



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:04 PM UTC

PDB ID : 7W4F / pdb_00007w4f
EMDB ID : EMD-32303
Title : Active state CI from Q1-NADH dataset, Subclass 4
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-27
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

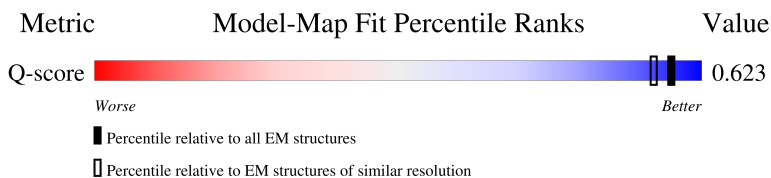
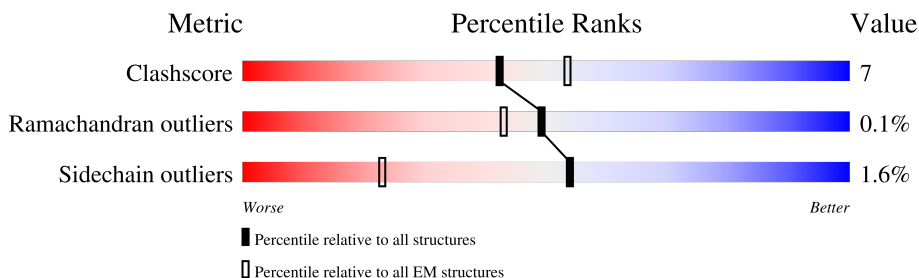
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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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	124	
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	202	-	-	X	-
52	CDL	l	702	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68192 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
			3328	2102	593	613	20		

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			703	453	104	141	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			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
			3456	2209	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
			1167	752	200	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			580	383	95	101	1		

- Molecule 23 is a protein called Complex I-B12.

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 Complex I-SGDH.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	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	S	0	0
			1062	691	182	189			

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

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

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

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

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

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

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

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

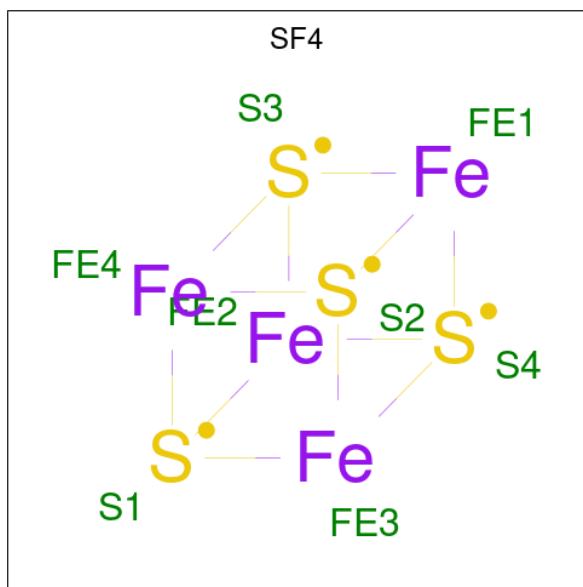
- Molecule 43 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1021	638	194	180	9		

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

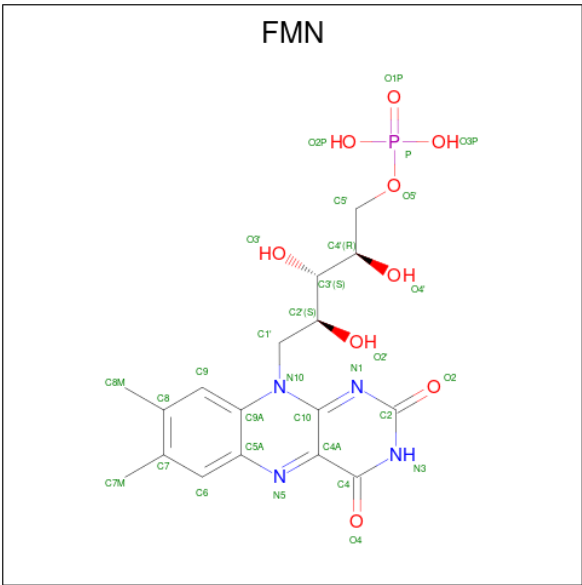
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



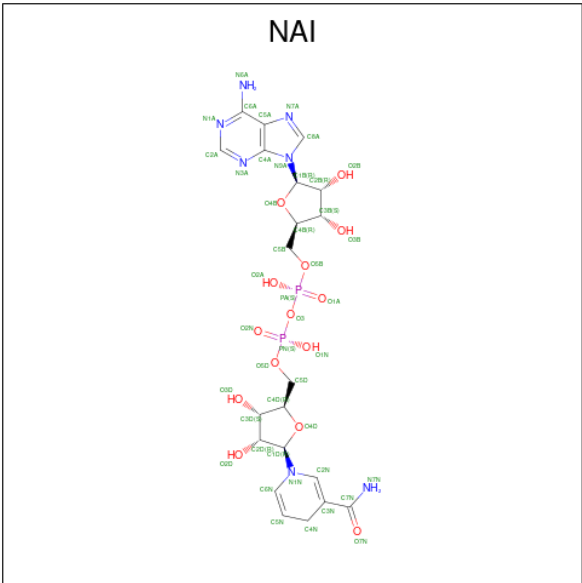
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

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



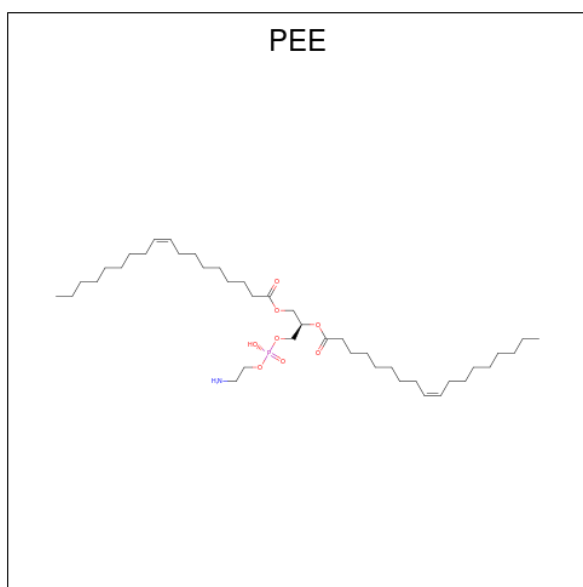
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).



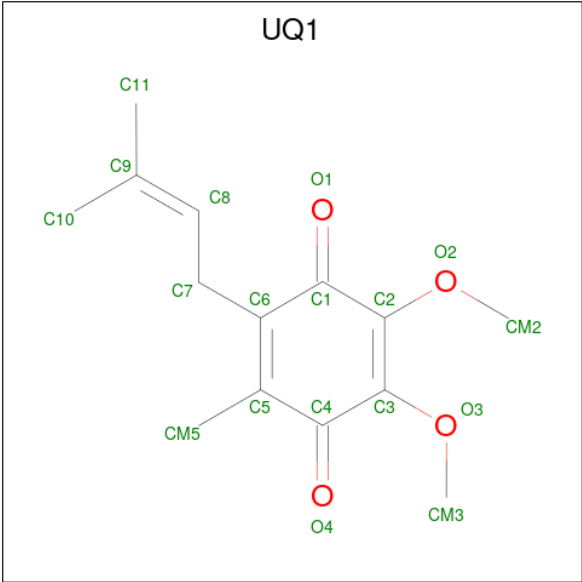
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- 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).



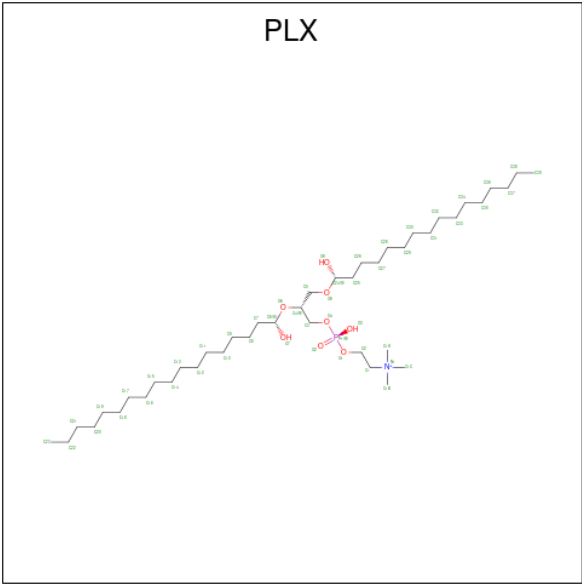
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41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

- Molecule 49 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄) (labeled as "Ligand of Interest" by depositor).



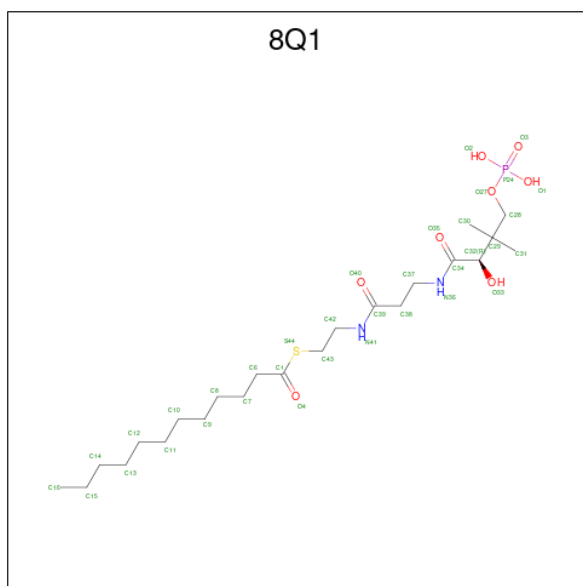
Mol	Chain	Residues	Atoms			AltConf
49	C	1	Total	C	O	0
			18	14	4	
49	Q	1	Total	C	O	0
			18	14	4	

- Molecule 50 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).



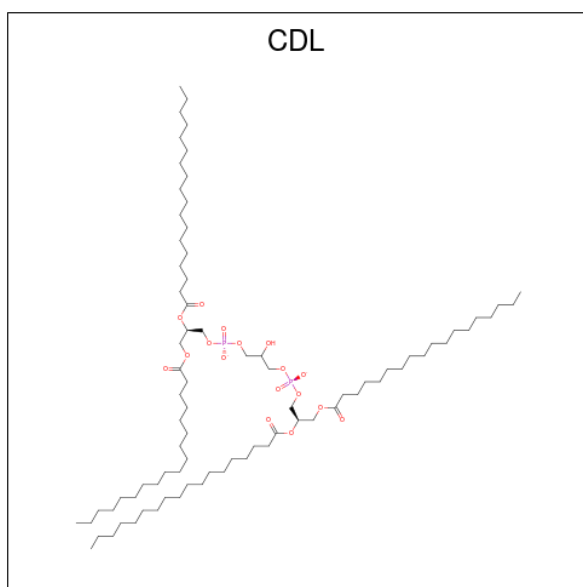
Mol	Chain	Residues	Atoms					AltConf
50	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
50	j	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



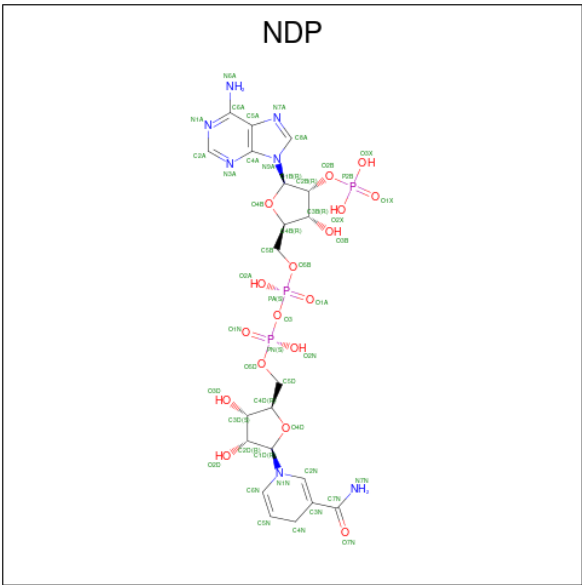
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total 35	C 23	N 2	O 8	P 1	S 1	0
51	X	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



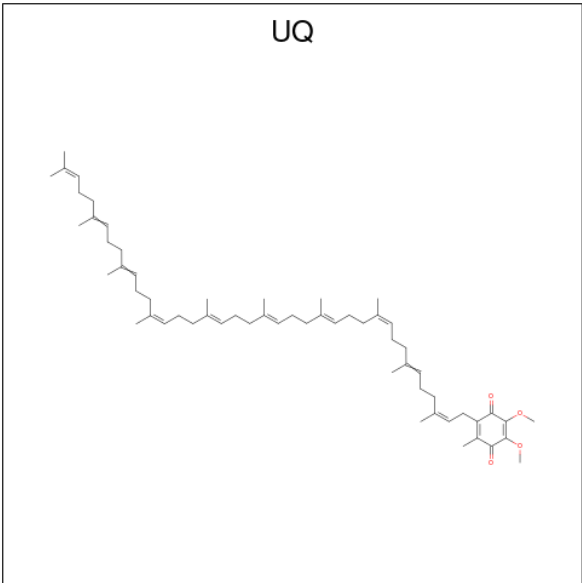
Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	g	1	Total	C	O	P	0
			100	81	17	2	
52	k	1	Total	C	O	P	0
			94	75	17	2	
52	l	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			100	81	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	
52	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



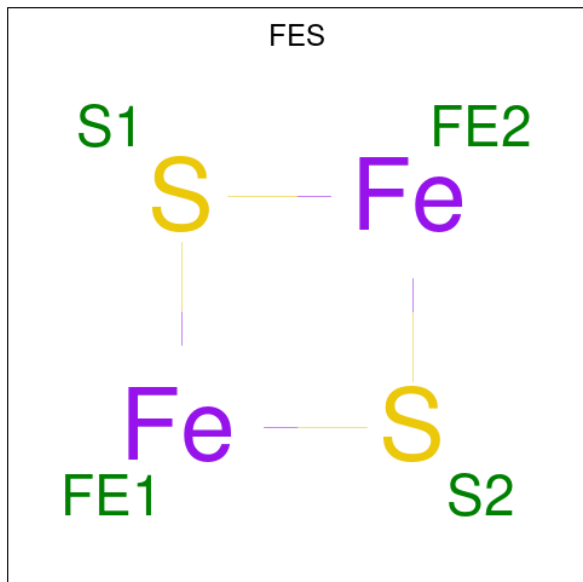
Mol	Chain	Residues	Atoms					AltConf
53	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 54 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
54	J	1	Total	C	O	0
			33	29	4	
54	s	1	Total	C	O	0
			38	34	4	

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

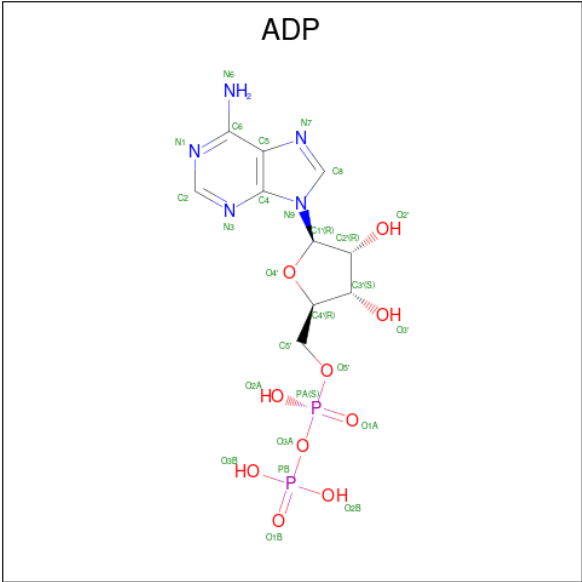
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- 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: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

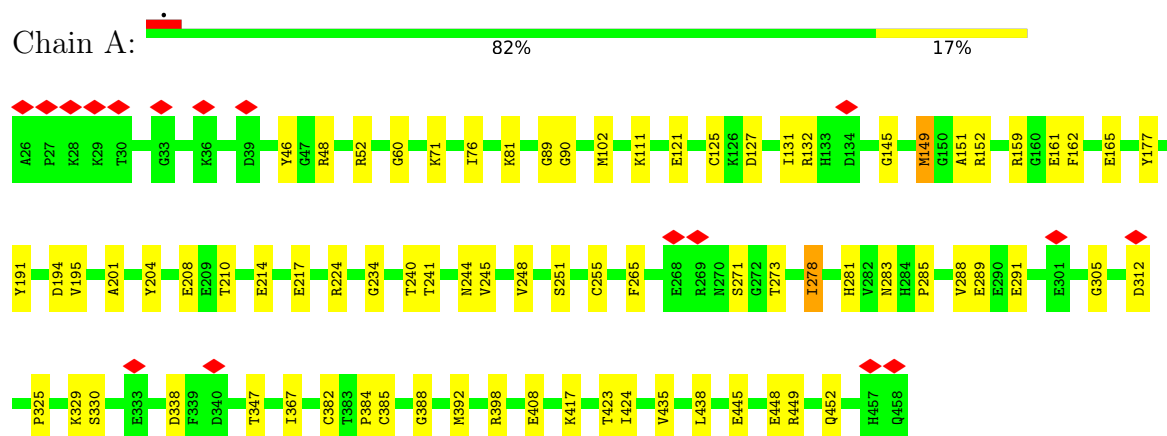


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

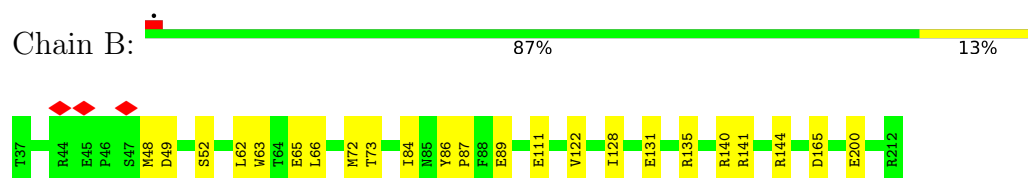
3 Residue-property plots

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

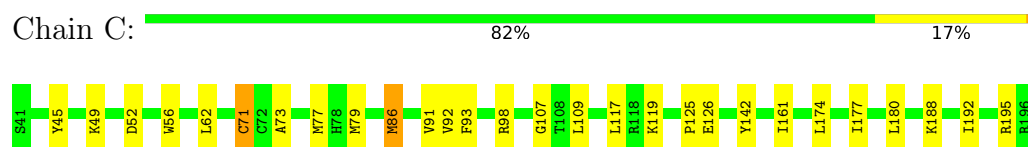
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



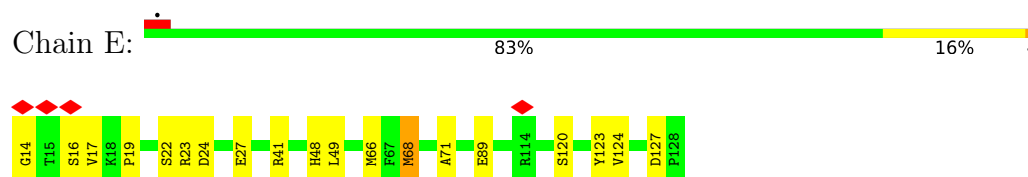
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



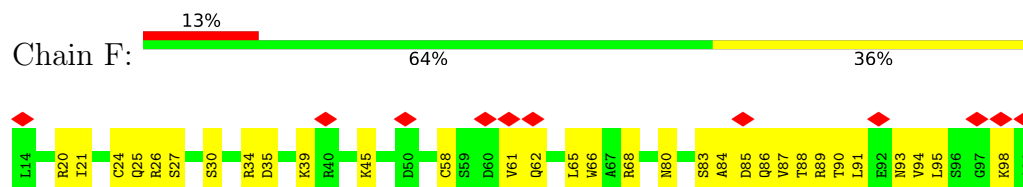
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



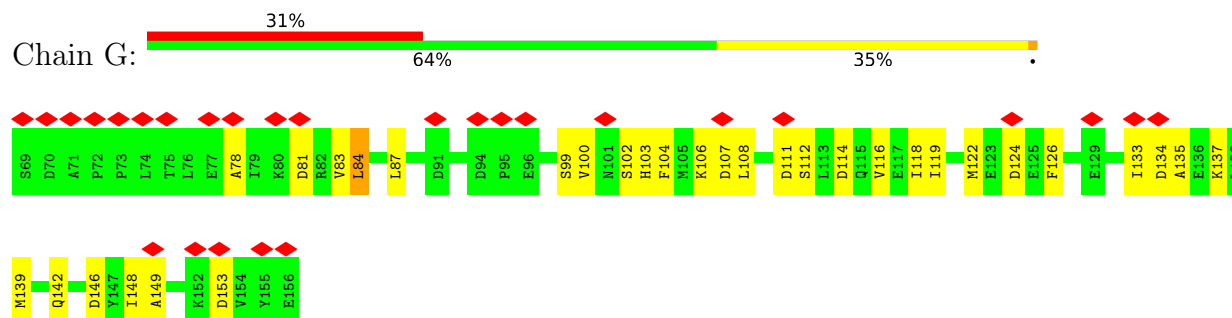
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



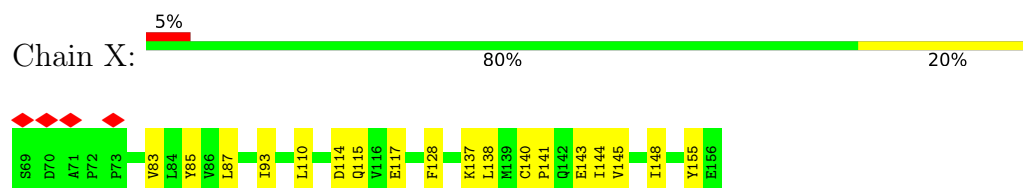
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



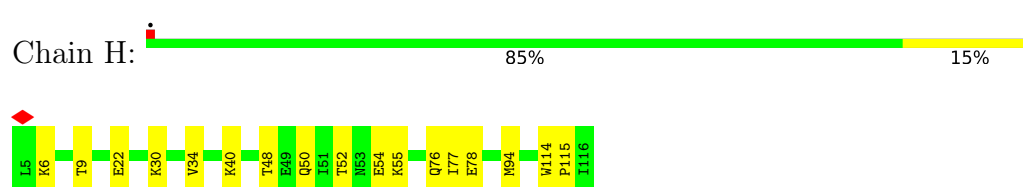
- Molecule 6: Acyl carrier protein



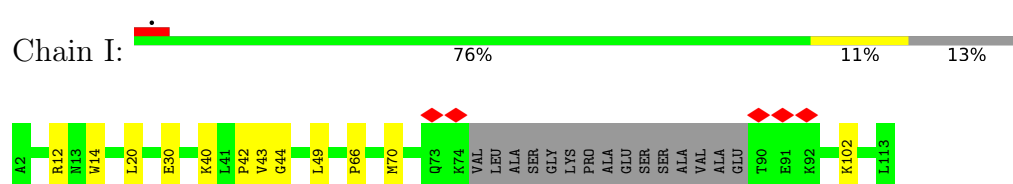
- Molecule 6: Acyl carrier protein



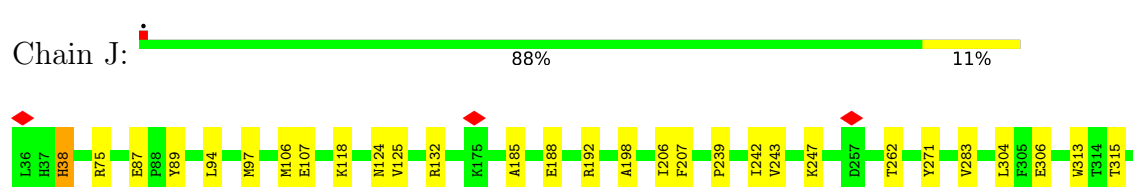
- Molecule 7: Complex I subunit B13



- Molecule 8: Complex I-B14.5a

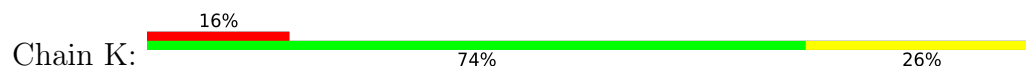


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

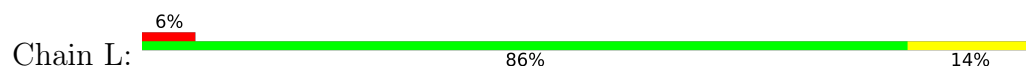




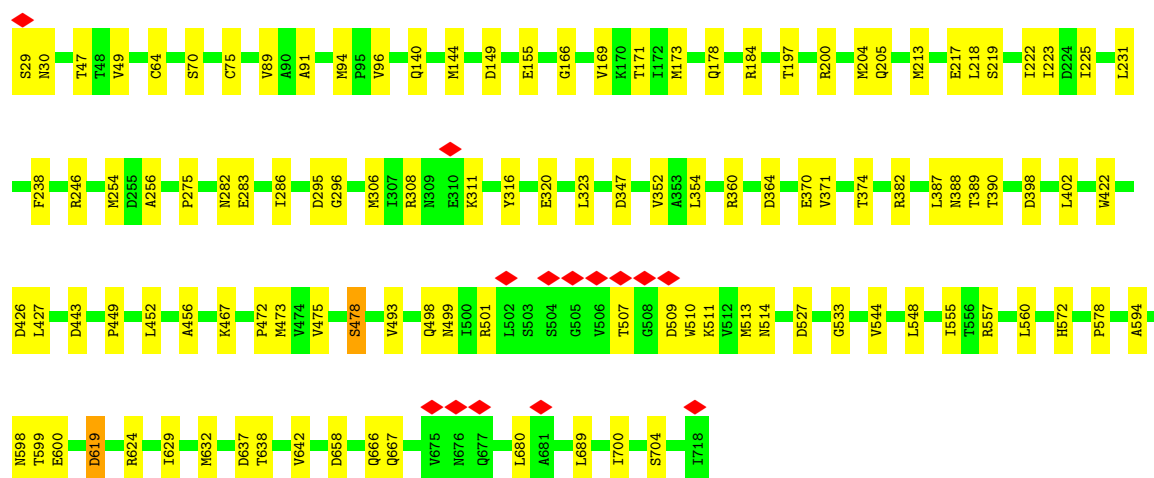
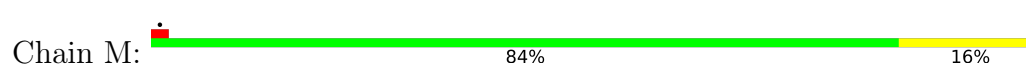
- Molecule 10: Complex I-9kD



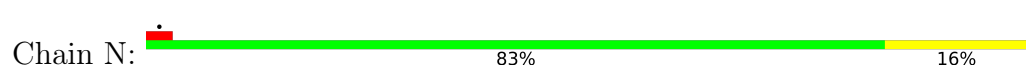
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



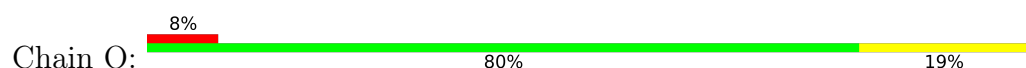
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

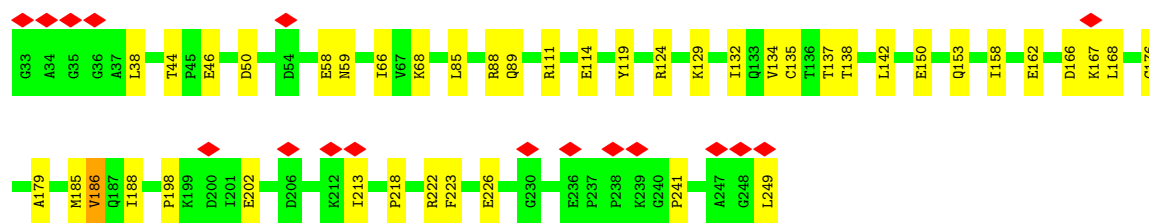


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



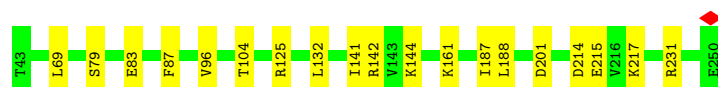
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





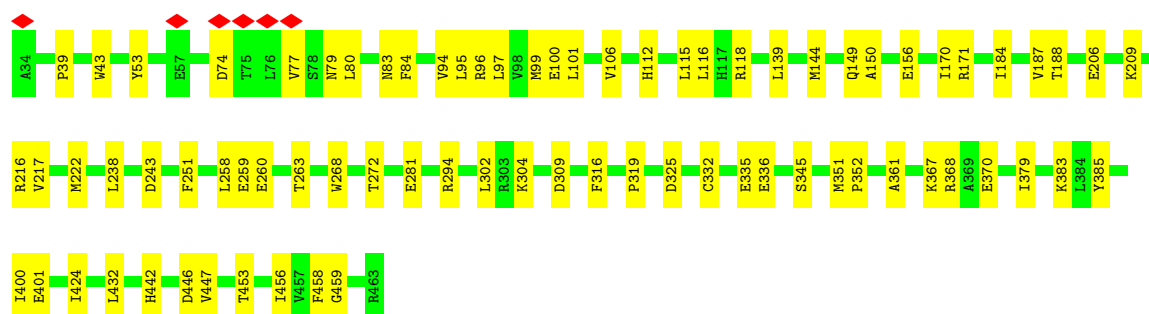
• Molecule 15: Complex I-30kD

Chain P: 91% 9%



• Molecule 16: Complex I-49kD

Chain Q: 82% 18%



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

Chain S: 87% 13%



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

Chain T: 5% 96% ..

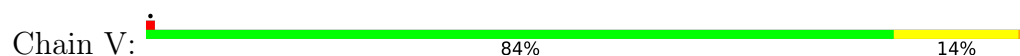


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

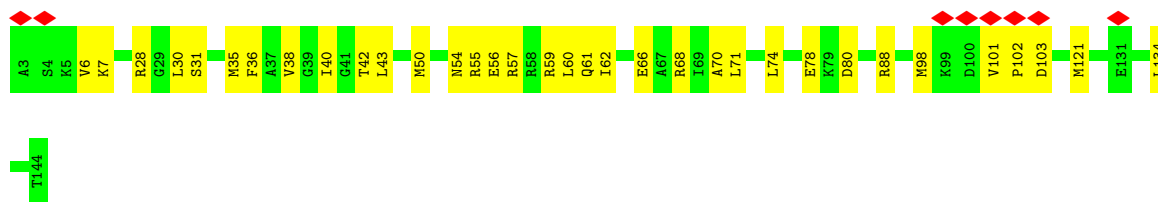
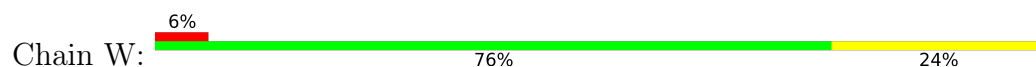
Chain U: 5% 88% 12%



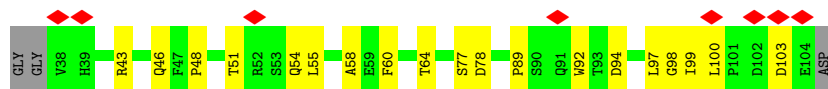
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



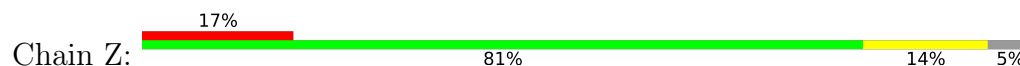
- Molecule 21: Complex I-B16.6



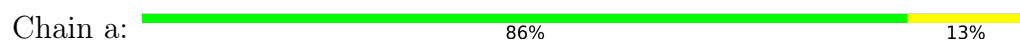
- Molecule 22: Complex I-AGGG



- Molecule 23: Complex I-B12

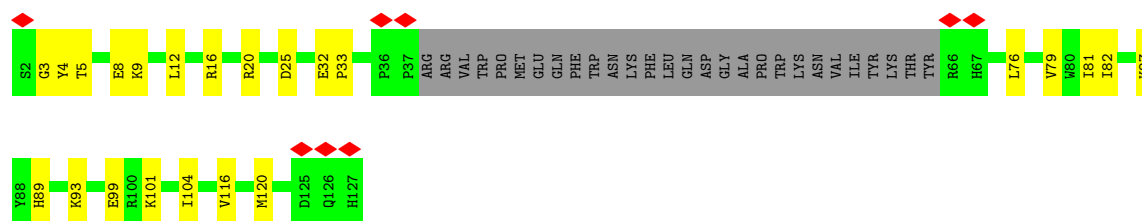


- Molecule 24: Complex I-SGDH

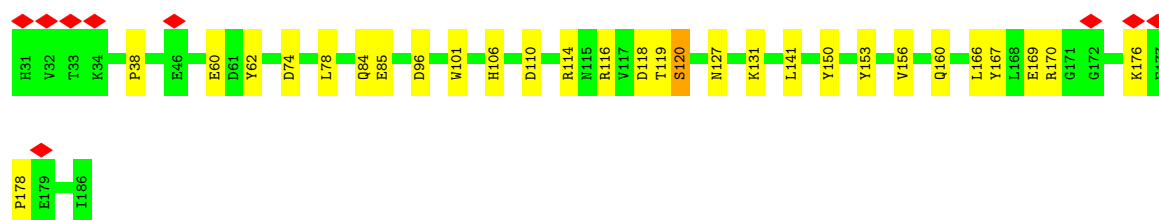
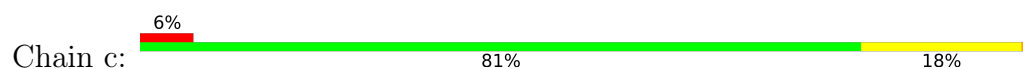


- Molecule 25: Complex I-B17

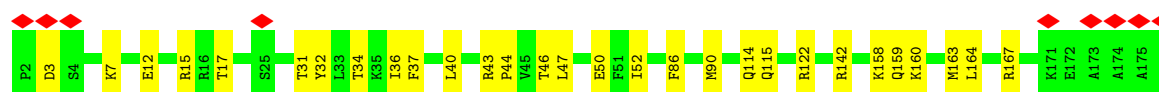
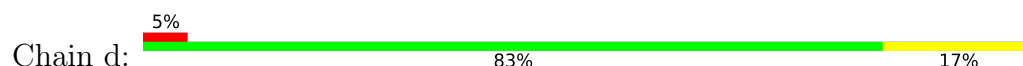




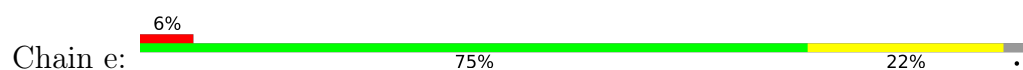
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



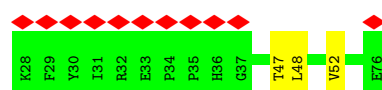
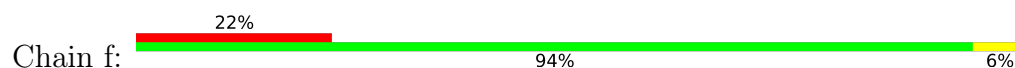
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



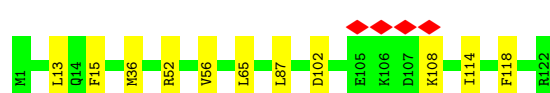
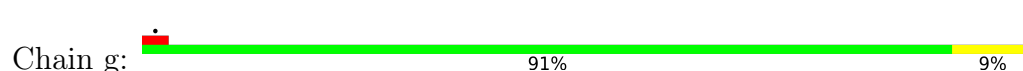
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



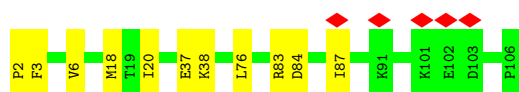
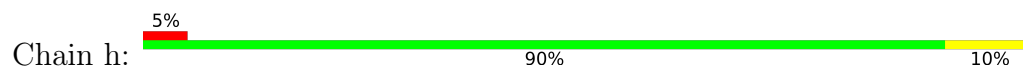
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



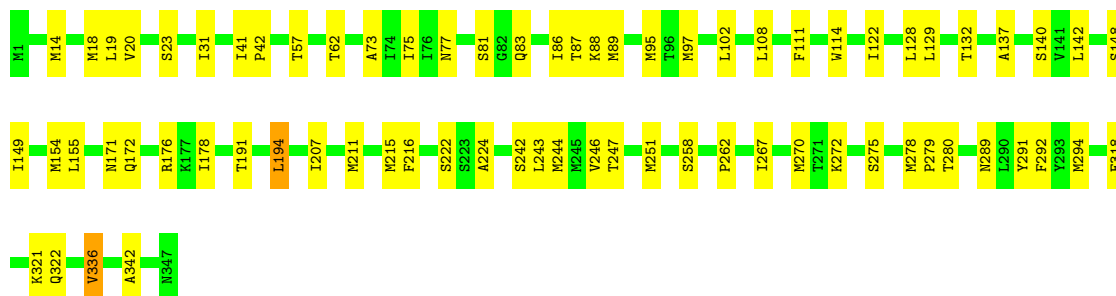
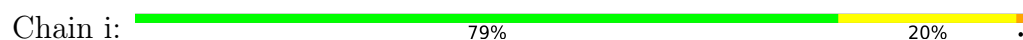
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



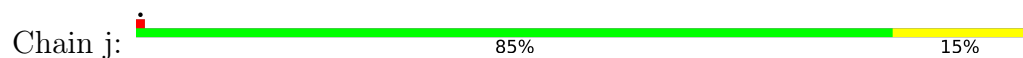
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



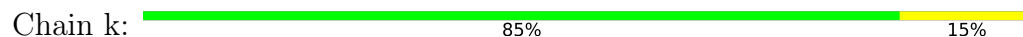
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



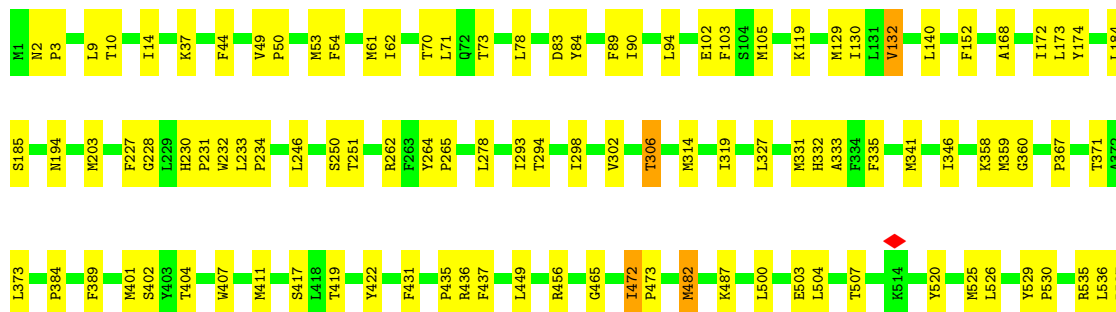
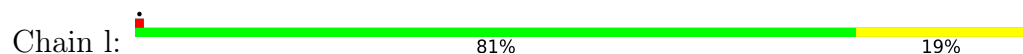
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

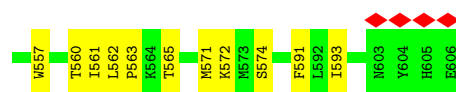


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

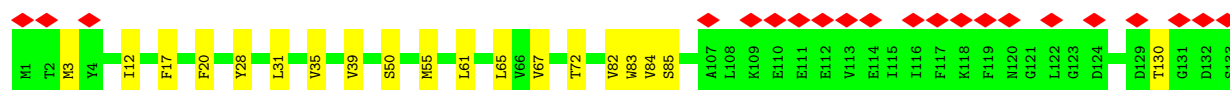
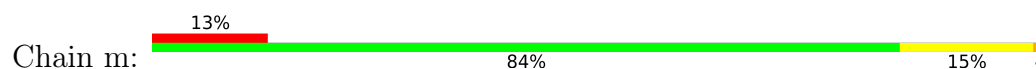


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

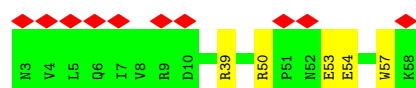




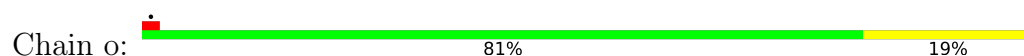
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



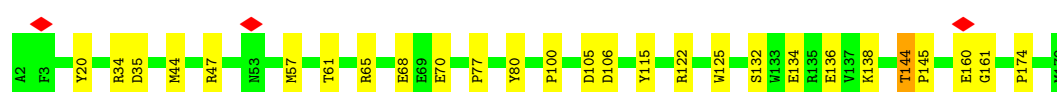
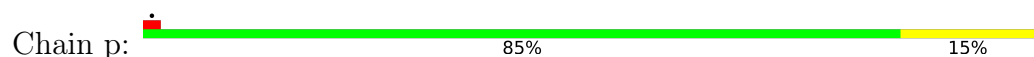
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



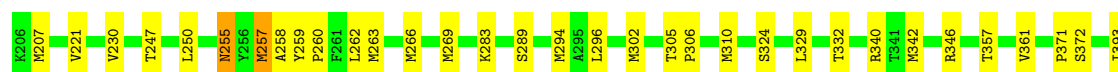
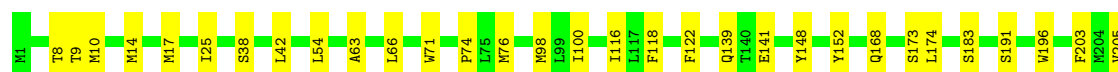
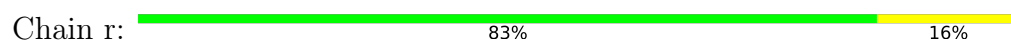
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



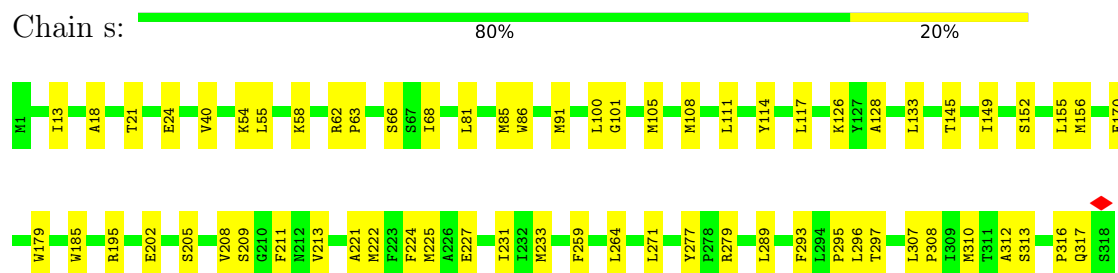
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



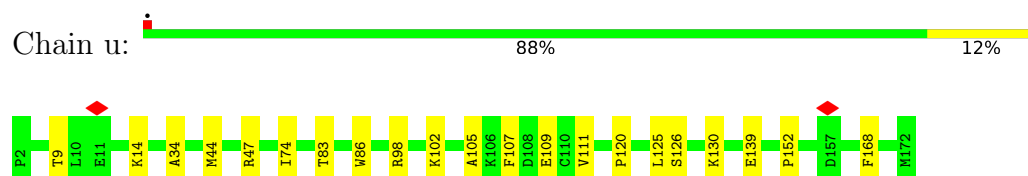
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



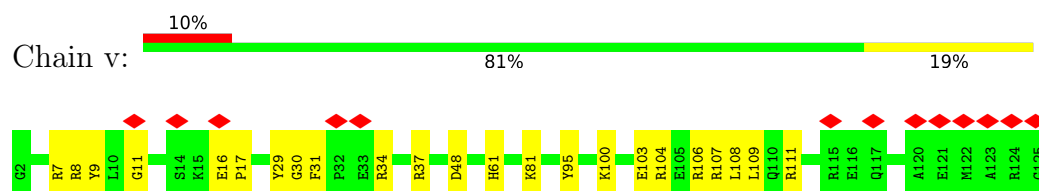
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



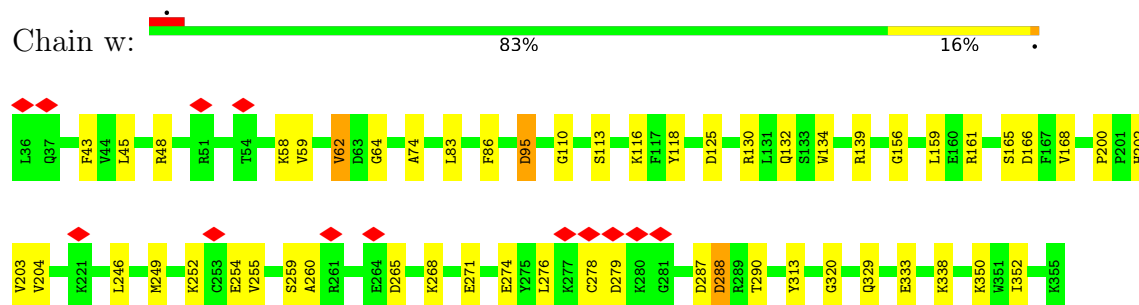
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 43: Complex I-B18



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91450	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	0.218	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0296	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, MG, 8Q1, ZN, ADP, NDP, UQ, FES, 2MR, SF4, PLX, UQ1, FMN, NAI, PEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/3404	0.32	0/4600
2	B	0.15	0/1443	0.32	0/1952
3	C	0.16	0/1279	0.30	0/1730
4	E	0.19	0/995	0.34	0/1340
5	F	0.13	0/698	0.34	0/940
6	G	0.14	0/705	0.43	0/956
6	X	0.14	0/715	0.36	0/967
7	H	0.15	0/929	0.37	0/1258
8	I	0.14	0/798	0.38	0/1079
9	J	0.14	0/2828	0.32	0/3834
10	K	0.12	0/377	0.32	0/509
11	L	0.14	0/1039	0.30	0/1403
12	M	0.15	0/5384	0.35	0/7295
13	N	0.17	0/1245	0.44	0/1694
14	O	0.13	0/1711	0.36	0/2328
15	P	0.16	0/1789	0.32	0/2436
16	Q	0.17	0/3535	0.34	0/4792
17	S	0.16	0/581	0.39	0/781
18	T	0.12	0/755	0.30	0/1018
19	U	0.12	0/664	0.30	0/912
20	V	0.20	0/1042	0.35	0/1411
21	W	0.16	0/1198	0.34	0/1617
22	Y	0.19	0/606	0.44	0/831
23	Z	0.12	0/660	0.30	0/892
24	a	0.15	0/1184	0.29	0/1603
25	b	0.15	0/844	0.36	0/1149
26	c	0.14	0/1371	0.33	0/1875
27	d	0.13	0/1494	0.27	0/2015
28	e	0.13	0/891	0.30	0/1210
29	f	0.13	0/386	0.28	0/523
30	g	0.14	0/1036	0.29	0/1401
31	h	0.15	0/889	0.33	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.17	0/2773	0.37	0/3768
33	j	0.15	0/938	0.32	0/1281
34	k	0.18	0/759	0.34	0/1029
35	l	0.18	0/4947	0.38	0/6728
36	m	0.17	0/1325	0.37	0/1800
37	n	0.12	0/491	0.27	0/663
38	o	0.14	0/1092	0.29	0/1481
39	p	0.17	0/1590	0.43	2/2155 (0.1%)
40	r	0.19	0/3723	0.39	2/5078 (0.0%)
41	s	0.18	0/2581	0.36	0/3529
42	u	0.15	0/1436	0.35	0/1938
43	v	0.15	0/1045	0.41	0/1403
44	w	0.13	0/2642	0.30	0/3580
All	All	0.16	0/67817	0.35	4/91974 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	r	257	MET	N-CA-C	7.37	119.40	111.36
39	p	144	THR	CA-C-N	7.10	127.69	120.38
39	p	144	THR	C-N-CA	7.10	127.69	120.38
40	r	258	ALA	N-CA-C	5.75	118.32	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3328	0	3287	52	0
2	B	1412	0	1363	17	0
3	C	1248	0	1254	22	0
4	E	971	0	975	16	0
5	F	687	0	700	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	693	0	671	19	0
6	X	703	0	693	14	0
7	H	910	0	950	10	0
8	I	780	0	808	10	0
9	J	2751	0	2773	27	0
10	K	366	0	338	10	0
11	L	1016	0	1016	13	0
12	M	5296	0	5326	71	0
13	N	1204	0	1162	21	0
14	O	1671	0	1673	29	0
15	P	1738	0	1693	13	0
16	Q	3456	0	3387	47	0
17	S	566	0	561	7	0
18	T	741	0	702	2	0
19	U	643	0	642	8	0
20	V	1021	0	1025	15	0
21	W	1167	0	1155	29	0
22	Y	580	0	525	21	0
23	Z	641	0	620	7	0
24	a	1151	0	1164	13	0
25	b	819	0	835	18	0
26	c	1315	0	1208	23	0
27	d	1461	0	1429	20	0
28	e	867	0	817	20	0
29	f	378	0	356	2	0
30	g	1005	0	999	12	0
31	h	867	0	871	8	0
32	i	2710	0	2874	49	0
33	j	914	0	951	15	0
34	k	748	0	799	12	0
35	l	4816	0	4955	78	0
36	m	1292	0	1261	25	0
37	n	479	0	486	4	0
38	o	1062	0	1072	18	0
39	p	1534	0	1470	24	0
40	r	3631	0	3839	50	0
41	s	2508	0	2607	46	0
42	u	1398	0	1374	17	0
43	v	1021	0	969	27	0
44	w	2582	0	2531	33	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	27	4	0
48	B	51	0	82	1	0
48	C	47	0	71	1	0
48	W	41	0	59	1	0
48	i	47	0	71	3	0
48	j	41	0	59	1	0
48	l	137	0	205	6	0
48	r	51	0	82	3	0
48	s	51	0	82	4	0
49	C	18	0	18	0	0
49	Q	18	0	18	3	0
50	C	52	0	88	3	0
50	J	52	0	88	4	0
50	a	52	0	88	0	0
50	e	52	0	88	6	0
50	g	52	0	88	5	0
50	j	52	0	88	3	0
51	G	35	0	0	2	0
51	X	35	0	0	0	0
52	I	51	0	46	0	0
52	V	94	0	138	5	0
52	a	100	0	156	3	0
52	g	100	0	156	11	0
52	k	94	0	141	5	0
52	l	199	0	307	43	0
52	o	100	0	156	4	0
52	s	89	0	125	5	0
52	u	55	0	54	0	0
53	J	48	0	24	2	0
54	J	33	0	39	3	0
54	s	38	0	47	4	0
55	M	4	0	0	0	0
55	O	4	0	0	0	0
56	M	1	0	0	0	0
57	T	1	0	0	0	0
58	w	27	0	11	2	0
All	All	68192	0	68887	917	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 (917) 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)
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.69	1.17
52:l:702:CDL:H312	52:l:702:CDL:H742	1.26	1.15
52:l:702:CDL:H611	52:l:702:CDL:H791	1.21	1.13
50:e:201:PLX:H222	52:l:702:CDL:OB7	1.48	1.12
52:l:702:CDL:HA62	52:l:702:CDL:H541	1.38	0.99
22:Y:98:GLY:O	43:v:30:GLY:HA3	1.63	0.97
52:l:702:CDL:H791	52:l:702:CDL:C61	2.02	0.90
41:s:24:GLU:HG3	41:s:271:LEU:HD22	1.57	0.86
52:l:702:CDL:H742	52:l:702:CDL:C31	2.05	0.85
33:j:90:MET:HE3	36:m:151:THR:HG23	1.57	0.84
52:l:702:CDL:H611	52:l:702:CDL:C79	2.06	0.84
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.61	0.83
43:v:7:ARG:O	43:v:11:GLY:HA3	1.79	0.82
4:E:68:MET:HA	4:E:68:MET:HE2	1.62	0.80
36:m:72:THR:HG21	41:s:133:LEU:HD21	1.62	0.79
52:l:702:CDL:H622	52:l:702:CDL:C66	2.14	0.78
13:N:144:TYR:HD1	13:N:144:TYR:H	1.31	0.76
5:F:25:GLN:HB3	5:F:26:ARG:HD2	1.68	0.76
52:l:702:CDL:H541	52:l:702:CDL:CA6	2.16	0.76
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.66	0.75
16:Q:99:MET:HE3	16:Q:101:LEU:HD21	1.69	0.74
35:l:3:PRO:HG2	35:l:53:MET:HE1	1.69	0.74
22:Y:97:LEU:HD23	43:v:107:ARG:HD2	1.69	0.74
50:e:201:PLX:H181	52:l:702:CDL:H801	1.68	0.74
52:l:702:CDL:H651	52:l:702:CDL:H852	1.70	0.74
52:l:702:CDL:HA62	52:l:702:CDL:C54	2.17	0.73
26:c:84:GLN:HG2	26:c:114:ARG:HB2	1.71	0.73
8:I:40:LYS:HB3	21:W:7:LYS:H	1.53	0.73
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.71	0.72
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.22	0.72
38:o:20:PRO:HB3	39:p:65:ARG:HH12	1.55	0.71
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.72	0.70
12:M:493:VAL:HG12	12:M:513:MET:HE1	1.72	0.70
21:W:121:MET:HG3	36:m:130:THR:HB	1.74	0.70
7:H:9:THR:O	7:H:76:GLN:NE2	2.24	0.69
31:h:18:MET:HE3	34:k:56:ALA:HA	1.74	0.69
4:E:68:MET:HE2	4:E:68:MET:CA	2.22	0.69
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.74	0.69
52:l:702:CDL:H861	52:l:702:CDL:H572	1.75	0.68
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:54:ARG:NH2	44:w:313:TYR:O	2.27	0.68
1:A:149:MET:HE3	1:A:241:THR:HB	1.75	0.68
48:j:201:PEE:O1P	41:s:62:ARG:NH2	2.27	0.68
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.77	0.67
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.77	0.67
16:Q:351:MET:HE3	16:Q:352:PRO:HD2	1.77	0.67
37:n:54:GLU:N	37:n:54:GLU:OE1	2.27	0.67
34:k:44:SER:HB2	34:k:59:MET:HE1	1.77	0.67
1:A:48:ARG:NH1	10:K:70:ASN:O	2.27	0.66
41:s:205:SER:OG	41:s:279:ARG:NH2	2.27	0.66
2:B:62:LEU:HD12	21:W:35:MET:HE3	1.77	0.66
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.61	0.66
9:J:192:ARG:NH1	9:J:198:ALA:O	2.29	0.66
42:u:105:ALA:O	42:u:109:GLU:HG2	1.96	0.66
3:C:126:GLU:OE1	33:j:33:LYS:NZ	2.28	0.66
43:v:16:GLU:HG3	43:v:17:PRO:HD2	1.76	0.66
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.78	0.65
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.35	0.65
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.77	0.65
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.29	0.65
7:H:55:LYS:HE3	15:P:104:THR:HG21	1.79	0.65
11:L:109:ASN:ND2	11:L:111:LEU:O	2.29	0.65
23:Z:33:GLN:HE22	23:Z:43:ASP:H	1.43	0.65
32:i:294:MET:HA	32:i:294:MET:HE2	1.79	0.65
41:s:62:ARG:HD3	41:s:68:ILE:HD13	1.78	0.65
44:w:125:ASP:O	44:w:130:ARG:NH2	2.30	0.65
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.28	0.65
13:N:4:VAL:O	13:N:8:ARG:HG2	1.97	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.29	0.64
41:s:63:PRO:HB2	41:s:66:SER:HB3	1.77	0.64
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.31	0.64
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.28	0.64
21:W:62:ILE:O	21:W:66:GLU:HG2	1.97	0.64
14:O:132:ILE:HG12	14:O:188:ILE:HG12	1.78	0.64
6:G:134:ASP:HA	6:G:137:LYS:HE2	1.77	0.64
26:c:38:PRO:HD3	38:o:67:ARG:HG2	1.79	0.64
35:l:525:MET:HE2	39:p:77:PRO:HB3	1.79	0.64
27:d:32:TYR:O	27:d:36:ILE:HG13	1.98	0.64
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.80	0.64
24:a:154:LEU:HD21	32:i:272:LYS:HG2	1.78	0.64
2:B:48:MET:HA	2:B:48:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:294:THR:HG22	52:l:703:CDL:HB62	1.78	0.63
21:W:55:ARG:HH21	41:s:312:ALA:HB3	1.63	0.63
44:w:62:VAL:HG11	44:w:74:ALA:HB2	1.79	0.63
12:M:256:ALA:O	12:M:598:ASN:ND2	2.32	0.63
4:E:23:ARG:HH22	11:L:51:GLN:HB2	1.61	0.63
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.32	0.63
35:l:227:PHE:O	35:l:230:HIS:ND1	2.32	0.63
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.79	0.63
36:m:82:VAL:HG22	36:m:85:SER:HB3	1.81	0.63
16:Q:83:ASN:HB2	33:j:38:GLU:HG2	1.80	0.63
26:c:60:GLU:OE1	26:c:60:GLU:N	2.24	0.63
32:i:14:MET:O	32:i:18:MET:HG2	1.99	0.62
1:A:285:PRO:O	14:O:222:ARG:NH2	2.33	0.62
19:U:16:GLU:HG3	48:s:401:PEE:H49	1.81	0.62
43:v:8:ARG:HB2	43:v:16:GLU:HG2	1.79	0.62
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.32	0.62
13:N:8:ARG:O	13:N:12:GLN:HG2	1.99	0.62
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.82	0.62
52:a:201:CDL:H191	52:a:201:CDL:H752	1.81	0.62
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.81	0.62
1:A:448:GLU:O	1:A:452:GLN:HG2	1.99	0.62
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.32	0.62
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.81	0.62
21:W:30:LEU:HD12	21:W:31:SER:H	1.65	0.62
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.31	0.61
22:Y:43:ARG:O	22:Y:46:GLN:NE2	2.33	0.61
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.82	0.61
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.80	0.61
1:A:288:VAL:HG22	1:A:289:GLU:N	2.15	0.61
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.81	0.61
2:B:128:ILE:O	15:P:231:ARG:NH2	2.34	0.61
14:O:198:PRO:O	14:O:202:GLU:HG2	2.00	0.61
17:S:66:LEU:HD21	42:u:74:ILE:HG22	1.83	0.61
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.83	0.61
9:J:107:GLU:O	9:J:118:LYS:NZ	2.34	0.61
44:w:139:ARG:NH1	44:w:166:ASP:OD2	2.34	0.60
50:e:201:PLX:H21	48:l:705:PEE:H2	1.82	0.60
22:Y:97:LEU:CD2	43:v:107:ARG:HD2	2.31	0.60
40:r:403:THR:HA	40:r:406:TYR:CE2	2.36	0.60
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.83	0.60
35:l:78:LEU:HD11	52:l:702:CDL:H261	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:501:ARG:NH2	12:M:666:GLN:OE1	2.35	0.60
16:Q:281:GLU:CD	16:Q:281:GLU:H	2.09	0.60
44:w:58:LYS:NZ	44:w:278:CYS:SG	2.75	0.60
52:g:202:CDL:H362	32:i:246:VAL:HG21	1.82	0.60
52:l:702:CDL:H601	52:l:702:CDL:H772	1.83	0.59
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.36	0.59
39:p:105:ASP:OD2	39:p:122:ARG:NH1	2.29	0.59
6:G:114:ASP:O	6:G:118:ILE:HG13	2.02	0.59
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.35	0.59
4:E:24:ASP:OD1	4:E:24:ASP:N	2.36	0.59
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.83	0.59
32:i:215:MET:HE1	32:i:244:MET:HG3	1.83	0.59
41:s:85:MET:SD	41:s:108:MET:HB2	2.43	0.59
21:W:61:GLN:NE2	41:s:317:GLN:OE1	2.35	0.59
9:J:283:VAL:HG22	9:J:369:VAL:HG21	1.83	0.59
26:c:166:LEU:HB3	26:c:169:GLU:HB2	1.85	0.59
43:v:7:ARG:O	43:v:11:GLY:CA	2.51	0.59
2:B:72:MET:HE3	16:Q:260:GLU:HG2	1.85	0.58
41:s:18:ALA:O	41:s:21:THR:OG1	2.20	0.58
6:G:142:GLN:NE2	6:G:146:ASP:OD1	2.36	0.58
21:W:80:ASP:OD2	42:u:47:ARG:NH1	2.36	0.58
28:e:129:ARG:NH1	28:e:136:LEU:O	2.36	0.58
26:c:85:GLU:OE2	26:c:119:THR:OG1	2.21	0.58
1:A:195:VAL:O	10:K:97:ARG:NH1	2.35	0.58
20:V:88:LEU:O	20:V:92:ILE:HD12	2.04	0.58
35:l:327:LEU:O	35:l:331:MET:HG2	2.03	0.58
14:O:38:LEU:O	14:O:124:ARG:NH2	2.37	0.58
52:s:402:CDL:HB61	52:s:402:CDL:H322	1.85	0.58
32:i:128:LEU:O	32:i:132:THR:OG1	2.21	0.58
44:w:43:PHE:O	44:w:48:ARG:NH1	2.36	0.58
24:a:166:GLY:O	24:a:170:GLN:NE2	2.37	0.57
40:r:269:MET:HE1	40:r:296:LEU:HD13	1.85	0.57
50:C:204:PLX:H102	50:C:204:PLX:H261	1.86	0.57
5:F:24:CYS:N	5:F:58:CYS:SG	2.77	0.57
27:d:46:THR:O	27:d:50:GLU:HG2	2.04	0.57
27:d:159:GLN:HG2	27:d:163:MET:HE2	1.85	0.57
21:W:134:LEU:HD21	36:m:3:MET:HG3	1.85	0.57
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.30	0.57
24:a:188:ASP:OD2	42:u:47:ARG:NH2	2.38	0.57
44:w:113:SER:HB3	44:w:116:LYS:HG2	1.86	0.57
52:V:201:CDL:H731	52:V:201:CDL:H601	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:g:202:CDL:H392	32:i:246:VAL:HG11	1.85	0.57
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.39	0.57
4:E:48:HIS:NE2	9:J:365:GLU:OE1	2.31	0.57
11:L:78:ARG:NH1	11:L:148:GLU:OE2	2.38	0.57
14:O:129:LYS:H	14:O:168:LEU:HA	1.70	0.56
27:d:160:LYS:NZ	30:g:114:ILE:O	2.37	0.56
28:e:57:GLU:HG2	44:w:320:GLY:HA3	1.85	0.56
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.87	0.56
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.85	0.56
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.28	0.56
1:A:283:ASN:ND2	1:A:305:GLY:O	2.39	0.56
2:B:65:GLU:N	2:B:65:GLU:OE1	2.35	0.56
50:J:403:PLX:H192	33:j:16:LEU:HD21	1.87	0.56
52:g:202:CDL:H221	52:g:202:CDL:H401	1.86	0.56
35:l:500:LEU:HD12	52:l:703:CDL:H562	1.87	0.56
1:A:248:VAL:O	1:A:251:SER:OG	2.23	0.56
1:A:278:ILE:HD12	1:A:278:ILE:N	2.20	0.56
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.88	0.56
1:A:325:PRO:O	1:A:347:THR:OG1	2.23	0.56
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.88	0.56
50:e:201:PLX:C22	52:l:702:CDL:OB7	2.38	0.56
30:g:52:ARG:NH2	44:w:338:LYS:O	2.38	0.56
32:i:207:ILE:HD13	32:i:262:PRO:HD3	1.88	0.56
52:l:702:CDL:H382	40:r:372:SER:HB3	1.88	0.56
12:M:282:ASN:O	12:M:283:GLU:HG2	2.05	0.56
52:g:202:CDL:H361	32:i:243:LEU:HD23	1.88	0.56
33:j:71:LEU:O	36:m:147:TYR:OH	2.21	0.56
12:M:472:PRO:O	12:M:510:TRP:NE1	2.32	0.56
16:Q:294:ARG:NH1	16:Q:336:GLU:OE2	2.39	0.56
50:e:201:PLX:H141	52:l:702:CDL:H802	1.87	0.56
30:g:52:ARG:NH1	32:i:318:GLU:OE1	2.38	0.56
12:M:509:ASP:N	12:M:509:ASP:OD1	2.37	0.56
16:Q:80:LEU:HD11	41:s:126:LYS:HE3	1.87	0.56
35:l:246:LEU:O	35:l:251:THR:OG1	2.23	0.56
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.88	0.55
16:Q:79:ASN:HB2	16:Q:100:GLU:HG2	1.87	0.55
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.22	0.55
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.87	0.55
3:C:52:ASP:HB3	50:C:204:PLX:H251	1.87	0.55
6:G:83:VAL:O	6:G:87:LEU:HD22	2.07	0.55
38:o:9:SER:OG	38:o:10:ARG:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:307:LEU:HA	41:s:310:MET:HE2	1.88	0.55
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.39	0.55
8:I:30:GLU:CD	8:I:30:GLU:H	2.15	0.55
40:r:266:MET:O	40:r:269:MET:HG2	2.05	0.55
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.89	0.55
20:V:36:VAL:HG22	52:V:201:CDL:H741	1.89	0.55
41:s:295:PRO:HB3	48:s:401:PEE:H26	1.87	0.55
3:C:71:CYS:HB2	45:C:202:SF4:S4	2.47	0.55
22:Y:97:LEU:O	43:v:104:ARG:HD2	2.07	0.55
5:F:91:LEU:O	5:F:95:LEU:HD12	2.06	0.55
9:J:370:LYS:HE2	9:J:370:LYS:HA	1.88	0.55
30:g:36:MET:HE1	50:g:201:PLX:H393	1.88	0.55
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.88	0.54
35:l:571:MET:HE3	35:l:572:LYS:HD3	1.89	0.54
35:l:367:PRO:O	35:l:371:THR:HG23	2.07	0.54
42:u:83:THR:HA	42:u:86:TRP:CD1	2.43	0.54
44:w:48:ARG:HD2	44:w:288:ASP:OD1	2.07	0.54
5:F:93:ASN:HD22	5:F:98:LYS:HD3	1.72	0.54
28:e:119:ARG:O	28:e:123:GLU:HG3	2.07	0.54
35:l:105:MET:HB3	35:l:449:LEU:HD13	1.88	0.54
1:A:338:ASP:OD1	1:A:338:ASP:N	2.39	0.54
21:W:103:ASP:OD1	21:W:103:ASP:N	2.39	0.54
26:c:116:ARG:HG2	48:l:704:PEE:H49	1.88	0.54
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.89	0.54
12:M:360:ARG:HG3	12:M:360:ARG:HH11	1.73	0.54
36:m:35:VAL:O	36:m:39:VAL:HG22	2.08	0.54
39:p:47:ARG:NH2	39:p:70:GLU:OE1	2.38	0.54
14:O:44:THR:HG22	14:O:46:GLU:H	1.73	0.54
24:a:78:THR:HG21	28:e:96:SER:HA	1.90	0.54
17:S:12:MET:HG2	41:s:264:LEU:HD21	1.90	0.54
22:Y:98:GLY:HA3	43:v:31:PHE:CE1	2.43	0.54
52:l:702:CDL:H391	40:r:371:PRO:HD2	1.90	0.54
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.33	0.54
6:G:103:HIS:ND1	6:G:106:LYS:HE3	2.23	0.54
35:l:130:ILE:HD13	52:l:702:CDL:H252	1.88	0.54
52:l:702:CDL:C66	52:l:702:CDL:H211	2.37	0.54
4:E:68:MET:CA	4:E:68:MET:CE	2.86	0.53
12:M:320:GLU:CD	12:M:320:GLU:H	2.16	0.53
31:h:20:ILE:HB	31:h:37:GLU:OE1	2.08	0.53
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.89	0.53
35:l:504:LEU:HD12	52:l:703:CDL:H511	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:598:ASN:HD22	12:M:599:THR:H	1.56	0.53
17:S:17:PHE:HB3	17:S:21:MET:HE3	1.91	0.53
52:g:202:CDL:H351	52:g:202:CDL:H201	1.90	0.53
32:i:31:ILE:HG21	36:m:156:VAL:HG11	1.89	0.53
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.89	0.53
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.91	0.53
36:m:141:MET:HE2	36:m:141:MET:HA	1.91	0.53
6:G:133:ILE:O	6:G:134:ASP:HB2	2.08	0.53
18:T:69:ASP:O	18:T:73:GLU:HG3	2.08	0.53
50:e:201:PLX:H282	40:r:446:LEU:HB3	1.90	0.53
44:w:200:PRO:HG3	44:w:252:LYS:HD3	1.90	0.53
44:w:271:GLU:HA	44:w:274:GLU:HG3	1.89	0.53
52:l:702:CDL:C66	52:l:702:CDL:C62	2.85	0.53
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.89	0.53
16:Q:170:ILE:HG13	16:Q:351:MET:HE1	1.91	0.53
41:s:81:LEU:HD11	41:s:111:LEU:HG	1.91	0.53
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.29	0.53
10:K:87:LEU:O	10:K:91:VAL:HG23	2.09	0.53
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.89	0.53
5:F:61:VAL:HG23	5:F:62:GLN:H	1.74	0.53
40:r:259:TYR:O	40:r:263:MET:HG2	2.08	0.53
1:A:89:GLY:O	47:A:503:NAI:H2N	2.08	0.53
4:E:23:ARG:HD2	11:L:53:ILE:HG22	1.90	0.53
6:G:111:ASP:OD1	6:G:111:ASP:N	2.42	0.53
8:I:70:MET:HE3	8:I:70:MET:O	2.08	0.53
9:J:106:MET:HE2	9:J:118:LYS:HD3	1.90	0.53
19:U:26:GLY:HA3	48:s:401:PEE:H38	1.90	0.53
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.90	0.53
35:l:419:THR:HA	35:l:422:TYR:CE2	2.43	0.53
38:o:91:ALA:O	38:o:95:ILE:HB	2.09	0.53
5:F:90:THR:O	5:F:94:VAL:HG23	2.08	0.53
52:l:703:CDL:H601	52:l:703:CDL:H361	1.90	0.53
3:C:77:MET:HE3	49:Q:501:UQ1:H113	1.91	0.52
7:H:48:THR:O	7:H:52:THR:OG1	2.23	0.52
41:s:222:MET:HA	41:s:225:MET:HE3	1.90	0.52
3:C:86:MET:HE1	3:C:93:PHE:CE2	2.44	0.52
5:F:27:SER:O	5:F:34:ARG:NH2	2.42	0.52
52:g:202:CDL:H412	52:g:202:CDL:H472	1.91	0.52
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.90	0.52
13:N:6:VAL:HG12	13:N:9:ARG:HH12	1.74	0.52
13:N:68:MET:SD	13:N:81:MET:HG2	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:94:VAL:HB	16:Q:115:LEU:HB2	1.91	0.52
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.90	0.52
13:N:65:THR:O	13:N:73:THR:OG1	2.28	0.52
21:W:38:VAL:O	21:W:42:THR:HG22	2.09	0.52
24:a:91:VAL:HG22	27:d:52:ILE:HD11	1.91	0.52
1:A:265:PHE:HB3	1:A:291:GLU:HG3	1.91	0.52
42:u:107:PHE:O	42:u:111:VAL:HG22	2.10	0.52
13:N:144:TYR:CD1	13:N:144:TYR:N	2.73	0.52
15:P:69:LEU:HD13	15:P:96:VAL:HG22	1.92	0.52
52:g:202:CDL:H232	52:g:202:CDL:H782	1.90	0.52
52:g:202:CDL:H562	40:r:17:MET:HE3	1.92	0.52
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.44	0.52
20:V:66:ILE:HD11	20:V:101:LEU:HB2	1.92	0.52
44:w:265:ASP:OD2	44:w:265:ASP:N	2.38	0.52
1:A:312:ASP:HA	1:A:329:LYS:NZ	2.25	0.52
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.75	0.52
21:W:50:MET:HB3	41:s:156:MET:HE2	1.91	0.51
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.92	0.51
5:F:21:ILE:HG12	5:F:65:LEU:HD12	1.91	0.51
10:K:83:THR:HG23	14:O:88:ARG:HE	1.75	0.51
8:I:14:TRP:O	21:W:28:ARG:NH1	2.43	0.51
9:J:304:LEU:HD11	50:J:403:PLX:H312	1.91	0.51
28:e:79:ASP:HB3	28:e:82:VAL:HB	1.92	0.51
41:s:209:SER:HB3	41:s:213:VAL:HA	1.92	0.51
44:w:95:ASP:OD1	44:w:95:ASP:N	2.41	0.51
15:P:201:ASP:OD1	15:P:201:ASP:N	2.37	0.51
24:a:56:ILE:HG22	24:a:58:LYS:HG2	1.91	0.51
36:m:61:LEU:O	41:s:114:TYR:OH	2.27	0.51
9:J:87:GLU:HG3	9:J:89:TYR:H	1.76	0.51
34:k:16:LEU:HA	34:k:36:MET:HE2	1.92	0.51
38:o:82:PRO:HB2	52:o:201:CDL:HB4	1.93	0.51
5:F:86:GLN:O	5:F:90:THR:HG22	2.11	0.51
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.51
30:g:15:PHE:HB2	50:g:201:PLX:H6	1.92	0.51
41:s:101:GLY:O	41:s:105:MET:HG2	2.11	0.51
43:v:103:GLU:O	43:v:107:ARG:HG2	2.10	0.51
13:N:8:ARG:HA	13:N:11:LEU:HD12	1.91	0.51
6:G:119:ILE:HG21	6:G:135:ALA:HB1	1.93	0.51
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.44	0.51
22:Y:99:ILE:O	22:Y:99:ILE:HG13	2.11	0.51
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:99:GLU:HG2	35:l:61:MET:HE2	1.93	0.51
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.39	0.51
39:p:160:GLU:HG2	39:p:161:GLY:N	2.26	0.51
3:C:98:ARG:NH2	33:j:35:SER:O	2.44	0.50
12:M:389:THR:HG21	12:M:473:MET:HE2	1.93	0.50
14:O:179:ALA:HB3	14:O:185:MET:HE3	1.92	0.50
20:V:70:PHE:O	20:V:74:SER:OG	2.27	0.50
10:K:87:LEU:HD22	14:O:66:ILE:HD11	1.93	0.50
26:c:96:ASP:N	26:c:96:ASP:OD1	2.44	0.50
39:p:132:SER:O	39:p:136:GLU:HG3	2.12	0.50
50:J:403:PLX:H121	33:j:20:ILE:HD13	1.93	0.50
14:O:137:THR:HG22	14:O:138:THR:H	1.75	0.50
22:Y:100:LEU:HB2	43:v:111:ARG:NH2	2.26	0.50
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.39	0.50
28:e:72:ASP:OD1	28:e:72:ASP:N	2.43	0.50
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.92	0.50
35:l:71:LEU:HD12	40:r:310:MET:HE1	1.94	0.50
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.29	0.50
12:M:390:THR:HA	12:M:600:GLU:HG2	1.93	0.50
6:X:140:CYS:SG	6:X:143:GLU:HG3	2.51	0.50
32:i:19:LEU:O	32:i:23:SER:OG	2.25	0.50
40:r:203:PHE:O	40:r:207:MET:HG2	2.11	0.50
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.92	0.50
22:Y:94:ASP:HB3	22:Y:99:ILE:HG12	1.93	0.50
12:M:295:ASP:OD1	12:M:704:SER:OG	2.21	0.50
12:M:389:THR:O	12:M:390:THR:OG1	2.26	0.50
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.92	0.50
1:A:210:THR:HB	1:A:224:ARG:HG2	1.94	0.49
9:J:313:TRP:CD1	54:J:402:UQ:H8	2.47	0.49
12:M:402:LEU:HD23	12:M:475:VAL:HB	1.94	0.49
18:T:47:ASP:OD1	18:T:47:ASP:N	2.44	0.49
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.94	0.49
44:w:204:VAL:HG21	44:w:249:MET:HG2	1.93	0.49
16:Q:367:LYS:HB2	16:Q:370:GLU:HG3	1.94	0.49
35:l:535:ARG:NH1	38:o:11:LEU:O	2.44	0.49
28:e:97:ILE:O	28:e:101:LEU:HB2	2.13	0.49
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.47	0.49
38:o:117:GLN:OE1	38:o:117:GLN:HA	2.13	0.49
48:r:501:PEE:H73	48:r:501:PEE:H29	1.93	0.49
22:Y:43:ARG:HA	23:Z:14:MET:HE1	1.94	0.49
25:b:89:HIS:O	25:b:93:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:OH	1:A:194:ASP:OD1	2.25	0.49
12:M:422:TRP:HA	12:M:427:LEU:HB3	1.93	0.49
6:X:128:PHE:HZ	6:X:148:ILE:HD12	1.77	0.49
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.93	0.49
3:C:195:ARG:HG3	3:C:195:ARG:HH11	1.76	0.49
14:O:218:PRO:HD2	14:O:223:PHE:HA	1.94	0.49
32:i:88:LYS:HG2	32:i:148:SER:HB3	1.93	0.49
1:A:102:MET:HE3	1:A:111:LYS:HE2	1.94	0.49
2:B:49:ASP:OD1	2:B:52:SER:OG	2.30	0.49
12:M:275:PRO:HG3	12:M:286:ILE:HG12	1.95	0.49
20:V:38:ALA:HA	52:k:101:CDL:H212	1.93	0.49
22:Y:58:ALA:HB1	35:l:371:THR:HG21	1.95	0.49
32:i:242:SER:O	32:i:246:VAL:HG23	2.11	0.49
1:A:152:ARG:NH2	10:K:99:PRO:O	2.46	0.49
32:i:95:MET:HE3	32:i:149:ILE:HD12	1.95	0.49
36:m:82:VAL:HG23	36:m:84:VAL:H	1.77	0.49
8:I:66:PRO:HB3	15:P:79:SER:HA	1.95	0.48
12:M:449:PRO:O	12:M:452:LEU:HB2	2.13	0.48
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.43	0.48
52:a:201:CDL:OB4	28:e:108:TYR:OH	2.24	0.48
25:b:120:MET:HE3	43:v:61:HIS:HB2	1.95	0.48
30:g:13:LEU:HA	50:g:201:PLX:H32	1.95	0.48
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.48	0.48
3:C:107:GLY:HA2	45:C:202:SF4:S1	2.53	0.48
36:m:173:ARG:HG3	36:m:173:ARG:HH11	1.79	0.48
40:r:141:GLU:CD	40:r:141:GLU:H	2.21	0.48
54:J:402:UQ:H111	54:J:402:UQ:H71	1.48	0.48
2:B:200:GLU:HG3	13:N:88:ARG:HD3	1.96	0.48
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.13	0.48
52:l:703:CDL:H751	52:l:703:CDL:H781	1.69	0.48
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.14	0.48
6:G:78:ALA:HA	6:G:81:ASP:OD1	2.14	0.48
12:M:619:ASP:N	12:M:619:ASP:OD2	2.47	0.48
13:N:21:ARG:HG3	13:N:21:ARG:HH11	1.78	0.48
32:i:122:ILE:O	32:i:176:ARG:NH1	2.44	0.48
9:J:124:ASN:OD1	9:J:125:VAL:HG23	2.14	0.48
12:M:456:ALA:O	12:M:499:ASN:ND2	2.46	0.48
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.96	0.48
41:s:152:SER:HA	41:s:155:LEU:HD12	1.95	0.48
6:G:99:SER:O	6:G:102:SER:OG	2.30	0.47
9:J:75:ARG:NH2	15:P:215:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:131:ARG:HB2	13:N:131:ARG:NH1	2.28	0.47
22:Y:89:PRO:HA	22:Y:92:TRP:CE3	2.49	0.47
32:i:270:MET:O	32:i:275:SER:HB3	2.13	0.47
14:O:58:GLU:OE1	14:O:58:GLU:N	2.39	0.47
43:v:103:GLU:HA	43:v:103:GLU:OE1	2.14	0.47
44:w:59:VAL:H	44:w:202:HIS:CD2	2.31	0.47
7:H:6:LYS:NZ	7:H:78:GLU:OE1	2.47	0.47
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.79	0.47
21:W:61:GLN:HE22	41:s:317:GLN:H	1.63	0.47
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.96	0.47
7:H:22:GLU:OE1	7:H:22:GLU:N	2.43	0.47
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.96	0.47
19:U:38:TYR:HB2	41:s:310:MET:O	2.15	0.47
19:U:66:VAL:O	42:u:130:LYS:HE3	2.14	0.47
6:X:115:GLN:NE2	6:X:138:LEU:O	2.47	0.47
50:g:201:PLX:H351	32:i:336:VAL:HG22	1.96	0.47
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.97	0.47
52:l:702:CDL:H601	52:l:702:CDL:H761	1.95	0.47
17:S:1:MET:O	17:S:4:GLU:HG3	2.15	0.47
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.50	0.47
32:i:172:GLN:HB2	32:i:178:ILE:HG13	1.96	0.47
40:r:255:ASN:N	40:r:255:ASN:OD1	2.47	0.47
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.97	0.47
3:C:79:MET:HE1	3:C:177:ILE:HG13	1.96	0.47
48:C:203:PEE:H32	48:C:203:PEE:H63	1.97	0.47
12:M:171:THR:HG23	12:M:173:MET:SD	2.54	0.47
20:V:141:VAL:O	24:a:161:ARG:NH1	2.39	0.47
24:a:186:THR:OG1	24:a:189:ASN:O	2.32	0.47
26:c:110:ASP:OD1	26:c:110:ASP:N	2.47	0.47
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.96	0.47
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.50	0.47
52:l:702:CDL:H472	40:r:445:LEU:HB2	1.96	0.47
41:s:91:MET:HG2	41:s:259:PHE:CE2	2.50	0.47
6:G:112:SER:O	6:G:116:VAL:HG23	2.15	0.47
12:M:347:ASP:OD2	12:M:347:ASP:N	2.47	0.47
35:l:557:TRP:O	35:l:561:ILE:HG12	2.15	0.47
52:l:703:CDL:H121	52:l:703:CDL:H321	1.97	0.47
9:J:94:LEU:HA	9:J:97:MET:HG3	1.96	0.47
35:l:571:MET:HE2	35:l:571:MET:HB3	1.77	0.47
44:w:165:SER:O	44:w:168:VAL:HG22	2.15	0.47
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:23:TYR:OH	39:p:68:GLU:HG3	2.15	0.47
39:p:138:LYS:HE3	39:p:138:LYS:HB3	1.73	0.47
4:E:14:GLY:C	4:E:16:SER:H	2.23	0.46
4:E:71:ALA:HB1	51:G:201:8Q1:C30	2.45	0.46
21:W:88:ARG:HH21	42:u:9:THR:HG22	1.80	0.46
25:b:16:ARG:HG2	25:b:20:ARG:NH1	2.30	0.46
26:c:160:GLN:OE1	43:v:37:ARG:NH2	2.48	0.46
40:r:14:MET:HE2	40:r:14:MET:HB3	1.86	0.46
1:A:278:ILE:HD12	1:A:278:ILE:H	1.80	0.46
44:w:139:ARG:HH12	58:w:401:ADP:HN61	1.62	0.46
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.55	0.46
9:J:132:ARG:NH1	53:J:401:NDP:O3X	2.47	0.46
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.44	0.46
12:M:666:GLN:HE21	12:M:666:GLN:HA	1.81	0.46
26:c:38:PRO:HG2	38:o:70:TYR:HD2	1.80	0.46
35:l:103:PHE:HB2	35:l:341:MET:HE3	1.97	0.46
35:l:359:MET:O	35:l:436:ARG:NH2	2.48	0.46
40:r:71:TRP:O	40:r:74:PRO:HD2	2.15	0.46
54:s:403:UQ:H221	54:s:403:UQ:H262	1.45	0.46
44:w:329:GLN:O	44:w:333:GLU:HG3	2.16	0.46
3:C:98:ARG:NH1	33:j:33:LYS:O	2.38	0.46
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.26	0.46
52:a:201:CDL:H321	48:l:705:PEE:H59	1.98	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.16	0.46
43:v:34:ARG:NH1	43:v:104:ARG:HH12	2.14	0.46
44:w:64:GLY:O	44:w:161:ARG:NH2	2.46	0.46
7:H:30:LYS:O	7:H:34:VAL:HG23	2.16	0.46
9:J:38:HIS:NE2	13:N:132:LYS:HE3	2.30	0.46
12:M:169:VAL:HG22	12:M:223:ILE:HD11	1.98	0.46
22:Y:103:ASP:OD1	22:Y:103:ASP:N	2.48	0.46
26:c:166:LEU:HB2	26:c:170:ARG:HH11	1.81	0.46
12:M:254:MET:HE1	12:M:700:ILE:HB	1.98	0.46
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.51	0.46
21:W:56:GLU:OE2	21:W:59:ARG:NH2	2.42	0.46
21:W:98:MET:HG3	21:W:101:VAL:HG11	1.96	0.46
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.16	0.46
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.97	0.46
4:E:19:PRO:HB3	11:L:53:ILE:HG21	1.97	0.46
12:M:323:LEU:HB3	12:M:629:ILE:HD12	1.97	0.46
16:Q:206:GLU:HA	16:Q:209:LYS:HE3	1.97	0.46
25:b:4:TYR:HB2	25:b:9:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.16	0.46
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.97	0.46
34:k:43:MET:HE3	34:k:47:ILE:HD11	1.97	0.46
6:X:138:LEU:HB3	6:X:144:ILE:HD12	1.98	0.46
22:Y:92:TRP:NE1	43:v:100:LYS:NZ	2.64	0.46
35:l:503:GLU:OE2	35:l:503:GLU:HA	2.15	0.46
52:l:702:CDL:HA62	52:l:702:CDL:H522	1.97	0.46
4:E:120:SER:O	4:E:124:VAL:HG22	2.17	0.46
12:M:200:ARG:HA	12:M:204:MET:HB2	1.98	0.46
22:Y:78:ASP:C	22:Y:78:ASP:OD1	2.59	0.46
52:g:202:CDL:H381	52:g:202:CDL:H352	1.75	0.46
40:r:42:LEU:HB3	40:r:453:MET:HE2	1.98	0.46
6:X:114:ASP:OD2	6:X:114:ASP:N	2.49	0.45
26:c:127:ASN:O	26:c:131:LYS:HE2	2.16	0.45
32:i:222:SER:O	32:i:224:ALA:N	2.49	0.45
52:l:703:CDL:H111	52:l:703:CDL:H142	1.66	0.45
40:r:116:ILE:HG21	42:u:168:PHE:HB3	1.98	0.45
40:r:294:MET:HE2	40:r:294:MET:HA	1.98	0.45
40:r:453:MET:HE3	40:r:453:MET:HA	1.97	0.45
44:w:246:LEU:HD22	44:w:255:VAL:HG11	1.98	0.45
1:A:76:ILE:HG23	1:A:255:CYS:SG	2.57	0.45
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.50	0.45
16:Q:96:ARG:HB3	16:Q:112:HIS:HB2	1.98	0.45
16:Q:294:ARG:NH2	16:Q:401:GLU:OE2	2.49	0.45
39:p:144:THR:HA	39:p:145:PRO:HD3	1.71	0.45
40:r:63:ALA:HA	40:r:66:LEU:HD12	1.97	0.45
1:A:159:ARG:HD3	1:A:161:GLU:HB2	1.98	0.45
1:A:288:VAL:CG2	1:A:289:GLU:N	2.79	0.45
5:F:84:ALA:O	5:F:88:THR:OG1	2.28	0.45
6:G:102:SER:H	6:G:102:SER:HG	1.56	0.45
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	1.99	0.45
35:l:184:LEU:HB2	40:r:393:ILE:HG12	1.99	0.45
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.98	0.45
19:U:41:TYR:O	19:U:45:ILE:HG13	2.16	0.45
27:d:15:ARG:O	27:d:15:ARG:HG2	2.16	0.45
39:p:35:ASP:OD2	39:p:35:ASP:N	2.49	0.45
39:p:134:GLU:H	39:p:134:GLU:CD	2.24	0.45
12:M:360:ARG:HG3	12:M:360:ARG:NH1	2.31	0.45
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.98	0.45
42:u:14:LYS:HE2	42:u:14:LYS:HB2	1.75	0.45
1:A:81:LYS:HB2	1:A:81:LYS:HE2	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:40:LYS:HE2	7:H:40:LYS:HB2	1.89	0.45
12:M:632:MET:H	12:M:632:MET:HG2	1.61	0.45
23:Z:60:ASN:OD1	23:Z:61:VAL:N	2.49	0.45
33:j:83:ASN:OD1	33:j:83:ASN:N	2.45	0.45
40:r:139:GLN:OE1	40:r:340:ARG:NH1	2.50	0.45
5:F:83:SER:O	5:F:87:VAL:HG13	2.16	0.45
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.99	0.45
20:V:25:SER:OG	20:V:67:GLY:O	2.30	0.45
48:W:201:PEE:H37	36:m:12:ILE:HD13	1.99	0.45
35:l:228:GLY:HA3	48:l:704:PEE:H38	1.97	0.45
52:l:702:CDL:H601	52:l:702:CDL:C77	2.47	0.45
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.81	0.45
35:l:407:TRP:CZ2	35:l:411:MET:HE3	2.52	0.45
52:l:702:CDL:H791	52:l:702:CDL:H582	1.98	0.45
52:l:702:CDL:H452	40:r:445:LEU:HB3	1.99	0.45
1:A:367:ILE:HG13	1:A:438:LEU:HD13	1.99	0.45
4:E:41:ARG:HH12	6:G:124:ASP:CG	2.23	0.45
10:K:87:LEU:HD13	14:O:85:LEU:HD13	1.98	0.45
52:l:702:CDL:H631	52:l:702:CDL:H811	1.99	0.45
13:N:3:LEU:O	13:N:6:VAL:HG22	2.17	0.45
28:e:137:MET:HE3	28:e:137:MET:HB2	1.76	0.45
52:l:703:CDL:H371	52:l:703:CDL:H401	1.78	0.45
44:w:259:SER:OG	44:w:260:ALA:N	2.50	0.45
1:A:217:GLU:CD	11:L:171:ARG:HH22	2.25	0.44
32:i:258:SER:HB2	32:i:336:VAL:HG12	1.99	0.44
32:i:321:LYS:HD2	32:i:322:GLN:N	2.32	0.44
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.51	0.44
52:l:702:CDL:H792	52:l:702:CDL:H762	1.91	0.44
16:Q:332:CYS:O	16:Q:336:GLU:HG3	2.17	0.44
31:h:84:ASP:HA	31:h:87:ILE:HG12	2.00	0.44
39:p:106:ASP:OD1	40:r:427:LYS:HD3	2.17	0.44
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.99	0.44
10:K:105:ARG:NH2	12:M:426:ASP:OD1	2.50	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.44
15:P:214:ASP:O	15:P:217:LYS:NZ	2.41	0.44
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.99	0.44
32:i:244:MET:HE2	32:i:244:MET:HB2	1.78	0.44
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.00	0.44
39:p:47:ARG:HH22	39:p:70:GLU:CD	2.25	0.44
41:s:170:GLU:CD	42:u:98:ARG:HH22	2.25	0.44
52:s:402:CDL:H771	52:s:402:CDL:H801	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:TYR:CZ	3:C:49:LYS:HE3	2.52	0.44
41:s:233:MET:HE3	41:s:233:MET:HB3	1.78	0.44
44:w:83:LEU:HD22	44:w:156:GLY:HA3	2.00	0.44
3:C:56:TRP:CE2	50:C:204:PLX:H112	2.52	0.44
12:M:443:ASP:OD1	12:M:443:ASP:N	2.50	0.44
23:Z:18:ASP:O	23:Z:21:GLN:HG2	2.18	0.44
27:d:86:PHE:O	27:d:90:MET:HG2	2.17	0.44
33:j:90:MET:HE1	50:j:202:PLX:H281	1.99	0.44
52:o:201:CDL:H622	52:o:201:CDL:H762	1.99	0.44
41:s:224:PHE:HZ	54:s:403:UQ:H72	1.82	0.44
42:u:139:GLU:CD	42:u:139:GLU:H	2.26	0.44
2:B:84:ILE:HA	13:N:58:ARG:HD3	1.98	0.44
9:J:262:THR:O	9:J:333:PRO:HD2	2.18	0.44
12:M:166:GLY:HA2	12:M:213:MET:HG2	2.00	0.44
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.99	0.44
21:W:36:PHE:O	21:W:40:ILE:HG12	2.18	0.44
21:W:66:GLU:OE2	42:u:126:SER:HB3	2.17	0.44
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.99	0.44
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.32	0.44
26:c:101:TRP:CZ3	38:o:46:GLU:HG2	2.53	0.44
32:i:247:THR:O	32:i:251:MET:HG3	2.18	0.44
10:K:100:GLN:NE2	14:O:68:LYS:O	2.50	0.44
12:M:370:GLU:OE2	12:M:478:SER:OG	2.30	0.44
27:d:163:MET:HE1	28:e:147:ILE:HG21	1.99	0.44
35:l:73:THR:HG22	35:l:194:ASN:HD21	1.83	0.44
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.53	0.44
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.52	0.44
38:o:95:ILE:HG23	38:o:99:PHE:CE2	2.53	0.44
40:r:148:TYR:O	40:r:152:TYR:HB2	2.17	0.44
40:r:262:LEU:HD21	40:r:302:MET:HB3	2.00	0.44
44:w:279:ASP:OD1	44:w:279:ASP:N	2.49	0.44
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.50	0.44
6:G:149:ALA:O	6:G:153:ASP:N	2.51	0.44
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.98	0.44
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.28	0.44
24:a:139:ILE:HG12	40:r:54:LEU:HD23	1.98	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	2.00	0.44
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.99	0.44
52:g:202:CDL:H742	52:g:202:CDL:H772	1.87	0.44
33:j:3:ILE:HA	33:j:6:THR:HG22	2.00	0.44
44:w:254:GLU:HG3	44:w:276:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ARG:HD3	2:B:141:ARG:HG3	1.99	0.43
3:C:79:MET:HE2	3:C:174:LEU:HD13	1.99	0.43
5:F:85:ASP:O	5:F:89:ARG:HG2	2.17	0.43
12:M:388:ASN:HB3	12:M:511:LYS:HD2	2.00	0.43
32:i:73:ALA:HB2	32:i:97:MET:HB3	1.99	0.43
13:N:101:LYS:HB2	13:N:101:LYS:HE2	1.59	0.43
17:S:1:MET:HE3	17:S:1:MET:HB3	1.80	0.43
50:j:202:PLX:H22	50:j:202:PLX:H1C3	1.80	0.43
35:l:373:LEU:HD22	35:l:431:PHE:CE1	2.53	0.43
1:A:382:CYS:HB3	1:A:424:ILE:HD12	2.00	0.43
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.86	0.43
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.70	0.43
50:J:403:PLX:H172	33:j:16:LEU:HD11	2.00	0.43
12:M:308:ARG:NH2	12:M:578:PRO:O	2.52	0.43
13:N:85:GLU:HG2	13:N:86:TRP:H	1.84	0.43
27:d:37:PHE:CE1	35:l:3:PRO:HB3	2.53	0.43
27:d:115:GLN:HG2	35:l:62:ILE:HG12	2.00	0.43
28:e:128:TYR:CD1	28:e:128:TYR:C	2.96	0.43
31:h:2:PRO:HB2	31:h:3:PHE:H	1.68	0.43
35:l:230:HIS:N	35:l:231:PRO:HD3	2.32	0.43
35:l:346:ILE:HD11	35:l:431:PHE:CZ	2.53	0.43
35:l:407:TRP:CE2	35:l:411:MET:HE3	2.53	0.43
52:s:402:CDL:H162	52:s:402:CDL:H191	1.78	0.43
44:w:45:LEU:O	44:w:45:LEU:HD12	2.18	0.43
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.54	0.43
33:j:73:LEU:HD12	36:m:55:MET:SD	2.57	0.43
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.54	0.43
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.54	0.43
8:I:43:VAL:HG23	8:I:44:GLY:H	1.84	0.43
11:L:132:GLU:OE2	11:L:132:GLU:N	2.47	0.43
12:M:222:ILE:HD12	12:M:231:LEU:HD13	2.00	0.43
12:M:557:ARG:HA	12:M:560:LEU:HD12	2.01	0.43
12:M:666:GLN:HA	12:M:666:GLN:NE2	2.33	0.43
15:P:187:ILE:HG23	15:P:188:LEU:HG	2.01	0.43
23:Z:23:LYS:HB3	23:Z:25:GLU:HG2	2.00	0.43
24:a:184:LYS:C	24:a:186:THR:H	2.27	0.43
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.99	0.43
28:e:92:PHE:O	28:e:96:SER:HB2	2.19	0.43
32:i:77:ASN:HB2	32:i:89:MET:HE3	2.00	0.43
32:i:267:ILE:HG12	32:i:279:PRO:HB3	2.00	0.43
52:l:702:CDL:H601	52:l:702:CDL:C76	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:28:TYR:CE2	36:m:82:VAL:HG12	2.53	0.43
1:A:201:ALA:O	14:O:119:TYR:HB3	2.19	0.43
14:O:222:ARG:NE	14:O:226:GLU:O	2.39	0.43
15:P:161:LYS:HA	15:P:161:LYS:HD2	1.67	0.43
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.34	0.43
19:U:46:ASN:ND2	33:j:81:THR:O	2.52	0.43
25:b:81:ILE:HG23	48:l:705:PEE:H58	2.01	0.43
27:d:163:MET:HE1	28:e:147:ILE:HD13	2.00	0.43
36:m:65:LEU:HD23	41:s:117:LEU:HD11	2.00	0.43
40:r:168:GLN:HG3	40:r:174:LEU:HG	2.01	0.43
43:v:109:LEU:HD12	43:v:109:LEU:HA	1.89	0.43
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.99	0.43
11:L:99:MET:HE3	11:L:128:PHE:CE1	2.54	0.43
26:c:167:TYR:CE2	26:c:178:PRO:HG3	2.54	0.43
28:e:62:GLU:H	28:e:62:GLU:CD	2.26	0.43
34:k:23:ARG:HG2	52:k:101:CDL:HB62	2.00	0.43
35:l:10:THR:O	35:l:14:ILE:HG23	2.18	0.43
35:l:90:ILE:HG12	35:l:129:MET:SD	2.58	0.43
40:r:342:MET:HE3	40:r:413:THR:HG21	2.00	0.43
40:r:357:THR:O	40:r:361:VAL:HG23	2.18	0.43
41:s:62:ARG:HB2	41:s:62:ARG:CZ	2.49	0.43
44:w:110:GLY:HA2	44:w:134:TRP:CE2	2.54	0.43
35:l:278:LEU:HD13	35:l:319:ILE:HG23	2.01	0.43
2:B:131:GLU:HB2	2:B:144:ARG:HB3	2.01	0.43
8:I:102:LYS:HD3	8:I:102:LYS:HA	1.90	0.43
54:J:402:UQ:H201	54:J:402:UQ:H221	1.70	0.43
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.87	0.43
35:l:78:LEU:CD1	52:l:702:CDL:H261	2.49	0.43
36:m:31:LEU:HD21	52:s:402:CDL:H542	2.01	0.43
38:o:50:GLN:O	38:o:56:ARG:HD3	2.19	0.43
39:p:34:ARG:HA	39:p:34:ARG:HD2	1.83	0.43
40:r:191:SER:HB3	48:r:501:PEE:H3	2.01	0.43
43:v:108:LEU:HD23	43:v:108:LEU:HA	1.89	0.43
4:E:66:MET:HB3	51:G:201:8Q1:C9	2.49	0.43
9:J:243:VAL:HG12	9:J:247:LYS:HE2	2.01	0.43
21:W:54:ASN:ND2	41:s:313:SER:O	2.52	0.43
21:W:57:ARG:HA	21:W:60:LEU:HD12	2.01	0.43
6:X:117:GLU:OE1	39:p:20:TYR:OH	2.31	0.43
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.54	0.43
35:l:89:PHE:CD2	35:l:132:VAL:HG21	2.54	0.43
35:l:472:ILE:HG13	35:l:473:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:520:TYR:CE1	52:l:703:CDL:HB22	2.53	0.43
40:r:329:LEU:O	40:r:332:THR:OG1	2.32	0.43
1:A:145:GLY:O	1:A:149:MET:HB2	2.19	0.42
6:G:103:HIS:NE2	6:G:139:MET:HB3	2.34	0.42
16:Q:144:MET:HE3	16:Q:222:MET:HB2	2.00	0.42
38:o:19:ASP:OD2	38:o:20:PRO:HD2	2.19	0.42
43:v:7:ARG:CZ	43:v:106:ARG:HH12	2.32	0.42
1:A:127:ASP:O	1:A:131:ILE:HG13	2.20	0.42
5:F:35:ASP:O	5:F:39:LYS:HG2	2.19	0.42
14:O:166:ASP:OD2	14:O:166:ASP:C	2.62	0.42
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.54	0.42
35:l:302:VAL:O	35:l:306:THR:HG22	2.19	0.42
35:l:560:THR:O	35:l:565:THR:OG1	2.36	0.42
40:r:10:MET:HE2	40:r:10:MET:HA	2.00	0.42
41:s:149:ILE:HG21	41:s:185:TRP:HB2	2.01	0.42
1:A:46:TYR:CE1	14:O:226:GLU:HA	2.54	0.42
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.49	0.42
9:J:344:PRO:HG2	9:J:347:LEU:HG	2.01	0.42
9:J:375:VAL:HG23	9:J:375:VAL:O	2.19	0.42
15:P:132:LEU:HB2	15:P:141:ILE:HG22	2.01	0.42
25:b:32:GLU:OE1	39:p:115:TYR:HA	2.19	0.42
27:d:31:THR:O	27:d:34:THR:HG22	2.19	0.42
30:g:108:LYS:HA	30:g:108:LYS:HD2	1.73	0.42
32:i:81:SER:O	32:i:83:GLN:N	2.49	0.42
35:l:401:MET:HG3	35:l:482:MET:SD	2.58	0.42
38:o:25:ILE:HD12	38:o:30:ARG:NH2	2.34	0.42
38:o:53:ASP:HB3	38:o:56:ARG:HB2	2.02	0.42
38:o:75:ASN:O	38:o:79:ASN:ND2	2.49	0.42
40:r:76:MET:SD	40:r:230:VAL:HB	2.60	0.42
1:A:151:ALA:O	1:A:191:TYR:OH	2.29	0.42
4:E:16:SER:HA	11:L:52:LEU:HD13	2.00	0.42
16:Q:74:ASP:OD1	16:Q:74:ASP:N	2.39	0.42
6:X:137:LYS:HA	25:b:3:GLY:HA2	2.00	0.42
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.19	0.42
54:s:403:UQ:H152	54:s:403:UQ:H121	1.78	0.42
3:C:188:LYS:HB2	3:C:188:LYS:HE2	1.70	0.42
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.71	0.42
16:Q:116:LEU:HD23	16:Q:459:GLY:HA2	2.02	0.42
20:V:126:LYS:HA	20:V:126:LYS:HD3	1.87	0.42
6:X:128:PHE:CZ	6:X:148:ILE:HD12	2.54	0.42
22:Y:55:LEU:HD13	35:l:367:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:18:MET:HE1	34:k:59:MET:HB2	2.01	0.42
38:o:18:LEU:HD23	38:o:18:LEU:HA	1.87	0.42
12:M:70:SER:O	12:M:184:ARG:NH1	2.50	0.42
16:Q:77:VAL:O	16:Q:77:VAL:HG23	2.20	0.42
16:Q:432:LEU:HD13	16:Q:456:ILE:HD13	2.00	0.42
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.01	0.42
26:c:118:ASP:CG	26:c:120:SER:HG	2.26	0.42
32:i:154:MET:HE2	32:i:154:MET:HB2	1.92	0.42
38:o:31:LYS:HB3	38:o:31:LYS:HE3	1.64	0.42
7:H:94:MET:HE3	7:H:94:MET:HB3	1.84	0.42
12:M:47:THR:O	12:M:96:VAL:HG22	2.20	0.42
12:M:219:SER:O	12:M:222:ILE:HG12	2.19	0.42
22:Y:89:PRO:HB3	22:Y:92:TRP:CZ3	2.55	0.42
26:c:78:LEU:HB2	26:c:106:HIS:CD2	2.55	0.42
50:j:202:PLX:H132	50:j:202:PLX:H161	1.40	0.42
40:r:98:MET:HE2	40:r:98:MET:HA	2.02	0.42
6:G:84:LEU:HD13	6:G:84:LEU:HA	1.93	0.42
14:O:185:MET:HE2	14:O:185:MET:HB2	1.93	0.42
16:Q:259:GLU:HG3	16:Q:263:THR:OG1	2.19	0.42
22:Y:60:PHE:O	22:Y:64:THR:HG22	2.19	0.42
52:l:703:CDL:H602	52:l:703:CDL:H571	1.81	0.42
1:A:71:LYS:HZ1	14:O:249:LEU:HA	1.84	0.42
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.93	0.42
20:V:106:ARG:HA	20:V:106:ARG:HD2	1.61	0.42
25:b:76:LEU:O	25:b:79:VAL:HG12	2.20	0.42
31:h:2:PRO:HA	32:i:140:SER:HB2	2.02	0.42
35:l:44:PHE:HB2	35:l:94:LEU:HB3	2.01	0.42
39:p:44:MET:HE2	39:p:44:MET:HB2	1.94	0.42
40:r:118:PHE:O	40:r:122:PHE:HB3	2.19	0.42
43:v:29:TYR:OH	43:v:111:ARG:NH1	2.32	0.42
44:w:268:LYS:O	44:w:271:GLU:HG2	2.20	0.42
14:O:134:VAL:HG22	14:O:186:VAL:HG22	2.01	0.42
20:V:107:SER:HB3	20:V:110:ILE:HB	2.01	0.42
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.54	0.42
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.55	0.42
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.54	0.42
35:l:562:LEU:HD21	48:r:501:PEE:H45	2.02	0.42
35:l:572:LYS:HD2	35:l:572:LYS:HA	1.88	0.42
52:l:702:CDL:H772	52:l:702:CDL:C60	2.47	0.42
39:p:144:THR:CG2	39:p:145:PRO:HD2	2.50	0.42
12:M:306:MET:HE1	13:N:139:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:184:ILE:O	16:Q:188:THR:OG1	2.26	0.41
21:W:101:VAL:HG23	21:W:102:PRO:HD2	2.02	0.41
23:Z:30:GLU:O	23:Z:34:GLU:HG3	2.20	0.41
27:d:142:ARG:NE	28:e:138:GLU:O	2.51	0.41
29:f:48:LEU:O	29:f:52:VAL:HG22	2.20	0.41
35:l:2:ASN:ND2	35:l:61:MET:HE1	2.35	0.41
40:r:8:THR:HG22	40:r:100:ILE:HG23	2.02	0.41
41:s:264:LEU:HD23	41:s:264:LEU:HA	1.91	0.41
42:u:102:LYS:HD3	42:u:102:LYS:N	2.35	0.41
1:A:52:ARG:NH1	10:K:77:GLN:OE1	2.53	0.41
2:B:111:GLU:O	2:B:141:ARG:NH1	2.53	0.41
12:M:49:VAL:HB	12:M:91:ALA:HA	2.02	0.41
12:M:197:THR:HA	12:M:205:GLN:O	2.20	0.41
20:V:104:ARG:HA	20:V:104:ARG:HD2	1.72	0.41
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.90	0.41
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.55	0.41
36:m:163:ILE:HD13	36:m:163:ILE:HA	1.85	0.41
40:r:346:ARG:O	40:r:419:TYR:HA	2.20	0.41
12:M:178:GLN:HG2	12:M:204:MET:HE2	2.02	0.41
12:M:296:GLY:O	12:M:572:HIS:NE2	2.46	0.41
12:M:387:LEU:HD12	12:M:514:ASN:HB3	2.03	0.41
26:c:176:LYS:HA	26:c:176:LYS:HD3	1.88	0.41
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.56	0.41
52:o:201:CDL:H872	52:o:201:CDL:H841	1.78	0.41
5:F:61:VAL:HG23	5:F:62:GLN:N	2.35	0.41
11:L:107:TRP:HH2	11:L:118:ALA:HB2	1.84	0.41
25:b:101:LYS:HB2	25:b:101:LYS:HE2	1.79	0.41
27:d:158:LYS:HG3	30:g:118:PHE:CE2	2.55	0.41
52:k:101:CDL:H191	52:k:101:CDL:H161	1.86	0.41
49:Q:501:UQ1:H72	49:Q:501:UQ1:HM51	1.87	0.41
21:W:71:LEU:HD23	21:W:71:LEU:HA	1.91	0.41
27:d:122:ARG:HD3	27:d:122:ARG:HA	1.76	0.41
35:l:37:LYS:HE3	35:l:37:LYS:HB3	1.80	0.41
40:r:221:VAL:HG22	40:r:283:LYS:HB3	2.02	0.41
3:C:73:ALA:HB1	49:Q:501:UQ1:H112	2.03	0.41
9:J:38:HIS:CD2	13:N:132:LYS:HE3	2.56	0.41
26:c:150:TYR:HD2	43:v:9:TYR:CD1	2.39	0.41
35:l:487:LYS:HD2	35:l:487:LYS:HA	1.86	0.41
41:s:145:THR:HG21	41:s:293:PHE:HB3	2.02	0.41
41:s:307:LEU:HB3	41:s:308:PRO:HD3	2.01	0.41
43:v:104:ARG:HE	43:v:108:LEU:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:HB3	1:A:165:GLU:HB2	2.02	0.41
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.03	0.41
9:J:206:ILE:HG21	9:J:242:ILE:HD12	2.02	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.41
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.83	0.41
19:U:53:TYR:CZ	42:u:44:MET:HG3	2.55	0.41
20:V:40:SER:HA	52:V:201:CDL:HB61	2.02	0.41
6:X:83:VAL:HG21	6:X:145:VAL:HG12	2.03	0.41
6:X:155:TYR:HA	25:b:20:ARG:HG2	2.02	0.41
27:d:3:ASP:OD1	27:d:7:LYS:NZ	2.53	0.41
52:g:202:CDL:H872	52:g:202:CDL:H841	1.90	0.41
31:h:38:LYS:HD3	31:h:38:LYS:C	2.46	0.41
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.33	0.41
36:m:28:TYR:HB3	36:m:83:TRP:CH2	2.56	0.41
40:r:289:SER:HB2	40:r:406:TYR:OH	2.21	0.41
41:s:128:ALA:HA	41:s:211:PHE:HA	2.02	0.41
41:s:293:PHE:O	41:s:297:THR:OG1	2.37	0.41
1:A:281:HIS:CE1	14:O:142:LEU:HD22	2.56	0.41
12:M:667:GLN:OE1	12:M:667:GLN:N	2.50	0.41
12:M:680:LEU:HD23	12:M:680:LEU:HA	1.95	0.41
14:O:158:ILE:HB	14:O:162:GLU:HB2	2.02	0.41
21:W:57:ARG:HB3	41:s:316:PRO:HG3	2.02	0.41
26:c:118:ASP:OD1	26:c:120:SER:OG	2.34	0.41
32:i:75:ILE:HD12	34:k:40:LEU:HD22	2.02	0.41
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.03	0.41
52:k:101:CDL:H192	35:l:593:ILE:HD11	2.03	0.41
35:l:293:ILE:HG13	35:l:294:THR:HG23	2.02	0.41
52:o:201:CDL:H761	52:o:201:CDL:H792	1.82	0.41
44:w:287:ASP:OD1	44:w:290:THR:HG23	2.21	0.41
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.55	0.41
3:C:195:ARG:HG3	3:C:195:ARG:NH1	2.36	0.41
9:J:271:TYR:OH	9:J:346:GLU:OE2	2.21	0.41
12:M:89:VAL:HB	12:M:94:MET:HE3	2.02	0.41
12:M:311:LYS:N	12:M:311:LYS:HD3	2.36	0.41
20:V:46:PRO:HB2	20:V:51:GLU:HG2	2.03	0.41
6:X:141:PRO:O	6:X:145:VAL:HG13	2.21	0.41
27:d:164:LEU:HD21	28:e:150:PRO:HD2	2.03	0.41
48:i:401:PEE:H27	48:i:401:PEE:H33	1.85	0.41
52:k:101:CDL:H362	52:k:101:CDL:H392	1.66	0.41
35:l:83:ASP:OD1	35:l:262:ARG:NH1	2.53	0.41
35:l:172:ILE:HG21	40:r:408:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:250:SER:HB2	35:l:333:ALA:HA	2.02	0.41
35:l:435:PRO:HB3	35:l:437:PHE:CZ	2.55	0.41
39:p:57:MET:O	39:p:61:THR:HG23	2.20	0.41
40:r:257:MET:O	40:r:260:PRO:HD2	2.21	0.41
41:s:105:MET:HE3	41:s:105:MET:HB3	1.97	0.41
1:A:388:GLY:O	1:A:392:MET:HG3	2.21	0.41
3:C:62:LEU:O	3:C:91:VAL:HA	2.20	0.41
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	2.03	0.41
32:i:87:THR:HG23	32:i:88:LYS:N	2.35	0.41
32:i:155:LEU:HD22	32:i:278:MET:HE2	2.02	0.41
35:l:526:LEU:HD12	35:l:530:PRO:HG2	2.01	0.41
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.03	0.40
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.84	0.40
22:Y:97:LEU:O	43:v:104:ARG:CD	2.70	0.40
31:h:83:ARG:HE	31:h:83:ARG:HB3	1.62	0.40
32:i:278:MET:HE3	32:i:278:MET:HB3	1.89	0.40
40:r:324:SER:OG	40:r:440:HIS:NE2	2.47	0.40
8:I:49:LEU:HD23	8:I:49:LEU:HA	1.93	0.40
16:Q:187:VAL:HG11	16:Q:258:LEU:HD21	2.03	0.40
16:Q:319:PRO:HG3	16:Q:335:GLU:HB3	2.03	0.40
20:V:67:GLY:HA2	52:V:201:CDL:H221	2.03	0.40
52:V:201:CDL:H472	52:V:201:CDL:H442	1.88	0.40
21:W:74:LEU:O	21:W:78:GLU:HG2	2.21	0.40
34:k:4:VAL:O	34:k:8:ILE:HG12	2.21	0.40
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.56	0.40
39:p:100:PRO:HD3	40:r:419:TYR:CE2	2.56	0.40
41:s:54:LYS:HE3	41:s:54:LYS:HB3	1.97	0.40
44:w:350:LYS:HA	44:w:350:LYS:HD3	1.87	0.40
3:C:119:LYS:HE2	3:C:119:LYS:HB2	1.70	0.40
6:G:126:PHE:CE2	6:G:148:ILE:HG21	2.57	0.40
12:M:382:ARG:HE	12:M:527:ASP:CG	2.30	0.40
16:Q:325:ASP:OD1	16:Q:325:ASP:N	2.54	0.40
19:U:30:ILE:HD12	48:s:401:PEE:H43	2.03	0.40
25:b:32:GLU:HB3	39:p:115:TYR:HD1	1.87	0.40
26:c:141:LEU:HD23	26:c:141:LEU:HA	1.94	0.40
32:i:57:THR:HA	34:k:77:LEU:HD13	2.02	0.40
35:l:331:MET:SD	35:l:465:GLY:HA2	2.61	0.40
52:s:402:CDL:H381	52:s:402:CDL:H742	2.03	0.40
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.54	0.40
7:H:50:GLN:O	7:H:54:GLU:HG3	2.21	0.40
14:O:135:CYS:SG	14:O:176:CYS:HA	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:53:TYR:HE1	48:i:401:PEE:H2	1.86	0.40
25:b:89:HIS:CE1	48:l:705:PEE:H48	2.56	0.40
32:i:171:ASN:HB2	35:l:574:SER:OG	2.21	0.40
32:i:291:TYR:CZ	48:i:401:PEE:H48	2.57	0.40
35:l:402:SER:O	35:l:404:THR:HG22	2.21	0.40
54:s:403:UQ:H202	54:s:403:UQ:H172	1.85	0.40
6:G:103:HIS:N	6:G:107:ASP:OD1	2.43	0.40
9:J:185:ALA:O	9:J:188:GLU:HG2	2.22	0.40
9:J:207:PHE:HD2	9:J:239:PRO:HB2	1.86	0.40
14:O:137:THR:HG22	14:O:138:THR:N	2.36	0.40
25:b:82:ILE:HD13	25:b:82:ILE:HA	1.89	0.40
50:g:201:PLX:H332	32:i:342:ALA:HB3	2.03	0.40
39:p:144:THR:HG22	39:p:145:PRO:HD2	2.03	0.40
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.56	0.40
41:s:13:ILE:HD12	41:s:86:TRP:CE2	2.57	0.40
43:v:81:LYS:HA	43:v:81:LYS:HD2	1.86	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%)	418 (97%)	13 (3%)	0	100	100
2	B	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
5	F	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
6	G	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	110/112 (98%)	101 (92%)	8 (7%)	1 (1%)	14	35
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	340/342 (99%)	327 (96%)	12 (4%)	1 (0%)	36	60
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	667 (97%)	21 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	203 (94%)	12 (6%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
24	a	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	84 (89%)	10 (11%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/107 (95%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	327 (95%)	18 (5%)	0	100	100
33	j	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	l	604/606 (100%)	580 (96%)	24 (4%)	0	100	100
36	m	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	44
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	36	60
42	u	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	21	44
43	v	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8175/8325 (98%)	7862 (96%)	308 (4%)	5 (0%)	49	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	s	208	VAL
9	J	38	HIS
7	H	77	ILE
39	p	174	PRO
42	u	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/346 (100%)	337 (98%)	8 (2%)	44	73
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	90
3	C	132/132 (100%)	127 (96%)	5 (4%)	29	58
4	E	107/107 (100%)	102 (95%)	5 (5%)	23	51
5	F	75/76 (99%)	73 (97%)	2 (3%)	39	69
6	G	76/81 (94%)	73 (96%)	3 (4%)	28	57
6	X	79/81 (98%)	79 (100%)	0	100	100
7	H	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	296/296 (100%)	296 (100%)	0	100	100
10	K	42/42 (100%)	40 (95%)	2 (5%)	23	50
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	87
12	M	580/580 (100%)	569 (98%)	11 (2%)	50	77
13	N	130/130 (100%)	128 (98%)	2 (2%)	57	81
14	O	183/183 (100%)	178 (97%)	5 (3%)	39	69
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	369/370 (100%)	366 (99%)	3 (1%)	73	88
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	77 (98%)	2 (2%)	42	71
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	82
20	V	101/101 (100%)	97 (96%)	4 (4%)	28	56
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	61/63 (97%)	60 (98%)	1 (2%)	55	80
23	Z	62/65 (95%)	62 (100%)	0	100	100
24	a	121/122 (99%)	119 (98%)	2 (2%)	53	79
25	b	90/119 (76%)	87 (97%)	3 (3%)	33	63
26	c	141/141 (100%)	140 (99%)	1 (1%)	76	90
27	d	155/155 (100%)	151 (97%)	4 (3%)	40	70
28	e	96/99 (97%)	96 (100%)	0	100	100
29	f	36/45 (80%)	36 (100%)	0	100	100
30	g	108/109 (99%)	108 (100%)	0	100	100
31	h	93/93 (100%)	91 (98%)	2 (2%)	45	74
32	i	311/311 (100%)	305 (98%)	6 (2%)	50	77
33	j	100/100 (100%)	96 (96%)	4 (4%)	28	56
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	540/540 (100%)	528 (98%)	12 (2%)	45	74
36	m	129/141 (92%)	127 (98%)	2 (2%)	55	80
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	402 (98%)	8 (2%)	48	76
41	s	275/275 (100%)	269 (98%)	6 (2%)	45	74
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	102/111 (92%)	102 (100%)	0	100	100
44	w	281/283 (99%)	276 (98%)	5 (2%)	51	78
All	All	7156/7249 (99%)	7044 (98%)	112 (2%)	54	80

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	CYS
1	A	149	MET
1	A	245	VAL
1	A	271	SER
1	A	273	THR
1	A	278	ILE
1	A	330	SER
1	A	435	VAL
2	B	73	THR
3	C	71	CYS
3	C	86	MET
3	C	92	VAL
3	C	142	TYR
3	C	192	ILE
4	E	17	VAL
4	E	49	LEU
4	E	68	MET
4	E	89	GLU
4	E	127	ASP
5	F	30	SER
5	F	80	ASN
6	G	84	LEU
6	G	100	VAL
6	G	122	MET
10	K	82	SER
10	K	107	SER
11	L	144	SER
12	M	352	VAL
12	M	374	THR

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Mol	Chain	Res	Type
12	M	398	ASP
12	M	467	LYS
12	M	478	SER
12	M	498	GLN
12	M	507	THR
12	M	544	VAL
12	M	555	ILE
12	M	619	ASP
12	M	658	ASP
13	N	4	VAL
13	N	144	TYR
14	O	50	ASP
14	O	150	GLU
14	O	167	LYS
14	O	186	VAL
14	O	213	ILE
16	Q	217	VAL
16	Q	345	SER
16	Q	453	THR
18	T	69	ASP
18	T	70	LEU
19	U	81	LEU
20	V	4	THR
20	V	69	ILE
20	V	74	SER
20	V	92	ILE
22	Y	77	SER
24	a	69	LYS
24	a	77	LEU
25	b	12	LEU
25	b	87	LYS
25	b	116	VAL
26	c	120	SER
27	d	12	GLU
27	d	17	THR
27	d	40	LEU
27	d	47	LEU
31	h	6	VAL
31	h	76	LEU
32	i	86	ILE
32	i	129	LEU
32	i	194	LEU

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Mol	Chain	Res	Type
32	i	211	MET
32	i	280	THR
32	i	336	VAL
33	j	13	LEU
33	j	26	GLN
33	j	31	SER
33	j	87	MET
35	l	9	LEU
35	l	70	THR
35	l	119	LYS
35	l	132	VAL
35	l	140	LEU
35	l	185	SER
35	l	306	THR
35	l	314	MET
35	l	417	SER
35	l	472	ILE
35	l	482	MET
35	l	507	THR
36	m	50	SER
36	m	156	VAL
38	o	59	VAL
40	r	9	THR
40	r	38	SER
40	r	183	SER
40	r	205	VAL
40	r	247	THR
40	r	255	ASN
40	r	305	THR
40	r	398	MET
41	s	40	VAL
41	s	100	LEU
41	s	202	GLU
41	s	227	GLU
41	s	289	LEU
41	s	296	LEU
44	w	62	VAL
44	w	95	ASP
44	w	203	VAL
44	w	288	ASP
44	w	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
4	E	70	ASN
4	E	126	HIS
5	F	48	ASN
7	H	71	GLN
7	H	73	GLN
8	I	47	HIS
9	J	128	ASN
9	J	166	HIS
10	K	79	HIS
11	L	71	HIS
12	M	123	ASN
12	M	260	ASN
12	M	464	GLN
12	M	598	ASN
12	M	676	ASN
13	N	113	HIS
13	N	135	GLN
14	O	90	ASN
14	O	131	HIS
14	O	187	GLN
14	O	246	GLN
15	P	55	HIS
15	P	75	GLN
15	P	228	GLN
16	Q	190	HIS
21	W	61	GLN
21	W	76	GLN
22	Y	46	GLN
23	Z	21	GLN
23	Z	33	GLN
26	c	31	HIS
27	d	23	GLN
27	d	124	ASN
27	d	134	GLN
27	d	149	HIS
28	e	132	ASN
28	e	140	ASN
29	f	61	GLN
29	f	73	ASN
30	g	63	GLN
31	h	21	GLN

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Mol	Chain	Res	Type
31	h	34	HIS
31	h	98	HIS
32	i	36	ASN
32	i	77	ASN
32	i	134	GLN
32	i	172	GLN
34	k	57	ASN
35	l	23	ASN
35	l	72	GLN
35	l	165	ASN
35	l	296	ASN
35	l	309	GLN
35	l	447	ASN
35	l	541	ASN
37	n	6	GLN
39	p	51	HIS
40	r	51	ASN
40	r	144	ASN
40	r	175	ASN
40	r	251	ASN
40	r	304	GLN
40	r	366	ASN
41	s	171	HIS
42	u	64	ASN
42	u	77	HIS
42	u	95	GLN
42	u	151	ASN
43	v	76	ASN
43	v	84	GLN
44	w	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	2.01	1 (10%)	5,13,15	6.04	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	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	12.30	130.75	119.48
16	Q	118	2MR	CD-NE-CZ	3.93	130.75	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.53	131.22	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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
52	CDL	V	201	-	93,93,99	1.14	8 (8%)	99,105,111	0.85	4 (4%)
48	PEE	i	401	-	46,46,50	1.22	6 (13%)	49,51,55	1.03	2 (4%)
49	UQ1	Q	501	-	18,18,18	2.32	6 (33%)	24,25,25	2.09	7 (29%)
48	PEE	l	701	-	39,39,50	1.33	6 (15%)	42,44,55	1.16	3 (7%)
48	PEE	s	401	-	50,50,50	1.17	6 (12%)	53,55,55	0.98	2 (3%)
52	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
48	PEE	j	201	-	40,40,50	1.18	5 (12%)	43,45,55	1.08	3 (6%)
52	CDL	I	201	-	50,50,99	1.42	8 (16%)	56,62,111	1.15	4 (7%)
52	CDL	g	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
50	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
52	CDL	k	101	-	93,93,99	1.14	8 (8%)	99,105,111	0.88	4 (4%)
55	FES	O	301	14	0,4,4	-	-	-	-	-
50	PLX	g	201	-	51,51,51	1.19	4 (7%)	53,59,59	0.66	1 (1%)
55	FES	M	803	12	0,4,4	-	-	-	-	-
50	PLX	C	204	-	51,51,51	1.19	3 (5%)	53,59,59	0.63	1 (1%)
52	CDL	l	702	-	98,98,99	0.92	4 (4%)	104,110,111	1.15	7 (6%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
52	CDL	o	201	-	99,99,99	1.10	8 (8%)	105,111,111	0.90	4 (3%)
50	PLX	J	403	-	51,51,51	1.21	4 (7%)	53,59,59	0.64	1 (1%)
58	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.92	9 (20%)
52	CDL	u	201	-	54,54,99	1.38	8 (14%)	60,66,111	1.10	4 (6%)
50	PLX	a	202	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	M	802	12	0,12,12	-	-	-		
54	UQ	J	402	-	33,33,63	3.51	10 (30%)	42,43,79	2.74	15 (35%)
48	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
45	SF4	C	202	3	0,12,12	-	-	-		
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
54	UQ	s	403	-	38,38,63	3.61	11 (28%)	48,49,79	2.79	17 (35%)
50	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.55	1 (1%)
51	8Q1	X	201	-	32,34,34	1.65	6 (18%)	39,43,43	1.62	7 (17%)
47	NAI	A	503	-	47,48,48	4.00	22 (46%)	64,73,73	1.70	12 (18%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.28	8 (16%)
53	NDP	J	401	-	51,52,52	4.27	25 (49%)	71,80,80	2.22	13 (18%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
52	CDL	l	703	-	99,99,99	1.11	9 (9%)	105,111,111	0.93	5 (4%)
51	8Q1	G	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.66	6 (15%)
45	SF4	A	501	1	0,12,12	-	-	-		
48	PEE	C	203	-	46,46,50	1.23	6 (13%)	49,51,55	0.98	2 (4%)
48	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
52	CDL	s	402	-	88,88,99	1.16	8 (9%)	94,100,111	0.94	4 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	UQ1	C	201	-	18,18,18	2.30	6 (33%)	24,25,25	1.63	5 (20%)

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
52	CDL	V	201	-	-	57/104/104/110	-
48	PEE	i	401	-	-	20/50/50/54	-
49	UQ1	Q	501	-	-	3/9/33/33	0/1/1/1
48	PEE	l	701	-	-	14/43/43/54	-
48	PEE	s	401	-	-	23/54/54/54	-
52	CDL	a	201	-	-	52/110/110/110	-
48	PEE	j	201	-	-	24/44/44/54	-
52	CDL	I	201	-	-	27/61/61/110	-
52	CDL	g	202	-	-	55/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PLX	j	202	-	-	25/55/55/55	-
52	CDL	k	101	-	-	43/104/104/110	-
45	SF4	M	801	12	-	-	0/6/5/5
55	FES	O	301	14	-	-	0/1/1/1
50	PLX	g	201	-	-	34/55/55/55	-
55	FES	M	803	12	-	-	0/1/1/1
50	PLX	C	204	-	-	27/55/55/55	-
52	CDL	l	702	-	-	43/109/109/110	-
52	CDL	o	201	-	-	49/110/110/110	-
45	SF4	B	302	2	-	-	0/6/5/5
50	PLX	J	403	-	-	34/55/55/55	-
58	ADP	w	401	-	-	5/16/32/32	0/3/3/3
52	CDL	u	201	-	-	27/65/65/110	-
50	PLX	a	202	-	-	29/55/55/55	-
45	SF4	M	802	12	-	-	0/6/5/5
54	UQ	J	402	-	-	17/27/51/87	0/1/1/1
48	PEE	l	705	-	-	13/49/49/54	-
45	SF4	C	202	3	-	-	0/6/5/5
48	PEE	r	501	-	-	26/54/54/54	-
48	PEE	W	201	-	-	17/44/44/54	-
54	UQ	s	403	-	-	9/33/57/87	0/1/1/1
50	PLX	e	201	-	-	33/55/55/55	-
51	8Q1	X	201	-	-	6/41/41/41	-
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3
53	NDP	J	401	-	-	8/34/77/77	0/5/5/5
48	PEE	B	303	-	-	26/54/54/54	-
52	CDL	l	703	-	-	58/110/110/110	-
51	8Q1	G	201	-	-	16/41/41/41	-
48	PEE	l	704	-	-	29/54/54/54	-
48	PEE	C	203	-	-	27/50/50/54	-
45	SF4	A	501	1	-	-	0/6/5/5
52	CDL	s	402	-	-	50/99/99/110	-
45	SF4	B	301	2	-	-	0/6/5/5
49	UQ1	C	201	-	-	2/9/33/33	0/1/1/1

All (262) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C3B-C2B	-13.23	1.24	1.53
53	J	401	NDP	O4D-C4D	10.78	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.44	1.26	1.53
54	s	403	UQ	C18-C19	10.05	1.56	1.33
53	J	401	NDP	C3D-C4D	-9.97	1.27	1.53
54	J	402	UQ	C18-C19	9.95	1.56	1.33
54	s	403	UQ	C13-C14	9.59	1.55	1.33
54	J	402	UQ	C13-C14	9.47	1.54	1.33
54	s	403	UQ	C23-C24	9.39	1.54	1.33
54	J	402	UQ	C8-C9	9.31	1.54	1.33
47	A	503	NAI	O4B-C1B	9.26	1.63	1.42
54	s	403	UQ	C8-C9	9.22	1.54	1.33
58	w	401	ADP	C3'-C4'	-8.98	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.37	1.26	1.45
53	J	401	NDP	O4B-C4B	-8.05	1.27	1.45
58	w	401	ADP	O4'-C4'	7.75	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.70	1.29	1.53
54	J	402	UQ	C23-C24	7.52	1.54	1.32
53	J	401	NDP	C2N-C3N	7.43	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.34	1.30	1.53
54	s	403	UQ	C28-C29	7.32	1.54	1.32
53	J	401	NDP	C6N-C5N	7.22	1.55	1.33
49	Q	501	UQ1	C8-C9	6.97	1.53	1.32
49	C	201	UQ1	C8-C9	6.93	1.53	1.32
47	A	503	NAI	O4D-C4D	6.86	1.60	1.45
53	J	401	NDP	PN-O3	6.46	1.66	1.59
58	w	401	ADP	PA-O3A	6.43	1.66	1.59
47	A	503	NAI	PA-O3	6.25	1.66	1.59
47	A	503	NAI	C2D-C3D	5.99	1.69	1.53
53	J	401	NDP	P2B-O2B	5.83	1.69	1.59
53	J	401	NDP	C6A-N6A	5.71	1.48	1.34
47	A	503	NAI	O4D-C1D	5.57	1.54	1.42
53	J	401	NDP	PA-O3	5.45	1.65	1.59
58	w	401	ADP	C6-N6	5.44	1.48	1.34
53	J	401	NDP	C3B-C4B	5.44	1.66	1.53
47	A	503	NAI	PN-O3	5.41	1.65	1.59
47	A	503	NAI	C4N-C3N	-5.32	1.39	1.50
47	A	503	NAI	C7N-N7N	5.27	1.48	1.33
51	X	201	8Q1	C39-N41	5.18	1.45	1.33
51	X	201	8Q1	C34-N36	5.16	1.45	1.33
47	A	503	NAI	C6A-N6A	5.08	1.47	1.34
51	G	201	8Q1	C34-N36	5.04	1.45	1.33
51	G	201	8Q1	C39-N41	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	O4D-C1D	-4.99	1.30	1.42
53	J	401	NDP	C6N-N1N	4.99	1.49	1.37
53	J	401	NDP	C1B-N9A	-4.64	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.59	1.31	1.42
53	J	401	NDP	O4B-C1B	4.58	1.52	1.42
47	A	503	NAI	O2B-C2B	4.30	1.53	1.43
52	l	702	CDL	OA8-CA7	4.26	1.45	1.33
52	l	702	CDL	OB8-CB7	4.19	1.45	1.33
52	l	702	CDL	OB6-CB5	4.12	1.45	1.34
52	l	702	CDL	OA6-CA5	4.00	1.45	1.34
53	J	401	NDP	O2D-C2D	-3.98	1.33	1.43
48	l	701	PEE	C18-C19	3.84	1.53	1.31
48	C	203	PEE	C18-C19	3.84	1.53	1.31
48	j	201	PEE	C18-C19	3.82	1.53	1.31
48	l	704	PEE	C18-C19	3.82	1.53	1.31
48	s	401	PEE	C18-C19	3.82	1.53	1.31
48	W	201	PEE	C18-C19	3.81	1.53	1.31
48	r	501	PEE	C18-C19	3.81	1.53	1.31
48	l	705	PEE	C18-C19	3.81	1.53	1.31
53	J	401	NDP	C7N-N7N	3.80	1.44	1.33
48	i	401	PEE	C18-C19	3.79	1.53	1.31
48	B	303	PEE	C18-C19	3.79	1.53	1.31
48	C	203	PEE	C39-C38	3.73	1.52	1.31
48	l	701	PEE	C39-C38	3.72	1.52	1.31
48	l	705	PEE	C39-C38	3.72	1.52	1.31
48	r	501	PEE	C39-C38	3.72	1.52	1.31
48	B	303	PEE	C39-C38	3.72	1.52	1.31
48	s	401	PEE	C39-C38	3.72	1.52	1.31
48	i	401	PEE	C39-C38	3.71	1.52	1.31
48	l	704	PEE	C39-C38	3.71	1.52	1.31
47	A	503	NAI	C7N-C3N	3.58	1.56	1.48
52	u	201	CDL	OA8-CA7	3.47	1.43	1.33
52	a	201	CDL	OA8-CA7	3.47	1.43	1.33
46	A	502	FMN	C4A-N5	3.45	1.38	1.30
52	I	201	CDL	OA8-CA7	3.45	1.43	1.33
52	V	201	CDL	OA8-CA7	3.44	1.43	1.33
52	o	201	CDL	OA8-CA7	3.44	1.43	1.33
52	s	402	CDL	OA8-CA7	3.42	1.43	1.33
52	l	703	CDL	OA8-CA7	3.42	1.43	1.33
58	w	401	ADP	C8-N9	-3.42	1.31	1.37
47	A	503	NAI	C4N-C5N	-3.38	1.40	1.49
52	k	101	CDL	OA8-CA7	3.38	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	g	202	CDL	OA8-CA7	3.36	1.43	1.33
52	k	101	CDL	OA6-CA5	3.27	1.43	1.34
58	w	401	ADP	O2'-C2'	-3.22	1.35	1.43
53	J	401	NDP	C8A-N9A	-3.21	1.32	1.37
52	V	201	CDL	OA6-CA5	3.12	1.43	1.34
52	g	202	CDL	OB6-CB5	3.09	1.43	1.34
52	s	402	CDL	OB6-CB5	3.07	1.42	1.34
52	I	201	CDL	OB8-CB7	3.06	1.42	1.33
52	a	201	CDL	OB6-CB5	3.04	1.42	1.34
52	a	201	CDL	OB8-CB7	3.02	1.42	1.33
52	l	703	CDL	OB8-CB7	3.02	1.42	1.33
52	l	703	CDL	OA6-CA5	3.01	1.42	1.34
52	V	201	CDL	OB6-CB5	3.01	1.42	1.34
52	g	202	CDL	OB8-CB7	3.00	1.42	1.33
52	k	101	CDL	OB6-CB5	3.00	1.42	1.34
52	u	201	CDL	OB6-CB5	3.00	1.42	1.34
50	C	204	PLX	O6-C4	-3.00	1.40	1.44
52	V	201	CDL	OB8-CB7	2.99	1.42	1.33
52	s	402	CDL	OA6-CA5	2.98	1.42	1.34
52	I	201	CDL	OB6-CB5	2.98	1.42	1.34
52	l	703	CDL	OB6-CB5	2.98	1.42	1.34
53	J	401	NDP	C5A-N7A	-2.97	1.33	1.39
52	o	201	CDL	OB6-CB5	2.96	1.42	1.34
50	a	202	PLX	O6-C4	-2.94	1.40	1.44
52	u	201	CDL	OB8-CB7	2.94	1.41	1.33
52	g	202	CDL	OA6-CA5	2.93	1.42	1.34
52	s	402	CDL	OB8-CB7	2.93	1.41	1.33
52	o	201	CDL	OA6-CA5	2.93	1.42	1.34
58	w	401	ADP	O3'-C3'	2.92	1.50	1.43
52	u	201	CDL	OA6-CA5	2.92	1.42	1.34
52	a	201	CDL	OA6-CA5	2.91	1.42	1.34
52	o	201	CDL	OB8-CB7	2.91	1.41	1.33
52	k	101	CDL	OB8-CB7	2.91	1.41	1.33
53	J	401	NDP	O3D-C3D	2.89	1.50	1.43
50	g	201	PLX	O6-C4	-2.89	1.40	1.44
53	J	401	NDP	C7N-C3N	2.89	1.54	1.48
52	I	201	CDL	OA6-CA5	2.89	1.42	1.34
50	e	201	PLX	O6-C4	-2.85	1.41	1.44
54	J	402	UQ	C6-C1	2.80	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.79	1.32	1.37
50	j	202	PLX	O6-C4	-2.72	1.41	1.44
49	Q	501	UQ1	C6-C1	2.70	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	W	201	PEE	O2-C2	-2.68	1.40	1.46
50	J	403	PLX	O6-C4	-2.67	1.41	1.44
52	I	201	CDL	OA6-CA4	-2.65	1.40	1.46
48	B	303	PEE	O2-C2	-2.64	1.40	1.46
48	i	401	PEE	O2-C2	-2.64	1.40	1.46
54	s	403	UQ	C6-C1	2.62	1.53	1.46
52	a	201	CDL	OA6-CA4	-2.60	1.40	1.46
48	j	201	PEE	O2-C2	-2.59	1.40	1.46
48	C	203	PEE	O2-C2	-2.58	1.40	1.46
52	g	202	CDL	OA6-CA4	-2.58	1.40	1.46
52	u	201	CDL	OA6-CA4	-2.57	1.40	1.46
52	o	201	CDL	OA6-CA4	-2.56	1.40	1.46
53	J	401	NDP	O2B-C2B	2.55	1.52	1.44
48	r	501	PEE	O2-C2	-2.54	1.40	1.46
48	l	701	PEE	O3-C30	2.51	1.40	1.33
52	s	402	CDL	OA6-CA4	-2.51	1.40	1.46
48	j	201	PEE	O3-C30	2.51	1.40	1.33
48	l	704	PEE	O2-C2	-2.49	1.40	1.46
48	l	701	PEE	O2-C2	-2.49	1.40	1.46
48	s	401	PEE	O2-C2	-2.48	1.40	1.46
51	X	201	8Q1	C1-S44	2.48	1.82	1.76
48	l	705	PEE	O2-C2	-2.46	1.40	1.46
58	w	401	ADP	C5-N7	-2.46	1.34	1.39
48	l	705	PEE	O3-C30	2.46	1.40	1.33
48	s	401	PEE	O3-C30	2.44	1.40	1.33
47	A	503	NAI	PN-O5D	2.44	1.68	1.59
51	G	201	8Q1	C1-S44	2.43	1.82	1.76
48	B	303	PEE	O3-C30	2.43	1.40	1.33
52	l	703	CDL	OA6-CA4	-2.43	1.40	1.46
49	C	201	UQ1	C6-C1	2.42	1.53	1.46
46	A	502	FMN	C10-N1	2.42	1.38	1.33
52	k	101	CDL	OB6-CB4	-2.42	1.40	1.46
51	G	201	8Q1	O40-C39	-2.41	1.18	1.23
50	e	201	PLX	C7-C6	2.40	1.55	1.50
47	A	503	NAI	O3B-C3B	-2.39	1.37	1.43
48	l	704	PEE	O3-C30	2.38	1.40	1.33
51	G	201	8Q1	O35-C34	-2.38	1.18	1.23
49	Q	501	UQ1	O2-CM2	-2.38	1.40	1.45
48	i	401	PEE	O3-C30	2.38	1.40	1.33
48	W	201	PEE	O3-C30	2.37	1.40	1.33
47	A	503	NAI	C6N-C5N	2.37	1.40	1.33
50	J	403	PLX	C7-C6	2.37	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	j	202	PLX	C7-C6	2.37	1.55	1.50
52	s	402	CDL	OB6-CB4	-2.36	1.41	1.46
52	I	201	CDL	OB6-CB4	-2.35	1.41	1.46
52	o	201	CDL	OB6-CB4	-2.35	1.41	1.46
51	X	201	8Q1	O40-C39	-2.34	1.18	1.23
48	r	501	PEE	O3-C30	2.34	1.40	1.33
51	X	201	8Q1	C6-C1	2.33	1.53	1.50
52	u	201	CDL	OB6-CB4	-2.33	1.41	1.46
52	V	201	CDL	OB6-CB4	-2.33	1.41	1.46
48	C	203	PEE	O3-C30	2.33	1.40	1.33
52	V	201	CDL	OA6-CA4	-2.32	1.41	1.46
48	l	705	PEE	O2-C10	2.32	1.40	1.34
52	l	703	CDL	OB6-CB4	-2.32	1.41	1.46
51	X	201	8Q1	O35-C34	-2.31	1.19	1.23
50	a	202	PLX	C7-C6	2.31	1.55	1.50
52	a	201	CDL	OB6-CB4	-2.31	1.41	1.46
48	l	704	PEE	O2-C10	2.29	1.40	1.34
50	g	201	PLX	C7-C6	2.29	1.55	1.50
47	A	503	NAI	C5B-C4B	2.29	1.58	1.51
52	o	201	CDL	PB2-OB2	2.28	1.68	1.59
48	l	701	PEE	O2-C10	2.27	1.40	1.34
50	C	204	PLX	C7-C6	2.26	1.55	1.50
48	j	201	PEE	O2-C10	2.26	1.40	1.34
52	V	201	CDL	PB2-OB2	2.26	1.68	1.59
52	u	201	CDL	PB2-OB2	2.25	1.68	1.59
52	V	201	CDL	PB2-OB5	2.25	1.68	1.59
48	W	201	PEE	O2-C10	2.25	1.40	1.34
52	g	202	CDL	OB6-CB4	-2.24	1.41	1.46
48	s	401	PEE	O2-C10	2.24	1.40	1.34
49	Q	501	UQ1	O3-CM3	-2.23	1.40	1.45
49	C	201	UQ1	O2-CM2	-2.23	1.40	1.45
49	C	201	UQ1	O3-CM3	-2.23	1.40	1.45
52	a	201	CDL	PB2-OB5	2.23	1.68	1.59
48	r	501	PEE	O3-C3	-2.23	1.40	1.45
48	C	203	PEE	O2-C10	2.23	1.40	1.34
48	C	203	PEE	O3-C3	-2.23	1.40	1.45
48	l	704	PEE	O3-C3	-2.22	1.40	1.45
51	G	201	8Q1	C6-C1	2.22	1.53	1.50
52	l	703	CDL	PB2-OB5	2.22	1.68	1.59
52	g	202	CDL	PB2-OB5	2.22	1.68	1.59
48	B	303	PEE	O2-C10	2.22	1.40	1.34
54	s	403	UQ	C7-C8	2.21	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	k	101	CDL	PB2-OB2	2.21	1.68	1.59
53	J	401	NDP	C2D-C3D	2.21	1.59	1.53
53	J	401	NDP	O7N-C7N	-2.21	1.19	1.24
54	J	402	UQ	C7-C8	2.20	1.54	1.50
48	W	201	PEE	O3-C3	-2.20	1.40	1.45
52	o	201	CDL	PB2-OB5	2.20	1.68	1.59
48	i	401	PEE	O3-C3	-2.20	1.40	1.45
52	a	201	CDL	PB2-OB2	2.19	1.68	1.59
52	u	201	CDL	PB2-OB5	2.18	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.18	1.35	1.39
48	i	401	PEE	O2-C10	2.18	1.40	1.34
52	g	202	CDL	PB2-OB2	2.18	1.67	1.59
48	r	501	PEE	O2-C10	2.17	1.40	1.34
52	l	703	CDL	PB2-OB2	2.17	1.67	1.59
50	a	202	PLX	P1-O4	2.17	1.67	1.59
48	l	705	PEE	O3-C3	-2.17	1.40	1.45
52	I	201	CDL	PB2-OB2	2.17	1.67	1.59
52	s	402	CDL	PB2-OB2	2.16	1.67	1.59
48	B	303	PEE	O3-C3	-2.16	1.40	1.45
50	e	201	PLX	P1-O4	2.15	1.67	1.59
52	I	201	CDL	PB2-OB5	2.15	1.67	1.59
52	s	402	CDL	PB2-OB5	2.15	1.67	1.59
50	j	202	PLX	P1-O4	2.15	1.67	1.59
48	j	201	PEE	O3-C3	-2.14	1.40	1.45
48	s	401	PEE	O3-C3	-2.13	1.40	1.45
50	g	201	PLX	P1-O4	2.13	1.67	1.59
49	C	201	UQ1	O4-C4	-2.12	1.18	1.23
52	k	101	CDL	PB2-OB5	2.12	1.67	1.59
54	J	402	UQ	O4-C4	-2.11	1.18	1.23
52	k	101	CDL	OA6-CA4	-2.11	1.41	1.46
50	J	403	PLX	P1-O4	2.11	1.67	1.59
49	Q	501	UQ1	O4-C4	-2.10	1.18	1.23
53	J	401	NDP	PA-O5B	2.10	1.67	1.59
50	C	204	PLX	P1-O4	2.09	1.67	1.59
49	C	201	UQ1	O1-C1	-2.09	1.18	1.23
48	l	701	PEE	O3-C3	-2.09	1.40	1.45
54	s	403	UQ	O3-CM3	-2.09	1.40	1.45
50	a	202	PLX	P1-O1	2.08	1.67	1.59
50	j	202	PLX	P1-O1	2.08	1.67	1.59
54	J	402	UQ	O3-CM3	-2.08	1.40	1.45
54	s	403	UQ	O4-C4	-2.07	1.18	1.23
54	J	402	UQ	C21-C19	2.07	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	403	PLX	P1-O1	2.04	1.67	1.59
50	e	201	PLX	P1-O1	2.04	1.67	1.59
49	Q	501	UQ1	O1-C1	-2.03	1.18	1.23
50	g	201	PLX	P1-O1	2.02	1.67	1.59
54	s	403	UQ	O1-C1	-2.02	1.18	1.23
50	e	201	PLX	C1-C2	2.02	1.57	1.51
52	l	703	CDL	C11-CA5	2.01	1.56	1.50
54	J	402	UQ	O1-C1	-2.01	1.18	1.23
54	s	403	UQ	C21-C19	2.01	1.55	1.51

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	s	403	UQ	C7-C8-C9	-7.94	113.15	126.83
54	J	402	UQ	C7-C8-C9	-7.92	113.19	126.83
53	J	401	NDP	C3N-C2N-N1N	-7.75	111.82	123.20
53	J	401	NDP	C1D-N1N-C2N	-7.03	109.56	121.14
53	J	401	NDP	C6N-N1N-C2N	-6.49	112.37	119.32
54	J	402	UQ	C12-C13-C14	-6.46	112.83	127.62
54	J	402	UQ	C17-C18-C19	-6.33	113.14	127.62
54	s	403	UQ	C17-C18-C19	-6.24	113.34	127.62
51	G	201	8Q1	C6-C1-S44	6.22	120.82	113.40
54	s	403	UQ	C12-C13-C14	-6.17	113.51	127.62
54	s	403	UQ	C22-C23-C24	-6.04	113.80	127.62
51	X	201	8Q1	C6-C1-S44	5.93	120.47	113.40
47	A	503	NAI	C5A-C4A-N3A	-5.46	119.19	126.72
53	J	401	NDP	C1D-N1N-C6N	-5.45	109.25	120.77
53	J	401	NDP	C5A-C4A-N3A	-5.44	119.23	126.72
58	w	401	ADP	C5-C4-N3	-5.43	119.24	126.72
49	Q	501	UQ1	C7-C6-C1	4.93	124.24	118.52
52	l	702	CDL	OA6-CA5-C11	4.78	121.83	111.48
49	C	201	UQ1	C7-C8-C9	-4.68	114.01	127.25
58	w	401	ADP	N3-C2-N1	-4.58	121.65	128.58
54	s	403	UQ	C27-C28-C29	-4.51	112.59	127.64
47	A	503	NAI	N3A-C2A-N1A	-4.43	121.88	128.58
49	Q	501	UQ1	C7-C6-C5	-4.43	117.30	124.89
54	J	402	UQ	C20-C19-C18	-4.40	112.31	123.63
54	J	402	UQ	C22-C23-C24	-4.40	112.97	127.64
54	J	402	UQ	C15-C14-C13	-4.39	112.36	123.63
54	s	403	UQ	C10-C9-C8	-4.34	112.47	123.63
48	l	701	PEE	O2-C10-C11	4.33	120.85	111.48
53	J	401	NDP	N3A-C2A-N1A	-4.33	122.03	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	l	702	CDL	OB6-CB5-C51	4.32	120.83	111.48
48	r	501	PEE	O2-C10-C11	4.27	120.72	111.48
48	j	201	PEE	O2-C10-C11	4.27	120.72	111.48
58	w	401	ADP	N3-C4-N9	4.21	134.33	127.17
49	Q	501	UQ1	C7-C8-C9	-4.19	115.40	127.25
54	J	402	UQ	C10-C9-C8	-4.18	112.89	123.63
54	s	403	UQ	C25-C24-C23	-4.18	112.89	123.63
52	s	402	CDL	OA6-CA5-C11	4.15	120.47	111.48
48	l	705	PEE	O2-C10-C11	4.14	120.44	111.48
48	s	401	PEE	O2-C10-C11	4.13	120.42	111.48
52	l	703	CDL	OA6-CA5-C11	4.12	120.40	111.48
52	a	201	CDL	OB6-CB5-C51	4.11	120.37	111.48
52	g	202	CDL	OB6-CB5-C51	4.08	120.30	111.48
52	l	703	CDL	OB6-CB5-C51	4.07	120.29	111.48
52	o	201	CDL	OA6-CA5-C11	4.03	120.20	111.48
52	o	201	CDL	OB6-CB5-C51	4.03	120.19	111.48
48	B	303	PEE	O2-C10-C11	4.02	120.19	111.48
54	s	403	UQ	C15-C14-C13	-4.01	113.34	123.63
54	J	402	UQ	C16-C14-C13	-3.97	112.26	121.17
52	a	201	CDL	OA6-CA5-C11	3.97	120.06	111.48
52	u	201	CDL	OA6-CA5-C11	3.96	120.04	111.48
52	g	202	CDL	OA6-CA5-C11	3.95	120.02	111.48
52	s	402	CDL	OB6-CB5-C51	3.94	120.01	111.48
52	u	201	CDL	OB6-CB5-C51	3.93	119.99	111.48
52	I	201	CDL	OA6-CA5-C11	3.93	119.98	111.48
54	s	403	UQ	C20-C19-C18	-3.88	113.67	123.63
52	I	201	CDL	OB6-CB5-C51	3.87	119.84	111.48
48	W	201	PEE	O2-C10-C11	3.83	119.77	111.48
52	k	101	CDL	OB6-CB5-C51	3.83	119.76	111.48
48	i	401	PEE	O2-C10-C11	3.83	119.76	111.48
54	s	403	UQ	C11-C9-C8	-3.82	112.60	121.17
51	G	201	8Q1	O4-C1-C6	-3.82	119.58	123.98
48	l	704	PEE	O2-C10-C11	3.82	119.74	111.48
47	A	503	NAI	N3A-C4A-N9A	3.81	133.65	127.17
51	X	201	8Q1	O4-C1-C6	-3.79	119.60	123.98
52	V	201	CDL	OB6-CB5-C51	3.77	119.64	111.48
53	J	401	NDP	N3A-C4A-N9A	3.77	133.57	127.17
52	V	201	CDL	OA6-CA5-C11	3.75	119.60	111.48
48	C	203	PEE	O2-C10-C11	3.74	119.57	111.48
54	J	402	UQ	C21-C19-C18	-3.74	112.77	121.17
47	A	503	NAI	C2A-N3A-C4A	3.69	120.83	111.83
53	J	401	NDP	C2A-N3A-C4A	3.67	120.79	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	w	401	ADP	C2-N3-C4	3.57	120.55	111.83
54	s	403	UQ	C16-C14-C13	-3.53	113.24	121.17
54	s	403	UQ	C21-C19-C18	-3.52	113.26	121.17
58	w	401	ADP	N9-C8-N7	-3.51	108.96	113.94
47	A	503	NAI	C4A-C5A-N7A	-3.50	106.58	110.58
54	s	403	UQ	C26-C24-C23	-3.43	113.47	121.17
47	A	503	NAI	C5A-N7A-C8A	3.41	108.82	103.45
46	A	502	FMN	C4-N3-C2	-3.39	119.62	125.64
54	J	402	UQ	C11-C9-C8	-3.38	113.59	121.17
54	s	403	UQ	C31-C29-C28	-3.33	112.68	122.66
53	J	401	NDP	C4A-C5A-N7A	-3.29	106.82	110.58
49	C	201	UQ1	C10-C9-C8	-3.28	112.81	122.66
49	Q	501	UQ1	C10-C9-C8	-3.27	112.83	122.66
51	X	201	8Q1	C37-C38-C39	3.27	117.84	112.39
54	J	402	UQ	C25-C24-C23	-3.27	112.85	122.66
54	s	403	UQ	C30-C29-C28	-3.27	112.85	122.66
47	A	503	NAI	N9A-C8A-N7A	-3.27	109.30	113.94
52	l	702	CDL	CA4-OA6-CA5	-3.24	110.03	117.80
52	k	101	CDL	OA6-CA5-C11	3.23	118.46	111.48
58	w	401	ADP	C5-N7-C8	3.22	108.52	103.45
47	A	503	NAI	C3D-C2D-C1D	3.22	107.56	101.46
53	J	401	NDP	N9A-C8A-N7A	-3.16	109.45	113.94
47	A	503	NAI	C4D-O4D-C1D	-3.15	102.50	109.47
54	J	402	UQ	C7-C6-C5	-3.15	119.50	124.89
54	J	402	UQ	C26-C24-C23	-3.14	113.23	122.66
58	w	401	ADP	C4-N9-C8	3.11	109.00	105.74
51	G	201	8Q1	C37-C38-C39	3.05	117.48	112.39
58	w	401	ADP	C4-C5-N7	-3.05	107.10	110.58
53	J	401	NDP	C5A-N7A-C8A	3.02	108.20	103.45
52	l	702	CDL	OA8-CA7-C31	2.97	120.90	111.83
48	B	303	PEE	O3-C30-C31	2.97	120.89	111.83
48	l	704	PEE	O3-C30-C31	2.96	120.86	111.83
52	k	101	CDL	OA8-CA7-C31	2.96	120.86	111.83
48	i	401	PEE	O3-C30-C31	2.93	120.76	111.83
49	C	201	UQ1	C11-C9-C8	-2.91	113.92	122.66
52	l	702	CDL	OB8-CB7-C71	2.91	120.71	111.83
52	l	703	CDL	OA8-CA7-C31	2.91	120.70	111.83
51	G	201	8Q1	C43-S44-C1	2.89	110.40	101.84
52	l	703	CDL	OB8-CB7-C71	2.88	120.62	111.83
52	a	201	CDL	OB8-CB7-C71	2.84	120.50	111.83
52	k	101	CDL	OB8-CB7-C71	2.82	120.44	111.83
48	j	201	PEE	O3-C30-C31	2.80	120.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	o	201	CDL	OB8-CB7-C71	2.80	120.37	111.83
52	I	201	CDL	OA8-CA7-C31	2.80	120.36	111.83
48	l	701	PEE	O3-C30-C31	2.79	120.33	111.83
52	s	402	CDL	OA8-CA7-C31	2.78	120.30	111.83
46	A	502	FMN	C4A-C4-N3	2.76	120.28	113.25
52	u	201	CDL	OB8-CB7-C71	2.75	120.23	111.83
52	u	201	CDL	OA8-CA7-C31	2.75	119.50	111.15
52	I	201	CDL	OB8-CB7-C71	2.73	120.17	111.83
52	g	202	CDL	OB8-CB7-C71	2.73	120.16	111.83
52	g	202	CDL	OA8-CA7-C31	2.73	120.15	111.83
52	V	201	CDL	OB8-CB7-C71	2.72	120.12	111.83
49	Q	501	UQ1	C11-C9-C8	-2.70	114.55	122.66
52	a	201	CDL	OA8-CA7-C31	2.69	120.04	111.83
48	W	201	PEE	O3-C30-C31	2.69	120.03	111.83
48	C	203	PEE	O3-C30-C31	2.69	120.03	111.83
48	r	501	PEE	O3-C30-C31	2.69	120.03	111.83
48	l	705	PEE	O3-C30-C31	2.63	119.86	111.83
46	A	502	FMN	C5A-C9A-N10	2.61	120.33	117.97
54	J	402	UQ	CM5-C5-C6	-2.59	120.20	124.45
46	A	502	FMN	O4-C4-C4A	-2.58	119.72	126.53
52	V	201	CDL	OA8-CA7-C31	2.58	119.69	111.83
48	s	401	PEE	O3-C30-C31	2.58	119.69	111.83
52	o	201	CDL	OA8-CA7-C31	2.54	119.58	111.83
49	C	201	UQ1	C7-C6-C5	-2.53	120.55	124.89
50	g	201	PLX	C1A-N1-C1	2.50	119.83	109.91
46	A	502	FMN	C9A-C5A-N5	-2.48	119.82	122.45
53	J	401	NDP	C4A-N9A-C8A	2.47	108.33	105.74
49	Q	501	UQ1	C6-C5-C4	2.46	121.11	119.17
52	s	402	CDL	OB8-CB7-C71	2.45	119.29	111.83
52	l	702	CDL	OA6-CA5-OA7	-2.44	118.01	123.70
51	X	201	8Q1	C43-S44-C1	2.43	109.03	101.84
51	G	201	8Q1	O4-C1-S44	-2.42	119.61	122.68
50	J	403	PLX	C1A-N1-C1	2.42	119.52	109.91
50	j	202	PLX	C1A-N1-C1	2.41	119.50	109.91
50	a	202	PLX	C1A-N1-C1	2.38	119.37	109.91
54	s	403	UQ	C7-C6-C5	-2.37	120.83	124.89
48	l	701	PEE	C20-C19-C18	-2.33	112.42	126.42
48	j	201	PEE	C2-O2-C10	-2.31	112.28	117.80
51	X	201	8Q1	C38-C39-N41	2.30	120.54	116.34
46	A	502	FMN	C4A-C10-N10	2.29	119.77	116.48
47	A	503	NAI	C4A-N9A-C8A	2.29	108.14	105.74
52	l	702	CDL	CB4-OB6-CB5	-2.28	112.33	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	204	PLX	C1A-N1-C1	2.28	118.96	109.91
53	J	401	NDP	C2B-C3B-C4B	2.27	106.88	101.99
49	Q	501	UQ1	CM5-C5-C6	-2.25	120.75	124.45
46	A	502	FMN	C4A-C10-N1	-2.23	119.11	124.59
47	A	503	NAI	C2D-C3D-C4D	2.21	106.88	102.61
51	G	201	8Q1	C38-C39-N41	2.20	120.34	116.34
46	A	502	FMN	C10-C4A-N5	-2.19	120.34	124.81
54	s	403	UQ	CM5-C5-C6	-2.19	120.86	124.45
51	X	201	8Q1	O4-C1-S44	-2.17	119.92	122.68
52	l	703	CDL	CB4-OB6-CB5	-2.17	112.61	117.80
51	X	201	8Q1	C32-C34-N36	2.14	120.54	116.48
50	e	201	PLX	C1A-N1-C1	2.12	118.35	109.91
47	A	503	NAI	C6N-N1N-C2N	2.12	121.58	119.32
58	w	401	ADP	C4'-O4'-C1'	-2.10	104.83	109.47
49	C	201	UQ1	CM5-C5-C6	-2.08	121.03	124.45
54	J	402	UQ	C7-C6-C1	2.01	120.86	118.52

There are no chirality outliers.

All (943) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	A	503	NAI	PN-O3-PA-O5B
48	B	303	PEE	C4-O4P-P-O3P
48	B	303	PEE	C4-O4P-P-O2P
48	C	203	PEE	C1-O3P-P-O1P
48	C	203	PEE	C1-O3P-P-O4P
48	C	203	PEE	C4-O4P-P-O3P
48	C	203	PEE	C4-O4P-P-O1P
48	W	201	PEE	C4-O4P-P-O1P
48	i	401	PEE	O4-C10-O2-C2
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	j	201	PEE	O4P-C4-C5-N
48	l	704	PEE	C11-C10-O2-C2
48	l	704	PEE	C4-O4P-P-O3P
48	l	704	PEE	C4-O4P-P-O2P
48	l	704	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O2P
48	r	501	PEE	C4-O4P-P-O1P
48	s	401	PEE	C1-O3P-P-O1P
48	s	401	PEE	C1-O3P-P-O4P
48	s	401	PEE	C4-O4P-P-O3P
49	Q	501	UQ1	C1-C6-C7-C8
49	Q	501	UQ1	C5-C6-C7-C8
50	C	204	PLX	O6-C6-C7-C8
50	C	204	PLX	C2-O1-P1-O4
50	C	204	PLX	C2-O1-P1-O2
50	J	403	PLX	O7-C6-O6-C4
50	J	403	PLX	C2-O1-P1-O2
50	J	403	PLX	N1-C1-C2-O1
50	J	403	PLX	C25-C24-O8-C5
50	a	202	PLX	O7-C6-O6-C4
50	a	202	PLX	C3-O4-P1-O1
50	a	202	PLX	C3-O4-P1-O2
50	a	202	PLX	C3-O4-P1-O3
50	a	202	PLX	C2-O1-P1-O4
50	a	202	PLX	C2-O1-P1-O2
50	a	202	PLX	N1-C1-C2-O1
50	a	202	PLX	O9-C24-C25-C26
50	e	201	PLX	O7-C6-O6-C4
50	e	201	PLX	C3-O4-P1-O1
50	e	201	PLX	C3-O4-P1-O2
50	e	201	PLX	C2-O1-P1-O4
50	e	201	PLX	O9-C24-O8-C5
50	e	201	PLX	O9-C24-C25-C26
50	g	201	PLX	C2-O1-P1-O4
50	g	201	PLX	C2-O1-P1-O2
50	g	201	PLX	C2-O1-P1-O3
50	g	201	PLX	C25-C24-O8-C5
50	j	202	PLX	O7-C6-C7-C8
50	j	202	PLX	O7-C6-O6-C4
50	j	202	PLX	O9-C24-O8-C5
51	G	201	8Q1	O27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
51	G	201	8Q1	O27-C28-C29-C31
51	G	201	8Q1	C28-C29-C32-C34
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	C28-O27-P24-O3
51	G	201	8Q1	C28-O27-P24-O2
51	G	201	8Q1	C28-O27-P24-O1
52	I	201	CDL	CB2-C1-CA2-OA2
52	I	201	CDL	CA2-OA2-PA1-OA3
52	I	201	CDL	CA2-OA2-PA1-OA4
52	I	201	CDL	CA2-OA2-PA1-OA5
52	I	201	CDL	OA5-CA3-CA4-OA6
52	I	201	CDL	CB2-OB2-PB2-OB3
52	I	201	CDL	CB2-OB2-PB2-OB5
52	I	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CA3-OA5-PA1-OA4
52	V	201	CDL	CB2-OB2-PB2-OB3
52	V	201	CDL	CB2-OB2-PB2-OB4
52	V	201	CDL	CB2-OB2-PB2-OB5
52	V	201	CDL	CB3-OB5-PB2-OB2
52	V	201	CDL	CB3-OB5-PB2-OB3
52	V	201	CDL	CB3-OB5-PB2-OB4
52	a	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CB2-OB2-PB2-OB3
52	a	201	CDL	CB2-OB2-PB2-OB5
52	a	201	CDL	OB7-CB5-OB6-CB4
52	a	201	CDL	C51-CB5-OB6-CB4
52	g	202	CDL	CA3-OA5-PA1-OA2
52	g	202	CDL	CB2-OB2-PB2-OB3
52	g	202	CDL	CB2-OB2-PB2-OB4
52	g	202	CDL	CB2-OB2-PB2-OB5
52	g	202	CDL	CB3-OB5-PB2-OB2
52	g	202	CDL	CB3-OB5-PB2-OB3
52	g	202	CDL	OB7-CB5-OB6-CB4
52	g	202	CDL	C51-CB5-OB6-CB4
52	k	101	CDL	CA3-OA5-PA1-OA2
52	k	101	CDL	CA3-OA5-PA1-OA3
52	k	101	CDL	CA3-OA5-PA1-OA4
52	l	702	CDL	CA2-OA2-PA1-OA3
52	l	702	CDL	CA3-OA5-PA1-OA2
52	l	702	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	CB2-OB2-PB2-OB3
52	l	702	CDL	CB2-OB2-PB2-OB5
52	l	702	CDL	CB3-OB5-PB2-OB2
52	l	702	CDL	CB3-OB5-PB2-OB3
52	l	702	CDL	CB3-OB5-PB2-OB4
52	l	703	CDL	CA2-OA2-PA1-OA4
52	l	703	CDL	CA2-OA2-PA1-OA5
52	l	703	CDL	CA3-OA5-PA1-OA2
52	l	703	CDL	CA3-OA5-PA1-OA4
52	l	703	CDL	CB2-OB2-PB2-OB3
52	l	703	CDL	CB2-OB2-PB2-OB4
52	l	703	CDL	CB2-OB2-PB2-OB5
52	l	703	CDL	CB3-OB5-PB2-OB2
52	l	703	CDL	CB3-OB5-PB2-OB3
52	l	703	CDL	CB3-OB5-PB2-OB4
52	o	201	CDL	CA2-C1-CB2-OB2
52	o	201	CDL	CA3-OA5-PA1-OA2
52	o	201	CDL	CA3-OA5-PA1-OA3
52	o	201	CDL	CA3-OA5-PA1-OA4
52	o	201	CDL	OB5-CB3-CB4-OB6
52	s	402	CDL	OA5-CA3-CA4-OA6
52	u	201	CDL	CB2-C1-CA2-OA2
52	u	201	CDL	CB2-OB2-PB2-OB4
52	u	201	CDL	CB2-OB2-PB2-OB5
53	J	401	NDP	C5B-O5B-PA-O1A
53	J	401	NDP	C2N-C3N-C7N-N7N
54	J	402	UQ	C7-C8-C9-C10
54	J	402	UQ	C12-C13-C14-C15
54	J	402	UQ	C12-C13-C14-C16
54	s	403	UQ	C7-C8-C9-C10
54	s	403	UQ	C7-C8-C9-C11
58	w	401	ADP	C5'-O5'-PA-O3A
52	s	402	CDL	OA9-CA7-OA8-CA6
49	Q	501	UQ1	C7-C8-C9-C10
52	s	402	CDL	C31-CA7-OA8-CA6
48	s	401	PEE	O5-C30-O3-C3
48	j	201	PEE	O4-C10-O2-C2
48	l	704	PEE	O4-C10-O2-C2
48	s	401	PEE	C31-C30-O3-C3
48	i	401	PEE	C11-C10-O2-C2
54	J	402	UQ	C12-C11-C9-C10
54	J	402	UQ	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
54	J	402	UQ	C18-C19-C21-C22
54	s	403	UQ	C18-C19-C21-C22
48	i	401	PEE	C31-C30-O3-C3
48	l	701	PEE	C31-C30-O3-C3
54	s	403	UQ	C22-C23-C24-C25
48	l	701	PEE	C17-C18-C19-C20
48	s	401	PEE	C17-C18-C19-C20
54	J	402	UQ	C17-C18-C19-C21
54	s	403	UQ	C17-C18-C19-C21
48	i	401	PEE	O5-C30-O3-C3
48	l	701	PEE	O5-C30-O3-C3
50	j	202	PLX	C13-C14-C15-C16
52	I	201	CDL	O1-C1-CA2-OA2
52	V	201	CDL	O1-C1-CA2-OA2
52	a	201	CDL	O1-C1-CB2-OB2
52	g	202	CDL	O1-C1-CA2-OA2
52	l	703	CDL	O1-C1-CA2-OA2
52	l	703	CDL	O1-C1-CB2-OB2
52	u	201	CDL	O1-C1-CA2-OA2
52	u	201	CDL	O1-C1-CB2-OB2
52	V	201	CDL	C31-CA7-OA8-CA6
52	l	702	CDL	C31-CA7-OA8-CA6
48	B	303	PEE	C11-C10-O2-C2
48	l	705	PEE	C11-C10-O2-C2
52	V	201	CDL	C11-CA5-OA6-CA4
54	J	402	UQ	C22-C23-C24-C26
47	A	503	NAI	C3D-C4D-C5D-O5D
53	J	401	NDP	O4D-C4D-C5D-O5D
58	w	401	ADP	O4'-C4'-C5'-O5'
54	J	402	UQ	C15-C14-C16-C17
54	J	402	UQ	C20-C19-C21-C22
54	s	403	UQ	C14-C16-C17-C18
52	V	201	CDL	C11-C12-C13-C14
54	s	403	UQ	C27-C28-C29-C31
52	V	201	CDL	OA9-CA7-OA8-CA6
52	l	702	CDL	OA9-CA7-OA8-CA6
48	r	501	PEE	C17-C18-C19-C20
54	s	403	UQ	C22-C23-C24-C26
52	V	201	CDL	C62-C63-C64-C65
52	l	703	CDL	C75-C76-C77-C78
48	B	303	PEE	O4-C10-O2-C2
48	l	705	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
52	V	201	CDL	CB2-C1-CA2-OA2
52	a	201	CDL	CA2-C1-CB2-OB2
52	g	202	CDL	CB2-C1-CA2-OA2
52	l	703	CDL	CB2-C1-CA2-OA2
48	W	201	PEE	C31-C30-O3-C3
52	l	703	CDL	C71-CB7-OB8-CB6
52	o	201	CDL	C31-CA7-OA8-CA6
50	C	204	PLX	C25-C26-C27-C28
52	l	703	CDL	C37-C38-C39-C40
52	a	201	CDL	O1-C1-CA2-OA2
52	l	703	CDL	OB9-CB7-OB8-CB6
52	o	201	CDL	OA9-CA7-OA8-CA6
52	V	201	CDL	OA7-CA5-OA6-CA4
52	s	402	CDL	C51-CB5-OB6-CB4
52	l	703	CDL	C61-C62-C63-C64
54	J	402	UQ	C17-C18-C19-C20
48	l	705	PEE	C34-C35-C36-C37
48	l	705	PEE	C37-C38-C39-C40
54	J	402	UQ	C7-C8-C9-C11
47	A	503	NAI	O4D-C4D-C5D-O5D
52	I	201	CDL	CA7-C31-C32-C33
52	k	101	CDL	CA5-C11-C12-C13
49	C	201	UQ1	C7-C8-C9-C11
54	J	402	UQ	C14-C16-C17-C18
52	g	202	CDL	C74-C75-C76-C77
52	l	703	CDL	C11-C12-C13-C14
50	g	201	PLX	C2-C1-N1-C1A
52	V	201	CDL	CA7-C31-C32-C33
52	V	201	CDL	CB7-C71-C72-C73
52	k	101	CDL	CA7-C31-C32-C33
48	W	201	PEE	O5-C30-O3-C3
52	o	201	CDL	C51-CB5-OB6-CB4
52	s	402	CDL	C14-C15-C16-C17
52	g	202	CDL	CB5-C51-C52-C53
52	l	702	CDL	CB5-C51-C52-C53
52	k	101	CDL	C43-C44-C45-C46
52	V	201	CDL	O1-C1-CB2-OB2
52	o	201	CDL	O1-C1-CB2-OB2
48	l	704	PEE	C31-C30-O3-C3
52	l	703	CDL	CB7-C71-C72-C73
52	s	402	CDL	CB7-C71-C72-C73
52	u	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
52	l	703	CDL	C51-C52-C53-C54
48	C	203	PEE	C11-C10-O2-C2
48	B	303	PEE	C34-C35-C36-C37
50	C	204	PLX	C27-C28-C29-C30
48	C	203	PEE	O4-C10-O2-C2
52	o	201	CDL	OB7-CB5-OB6-CB4
52	s	402	CDL	OB7-CB5-OB6-CB4
52	V	201	CDL	CA2-C1-CB2-OB2
52	l	703	CDL	CA2-C1-CB2-OB2
50	g	201	PLX	C2-C1-N1-C1B
52	l	702	CDL	C32-C33-C34-C35
48	B	303	PEE	C17-C18-C19-C20
52	s	402	CDL	O1-C1-CA2-OA2
52	g	202	CDL	CB7-C71-C72-C73
52	a	201	CDL	C34-C35-C36-C37
48	l	704	PEE	O5-C30-O3-C3
48	l	701	PEE	C11-C10-O2-C2
52	I	201	CDL	CB7-C71-C72-C73
48	i	401	PEE	C12-C13-C14-C15
48	r	501	PEE	C31-C32-C33-C34
50	j	202	PLX	C14-C15-C16-C17
51	X	201	8Q1	C12-C13-C14-C15
52	V	201	CDL	C37-C38-C39-C40
52	a	201	CDL	C62-C63-C64-C65
52	o	201	CDL	C14-C15-C16-C17
52	u	201	CDL	C75-C76-C77-C78
50	J	403	PLX	C34-C35-C36-C37
52	V	201	CDL	C73-C74-C75-C76
50	C	204	PLX	O7-C6-C7-C8
50	J	403	PLX	O9-C24-C25-C26
48	l	705	PEE	C13-C14-C15-C16
50	J	403	PLX	C14-C15-C16-C17
50	J	403	PLX	C26-C27-C28-C29
52	V	201	CDL	C32-C33-C34-C35
52	a	201	CDL	C21-C22-C23-C24
52	a	201	CDL	C60-C61-C62-C63
52	k	101	CDL	C37-C38-C39-C40
52	l	703	CDL	C32-C33-C34-C35
48	l	701	PEE	O4-C10-O2-C2
48	r	501	PEE	C20-C21-C22-C23
50	a	202	PLX	C31-C32-C33-C34
52	l	703	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
50	C	204	PLX	C14-C15-C16-C17
52	u	201	CDL	C55-C56-C57-C58
52	I	201	CDL	C11-C12-C13-C14
50	C	204	PLX	C10-C11-C12-C13
50	g	201	PLX	C30-C31-C32-C33
48	l	705	PEE	C10-C11-C12-C13
52	s	402	CDL	CA7-C31-C32-C33
53	J	401	NDP	C3D-C4D-C5D-O5D
58	w	401	ADP	C3'-C4'-C5'-O5'
48	C	203	PEE	C11-C12-C13-C14
48	j	201	PEE	C12-C13-C14-C15
50	C	204	PLX	C28-C29-C30-C31
50	e	201	PLX	C25-C26-C27-C28
52	g	202	CDL	C83-C84-C85-C86
50	a	202	PLX	C12-C13-C14-C15
51	X	201	8Q1	C11-C10-C9-C8
52	k	101	CDL	C36-C37-C38-C39
52	o	201	CDL	C59-C60-C61-C62
52	o	201	CDL	CA5-C11-C12-C13
52	g	202	CDL	C14-C15-C16-C17
48	j	201	PEE	C11-C12-C13-C14
50	e	201	PLX	C29-C30-C31-C32
50	j	202	PLX	C12-C13-C14-C15
52	a	201	CDL	C22-C23-C24-C25
52	u	201	CDL	C71-C72-C73-C74
52	l	703	CDL	CA3-CA4-CA6-OA8
48	j	201	PEE	C23-C24-C25-C26
50	J	403	PLX	C31-C32-C33-C34
50	j	202	PLX	C7-C8-C9-C10
52	V	201	CDL	C75-C76-C77-C78
52	g	202	CDL	C62-C63-C64-C65
48	r	501	PEE	C23-C24-C25-C26
48	s	401	PEE	C11-C12-C13-C14
50	J	403	PLX	C13-C14-C15-C16
50	j	202	PLX	C33-C34-C35-C36
52	g	202	CDL	C43-C44-C45-C46
52	l	702	CDL	C75-C76-C77-C78
52	o	201	CDL	C11-C12-C13-C14
52	o	201	CDL	C17-C18-C19-C20
52	o	201	CDL	C42-C43-C44-C45
48	B	303	PEE	C20-C21-C22-C23
50	g	201	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
52	a	201	CDL	C51-C52-C53-C54
48	r	501	PEE	C14-C15-C16-C17
50	g	201	PLX	C9-C10-C11-C12
50	g	201	PLX	C28-C29-C30-C31
52	s	402	CDL	C35-C36-C37-C38
48	l	704	PEE	C21-C22-C23-C24
48	l	704	PEE	C32-C33-C34-C35
50	C	204	PLX	C11-C12-C13-C14
52	V	201	CDL	C56-C57-C58-C59
52	g	202	CDL	C34-C35-C36-C37
50	J	403	PLX	C7-C8-C9-C10
52	V	201	CDL	C55-C56-C57-C58
52	s	402	CDL	C11-CA5-OA6-CA4
48	s	401	PEE	C36-C37-C38-C39
48	l	705	PEE	C19-C20-C21-C22
48	j	201	PEE	C31-C30-O3-C3
50	g	201	PLX	C11-C10-C9-C8
52	a	201	CDL	C54-C55-C56-C57
52	s	402	CDL	C32-C33-C34-C35
48	s	401	PEE	C10-C11-C12-C13
52	u	201	CDL	CB7-C71-C72-C73
52	k	101	CDL	C33-C34-C35-C36
52	l	703	CDL	C72-C73-C74-C75
52	s	402	CDL	C71-C72-C73-C74
52	s	402	CDL	C73-C74-C75-C76
52	s	402	CDL	C82-C83-C84-C85
50	C	204	PLX	C11-C10-C9-C8
52	k	101	CDL	C42-C43-C44-C45
52	o	201	CDL	C75-C76-C77-C78
52	V	201	CDL	C52-C53-C54-C55
52	g	202	CDL	C54-C55-C56-C57
52	g	202	CDL	C77-C78-C79-C80
52	l	703	CDL	C55-C56-C57-C58
50	a	202	PLX	C14-C15-C16-C17
52	g	202	CDL	C57-C58-C59-C60
52	k	101	CDL	C15-C16-C17-C18
52	o	201	CDL	C60-C61-C62-C63
52	a	201	CDL	CA5-C11-C12-C13
52	a	201	CDL	C71-CB7-OB8-CB6
52	a	201	CDL	C11-C12-C13-C14
52	k	101	CDL	C21-C22-C23-C24
52	k	101	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C58-C59-C60-C61
50	J	403	PLX	C20-C21-C22-C23
52	l	702	CDL	C71-C72-C73-C74
52	s	402	CDL	C75-C76-C77-C78
48	s	401	PEE	C12-C13-C14-C15
50	g	201	PLX	C14-C15-C16-C17
50	a	202	PLX	C7-C8-C9-C10
51	X	201	8Q1	C11-C12-C13-C14
52	s	402	CDL	C52-C53-C54-C55
52	g	202	CDL	CA7-C31-C32-C33
50	j	202	PLX	C9-C10-C11-C12
50	e	201	PLX	C14-C15-C16-C17
50	e	201	PLX	C13-C14-C15-C16
50	e	201	PLX	C28-C29-C30-C31
52	o	201	CDL	C12-C13-C14-C15
52	o	201	CDL	C37-C38-C39-C40
52	l	702	CDL	C11-CA5-OA6-CA4
52	l	703	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	C31-C32-C33-C34
48	W	201	PEE	C19-C20-C21-C22
48	i	401	PEE	C19-C20-C21-C22
48	C	203	PEE	C42-C43-C44-C45
50	a	202	PLX	C13-C14-C15-C16
48	B	303	PEE	C12-C13-C14-C15
50	C	204	PLX	C33-C34-C35-C36
50	J	403	PLX	C33-C34-C35-C36
52	a	201	CDL	C81-C82-C83-C84
47	A	503	NAI	O4B-C4B-C5B-O5B
52	k	101	CDL	C20-C21-C22-C23
52	o	201	CDL	C55-C56-C57-C58
50	g	201	PLX	C2-C1-N1-C1C
52	k	101	CDL	C34-C35-C36-C37
52	l	702	CDL	C51-C52-C53-C54
50	J	403	PLX	C27-C28-C29-C30
52	k	101	CDL	C78-C79-C80-C81
52	u	201	CDL	C56-C57-C58-C59
52	u	201	CDL	C73-C74-C75-C76
52	g	202	CDL	C35-C36-C37-C38
52	g	202	CDL	C41-C42-C43-C44
48	l	704	PEE	O3P-C1-C2-O2
52	k	101	CDL	OA5-CA3-CA4-OA6
48	r	501	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
52	k	101	CDL	C11-C12-C13-C14
52	o	201	CDL	C32-C33-C34-C35
50	g	201	PLX	C10-C11-C12-C13
52	V	201	CDL	C31-C32-C33-C34
52	l	703	CDL	CA7-C31-C32-C33
52	g	202	CDL	C75-C76-C77-C78
48	B	303	PEE	C35-C36-C37-C38
52	l	703	CDL	OA6-CA4-CA6-OA8
52	o	201	CDL	OB6-CB4-CB6-OB8
52	s	402	CDL	OB6-CB4-CB6-OB8
52	l	703	CDL	C40-C41-C42-C43
48	j	201	PEE	O5-C30-O3-C3
50	J	403	PLX	C30-C31-C32-C33
52	a	201	CDL	C33-C34-C35-C36
52	o	201	CDL	C74-C75-C76-C77
52	s	402	CDL	C51-C52-C53-C54
48	i	401	PEE	C18-C19-C20-C21
48	r	501	PEE	C36-C37-C38-C39
50	a	202	PLX	C15-C16-C17-C18
52	V	201	CDL	C43-C44-C45-C46
52	V	201	CDL	C1-CB2-OB2-PB2
52	V	201	CDL	C71-C72-C73-C74
52	u	201	CDL	CA2-C1-CB2-OB2
48	C	203	PEE	C13-C14-C15-C16
48	C	203	PEE	C32-C33-C34-C35
52	g	202	CDL	C11-C12-C13-C14
50	J	403	PLX	C35-C36-C37-C38
50	C	204	PLX	C7-C8-C9-C10
52	o	201	CDL	C54-C55-C56-C57
52	a	201	CDL	OB9-CB7-OB8-CB6
50	j	202	PLX	C30-C31-C32-C33
52	a	201	CDL	C32-C33-C34-C35
52	u	201	CDL	C74-C75-C76-C77
48	W	201	PEE	C15-C16-C17-C18
52	o	201	CDL	C34-C35-C36-C37
52	I	201	CDL	OA5-CA3-CA4-CA6
52	l	703	CDL	OB5-CB3-CB4-CB6
52	l	702	CDL	OA7-CA5-OA6-CA4
52	l	703	CDL	OB7-CB5-OB6-CB4
52	s	402	CDL	OA7-CA5-OA6-CA4
52	k	101	CDL	C75-C76-C77-C78
52	k	101	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
52	l	703	CDL	C59-C60-C61-C62
50	a	202	PLX	C34-C35-C36-C37
52	a	201	CDL	C53-C54-C55-C56
47	A	503	NAI	C3B-C4B-C5B-O5B
53	J	401	NDP	O4B-C4B-C5B-O5B
52	o	201	CDL	C40-C41-C42-C43
49	C	201	UQ1	C7-C8-C9-C10
52	k	101	CDL	C32-C33-C34-C35
50	J	403	PLX	O8-C24-C25-C26
48	W	201	PEE	C22-C23-C24-C25
52	V	201	CDL	C14-C15-C16-C17
52	k	101	CDL	C71-CB7-OB8-CB6
52	s	402	CDL	C12-C13-C14-C15
48	r	501	PEE	O4-C10-O2-C2
48	W	201	PEE	C1-C2-C3-O3
50	a	202	PLX	C3-C4-C5-O8
50	e	201	PLX	C3-C4-C5-O8
52	g	202	CDL	CA3-CA4-CA6-OA8
52	s	402	CDL	CB3-CB4-CB6-OB8
48	C	203	PEE	C15-C16-C17-C18
48	r	501	PEE	C39-C40-C41-C42
48	s	401	PEE	C23-C24-C25-C26
52	V	201	CDL	C51-C52-C53-C54
52	s	402	CDL	C37-C38-C39-C40
50	g	201	PLX	C32-C33-C34-C35
52	g	202	CDL	C60-C61-C62-C63
52	s	402	CDL	C17-C18-C19-C20
52	k	101	CDL	C81-C82-C83-C84
52	l	702	CDL	C74-C75-C76-C77
48	r	501	PEE	C22-C23-C24-C25
46	A	502	FMN	C5'-O5'-P-O1P
52	o	201	CDL	C77-C78-C79-C80
48	l	704	PEE	C44-C45-C46-C47
52	a	201	CDL	C52-C53-C54-C55
52	V	201	CDL	C44-C45-C46-C47
50	e	201	PLX	C7-C8-C9-C10
50	e	201	PLX	C30-C31-C32-C33
52	u	201	CDL	C72-C73-C74-C75
48	r	501	PEE	C15-C16-C17-C18
48	s	401	PEE	C19-C20-C21-C22
48	s	401	PEE	C35-C36-C37-C38
50	a	202	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
50	a	202	PLX	C27-C28-C29-C30
50	e	201	PLX	C10-C11-C12-C13
52	a	201	CDL	C37-C38-C39-C40
52	V	201	CDL	OA5-CA3-CA4-OA6
52	l	703	CDL	OA5-CA3-CA4-OA6
52	g	202	CDL	C37-C38-C39-C40
48	B	303	PEE	C31-C30-O3-C3
48	W	201	PEE	C11-C10-O2-C2
52	k	101	CDL	C84-C85-C86-C87
50	e	201	PLX	C11-C12-C13-C14
50	a	202	PLX	C25-C26-C27-C28
52	s	402	CDL	C33-C34-C35-C36
51	X	201	8Q1	C7-C8-C9-C10
52	I	201	CDL	C51-C52-C53-C54
52	V	201	CDL	C57-C58-C59-C60
52	a	201	CDL	C71-C72-C73-C74
50	C	204	PLX	O6-C4-C5-O8
52	g	202	CDL	OA6-CA4-CA6-OA8
53	J	401	NDP	C2D-C1D-N1N-C6N
48	j	201	PEE	C21-C22-C23-C24
50	a	202	PLX	C16-C17-C18-C19
52	g	202	CDL	C32-C33-C34-C35
48	C	203	PEE	C39-C40-C41-C42
51	G	201	8Q1	C31-C29-C32-O33
52	l	703	CDL	C73-C74-C75-C76
52	l	703	CDL	C38-C39-C40-C41
52	g	202	CDL	C64-C65-C66-C67
52	o	201	CDL	C84-C85-C86-C87
48	i	401	PEE	C37-C38-C39-C40
48	s	401	PEE	C37-C38-C39-C40
52	V	201	CDL	C53-C54-C55-C56
52	s	402	CDL	C36-C37-C38-C39
52	a	201	CDL	C64-C65-C66-C67
48	C	203	PEE	C34-C35-C36-C37
48	r	501	PEE	C12-C13-C14-C15
50	e	201	PLX	C12-C13-C14-C15
50	e	201	PLX	C31-C32-C33-C34
52	g	202	CDL	C59-C60-C61-C62
48	B	303	PEE	C38-C39-C40-C41
52	o	201	CDL	C1-CB2-OB2-PB2
50	g	201	PLX	C12-C13-C14-C15
48	s	401	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
50	C	204	PLX	C13-C14-C15-C16
51	G	201	8Q1	C11-C10-C9-C8
52	I	201	CDL	C12-C13-C14-C15
48	B	303	PEE	O3P-C1-C2-C3
48	i	401	PEE	O3P-C1-C2-C3
48	l	704	PEE	O3P-C1-C2-C3
52	I	201	CDL	OB5-CB3-CB4-CB6
52	k	101	CDL	OA5-CA3-CA4-CA6
52	s	402	CDL	OA5-CA3-CA4-CA6
52	k	101	CDL	OB9-CB7-OB8-CB6
48	s	401	PEE	C44-C45-C46-C47
48	r	501	PEE	C24-C25-C26-C27
50	j	202	PLX	C34-C35-C36-C37
52	a	201	CDL	C35-C36-C37-C38
48	C	203	PEE	C20-C21-C22-C23
48	B	303	PEE	C23-C24-C25-C26
52	l	703	CDL	C71-C72-C73-C74
52	l	702	CDL	C71-CB7-OB8-CB6
52	g	202	CDL	C84-C85-C86-C87
48	l	704	PEE	C13-C14-C15-C16
51	G	201	8Q1	C9-C10-C11-C12
48	l	704	PEE	C15-C16-C17-C18
52	k	101	CDL	C14-C15-C16-C17
52	l	702	CDL	C36-C37-C38-C39
52	s	402	CDL	C59-C60-C61-C62
52	I	201	CDL	C31-CA7-OA8-CA6
50	e	201	PLX	C27-C28-C29-C30
48	C	203	PEE	C1-C2-C3-O3
48	j	201	PEE	C1-C2-C3-O3
48	l	704	PEE	C1-C2-C3-O3
48	l	705	PEE	C1-C2-C3-O3
50	j	202	PLX	C3-C4-C5-O8
52	V	201	CDL	CA3-CA4-CA6-OA8
52	o	201	CDL	CB3-CB4-CB6-OB8
52	u	201	CDL	C54-C55-C56-C57
48	l	701	PEE	C31-C32-C33-C34
52	V	201	CDL	C72-C73-C74-C75
52	a	201	CDL	C14-C15-C16-C17
52	l	703	CDL	C80-C81-C82-C83
52	g	202	CDL	C12-C13-C14-C15
52	l	702	CDL	C53-C54-C55-C56
52	s	402	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
52	l	703	CDL	C64-C65-C66-C67
48	B	303	PEE	C13-C14-C15-C16
52	s	402	CDL	C54-C55-C56-C57
48	C	203	PEE	C12-C13-C14-C15
52	g	202	CDL	C1-CB2-OB2-PB2
52	l	702	CDL	C56-C57-C58-C59
50	J	403	PLX	C36-C37-C38-C39
52	l	702	CDL	C16-C17-C18-C19
52	s	402	CDL	C55-C56-C57-C58
52	V	201	CDL	C74-C75-C76-C77
52	s	402	CDL	C61-C62-C63-C64
48	B	303	PEE	C40-C41-C42-C43
48	C	203	PEE	O2-C2-C3-O3
48	l	705	PEE	O2-C2-C3-O3
50	j	202	PLX	O6-C4-C5-O8
52	V	201	CDL	OA6-CA4-CA6-OA8
52	k	101	CDL	OB6-CB4-CB6-OB8
52	l	702	CDL	C81-C82-C83-C84
48	B	303	PEE	O5-C30-O3-C3
52	a	201	CDL	C17-C18-C19-C20
48	s	401	PEE	C21-C22-C23-C24
50	a	202	PLX	O8-C24-C25-C26
50	e	201	PLX	O8-C24-C25-C26
48	r	501	PEE	C21-C22-C23-C24
50	C	204	PLX	C31-C32-C33-C34
50	a	202	PLX	C11-C12-C13-C14
48	l	701	PEE	C10-C11-C12-C13
48	i	401	PEE	C24-C25-C26-C27
48	j	201	PEE	C15-C16-C17-C18
50	g	201	PLX	C25-C26-C27-C28
50	g	201	PLX	C13-C14-C15-C16
48	l	704	PEE	C11-C12-C13-C14
50	g	201	PLX	C33-C34-C35-C36
48	l	704	PEE	C30-C31-C32-C33
52	V	201	CDL	C64-C65-C66-C67
48	W	201	PEE	C13-C14-C15-C16
52	l	703	CDL	C44-C45-C46-C47
50	j	202	PLX	C28-C29-C30-C31
52	o	201	CDL	CB2-C1-CA2-OA2
52	V	201	CDL	C54-C55-C56-C57
52	l	703	CDL	C62-C63-C64-C65
50	J	403	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
50	J	403	PLX	O4-C3-C4-C5
52	V	201	CDL	OA5-CA3-CA4-CA6
52	l	703	CDL	OA5-CA3-CA4-CA6
52	o	201	CDL	OB5-CB3-CB4-CB6
52	g	202	CDL	C52-C53-C54-C55
48	r	501	PEE	C38-C39-C40-C41
50	a	202	PLX	C36-C37-C38-C39
52	s	402	CDL	C57-C58-C59-C60
52	o	201	CDL	C53-C54-C55-C56
51	X	201	8Q1	C28-O27-P24-O2
48	j	201	PEE	C22-C23-C24-C25
52	l	703	CDL	C57-C58-C59-C60
52	a	201	CDL	C11-CA5-OA6-CA4
48	W	201	PEE	O4-C10-O2-C2
50	j	202	PLX	C10-C11-C12-C13
48	j	201	PEE	C13-C14-C15-C16
52	o	201	CDL	C76-C77-C78-C79
52	o	201	CDL	C83-C84-C85-C86
50	J	403	PLX	C19-C20-C21-C22
50	e	201	PLX	C35-C36-C37-C38
52	V	201	CDL	CA6-CA4-OA6-CA5
52	a	201	CDL	C84-C85-C86-C87
50	g	201	PLX	C7-C8-C9-C10
48	B	303	PEE	O3P-C1-C2-O2
48	i	401	PEE	O3P-C1-C2-O2
50	J	403	PLX	O4-C3-C4-O6
52	l	703	CDL	OB5-CB3-CB4-OB6
50	g	201	PLX	C18-C19-C20-C21
52	k	101	CDL	CB3-CB4-CB6-OB8
52	I	201	CDL	C51-CB5-OB6-CB4
50	J	403	PLX	C9-C10-C11-C12
52	g	202	CDL	C44-C45-C46-C47
48	r	501	PEE	C5-C4-O4P-P
50	J	403	PLX	C1-C2-O1-P1
54	J	402	UQ	C1-C6-C7-C8
52	I	201	CDL	OA9-CA7-OA8-CA6
48	W	201	PEE	O2-C2-C3-O3
48	j	201	PEE	O2-C2-C3-O3
48	l	704	PEE	O2-C2-C3-O3
50	J	403	PLX	O6-C4-C5-O8
50	a	202	PLX	O6-C4-C5-O8
52	u	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
52	g	202	CDL	C71-C72-C73-C74
48	l	704	PEE	C24-C25-C26-C27
50	j	202	PLX	C7-C6-O6-C4
52	k	101	CDL	C74-C75-C76-C77
52	u	201	CDL	C52-C53-C54-C55
48	B	303	PEE	C44-C45-C46-C47
50	C	204	PLX	N1-C1-C2-O1
48	l	704	PEE	C31-C32-C33-C34
52	s	402	CDL	CA2-C1-CB2-OB2
52	g	202	CDL	C58-C59-C60-C61
48	W	201	PEE	C17-C18-C19-C20
48	W	201	PEE	C12-C13-C14-C15
52	l	702	CDL	C82-C83-C84-C85
50	C	204	PLX	C25-C24-O8-C5
50	a	202	PLX	C25-C24-O8-C5
50	j	202	PLX	C16-C17-C18-C19
52	s	402	CDL	C80-C81-C82-C83
52	I	201	CDL	OB7-CB5-OB6-CB4
52	a	201	CDL	OA7-CA5-OA6-CA4
51	G	201	8Q1	C11-C12-C13-C14
52	o	201	CDL	O1-C1-CA2-OA2
50	e	201	PLX	C16-C17-C18-C19
52	g	202	CDL	C15-C16-C17-C18
52	l	702	CDL	OB9-CB7-OB8-CB6
51	X	201	8Q1	C42-C43-S44-C1
48	r	501	PEE	C44-C45-C46-C47
52	I	201	CDL	OB5-CB3-CB4-OB6
52	g	202	CDL	C17-C18-C19-C20
52	k	101	CDL	C40-C41-C42-C43
52	g	202	CDL	C39-C40-C41-C42
48	B	303	PEE	C41-C42-C43-C44
50	j	202	PLX	C11-C12-C13-C14
52	a	201	CDL	C82-C83-C84-C85
52	s	402	CDL	OB9-CB7-OB8-CB6
48	i	401	PEE	O2-C2-C3-O3
50	e	201	PLX	O6-C4-C5-O8
52	k	101	CDL	C22-C23-C24-C25
52	a	201	CDL	C44-C45-C46-C47
50	C	204	PLX	C16-C17-C18-C19
52	s	402	CDL	C74-C75-C76-C77
52	s	402	CDL	C71-CB7-OB8-CB6
52	k	101	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
50	a	202	PLX	C10-C11-C12-C13
52	a	201	CDL	C57-C58-C59-C60
52	l	703	CDL	C43-C44-C45-C46
47	A	503	NAI	C5B-O5B-PA-O2A
48	C	203	PEE	C1-O3P-P-O2P
48	C	203	PEE	C4-O4P-P-O2P
48	i	401	PEE	C1-O3P-P-O1P
48	l	704	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O2P
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
50	C	204	PLX	C2-O1-P1-O3
50	J	403	PLX	C3-C4-O6-C6
50	J	403	PLX	C5-C4-O6-C6
50	J	403	PLX	C2-O1-P1-O4
50	J	403	PLX	C2-O1-P1-O3
50	g	201	PLX	C3-O4-P1-O1
50	g	201	PLX	C3-O4-P1-O3
51	G	201	8Q1	C28-C29-C32-O33
52	I	201	CDL	CB2-OB2-PB2-OB4
52	I	201	CDL	CB3-OB5-PB2-OB2
52	I	201	CDL	CB3-OB5-PB2-OB4
52	V	201	CDL	CA3-OA5-PA1-OA2
52	V	201	CDL	CA3-OA5-PA1-OA3
52	a	201	CDL	CA2-OA2-PA1-OA3
52	a	201	CDL	CB2-OB2-PB2-OB4
52	a	201	CDL	CB3-OB5-PB2-OB2
52	a	201	CDL	CB3-OB5-PB2-OB3
52	g	202	CDL	CA2-OA2-PA1-OA4
52	g	202	CDL	CA2-OA2-PA1-OA5
52	g	202	CDL	CA3-OA5-PA1-OA3
52	g	202	CDL	CB3-OB5-PB2-OB4
52	k	101	CDL	CB3-OB5-PB2-OB4
52	l	702	CDL	CA3-OA5-PA1-OA4
52	l	702	CDL	CB2-OB2-PB2-OB4
52	o	201	CDL	CB2-OB2-PB2-OB3
52	u	201	CDL	CA3-OA5-PA1-OA2
52	u	201	CDL	CA3-OA5-PA1-OA3
52	u	201	CDL	CB3-OB5-PB2-OB3
58	w	401	ADP	C5'-O5'-PA-O2A
50	j	202	PLX	C29-C30-C31-C32
52	l	702	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
48	s	401	PEE	O2-C10-C11-C12
48	l	701	PEE	C36-C37-C38-C39
52	k	101	CDL	CA6-CA4-OA6-CA5
52	l	703	CDL	C12-C11-CA5-OA6
54	s	403	UQ	C9-C11-C12-C13
52	l	702	CDL	CA5-C11-C12-C13
52	k	101	CDL	C71-C72-C73-C74
48	l	704	PEE	C14-C15-C16-C17
48	s	401	PEE	C22-C23-C24-C25
52	a	201	CDL	C23-C24-C25-C26
48	j	201	PEE	C18-C19-C20-C21
53	J	401	NDP	O4D-C1D-N1N-C6N
52	k	101	CDL	C16-C17-C18-C19
48	l	701	PEE	O2-C2-C3-O3
52	o	201	CDL	C24-C25-C26-C27
48	l	701	PEE	C18-C19-C20-C21
52	g	202	CDL	C51-C52-C53-C54
48	j	201	PEE	C24-C25-C26-C27
50	J	403	PLX	C2-C1-N1-C1A
50	g	201	PLX	C34-C35-C36-C37
50	J	403	PLX	C17-C18-C19-C20
52	k	101	CDL	C58-C59-C60-C61
50	C	204	PLX	C3-C4-C5-O8
50	J	403	PLX	C3-C4-C5-O8
48	l	701	PEE	O3-C30-C31-C32
52	V	201	CDL	C32-C31-CA7-OA8
52	s	402	CDL	C56-C57-C58-C59
48	l	704	PEE	C36-C37-C38-C39
54	J	402	UQ	C5-C6-C7-C8
50	e	201	PLX	C24-C25-C26-C27
52	s	402	CDL	C16-C17-C18-C19
50	j	202	PLX	O6-C6-C7-C8
52	s	402	CDL	C34-C35-C36-C37
52	s	402	CDL	CB2-C1-CA2-OA2
48	l	705	PEE	C14-C15-C16-C17
50	g	201	PLX	C31-C32-C33-C34
52	l	703	CDL	C60-C61-C62-C63
48	i	401	PEE	C11-C12-C13-C14
52	l	702	CDL	C14-C15-C16-C17
48	C	203	PEE	C44-C45-C46-C47
48	s	401	PEE	C38-C39-C40-C41
52	g	202	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
48	C	203	PEE	C16-C17-C18-C19
52	V	201	CDL	C36-C37-C38-C39
52	s	402	CDL	C77-C78-C79-C80
52	k	101	CDL	CA4-CA3-OA5-PA1
50	g	201	PLX	C19-C20-C21-C22
52	s	402	CDL	C31-C32-C33-C34
52	I	201	CDL	C52-C53-C54-C55
52	o	201	CDL	C33-C34-C35-C36
48	l	705	PEE	C16-C17-C18-C19
50	g	201	PLX	C11-C12-C13-C14
48	B	303	PEE	C21-C22-C23-C24
48	l	704	PEE	C3-C2-O2-C10
48	s	401	PEE	C41-C42-C43-C44
47	A	503	NAI	O4D-C1D-N1N-C2N
52	u	201	CDL	C51-C52-C53-C54
48	i	401	PEE	C22-C23-C24-C25
48	s	401	PEE	C31-C32-C33-C34
52	o	201	CDL	CA7-C31-C32-C33
50	g	201	PLX	C17-C18-C19-C20
52	l	702	CDL	C76-C77-C78-C79
48	i	401	PEE	C2-C1-O3P-P
48	W	201	PEE	C23-C24-C25-C26
52	g	202	CDL	C33-C34-C35-C36
50	e	201	PLX	C19-C20-C21-C22
50	C	204	PLX	C32-C33-C34-C35
52	k	101	CDL	C56-C57-C58-C59
52	l	703	CDL	C82-C83-C84-C85
52	a	201	CDL	C18-C19-C20-C21
50	e	201	PLX	C26-C27-C28-C29
48	C	203	PEE	C36-C37-C38-C39
48	i	401	PEE	C38-C39-C40-C41
48	l	704	PEE	C16-C17-C18-C19
52	l	703	CDL	C13-C14-C15-C16
50	e	201	PLX	C2-C1-N1-C1B
48	l	704	PEE	C42-C43-C44-C45
53	J	401	NDP	C2B-O2B-P2B-O1X
48	s	401	PEE	C34-C35-C36-C37
50	C	204	PLX	C26-C27-C28-C29
50	g	201	PLX	O6-C6-C7-C8
52	k	101	CDL	C31-C32-C33-C34
52	l	703	CDL	C17-C18-C19-C20
52	V	201	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C33-C34-C35-C36
52	u	201	CDL	CA3-CA4-CA6-OA8
50	C	204	PLX	O9-C24-C25-C26
52	g	202	CDL	C72-C71-CB7-OB8
50	e	201	PLX	C36-C37-C38-C39
48	l	704	PEE	C23-C24-C25-C26
52	a	201	CDL	OA5-CA3-CA4-OA6
52	g	202	CDL	C80-C81-C82-C83
52	V	201	CDL	C60-C61-C62-C63
48	l	704	PEE	C38-C39-C40-C41
48	j	201	PEE	O3-C30-C31-C32
52	a	201	CDL	OA5-CA3-CA4-CA6
48	B	303	PEE	C18-C19-C20-C21
48	W	201	PEE	C16-C17-C18-C19
52	o	201	CDL	C52-C53-C54-C55
52	a	201	CDL	C20-C21-C22-C23
52	l	703	CDL	C74-C75-C76-C77
52	s	402	CDL	O1-C1-CB2-OB2
47	A	503	NAI	C2D-C1D-N1N-C2N
52	s	402	CDL	C84-C85-C86-C87
52	l	702	CDL	C31-C32-C33-C34
52	V	201	CDL	C76-C77-C78-C79
52	o	201	CDL	C31-C32-C33-C34
52	l	703	CDL	C58-C59-C60-C61
52	l	703	CDL	C52-C53-C54-C55
48	i	401	PEE	C36-C37-C38-C39
50	j	202	PLX	C19-C20-C21-C22
51	G	201	8Q1	C13-C14-C15-C16
52	k	101	CDL	C83-C84-C85-C86
50	e	201	PLX	C2-C1-N1-C1C
48	C	203	PEE	C43-C44-C45-C46
48	l	701	PEE	C16-C17-C18-C19
48	j	201	PEE	C31-C32-C33-C34
52	s	402	CDL	C11-C12-C13-C14
48	C	203	PEE	C18-C19-C20-C21
48	j	201	PEE	C16-C17-C18-C19
48	l	705	PEE	C2-C1-O3P-P
48	C	203	PEE	C19-C20-C21-C22
48	i	401	PEE	C1-C2-C3-O3
54	J	402	UQ	C9-C11-C12-C13
52	o	201	CDL	C72-C73-C74-C75
52	o	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
52	s	402	CDL	C15-C16-C17-C18
48	B	303	PEE	C16-C17-C18-C19
48	l	701	PEE	C38-C39-C40-C41
48	l	705	PEE	C38-C39-C40-C41
50	j	202	PLX	C36-C37-C38-C39
52	o	201	CDL	C64-C65-C66-C67
50	g	201	PLX	C6-C7-C8-C9
52	a	201	CDL	C61-C62-C63-C64
48	l	704	PEE	C19-C20-C21-C22
48	r	501	PEE	C16-C17-C18-C19
50	a	202	PLX	C29-C30-C31-C32
50	e	201	PLX	C11-C10-C9-C8
52	g	202	CDL	C42-C43-C44-C45
50	e	201	PLX	C2-C1-N1-C1A
50	j	202	PLX	C24-C25-C26-C27
50	C	204	PLX	C19-C20-C21-C22
52	V	201	CDL	CA4-CA3-OA5-PA1
54	J	402	UQ	C19-C21-C22-C23
58	w	401	ADP	PB-O3A-PA-O2A
52	a	201	CDL	C12-C11-CA5-OA6
52	l	702	CDL	C52-C51-CB5-OB6
52	u	201	CDL	C52-C51-CB5-OB6
52	u	201	CDL	C72-C71-CB7-OB8
52	l	703	CDL	C35-C36-C37-C38
52	l	702	CDL	C12-C11-CA5-OA6
52	V	201	CDL	OB7-CB5-OB6-CB4
48	C	203	PEE	O5-C30-O3-C3
52	l	702	CDL	OA5-CA3-CA4-OA6
52	V	201	CDL	C59-C60-C61-C62
50	a	202	PLX	C28-C29-C30-C31
52	a	201	CDL	C32-C31-CA7-OA8
50	e	201	PLX	C9-C10-C11-C12
48	W	201	PEE	C34-C35-C36-C37
50	J	403	PLX	C2-C1-N1-C1C
50	J	403	PLX	C2-C1-N1-C1B
50	e	201	PLX	C25-C24-O8-C5
50	j	202	PLX	C25-C24-O8-C5
48	B	303	PEE	C24-C25-C26-C27
52	l	702	CDL	C55-C56-C57-C58
52	k	101	CDL	C17-C18-C19-C20
52	g	202	CDL	CA5-C11-C12-C13
52	I	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
52	l	702	CDL	C72-C71-CB7-OB8
52	g	202	CDL	C55-C56-C57-C58
52	o	201	CDL	C41-C42-C43-C44
48	B	303	PEE	C33-C34-C35-C36
52	V	201	CDL	C39-C40-C41-C42
52	V	201	CDL	C12-C13-C14-C15
52	o	201	CDL	C15-C16-C17-C18
48	C	203	PEE	C31-C30-O3-C3
52	a	201	CDL	C42-C43-C44-C45
48	r	501	PEE	C34-C35-C36-C37
52	l	702	CDL	C38-C39-C40-C41
50	j	202	PLX	C31-C32-C33-C34
52	s	402	CDL	C76-C77-C78-C79
50	g	201	PLX	O8-C24-C25-C26
50	a	202	PLX	C30-C31-C32-C33
50	C	204	PLX	O9-C24-O8-C5
50	g	201	PLX	O9-C24-O8-C5
52	V	201	CDL	C51-CB5-OB6-CB4
52	a	201	CDL	C12-C11-CA5-OA7
52	l	702	CDL	C52-C51-CB5-OB7
52	l	702	CDL	C12-C11-CA5-OA7
52	u	201	CDL	C52-C51-CB5-OB7
48	l	701	PEE	C1-C2-C3-O3
50	g	201	PLX	C36-C37-C38-C39
52	l	703	CDL	C72-C71-CB7-OB8
52	u	201	CDL	C72-C71-CB7-OB9
51	G	201	8Q1	O27-C28-C29-C32
50	C	204	PLX	C15-C16-C17-C18
52	I	201	CDL	C72-C71-CB7-OB9
52	l	702	CDL	C72-C71-CB7-OB9
48	W	201	PEE	C24-C25-C26-C27
52	a	201	CDL	C32-C31-CA7-OA9
52	a	201	CDL	C55-C56-C57-C58
52	o	201	CDL	C44-C45-C46-C47
48	B	303	PEE	O2-C10-C11-C12
52	l	703	CDL	C32-C31-CA7-OA8
52	s	402	CDL	C72-C71-CB7-OB8
48	i	401	PEE	C35-C36-C37-C38
50	g	201	PLX	C29-C30-C31-C32
52	l	703	CDL	C39-C40-C41-C42

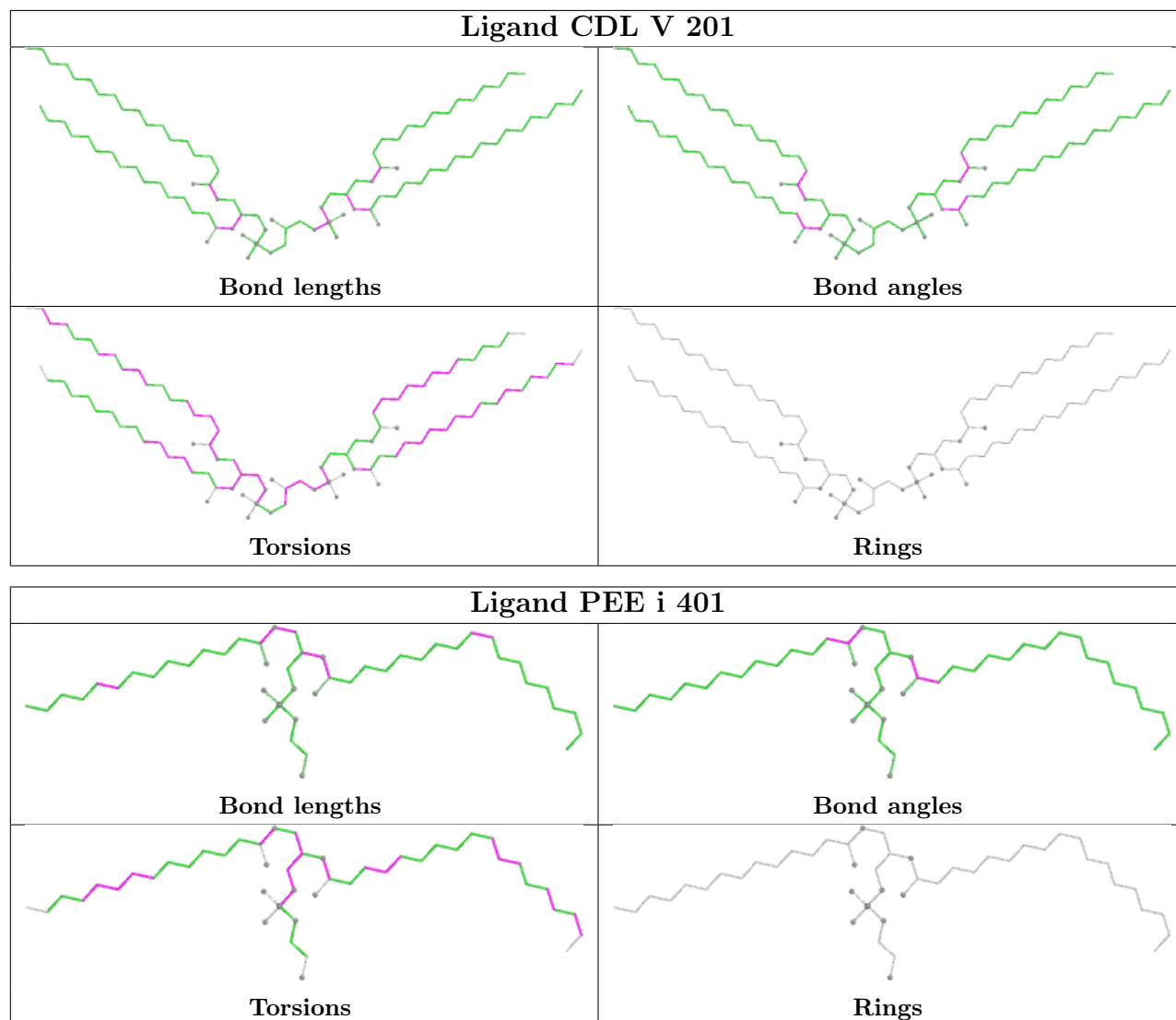
There are no ring outliers.

32 monomers are involved in 138 short contacts:

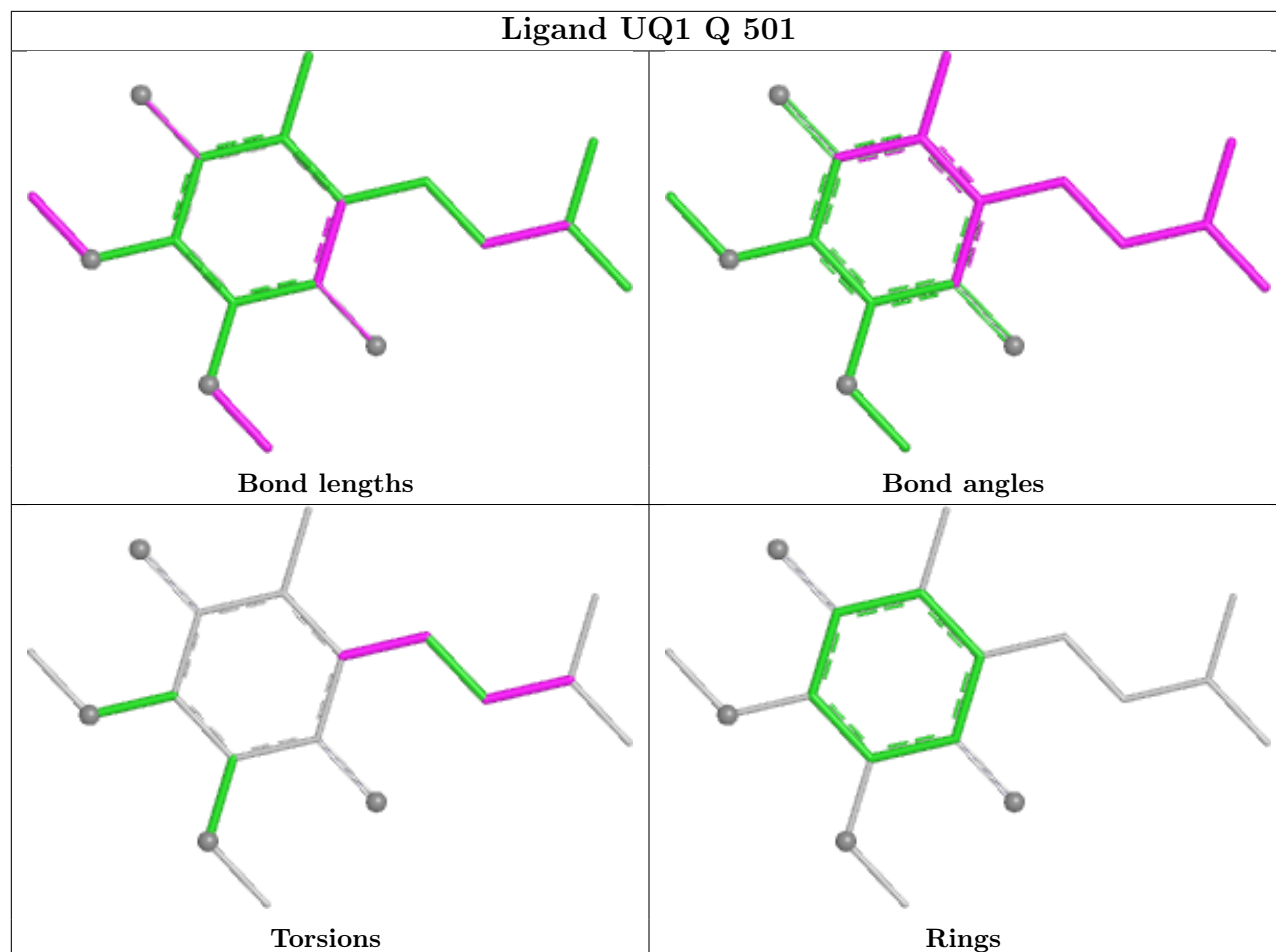
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	V	201	CDL	5	0
48	i	401	PEE	3	0
49	Q	501	UQ1	3	0
48	s	401	PEE	4	0
52	a	201	CDL	3	0
48	j	201	PEE	1	0
52	g	202	CDL	11	0
50	j	202	PLX	3	0
52	k	101	CDL	5	0
50	g	201	PLX	5	0
50	C	204	PLX	3	0
52	l	702	CDL	33	0
52	o	201	CDL	4	0
50	J	403	PLX	4	0
58	w	401	ADP	2	0
54	J	402	UQ	3	0
48	l	705	PEE	4	0
45	C	202	SF4	2	0
48	r	501	PEE	3	0
48	W	201	PEE	1	0
54	s	403	UQ	4	0
50	e	201	PLX	6	0
47	A	503	NAI	4	0
46	A	502	FMN	3	0
53	J	401	NDP	2	0
48	B	303	PEE	1	0
52	l	703	CDL	10	0
51	G	201	8Q1	2	0
45	A	501	SF4	2	0
48	C	203	PEE	1	0
48	l	704	PEE	2	0
52	s	402	CDL	5	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

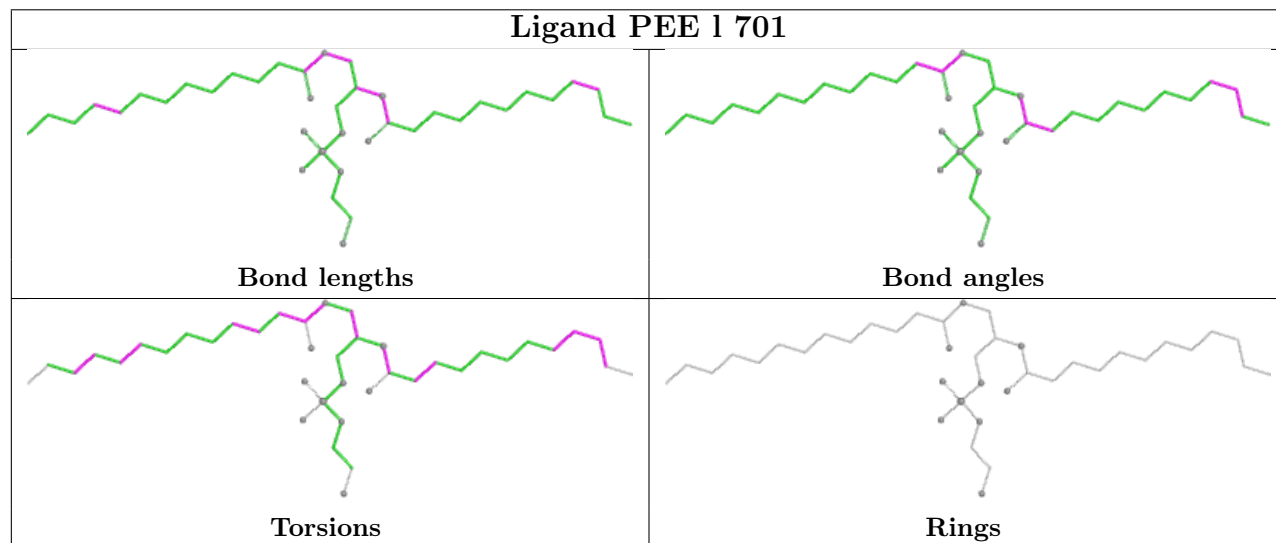
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

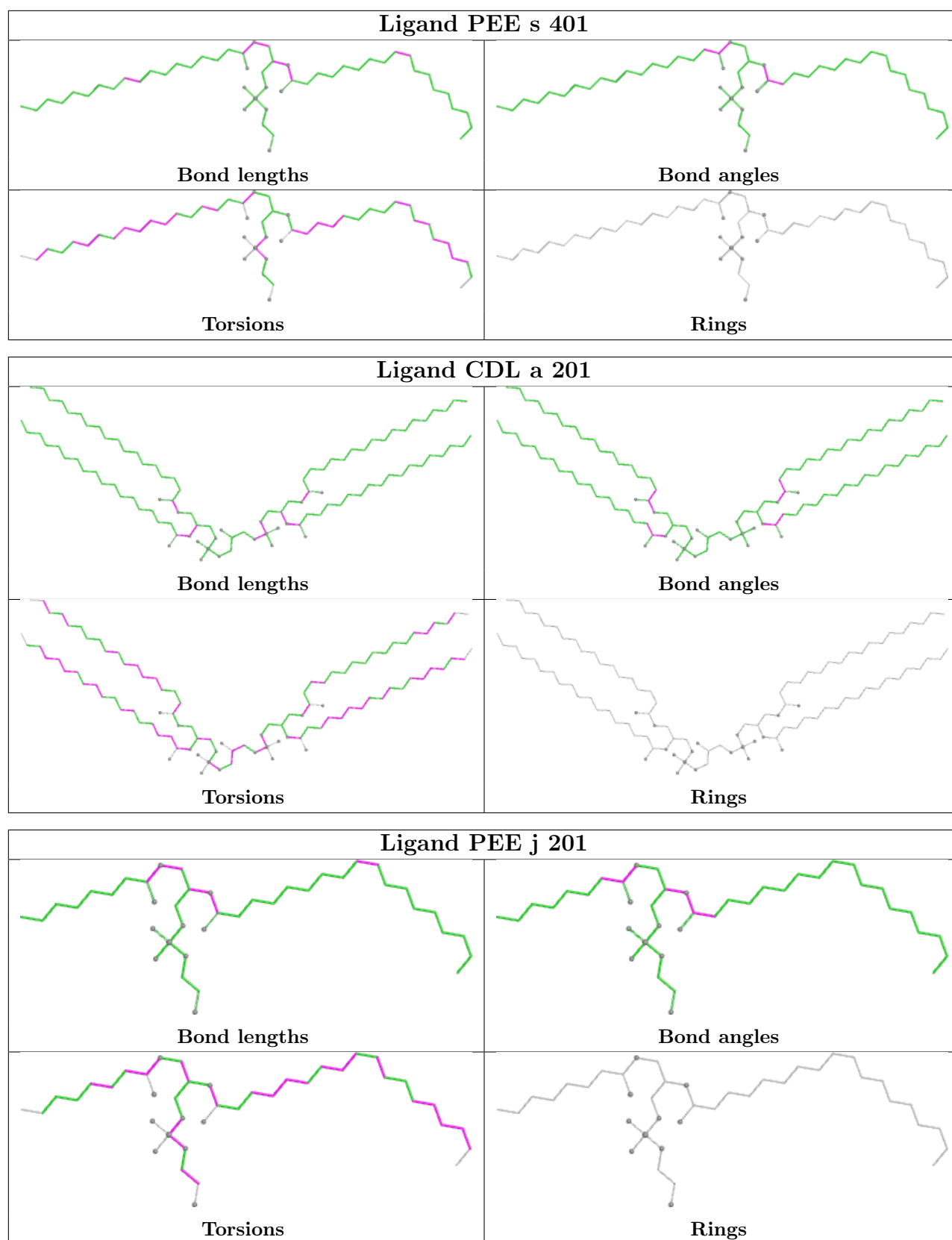


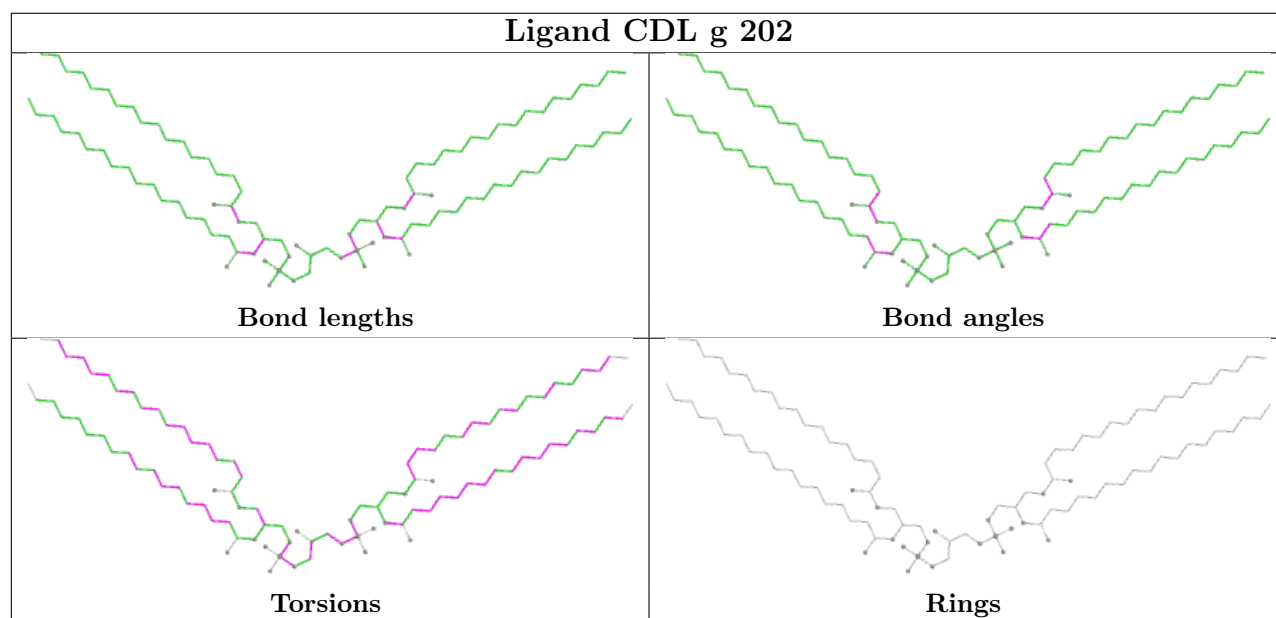
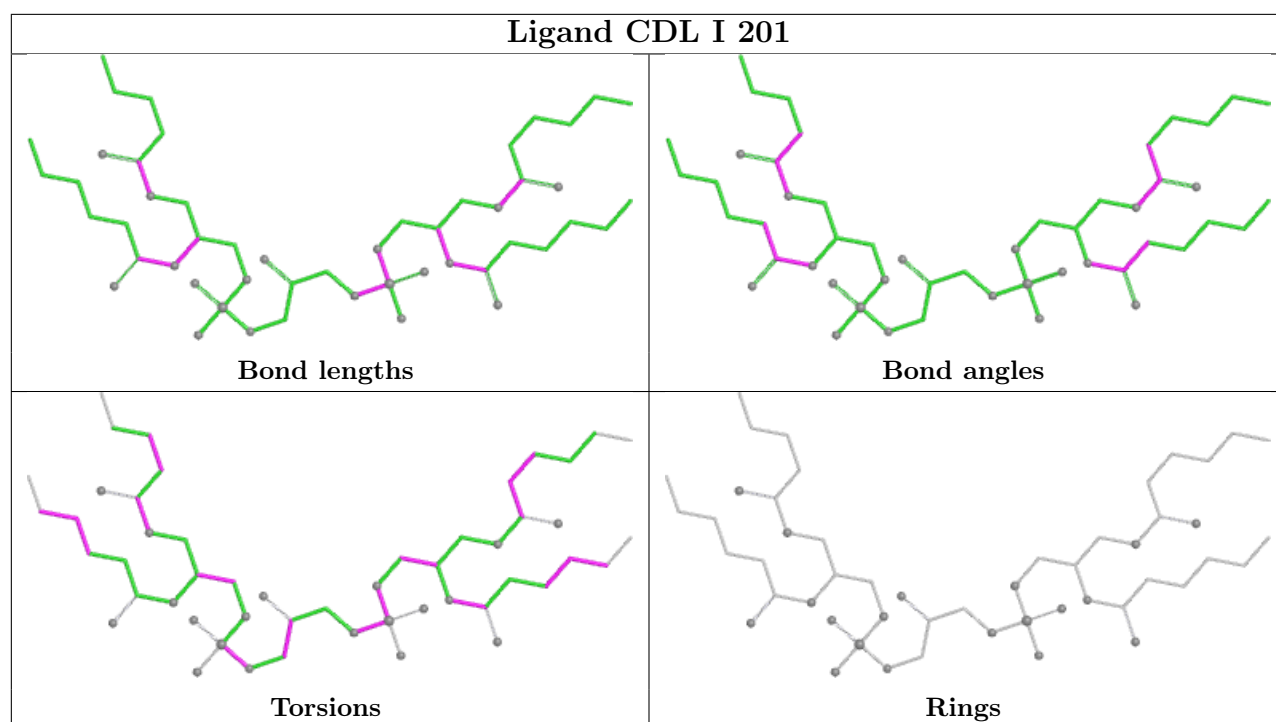
Ligand UQ1 Q 501

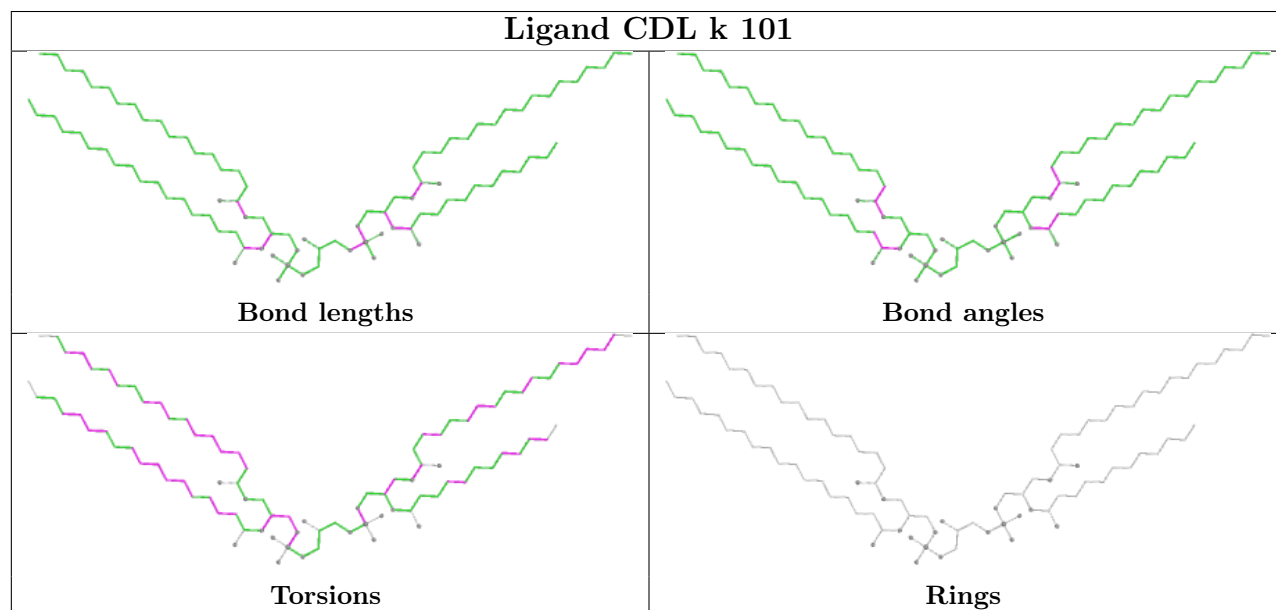
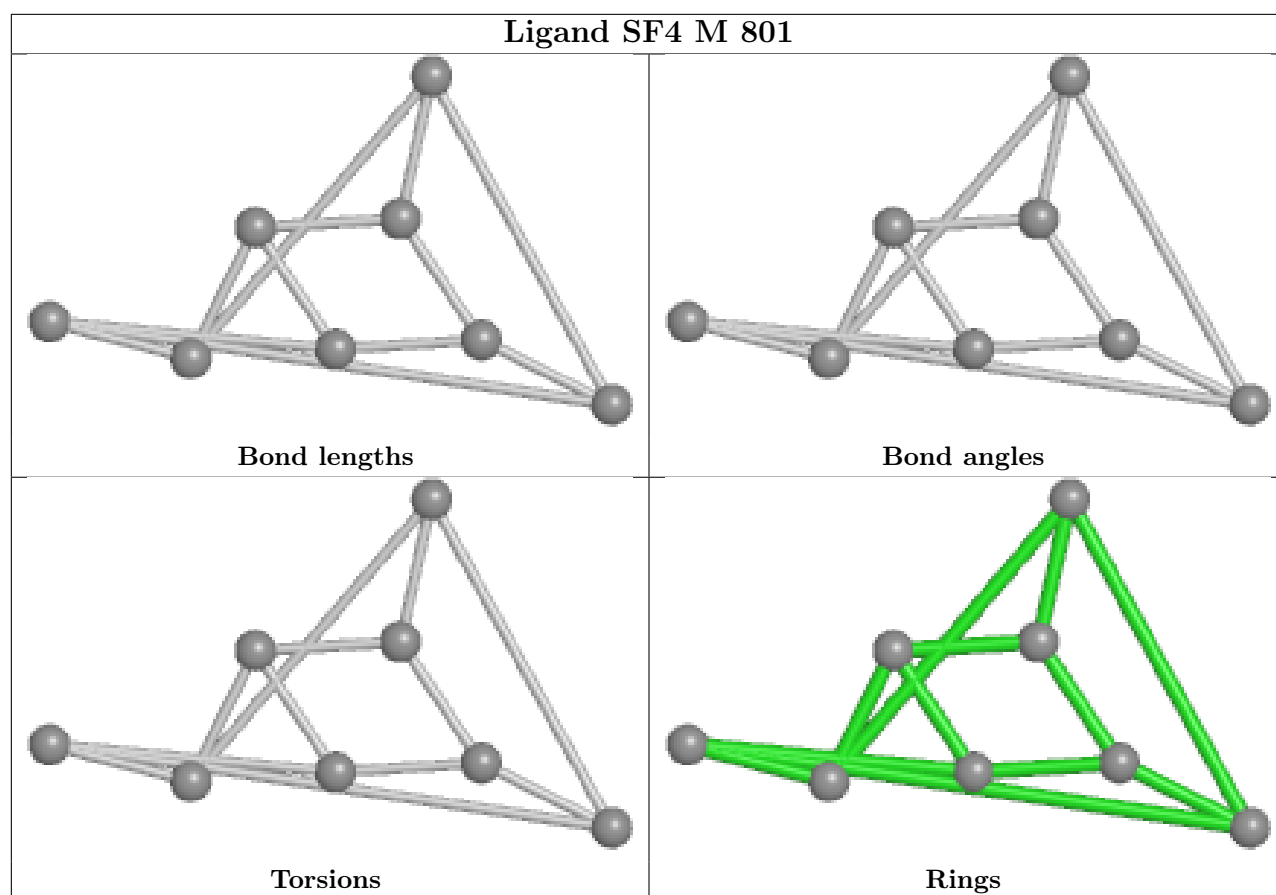


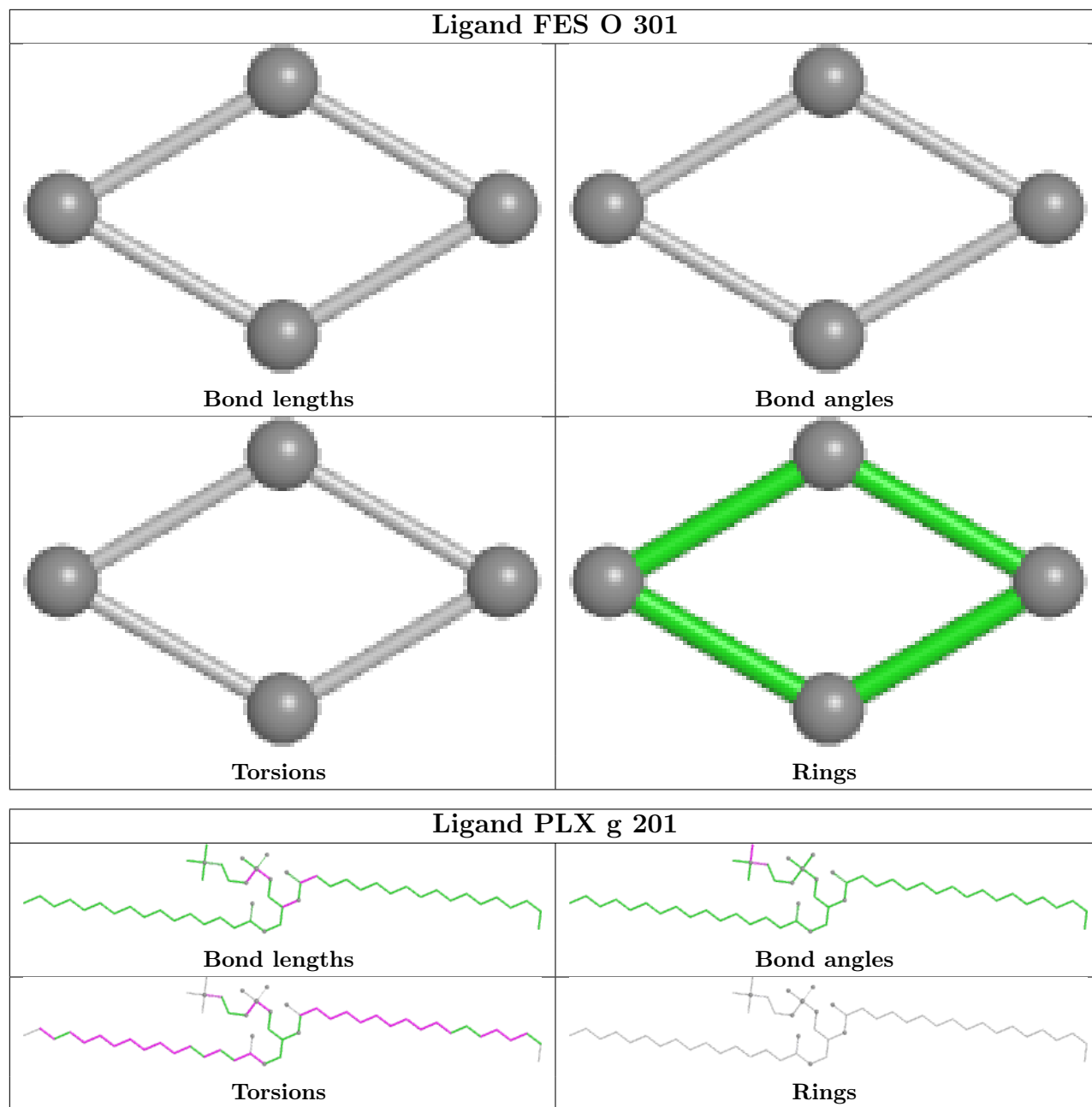
Ligand PEE 1 701

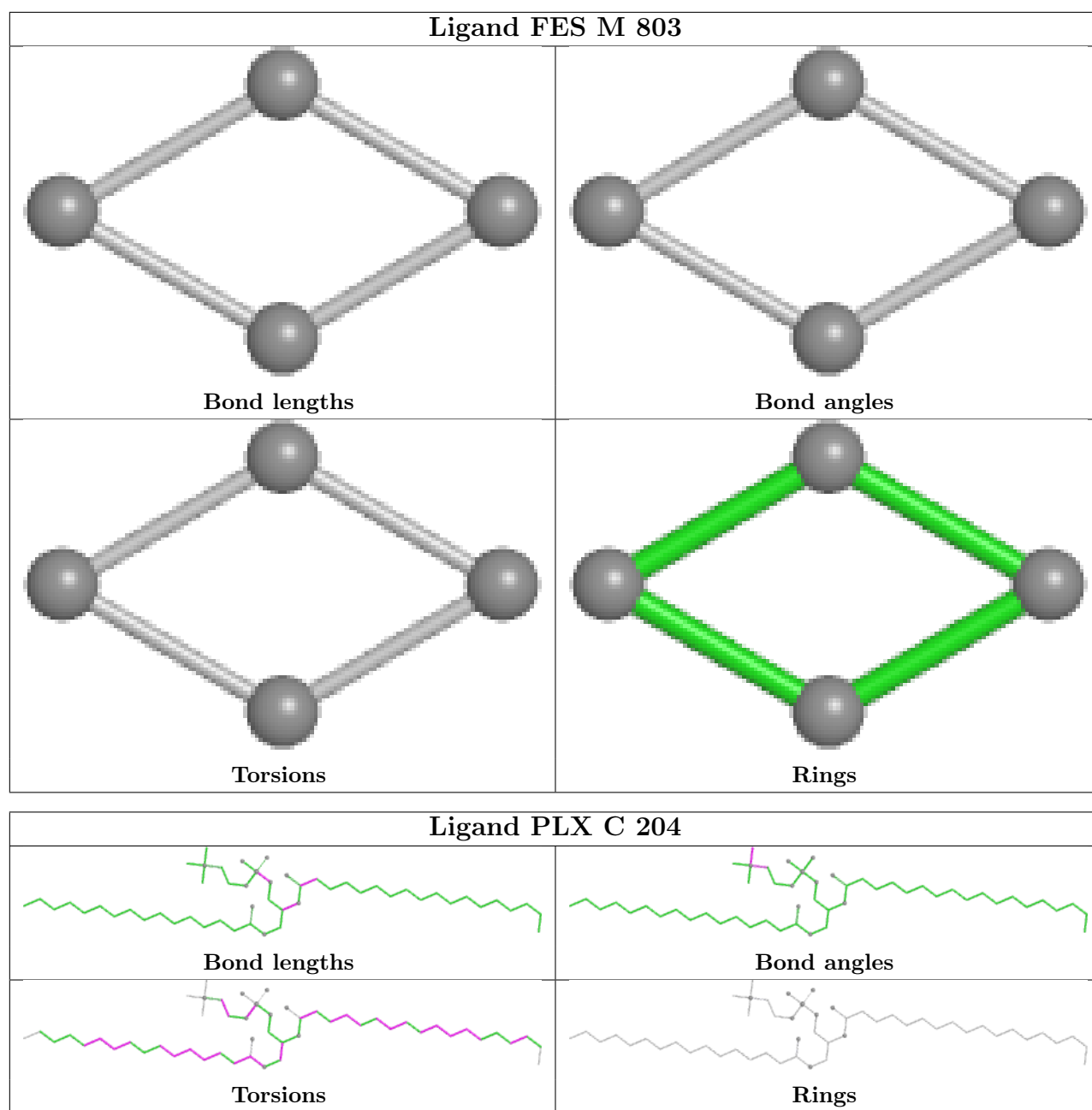


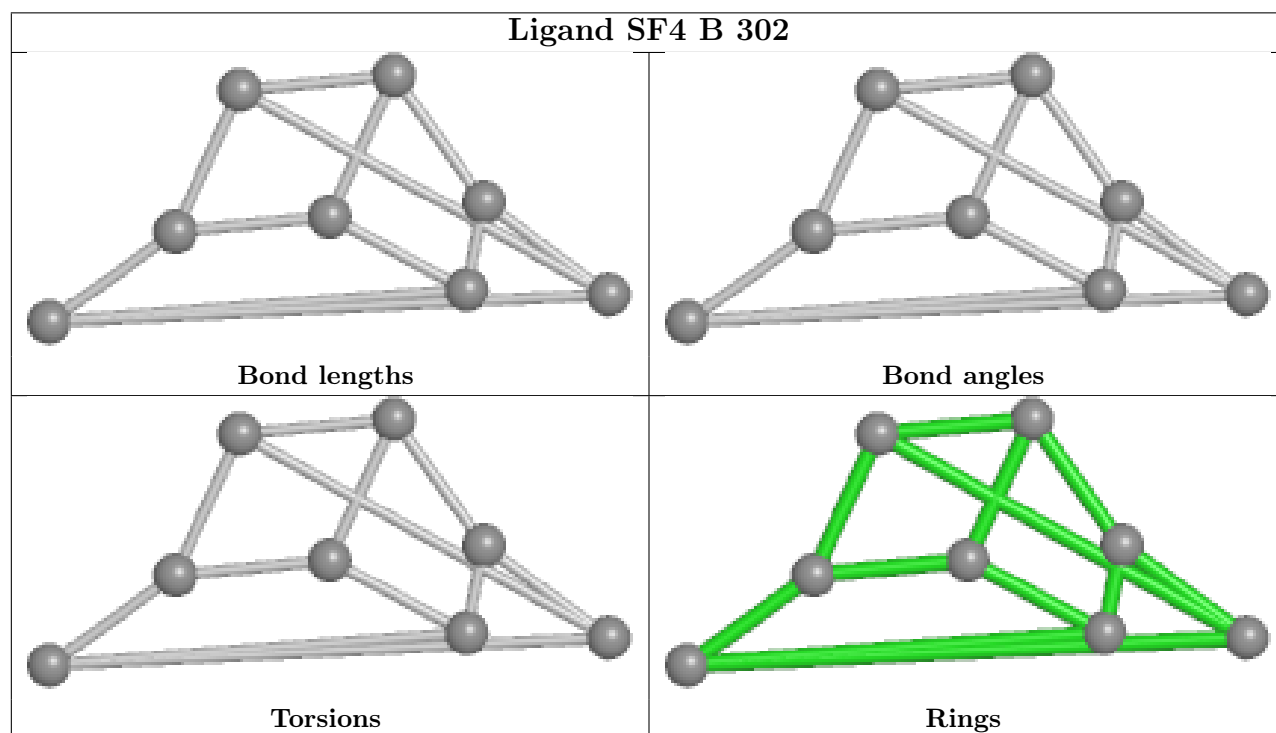
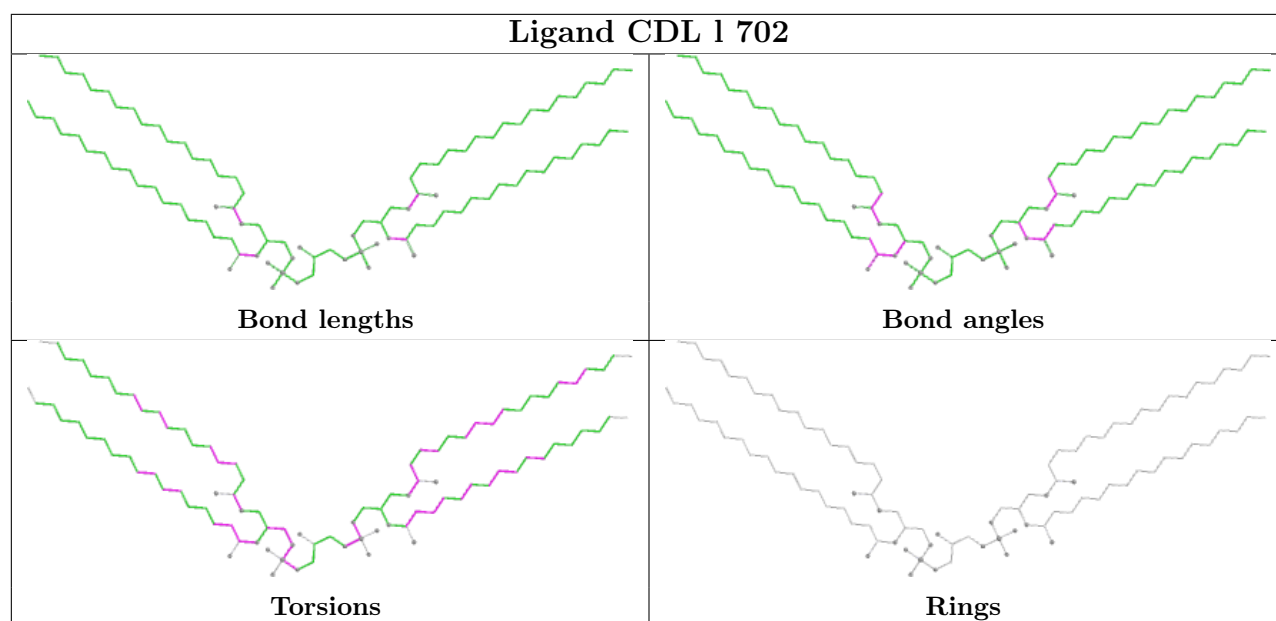


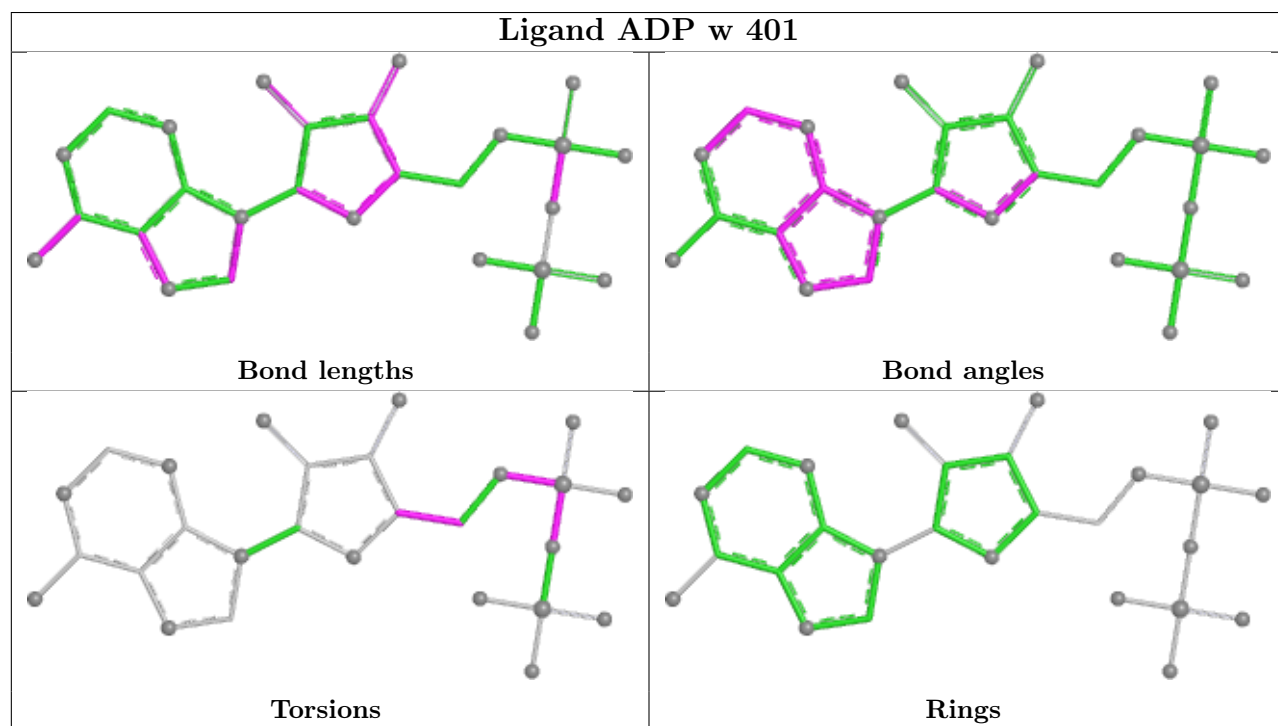
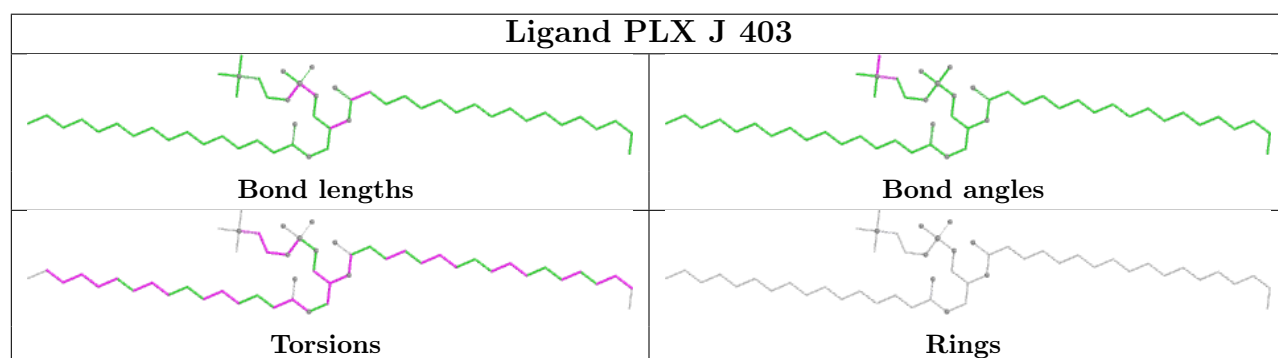
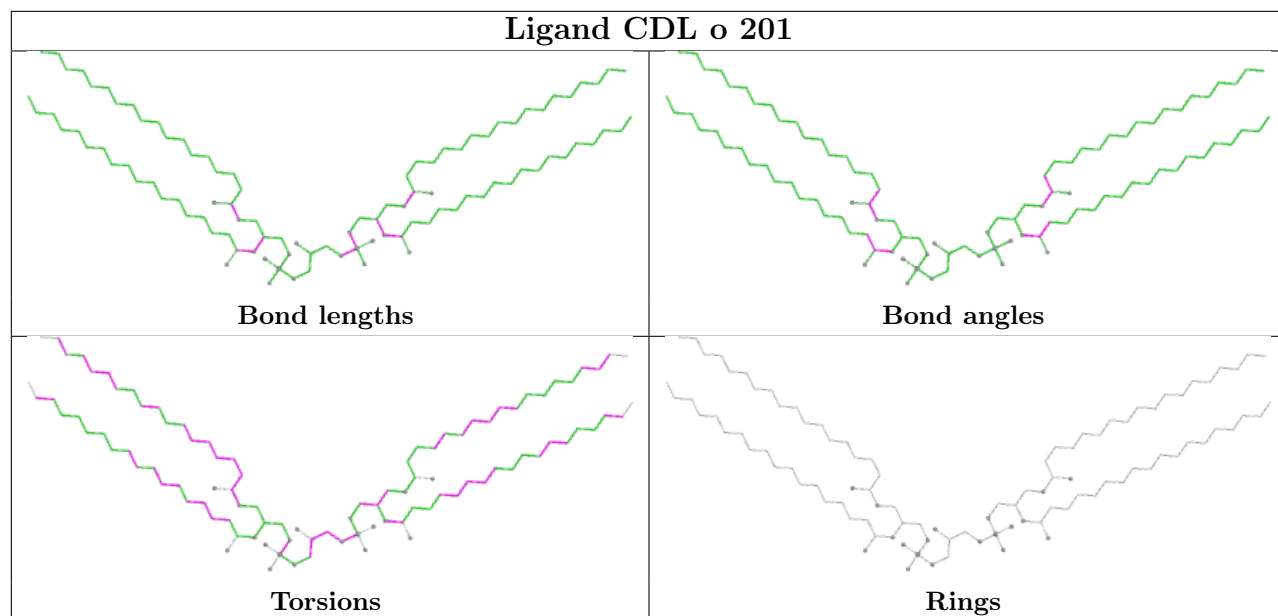


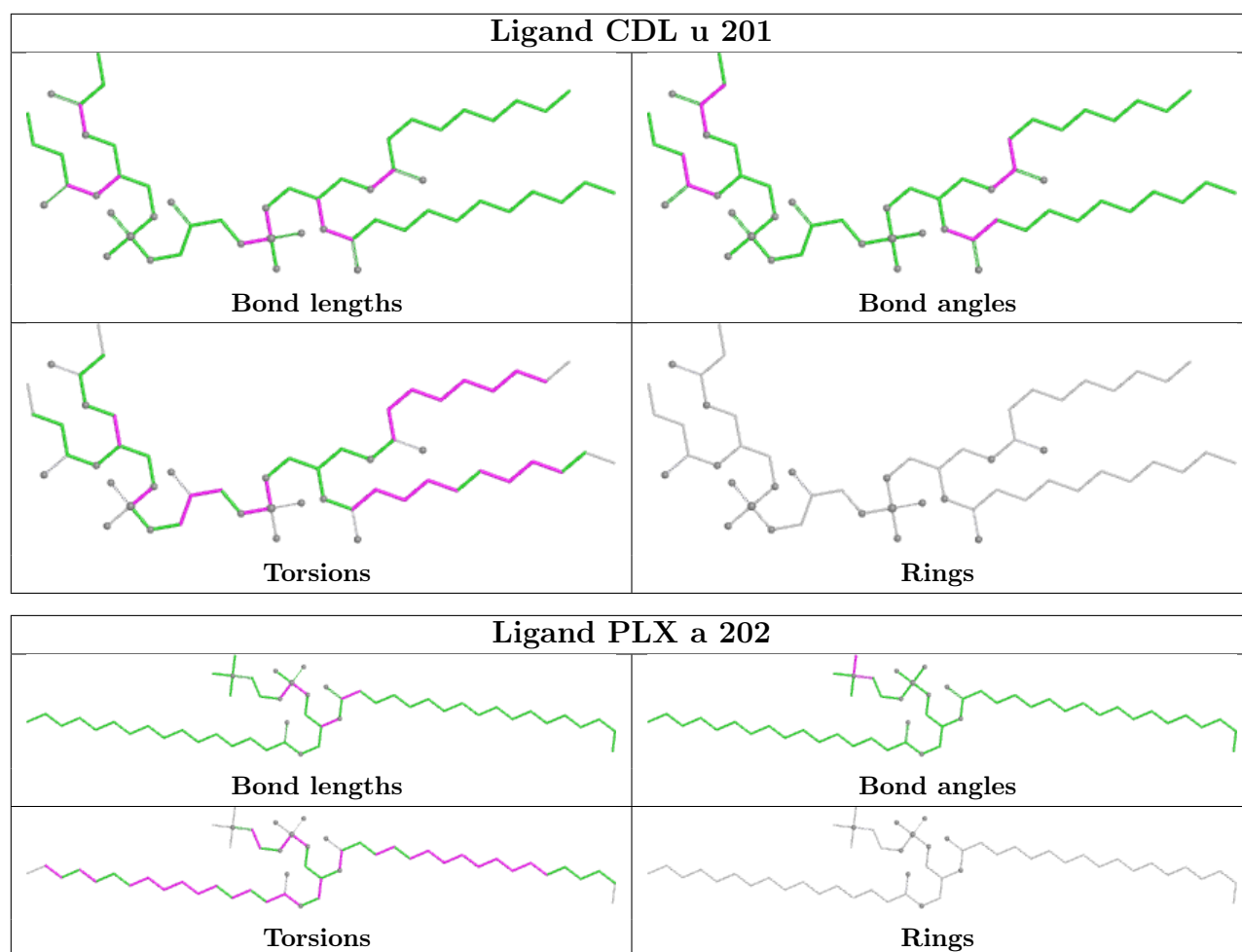


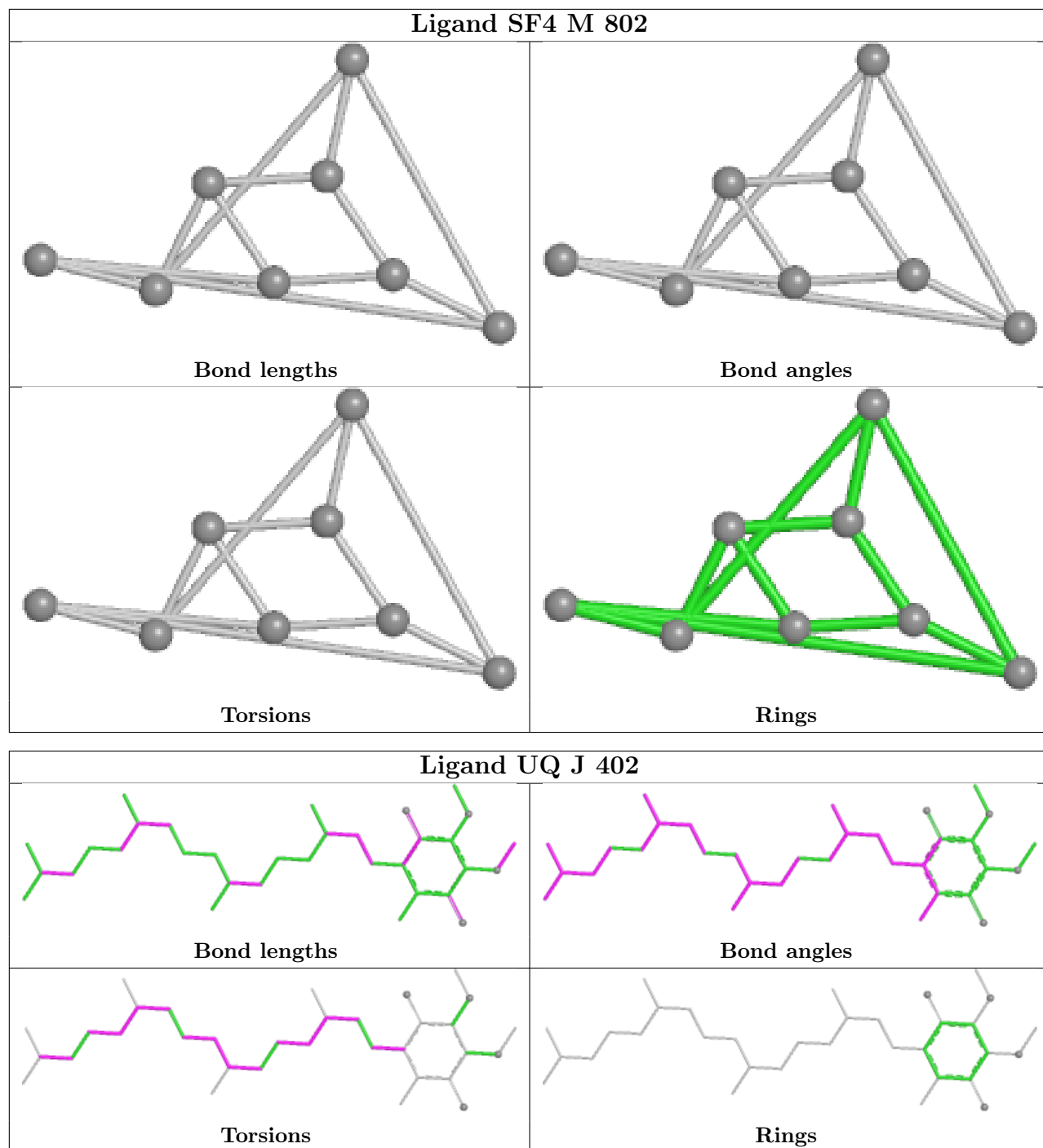


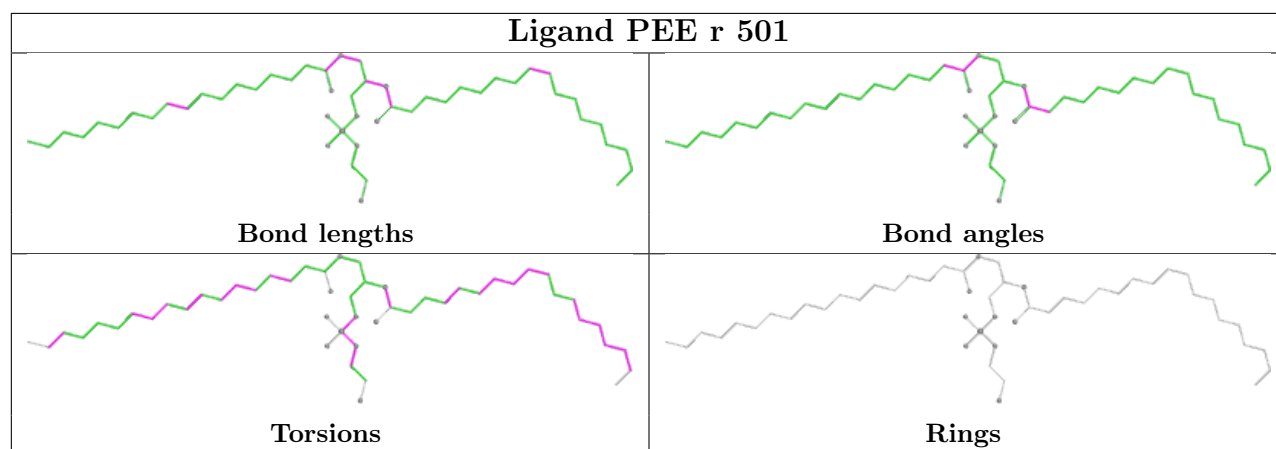
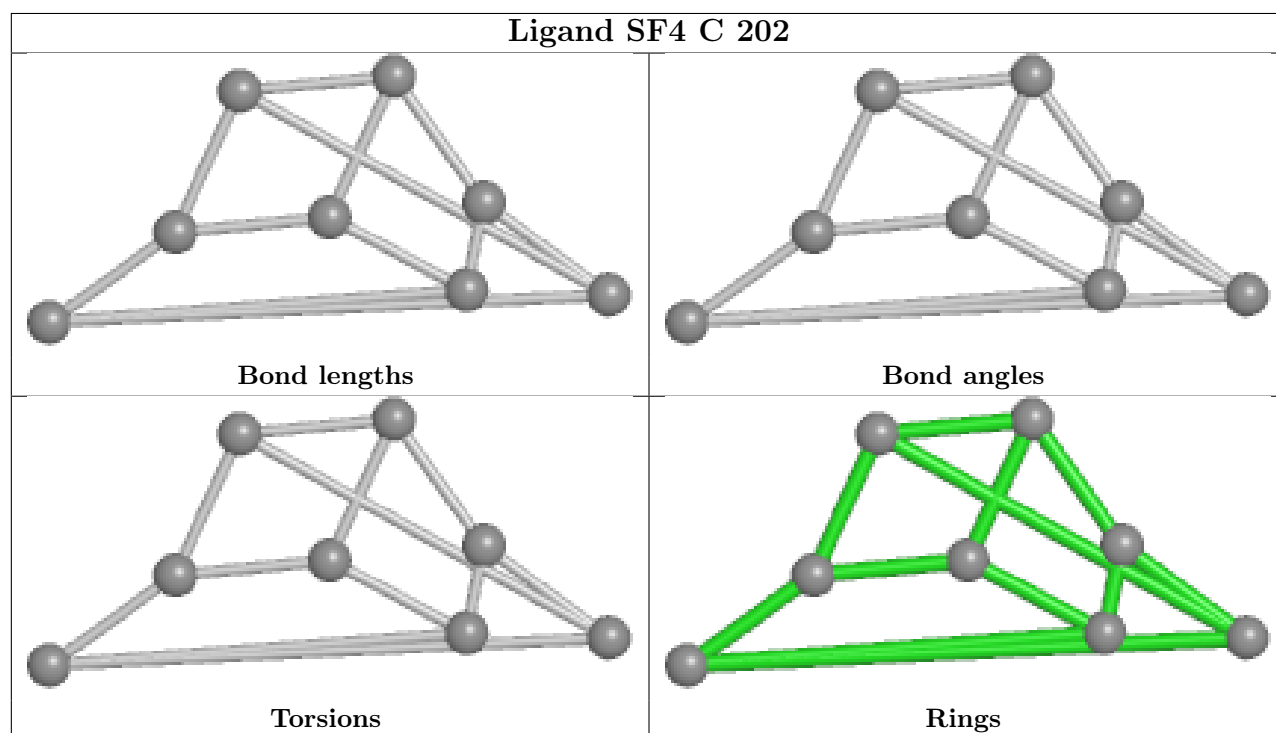
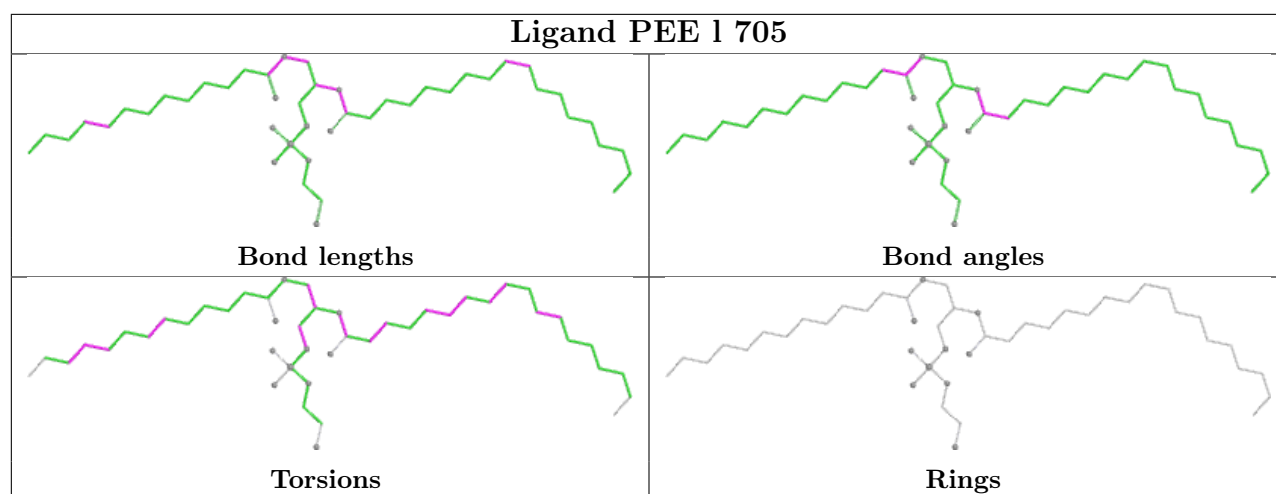


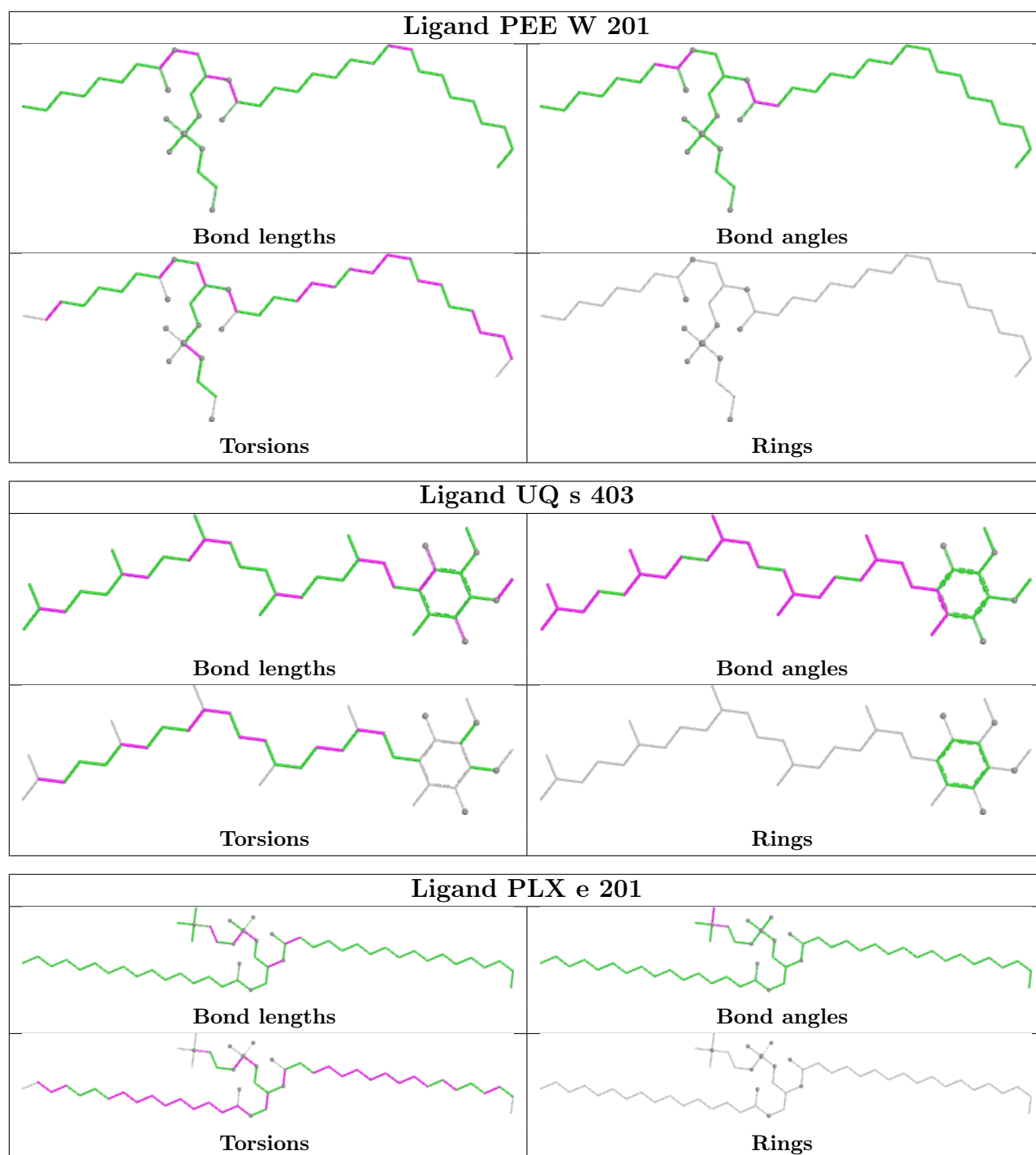


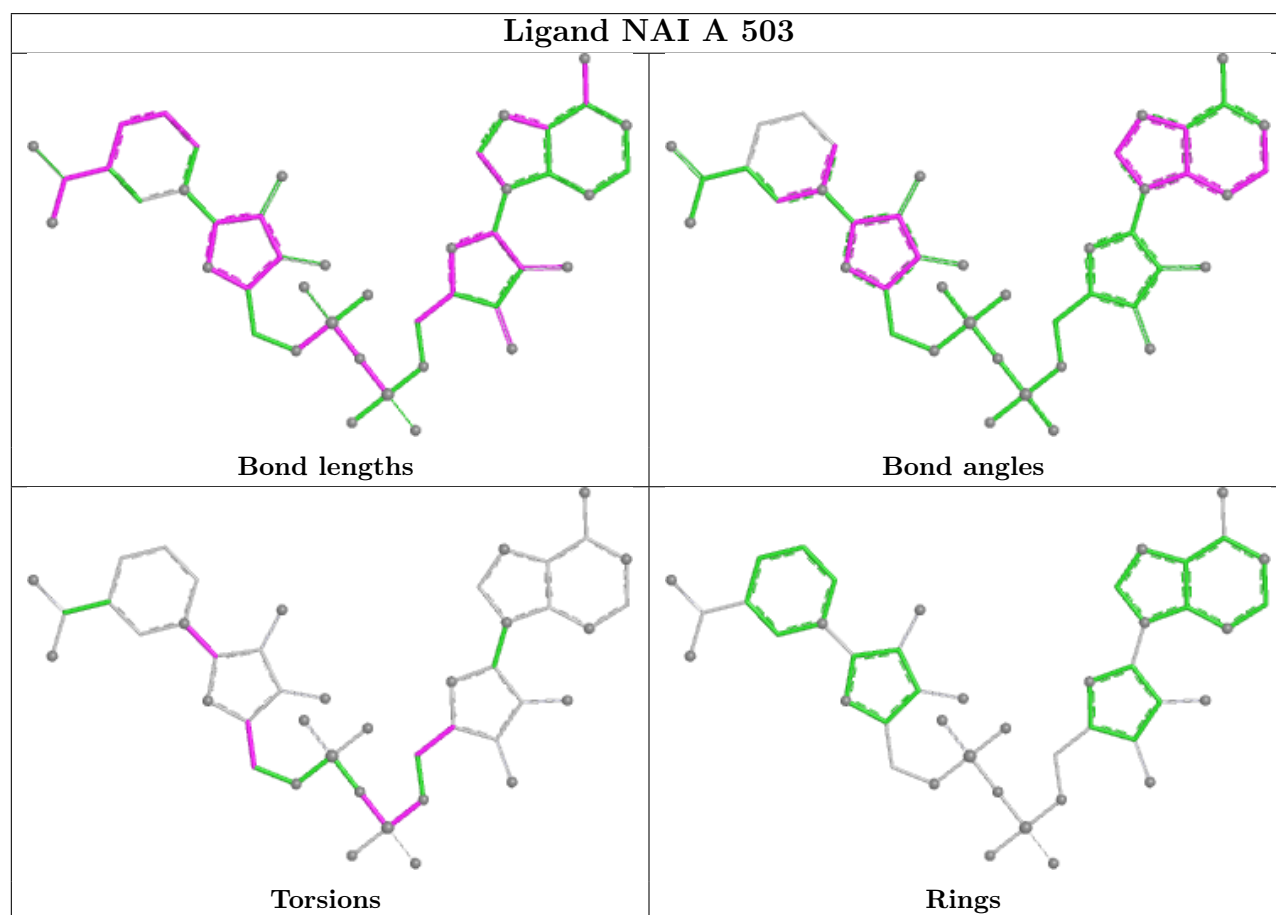
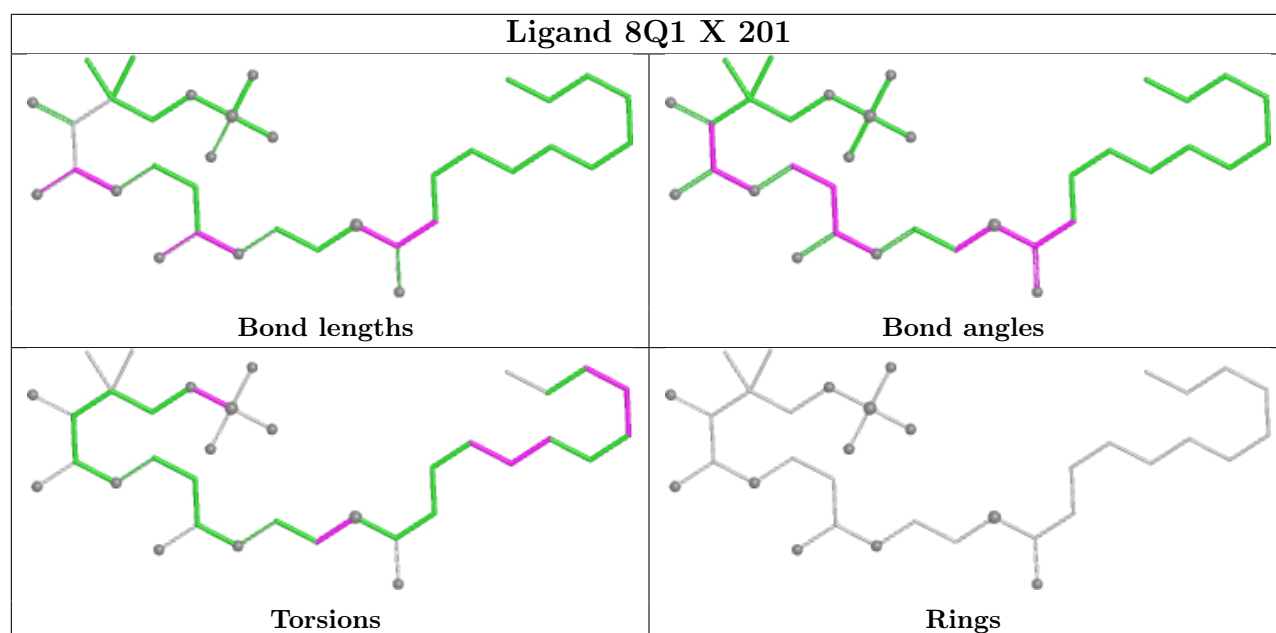


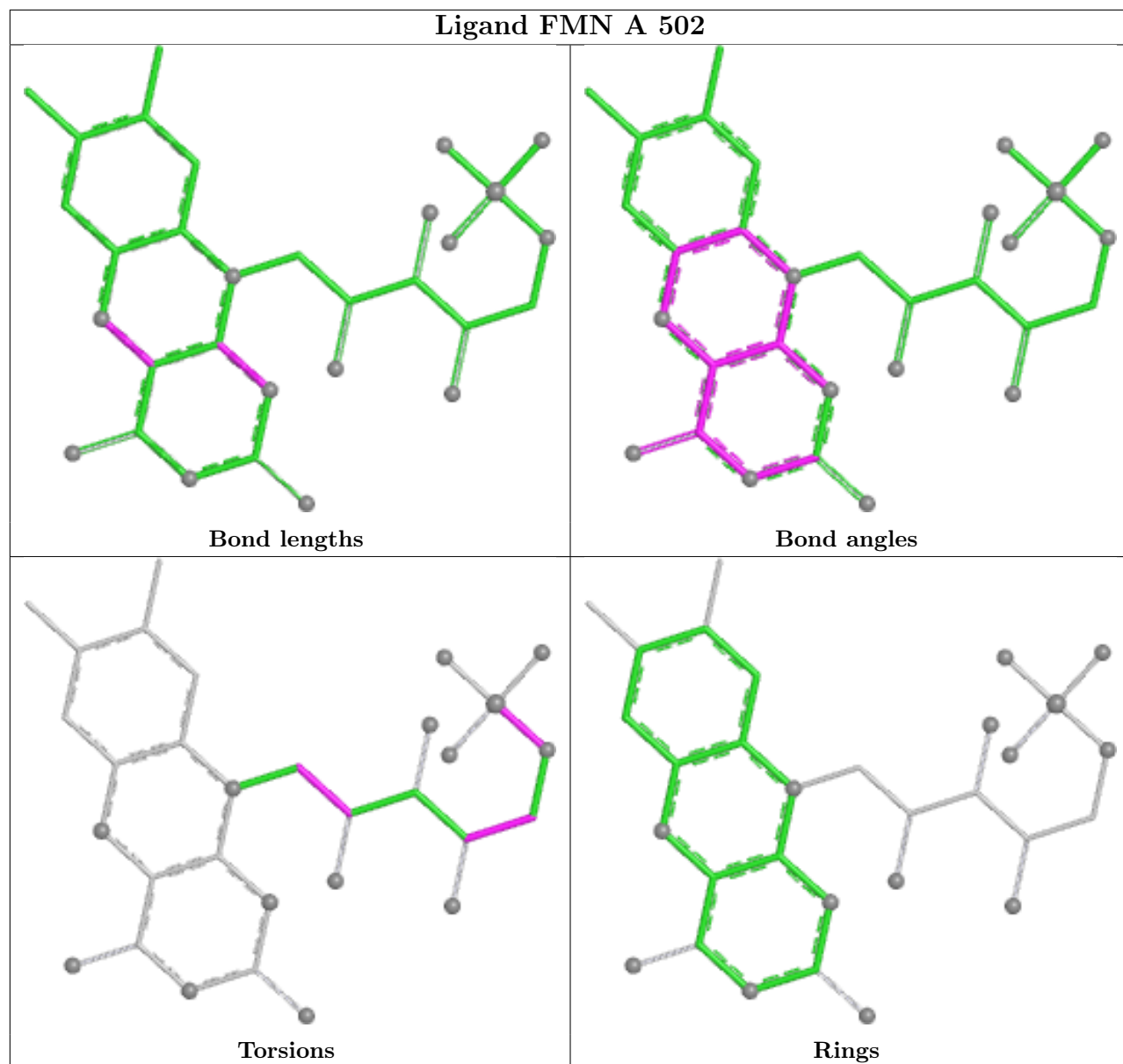




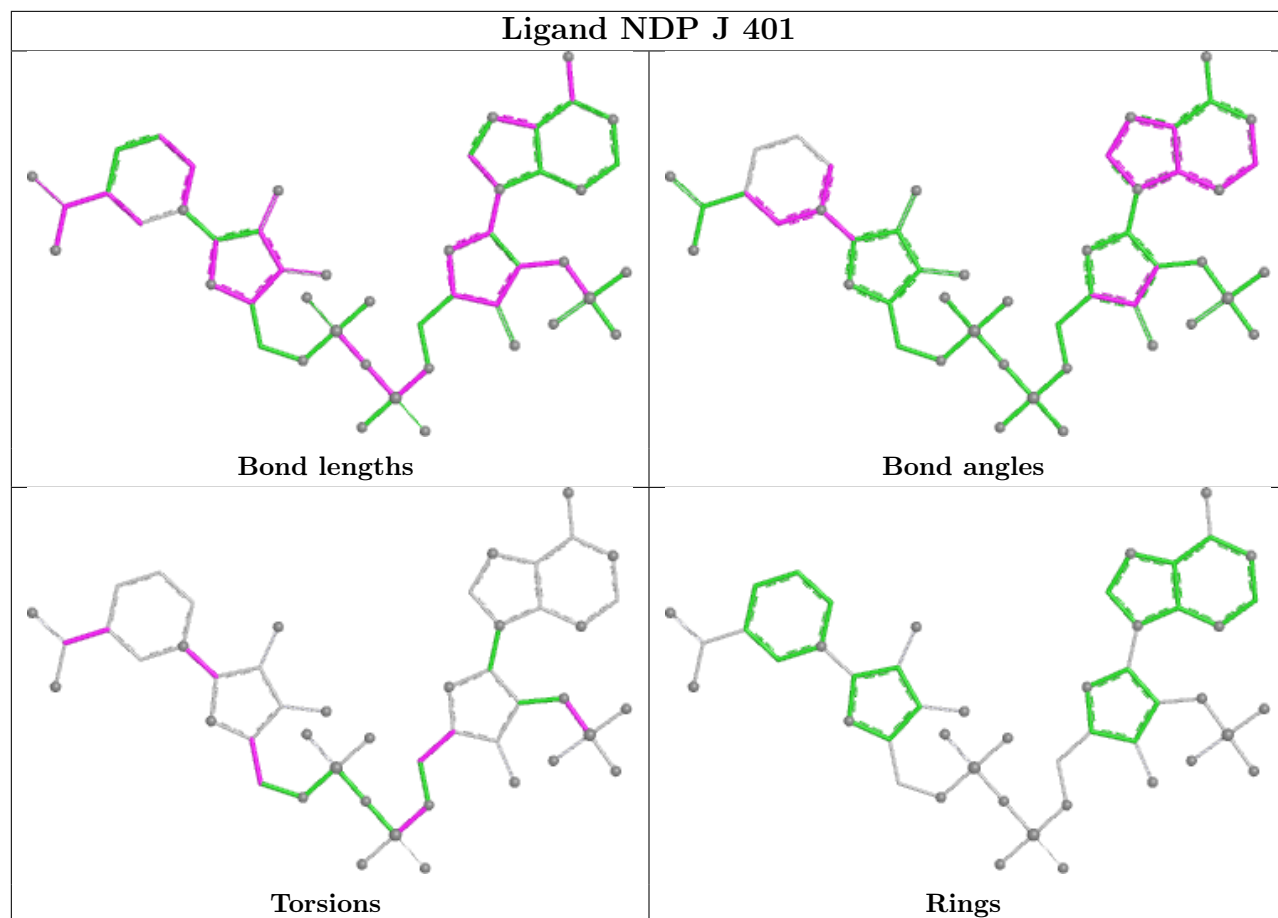




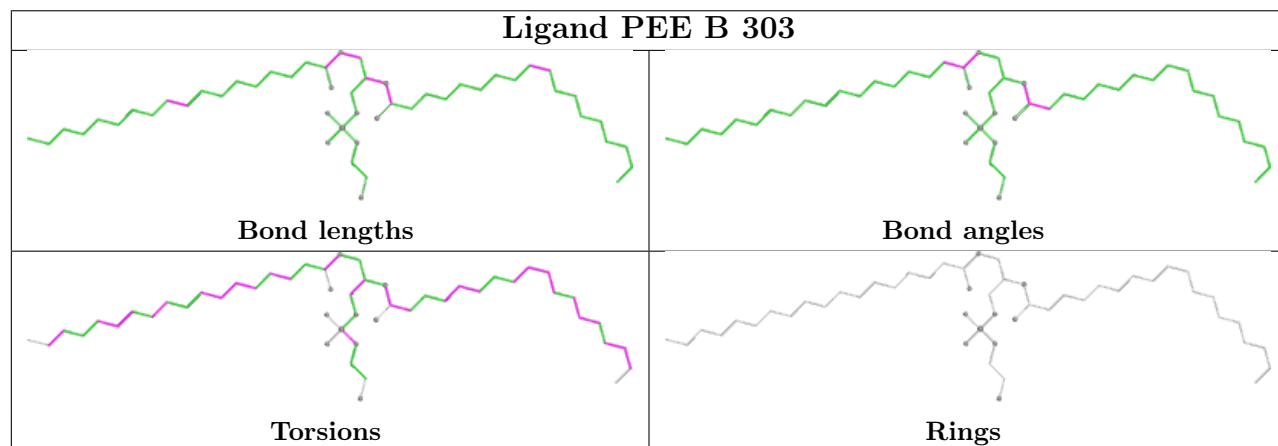


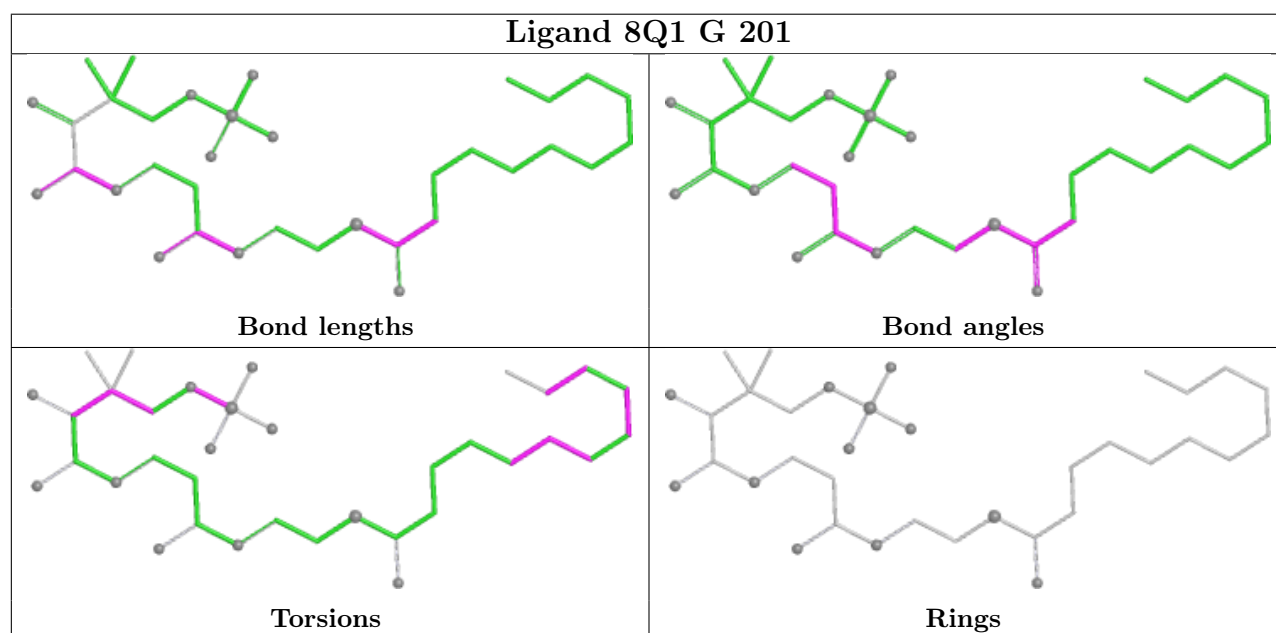
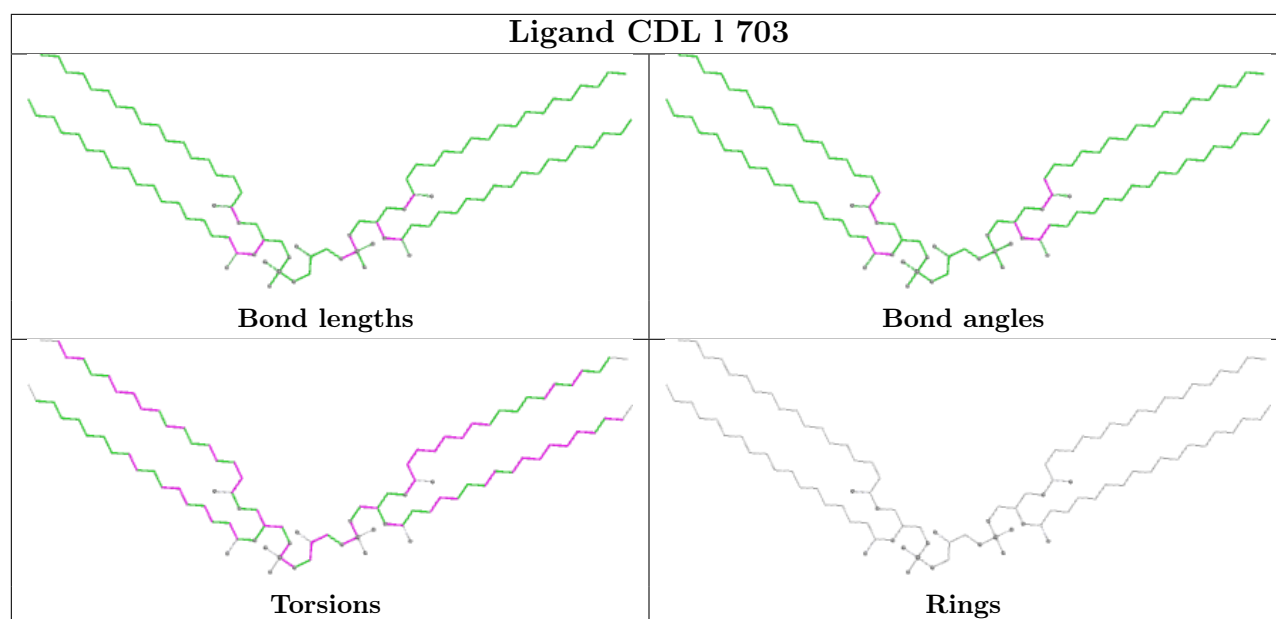


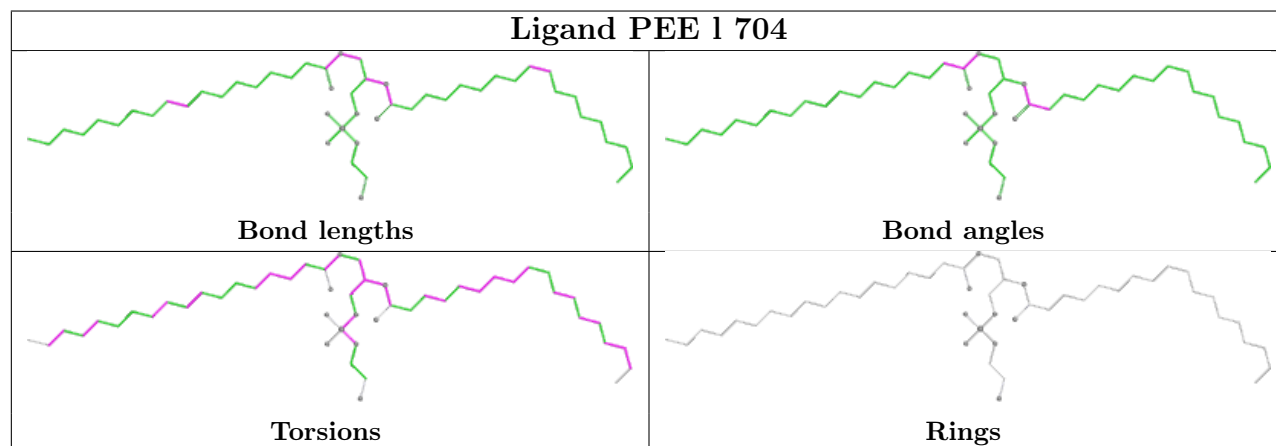
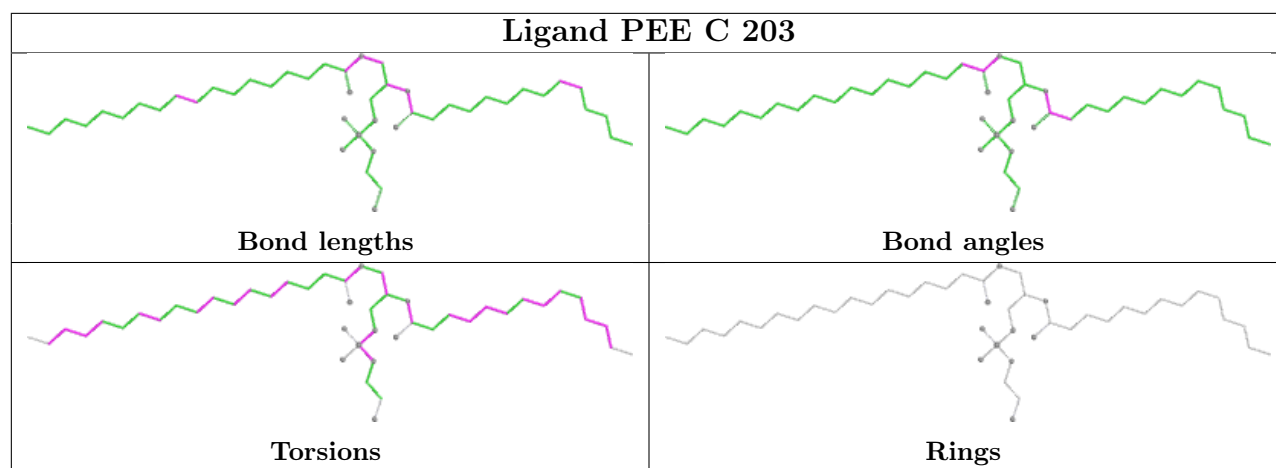
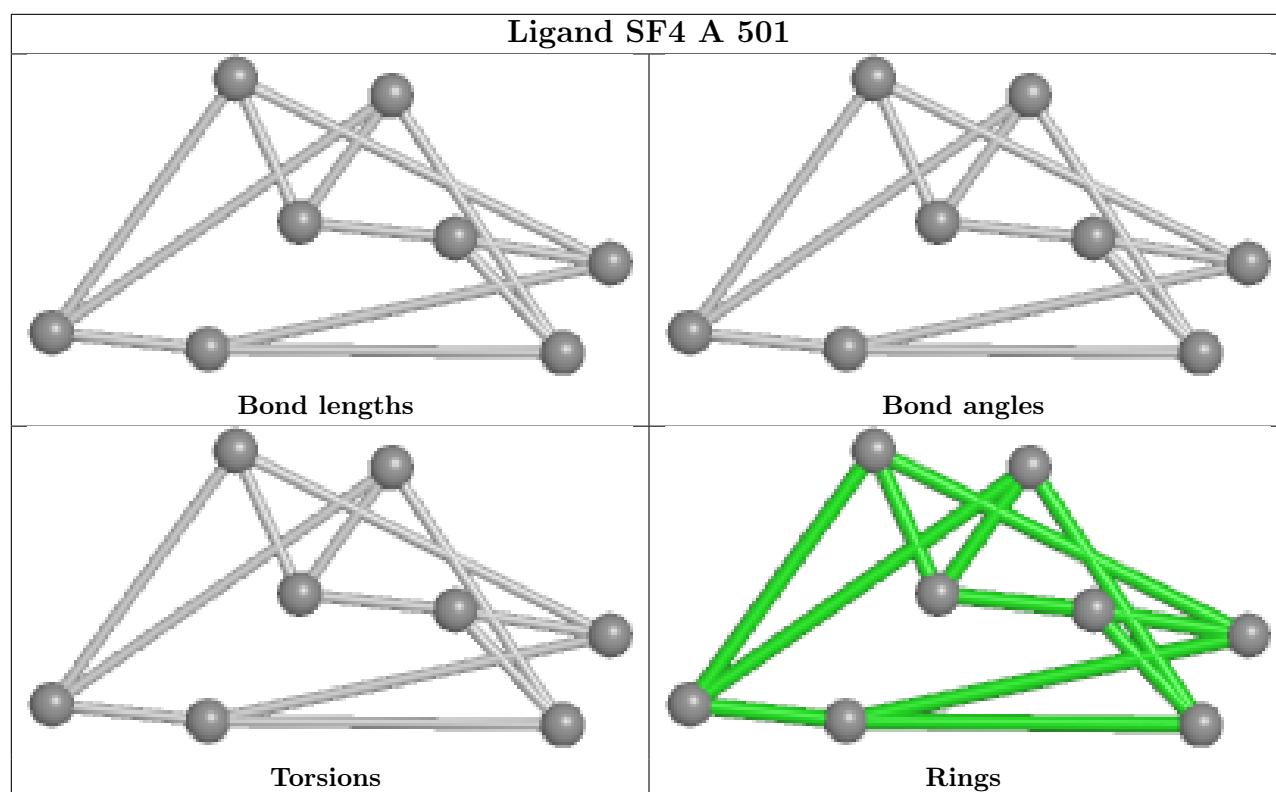
Ligand NDP J 401

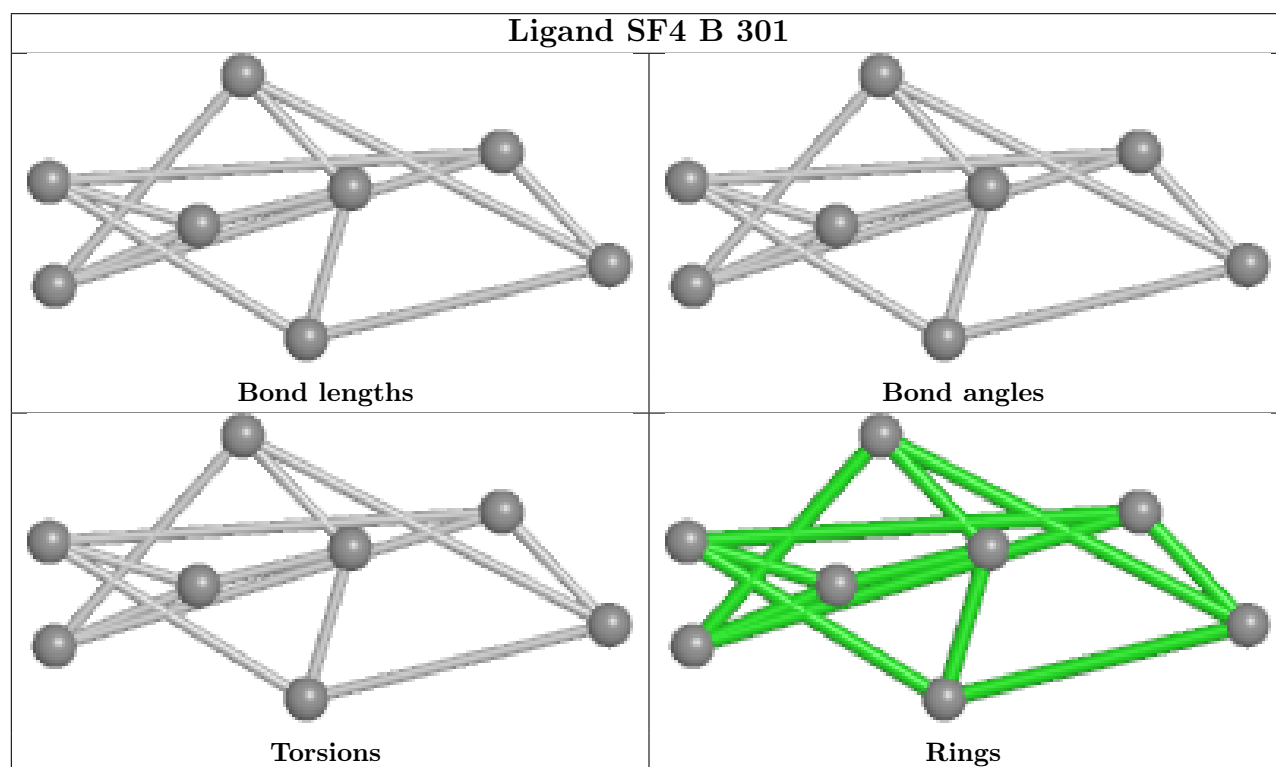
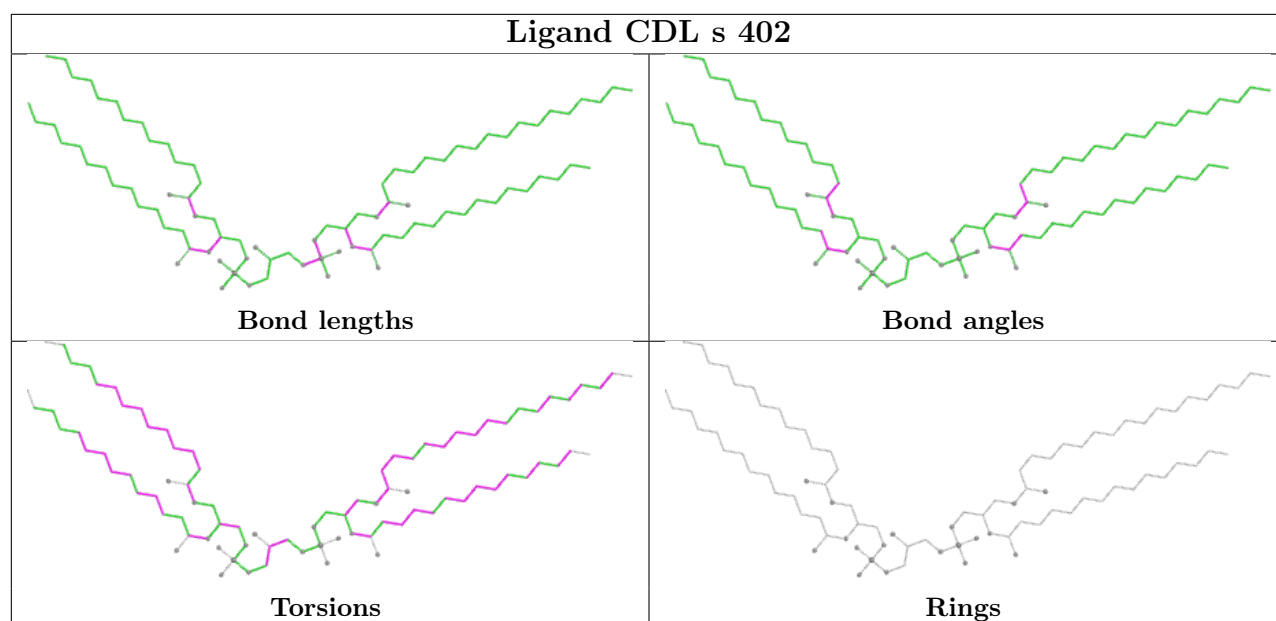


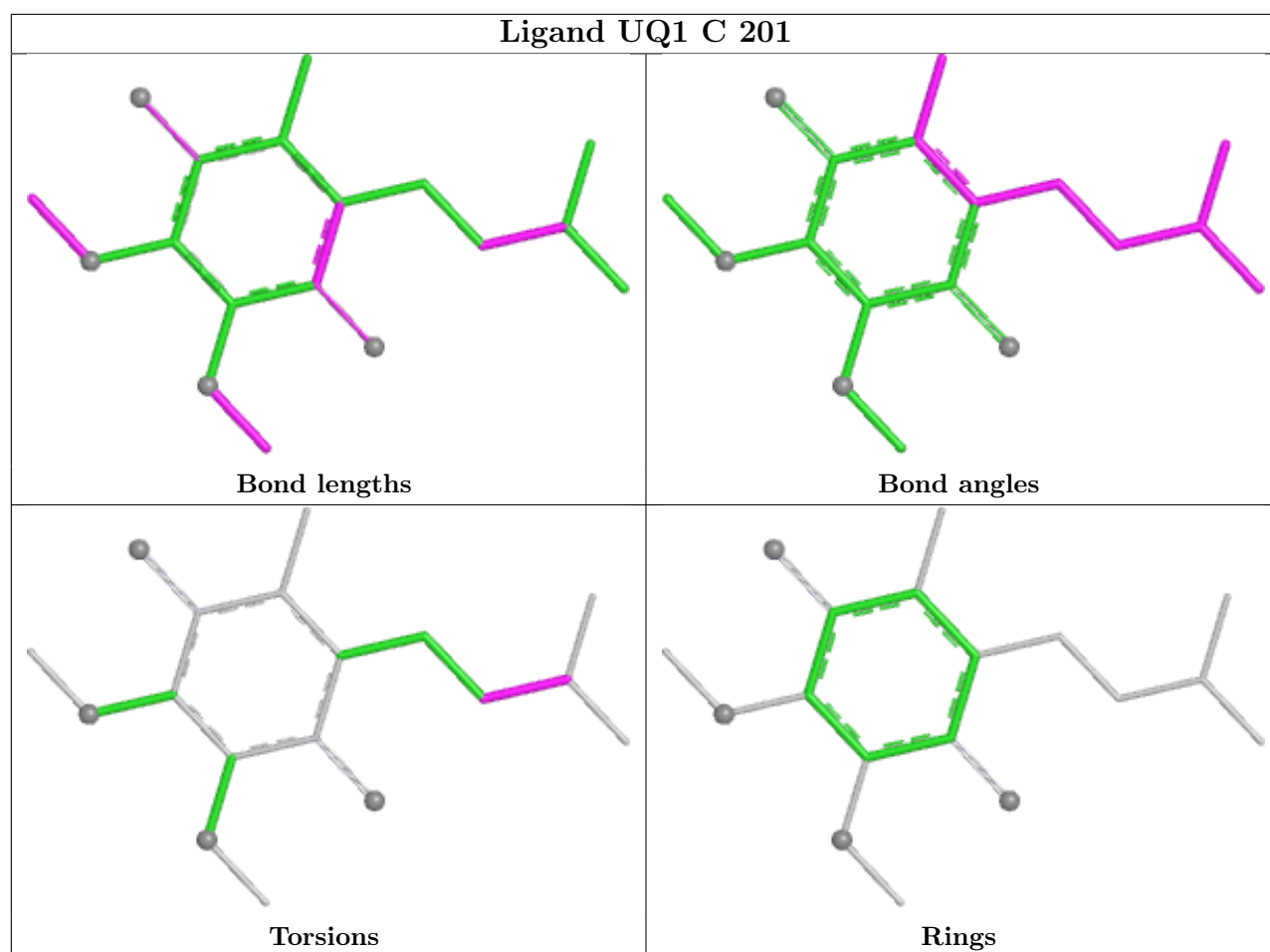
Ligand PEE B 303











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.

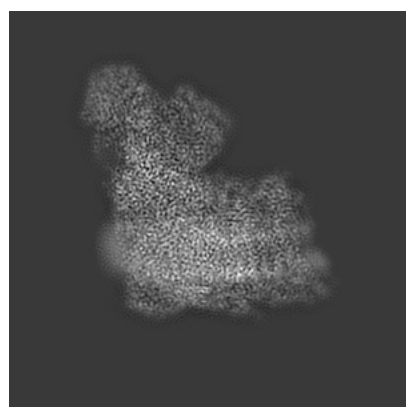
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32303. These allow visual inspection of the internal detail of the map and identification of artifacts.

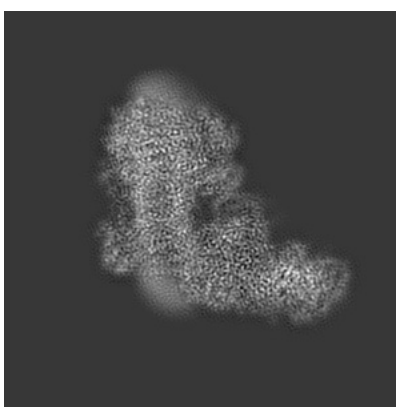
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

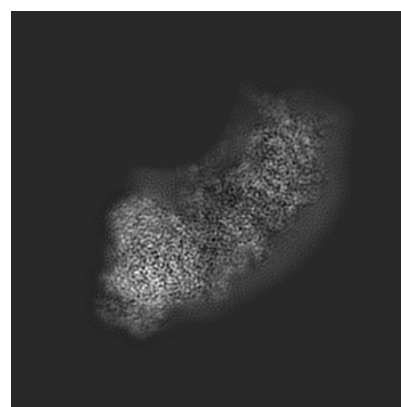
6.1.1 Primary map



X



Y

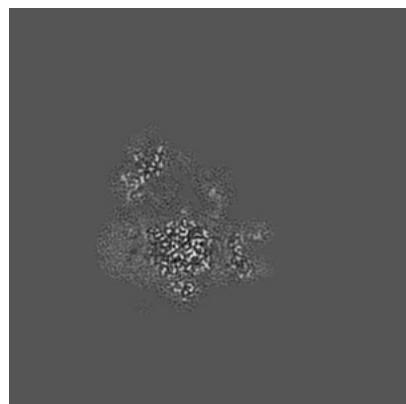


Z

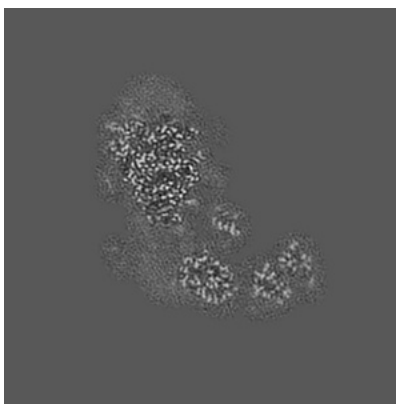
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

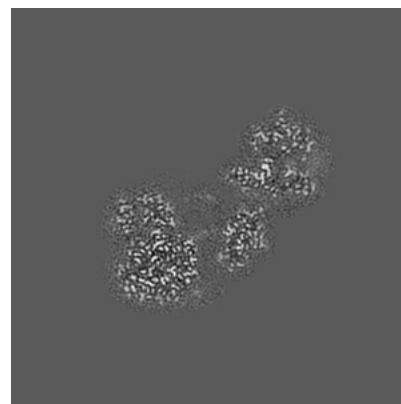
6.2.1 Primary map



X Index: 152



Y Index: 152

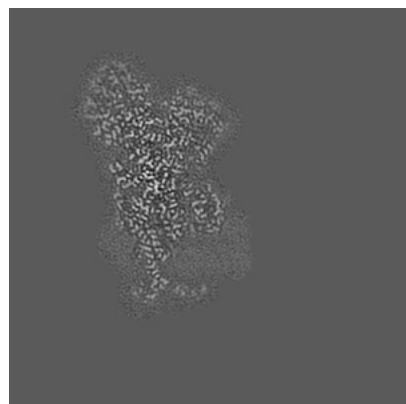


Z Index: 152

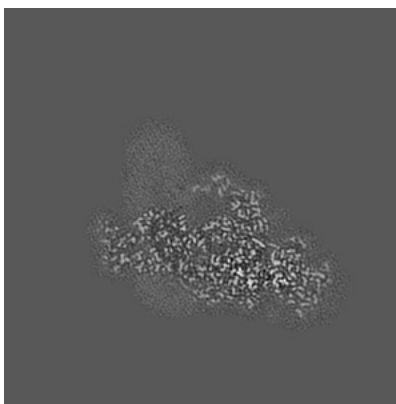
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

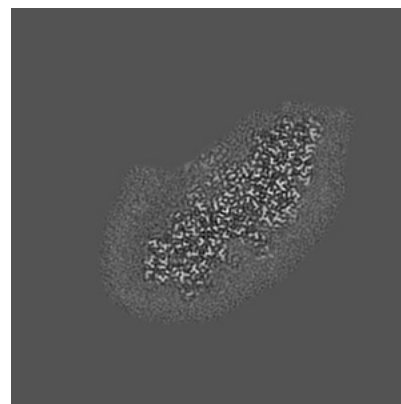
6.3.1 Primary map



X Index: 105



Y Index: 105

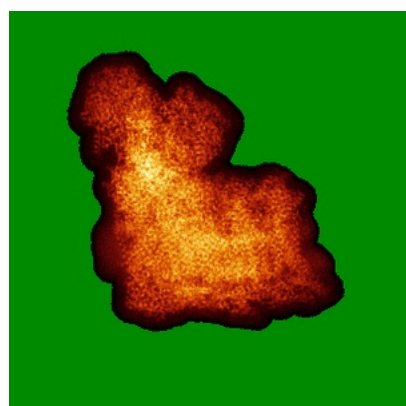


Z Index: 129

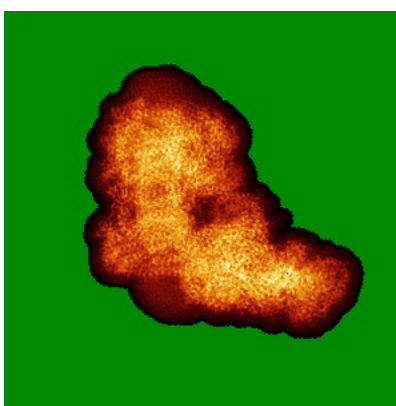
The images above show the largest variance slices of the map in three orthogonal directions.

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

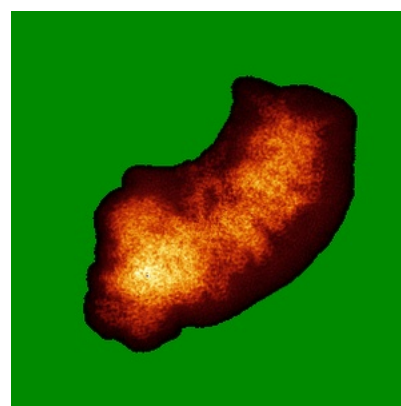
6.4.1 Primary map



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.

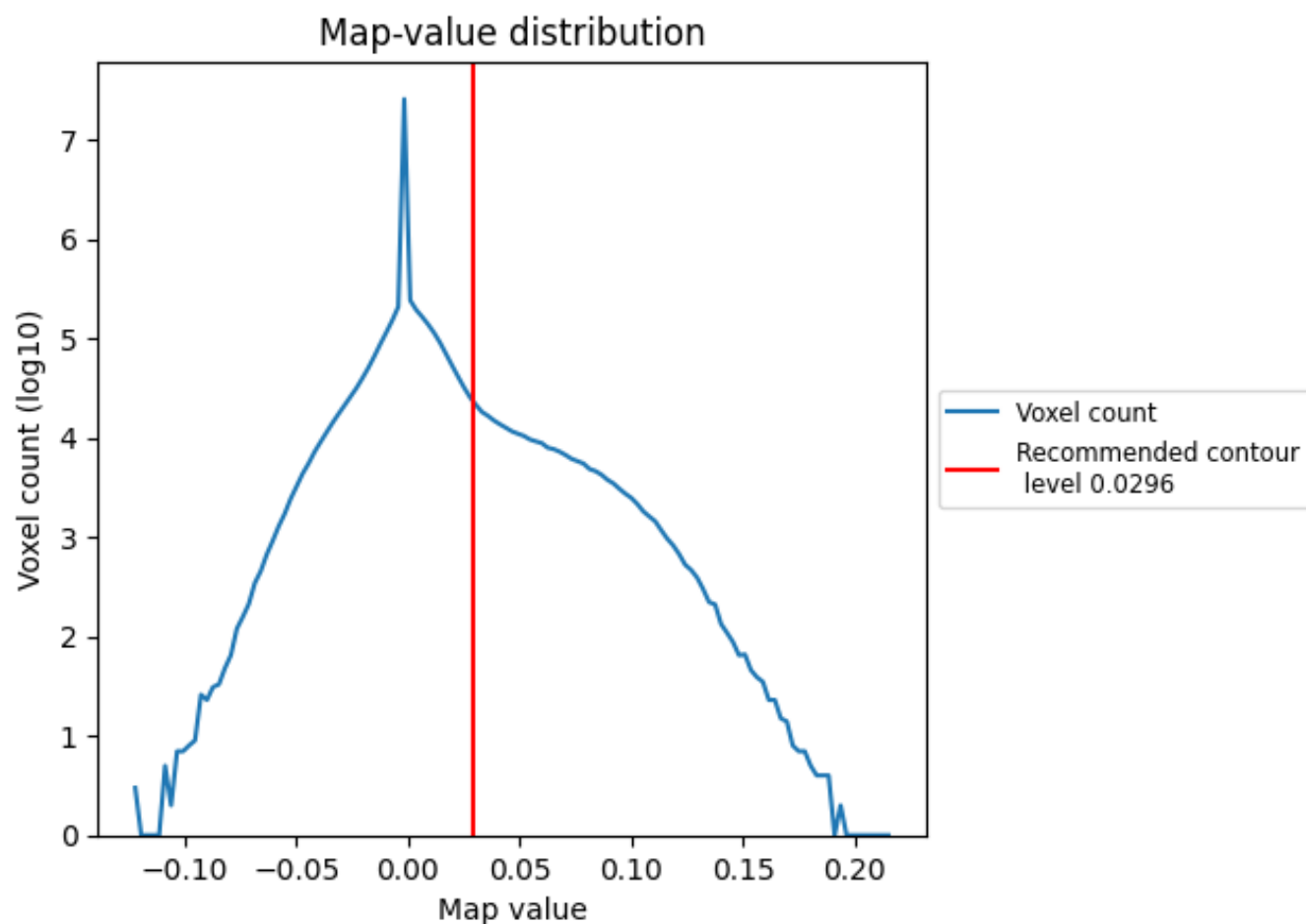
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

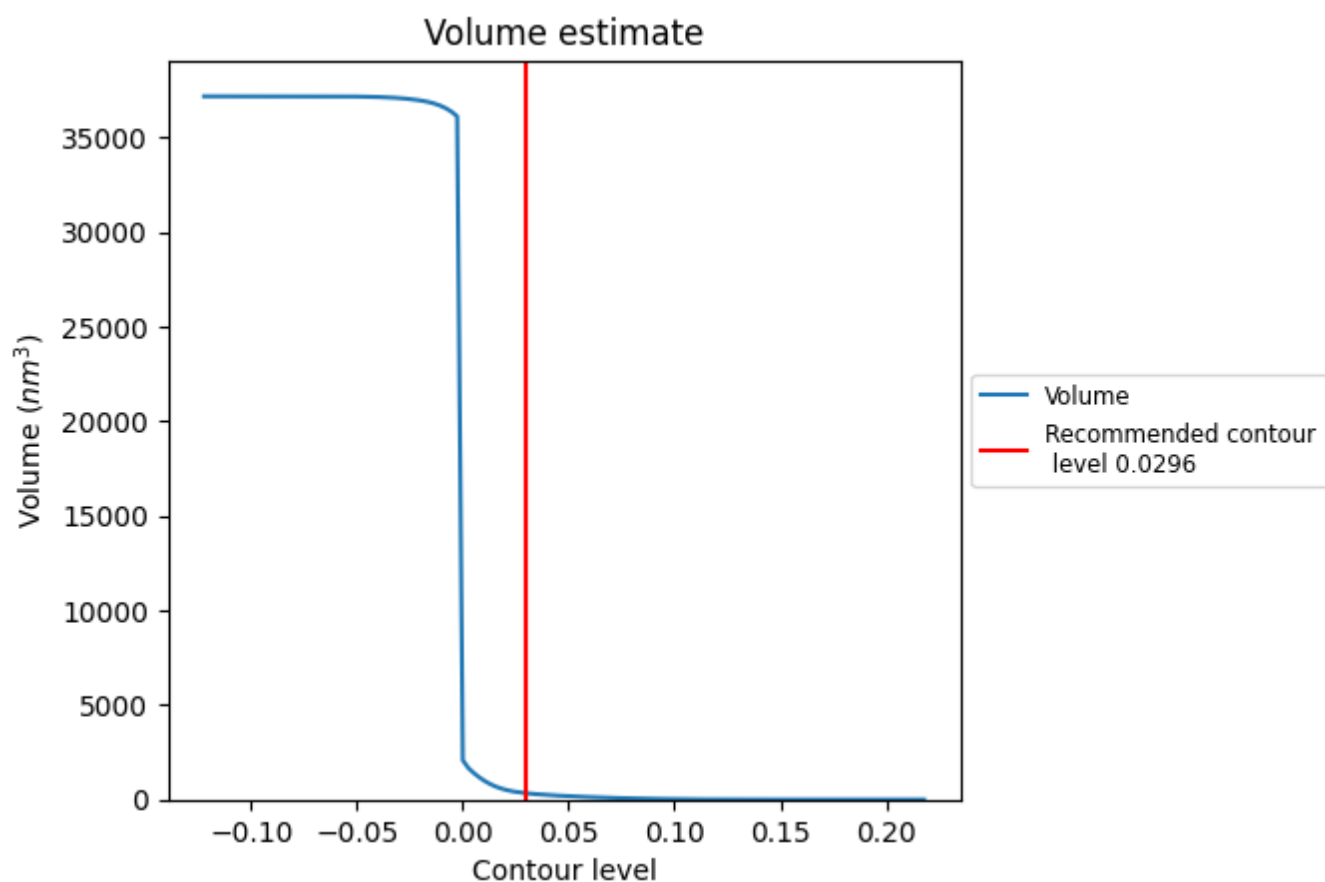
This section contains the results of statistical analysis of the map.

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.

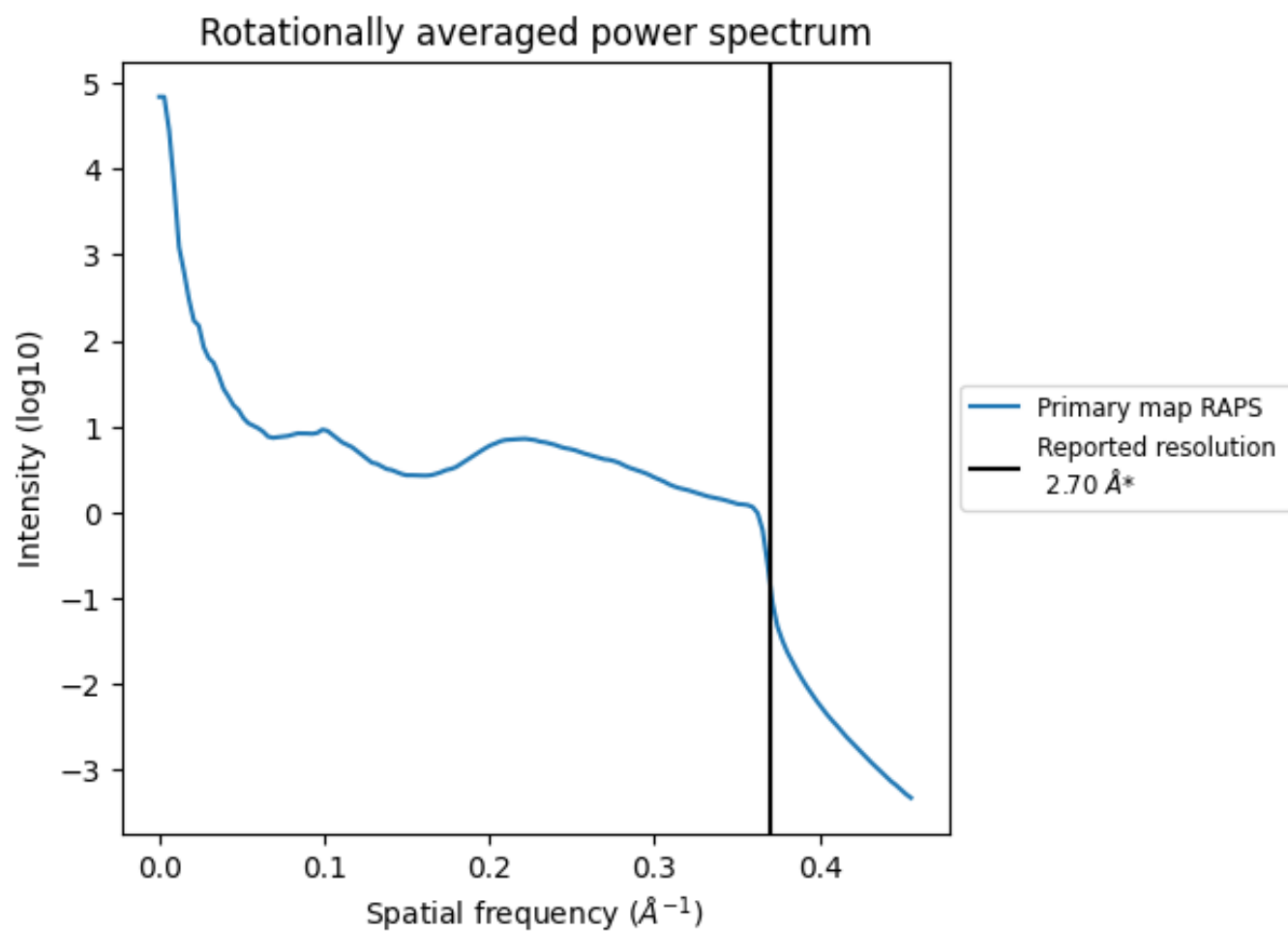
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 340 nm³; this corresponds to an approximate mass of 307 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 0.370 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

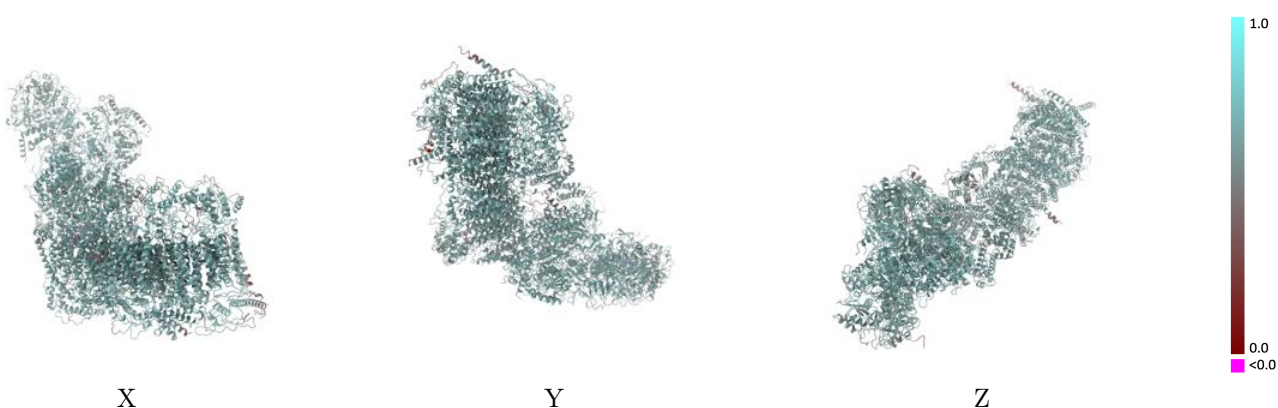
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32303 and PDB model 7W4F. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)

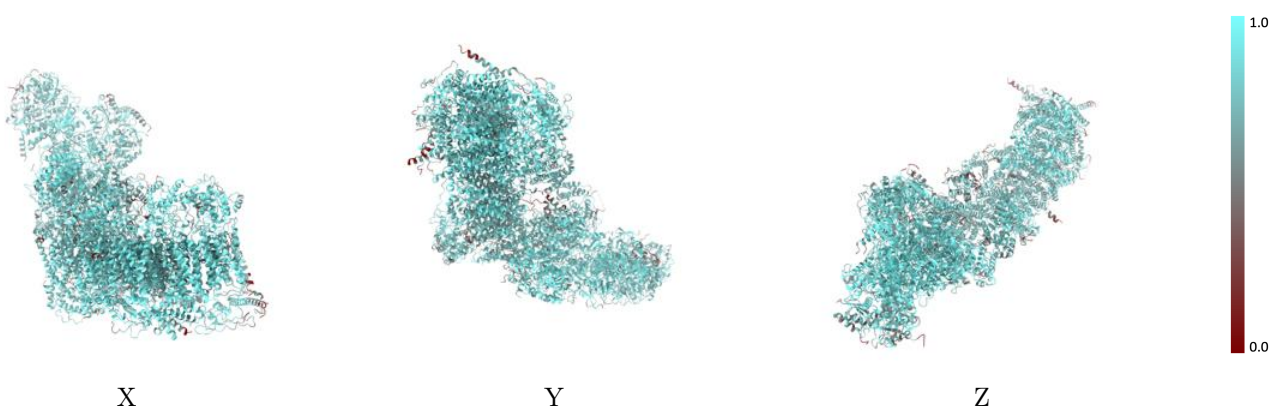
This section was not generated.

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



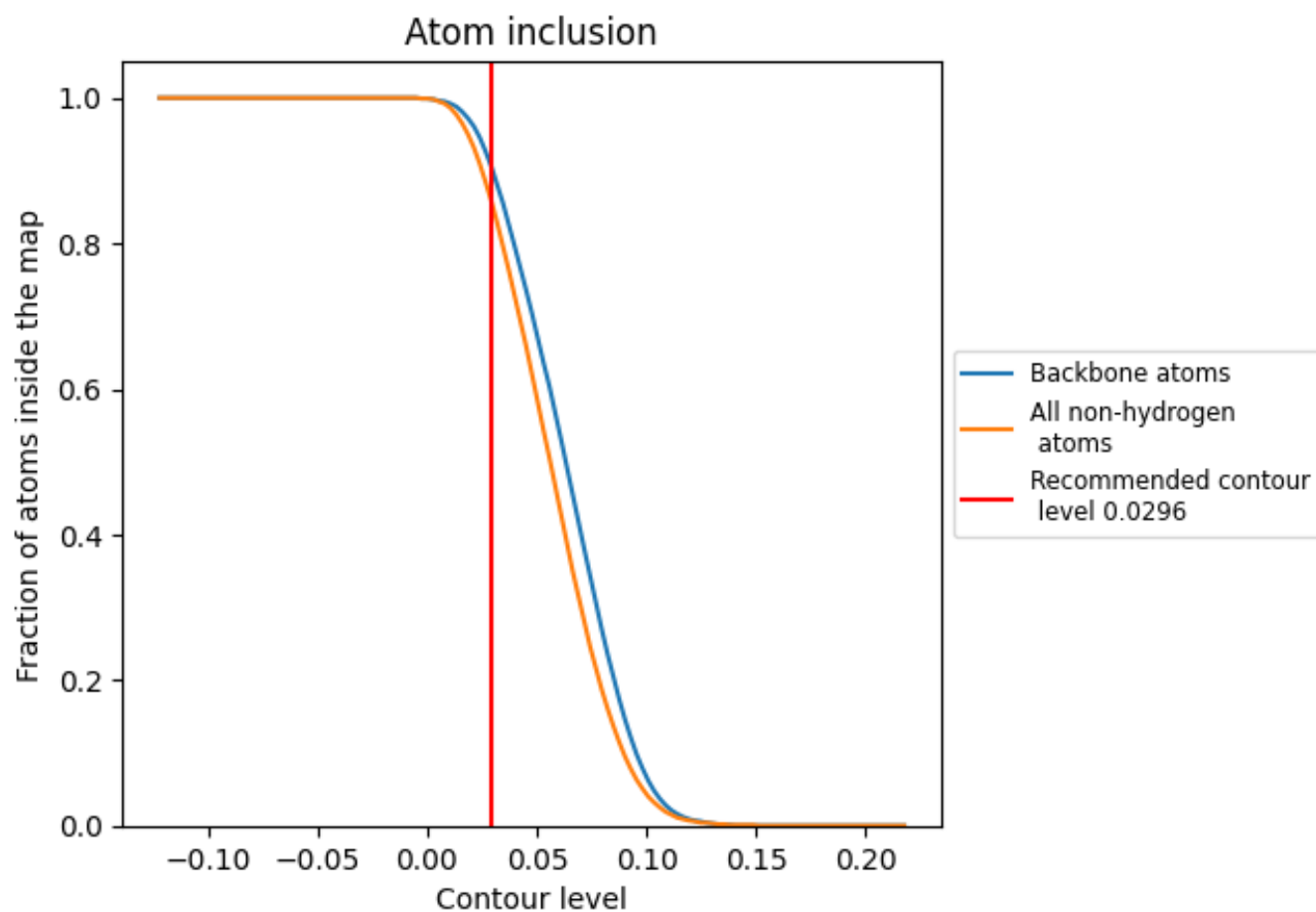
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0296) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.6230
A	 0.7960	 0.5970
B	 0.9380	 0.6590
C	 0.9270	 0.6590
E	 0.8680	 0.6310
F	 0.6990	 0.5520
G	 0.5850	 0.5110
H	 0.8400	 0.6080
I	 0.8030	 0.6150
J	 0.8670	 0.6290
K	 0.7040	 0.5660
L	 0.8800	 0.6450
M	 0.8770	 0.6280
N	 0.8640	 0.6340
O	 0.7730	 0.5890
P	 0.9430	 0.6610
Q	 0.9350	 0.6550
S	 0.9090	 0.6410
T	 0.8530	 0.6340
U	 0.8430	 0.6120
V	 0.7940	 0.6170
W	 0.8330	 0.6110
X	 0.7980	 0.5980
Y	 0.7540	 0.5830
Z	 0.6770	 0.5370
a	 0.8520	 0.6330
b	 0.7910	 0.5900
c	 0.8510	 0.6240
d	 0.8210	 0.6120
e	 0.7920	 0.6020
f	 0.6680	 0.5490
g	 0.8360	 0.6240
h	 0.8350	 0.6160
i	 0.9490	 0.6530
j	 0.8630	 0.6380



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Chain	Atom inclusion	Q-score
k	 0.8960	 0.6410
l	 0.8760	 0.6330
m	 0.8030	 0.5980
n	 0.7220	 0.5770
o	 0.8180	 0.6180
p	 0.8540	 0.6190
r	 0.9410	 0.6490
s	 0.9110	 0.6440
u	 0.8370	 0.6150
v	 0.7330	 0.5720
w	 0.8140	 0.6020