL	CB2-C1-CA2-OA2
56	l	702	CDL	C17-C18-C19-C20
56	a	201	CDL	C36-C37-C38-C39
56	V	201	CDL	C56-C57-C58-C59
56	V	201	CDL	C62-C63-C64-C65
56	l	701	CDL	C37-C38-C39-C40
56	l	702	CDL	C11-CA5-OA6-CA4
48	W	201	PEE	C13-C14-C15-C16
48	j	201	PEE	C12-C13-C14-C15
49	C	303	PLX	C9-C10-C11-C12
49	J	403	PLX	C7-C8-C9-C10
49	J	403	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C11-C10-C9-C8
56	V	201	CDL	C31-C32-C33-C34
56	V	201	CDL	C34-C35-C36-C37
56	k	101	CDL	C76-C77-C78-C79
56	l	701	CDL	C11-C12-C13-C14
56	l	701	CDL	C31-C32-C33-C34
56	s	401	CDL	C71-C72-C73-C74
56	s	401	CDL	C73-C74-C75-C76
48	r	501	PEE	C14-C15-C16-C17
49	g	201	PLX	C28-C29-C30-C31
51	X	201	8Q1	C9-C10-C11-C12
56	a	201	CDL	C62-C63-C64-C65
56	l	701	CDL	C73-C74-C75-C76
56	l	702	CDL	C80-C81-C82-C83
56	l	701	CDL	CA7-C31-C32-C33
48	C	302	PEE	C13-C14-C15-C16
48	i	401	PEE	C11-C12-C13-C14
49	a	202	PLX	C12-C13-C14-C15
49	j	202	PLX	C14-C15-C16-C17
51	X	201	8Q1	C11-C12-C13-C14
56	V	201	CDL	C40-C41-C42-C43
56	l	701	CDL	C59-C60-C61-C62
56	n	101	CDL	C74-C75-C76-C77
56	o	201	CDL	C82-C83-C84-C85
48	r	501	PEE	C20-C21-C22-C23
49	g	201	PLX	C10-C11-C12-C13
49	r	502	PLX	C33-C34-C35-C36
49	r	503	PLX	C32-C33-C34-C35
56	V	201	CDL	C75-C76-C77-C78
56	i	402	CDL	C80-C81-C82-C83
56	l	702	CDL	C11-C12-C13-C14
56	o	201	CDL	C75-C76-C77-C78
56	n	101	CDL	O1-C1-CB2-OB2
49	a	202	PLX	C10-C11-C12-C13
49	g	201	PLX	C12-C13-C14-C15
56	l	701	CDL	C62-C63-C64-C65
56	s	401	CDL	C32-C33-C34-C35
49	C	303	PLX	C11-C12-C13-C14
49	C	303	PLX	C10-C11-C12-C13
49	g	201	PLX	C27-C28-C29-C30
56	i	402	CDL	C31-C32-C33-C34
56	l	702	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C33-C34-C35-C36
49	j	202	PLX	C11-C12-C13-C14
49	j	202	PLX	C33-C34-C35-C36
49	r	502	PLX	C28-C29-C30-C31
56	a	201	CDL	C52-C53-C54-C55
56	l	702	CDL	C59-C60-C61-C62
48	i	401	PEE	C21-C22-C23-C24
48	i	401	PEE	C14-C15-C16-C17
49	J	403	PLX	C28-C29-C30-C31
49	J	403	PLX	C30-C31-C32-C33
49	a	202	PLX	C13-C14-C15-C16
49	g	201	PLX	C14-C15-C16-C17
49	g	201	PLX	C13-C14-C15-C16
49	j	202	PLX	C27-C28-C29-C30
49	r	502	PLX	C27-C28-C29-C30
56	a	201	CDL	C60-C61-C62-C63
56	i	402	CDL	C13-C14-C15-C16
56	l	701	CDL	C75-C76-C77-C78
56	l	702	CDL	C13-C14-C15-C16
56	o	201	CDL	C37-C38-C39-C40
49	C	303	PLX	C30-C31-C32-C33
49	a	202	PLX	C33-C34-C35-C36
49	g	201	PLX	C32-C33-C34-C35
56	i	402	CDL	C14-C15-C16-C17
56	l	702	CDL	C31-C32-C33-C34
48	B	303	PEE	O4-C10-O2-C2
56	l	702	CDL	OA7-CA5-OA6-CA4
48	B	303	PEE	C11-C10-O2-C2
48	U	101	PEE	C11-C12-C13-C14
49	j	202	PLX	C25-C26-C27-C28
49	r	503	PLX	C25-C26-C27-C28
56	o	201	CDL	C55-C56-C57-C58
56	o	201	CDL	C60-C61-C62-C63
56	s	401	CDL	C51-C52-C53-C54
48	B	303	PEE	C35-C36-C37-C38
48	U	101	PEE	C35-C36-C37-C38
48	r	501	PEE	C15-C16-C17-C18
48	i	401	PEE	C10-C11-C12-C13
56	l	702	CDL	CB7-C71-C72-C73
48	B	303	PEE	C23-C24-C25-C26
48	W	201	PEE	C21-C22-C23-C24
48	j	201	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C10-C11-C12-C13
56	V	201	CDL	C71-C72-C73-C74
56	V	201	CDL	C72-C73-C74-C75
56	a	201	CDL	C17-C18-C19-C20
56	a	201	CDL	C73-C74-C75-C76
56	a	201	CDL	C75-C76-C77-C78
56	i	402	CDL	C32-C33-C34-C35
56	i	402	CDL	C52-C53-C54-C55
56	i	402	CDL	C55-C56-C57-C58
56	k	101	CDL	C11-C12-C13-C14
56	k	101	CDL	C75-C76-C77-C78
56	o	201	CDL	C17-C18-C19-C20
49	j	202	PLX	C16-C17-C18-C19
51	X	201	8Q1	C7-C8-C9-C10
56	a	201	CDL	C22-C23-C24-C25
56	l	701	CDL	C36-C37-C38-C39
56	l	701	CDL	C52-C53-C54-C55
56	n	101	CDL	C52-C53-C54-C55
56	s	401	CDL	C37-C38-C39-C40
56	s	401	CDL	C59-C60-C61-C62
48	W	201	PEE	O4P-C4-C5-N
49	a	202	PLX	C9-C10-C11-C12
49	r	503	PLX	C28-C29-C30-C31
56	V	201	CDL	C59-C60-C61-C62
56	k	101	CDL	C71-C72-C73-C74
56	o	201	CDL	C53-C54-C55-C56
49	r	503	PLX	C14-C15-C16-C17
49	r	503	PLX	C7-C8-C9-C10
56	N	201	CDL	C71-C72-C73-C74
56	n	101	CDL	C55-C56-C57-C58
56	l	701	CDL	C71-CB7-OB8-CB6
56	V	201	CDL	C35-C36-C37-C38
56	a	201	CDL	C37-C38-C39-C40
56	i	402	CDL	C36-C37-C38-C39
56	i	402	CDL	C43-C44-C45-C46
46	A	502	FMN	O4'-C4'-C5'-O5'
48	U	101	PEE	C22-C23-C24-C25
49	C	303	PLX	C15-C16-C17-C18
49	a	202	PLX	C7-C8-C9-C10
48	l	703	PEE	C30-C31-C32-C33
49	J	403	PLX	C31-C32-C33-C34
56	V	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
56	a	201	CDL	C35-C36-C37-C38
56	i	402	CDL	C41-C42-C43-C44
48	i	401	PEE	C37-C38-C39-C40
49	r	502	PLX	C25-C26-C27-C28
56	a	201	CDL	C71-C72-C73-C74
56	l	701	CDL	C82-C83-C84-C85
56	s	401	CDL	C52-C53-C54-C55
56	s	401	CDL	C31-CA7-OA8-CA6
48	W	201	PEE	C11-C10-O2-C2
56	V	201	CDL	C51-CB5-OB6-CB4
49	j	202	PLX	C10-C11-C12-C13
56	k	101	CDL	C81-C82-C83-C84
49	g	201	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-C7-C8
49	g	201	PLX	C11-C10-C9-C8
49	r	502	PLX	C14-C15-C16-C17
56	l	701	CDL	C14-C15-C16-C17
56	l	701	CDL	C71-C72-C73-C74
56	n	101	CDL	C73-C74-C75-C76
56	s	401	CDL	C75-C76-C77-C78
48	l	703	PEE	C15-C16-C17-C18
48	U	101	PEE	C36-C37-C38-C39
49	a	202	PLX	C27-C28-C29-C30
49	j	202	PLX	C7-C8-C9-C10
56	a	201	CDL	C11-C12-C13-C14
56	a	201	CDL	C82-C83-C84-C85
48	B	303	PEE	O5-C30-O3-C3
56	V	201	CDL	C52-C53-C54-C55
56	i	402	CDL	C59-C60-C61-C62
48	W	201	PEE	O4-C10-O2-C2
56	o	201	CDL	C12-C13-C14-C15
49	r	502	PLX	C30-C31-C32-C33
49	g	201	PLX	C2-C1-N1-C1C
49	a	202	PLX	C34-C35-C36-C37
48	W	201	PEE	C31-C30-O3-C3
56	N	201	CDL	C71-CB7-OB8-CB6
56	o	201	CDL	C57-C58-C59-C60
48	l	704	PEE	C13-C14-C15-C16
48	j	201	PEE	C13-C14-C15-C16
49	j	202	PLX	C15-C16-C17-C18
56	V	201	CDL	C55-C56-C57-C58
56	a	201	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
56	l	702	CDL	C39-C40-C41-C42
56	l	701	CDL	OB9-CB7-OB8-CB6
56	s	401	CDL	OA9-CA7-OA8-CA6
49	r	502	PLX	C13-C14-C15-C16
48	i	401	PEE	C19-C20-C21-C22
48	r	501	PEE	O4-C10-O2-C2
56	V	201	CDL	OB7-CB5-OB6-CB4
48	C	302	PEE	C31-C30-O3-C3
48	l	703	PEE	C31-C32-C33-C34
56	l	701	CDL	C35-C36-C37-C38
56	k	101	CDL	CB7-C71-C72-C73
56	l	702	CDL	CA7-C31-C32-C33
48	W	201	PEE	C12-C13-C14-C15
56	o	201	CDL	C14-C15-C16-C17
56	o	201	CDL	C54-C55-C56-C57
48	C	302	PEE	C42-C43-C44-C45
56	V	201	CDL	C78-C79-C80-C81
56	k	101	CDL	C23-C24-C25-C26
56	a	201	CDL	C31-CA7-OA8-CA6
49	a	202	PLX	C17-C18-C19-C20
49	r	503	PLX	C13-C14-C15-C16
56	o	201	CDL	C36-C37-C38-C39
56	s	401	CDL	C35-C36-C37-C38
48	r	501	PEE	C11-C10-O2-C2
56	N	201	CDL	C51-CB5-OB6-CB4
56	l	701	CDL	C51-CB5-OB6-CB4
49	C	303	PLX	O4-C3-C4-O6
56	o	201	CDL	OB5-CB3-CB4-OB6
49	g	201	PLX	C30-C31-C32-C33
49	r	503	PLX	C11-C12-C13-C14
51	X	201	8Q1	C6-C7-C8-C9
56	s	401	CDL	C16-C17-C18-C19
49	a	202	PLX	C30-C31-C32-C33
56	l	701	CDL	OB7-CB5-OB6-CB4
49	C	303	PLX	C13-C14-C15-C16
49	g	201	PLX	C25-C26-C27-C28
56	o	201	CDL	OA6-CA4-CA6-OA8
56	o	201	CDL	OB6-CB4-CB6-OB8
56	k	101	CDL	C52-C53-C54-C55
56	l	702	CDL	C82-C83-C84-C85
56	s	401	CDL	C12-C13-C14-C15
48	l	703	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
56	l	701	CDL	C56-C57-C58-C59
56	l	702	CDL	C32-C33-C34-C35
48	C	302	PEE	C19-C20-C21-C22
48	l	703	PEE	C19-C20-C21-C22
48	U	101	PEE	C31-C32-C33-C34
48	r	501	PEE	C17-C18-C19-C20
56	V	201	CDL	C51-C52-C53-C54
48	W	201	PEE	O5-C30-O3-C3
56	N	201	CDL	OB9-CB7-OB8-CB6
56	N	201	CDL	OB7-CB5-OB6-CB4
49	C	303	PLX	C11-C10-C9-C8
56	o	201	CDL	C72-C73-C74-C75
48	B	303	PEE	C38-C39-C40-C41
48	j	201	PEE	C4-O4P-P-O3P
49	r	502	PLX	C3-O4-P1-O1
56	i	402	CDL	CA2-OA2-PA1-OA5
56	l	701	CDL	CB3-OB5-PB2-OB2
56	o	201	CDL	CA3-OA5-PA1-OA2
49	j	202	PLX	C19-C20-C21-C22
48	U	101	PEE	C21-C22-C23-C24
48	C	302	PEE	O3P-C1-C2-C3
56	V	201	CDL	OB5-CB3-CB4-CB6
56	i	402	CDL	C15-C16-C17-C18
49	j	202	PLX	C11-C10-C9-C8
49	J	403	PLX	C12-C13-C14-C15
56	k	101	CDL	C18-C19-C20-C21
48	C	302	PEE	C15-C16-C17-C18
48	l	703	PEE	C11-C12-C13-C14
56	k	101	CDL	C12-C13-C14-C15
56	l	702	CDL	C16-C17-C18-C19
56	o	201	CDL	C35-C36-C37-C38
48	j	201	PEE	C31-C30-O3-C3
56	s	401	CDL	C71-CB7-OB8-CB6
49	J	403	PLX	C13-C14-C15-C16
56	i	402	CDL	C72-C73-C74-C75
48	r	501	PEE	C11-C12-C13-C14
56	i	402	CDL	C71-C72-C73-C74
56	V	201	CDL	CB7-C71-C72-C73
48	C	302	PEE	O5-C30-O3-C3
49	r	502	PLX	C16-C17-C18-C19
48	r	501	PEE	C1-C2-C3-O3
49	a	202	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C3-C4-C5-O8
56	V	201	CDL	CA3-CA4-CA6-OA8
56	V	201	CDL	CB3-CB4-CB6-OB8
56	i	402	CDL	CB3-CB4-CB6-OB8
56	s	401	CDL	CB3-CB4-CB6-OB8
56	k	101	CDL	C17-C18-C19-C20
48	r	501	PEE	C10-C11-C12-C13
56	a	201	CDL	CB5-C51-C52-C53
49	r	502	PLX	C34-C35-C36-C37
49	a	202	PLX	O6-C6-C7-C8
49	g	201	PLX	O6-C6-C7-C8
48	i	401	PEE	C35-C36-C37-C38
48	j	201	PEE	C19-C20-C21-C22
56	N	201	CDL	C52-C53-C54-C55
56	n	101	CDL	C51-CB5-OB6-CB4
56	a	201	CDL	OA9-CA7-OA8-CA6
48	C	302	PEE	C44-C45-C46-C47
49	J	403	PLX	C11-C12-C13-C14
49	r	502	PLX	C12-C13-C14-C15
56	V	201	CDL	CA6-CA4-OA6-CA5
56	V	201	CDL	CB5-C51-C52-C53
48	U	101	PEE	C12-C13-C14-C15
56	i	402	CDL	C82-C83-C84-C85
56	V	201	CDL	C57-C58-C59-C60
56	N	201	CDL	OA5-CA3-CA4-OA6
56	l	701	CDL	OB5-CB3-CB4-OB6
56	l	702	CDL	OB5-CB3-CB4-OB6
49	C	303	PLX	C19-C20-C21-C22
49	C	303	PLX	C14-C15-C16-C17
51	X	201	8Q1	C11-C10-C9-C8
56	i	402	CDL	C35-C36-C37-C38
56	o	201	CDL	C32-C31-CA7-OA8
56	i	402	CDL	OB6-CB4-CB6-OB8
48	j	201	PEE	O5-C30-O3-C3
56	s	401	CDL	OB9-CB7-OB8-CB6
51	X	201	8Q1	C31-C29-C32-O33
48	j	201	PEE	C11-C12-C13-C14
48	r	501	PEE	C21-C22-C23-C24
56	l	702	CDL	C38-C39-C40-C41
52	J	401	NDP	PN-O3-PA-O1A
56	o	201	CDL	C62-C63-C64-C65
49	C	303	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
56	k	101	CDL	C32-C33-C34-C35
56	l	702	CDL	C44-C45-C46-C47
56	l	701	CDL	C16-C17-C18-C19
52	J	401	NDP	C3B-C4B-C5B-O5B
49	C	303	PLX	O4-C3-C4-C5
56	N	201	CDL	OB5-CB3-CB4-CB6
56	k	101	CDL	OA5-CA3-CA4-CA6
56	l	702	CDL	OB5-CB3-CB4-CB6
56	o	201	CDL	OB5-CB3-CB4-CB6
56	l	701	CDL	C74-C75-C76-C77
48	l	704	PEE	O4P-C4-C5-N
56	k	101	CDL	C31-CA7-OA8-CA6
56	V	201	CDL	C58-C59-C60-C61
56	V	201	CDL	C14-C15-C16-C17
48	r	501	PEE	C36-C37-C38-C39
56	i	402	CDL	C73-C74-C75-C76
48	C	302	PEE	C12-C13-C14-C15
56	a	201	CDL	C14-C15-C16-C17
56	n	101	CDL	C54-C55-C56-C57
48	i	401	PEE	C1-C2-C3-O3
48	j	201	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
49	C	303	PLX	C3-C4-C5-O8
49	J	403	PLX	C3-C4-C5-O8
49	j	202	PLX	C3-C4-C5-O8
56	o	201	CDL	CA3-CA4-CA6-OA8
56	o	201	CDL	CB3-CB4-CB6-OB8
56	s	401	CDL	CA3-CA4-CA6-OA8
48	r	501	PEE	C31-C32-C33-C34
49	j	202	PLX	C34-C35-C36-C37
49	r	503	PLX	C16-C17-C18-C19
56	V	201	CDL	C63-C64-C65-C66
49	r	503	PLX	C27-C28-C29-C30
49	J	403	PLX	C3-C4-O6-C6
49	r	503	PLX	C5-C4-O6-C6
49	r	503	PLX	C3-O4-P1-O1
56	a	201	CDL	CA2-OA2-PA1-OA5
48	l	703	PEE	C10-C11-C12-C13
56	k	101	CDL	C53-C54-C55-C56
49	C	303	PLX	O9-C24-C25-C26
48	l	704	PEE	C23-C24-C25-C26
48	r	501	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
56	o	201	CDL	C51-C52-C53-C54
56	i	402	CDL	C39-C40-C41-C42
48	i	401	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
56	k	101	CDL	OB6-CB4-CB6-OB8
49	r	503	PLX	C11-C10-C9-C8
56	V	201	CDL	C53-C54-C55-C56
49	j	202	PLX	C12-C13-C14-C15
56	i	402	CDL	C21-C22-C23-C24
56	l	701	CDL	C84-C85-C86-C87
56	s	401	CDL	C15-C16-C17-C18
56	o	201	CDL	C1-CB2-OB2-PB2
56	l	701	CDL	C81-C82-C83-C84
56	a	201	CDL	C56-C57-C58-C59
48	r	501	PEE	C38-C39-C40-C41
51	X	201	8Q1	O4-C1-S44-C43
56	n	101	CDL	OB7-CB5-OB6-CB4
48	l	704	PEE	C11-C12-C13-C14
48	C	302	PEE	C41-C42-C43-C44
49	g	201	PLX	O8-C24-C25-C26
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	O8-C24-C25-C26
48	r	501	PEE	C34-C35-C36-C37
48	l	703	PEE	O3P-C1-C2-C3
56	o	201	CDL	OA5-CA3-CA4-CA6
56	s	401	CDL	OA5-CA3-CA4-CA6
56	s	401	CDL	C39-C40-C41-C42
48	C	302	PEE	C16-C17-C18-C19
48	l	704	PEE	C18-C19-C20-C21
48	r	501	PEE	C33-C34-C35-C36
49	r	503	PLX	C30-C31-C32-C33
56	a	201	CDL	C42-C43-C44-C45
48	B	303	PEE	C20-C21-C22-C23
56	l	701	CDL	C17-C18-C19-C20
48	i	401	PEE	C24-C25-C26-C27
56	V	201	CDL	CA7-C31-C32-C33
56	i	402	CDL	CB5-C51-C52-C53
49	r	502	PLX	C31-C32-C33-C34
56	k	101	CDL	C82-C83-C84-C85
56	o	201	CDL	C64-C65-C66-C67
49	J	403	PLX	C34-C35-C36-C37
49	a	202	PLX	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C11-C12-C13-C14
51	X	201	8Q1	C6-C1-S44-C43
49	r	503	PLX	C26-C27-C28-C29
49	r	503	PLX	C33-C34-C35-C36
56	l	701	CDL	C54-C55-C56-C57
56	V	201	CDL	C44-C45-C46-C47
49	j	202	PLX	C20-C21-C22-C23
48	W	201	PEE	C1-C2-C3-O3
56	k	101	CDL	CB3-CB4-CB6-OB8
56	k	101	CDL	OA9-CA7-OA8-CA6
49	r	503	PLX	C29-C30-C31-C32
49	r	503	PLX	C34-C35-C36-C37
48	C	302	PEE	O3P-C1-C2-O2
49	g	201	PLX	O4-C3-C4-O6
56	V	201	CDL	OA5-CA3-CA4-OA6
56	s	401	CDL	OA5-CA3-CA4-OA6
48	U	101	PEE	C23-C24-C25-C26
56	i	402	CDL	C19-C20-C21-C22
48	B	303	PEE	C36-C37-C38-C39
48	j	201	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	J	403	PLX	O6-C4-C5-O8
49	a	202	PLX	O6-C4-C5-O8
49	j	202	PLX	O6-C4-C5-O8
49	r	503	PLX	O6-C4-C5-O8
56	V	201	CDL	OA6-CA4-CA6-OA8
56	s	401	CDL	OA6-CA4-CA6-OA8
47	A	503	NAI	C5B-O5B-PA-O3
56	i	402	CDL	C37-C38-C39-C40
56	o	201	CDL	C59-C60-C61-C62
48	W	201	PEE	C19-C20-C21-C22
48	l	704	PEE	C15-C16-C17-C18
48	i	401	PEE	C32-C33-C34-C35
51	X	201	8Q1	C12-C13-C14-C15
56	N	201	CDL	CA5-C11-C12-C13
56	i	402	CDL	C62-C63-C64-C65
49	g	201	PLX	C16-C17-C18-C19
56	a	201	CDL	C20-C21-C22-C23
56	i	402	CDL	C64-C65-C66-C67
56	k	101	CDL	C77-C78-C79-C80
56	o	201	CDL	CA7-C31-C32-C33
49	C	303	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
49	J	403	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O4
52	J	401	NDP	O4D-C1D-N1N-C6N
56	N	201	CDL	CB3-OB5-PB2-OB2
49	r	503	PLX	C12-C13-C14-C15
56	k	101	CDL	C54-C55-C56-C57
48	i	401	PEE	C2-C1-O3P-P
56	i	402	CDL	C1-CB2-OB2-PB2
53	s	402	UQ	C13-C14-C16-C17
56	i	402	CDL	C76-C77-C78-C79
48	C	302	PEE	C4-O4P-P-O2P
48	C	302	PEE	C4-O4P-P-O1P
48	U	101	PEE	C1-O3P-P-O1P
48	W	201	PEE	C4-O4P-P-O2P
48	i	401	PEE	C1-O3P-P-O1P
48	j	201	PEE	C4-O4P-P-O1P
49	C	303	PLX	C3-O4-P1-O3
49	C	303	PLX	C2-O1-P1-O2
49	C	303	PLX	C2-O1-P1-O3
49	J	403	PLX	C2-O1-P1-O3
49	a	202	PLX	C3-O4-P1-O2
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C2-O1-P1-O3
56	N	201	CDL	CB3-OB5-PB2-OB4
56	V	201	CDL	CA3-OA5-PA1-OA3
56	V	201	CDL	CB2-OB2-PB2-OB4
56	a	201	CDL	CA2-OA2-PA1-OA4
56	a	201	CDL	CB2-OB2-PB2-OB4
56	a	201	CDL	CB3-OB5-PB2-OB3
56	i	402	CDL	CA2-OA2-PA1-OA4
56	i	402	CDL	CB2-OB2-PB2-OB3
56	i	402	CDL	CB2-OB2-PB2-OB4
56	i	402	CDL	CB3-OB5-PB2-OB4
56	k	101	CDL	CA3-OA5-PA1-OA4
56	k	101	CDL	CB2-OB2-PB2-OB4
56	l	701	CDL	CB2-OB2-PB2-OB3
56	l	701	CDL	CB3-OB5-PB2-OB4
56	l	702	CDL	CB2-OB2-PB2-OB3
56	n	101	CDL	CA2-OA2-PA1-OA4
56	o	201	CDL	CB2-OB2-PB2-OB4
56	s	401	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	i	401	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
49	r	503	PLX	O4-C3-C4-C5
56	N	201	CDL	OA5-CA3-CA4-CA6
56	V	201	CDL	OA5-CA3-CA4-CA6
56	l	701	CDL	OB5-CB3-CB4-CB6
53	s	402	UQ	C22-C23-C24-C25
48	W	201	PEE	C23-C24-C25-C26
49	j	202	PLX	C30-C31-C32-C33
56	a	201	CDL	C44-C45-C46-C47
49	C	303	PLX	C25-C24-O8-C5
49	J	403	PLX	C25-C24-O8-C5
49	g	201	PLX	C25-C24-O8-C5
48	r	501	PEE	C39-C40-C41-C42
56	V	201	CDL	C33-C34-C35-C36
56	a	201	CDL	C84-C85-C86-C87
49	r	503	PLX	O4-C3-C4-O6
56	N	201	CDL	OB5-CB3-CB4-OB6
56	k	101	CDL	CA5-C11-C12-C13
56	o	201	CDL	OA5-CA3-CA4-OA6
56	l	701	CDL	C21-C22-C23-C24
47	A	503	NAI	C2D-C1D-N1N-C2N
48	C	302	PEE	C1-C2-C3-O3
51	X	201	8Q1	O27-C28-C29-C32
48	C	302	PEE	O2-C2-C3-O3
48	W	201	PEE	O2-C2-C3-O3
48	l	703	PEE	O2-C2-C3-O3
48	r	501	PEE	C23-C24-C25-C26
48	l	704	PEE	C17-C18-C19-C20
49	a	202	PLX	O8-C24-C25-C26
49	j	202	PLX	O6-C6-C7-C8
56	a	201	CDL	C74-C75-C76-C77
48	C	302	PEE	C38-C39-C40-C41
48	l	703	PEE	C24-C25-C26-C27
56	a	201	CDL	C41-C42-C43-C44
56	V	201	CDL	C64-C65-C66-C67
47	A	503	NAI	O4D-C1D-N1N-C2N
56	k	101	CDL	C80-C81-C82-C83
56	i	402	CDL	C11-C12-C13-C14
56	i	402	CDL	C83-C84-C85-C86
56	o	201	CDL	C77-C78-C79-C80
51	X	201	8Q1	O27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
58	w	401	ADP	PA-O3A-PB-O1B
56	k	101	CDL	C14-C15-C16-C17
56	k	101	CDL	CA6-CA4-OA6-CA5
49	C	303	PLX	C7-C8-C9-C10
49	C	303	PLX	C33-C34-C35-C36
48	U	101	PEE	C41-C42-C43-C44
56	s	401	CDL	C80-C81-C82-C83
56	n	101	CDL	C56-C57-C58-C59
48	l	704	PEE	C2-C1-O3P-P
48	l	704	PEE	O5-C30-O3-C3
49	j	202	PLX	O4-C3-C4-O6
48	l	704	PEE	C32-C33-C34-C35
56	s	401	CDL	C17-C18-C19-C20
56	s	401	CDL	C40-C41-C42-C43
56	s	401	CDL	C55-C56-C57-C58
48	l	704	PEE	C31-C30-O3-C3
48	C	302	PEE	C34-C35-C36-C37
48	i	401	PEE	C18-C19-C20-C21
56	l	702	CDL	C64-C65-C66-C67
48	B	303	PEE	C1-O3P-P-O4P
48	l	704	PEE	C4-O4P-P-O3P
56	V	201	CDL	CA2-OA2-PA1-OA5
56	l	701	CDL	CA2-OA2-PA1-OA5
56	n	101	CDL	CB2-OB2-PB2-OB5
56	s	401	CDL	CA2-OA2-PA1-OA5
56	s	401	CDL	CA3-OA5-PA1-OA2
49	r	503	PLX	C31-C32-C33-C34
48	l	703	PEE	C33-C34-C35-C36
56	o	201	CDL	C38-C39-C40-C41
56	n	101	CDL	C32-C31-CA7-OA8
48	r	501	PEE	C41-C42-C43-C44
56	o	201	CDL	C15-C16-C17-C18
56	a	201	CDL	C34-C35-C36-C37
48	j	201	PEE	C18-C19-C20-C21
48	l	703	PEE	C38-C39-C40-C41
56	a	201	CDL	C64-C65-C66-C67
56	l	702	CDL	C62-C63-C64-C65
49	r	503	PLX	C24-C25-C26-C27
48	B	303	PEE	C10-C11-C12-C13
49	a	202	PLX	C11-C10-C9-C8
56	i	402	CDL	C54-C55-C56-C57
49	J	403	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
56	a	201	CDL	C53-C54-C55-C56
48	B	303	PEE	O3P-C1-C2-O2
56	k	101	CDL	OB5-CB3-CB4-OB6
56	l	701	CDL	OA5-CA3-CA4-OA6
48	W	201	PEE	C22-C23-C24-C25
56	k	101	CDL	C84-C85-C86-C87
53	J	402	UQ	C13-C14-C16-C17
56	o	201	CDL	OB9-CB7-OB8-CB6
56	l	701	CDL	C24-C25-C26-C27
56	N	201	CDL	O1-C1-CB2-OB2
56	n	101	CDL	C32-C31-CA7-OA9
56	n	101	CDL	C72-C71-CB7-OB8
56	s	401	CDL	C13-C14-C15-C16
56	i	402	CDL	C17-C18-C19-C20
48	r	501	PEE	C12-C13-C14-C15
51	X	201	8Q1	O27-C28-C29-C30
56	i	402	CDL	C20-C21-C22-C23
56	o	201	CDL	C71-CB7-OB8-CB6
48	l	703	PEE	C3-C2-O2-C10
53	J	402	UQ	C15-C14-C16-C17
56	l	702	CDL	C55-C56-C57-C58
56	a	201	CDL	CB3-OB5-PB2-OB2
56	k	101	CDL	C21-C22-C23-C24
49	a	202	PLX	C24-C25-C26-C27
48	C	302	PEE	C35-C36-C37-C38
56	o	201	CDL	C83-C84-C85-C86
49	j	202	PLX	C18-C19-C20-C21
56	a	201	CDL	C39-C40-C41-C42
49	j	202	PLX	C31-C32-C33-C34
56	s	401	CDL	C11-C12-C13-C14
49	g	201	PLX	C33-C34-C35-C36
56	k	101	CDL	OA6-CA4-CA6-OA8
48	B	303	PEE	C42-C43-C44-C45
48	l	703	PEE	C37-C38-C39-C40
51	G	201	8Q1	C12-C13-C14-C15
47	A	503	NAI	C2D-C1D-N1N-C6N
53	s	402	UQ	C12-C13-C14-C15
56	i	402	CDL	C16-C17-C18-C19
56	l	702	CDL	C81-C82-C83-C84
48	l	703	PEE	C2-C1-O3P-P
56	o	201	CDL	C32-C31-CA7-OA9
48	B	303	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
48	W	201	PEE	C16-C17-C18-C19
48	l	703	PEE	C1-C2-C3-O3
56	s	401	CDL	C82-C83-C84-C85
58	w	401	ADP	O4'-C4'-C5'-O5'
56	l	702	CDL	C79-C80-C81-C82
51	X	201	8Q1	C10-C11-C12-C13
48	W	201	PEE	C15-C16-C17-C18
56	n	101	CDL	C53-C54-C55-C56
48	i	401	PEE	C16-C17-C18-C19
48	l	703	PEE	C18-C19-C20-C21
48	B	303	PEE	C44-C45-C46-C47
49	j	202	PLX	O8-C24-C25-C26
48	i	401	PEE	O4P-C4-C5-N
48	l	703	PEE	O4P-C4-C5-N
56	i	402	CDL	C44-C45-C46-C47
56	l	701	CDL	C20-C21-C22-C23
56	l	702	CDL	C33-C34-C35-C36
56	n	101	CDL	CA5-C11-C12-C13
49	r	502	PLX	O6-C4-C5-O8
49	a	202	PLX	C6-C7-C8-C9
48	B	303	PEE	C12-C13-C14-C15
56	s	401	CDL	C72-C71-CB7-OB8
56	l	701	CDL	C63-C64-C65-C66
56	s	401	CDL	C57-C58-C59-C60
48	C	302	PEE	C18-C19-C20-C21
51	G	201	8Q1	C28-O27-P24-O2
49	J	403	PLX	C14-C15-C16-C17
53	J	402	UQ	C20-C19-C21-C22
48	j	201	PEE	C1-O3P-P-O4P
56	N	201	CDL	CA3-OA5-PA1-OA2
49	a	202	PLX	C11-C12-C13-C14
56	s	401	CDL	C54-C55-C56-C57
56	V	201	CDL	C32-C31-CA7-OA8
56	l	702	CDL	C32-C31-CA7-OA8
48	U	101	PEE	C16-C17-C18-C19
48	j	201	PEE	C16-C17-C18-C19
48	l	703	PEE	C1-C2-O2-C10
56	V	201	CDL	C12-C13-C14-C15
56	l	702	CDL	C61-C62-C63-C64
56	l	702	CDL	C73-C74-C75-C76
48	r	501	PEE	C30-C31-C32-C33
48	j	201	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
56	o	201	CDL	C76-C77-C78-C79
56	a	201	CDL	C15-C16-C17-C18
56	s	401	CDL	C56-C57-C58-C59
56	l	701	CDL	C52-C51-CB5-OB6
48	W	201	PEE	C24-C25-C26-C27
56	i	402	CDL	C42-C43-C44-C45
48	B	303	PEE	C16-C17-C18-C19
48	W	201	PEE	C18-C19-C20-C21
48	l	703	PEE	C36-C37-C38-C39
49	r	502	PLX	C3-C4-C5-O8
56	l	702	CDL	C51-C52-C53-C54
56	a	201	CDL	C12-C11-CA5-OA6
56	n	101	CDL	C52-C51-CB5-OB6
48	r	501	PEE	C40-C41-C42-C43
48	B	303	PEE	C24-C25-C26-C27
56	k	101	CDL	C74-C75-C76-C77
56	l	701	CDL	C78-C79-C80-C81
58	w	401	ADP	PA-O3A-PB-O2B
58	w	401	ADP	PA-O3A-PB-O3B
48	U	101	PEE	C19-C20-C21-C22
48	B	303	PEE	O3P-C1-C2-C3
56	l	702	CDL	C72-C71-CB7-OB8
56	s	401	CDL	C12-C11-CA5-OA6
56	l	702	CDL	OA6-CA4-CA6-OA8
49	J	403	PLX	C11-C10-C9-C8
49	C	303	PLX	O7-C6-C7-C8
52	J	401	NDP	C2B-O2B-P2B-O2X
56	a	201	CDL	C57-C58-C59-C60
48	C	302	PEE	O3-C30-C31-C32
48	U	101	PEE	C15-C16-C17-C18
56	l	702	CDL	C74-C75-C76-C77
56	o	201	CDL	C44-C45-C46-C47
48	l	704	PEE	C38-C39-C40-C41
56	N	201	CDL	C52-C51-CB5-OB6
49	a	202	PLX	C35-C36-C37-C38
56	N	201	CDL	C72-C71-CB7-OB8
52	J	401	NDP	PN-O3-PA-O2A
56	o	201	CDL	C79-C80-C81-C82
48	U	101	PEE	C38-C39-C40-C41
49	g	201	PLX	C31-C32-C33-C34
48	i	401	PEE	C38-C39-C40-C41
48	C	302	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
56	n	101	CDL	C52-C51-CB5-OB7
56	V	201	CDL	C38-C39-C40-C41
48	U	101	PEE	C4-O4P-P-O2P
48	W	201	PEE	C4-O4P-P-O1P
49	J	403	PLX	C3-O4-P1-O2
49	j	202	PLX	C2-O1-P1-O2
49	r	502	PLX	C3-O4-P1-O3
49	r	503	PLX	C2-C1-N1-C1C
56	N	201	CDL	CB3-OB5-PB2-OB3
56	l	701	CDL	CA2-OA2-PA1-OA3
56	l	702	CDL	CA2-OA2-PA1-OA4
56	n	101	CDL	CB2-OB2-PB2-OB3
56	N	201	CDL	C52-C51-CB5-OB7
56	s	401	CDL	C12-C11-CA5-OA7
49	j	202	PLX	O4-C3-C4-C5
56	i	402	CDL	OB5-CB3-CB4-CB6
56	s	401	CDL	OB5-CB3-CB4-CB6
56	N	201	CDL	C72-C71-CB7-OB9
56	a	201	CDL	C12-C11-CA5-OA7
56	a	201	CDL	C12-C13-C14-C15
56	l	701	CDL	C52-C51-CB5-OB7
47	A	503	NAI	O4D-C1D-N1N-C6N
48	i	401	PEE	C5-C4-O4P-P
48	r	501	PEE	C5-C4-O4P-P
49	J	403	PLX	C1-C2-O1-P1
49	j	202	PLX	C25-C24-O8-C5
50	C	304	970	C01-C02-C04-C05
50	C	304	970	C01-C02-C04-O08
56	l	702	CDL	C54-C55-C56-C57
49	r	503	PLX	C2-C1-N1-C1B
49	r	503	PLX	C2-C1-N1-C1A
48	r	501	PEE	C16-C17-C18-C19
48	U	101	PEE	O3-C30-C31-C32
56	N	201	CDL	C12-C11-CA5-OA6
56	k	101	CDL	C32-C31-CA7-OA8
56	k	101	CDL	C52-C51-CB5-OB6
56	l	702	CDL	C72-C71-CB7-OB9
48	C	302	PEE	O2-C10-C11-C12
56	k	101	CDL	C12-C11-CA5-OA6
48	C	302	PEE	O5-C30-C31-C32
48	U	101	PEE	C24-C25-C26-C27
56	V	201	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C36-C37-C38-C39
48	j	201	PEE	O3-C30-C31-C32
48	r	501	PEE	O2-C10-C11-C12
56	a	201	CDL	C61-C62-C63-C64
48	U	101	PEE	O5-C30-C31-C32
56	l	702	CDL	C12-C11-CA5-OA6
56	i	402	CDL	C23-C24-C25-C26
49	r	503	PLX	C6-C7-C8-C9
48	B	303	PEE	C30-C31-C32-C33

There are no ring outliers.

32 monomers are involved in 117 short contacts:

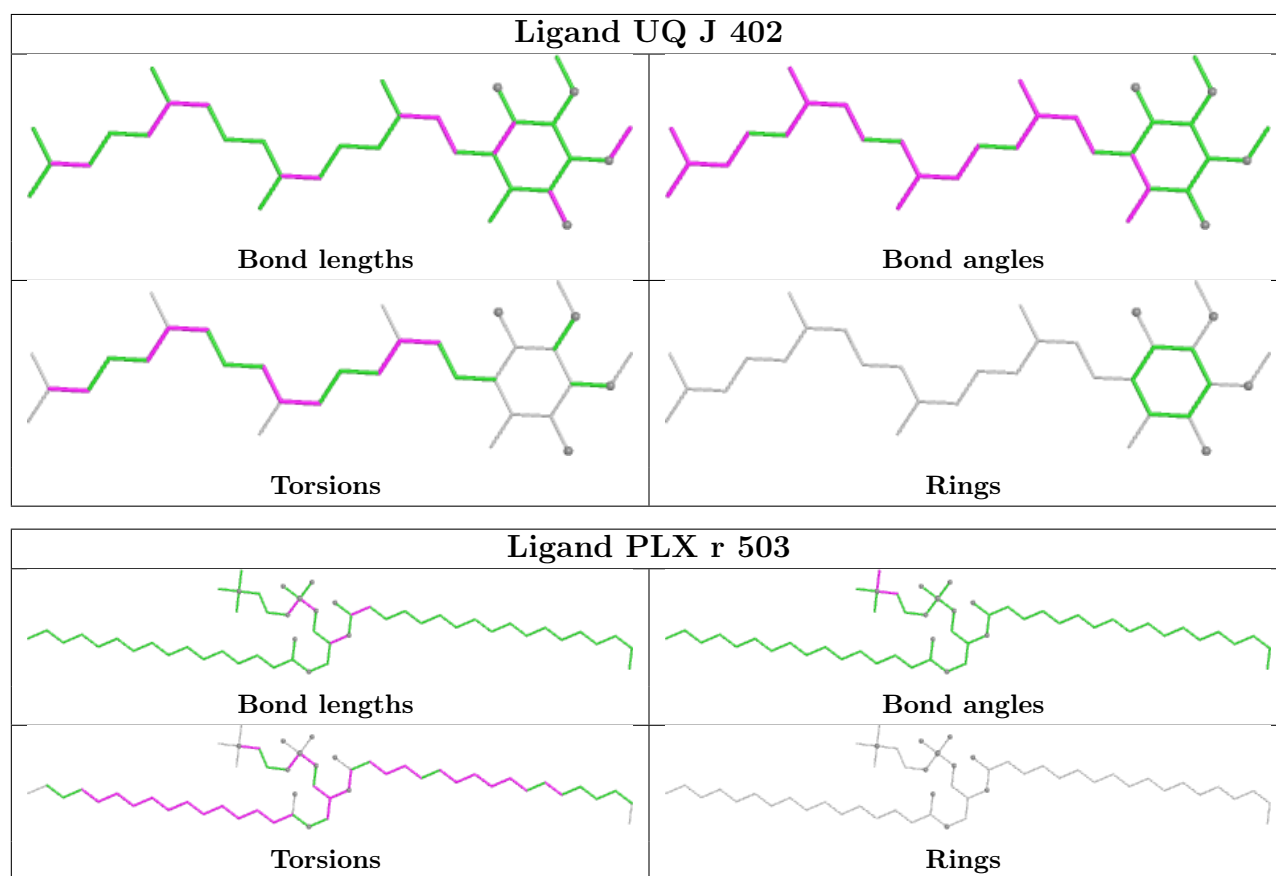
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53	J	402	UQ	2	0
49	r	503	PLX	1	0
48	U	101	PEE	4	0
48	B	303	PEE	6	0
49	j	202	PLX	3	0
56	o	201	CDL	6	0
52	J	401	NDP	2	0
58	w	401	ADP	2	0
56	a	201	CDL	5	0
56	l	702	CDL	6	0
49	g	201	PLX	6	0
47	A	503	NAI	4	0
48	C	302	PEE	2	0
48	j	201	PEE	2	0
49	J	403	PLX	3	0
56	k	101	CDL	4	0
48	l	704	PEE	4	0
48	i	401	PEE	2	0
45	C	301	SF4	2	0
49	C	303	PLX	2	0
48	l	703	PEE	3	0
46	A	502	FMN	4	0
56	s	401	CDL	8	0
56	n	101	CDL	2	0
49	r	502	PLX	5	0
56	N	201	CDL	1	0
56	l	701	CDL	10	0
45	A	501	SF4	2	0

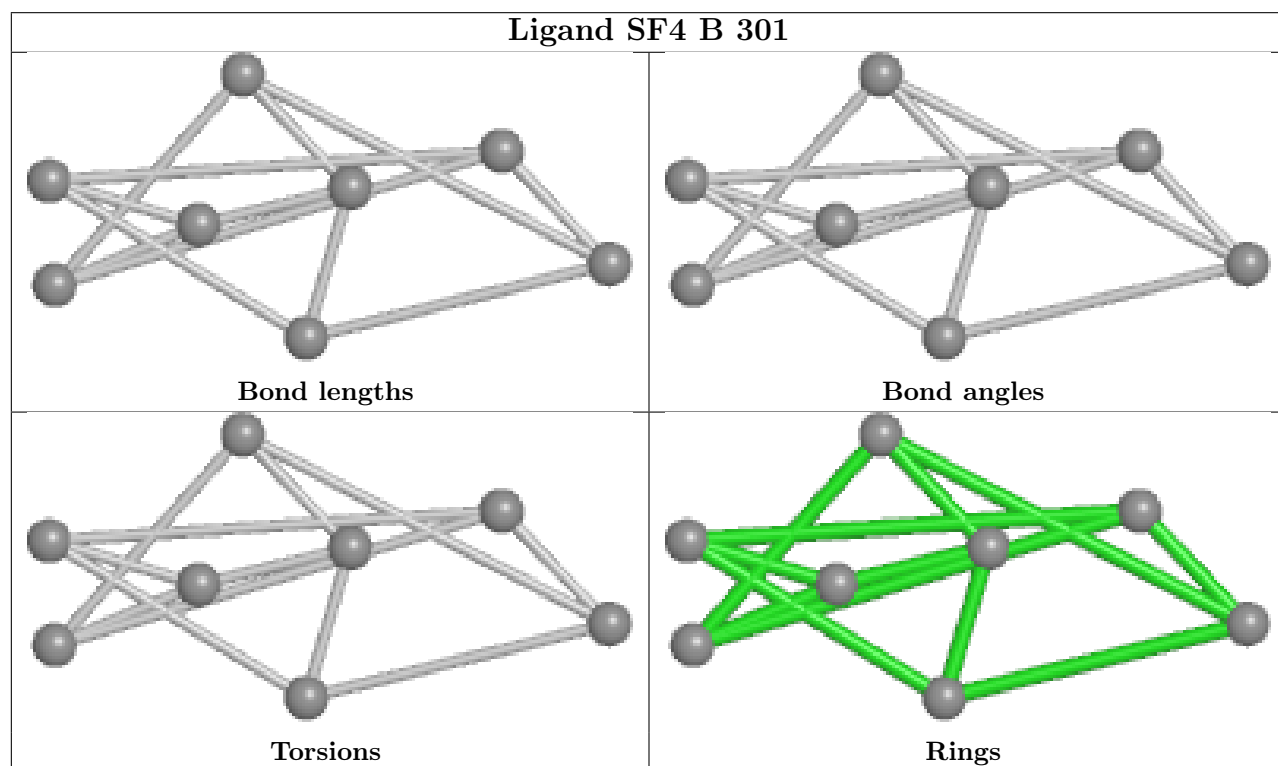
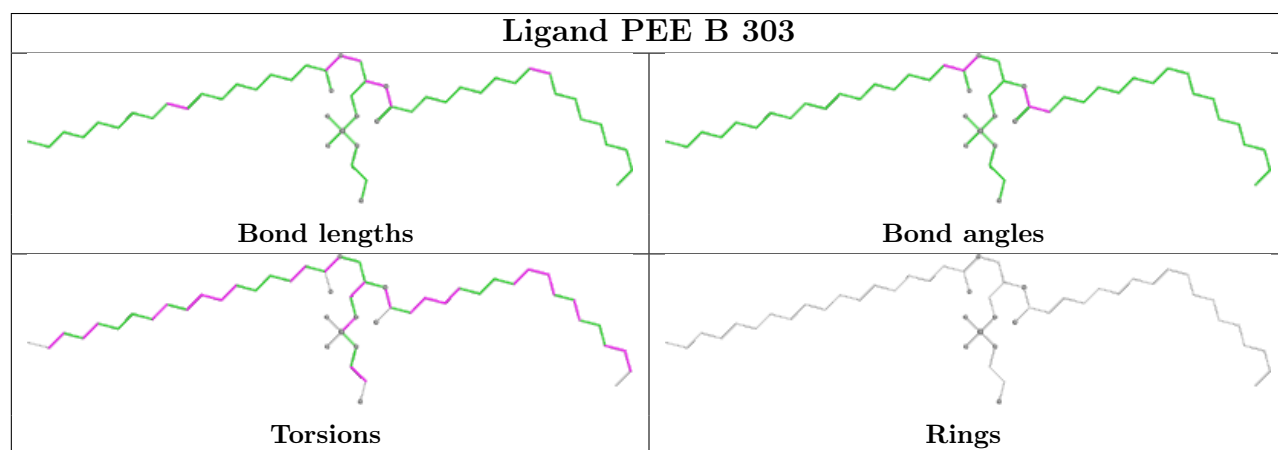
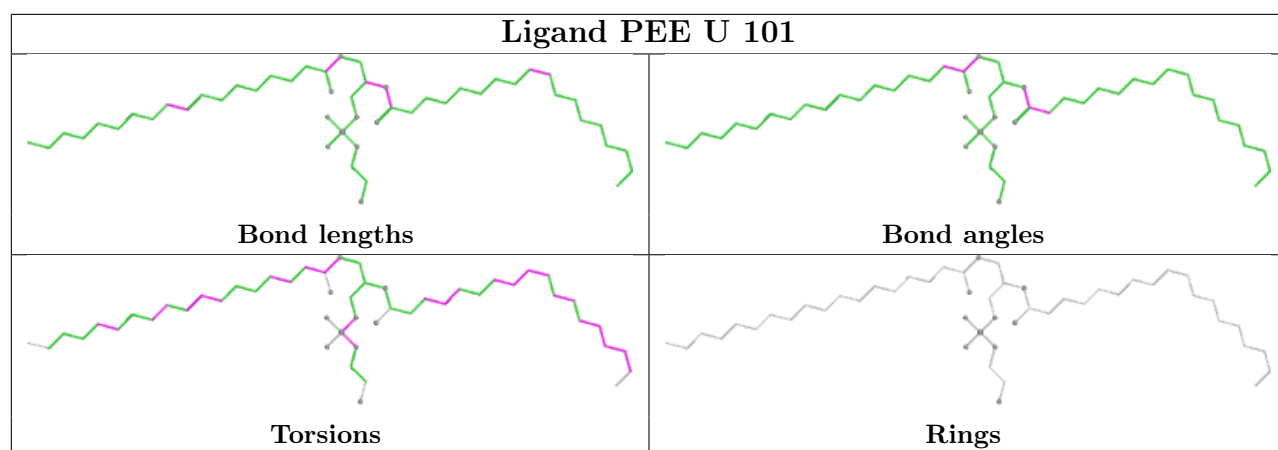
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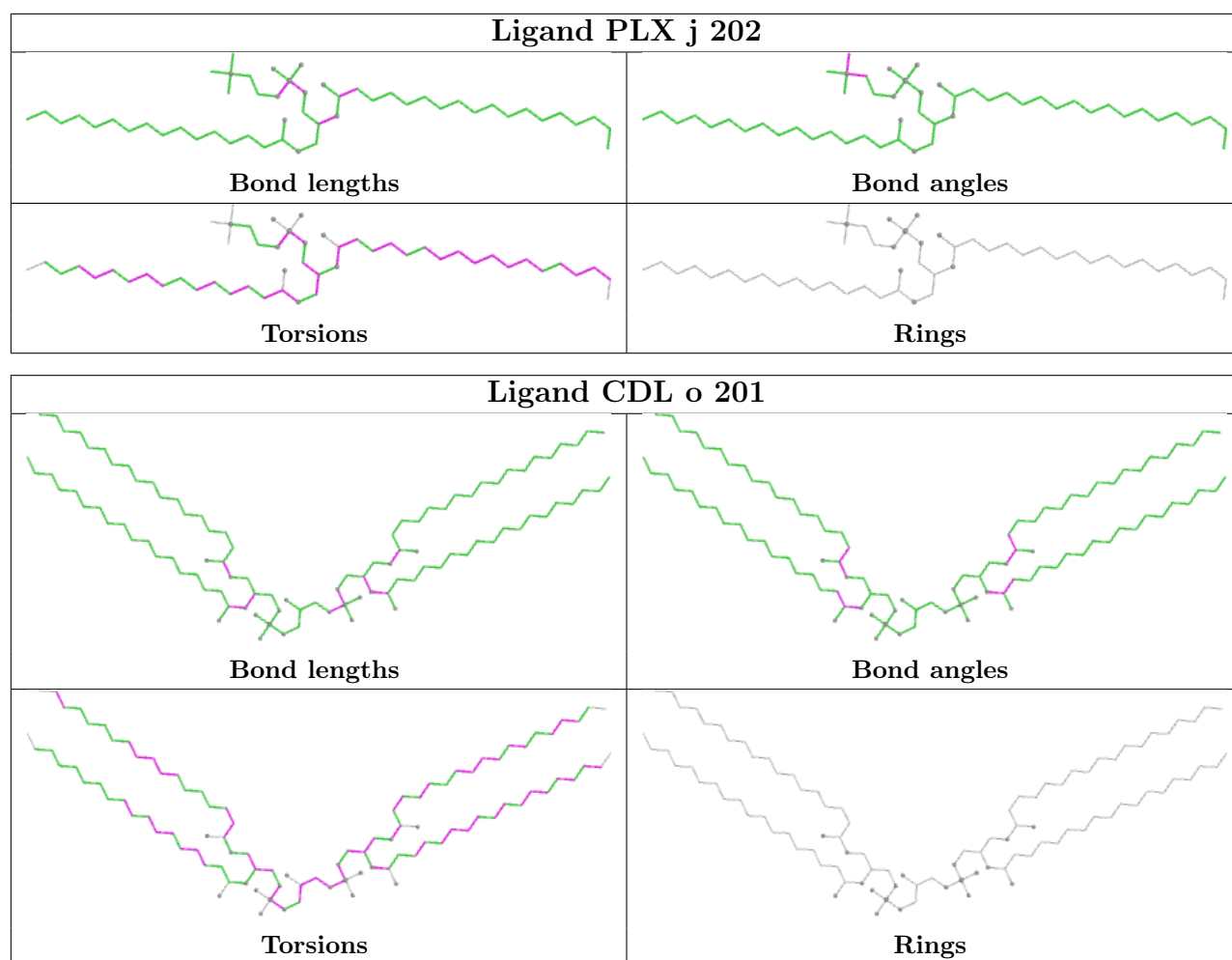
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	s	402	UQ	5	0
56	V	201	CDL	4	0
48	r	501	PEE	3	0
56	i	402	CDL	9	0

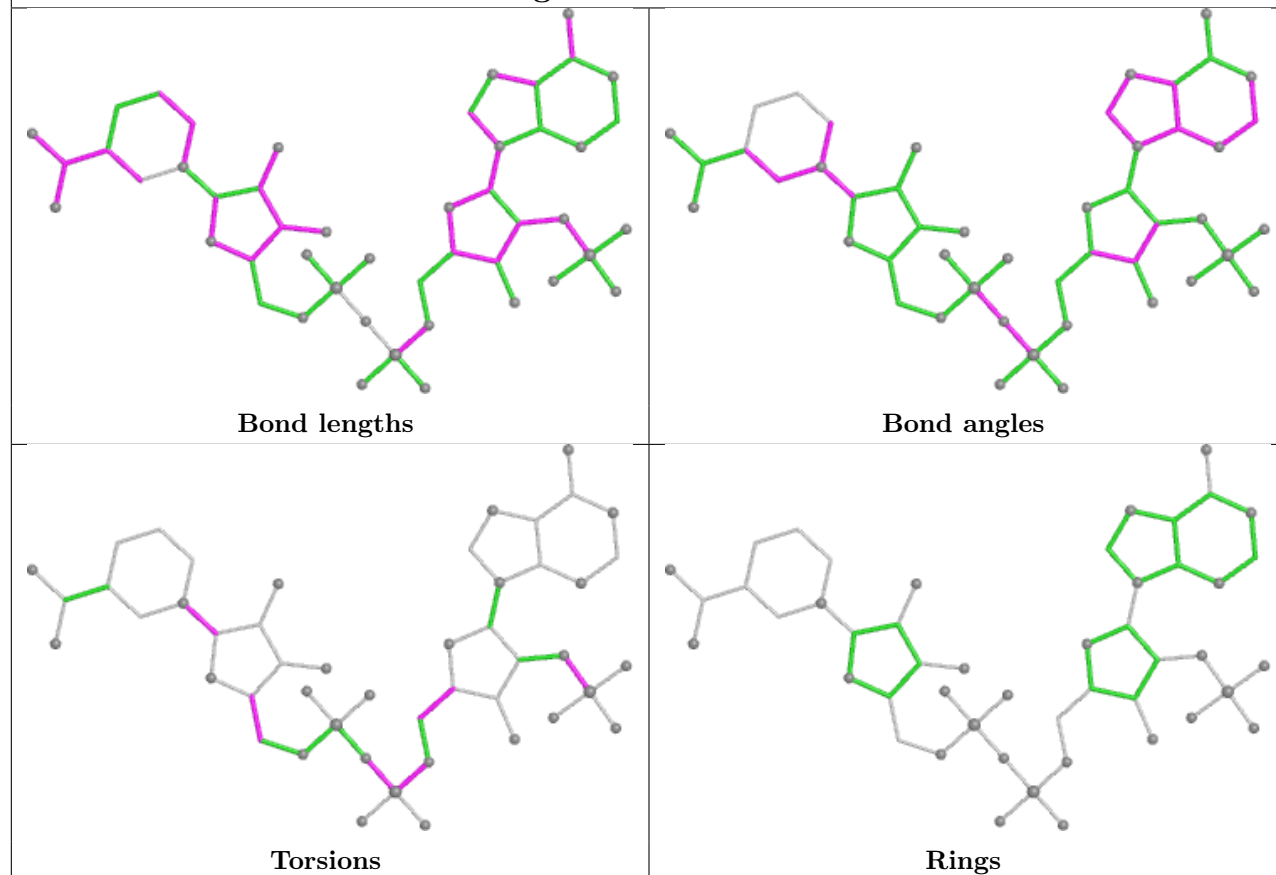
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



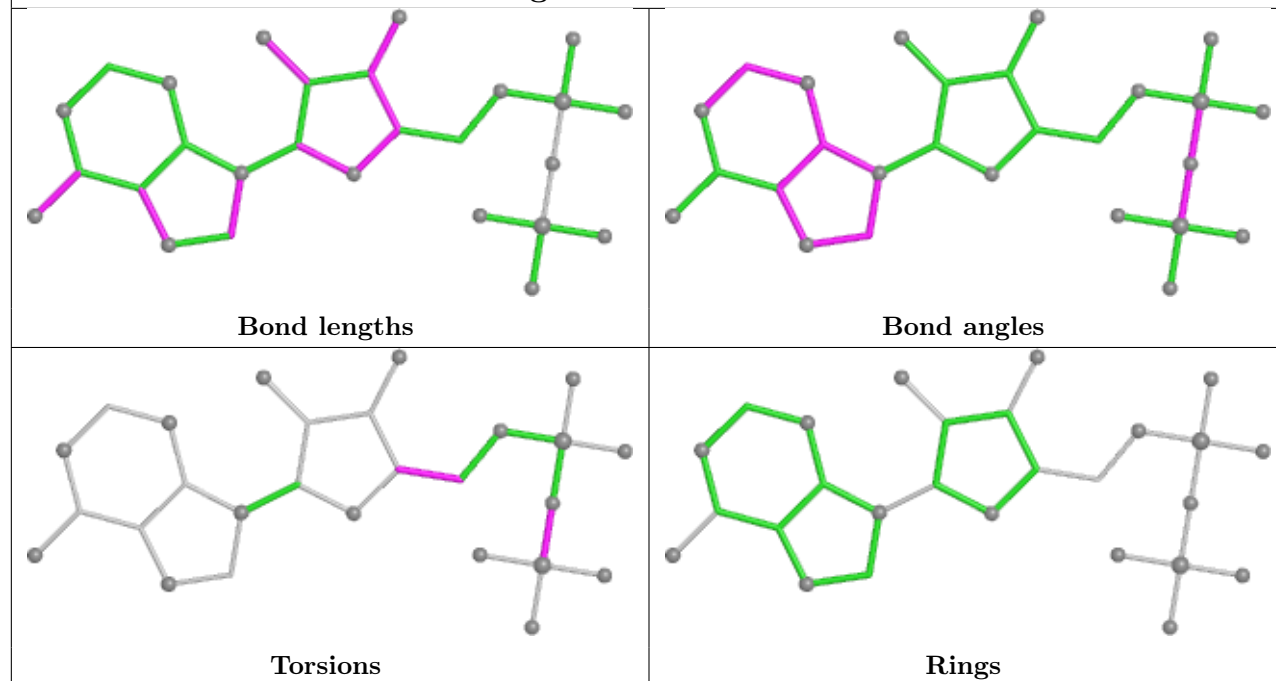


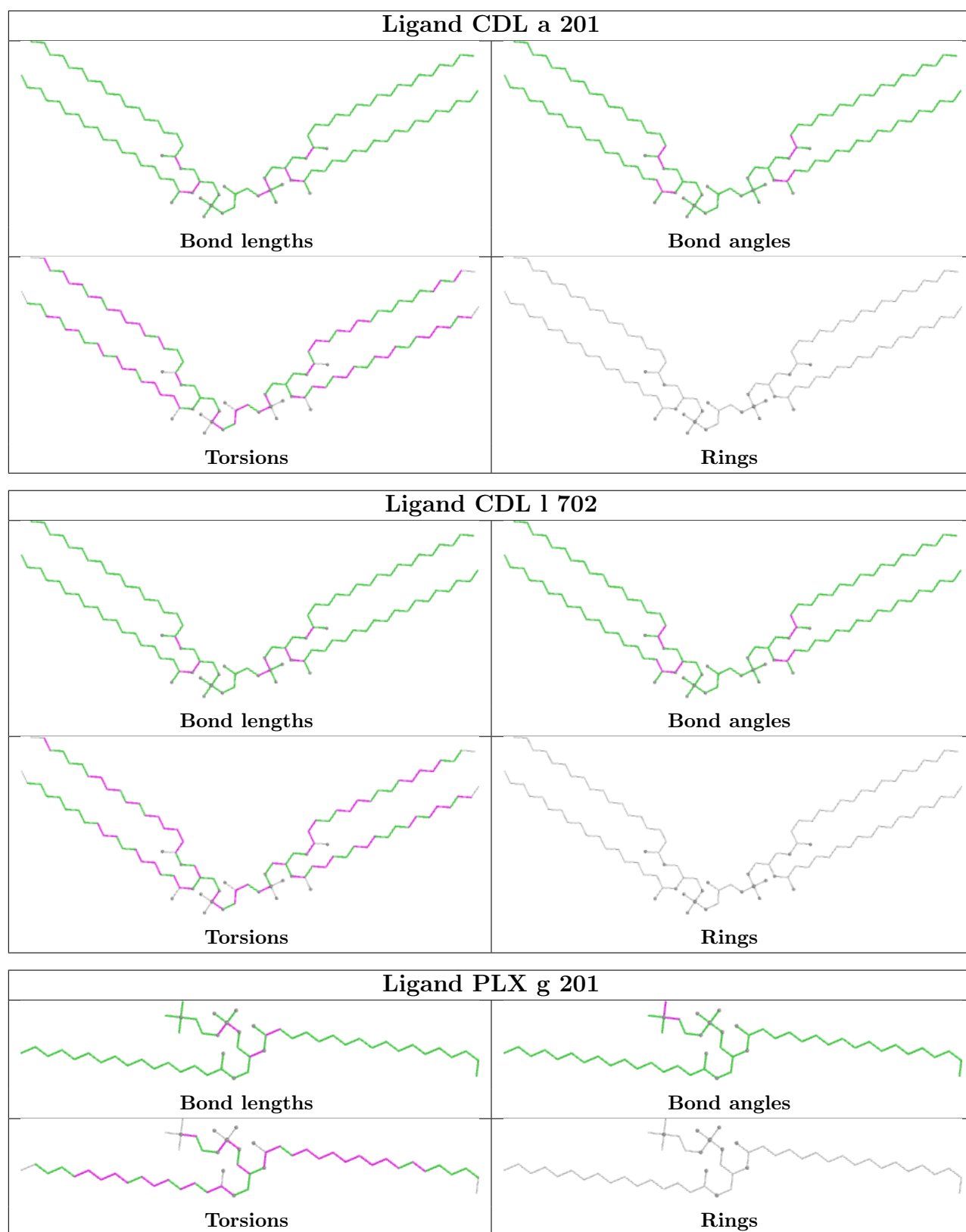


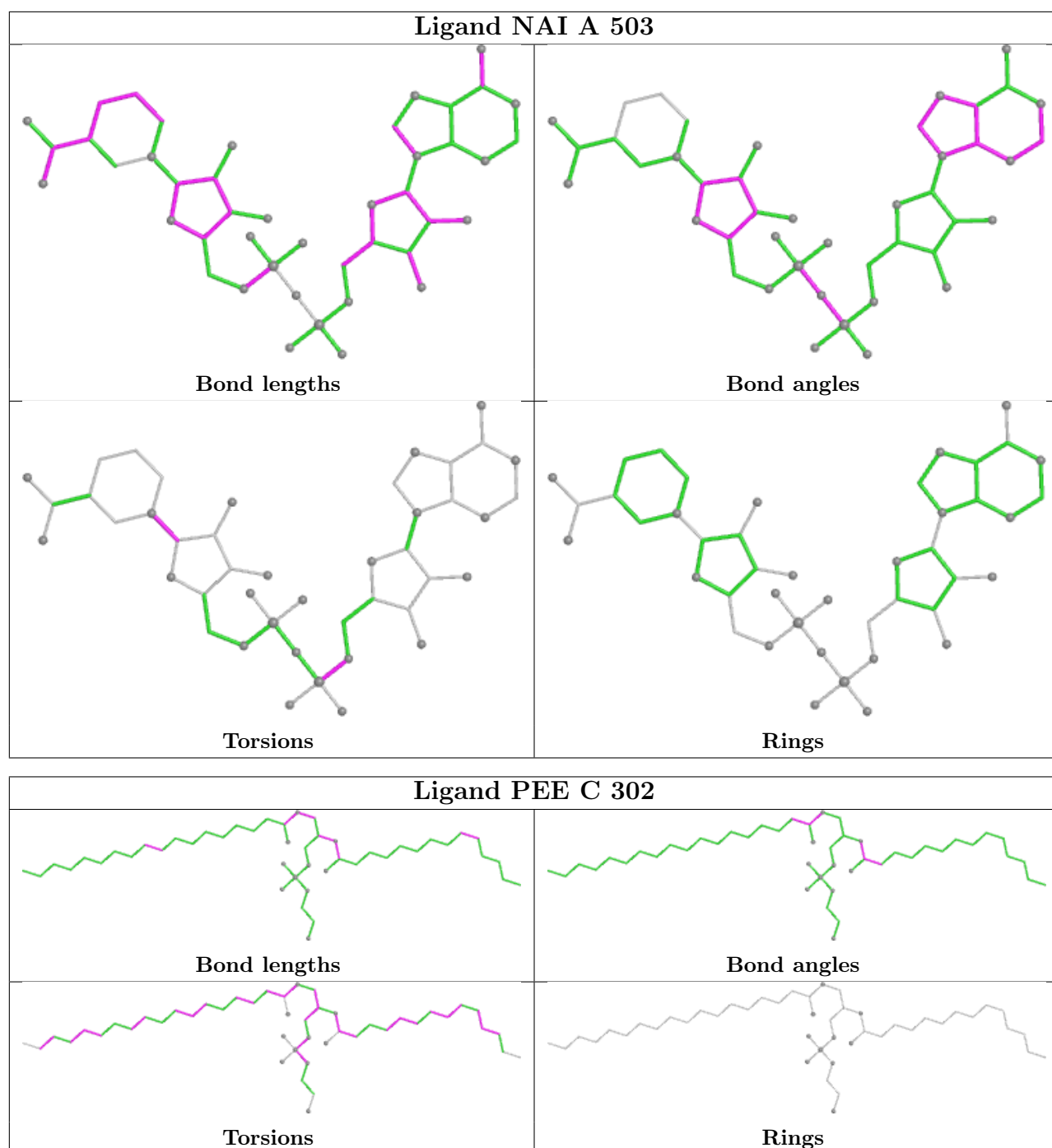
Ligand NDP J 401

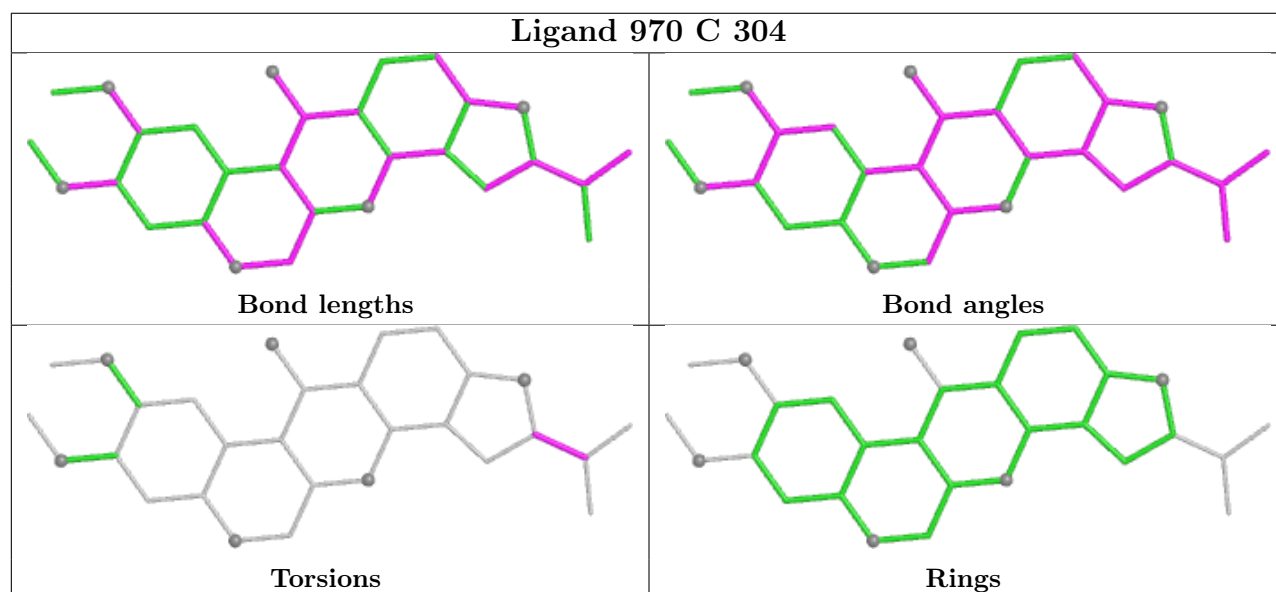
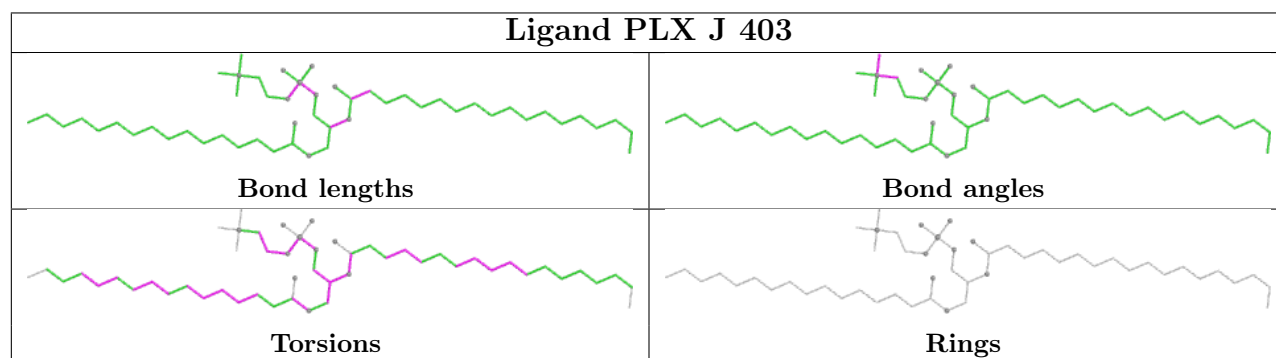
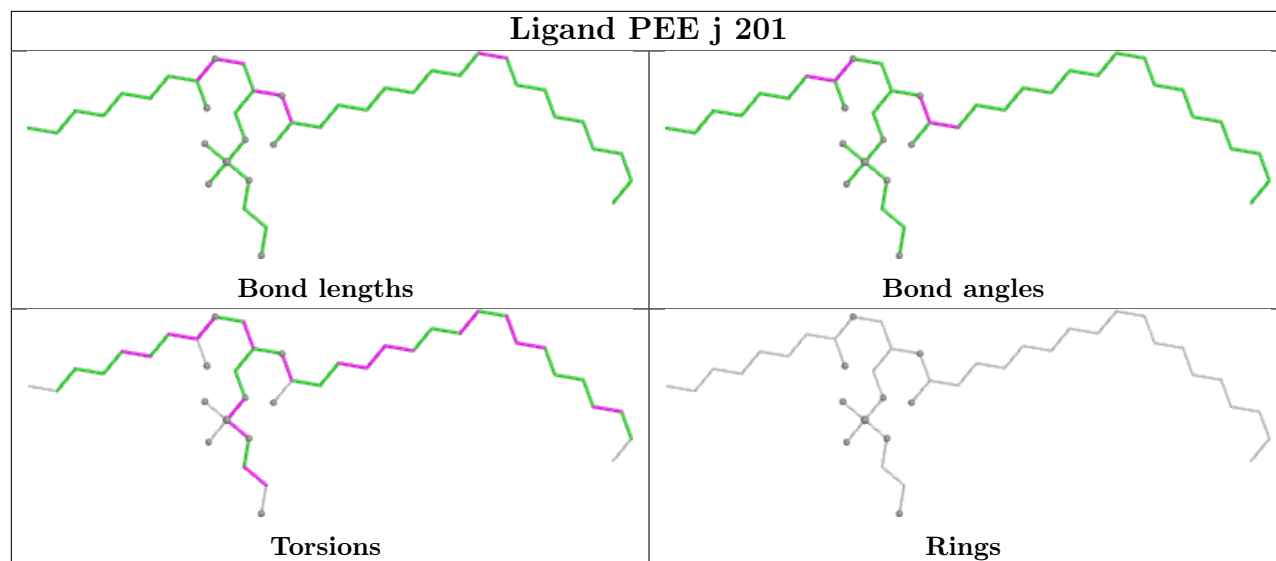


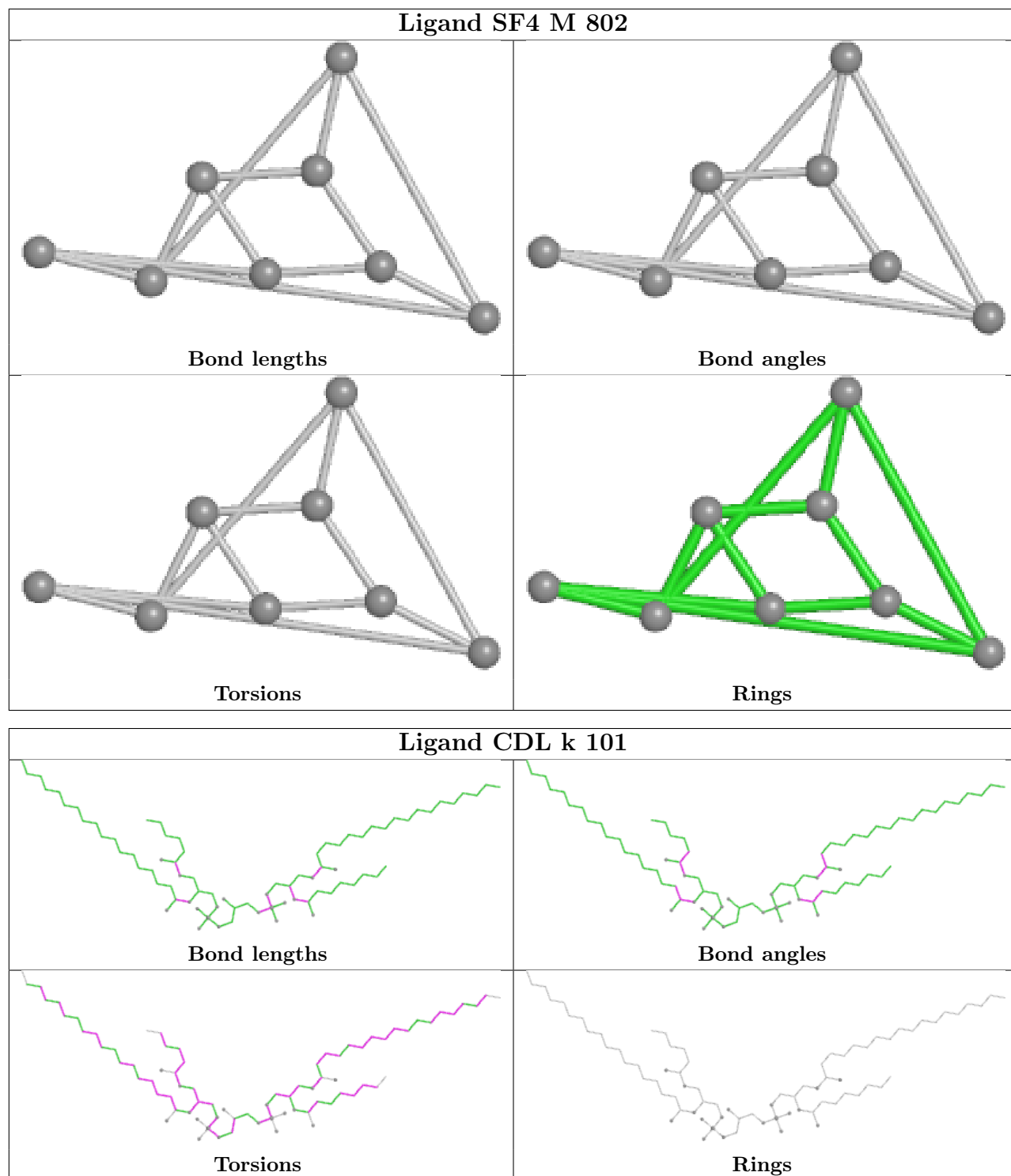
Ligand ADP w 401

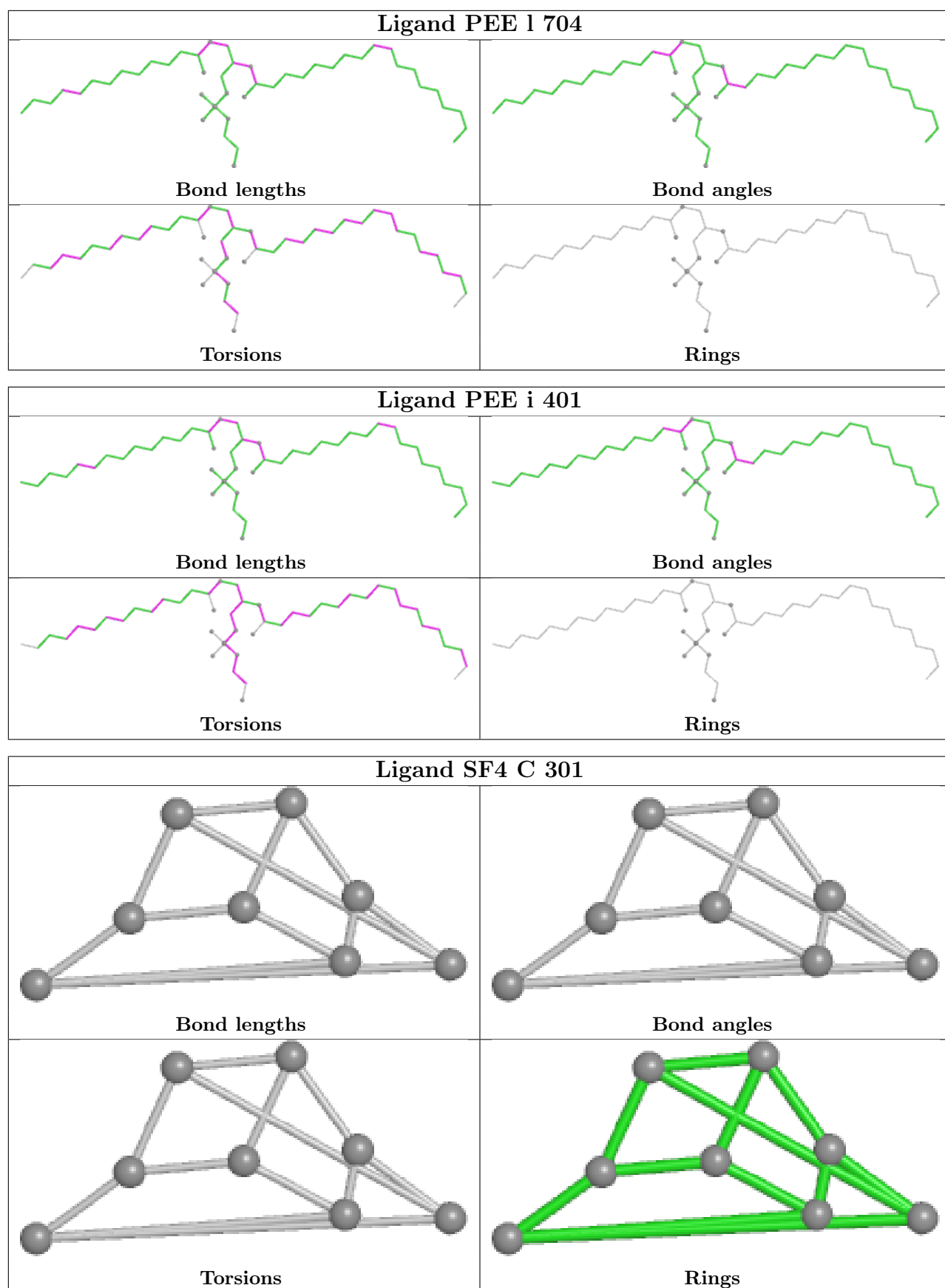


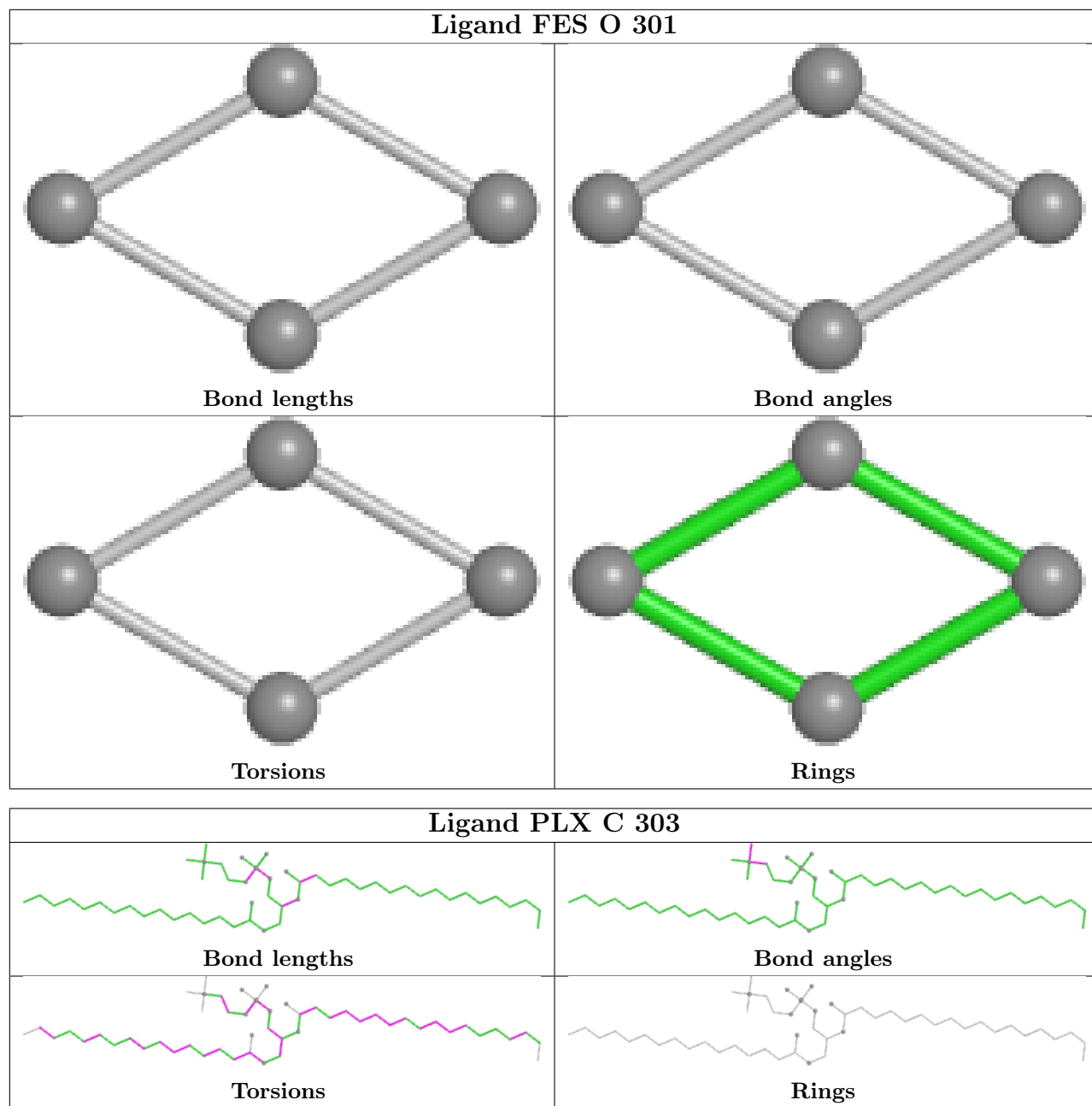


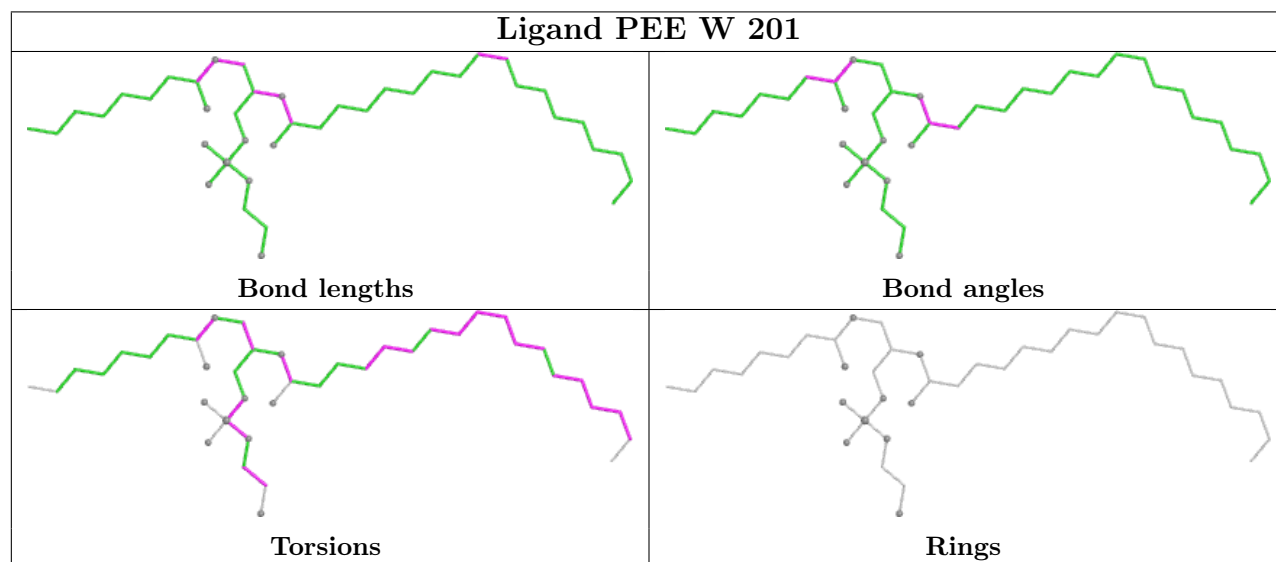
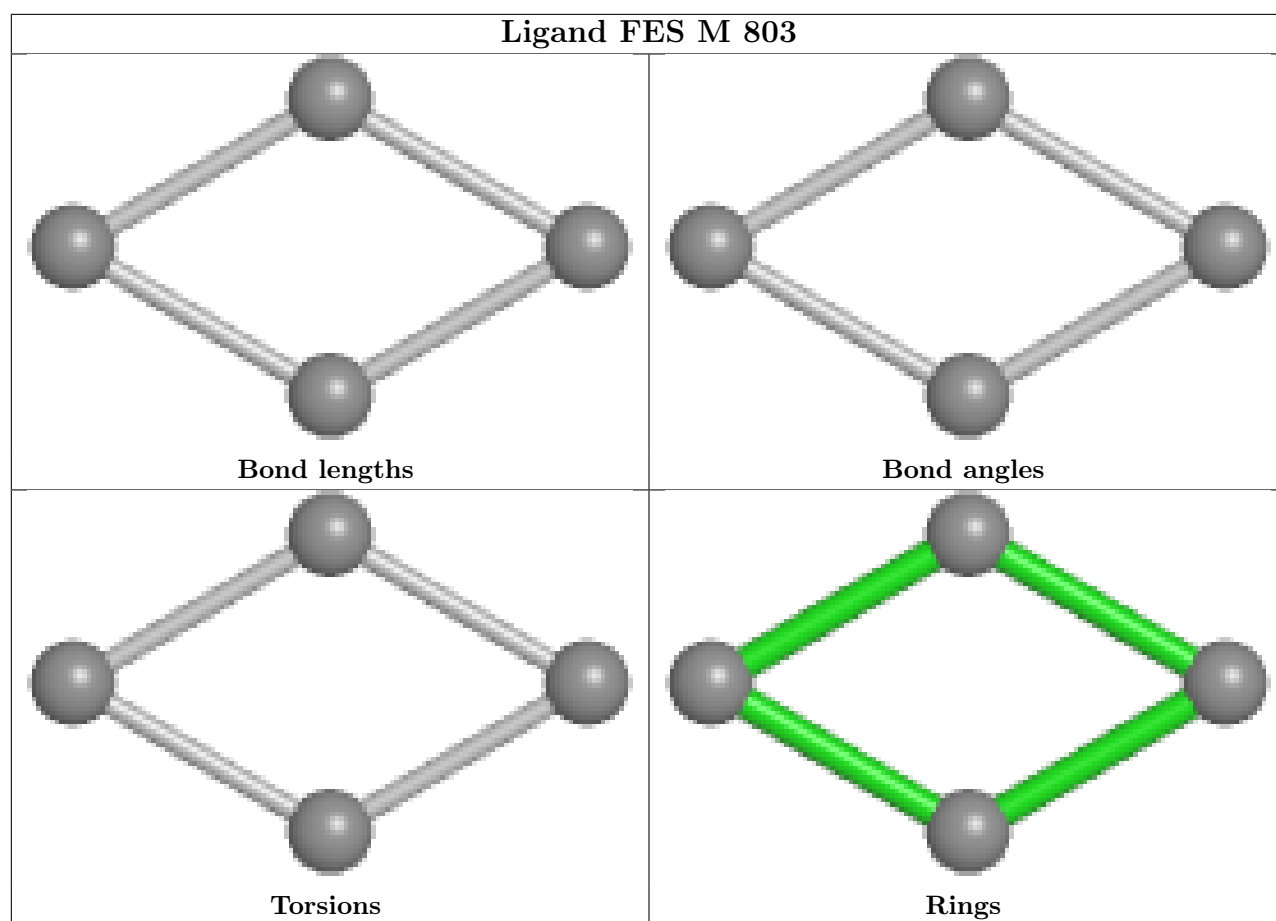


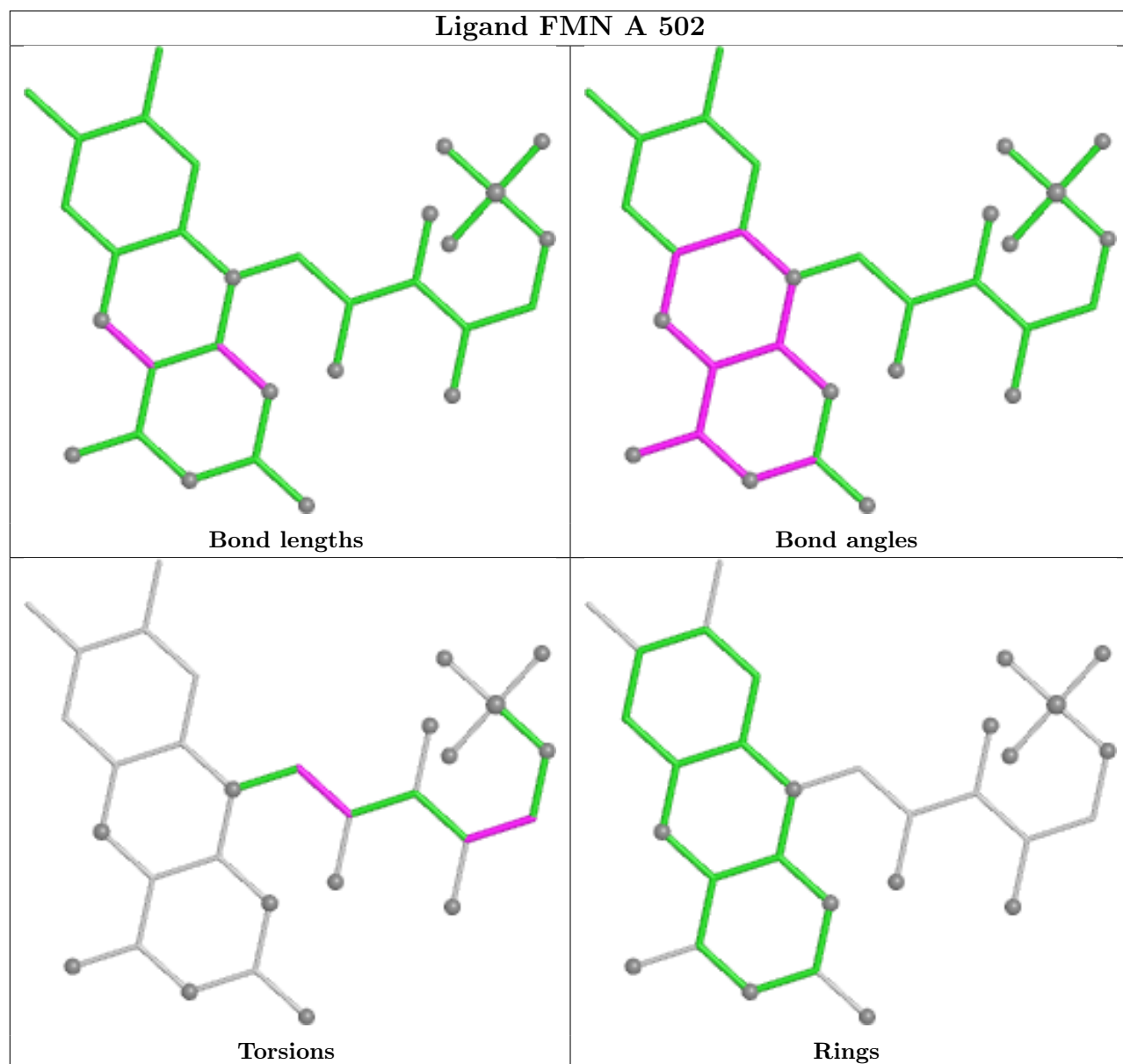
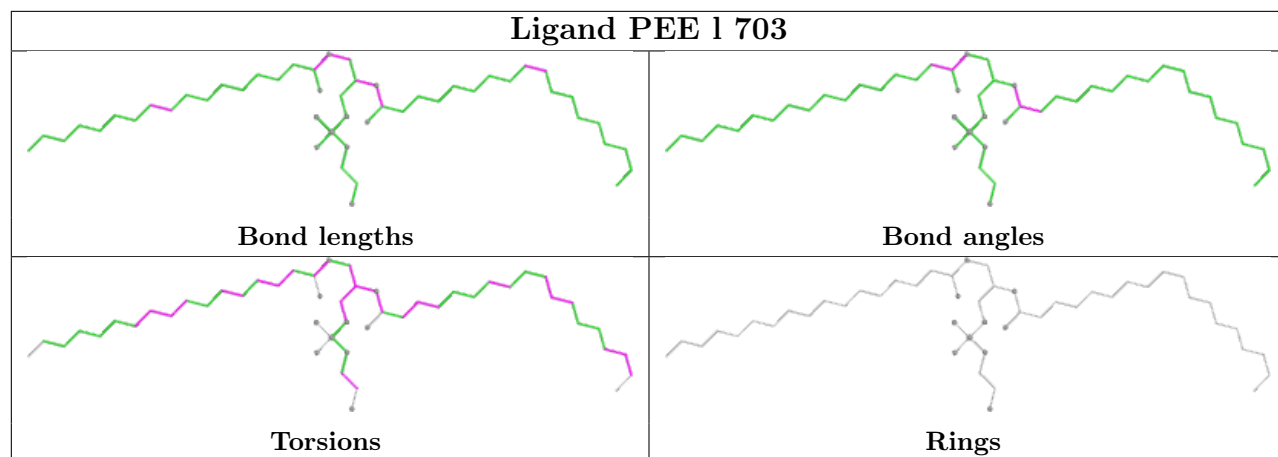


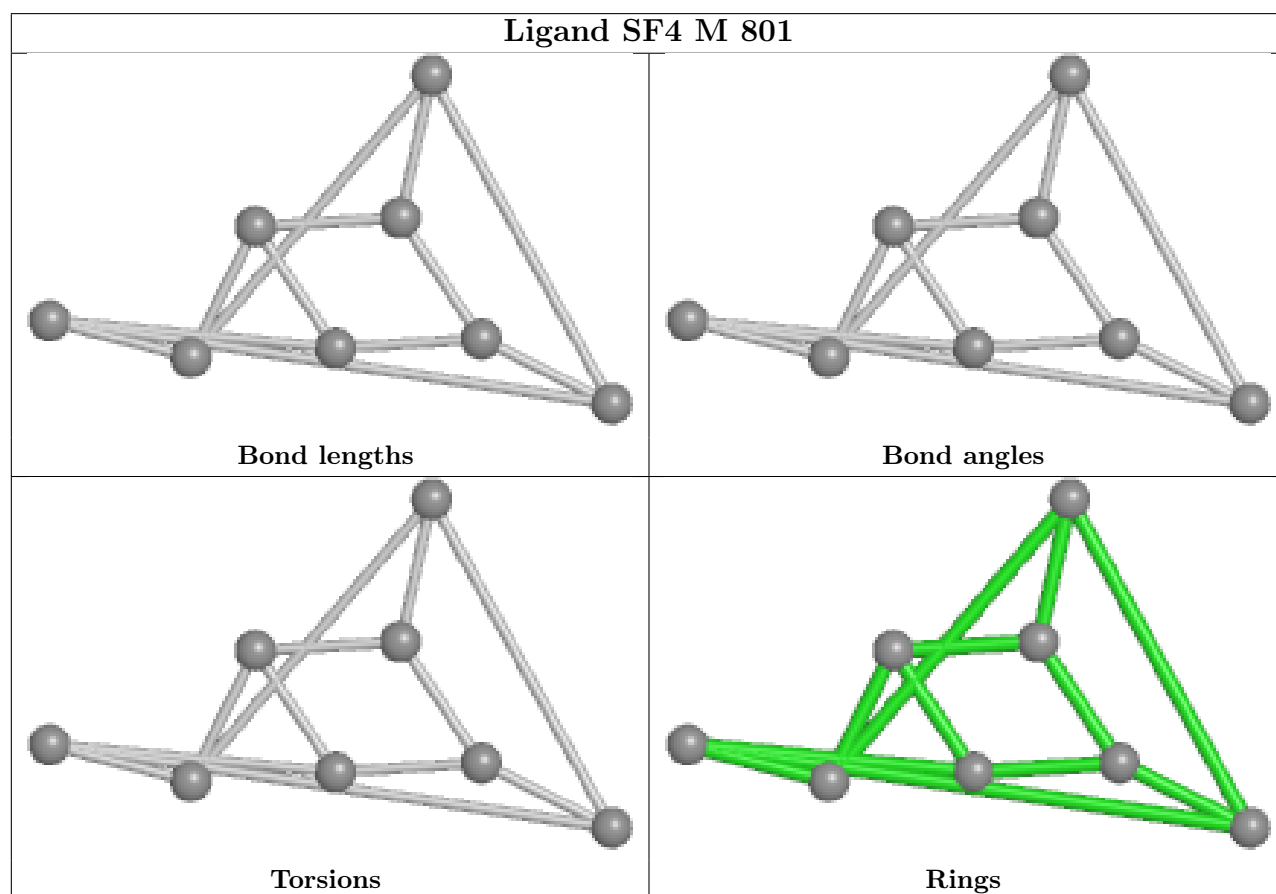
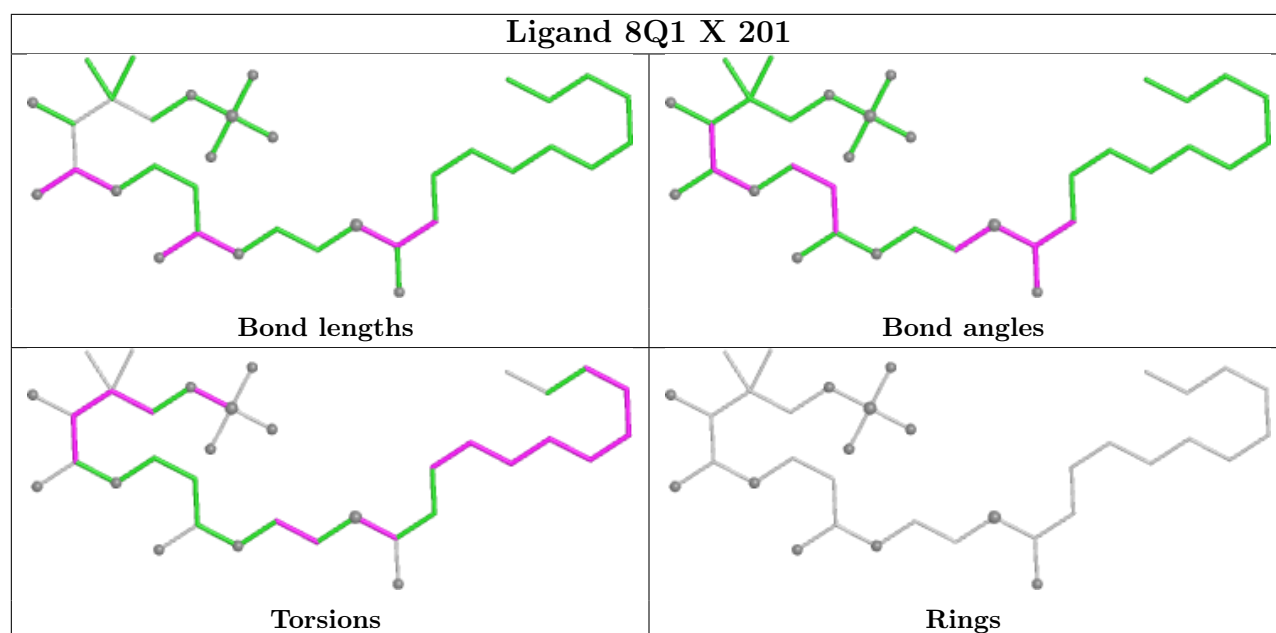


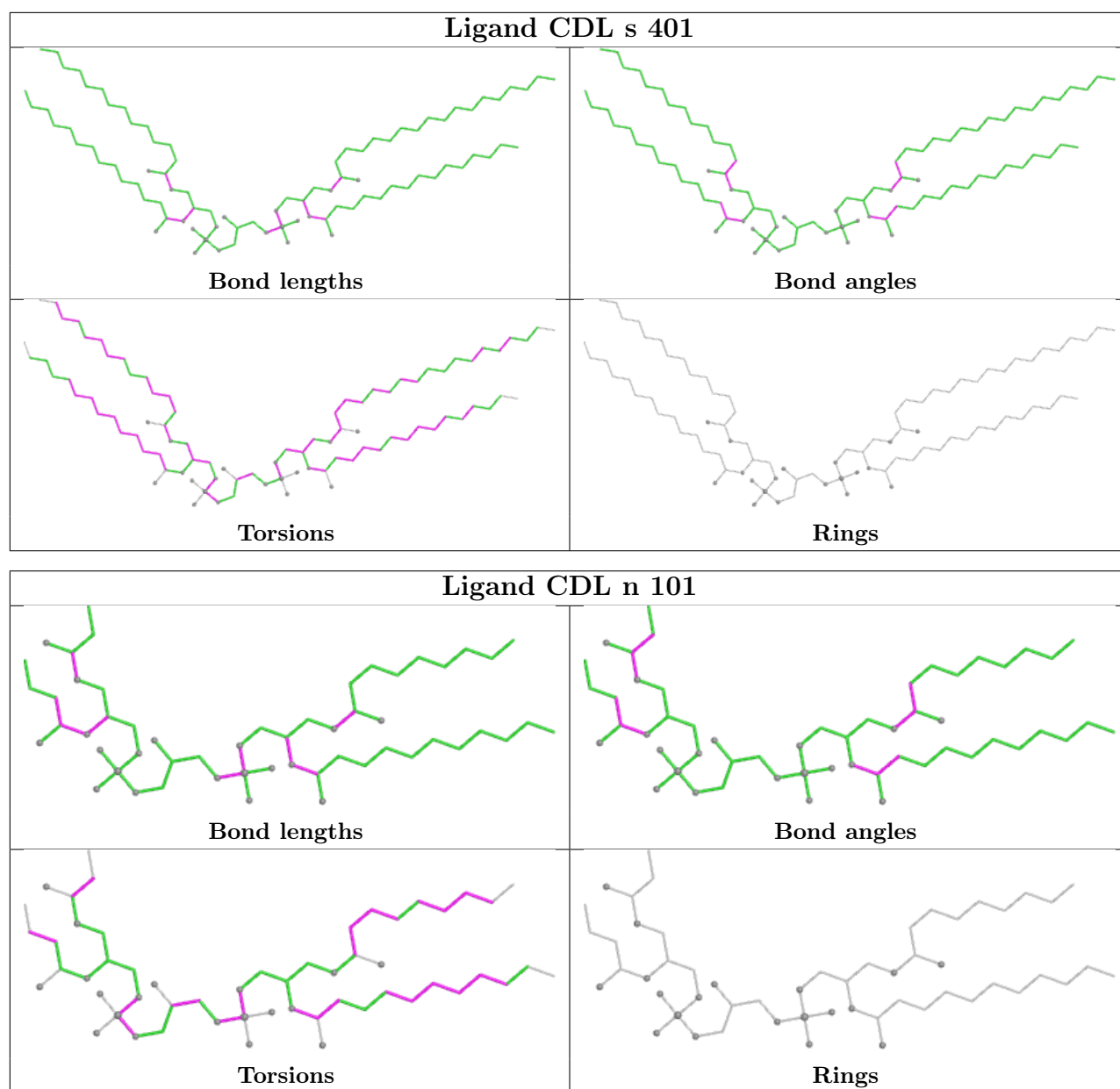


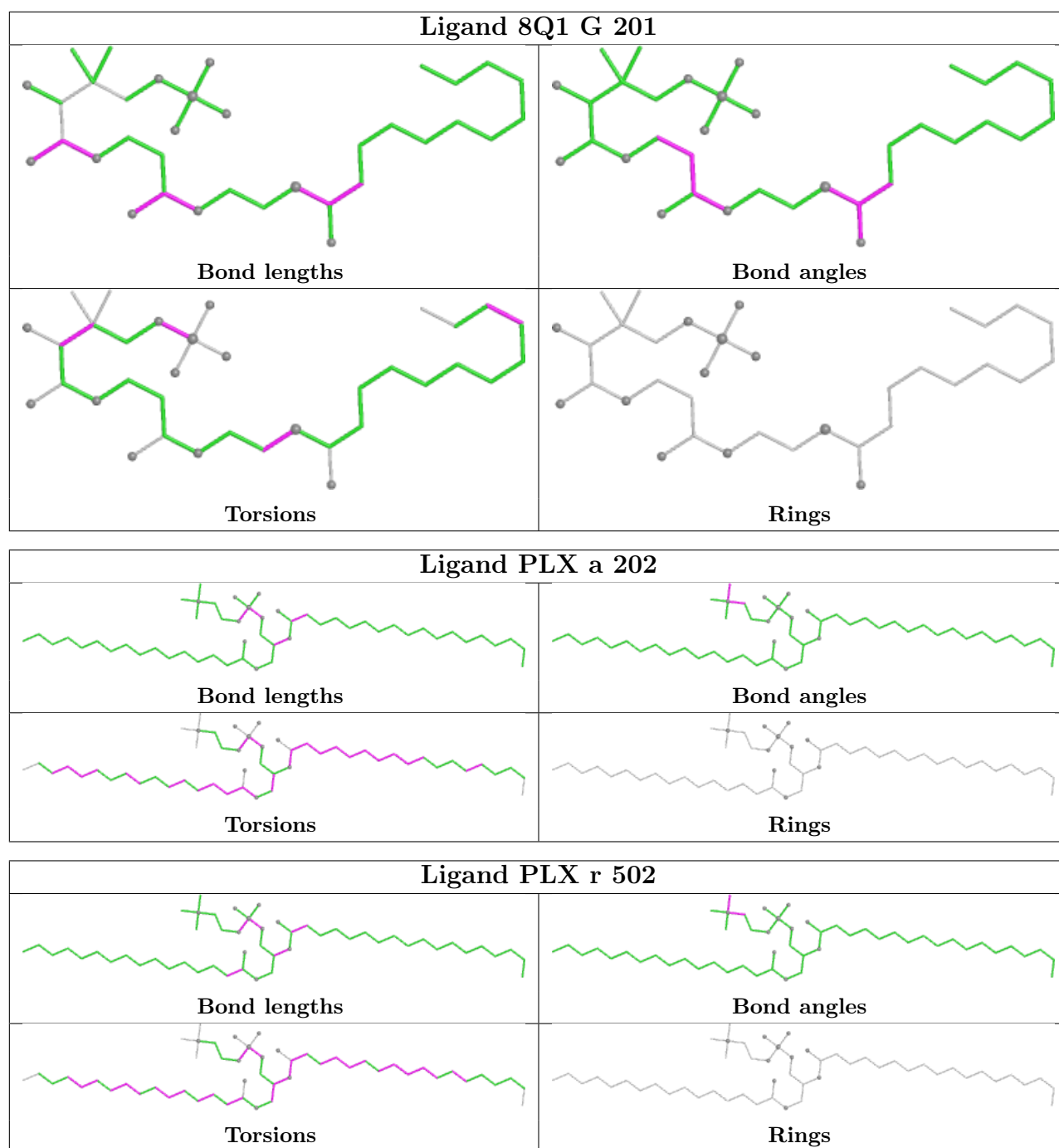


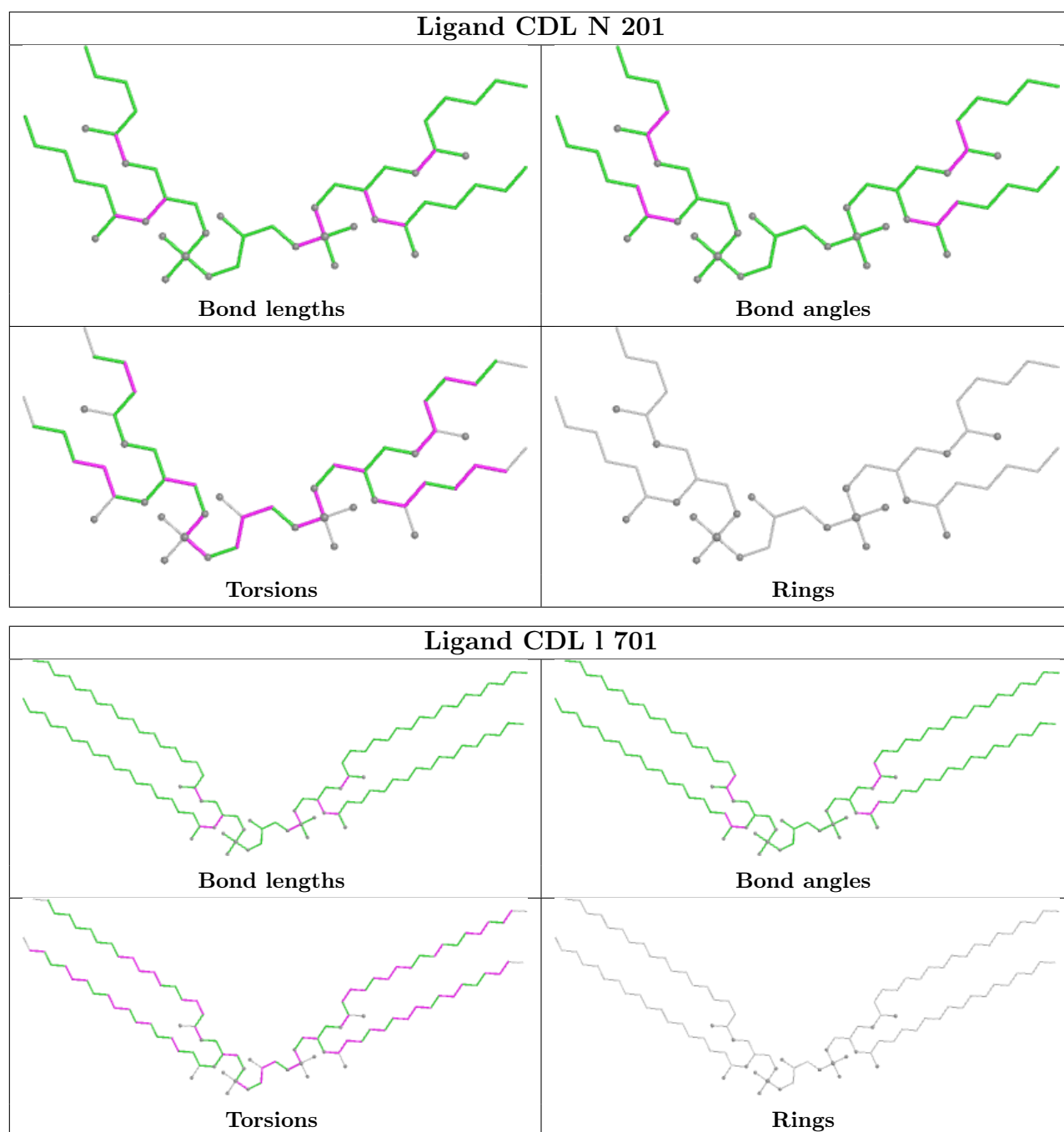




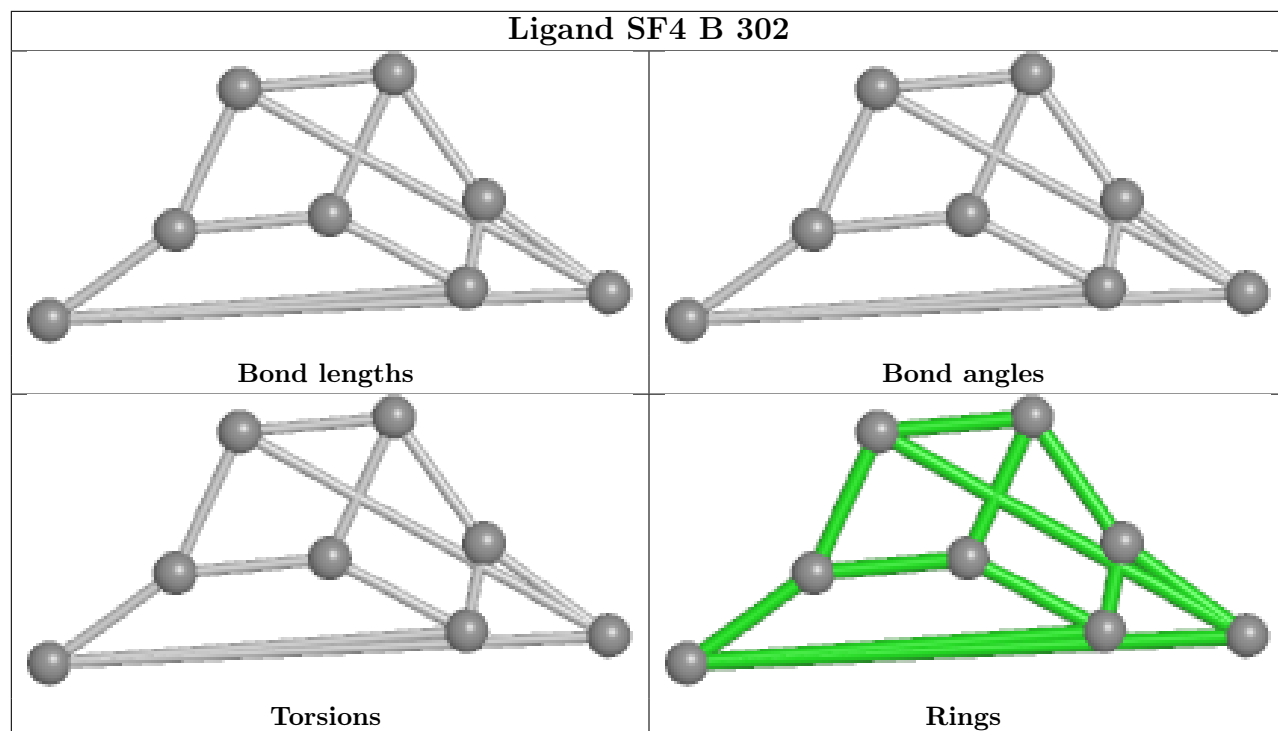




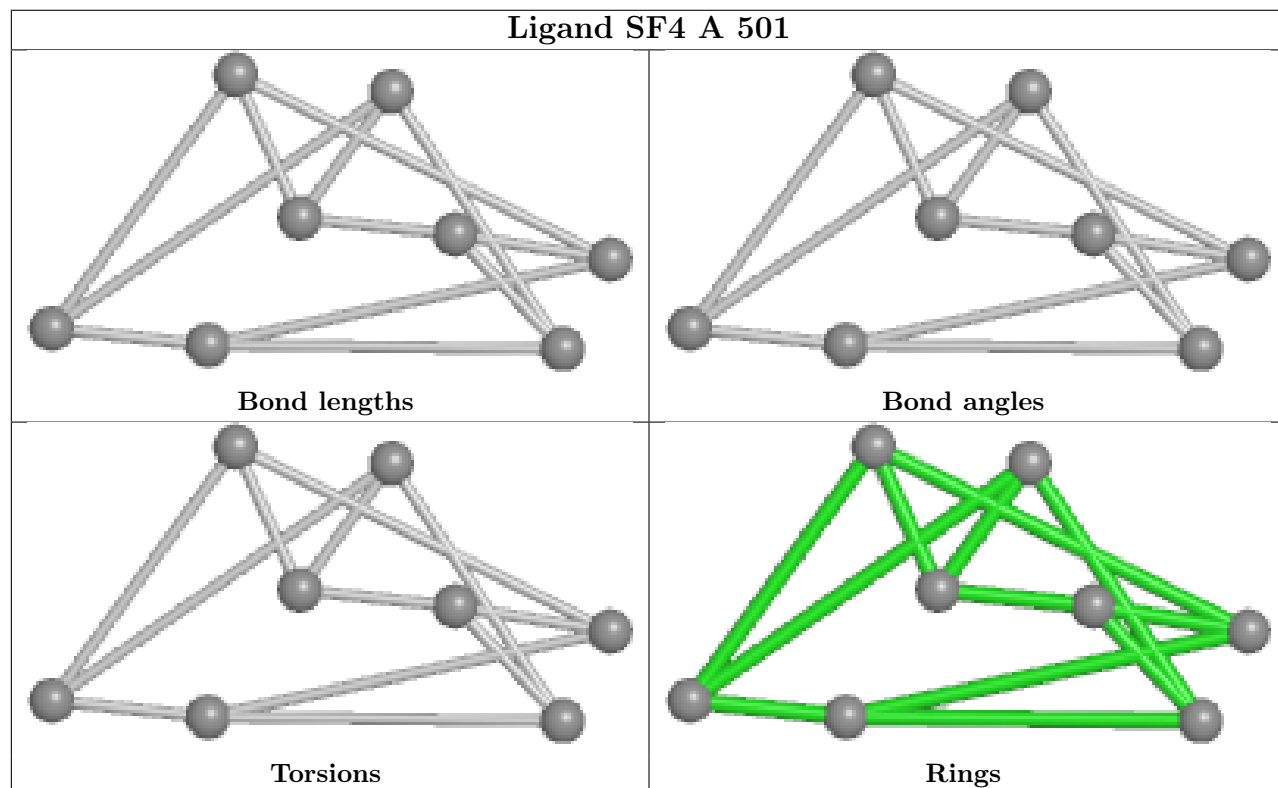


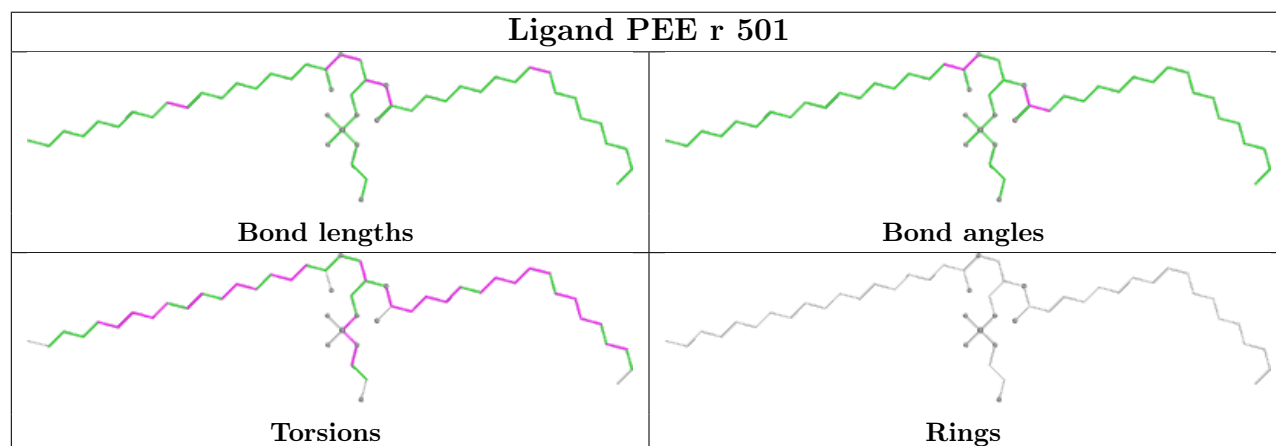
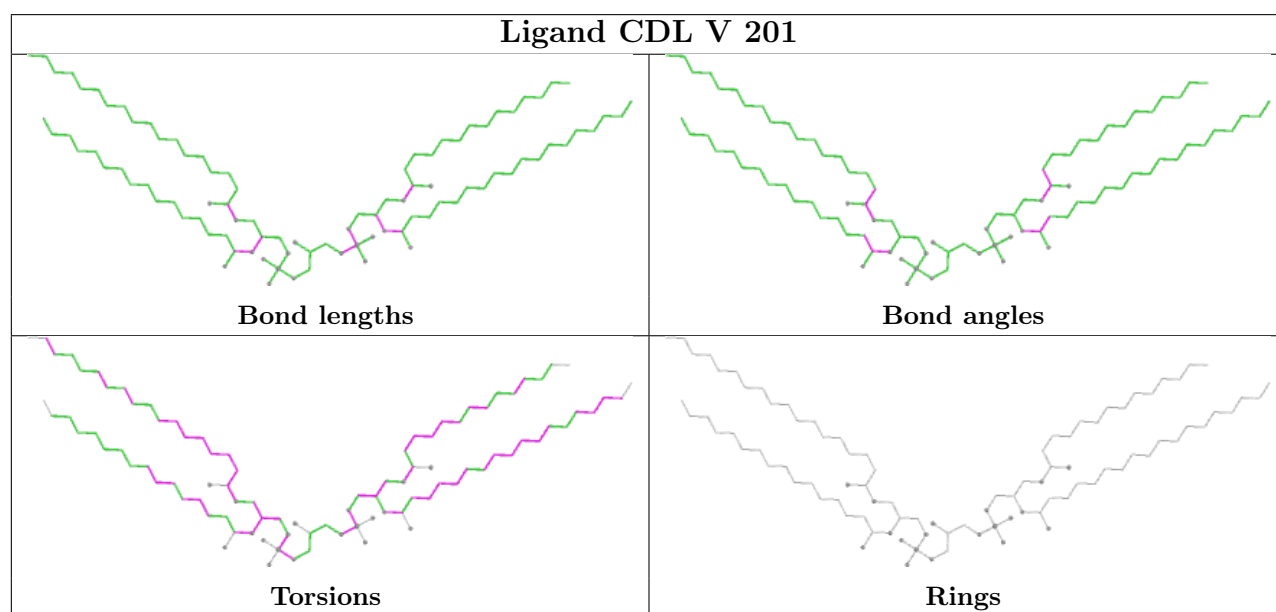
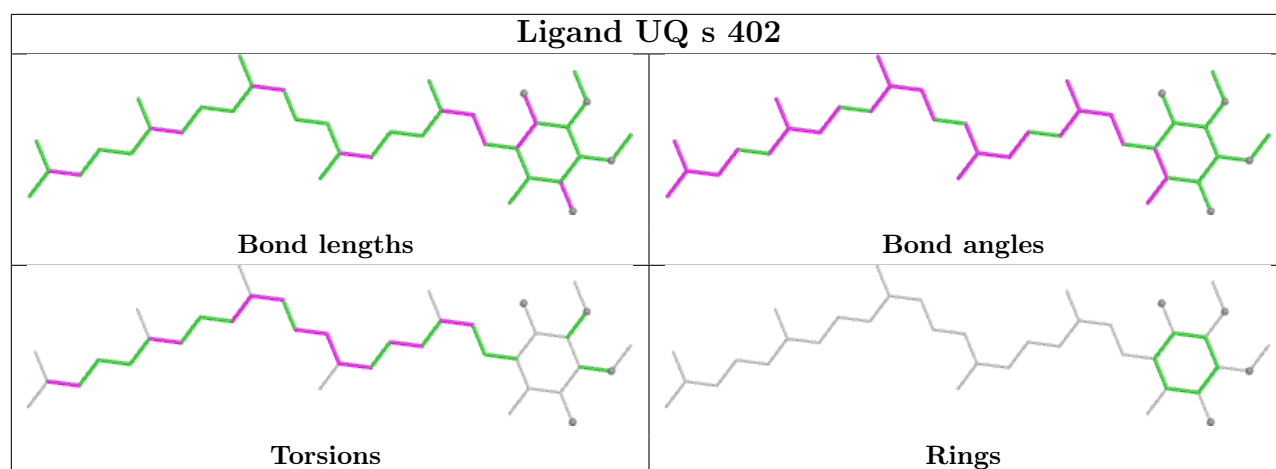


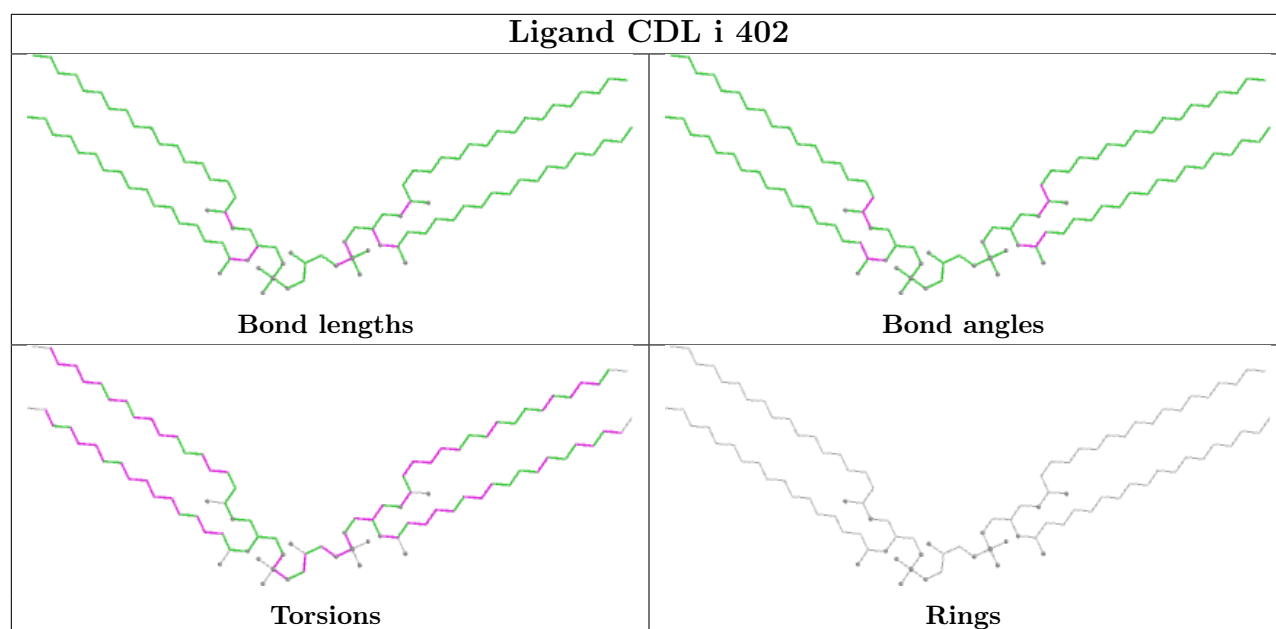
Ligand SF4 B 302



Ligand SF4 A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

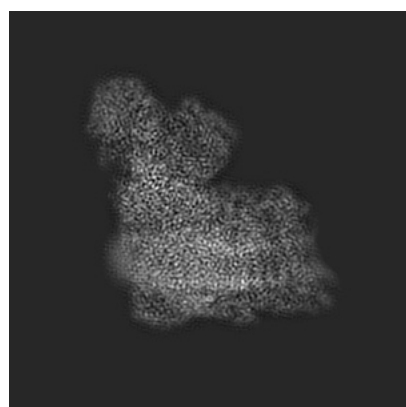
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32260. These allow visual inspection of the internal detail of the map and identification of artifacts.

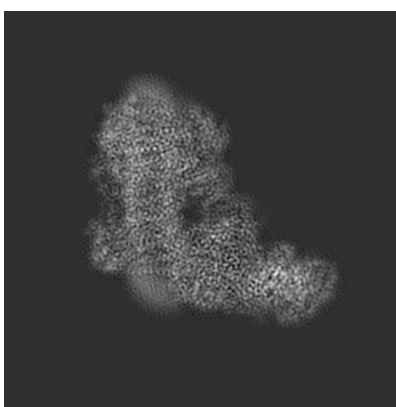
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

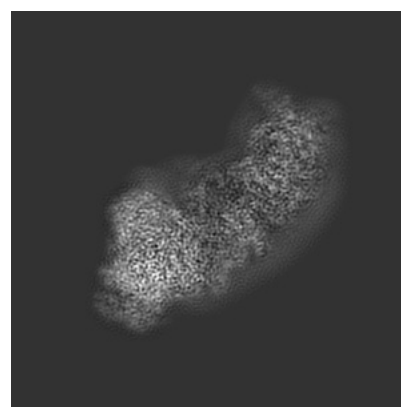
6.1.1 Primary map



X



Y

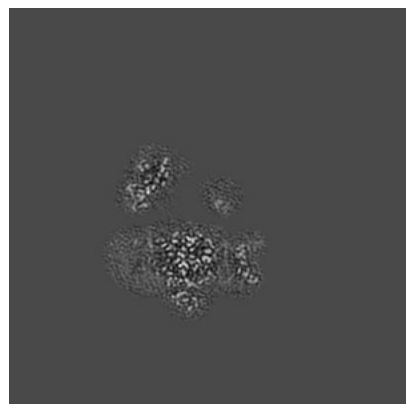


Z

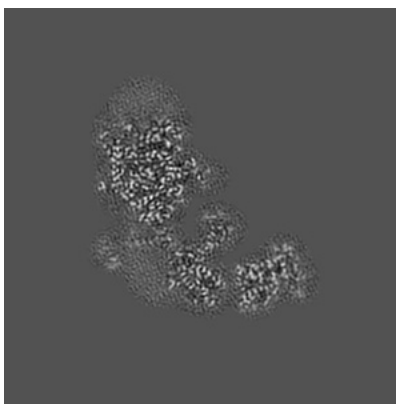
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

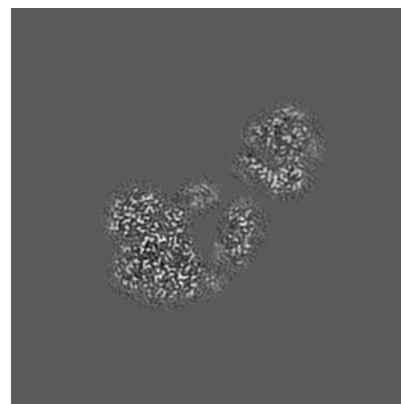
6.2.1 Primary map



X Index: 155



Y Index: 155

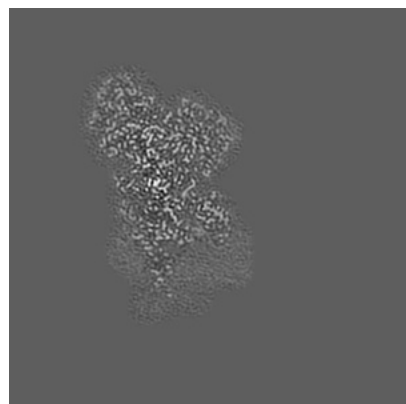


Z Index: 155

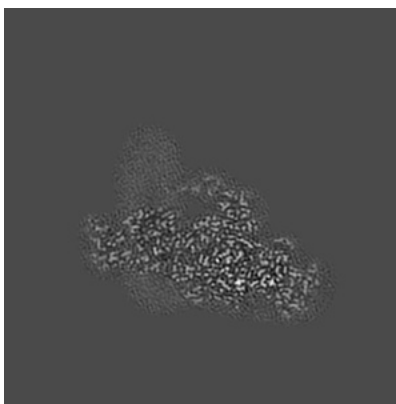
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

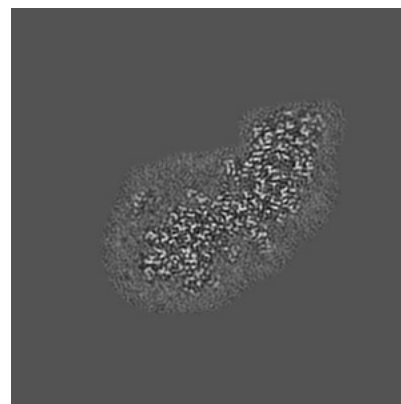
6.3.1 Primary map



X Index: 105



Y Index: 111

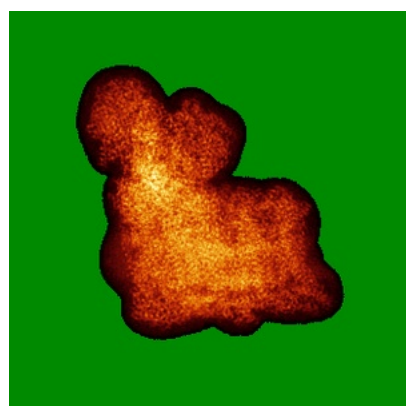


Z Index: 127

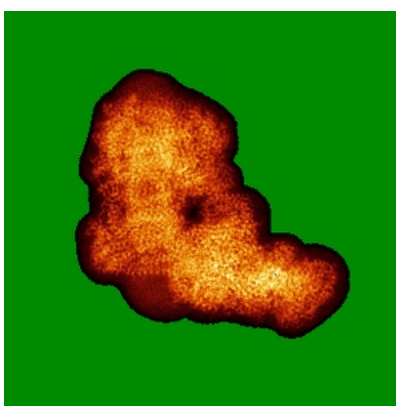
The images above show the largest variance slices of the map in three orthogonal directions.

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

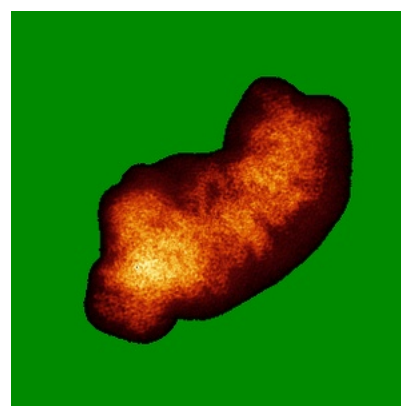
6.4.1 Primary map



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 0.0296. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

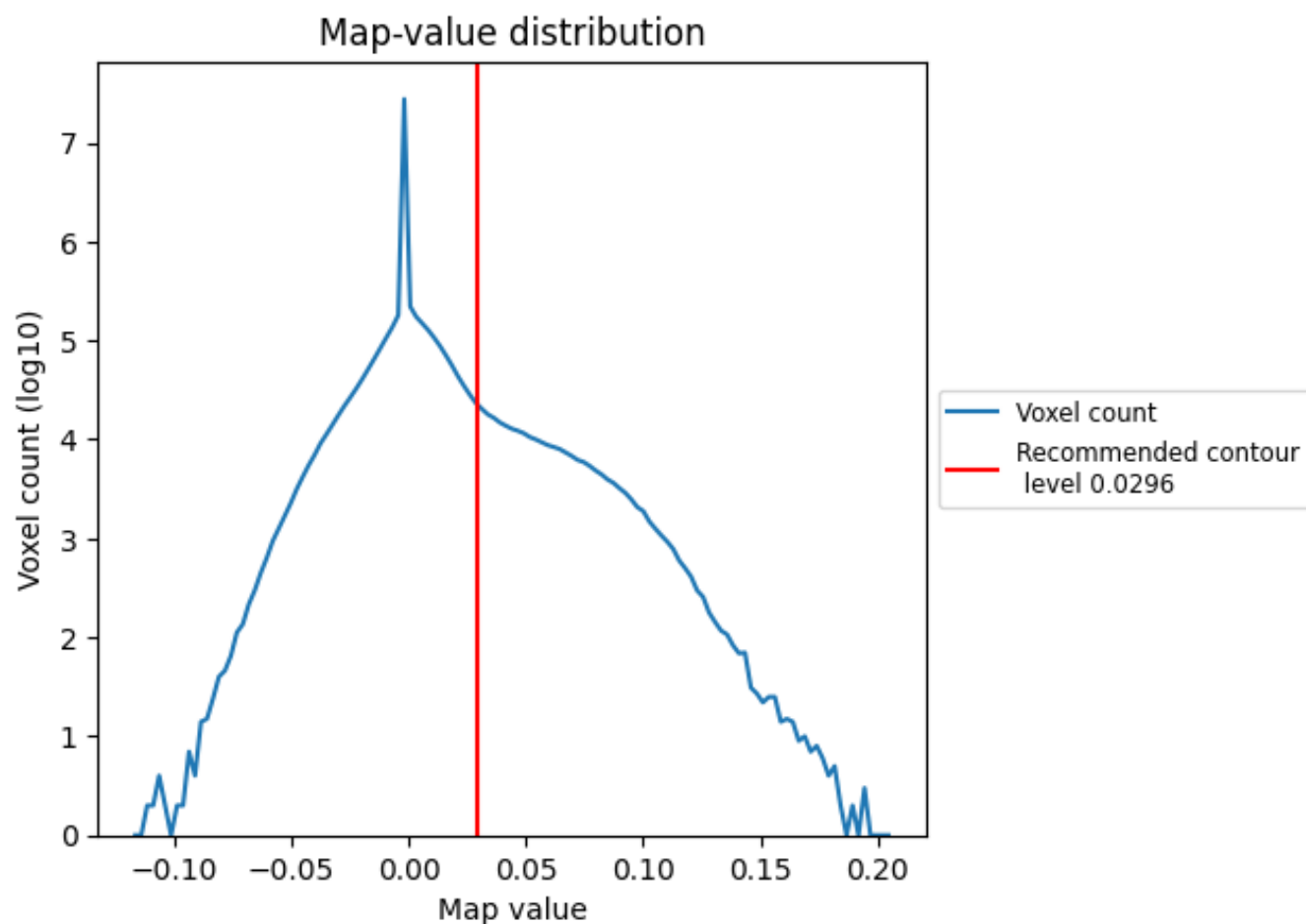
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

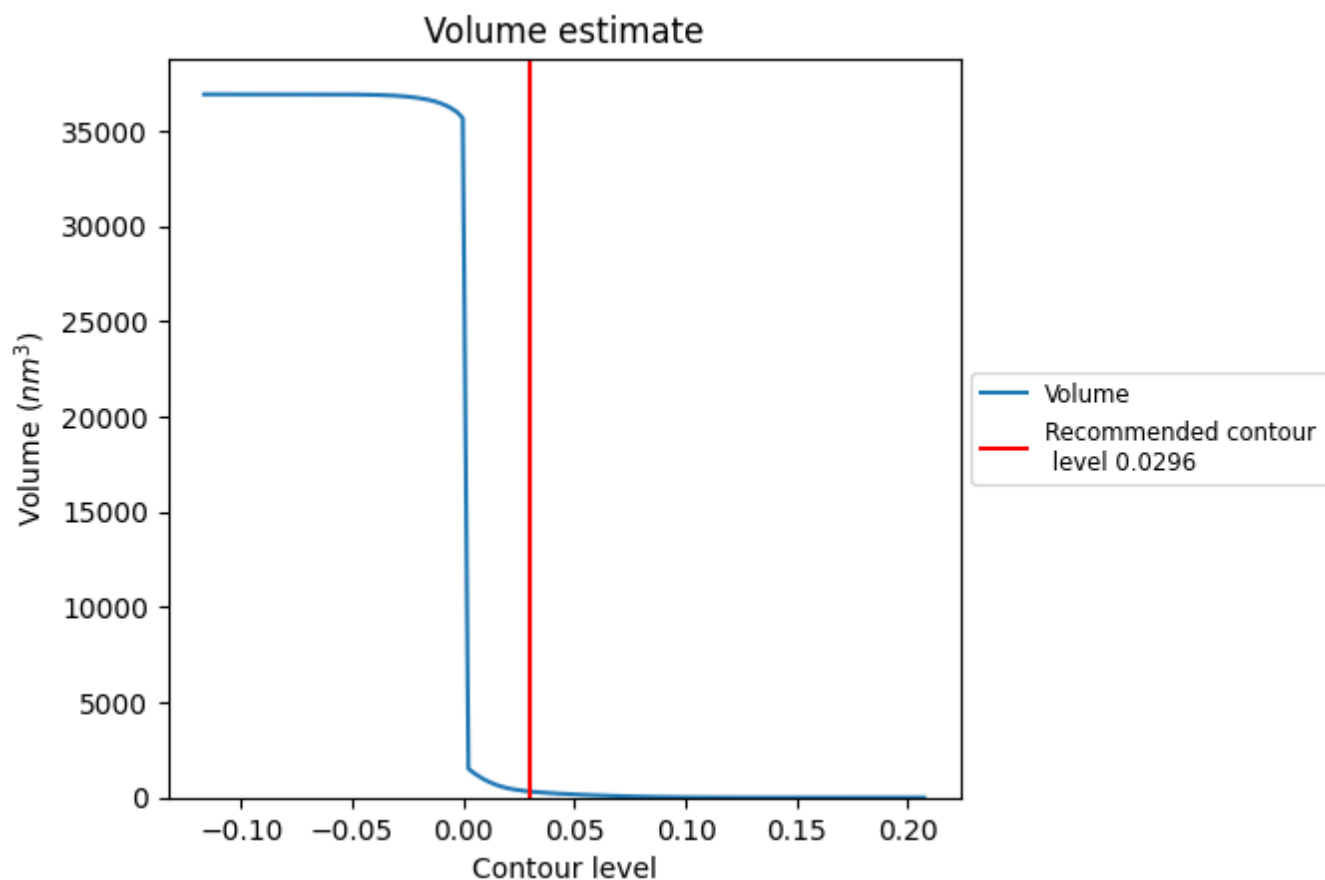
This section contains the results of statistical analysis of the map.

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.

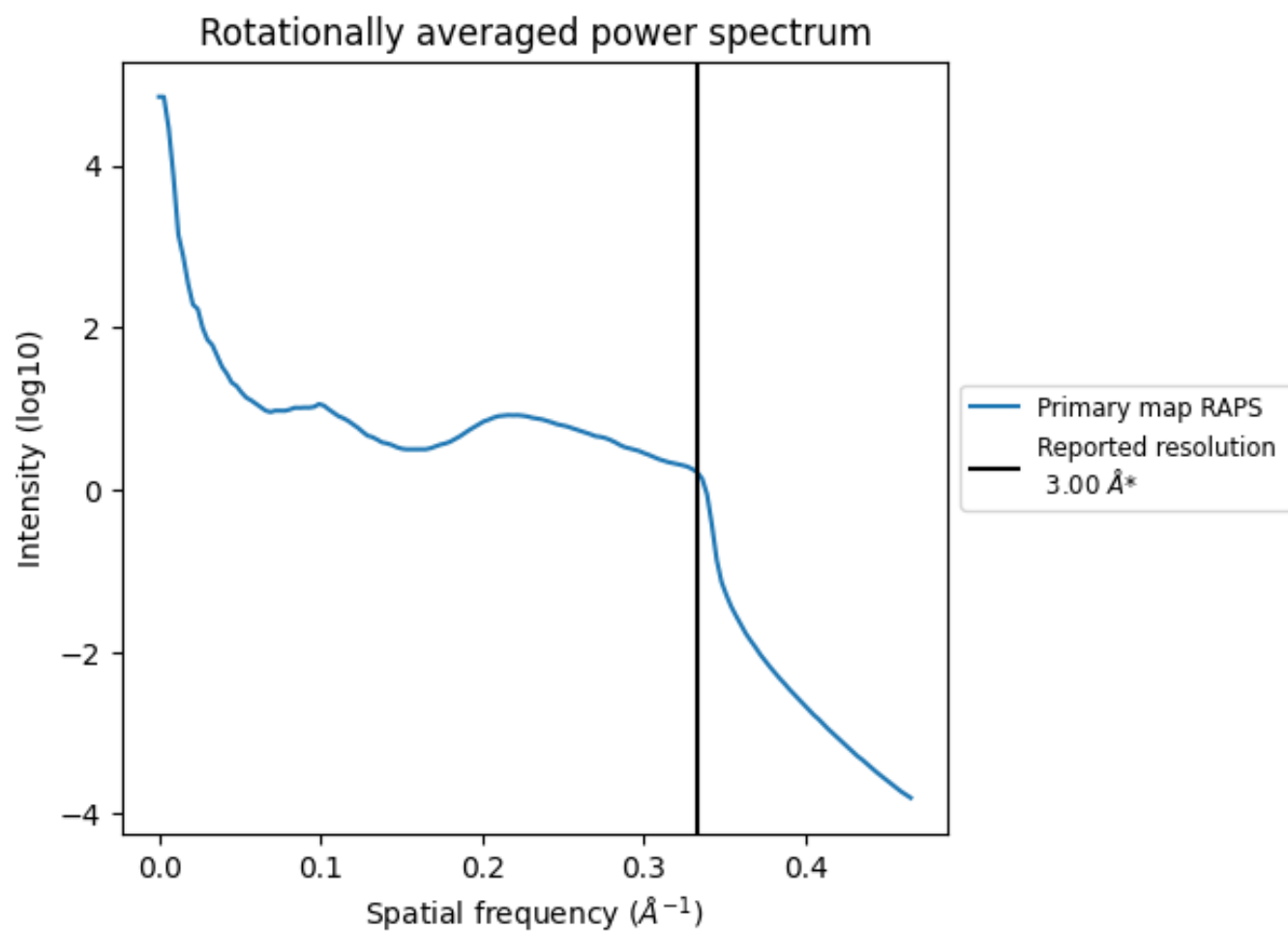
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323 nm³; this corresponds to an approximate mass of 292 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 0.333 Å⁻¹

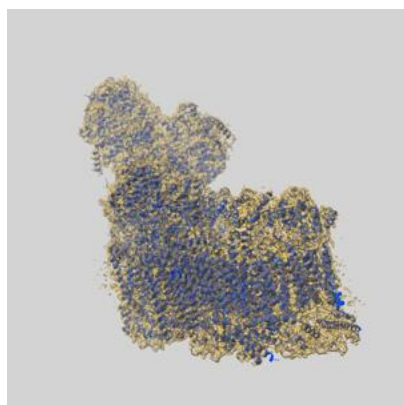
8 Fourier-Shell correlation

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

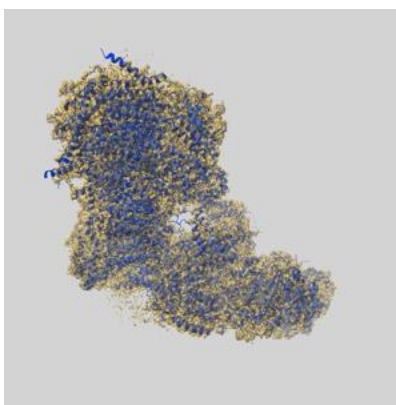
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32260 and PDB model 7W20. Per-residue inclusion information can be found in section 3 on page 21.

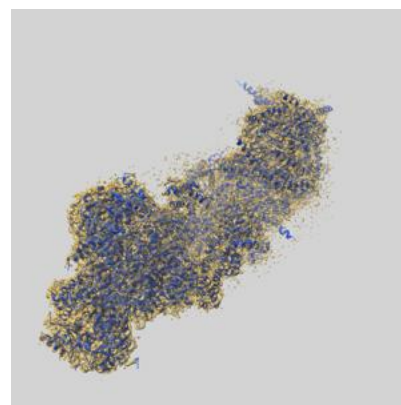
9.1 Map-model overlay [i](#)



X



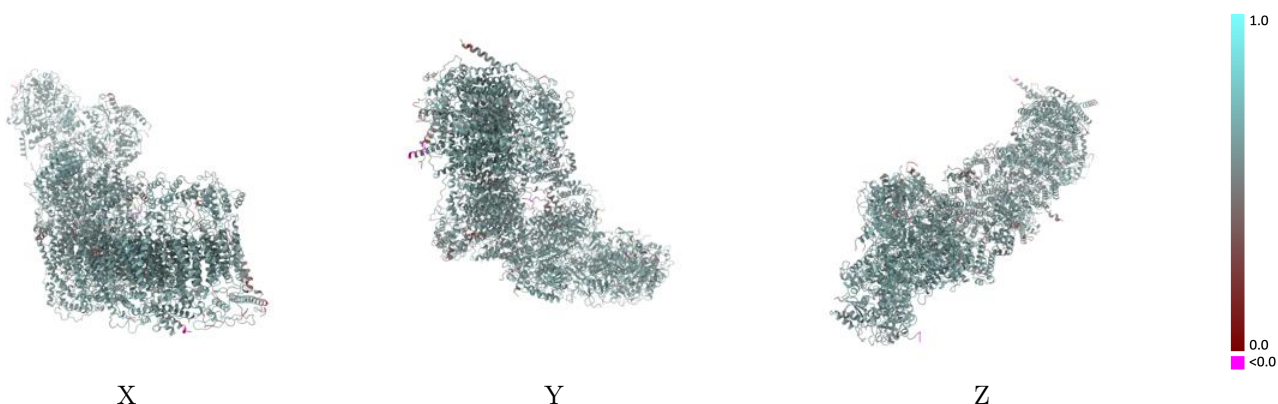
Y



Z

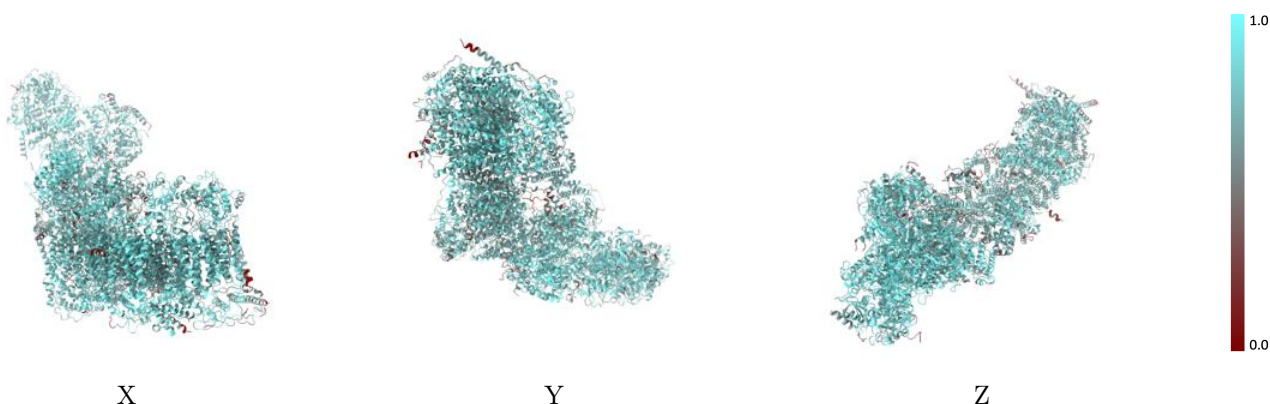
The images above show the 3D surface view of the map at the recommended contour level 0.0296 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



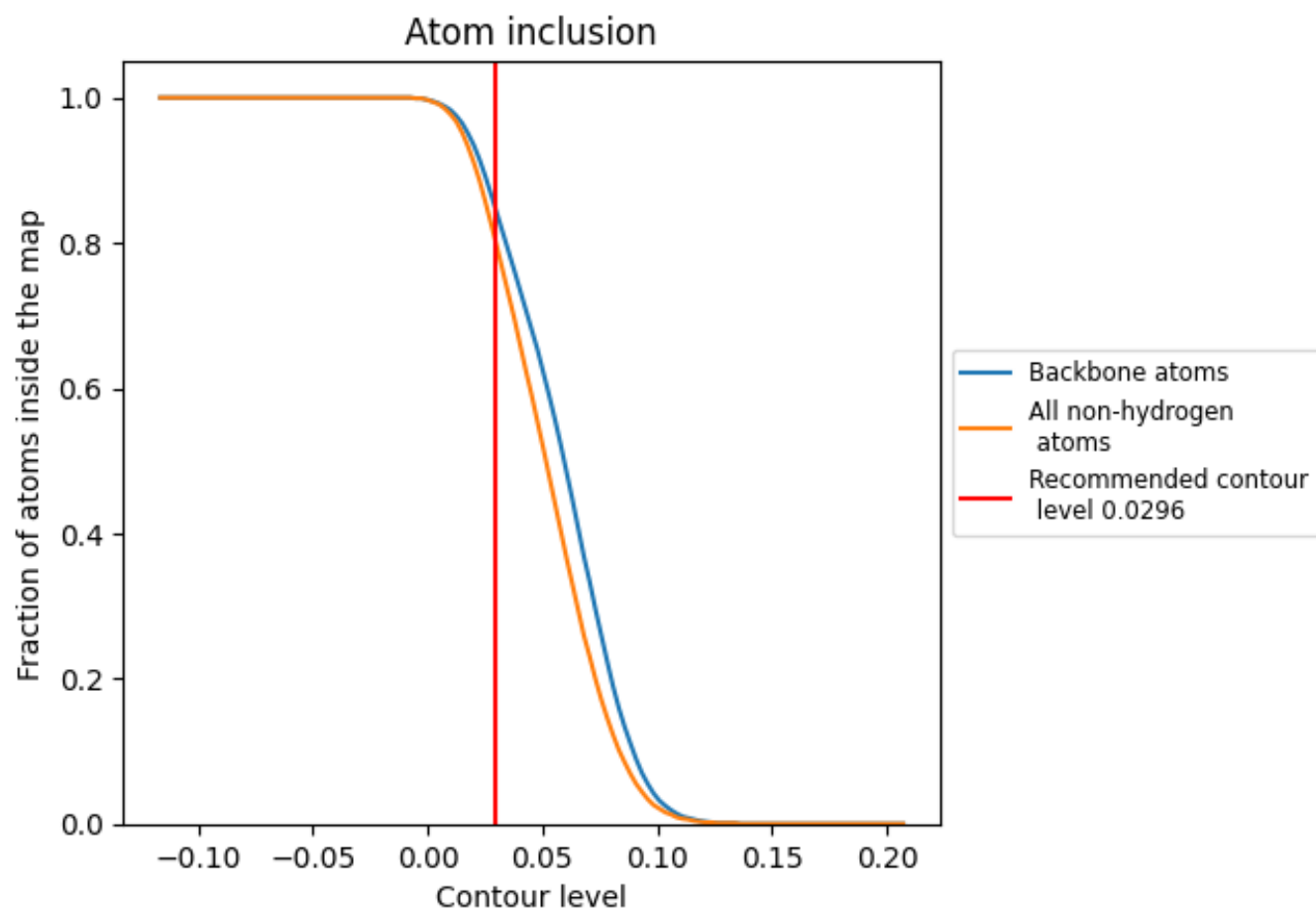
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0296).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.0296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.5910
A	 0.8090	 0.5840
B	 0.9060	 0.6290
C	 0.8890	 0.6220
E	 0.8030	 0.5950
F	 0.6960	 0.5340
G	 0.5280	 0.4710
H	 0.8190	 0.5910
I	 0.7250	 0.5720
J	 0.8270	 0.6000
K	 0.7300	 0.5650
L	 0.8330	 0.6110
M	 0.8380	 0.6030
N	 0.7450	 0.5940
O	 0.7700	 0.5690
P	 0.9050	 0.6320
Q	 0.8850	 0.6200
S	 0.8410	 0.6090
T	 0.7940	 0.5970
U	 0.7460	 0.5590
V	 0.7000	 0.5690
W	 0.7830	 0.5760
X	 0.7350	 0.5760
Y	 0.6840	 0.5380
Z	 0.6060	 0.5160
a	 0.8170	 0.6060
b	 0.7490	 0.5680
c	 0.7970	 0.5910
d	 0.7670	 0.5730
e	 0.7320	 0.5690
f	 0.6100	 0.5270
g	 0.8110	 0.5990
h	 0.7870	 0.5780
i	 0.8610	 0.6140
j	 0.7720	 0.5970



Continued on next page...

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Chain	Atom inclusion	Q-score
k	 0.8320	 0.6080
l	 0.7990	 0.5970
m	 0.7470	 0.5600
n	 0.6530	 0.5400
o	 0.7330	 0.5660
p	 0.8130	 0.5930
r	 0.8620	 0.6120
s	 0.8530	 0.6090
u	 0.7980	 0.5820
v	 0.6870	 0.5410
w	 0.7590	 0.5710