



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:36 AM UTC

PDB ID : 7W4J / pdb_00007w4j
EMDB ID : EMD-32305
Title : Deactive state CI from Q1-NADH dataset, Subclass 1
Authors : Gu, J.; Yang, M.
Deposited on : 2021-11-28
Resolution : 3.20 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

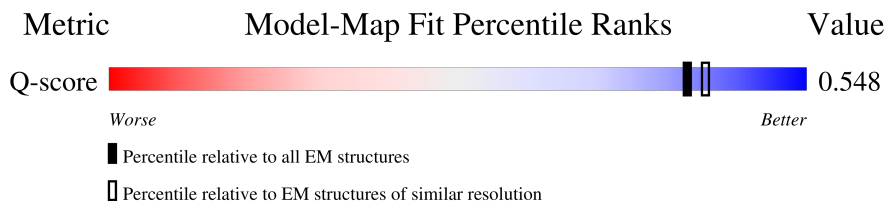
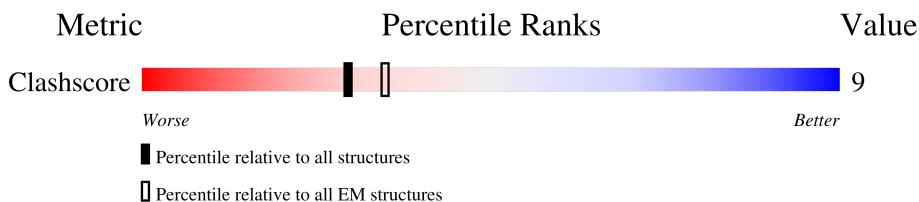
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

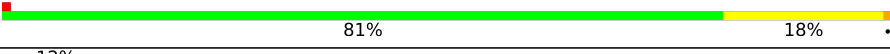
The reported resolution of this entry is 3.20 Å.

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	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	

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Mol	Chain	Length	Quality of chain
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	
29	f	49	
30	g	122	

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Mol	Chain	Length	Quality of chain
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	603	
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	

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66607 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	431	Total	C	N	O	S	0	0
			3318	2095	591	612	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
			1244	792	227	211	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
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2359	1514	421	416	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	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	419	Total	C	N	O	S	0	0
			3377	2162	578	613	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
			567	364	104	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
			1009	645	168	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
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			671	436	116	118	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			868	567	157	143	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	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- 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	603	Total	C	N	O	S	0	0
			4780	3172	740	817	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			948	636	138	166	8		

- 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
			1058	689	182	187			

- 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	303	Total	C	N	O	S	0	0
			2394	1607	369	397	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
			1028	642	195	182	9		

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

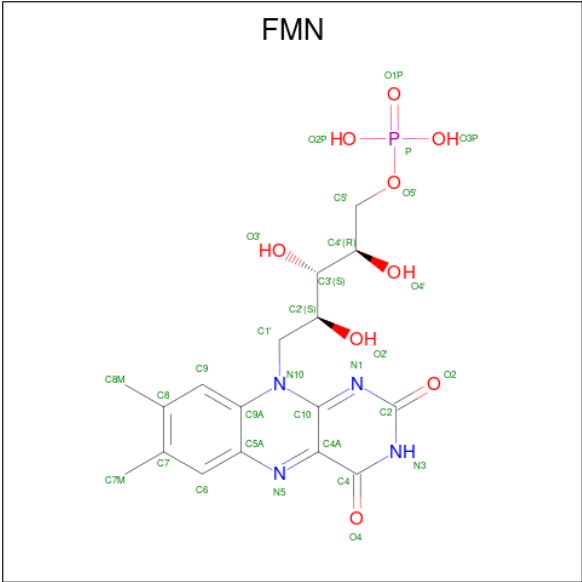
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



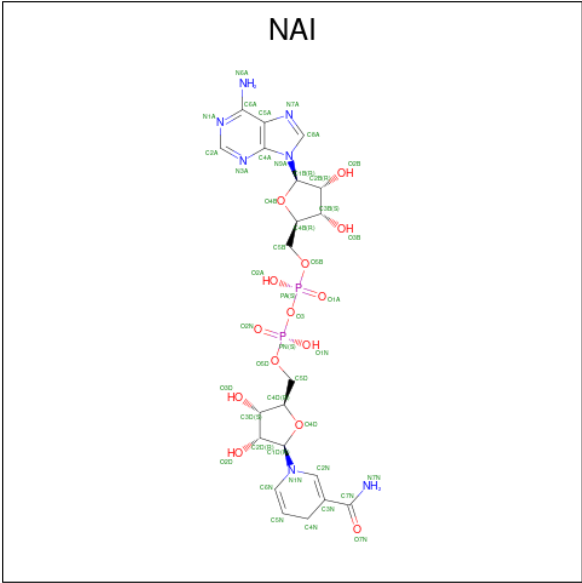
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- 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	

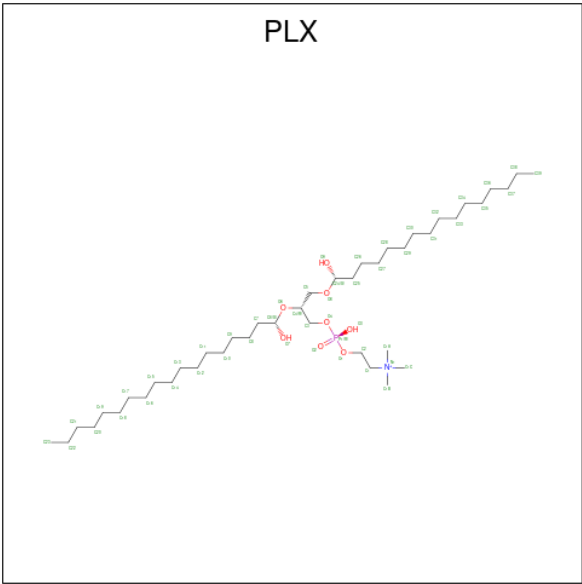
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

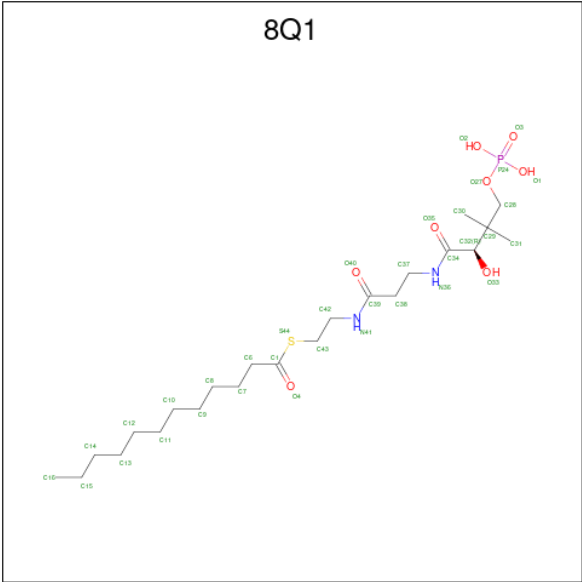
- Molecule 48 is (9R,11S)-9-([(1S)-1-HYDROXYHEXADECYL]OXY)METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-

6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



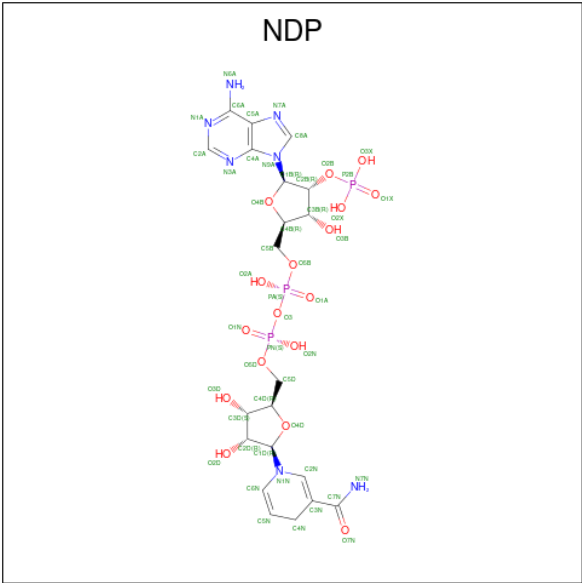
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	l	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



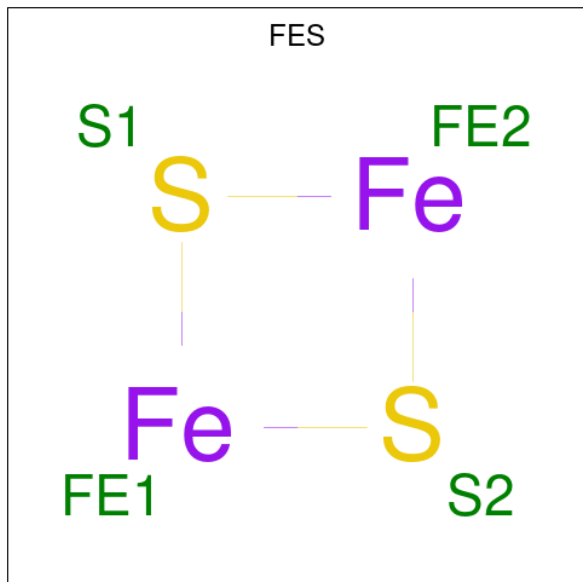
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 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
50	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

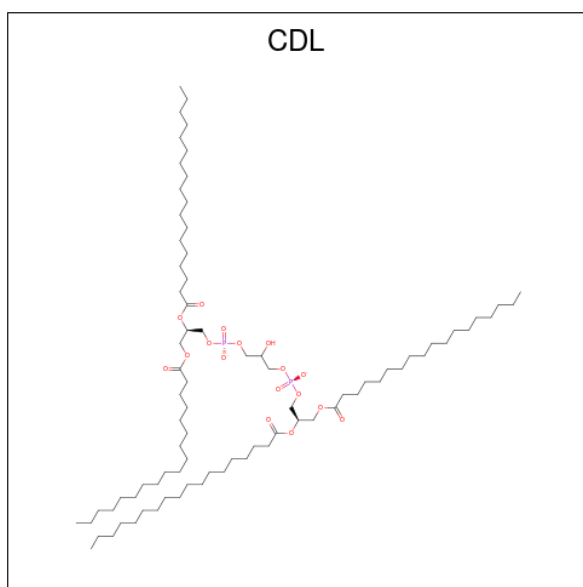


Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	Fe	S	0
			4	2	2	
51	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

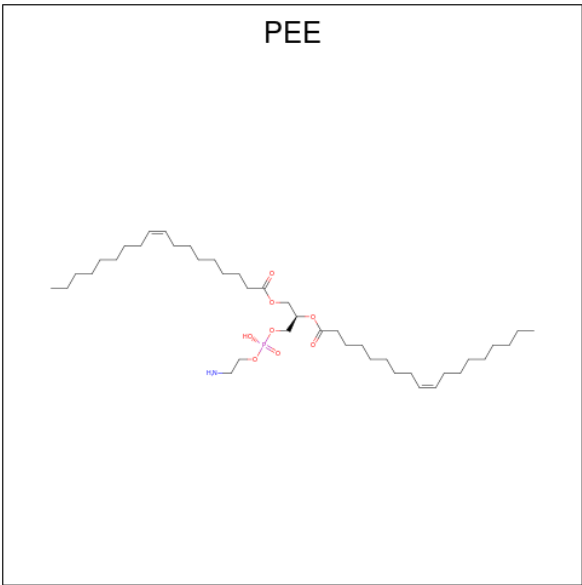


Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	V	1	Total	C	O	P	0
			71	52	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			100	81	17	2	
53	r	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

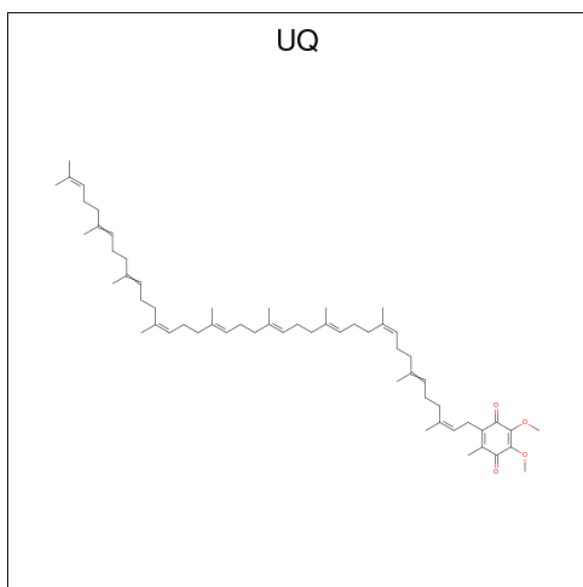
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



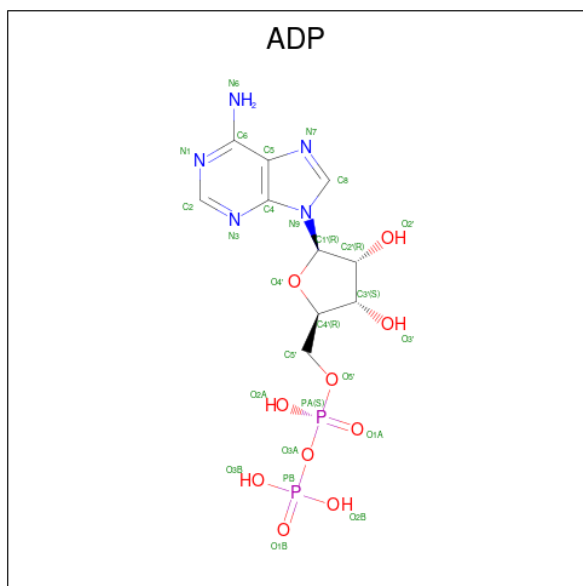
Mol	Chain	Residues	Atoms					AltConf
55	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 56 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
56	s	1	Total	C	O	0
			28	24	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

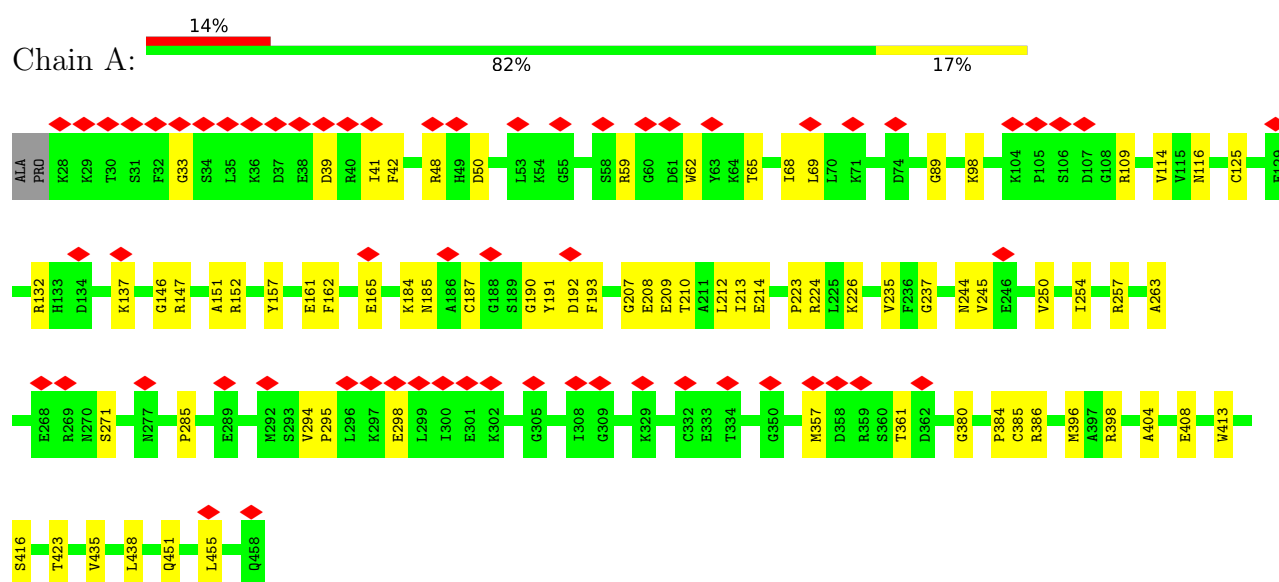


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

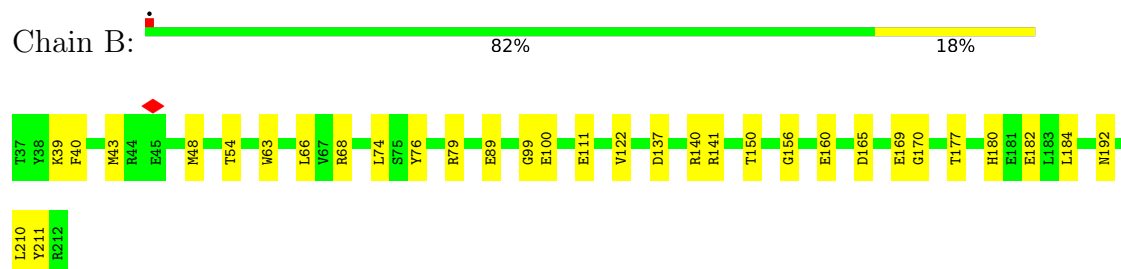
3 Residue-property plots

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

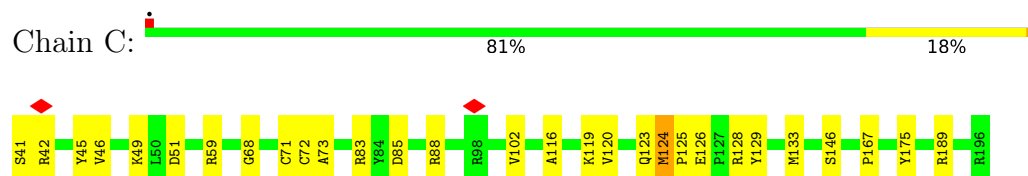
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



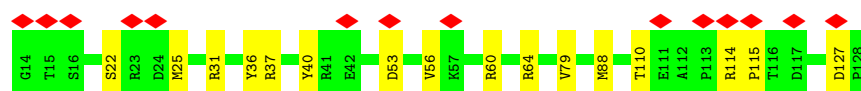
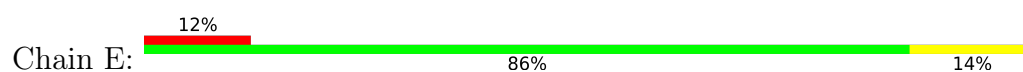
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



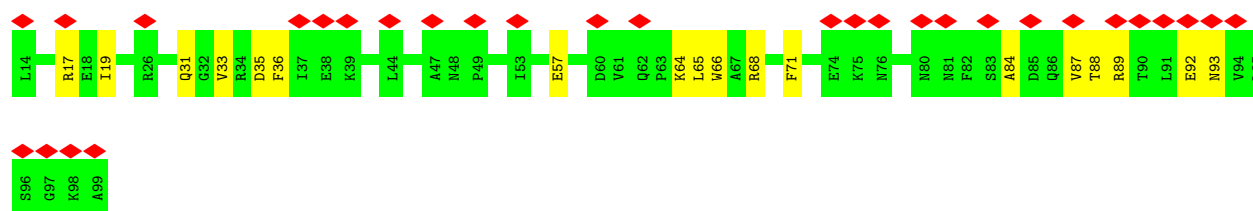
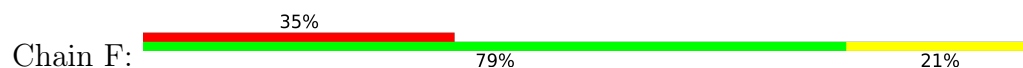
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



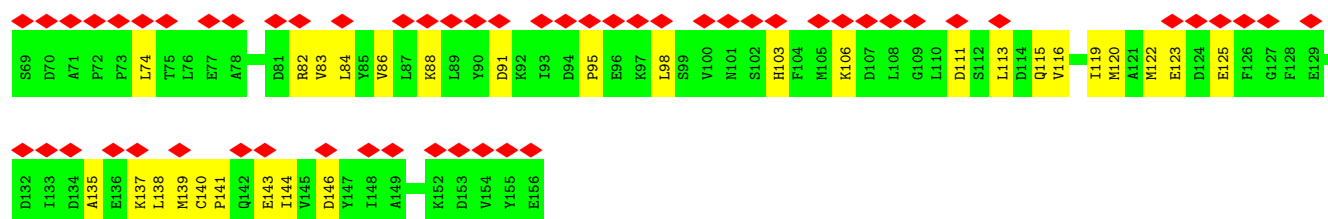
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



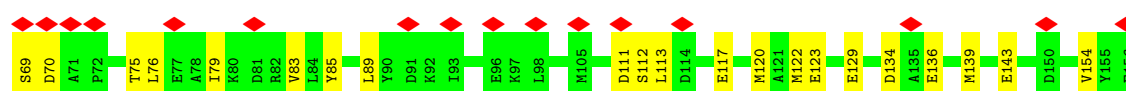
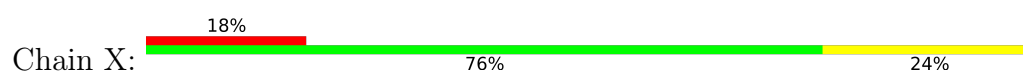
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



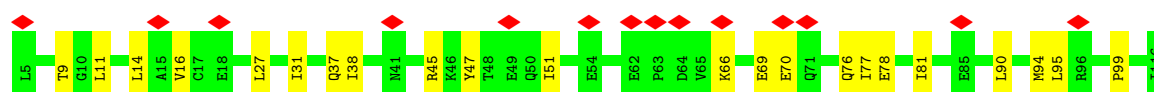
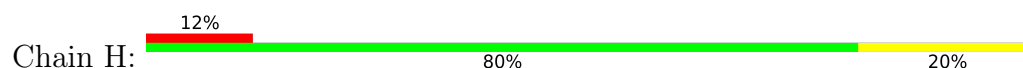
- Molecule 6: Acyl carrier protein



- Molecule 6: Acyl carrier protein



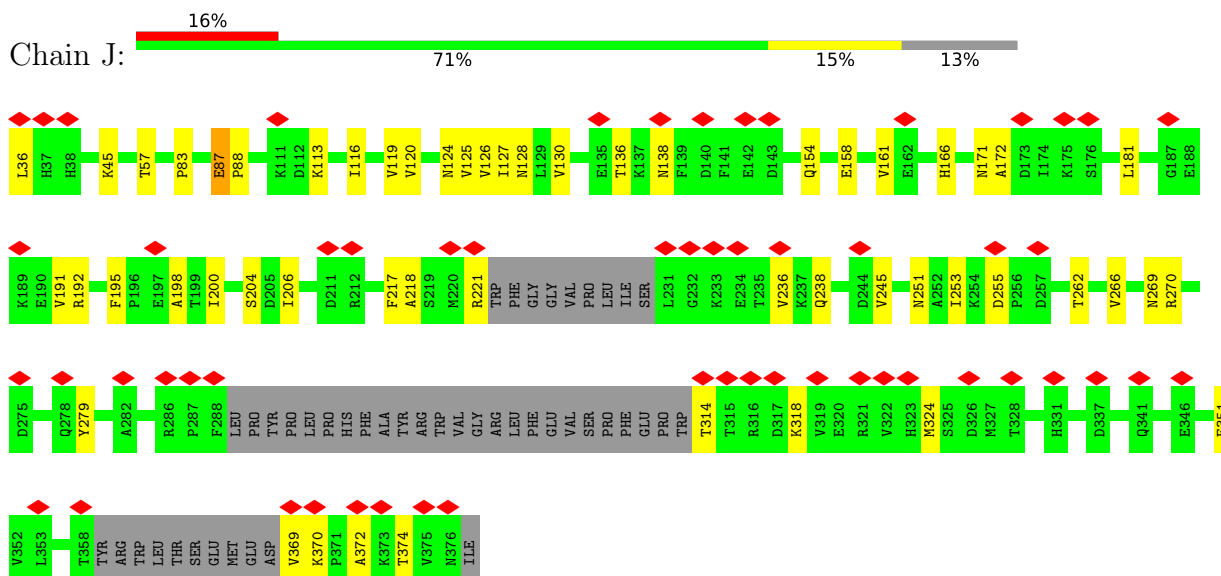
- Molecule 7: Complex I subunit B13



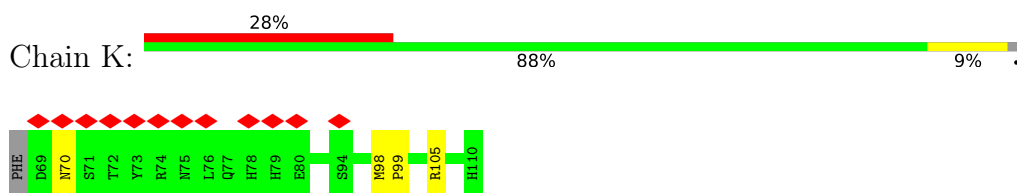
- Molecule 8: Complex I-B14.5a



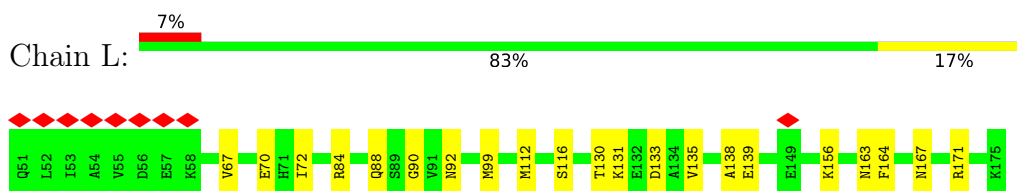
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



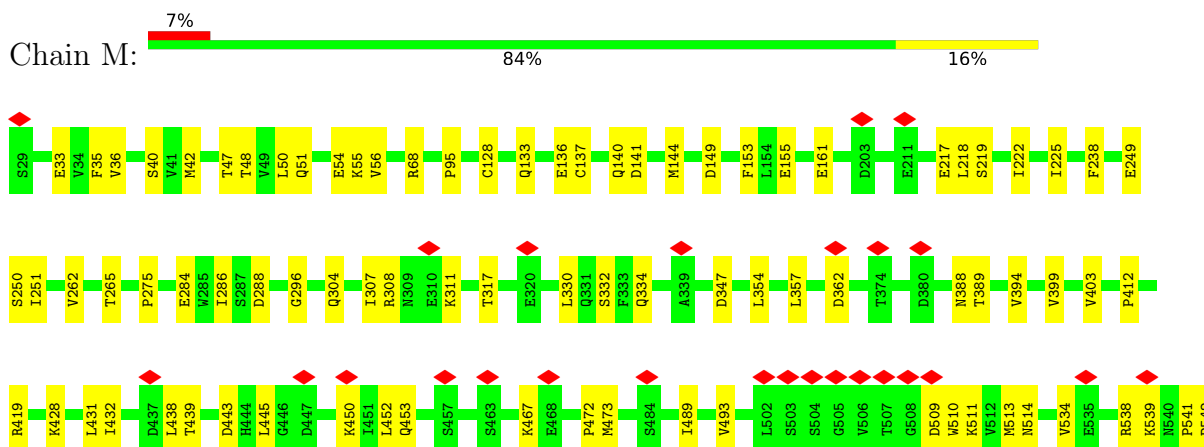
- Molecule 10: Complex I-9kD

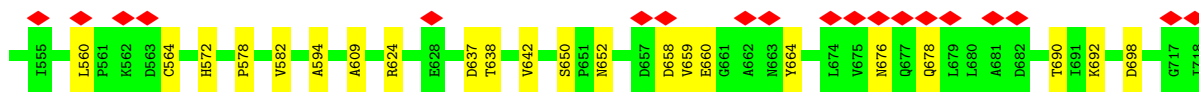


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

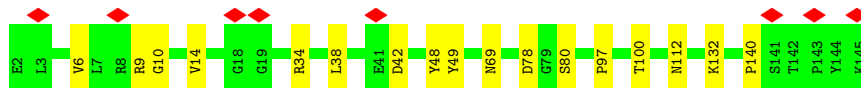
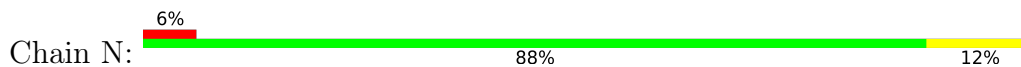


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

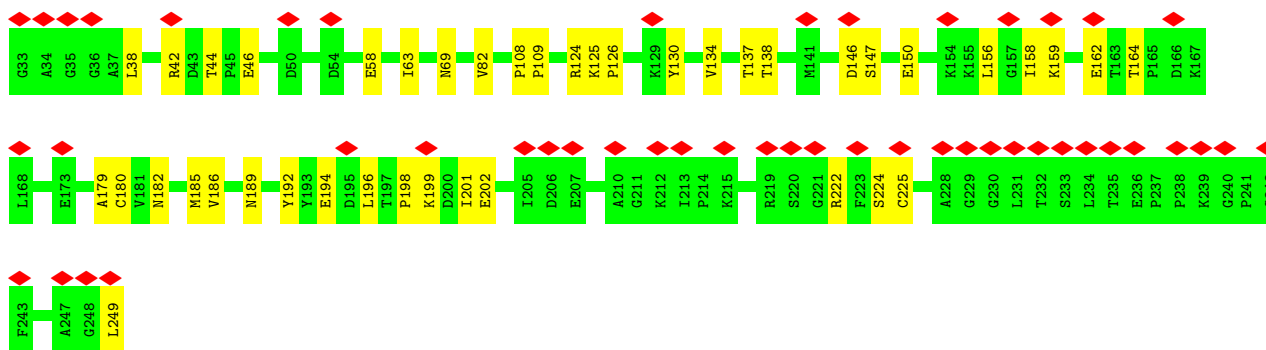
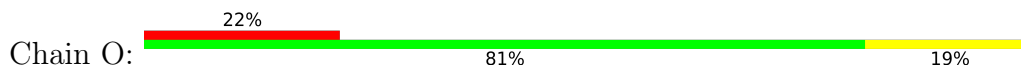




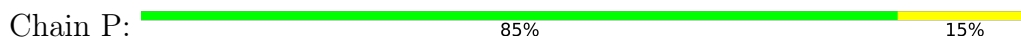
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



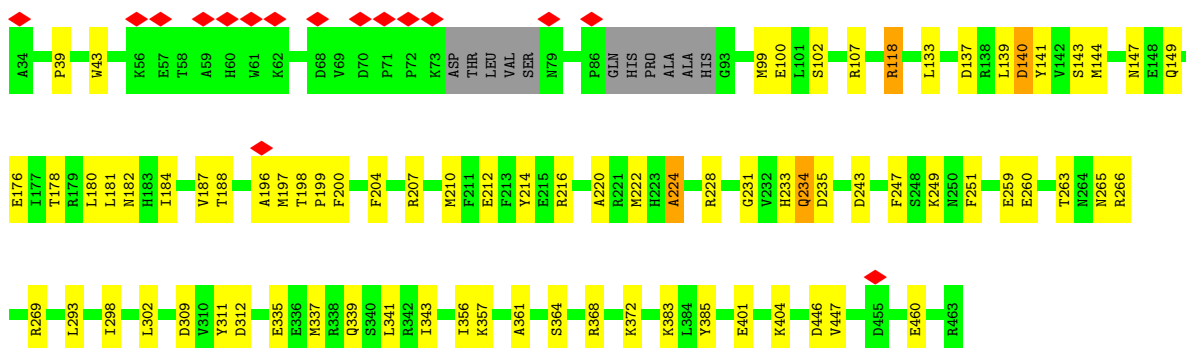
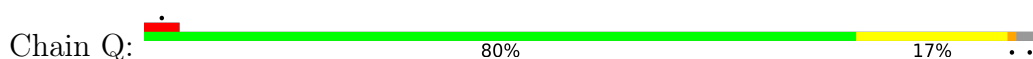
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



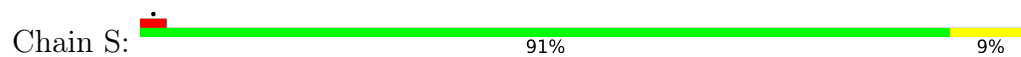
- Molecule 15: Complex I-30kD



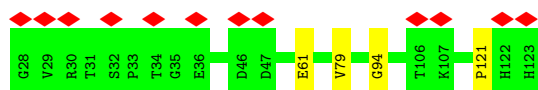
- Molecule 16: Complex I-49kD



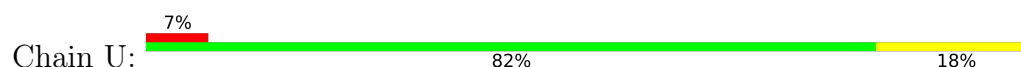
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



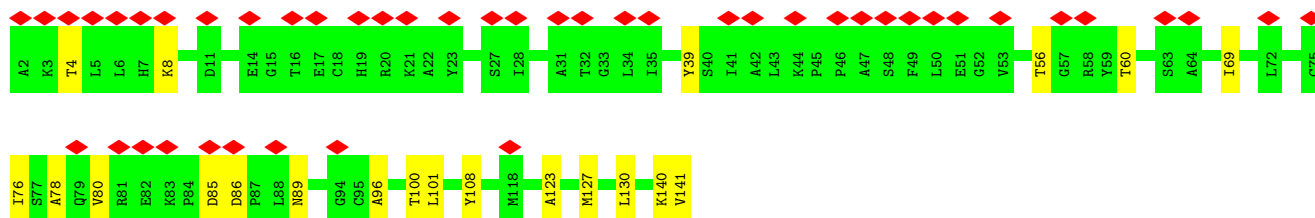
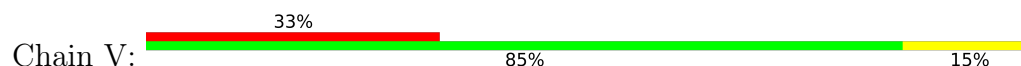
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



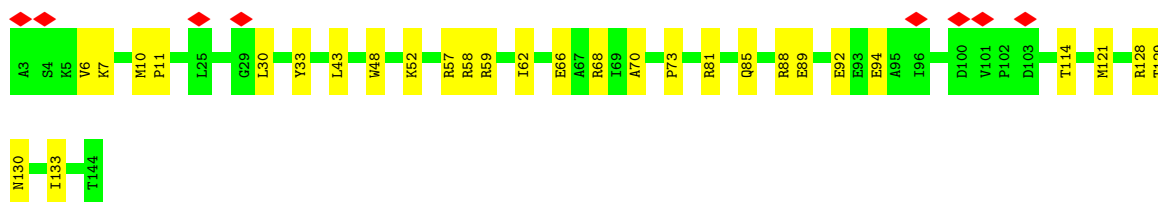
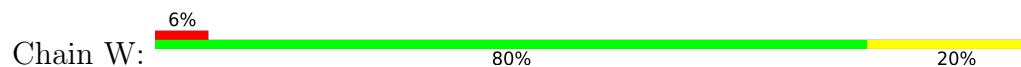
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



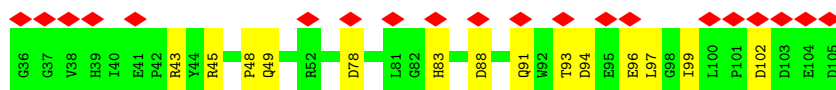
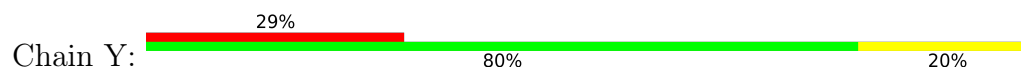
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



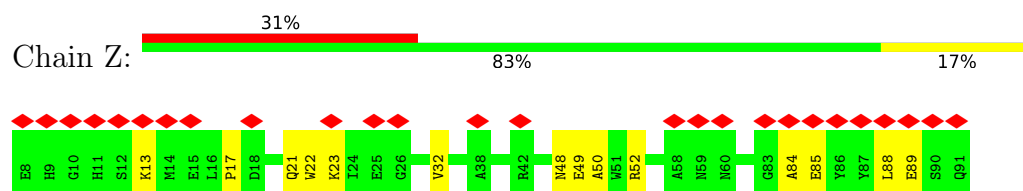
- Molecule 21: Complex I-B16.6



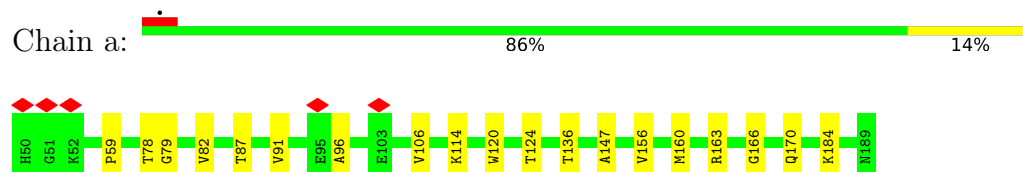
- Molecule 22: Complex I-AGGG



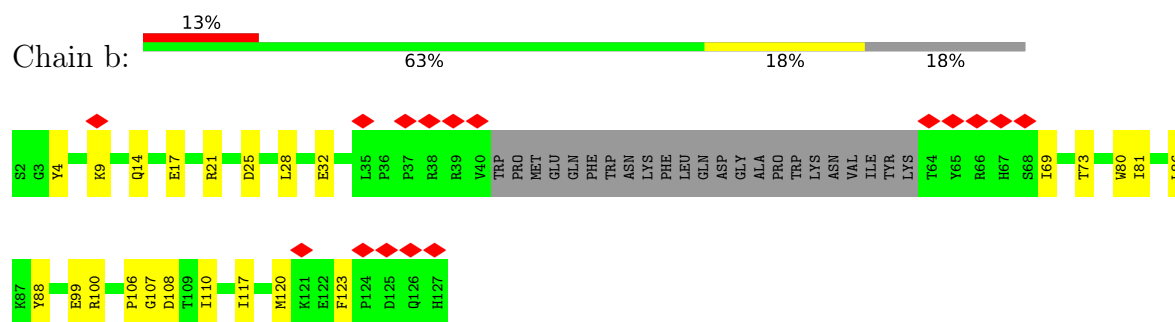
- Molecule 23: Complex I-B12



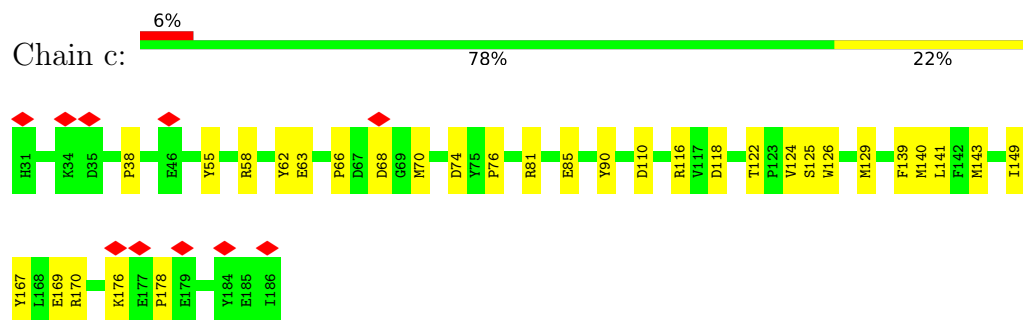
- Molecule 24: Complex I-SGDH



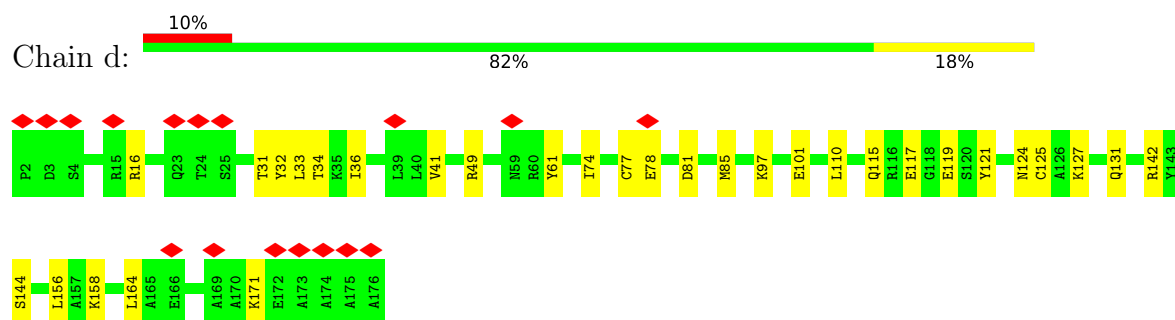
- Molecule 25: Complex I-B17



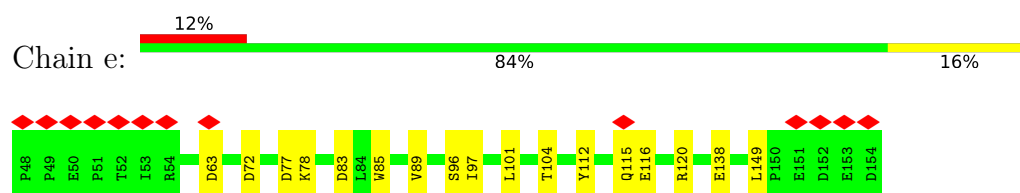
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



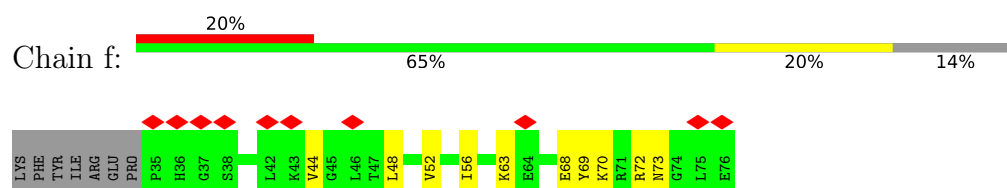
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



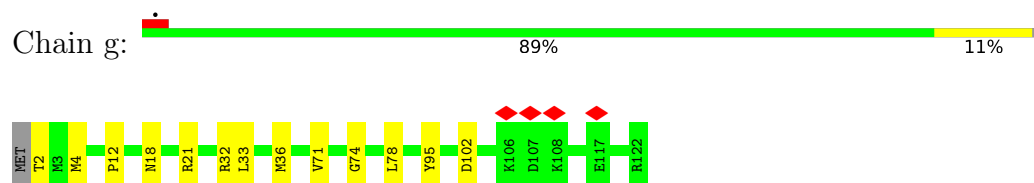
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



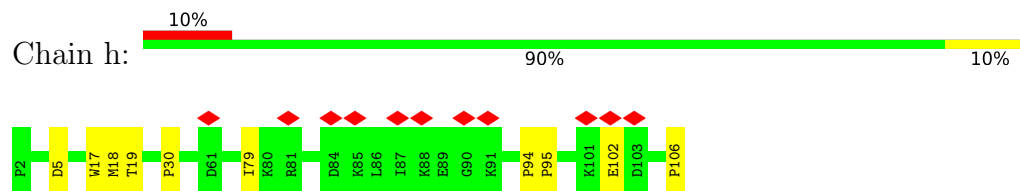
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



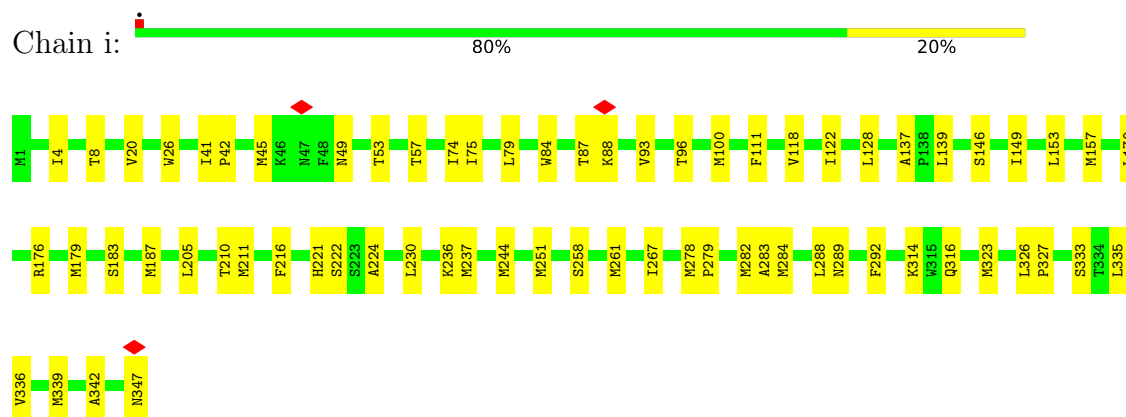
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

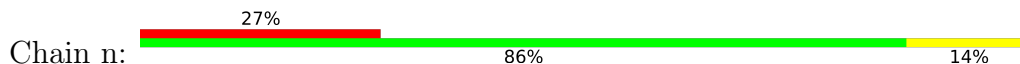


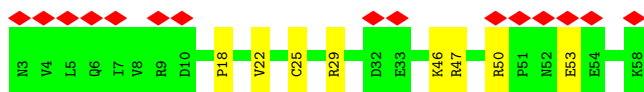
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



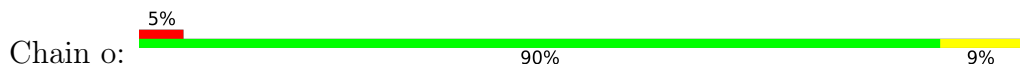
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



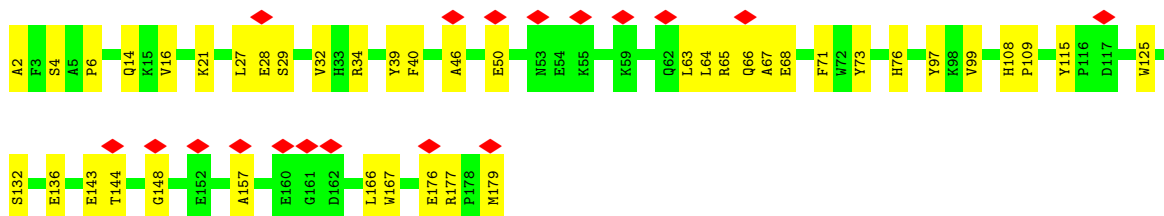
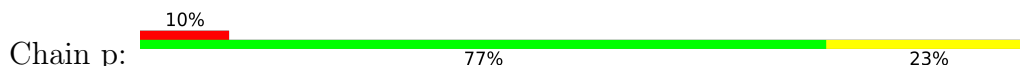




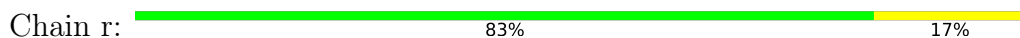
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



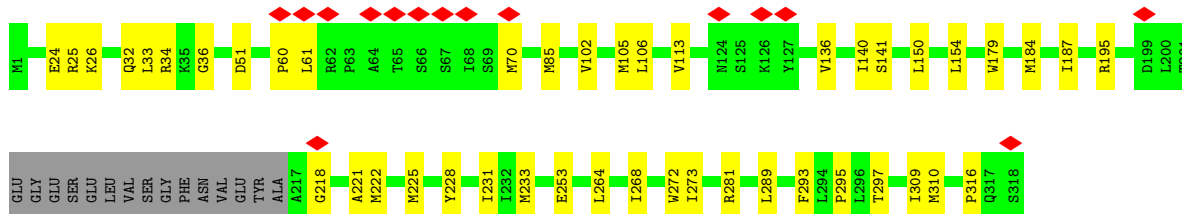
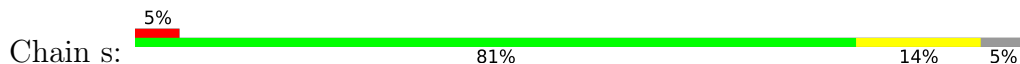
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

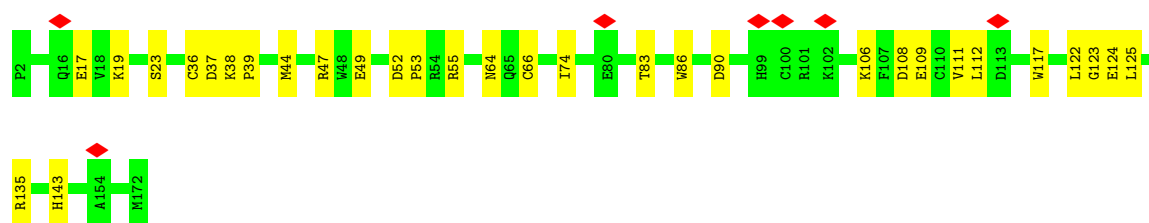


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



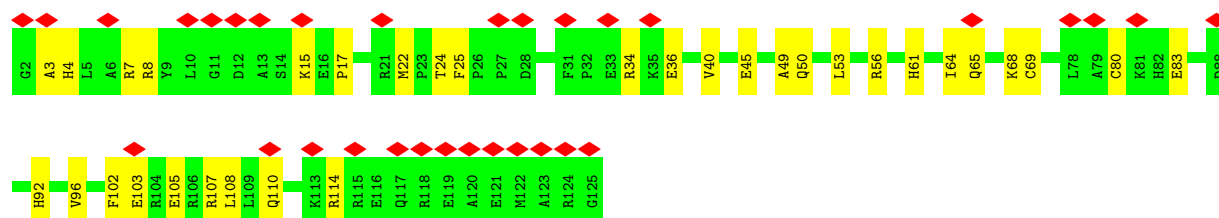
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  82% 18%



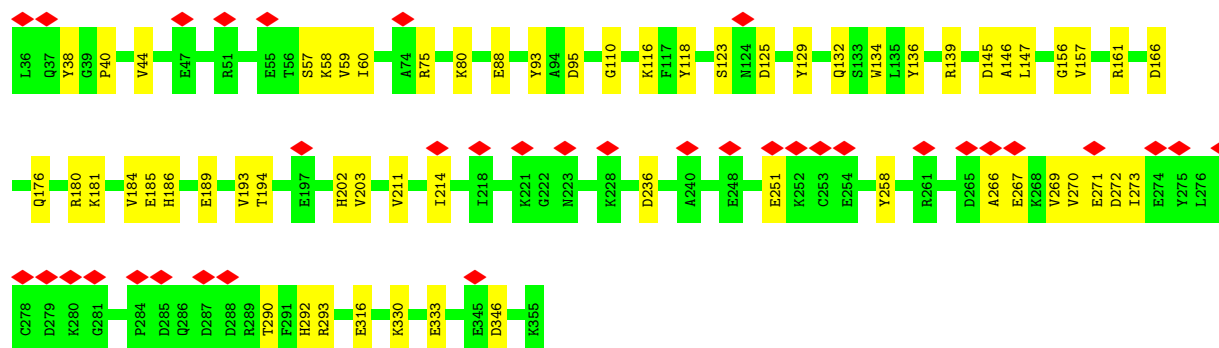
• Molecule 43: Complex I-B18

Chain v:  26% 73% 27%



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

Chain w:  11% 82% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32329	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	0.228	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0298	Depositor
Map size ($\text{\AA}$)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: FES, ADP, UQ, SF4, 8Q1, PLX, 2MR, CDL, MG, PEE, ZN, NDP, NAI, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3393	0.35	0/4584
2	B	0.11	0/1443	0.28	0/1952
3	C	0.14	0/1275	0.41	2/1725 (0.1%)
4	E	0.11	0/995	0.28	0/1340
5	F	0.12	0/702	0.33	0/945
6	G	0.18	0/705	0.44	0/956
6	X	0.11	0/708	0.31	0/959
7	H	0.12	0/929	0.35	0/1258
8	I	0.14	0/798	0.37	0/1079
9	J	0.13	0/2411	0.34	2/3254 (0.1%)
10	K	0.09	0/365	0.27	0/493
11	L	0.10	0/1039	0.28	0/1403
12	M	0.11	0/5384	0.31	0/7295
13	N	0.10	0/1245	0.29	0/1694
14	O	0.12	0/1711	0.36	0/2328
15	P	0.12	0/1789	0.33	0/2436
16	Q	0.19	0/3451	0.49	6/4672 (0.1%)
17	S	0.15	0/582	0.37	0/783
18	T	0.08	0/755	0.25	0/1018
19	U	0.11	0/664	0.34	0/912
20	V	0.21	0/1030	0.49	2/1397 (0.1%)
21	W	0.13	0/1204	0.28	0/1624
22	Y	0.13	0/623	0.32	0/853
23	Z	0.10	0/692	0.33	0/935
24	a	0.12	0/1199	0.34	0/1623
25	b	0.14	0/895	0.45	0/1219
26	c	0.15	0/1371	0.35	0/1875
27	d	0.19	0/1494	0.44	2/2015 (0.1%)
28	e	0.16	0/916	0.46	0/1246
29	f	0.14	0/350	0.34	0/473
30	g	0.11	0/1031	0.26	0/1394
31	h	0.12	0/889	0.30	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.14	0/2773	0.33	0/3768
33	j	0.17	0/819	0.42	0/1117
34	k	0.16	0/759	0.36	0/1029
35	l	0.15	0/4909	0.39	2/6677 (0.0%)
36	m	0.15	0/970	0.40	0/1316
37	n	0.18	0/491	0.39	0/663
38	o	0.15	0/1088	0.45	2/1476 (0.1%)
39	p	0.15	0/1590	0.49	7/2155 (0.3%)
40	r	0.15	0/3723	0.36	2/5078 (0.0%)
41	s	0.15	0/2464	0.36	0/3369
42	u	0.12	0/1436	0.34	0/1938
43	v	0.14	0/1052	0.38	0/1411
44	w	0.12	0/2642	0.32	0/3580
All	All	0.14	0/66754	0.37	27/90507 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	233	HIS	N-CA-C	10.10	122.29	111.28
16	Q	140	ASP	N-CA-C	-7.71	95.70	108.34
35	l	429	PHE	N-CA-C	6.75	118.72	111.36
16	Q	224	ALA	N-CA-C	6.61	118.56	111.36
35	l	432	LEU	N-CA-C	6.51	118.38	111.28
39	p	144	THR	CA-C-N	6.46	127.04	120.38
39	p	144	THR	C-N-CA	6.46	127.04	120.38
20	V	86	ASP	CA-C-N	6.27	126.01	119.05
20	V	86	ASP	C-N-CA	6.27	126.01	119.05
40	r	246	ILE	N-CA-C	6.12	118.73	111.09
38	o	19	ASP	CA-C-N	6.06	125.78	119.05
38	o	19	ASP	C-N-CA	6.06	125.78	119.05
39	p	148	GLY	CA-C-N	6.00	125.76	119.76
39	p	148	GLY	C-N-CA	6.00	125.76	119.76
27	d	124	ASN	N-CA-C	5.93	117.83	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	124	MET	CA-C-N	5.87	125.78	119.85
3	C	124	MET	C-N-CA	5.87	125.78	119.85
39	p	66	GLN	N-CA-C	-5.72	105.05	111.28
9	J	87	GLU	CA-C-N	5.68	125.35	119.05
9	J	87	GLU	C-N-CA	5.68	125.35	119.05
27	d	121	TYR	N-CA-C	5.47	117.24	111.28
16	Q	231	GLY	N-CA-C	5.44	118.67	111.70
16	Q	187	VAL	N-CA-C	5.35	115.56	110.53
39	p	143	GLU	N-CA-C	5.28	117.03	111.28
40	r	247	THR	N-CA-C	5.10	116.84	111.28
39	p	144	THR	N-CA-C	5.06	116.06	109.64
16	Q	234	GLN	N-CA-C	5.04	120.29	114.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	51	0
2	B	1412	0	1363	26	0
3	C	1244	0	1250	22	0
4	E	971	0	975	12	0
5	F	691	0	704	11	0
6	G	693	0	671	33	0
6	X	696	0	680	16	0
7	H	910	0	950	13	0
8	I	780	0	808	16	0
9	J	2359	0	2402	31	0
10	K	355	0	329	4	0
11	L	1016	0	1016	16	0
12	M	5296	0	5326	71	0
13	N	1204	0	1162	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	O	1671	0	1673	28	0
15	P	1738	0	1693	23	0
16	Q	3377	0	3319	52	0
17	S	567	0	565	5	0
18	T	741	0	702	3	0
19	U	643	0	642	14	0
20	V	1009	0	1005	16	0
21	W	1173	0	1166	25	0
22	Y	597	0	537	9	0
23	Z	671	0	641	9	0
24	a	1165	0	1174	17	0
25	b	868	0	882	26	0
26	c	1315	0	1208	28	0
27	d	1461	0	1431	31	0
28	e	890	0	837	16	0
29	f	342	0	341	8	0
30	g	1000	0	994	10	0
31	h	867	0	871	10	0
32	i	2710	0	2874	48	0
33	j	800	0	855	15	0
34	k	748	0	799	18	0
35	l	4780	0	4923	116	0
36	m	948	0	960	23	0
37	n	479	0	486	6	0
38	o	1058	0	1068	10	0
39	p	1534	0	1470	32	0
40	r	3631	0	3839	53	0
41	s	2394	0	2508	39	0
42	u	1398	0	1378	23	0
43	v	1028	0	980	32	0
44	w	2582	0	2531	36	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	6	0
47	A	44	0	27	2	0
48	C	52	0	88	4	0
48	a	52	0	88	1	0
48	i	52	0	88	4	0
48	j	52	0	88	3	0
48	l	52	0	88	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	r	52	0	88	2	0
49	G	35	0	0	0	0
49	X	35	0	0	6	0
50	J	48	0	24	1	0
51	M	4	0	0	0	0
51	O	4	0	0	0	0
52	M	1	0	0	0	0
53	N	51	0	46	0	0
53	V	71	0	92	7	0
53	a	91	0	132	4	0
53	i	66	0	76	2	0
53	l	100	0	156	5	0
53	r	100	0	156	7	0
54	T	1	0	0	0	0
55	U	51	0	82	5	0
55	i	47	0	71	5	0
55	j	47	0	71	2	0
55	l	92	0	138	4	0
55	m	41	0	59	0	0
55	r	51	0	82	2	0
55	s	51	0	82	8	0
56	s	28	0	31	2	0
57	w	27	0	11	2	0
All	All	66607	0	67151	977	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 9.

All (977) 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)
6:X:112:SER:CB	49:X:201:8Q1:O1	1.66	1.42
50:J:401:NDP:O4D	50:J:401:NDP:C4D	1.69	1.12
16:Q:235:ASP:HB2	16:Q:356:ILE:HD13	1.40	1.01
27:d:125:CYS:CB	35:l:203:MET:HE1	1.93	0.97
25:b:123:PHE:CD2	43:v:40:VAL:HG11	2.02	0.95
27:d:125:CYS:HB2	35:l:203:MET:HE1	1.52	0.90
21:W:57:ARG:HG2	41:s:316:PRO:HG3	1.55	0.88
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.57	0.86
38:o:23:TYR:OH	39:p:68:GLU:HG3	1.75	0.86
20:V:108:TYR:HB2	53:V:201:CDL:HB32	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:22:MET:HE1	43:v:102:PHE:HA	1.61	0.83
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.62	0.82
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.45	0.82
41:s:273:ILE:HD11	55:s:401:PEE:H64	1.63	0.81
40:r:207:MET:HE2	40:r:243:MET:HE2	1.63	0.80
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.64	0.79
27:d:125:CYS:CB	35:l:203:MET:CE	2.61	0.78
12:M:307:ILE:HG22	12:M:582:VAL:HG22	1.66	0.78
40:r:207:MET:HE2	40:r:243:MET:CE	2.14	0.78
27:d:110:LEU:HD11	35:l:203:MET:HG2	1.65	0.76
19:U:78:LEU:HD13	42:u:123:GLY:HA3	1.68	0.76
27:d:119:GLU:HB2	43:v:50:GLN:HB2	1.68	0.75
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.50	0.74
39:p:64:LEU:O	39:p:68:GLU:CG	2.35	0.74
25:b:106:PRO:HG2	25:b:120:MET:HE2	1.70	0.74
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.74
9:J:154:GLN:NE2	9:J:158:GLU:OE1	2.21	0.73
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.70	0.73
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.22	0.72
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.71	0.72
1:A:396:MET:HE3	1:A:435:VAL:HG22	1.69	0.72
12:M:539:LYS:HE3	12:M:539:LYS:HA	1.70	0.72
3:C:125:PRO:HG3	41:s:61:LEU:HD11	1.71	0.72
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.70	0.72
6:G:138:LEU:HD23	6:G:144:ILE:HG23	1.71	0.72
1:A:208:GLU:OE1	1:A:223:PRO:HB3	1.90	0.71
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.23	0.71
16:Q:266:ARG:NH1	55:s:401:PEE:O1P	2.23	0.71
5:F:89:ARG:O	5:F:93:ASN:ND2	2.24	0.71
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.71	0.71
32:i:87:THR:HG22	32:i:88:LYS:H	1.56	0.71
26:c:126:TRP:HA	26:c:129:MET:HE2	1.73	0.70
26:c:116:ARG:HG2	55:l:703:PEE:H49	1.72	0.70
53:r:503:CDL:H742	53:r:503:CDL:H271	1.73	0.70
20:V:85:ASP:HB2	20:V:130:LEU:HD21	1.72	0.70
16:Q:140:ASP:HB3	16:Q:147:ASN:HD21	1.55	0.70
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.72	0.70
41:s:273:ILE:HD11	55:s:401:PEE:C39	2.22	0.69
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.74	0.69
40:r:247:THR:O	40:r:249:ILE:N	2.25	0.69
28:e:72:ASP:OD1	39:p:108:HIS:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG12	14:O:249:LEU:HD11	1.73	0.69
27:d:125:CYS:HB2	35:l:203:MET:CE	2.23	0.69
28:e:112:TYR:HB3	40:r:45:LEU:HG	1.75	0.69
32:i:236:LYS:HE3	32:i:237:MET:HE2	1.75	0.69
6:G:103:HIS:CD2	6:G:139:MET:HG3	2.27	0.68
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.34	0.68
25:b:120:MET:CE	43:v:64:ILE:HG21	2.22	0.68
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.74	0.68
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.59	0.68
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.74	0.68
1:A:285:PRO:O	14:O:222:ARG:NH2	2.27	0.68
41:s:187:ILE:HD12	55:s:401:PEE:H57	1.75	0.67
12:M:33:GLU:HG3	12:M:42:MET:HE1	1.77	0.67
3:C:72:CYS:HB3	3:C:133:MET:HE2	1.76	0.67
7:H:27:LEU:O	7:H:31:ILE:HG13	1.94	0.67
8:I:51:ASN:ND2	8:I:51:ASN:O	2.28	0.67
25:b:108:ASP:OD1	43:v:68:LYS:NZ	2.28	0.67
33:j:79:SER:HA	33:j:87:MET:HE2	1.77	0.66
2:B:111:GLU:O	2:B:141:ARG:NH1	2.28	0.66
6:X:112:SER:CB	49:X:201:8Q1:P24	2.83	0.66
32:i:26:TRP:HB3	32:i:74:ILE:HD13	1.78	0.66
6:G:139:MET:N	6:G:143:GLU:OE2	2.20	0.66
40:r:229:MET:HE3	40:r:328:CYS:SG	2.36	0.66
1:A:33:GLY:HA2	1:A:294:VAL:HG12	1.76	0.66
27:d:81:ASP:O	27:d:85:MET:HG3	1.97	0.65
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.79	0.65
5:F:19:ILE:HD11	5:F:65:LEU:HD21	1.77	0.65
32:i:45:MET:HE3	32:i:53:THR:HG22	1.78	0.65
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.30	0.65
4:E:22:SER:OG	4:E:31:ARG:NH1	2.29	0.65
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.79	0.65
27:d:125:CYS:SG	35:l:203:MET:HE1	2.36	0.65
8:I:23:LYS:NZ	16:Q:249:LYS:O	2.30	0.65
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.78	0.65
35:l:370:THR:O	35:l:374:ILE:HG12	1.97	0.64
16:Q:133:LEU:CD2	16:Q:228:ARG:HD3	2.27	0.64
35:l:331:MET:HB3	35:l:387:THR:HG22	1.80	0.64
12:M:493:VAL:HG23	12:M:513:MET:HE1	1.80	0.64
38:o:19:ASP:OD1	38:o:20:PRO:HD2	1.98	0.64
41:s:187:ILE:CD1	55:s:401:PEE:H57	2.28	0.64
29:f:48:LEU:O	29:f:52:VAL:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:106:VAL:HG13	37:n:50:ARG:HH21	1.62	0.64
9:J:238:GLN:HE21	9:J:266:VAL:HB	1.63	0.63
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.30	0.63
35:l:559:GLU:OE1	35:l:564:LYS:NZ	2.30	0.63
9:J:113:LYS:HA	9:J:116:ILE:HD12	1.80	0.63
44:w:267:GLU:O	44:w:271:GLU:HG3	1.99	0.63
32:i:53:THR:O	32:i:57:THR:HG23	1.99	0.63
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.81	0.63
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.31	0.63
19:U:27:GLY:O	19:U:31:ILE:HG12	1.99	0.63
25:b:99:GLU:HB2	35:l:61:MET:HE2	1.80	0.63
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.81	0.62
35:l:499:MET:O	35:l:503:GLU:HG3	1.99	0.62
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.80	0.62
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.81	0.62
2:B:68:ARG:NH2	16:Q:260:GLU:OE1	2.32	0.62
24:a:120:TRP:O	24:a:124:THR:HG22	1.99	0.62
9:J:136:THR:HG22	9:J:138:ASN:H	1.65	0.62
9:J:218:ALA:O	9:J:221:ARG:NH1	2.32	0.62
21:W:10:MET:HE3	21:W:11:PRO:HD2	1.80	0.62
6:G:103:HIS:ND1	6:G:106:LYS:HE3	2.15	0.61
1:A:451:GLN:O	1:A:455:LEU:HD13	2.00	0.61
35:l:327:LEU:O	35:l:331:MET:HG2	1.99	0.61
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.82	0.61
26:c:155:PRO:HD3	43:v:4:HIS:CE1	2.34	0.61
35:l:331:MET:HE1	35:l:465:GLY:HA2	1.83	0.61
5:F:31:GLN:NE2	5:F:35:ASP:OD1	2.34	0.61
24:a:78:THR:OG1	28:e:96:SER:HB2	2.01	0.61
44:w:176:GLN:NE2	44:w:236:ASP:OD2	2.34	0.61
1:A:244:ASN:OD1	1:A:245:VAL:N	2.33	0.61
35:l:504:LEU:HD13	53:l:702:CDL:H522	1.82	0.61
33:j:7:LEU:O	33:j:11:VAL:HG23	2.00	0.61
6:G:122:MET:HA	6:G:122:MET:HE3	1.83	0.61
6:X:134:ASP:OD2	39:p:2:ALA:N	2.34	0.60
35:l:391:SER:O	35:l:395:ILE:HG12	2.01	0.60
41:s:85:MET:HE2	41:s:233:MET:HE2	1.82	0.60
15:P:104:THR:O	15:P:107:GLN:NE2	2.33	0.60
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.83	0.60
1:A:62:TRP:HE3	1:A:65:THR:HG21	1.66	0.60
5:F:88:THR:O	5:F:92:GLU:HG2	2.02	0.60
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:117:GLU:OE2	27:d:117:GLU:HA	2.01	0.60
35:l:362:LEU:HD12	35:l:430:ALA:O	2.01	0.60
20:V:56:THR:O	20:V:60:THR:HG22	2.01	0.60
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.84	0.60
4:E:40:TYR:HB3	6:G:120:MET:HE1	1.83	0.60
12:M:403:VAL:HG11	12:M:452:LEU:HD11	1.83	0.60
1:A:413:TRP:O	1:A:416:SER:OG	2.20	0.60
3:C:41:SER:OG	3:C:42:ARG:N	2.35	0.59
40:r:269:MET:HE1	40:r:296:LEU:HD12	1.84	0.59
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.59
7:H:94:MET:SD	7:H:99:PRO:HG3	2.42	0.59
14:O:198:PRO:O	14:O:201:ILE:HG22	2.02	0.59
12:M:428:LYS:NZ	12:M:443:ASP:OD2	2.34	0.59
26:c:110:ASP:OD1	26:c:110:ASP:N	2.36	0.59
35:l:227:PHE:O	35:l:230:HIS:ND1	2.35	0.59
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.31	0.59
23:Z:21:GLN:O	23:Z:23:LYS:NZ	2.34	0.59
40:r:452:LYS:HA	40:r:455:LEU:HD12	1.83	0.59
1:A:209:GLU:OE2	1:A:226:LYS:NZ	2.26	0.59
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.83	0.59
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.34	0.59
55:U:101:PEE:H26	41:s:295:PRO:HB3	1.83	0.59
25:b:123:PHE:HB3	43:v:40:VAL:CG2	2.33	0.59
24:a:166:GLY:O	24:a:170:GLN:NE2	2.35	0.59
41:s:70:MET:HE3	41:s:70:MET:HA	1.85	0.59
1:A:152:ARG:NH2	10:K:99:PRO:O	2.36	0.59
11:L:131:LYS:O	11:L:135:VAL:HG23	2.03	0.59
40:r:337:VAL:HG21	40:r:345:ALA:HB2	1.84	0.59
24:a:96:ALA:O	24:a:114:LYS:NZ	2.36	0.58
20:V:69:ILE:HG21	20:V:100:THR:HG21	1.86	0.58
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.58
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.38	0.58
35:l:419:THR:HA	35:l:422:TYR:CE2	2.39	0.58
6:G:120:MET:HA	6:G:123:GLU:HG3	1.84	0.58
7:H:9:THR:HG23	7:H:16:VAL:HG22	1.86	0.58
12:M:388:ASN:O	12:M:511:LYS:NZ	2.31	0.58
27:d:164:LEU:HD23	28:e:149:LEU:HD13	1.85	0.58
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.32	0.58
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.85	0.58
21:W:73:PRO:HA	42:u:44:MET:HE2	1.86	0.58
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:18:ASN:OD1	30:g:21:ARG:NH2	2.37	0.58
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.85	0.58
6:X:69:SER:OG	6:X:70:ASP:N	2.35	0.58
35:l:151:SER:HG	35:l:248:HIS:HE2	1.50	0.58
27:d:32:TYR:O	27:d:36:ILE:HG23	2.04	0.58
1:A:116:ASN:ND2	1:A:207:GLY:O	2.30	0.57
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.86	0.57
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.85	0.57
55:i:403:PEE:H37	55:i:403:PEE:H60	1.85	0.57
10:K:105:ARG:NH1	11:L:167:ASN:O	2.36	0.57
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.86	0.57
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.33	0.57
22:Y:102:ASP:OD2	43:v:114:ARG:NH1	2.35	0.57
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.36	0.57
16:Q:133:LEU:HD22	16:Q:228:ARG:HD3	1.84	0.57
44:w:139:ARG:NH1	44:w:166:ASP:OD1	2.38	0.57
2:B:76:TYR:HE1	41:s:33:LEU:HB2	1.68	0.57
7:H:47:TYR:O	7:H:51:ILE:HG12	2.05	0.57
44:w:132:GLN:OE1	57:w:401:ADP:N6	2.35	0.57
30:g:32:ARG:O	30:g:36:MET:HG2	2.05	0.57
32:i:122:ILE:O	32:i:176:ARG:NH1	2.36	0.57
11:L:156:LYS:HE2	12:M:68:ARG:HE	1.70	0.57
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.40	0.57
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.87	0.57
7:H:90:LEU:HB2	15:P:102:ASP:HB3	1.86	0.56
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.86	0.56
34:k:67:ALA:O	34:k:70:GLU:HG2	2.04	0.56
33:j:90:MET:HE1	48:j:202:PLX:H281	1.87	0.56
48:l:701:PLX:H321	40:r:39:LEU:HD11	1.85	0.56
40:r:312:ALA:O	40:r:316:MET:HG3	2.06	0.56
12:M:219:SER:OG	12:M:288:ASP:OD2	2.23	0.56
35:l:290:LEU:O	35:l:523:SER:OG	2.23	0.56
40:r:403:THR:HA	40:r:406:TYR:CE2	2.40	0.56
3:C:125:PRO:HG3	41:s:61:LEU:CD1	2.34	0.56
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.33	0.56
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.86	0.56
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.28	0.56
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.87	0.56
1:A:157:TYR:HB3	1:A:212:LEU:HD11	1.87	0.56
7:H:38:ILE:O	7:H:45:ARG:NH1	2.33	0.56
22:Y:97:LEU:HD12	43:v:107:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:93:VAL:HG13	35:l:599:MET:HE1	1.87	0.56
34:k:25:HIS:O	34:k:28:SER:N	2.38	0.56
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.39	0.56
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.65	0.56
5:F:84:ALA:O	5:F:88:THR:OG1	2.20	0.55
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.87	0.55
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.38	0.55
6:X:139:MET:N	6:X:143:GLU:OE2	2.27	0.55
42:u:83:THR:HA	42:u:86:TRP:CD1	2.41	0.55
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.87	0.55
12:M:36:VAL:HB	12:M:56:VAL:HG21	1.86	0.55
12:M:650:SER:OG	12:M:652:ASN:OD1	2.23	0.55
26:c:124:VAL:HG23	35:l:525:MET:HE1	1.87	0.55
8:I:40:LYS:HB3	21:W:7:LYS:H	1.71	0.55
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.86	0.55
35:l:387:THR:OG1	35:l:461:SER:O	2.20	0.55
12:M:419:ARG:NH1	12:M:439:THR:O	2.38	0.55
4:E:64:ARG:NH2	6:G:111:ASP:OD2	2.39	0.55
19:U:41:TYR:O	19:U:45:ILE:HG13	2.06	0.55
27:d:125:CYS:HB3	35:l:203:MET:HE3	1.89	0.55
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.71	0.55
27:d:115:GLN:OE1	35:l:62:ILE:HD11	2.07	0.55
33:j:16:LEU:O	33:j:20:ILE:HG23	2.06	0.55
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.21	0.55
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.89	0.55
2:B:48:MET:O	19:U:10:LYS:NZ	2.30	0.55
35:l:102:GLU:OE2	35:l:456:ARG:NH2	2.34	0.55
11:L:135:VAL:O	11:L:139:GLU:HG3	2.07	0.55
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.89	0.55
20:V:123:ALA:O	20:V:127:MET:HG3	2.06	0.55
22:Y:43:ARG:HH11	22:Y:49:GLN:HG2	1.72	0.55
44:w:38:TYR:HH	44:w:292:HIS:HD1	1.53	0.55
9:J:171:ASN:HB3	9:J:324:MET:HE2	1.89	0.54
6:X:136:GLU:OE2	39:p:14:GLN:NE2	2.40	0.54
55:r:501:PEE:H71	55:r:501:PEE:H32	1.88	0.54
3:C:45:TYR:O	3:C:49:LYS:HG2	2.08	0.54
16:Q:100:GLU:HG2	16:Q:107:ARG:HB2	1.88	0.54
40:r:237:LYS:NZ	40:r:316:MET:O	2.40	0.54
41:s:221:ALA:O	41:s:225:MET:HG2	2.08	0.54
1:A:185:ASN:OD1	1:A:190:GLY:N	2.31	0.54
4:E:56:VAL:HG12	4:E:60:ARG:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.40	0.54
16:Q:372:LYS:NZ	18:T:94:GLY:O	2.39	0.54
23:Z:84:ALA:O	23:Z:88:LEU:HG	2.07	0.54
36:m:25:SER:O	36:m:28:TYR:N	2.40	0.54
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.89	0.54
1:A:398:ARG:HE	1:A:404:ALA:HB2	1.73	0.54
21:W:62:ILE:O	21:W:66:GLU:HG2	2.07	0.54
40:r:105:PHE:O	40:r:109:THR:OG1	2.25	0.54
5:F:57:GLU:OE2	12:M:664:TYR:OH	2.26	0.54
12:M:450:LYS:O	12:M:453:GLN:HG2	2.07	0.53
25:b:17:GLU:O	25:b:21:ARG:HG3	2.08	0.53
28:e:77:ASP:HB3	28:e:83:ASP:HB2	1.89	0.53
31:h:18:MET:HE3	34:k:56:ALA:HA	1.91	0.53
6:G:143:GLU:HA	6:G:146:ASP:OD2	2.07	0.53
40:r:82:SER:OG	40:r:335:GLU:OE2	2.20	0.53
13:N:69:ASN:OD1	13:N:112:ASN:ND2	2.41	0.53
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.41	0.53
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.07	0.53
32:i:236:LYS:HD2	32:i:314:LYS:HB3	1.91	0.53
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.89	0.53
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.30	0.53
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.91	0.53
4:E:37:ARG:HG3	6:G:120:MET:SD	2.49	0.53
26:c:122:THR:OG1	26:c:124:VAL:O	2.26	0.53
32:i:183:SER:O	32:i:187:MET:HG2	2.09	0.53
35:l:150:MET:HE3	35:l:150:MET:HA	1.90	0.53
2:B:100:GLU:O	2:B:170:GLY:N	2.37	0.53
33:j:103:ALA:O	33:j:107:THR:HG23	2.09	0.53
6:G:74:LEU:H	6:G:74:LEU:HD23	1.74	0.53
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.39	0.53
35:l:231:PRO:HA	35:l:234:PRO:HG2	1.89	0.53
44:w:266:ALA:O	44:w:270:VAL:HG23	2.09	0.53
9:J:269:ASN:HB3	9:J:374:THR:HG21	1.91	0.52
35:l:374:ILE:CD1	35:l:427:ILE:HD12	2.39	0.52
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.91	0.52
32:i:4:ILE:O	32:i:8:THR:HG23	2.09	0.52
38:o:48:LEU:HB3	39:p:166:LEU:HD13	1.91	0.52
39:p:132:SER:O	39:p:136:GLU:HG3	2.09	0.52
6:X:89:LEU:HD22	23:Z:48:ASN:HA	1.91	0.52
41:s:106:LEU:HD13	41:s:150:LEU:HD23	1.91	0.52
1:A:184:LYS:NZ	1:A:192:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:52:VAL:O	29:f:56:ILE:HG12	2.10	0.52
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.91	0.52
6:G:91:ASP:N	6:G:91:ASP:OD1	2.42	0.52
20:V:101:LEU:HD23	20:V:101:LEU:O	2.08	0.52
26:c:66:PRO:O	26:c:68:ASP:N	2.40	0.52
1:A:125:CYS:SG	14:O:180:CYS:N	2.83	0.52
12:M:308:ARG:NH2	12:M:578:PRO:O	2.42	0.52
16:Q:176:GLU:OE2	16:Q:311:TYR:OH	2.22	0.52
4:E:114:ARG:HD3	4:E:115:PRO:HD2	1.90	0.52
23:Z:85:GLU:OE2	23:Z:89:GLU:HG3	2.09	0.52
3:C:167:PRO:HG3	16:Q:222:MET:SD	2.50	0.52
35:l:20:MET:HG2	48:l:701:PLX:H182	1.92	0.52
39:p:176:GLU:HG3	39:p:177:ARG:HG2	1.92	0.52
43:v:24:THR:OG1	43:v:105:GLU:OE2	2.27	0.52
1:A:250:VAL:O	1:A:254:ILE:HG12	2.09	0.52
34:k:37:MET:HG3	34:k:67:ALA:CB	2.40	0.52
35:l:534:HIS:CD2	55:l:703:PEE:H13	2.45	0.52
37:n:47:ARG:NH1	37:n:53:GLU:OE1	2.37	0.52
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.45	0.51
19:U:81:LEU:O	21:W:59:ARG:NH1	2.43	0.51
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.92	0.51
1:A:41:ILE:HG21	1:A:250:VAL:HG12	1.91	0.51
1:A:98:LYS:NZ	46:A:502:FMN:O3P	2.42	0.51
5:F:17:ARG:HB2	5:F:68:ARG:HE	1.75	0.51
9:J:87:GLU:CD	9:J:88:PRO:HD2	2.36	0.51
12:M:249:GLU:HG3	12:M:262:VAL:HG22	1.92	0.51
26:c:170:ARG:HG2	43:v:53:LEU:HD13	1.92	0.51
40:r:370:PRO:HD3	40:r:375:LEU:HD13	1.91	0.51
2:B:63:TRP:HE1	55:s:401:PEE:H1	1.75	0.51
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.93	0.51
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.91	0.51
43:v:103:GLU:O	43:v:107:ARG:HG2	2.10	0.51
20:V:140:LYS:HG2	20:V:141:VAL:HG13	1.92	0.51
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.43	0.51
14:O:186:VAL:HG22	14:O:196:LEU:HD11	1.93	0.51
14:O:222:ARG:NE	14:O:225:CYS:HA	2.26	0.51
29:f:44:VAL:O	29:f:48:LEU:HD22	2.10	0.51
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.92	0.51
34:k:2:PRO:HD2	34:k:5:TYR:CD2	2.46	0.51
6:G:119:ILE:HD13	6:G:135:ALA:HB1	1.93	0.51
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:66:LEU:O	17:S:69:ILE:HG22	2.11	0.51
34:k:19:LEU:HD22	34:k:36:MET:HE1	1.93	0.51
20:V:4:THR:O	20:V:8:LYS:HG2	2.11	0.51
20:V:76:ILE:O	20:V:80:VAL:HG23	2.10	0.51
23:Z:17:PRO:HB2	23:Z:21:GLN:NE2	2.26	0.51
32:i:118:VAL:O	32:i:122:ILE:HG12	2.10	0.51
1:A:210:THR:HB	1:A:224:ARG:H	1.75	0.51
6:G:84:LEU:O	6:G:88:LYS:HG2	2.11	0.51
6:G:103:HIS:HD2	6:G:139:MET:HG3	1.75	0.51
12:M:161:GLU:OE1	14:O:42:ARG:NH2	2.44	0.51
44:w:251:GLU:OE1	44:w:251:GLU:N	2.37	0.51
36:m:41:CYS:SG	36:m:57:PHE:HD2	2.34	0.51
38:o:83:THR:HG22	38:o:85:LYS:H	1.76	0.51
41:s:85:MET:HE3	41:s:105:MET:HE3	1.92	0.51
42:u:52:ASP:HB3	42:u:55:ARG:HG2	1.92	0.51
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.45	0.51
14:O:156:LEU:HD12	14:O:164:THR:HG21	1.93	0.50
49:X:201:8Q1:S44	39:p:63:LEU:HB3	2.50	0.50
22:Y:94:ASP:OD1	22:Y:99:ILE:HB	2.10	0.50
24:a:163:ARG:NH1	30:g:102:ASP:OD2	2.28	0.50
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.76	0.50
2:B:39:LYS:NZ	8:I:110:GLN:OE1	2.43	0.50
3:C:146:SER:OG	16:Q:118:2MR:O	2.26	0.50
12:M:250:SER:OG	12:M:251:ILE:N	2.44	0.50
17:S:46:ASN:ND2	36:m:132:ASP:HB3	2.27	0.50
32:i:278:MET:O	32:i:282:MET:HG3	2.11	0.50
55:j:201:PEE:H32	55:j:201:PEE:H63	1.93	0.50
40:r:139:GLN:OE1	40:r:340:ARG:NH1	2.38	0.50
9:J:251:ASN:O	9:J:255:ASP:N	2.45	0.50
12:M:128:CYS:SG	12:M:140:GLN:NE2	2.79	0.50
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.33	0.50
6:X:85:TYR:O	6:X:89:LEU:HD12	2.12	0.50
25:b:100:ARG:NH2	27:d:119:GLU:HG2	2.27	0.50
27:d:74:ILE:HA	27:d:77:CYS:SG	2.52	0.50
35:l:208:CYS:SG	35:l:266:LEU:HD23	2.51	0.50
40:r:247:THR:C	40:r:249:ILE:N	2.69	0.50
19:U:14:ALA:O	19:U:15:LYS:HG2	2.10	0.50
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.93	0.50
35:l:559:GLU:O	35:l:563:PRO:HD2	2.12	0.50
44:w:59:VAL:HG12	44:w:202:HIS:CE1	2.47	0.50
1:A:42:PHE:HA	1:A:137:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:78:ASP:OD2	13:N:80:SER:OG	2.21	0.50
14:O:137:THR:HG22	14:O:138:THR:H	1.77	0.50
25:b:4:TYR:HB2	25:b:9:LYS:HE3	1.93	0.50
27:d:127:LYS:HE3	27:d:131:GLN:NE2	2.26	0.50
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.44	0.50
3:C:119:LYS:NZ	3:C:123:GLN:NE2	2.59	0.50
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.92	0.50
35:l:51:LEU:O	35:l:55:MET:HG3	2.12	0.50
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.43	0.50
26:c:118:ASP:OD1	26:c:118:ASP:N	2.44	0.50
35:l:241:THR:HG21	35:l:344:GLY:HA3	1.94	0.50
2:B:40:PHE:HB3	2:B:43:MET:HB2	1.93	0.50
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	1.94	0.50
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.34	0.50
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	1.93	0.50
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.93	0.50
33:j:55:PHE:HB3	36:m:70:TYR:OH	2.12	0.50
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.50
9:J:314:THR:HA	9:J:318:LYS:HB3	1.94	0.49
16:Q:180:LEU:O	16:Q:184:ILE:HG13	2.12	0.49
6:X:111:ASP:OD1	6:X:112:SER:N	2.42	0.49
24:a:79:GLY:HA3	53:a:201:CDL:H222	1.93	0.49
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.30	0.49
5:F:33:VAL:HG22	5:F:87:VAL:HG11	1.93	0.49
44:w:88:GLU:OE2	44:w:161:ARG:NH1	2.45	0.49
12:M:489:ILE:O	12:M:493:VAL:HG13	2.12	0.49
21:W:129:THR:O	21:W:133:ILE:HG13	2.12	0.49
35:l:313:MET:HE3	35:l:329:ILE:HG12	1.93	0.49
53:a:201:CDL:H722	48:l:701:PLX:H51	1.94	0.49
27:d:144:SER:O	27:d:158:LYS:NZ	2.35	0.49
43:v:17:PRO:HB3	43:v:105:GLU:OE1	2.12	0.49
43:v:25:PHE:HD2	43:v:108:LEU:HD13	1.76	0.49
7:H:51:ILE:HD11	8:I:94:ALA:HB3	1.95	0.49
12:M:698:ASP:OD1	12:M:698:ASP:N	2.44	0.49
20:V:101:LEU:C	20:V:101:LEU:CD2	2.86	0.49
21:W:85:GLN:O	21:W:89:GLU:HG3	2.11	0.49
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.13	0.49
12:M:354:LEU:HD12	12:M:357:LEU:HD23	1.94	0.49
36:m:10:SER:O	36:m:14:VAL:HG23	2.12	0.49
1:A:109:ARG:NH1	1:A:237:GLY:O	2.45	0.49
11:L:84:ARG:NH1	11:L:88:GLN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:116:SER:OG	15:P:227:ALA:O	2.29	0.49
44:w:80:LYS:HZ3	44:w:267:GLU:HG3	1.76	0.49
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.94	0.49
35:l:467:ILE:O	35:l:471:ASN:HB2	2.12	0.49
43:v:34:ARG:NH1	43:v:36:GLU:OE2	2.46	0.49
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.94	0.49
5:F:36:PHE:CD1	5:F:36:PHE:C	2.90	0.49
7:H:11:LEU:HD12	7:H:14:LEU:HD22	1.95	0.49
16:Q:139:LEU:O	16:Q:460:GLU:N	2.45	0.49
25:b:110:ILE:HD12	27:d:16:ARG:HB3	1.95	0.49
3:C:102:VAL:HG23	3:C:129:TYR:O	2.12	0.48
16:Q:198:THR:OG1	16:Q:199:PRO:HD3	2.12	0.48
24:a:78:THR:HG21	28:e:96:SER:O	2.13	0.48
40:r:306:PRO:O	40:r:310:MET:HG3	2.12	0.48
6:G:86:VAL:HG11	6:G:125:GLU:HG2	1.95	0.48
24:a:160:MET:HE2	30:g:95:TYR:CD1	2.48	0.48
40:r:97:THR:HG21	53:r:503:CDL:H242	1.94	0.48
41:s:25:ARG:HD2	56:s:402:UQ:HM21	1.95	0.48
12:M:472:PRO:O	12:M:510:TRP:NE1	2.36	0.48
35:l:257:VAL:HG21	35:l:313:MET:HE2	1.96	0.48
35:l:298:ILE:O	35:l:302:VAL:HG23	2.13	0.48
35:l:373:LEU:HD13	35:l:431:PHE:HZ	1.78	0.48
44:w:123:SER:OG	44:w:125:ASP:OD1	2.26	0.48
2:B:210:LEU:HD12	8:I:38:PRO:HB3	1.94	0.48
3:C:119:LYS:HZ2	3:C:123:GLN:NE2	2.11	0.48
14:O:44:THR:HG22	14:O:46:GLU:H	1.78	0.48
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.95	0.48
32:i:261:MET:HE1	48:i:402:PLX:H342	1.95	0.48
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.48	0.48
9:J:128:ASN:OD1	9:J:130:VAL:HG12	2.14	0.48
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.38	0.48
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.48	0.48
3:C:51:ASP:OD2	3:C:189:ARG:N	2.47	0.48
32:i:283:ALA:HB1	40:r:158:LEU:HD22	1.95	0.48
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.49	0.48
6:G:82:ARG:O	6:G:86:VAL:HG13	2.14	0.48
6:G:141:PRO:HA	6:G:144:ILE:HD12	1.95	0.48
12:M:68:ARG:NH1	12:M:284:GLU:HB2	2.29	0.48
24:a:87:THR:O	24:a:91:VAL:HG13	2.14	0.48
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.96	0.48
44:w:211:VAL:HA	44:w:214:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:432:ILE:HD11	12:M:445:LEU:HD12	1.95	0.48
35:l:362:LEU:HB2	35:l:431:PHE:HD1	1.78	0.48
40:r:433:GLU:O	40:r:437:MET:HG2	2.14	0.48
53:r:503:CDL:H741	53:r:503:CDL:H772	1.52	0.48
13:N:10:GLY:O	13:N:14:VAL:HG23	2.14	0.48
26:c:90:TYR:HE1	39:p:6:PRO:HG3	1.79	0.48
37:n:25:CYS:O	37:n:29:ARG:HG3	2.14	0.48
48:C:302:PLX:H311	48:C:302:PLX:H281	1.69	0.48
6:X:83:VAL:HG13	6:X:122:MET:HE1	1.96	0.48
30:g:2:THR:HG22	30:g:4:MET:HG3	1.96	0.48
32:i:316:GLN:NE2	44:w:95:ASP:OD1	2.43	0.48
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.95	0.47
14:O:224:SER:O	14:O:224:SER:OG	2.26	0.47
16:Q:210:MET:HE2	16:Q:247:PHE:HZ	1.79	0.47
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	1.96	0.47
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.95	0.47
43:v:3:ALA:O	43:v:7:ARG:HG3	2.14	0.47
14:O:38:LEU:O	14:O:124:ARG:NH2	2.47	0.47
25:b:123:PHE:CE2	43:v:40:VAL:HG11	2.46	0.47
25:b:123:PHE:CB	43:v:40:VAL:HG21	2.43	0.47
32:i:146:SER:HA	32:i:149:ILE:HD12	1.95	0.47
19:U:38:TYR:HB2	41:s:310:MET:O	2.14	0.47
26:c:149:ILE:O	26:c:151:PRO:HD3	2.14	0.47
42:u:23:SER:OG	42:u:90:ASP:OD1	2.28	0.47
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.96	0.47
1:A:48:ARG:HB3	10:K:70:ASN:HA	1.96	0.47
35:l:554:ASP:OD1	40:r:213:HIS:NE2	2.47	0.47
40:r:285:LEU:HD22	40:r:410:MET:HE2	1.96	0.47
43:v:92:HIS:O	43:v:96:VAL:HG12	2.14	0.47
35:l:79:SER:HB3	35:l:135:ASN:HB3	1.97	0.47
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.41	0.47
49:X:201:8Q1:C10	39:p:67:ALA:HB1	2.45	0.47
30:g:12:PRO:HB3	31:h:5:ASP:HB3	1.96	0.47
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.96	0.47
16:Q:107:ARG:HA	16:Q:107:ARG:HD3	1.70	0.47
21:W:70:ALA:HB2	42:u:125:LEU:HD21	1.97	0.47
25:b:80:TRP:HD1	27:d:41:VAL:HG13	1.78	0.47
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.96	0.47
32:i:230:LEU:HD11	32:i:244:MET:HE1	1.96	0.47
48:l:701:PLX:H382	40:r:67:VAL:HG12	1.97	0.47
36:m:63:GLY:O	36:m:66:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:63:ILE:HG12	14:O:82:VAL:HG22	1.96	0.47
19:U:48:ALA:HB1	19:U:78:LEU:HD21	1.97	0.47
53:i:401:CDL:H122	53:i:401:CDL:H151	1.72	0.47
35:l:456:ARG:O	35:l:459:ILE:HG12	2.15	0.47
41:s:24:GLU:OE1	41:s:228:TYR:OH	2.20	0.47
11:L:163:ASN:O	11:L:171:ARG:HA	2.14	0.47
12:M:55:LYS:HB3	12:M:55:LYS:HE3	1.61	0.47
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.79	0.47
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.96	0.47
49:X:201:8Q1:C14	39:p:71:PHE:HA	2.45	0.47
34:k:61:ILE:HD11	36:m:51:PHE:HE2	1.79	0.47
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.97	0.47
43:v:61:HIS:O	43:v:65:GLN:HG2	2.15	0.47
3:C:85:ASP:O	3:C:88:ARG:HG2	2.15	0.47
4:E:127:ASP:OD2	9:J:45:LYS:NZ	2.42	0.47
35:l:143:GLY:O	35:l:147:VAL:HG22	2.15	0.47
35:l:332:HIS:HA	35:l:335:PHE:CZ	2.50	0.47
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.50	0.47
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.44	0.47
17:S:21:MET:HG2	41:s:253:GLU:HG3	1.96	0.46
6:X:75:THR:OG1	6:X:76:LEU:N	2.48	0.46
32:i:347:ASN:N	32:i:347:ASN:OD1	2.48	0.46
35:l:409:LEU:HD12	35:l:409:LEU:H	1.80	0.46
40:r:260:PRO:HG3	48:r:502:PLX:H132	1.96	0.46
1:A:263:ALA:HA	1:A:271:SER:HB2	1.96	0.46
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.97	0.46
1:A:380:GLY:O	1:A:386:ARG:NH1	2.49	0.46
4:E:110:THR:HG21	15:P:220:VAL:HG11	1.96	0.46
21:W:94:GLU:HG3	31:h:79:ILE:HD13	1.96	0.46
30:g:33:LEU:HD22	30:g:71:VAL:HG13	1.96	0.46
53:i:401:CDL:H142	53:i:401:CDL:H171	1.57	0.46
41:s:184:MET:HE3	55:s:401:PEE:H13	1.97	0.46
41:s:264:LEU:O	41:s:268:ILE:HG12	2.15	0.46
15:P:211:ARG:NH2	15:P:222:GLU:OE2	2.48	0.46
16:Q:335:GLU:O	16:Q:339:GLN:HG2	2.15	0.46
35:l:406:ALA:HA	35:l:409:LEU:HD13	1.98	0.46
42:u:106:LYS:O	42:u:109:GLU:HG2	2.16	0.46
9:J:124:ASN:OD1	9:J:125:VAL:HG23	2.15	0.46
16:Q:102:SER:O	16:Q:102:SER:OG	2.29	0.46
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.96	0.46
8:I:66:PRO:HB3	15:P:79:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:217:PHE:CD1	9:J:217:PHE:N	2.81	0.46
14:O:159:LYS:HB2	14:O:162:GLU:HG3	1.98	0.46
27:d:78:GLU:HB2	27:d:81:ASP:HB2	1.96	0.46
32:i:221:HIS:HB2	32:i:323:MET:HE1	1.96	0.46
48:i:402:PLX:H72	48:i:402:PLX:H101	1.62	0.46
35:l:305:SER:OG	35:l:336:LYS:NZ	2.49	0.46
42:u:74:ILE:HD11	42:u:117:TRP:HZ3	1.81	0.46
2:B:137:ASP:OD1	2:B:137:ASP:N	2.43	0.46
12:M:676:ASN:O	12:M:678:GLN:NE2	2.48	0.46
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.98	0.46
20:V:108:TYR:HB2	53:V:201:CDL:CB3	2.39	0.46
26:c:125:SER:O	26:c:129:MET:HG3	2.16	0.46
35:l:7:LEU:O	35:l:11:THR:HG23	2.15	0.46
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.46	0.46
17:S:53:ARG:NH1	31:h:106:PRO:O	2.48	0.46
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.40	0.46
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.98	0.46
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.51	0.46
21:W:30:LEU:HD12	21:W:30:LEU:HA	1.85	0.46
24:a:184:LYS:HB3	31:h:30:PRO:HB3	1.97	0.46
35:l:226:GLN:NE2	35:l:314:MET:HE3	2.31	0.46
35:l:595:ILE:O	35:l:599:MET:HG2	2.16	0.46
1:A:50:ASP:O	1:A:59:ARG:NH2	2.38	0.45
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.97	0.45
55:i:403:PEE:H35	55:i:403:PEE:H42	1.72	0.45
6:G:115:GLN:O	6:G:119:ILE:HG13	2.15	0.45
55:U:101:PEE:H35	55:U:101:PEE:H30	1.85	0.45
27:d:117:GLU:HG3	27:d:125:CYS:SG	2.57	0.45
48:C:302:PLX:H181	48:C:302:PLX:H212	1.78	0.45
8:I:42:PRO:HB3	21:W:6:VAL:HG21	1.99	0.45
12:M:431:LEU:HD13	12:M:438:LEU:HD11	1.99	0.45
20:V:78:ALA:HA	20:V:89:ASN:ND2	2.31	0.45
27:d:97:LYS:NZ	28:e:115:GLN:OE1	2.47	0.45
27:d:115:GLN:CG	35:l:62:ILE:HD12	2.44	0.45
28:e:116:GLU:O	28:e:120:ARG:HG3	2.17	0.45
48:j:202:PLX:H322	48:j:202:PLX:H381	1.97	0.45
40:r:121:LEU:O	40:r:125:THR:HG23	2.17	0.45
44:w:258:TYR:HE2	44:w:269:VAL:HG13	1.82	0.45
6:G:88:LYS:HE3	6:G:95:PRO:HB3	1.97	0.45
19:U:26:GLY:HA3	55:U:101:PEE:H38	1.98	0.45
24:a:59:PRO:HD3	39:p:99:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:75:ILE:HD11	34:k:59:MET:HE1	1.99	0.45
39:p:46:ALA:O	39:p:50:GLU:HG3	2.17	0.45
44:w:290:THR:HG22	44:w:293:ARG:HH21	1.82	0.45
1:A:62:TRP:CE3	1:A:65:THR:HG21	2.49	0.45
46:A:502:FMN:O2'	47:A:503:NAI:O2N	2.34	0.45
53:V:201:CDL:HA62	53:V:201:CDL:H312	1.62	0.45
26:c:81:ARG:HB3	26:c:85:GLU:OE1	2.17	0.45
35:l:367:PRO:O	35:l:371:THR:HG22	2.16	0.45
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.52	0.45
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.47	0.45
6:G:120:MET:HA	6:G:123:GLU:CG	2.45	0.45
12:M:560:LEU:HD23	12:M:564:CYS:SG	2.56	0.45
14:O:185:MET:HE1	14:O:192:TYR:HE1	1.81	0.45
53:a:201:CDL:H531	55:l:704:PEE:H56	1.98	0.45
27:d:31:THR:HA	27:d:34:THR:HG22	1.97	0.45
33:j:5:LEU:O	33:j:9:THR:OG1	2.31	0.45
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.51	0.45
6:X:134:ASP:OD1	39:p:4:SER:OG	2.28	0.45
25:b:107:GLY:H	25:b:117:ILE:HB	1.82	0.45
28:e:77:ASP:OD1	28:e:78:LYS:N	2.48	0.45
35:l:383:MET:HG3	35:l:384:PRO:HD2	1.99	0.45
40:r:325:MET:HG3	40:r:440:HIS:HB3	1.99	0.45
3:C:175:TYR:HE1	13:N:78:ASP:HB2	1.82	0.45
26:c:141:LEU:HD23	26:c:141:LEU:HA	1.86	0.45
27:d:74:ILE:HG23	27:d:156:LEU:HD22	1.98	0.45
32:i:326:LEU:HB3	32:i:327:PRO:HD3	1.99	0.45
35:l:303:ALA:O	35:l:306:THR:HG22	2.17	0.45
39:p:16:VAL:HG22	39:p:64:LEU:HD13	1.98	0.45
40:r:127:VAL:HB	40:r:128:PRO:HD3	1.98	0.45
1:A:213:ILE:HD12	1:A:235:VAL:HB	1.98	0.45
2:B:76:TYR:CE1	41:s:33:LEU:HB2	2.51	0.45
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.98	0.45
25:b:88:TYR:CE1	27:d:49:ARG:HG2	2.52	0.45
28:e:85:TRP:O	28:e:89:VAL:HG22	2.17	0.45
33:j:84:LEU:HD13	41:s:309:ILE:HG23	1.99	0.45
35:l:378:LEU:HD12	35:l:383:MET:SD	2.57	0.45
39:p:97:TYR:HB3	39:p:179:MET:HE3	1.98	0.45
43:v:80:CYS:HB3	43:v:83:GLU:OE2	2.16	0.45
1:A:39:ASP:OD1	1:A:257:ARG:NH2	2.47	0.45
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.32	0.45
26:c:129:MET:HB3	35:l:528:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.98	0.45
8:I:70:MET:HE2	15:P:66:ALA:HB1	1.99	0.44
44:w:269:VAL:O	44:w:273:ILE:HG12	2.16	0.44
1:A:161:GLU:OE1	1:A:161:GLU:N	2.47	0.44
3:C:124:MET:HA	3:C:125:PRO:HD3	1.77	0.44
6:X:113:LEU:O	6:X:117:GLU:HG3	2.17	0.44
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.98	0.44
22:Y:88:ASP:HB3	22:Y:91:GLN:HB2	1.99	0.44
34:k:23:ARG:HG2	36:m:23:LYS:HE2	1.98	0.44
35:l:137:LEU:HD13	35:l:186:MET:HG3	1.98	0.44
53:l:702:CDL:H622	53:l:702:CDL:H591	1.52	0.44
39:p:176:GLU:HG3	39:p:177:ARG:N	2.33	0.44
44:w:116:LYS:HB3	44:w:116:LYS:HE2	1.77	0.44
44:w:185:GLU:O	44:w:189:GLU:HG3	2.17	0.44
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.99	0.44
6:X:120:MET:HG2	39:p:21:LYS:HZ3	1.83	0.44
48:a:202:PLX:H22	48:a:202:PLX:H1C3	1.80	0.44
27:d:33:LEU:HD23	27:d:33:LEU:HA	1.85	0.44
31:h:18:MET:O	31:h:18:MET:HG2	2.17	0.44
35:l:357:ARG:HG3	39:p:32:VAL:HG22	1.99	0.44
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.98	0.44
21:W:81:ARG:NH2	42:u:64:ASN:OD1	2.50	0.44
28:e:63:ASP:OD1	28:e:63:ASP:N	2.50	0.44
40:r:12:LEU:HB2	40:r:13:PRO:HD3	2.00	0.44
41:s:141:SER:HB3	41:s:289:LEU:HD22	2.00	0.44
42:u:108:ASP:O	42:u:111:VAL:HG22	2.17	0.44
42:u:112:LEU:HD12	42:u:112:LEU:HA	1.82	0.44
1:A:224:ARG:HD3	11:L:164:PHE:CE2	2.53	0.44
1:A:396:MET:HE1	1:A:438:LEU:HD23	2.00	0.44
7:H:37:GLN:HB2	7:H:95:LEU:HD11	2.00	0.44
12:M:658:ASP:OD1	12:M:660:GLU:N	2.46	0.44
14:O:179:ALA:HB3	14:O:185:MET:SD	2.58	0.44
25:b:123:PHE:HD2	43:v:40:VAL:CG1	2.29	0.44
26:c:176:LYS:HA	26:c:176:LYS:HD3	1.85	0.44
40:r:13:PRO:HB3	53:r:503:CDL:H581	1.98	0.44
40:r:371:PRO:O	40:r:448:THR:OG1	2.35	0.44
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.53	0.44
14:O:58:GLU:H	14:O:58:GLU:CD	2.25	0.44
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.35	0.44
19:U:82:LYS:HD3	42:u:122:LEU:HD22	2.00	0.44
20:V:96:ALA:O	20:V:100:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:27:TYR:O	35:l:115:ASN:ND2	2.47	0.44
14:O:222:ARG:HE	14:O:225:CYS:HA	1.82	0.44
26:c:63:GLU:O	26:c:76:PRO:HA	2.18	0.44
35:l:373:LEU:HD13	35:l:431:PHE:CZ	2.52	0.44
1:A:151:ALA:O	1:A:191:TYR:OH	2.25	0.44
9:J:57:THR:HG21	9:J:120:VAL:HG12	2.00	0.44
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.53	0.44
53:l:702:CDL:H711	53:l:702:CDL:H742	1.51	0.44
5:F:71:PHE:CD1	12:M:362:ASP:HB2	2.53	0.44
6:G:86:VAL:HG21	6:G:122:MET:HE1	2.00	0.44
6:G:116:VAL:O	6:G:120:MET:HG3	2.18	0.44
7:H:69:GLU:HG3	7:H:77:ILE:HG12	2.00	0.44
9:J:127:ILE:HD11	9:J:253:ILE:HD11	2.00	0.44
18:T:79:VAL:O	18:T:121:PRO:HD3	2.18	0.44
53:V:201:CDL:H721	53:V:201:CDL:H561	2.00	0.44
25:b:106:PRO:HG2	25:b:120:MET:HE3	1.99	0.44
26:c:58:ARG:HD2	38:o:36:ARG:HG3	2.00	0.44
29:f:69:TYR:CE1	29:f:73:ASN:ND2	2.86	0.44
35:l:88:MET:HB3	35:l:326:PHE:CE2	2.52	0.44
35:l:237:MET:HB3	35:l:299:LYS:HE2	1.99	0.44
35:l:277:THR:HG23	35:l:314:MET:HG3	2.00	0.44
40:r:300:ALA:O	40:r:308:SER:HB3	2.18	0.44
44:w:330:LYS:O	44:w:333:GLU:HG2	2.18	0.44
12:M:133:GLN:HG3	12:M:136:GLU:HG3	2.00	0.43
16:Q:265:ASN:O	16:Q:269:ARG:HG3	2.18	0.43
35:l:257:VAL:O	35:l:261:ILE:HG13	2.18	0.43
44:w:75:ARG:HE	44:w:75:ARG:HB2	1.58	0.43
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.53	0.43
9:J:36:LEU:HB3	12:M:304:GLN:NE2	2.33	0.43
9:J:204:SER:OG	9:J:238:GLN:O	2.33	0.43
13:N:38:LEU:HD13	13:N:49:TYR:CE2	2.54	0.43
19:U:70:PRO:HD3	42:u:37:ASP:OD2	2.18	0.43
21:W:43:LEU:HD13	41:s:179:TRP:NE1	2.33	0.43
22:Y:78:ASP:HB2	22:Y:83:HIS:HB2	1.98	0.43
26:c:140:MET:HE1	35:l:411:MET:SD	2.57	0.43
48:j:202:PLX:H312	48:j:202:PLX:H282	1.50	0.43
40:r:329:LEU:HD23	40:r:437:MET:HE3	2.00	0.43
12:M:296:GLY:O	12:M:572:HIS:NE2	2.44	0.43
13:N:132:LYS:HB3	13:N:132:LYS:HE2	1.77	0.43
27:d:171:LYS:HE3	27:d:171:LYS:HB2	1.66	0.43
29:f:63:LYS:HA	29:f:63:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:187:MET:HE3	32:i:187:MET:HB3	1.85	0.43
36:m:41:CYS:SG	36:m:57:PHE:CD2	3.11	0.43
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.53	0.43
15:P:44:ARG:NE	15:P:45:PRO:HD3	2.30	0.43
55:U:101:PEE:H59	55:U:101:PEE:H64	1.73	0.43
26:c:55:TYR:OH	26:c:74:ASP:O	2.24	0.43
27:d:97:LYS:O	27:d:101:GLU:HG2	2.18	0.43
34:k:5:TYR:O	34:k:9:ILE:HG13	2.19	0.43
41:s:26:LYS:HD2	41:s:36:GLY:HA3	2.00	0.43
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.81	0.43
32:i:96:THR:O	32:i:100:MET:HG2	2.19	0.43
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.54	0.43
35:l:305:SER:HB2	35:l:422:TYR:CZ	2.53	0.43
41:s:218:GLY:O	41:s:222:MET:HE2	2.19	0.43
12:M:133:GLN:O	12:M:137:CYS:HB2	2.19	0.43
16:Q:184:ILE:HG12	16:Q:337:MET:HE3	2.00	0.43
32:i:179:MET:HE2	32:i:179:MET:HA	2.00	0.43
35:l:159:HIS:HB2	40:r:416:ARG:HG3	2.00	0.43
6:G:83:VAL:HG22	6:G:122:MET:HE2	2.00	0.43
9:J:206:ILE:HG12	9:J:245:VAL:HG21	2.01	0.43
14:O:199:LYS:HA	14:O:202:GLU:OE1	2.19	0.43
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.01	0.43
19:U:70:PRO:O	42:u:124:GLU:HG2	2.18	0.43
35:l:230:HIS:O	35:l:234:PRO:HD2	2.19	0.43
35:l:400:ASN:ND2	35:l:489:THR:HG21	2.33	0.43
4:E:88:MET:HE2	15:P:184:LEU:O	2.18	0.43
6:G:111:ASP:OD1	6:G:111:ASP:C	2.62	0.43
12:M:388:ASN:HB3	12:M:511:LYS:HB3	2.01	0.43
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	2.00	0.43
53:V:201:CDL:H792	35:l:561:ILE:HD11	2.01	0.43
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.34	0.43
43:v:15:LYS:HG3	43:v:110:GLN:OE1	2.18	0.43
44:w:189:GLU:O	44:w:193:VAL:HG22	2.19	0.43
1:A:69:LEU:HD13	1:A:147:ARG:HG2	2.01	0.43
6:G:143:GLU:HA	6:G:146:ASP:CG	2.44	0.43
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.34	0.43
44:w:181:LYS:O	44:w:184:VAL:HG22	2.19	0.43
1:A:357:MET:HB3	1:A:361:THR:HG21	2.01	0.43
11:L:67:VAL:HB	11:L:72:ILE:HD11	2.00	0.43
12:M:330:LEU:HD12	12:M:330:LEU:HA	1.83	0.43
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:70:MET:SD	26:c:70:MET:N	2.92	0.43
31:h:17:TRP:HH2	34:k:58:MET:HE1	1.83	0.43
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.54	0.43
35:l:261:ILE:HG13	35:l:317:ILE:HD11	2.00	0.43
35:l:313:MET:HE3	35:l:329:ILE:CG1	2.48	0.43
53:V:201:CDL:H591	53:V:201:CDL:H751	2.01	0.42
21:W:58:ARG:HD2	21:W:58:ARG:HA	1.87	0.42
39:p:28:GLU:OE2	39:p:34:ARG:NH1	2.43	0.42
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.54	0.42
12:M:332:SER:O	12:M:334:GLN:NE2	2.52	0.42
14:O:147:SER:O	14:O:150:GLU:HG3	2.18	0.42
16:Q:312:ASP:OD1	16:Q:312:ASP:N	2.49	0.42
19:U:70:PRO:HB3	42:u:124:GLU:O	2.19	0.42
23:Z:49:GLU:HG2	23:Z:52:ARG:HE	1.84	0.42
32:i:153:LEU:O	32:i:157:MET:HG3	2.18	0.42
35:l:128:MET:HE2	35:l:251:THR:O	2.19	0.42
44:w:40:PRO:O	44:w:44:VAL:HG13	2.19	0.42
46:A:502:FMN:H1'1	46:A:502:FMN:H9	1.81	0.42
6:G:140:CYS:O	6:G:144:ILE:HG13	2.19	0.42
9:J:126:VAL:HG23	9:J:161:VAL:HG11	2.01	0.42
22:Y:93:THR:OG1	22:Y:96:GLU:OE1	2.35	0.42
32:i:210:THR:HG22	32:i:333:SER:HB3	2.02	0.42
41:s:51:ASP:HB3	56:s:402:UQ:H8	2.01	0.42
3:C:102:VAL:HA	3:C:129:TYR:O	2.19	0.42
20:V:39:TYR:OH	35:l:594:THR:HB	2.20	0.42
35:l:464:ALA:HA	35:l:467:ILE:HG22	2.01	0.42
53:V:201:CDL:H562	53:V:201:CDL:H592	1.80	0.42
31:h:19:THR:HA	32:i:84:TRP:HB2	2.01	0.42
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.85	0.42
35:l:144:TRP:CE2	35:l:223:LYS:HD2	2.54	0.42
35:l:559:GLU:HG3	35:l:564:LYS:HG2	2.02	0.42
55:r:501:PEE:H28	55:r:501:PEE:H21	1.76	0.42
6:G:135:ALA:HA	6:G:138:LEU:HD13	2.02	0.42
8:I:28:TYR:O	8:I:31:ILE:HG12	2.20	0.42
12:M:658:ASP:OD1	12:M:659:VAL:N	2.52	0.42
26:c:143:MET:HE3	26:c:143:MET:HA	2.02	0.42
28:e:97:ILE:O	28:e:101:LEU:HB2	2.19	0.42
41:s:293:PHE:O	41:s:297:THR:OG1	2.23	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.42
12:M:509:ASP:OD1	12:M:509:ASP:N	2.45	0.42
34:k:14:ILE:HD13	36:m:18:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:l:702:CDL:H541	53:l:702:CDL:H572	1.72	0.42
37:n:46:LYS:HA	37:n:46:LYS:HD2	1.76	0.42
40:r:445:LEU:O	40:r:448:THR:HG22	2.19	0.42
42:u:36:CYS:HB3	42:u:66:CYS:SG	2.60	0.42
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.55	0.42
7:H:66:LYS:O	7:H:70:GLU:HG2	2.20	0.42
9:J:166:HIS:CD2	9:J:191:VAL:HG21	2.55	0.42
12:M:50:LEU:O	12:M:54:GLU:HG3	2.20	0.42
12:M:541:PRO:HA	12:M:542:PRO:HD3	1.90	0.42
21:W:130:ASN:HD22	36:m:1:MET:HB2	1.85	0.42
32:i:4:ILE:HD13	32:i:4:ILE:HA	1.91	0.42
32:i:222:SER:O	32:i:224:ALA:N	2.52	0.42
42:u:17:GLU:HB2	42:u:19:LYS:HD3	2.02	0.42
44:w:147:LEU:HD23	44:w:147:LEU:HA	1.92	0.42
2:B:76:TYR:HA	2:B:79:ARG:NE	2.35	0.42
3:C:124:MET:HE3	3:C:128:ARG:HB2	2.01	0.42
5:F:64:LYS:HD2	5:F:66:TRP:NE1	2.35	0.42
12:M:311:LYS:HA	12:M:311:LYS:HD2	1.78	0.42
12:M:467:LYS:HD3	12:M:467:LYS:N	2.34	0.42
14:O:134:VAL:HG22	14:O:186:VAL:HG12	2.02	0.42
19:U:19:LEU:HD23	19:U:19:LEU:HA	1.93	0.42
21:W:88:ARG:O	21:W:92:GLU:HG2	2.20	0.42
30:g:32:ARG:HB2	30:g:78:LEU:HD11	2.02	0.42
30:g:74:GLY:O	30:g:78:LEU:HG	2.20	0.42
32:i:284:MET:HE3	55:i:403:PEE:H46	2.01	0.42
32:i:339:MET:HE3	32:i:339:MET:HB3	1.91	0.42
36:m:23:LYS:N	36:m:24:PRO:HD3	2.35	0.42
37:n:18:PRO:O	37:n:22:VAL:HG23	2.20	0.42
1:A:185:ASN:C	1:A:187:CYS:H	2.28	0.42
12:M:48:THR:HA	12:M:95:PRO:HA	2.01	0.42
53:r:503:CDL:H832	53:r:503:CDL:H861	1.84	0.42
12:M:275:PRO:HB3	12:M:286:ILE:HG23	2.02	0.41
14:O:69:ASN:HD22	14:O:69:ASN:HA	1.66	0.41
16:Q:196:ALA:O	16:Q:197:MET:HG3	2.20	0.41
33:j:28:ASN:HD22	55:j:201:PEE:H49	1.84	0.41
35:l:533:MET:HE3	35:l:537:PRO:HG2	2.02	0.41
35:l:572:LYS:HE2	35:l:572:LYS:HB3	1.67	0.41
53:l:702:CDL:H391	53:l:702:CDL:H421	1.71	0.41
36:m:7:PHE:O	36:m:11:THR:HG23	2.20	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.41
1:A:207:GLY:HA3	46:A:502:FMN:N5	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:141:PRO:HA	6:G:144:ILE:CD1	2.50	0.41
7:H:77:ILE:O	7:H:81:ILE:HG13	2.19	0.41
12:M:638:THR:O	12:M:642:VAL:HG23	2.20	0.41
14:O:158:ILE:HD13	14:O:164:THR:HG23	2.01	0.41
16:Q:235:ASP:CB	16:Q:356:ILE:HD13	2.30	0.41
53:a:201:CDL:H311	53:a:201:CDL:H342	1.58	0.41
27:d:142:ARG:NE	28:e:138:GLU:O	2.53	0.41
38:o:57:LEU:HD23	38:o:57:LEU:O	2.20	0.41
40:r:14:MET:HE2	40:r:30:HIS:ND1	2.34	0.41
1:A:295:PRO:HB2	1:A:298:GLU:HB3	2.02	0.41
8:I:93:LYS:HB3	8:I:93:LYS:HE2	1.84	0.41
10:K:98:MET:HE3	10:K:98:MET:HB3	1.95	0.41
12:M:35:PHE:CE1	12:M:40:SER:HB2	2.55	0.41
12:M:438:LEU:O	12:M:439:THR:OG1	2.37	0.41
32:i:57:THR:HG22	34:k:77:LEU:HB3	2.03	0.41
35:l:336:LYS:HD3	35:l:336:LYS:HA	1.84	0.41
41:s:85:MET:HE1	41:s:105:MET:O	2.20	0.41
55:s:401:PEE:H21	55:s:401:PEE:H16	1.73	0.41
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.54	0.41
43:v:69:CYS:HB3	43:v:80:CYS:HB2	2.00	0.41
1:A:213:ILE:HG23	1:A:235:VAL:HA	2.01	0.41
11:L:92:ASN:HB3	15:P:238:PRO:HA	2.02	0.41
14:O:125:LYS:HG3	14:O:126:PRO:HD2	2.01	0.41
16:Q:339:GLN:O	16:Q:343:ILE:HG13	2.20	0.41
55:U:101:PEE:H67	55:U:101:PEE:H72	1.90	0.41
26:c:139:PHE:O	26:c:143:MET:HG2	2.19	0.41
32:i:100:MET:HE3	32:i:111:PHE:HZ	1.85	0.41
38:o:4:PRO:HG2	39:p:73:TYR:CE1	2.56	0.41
46:A:502:FMN:O2'	46:A:502:FMN:O4'	2.32	0.41
3:C:42:ARG:O	3:C:46:VAL:HG12	2.20	0.41
12:M:265:THR:HG21	12:M:609:ALA:HB1	2.02	0.41
35:l:20:MET:HA	48:l:701:PLX:H211	2.02	0.41
35:l:51:LEU:HD11	35:l:55:MET:HE3	2.03	0.41
44:w:136:TYR:OH	44:w:194:THR:OG1	2.25	0.41
1:A:114:VAL:CG1	1:A:212:LEU:HD21	2.51	0.41
3:C:116:ALA:O	3:C:120:VAL:HG23	2.20	0.41
9:J:87:GLU:OE1	9:J:88:PRO:HD2	2.20	0.41
12:M:690:THR:HG23	12:M:692:LYS:HG2	2.03	0.41
13:N:6:VAL:HA	13:N:9:ARG:HG2	2.01	0.41
31:h:94:PRO:HA	31:h:95:PRO:HD3	1.91	0.41
35:l:277:THR:HG21	35:l:317:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.03	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.35	0.41
48:C:302:PLX:H52	48:C:302:PLX:H252	1.84	0.41
4:E:53:ASP:OD2	9:J:351:GLU:HB2	2.20	0.41
6:G:119:ILE:O	6:G:123:GLU:HG2	2.21	0.41
12:M:399:VAL:HG23	12:M:428:LYS:HB3	2.02	0.41
32:i:211:MET:HB3	32:i:251:MET:HG2	2.01	0.41
33:j:1:MET:HE3	33:j:1:MET:HB3	1.90	0.41
39:p:63:LEU:C	39:p:65:ARG:H	2.28	0.41
42:u:37:ASP:OD1	42:u:37:ASP:C	2.63	0.41
43:v:25:PHE:CE2	43:v:108:LEU:HB3	2.56	0.41
44:w:58:LYS:HA	44:w:202:HIS:ND1	2.36	0.41
4:E:36:TYR:CE2	6:G:113:LEU:HD13	2.56	0.41
12:M:578:PRO:HB3	13:N:140:PRO:HG3	2.03	0.41
14:O:146:ASP:OD1	14:O:146:ASP:N	2.52	0.41
15:P:51:ASN:OD1	15:P:51:ASN:C	2.64	0.41
16:Q:137:ASP:OD1	16:Q:144:MET:HB3	2.21	0.41
34:k:57:ASN:O	34:k:60:PRO:HD2	2.21	0.41
35:l:362:LEU:HD22	35:l:366:MET:SD	2.61	0.41
35:l:410:LEU:HD12	35:l:410:LEU:HA	1.91	0.41
40:r:17:MET:HE3	40:r:17:MET:HA	2.03	0.41
53:r:503:CDL:H392	53:r:503:CDL:H362	1.88	0.41
1:A:157:TYR:CD2	1:A:212:LEU:CD1	3.04	0.41
3:C:68:GLY:HA2	3:C:73:ALA:HB2	2.03	0.41
6:G:137:LYS:HE2	6:G:137:LYS:HB3	1.87	0.41
11:L:99:MET:HE2	11:L:138:ALA:HB2	2.03	0.41
12:M:307:ILE:HD11	12:M:317:THR:HG21	2.03	0.41
12:M:534:VAL:CG1	12:M:538:ARG:HH21	2.34	0.41
16:Q:188:THR:HB	16:Q:200:PHE:HA	2.02	0.41
21:W:121:MET:HE2	21:W:121:MET:HB2	1.98	0.41
26:c:38:PRO:HG2	38:o:71:ALA:HB2	2.03	0.41
26:c:167:TYR:CE2	26:c:178:PRO:HG3	2.56	0.41
28:e:83:ASP:OD1	28:e:83:ASP:C	2.64	0.41
35:l:51:LEU:HD22	35:l:91:PRO:HG2	2.02	0.41
35:l:169:LEU:HD12	35:l:169:LEU:HA	1.90	0.41
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.56	0.41
35:l:345:SER:HB2	35:l:450:LEU:HD21	2.03	0.41
35:l:455:LYS:O	35:l:459:ILE:HG23	2.21	0.41
39:p:136:GLU:OE1	39:p:167:TRP:NE1	2.54	0.41
40:r:299:VAL:O	40:r:303:ILE:HG12	2.21	0.41
42:u:83:THR:HA	42:u:86:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:76:GLN:O	7:H:78:GLU:N	2.54	0.41
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.29	0.41
29:f:72:ARG:HH22	30:g:18:ASN:ND2	2.19	0.41
32:i:139:LEU:HD13	32:i:205:LEU:HD22	2.03	0.41
32:i:258:SER:OG	32:i:336:VAL:HG22	2.21	0.41
32:i:288:LEU:HD23	55:i:403:PEE:H54	2.03	0.41
35:l:88:MET:HB3	35:l:326:PHE:HE2	1.86	0.41
35:l:170:GLN:NE2	35:l:534:HIS:CE1	2.89	0.41
41:s:105:MET:HE2	41:s:105:MET:HB3	1.88	0.41
44:w:258:TYR:OH	44:w:272:ASP:OD2	2.40	0.41
44:w:346:ASP:OD1	44:w:346:ASP:C	2.64	0.41
2:B:177:THR:OG1	2:B:182:GLU:OE1	2.39	0.40
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.02	0.40
21:W:48:TRP:O	21:W:52:LYS:HG2	2.21	0.40
25:b:81:ILE:HG23	55:l:704:PEE:H58	2.02	0.40
55:i:403:PEE:H25	55:i:403:PEE:H20	1.79	0.40
35:l:123:LEU:O	35:l:127:THR:HG23	2.21	0.40
35:l:176:ARG:HD2	35:l:176:ARG:HA	1.85	0.40
36:m:25:SER:HB3	36:m:28:TYR:HD2	1.86	0.40
48:r:502:PLX:H331	48:r:502:PLX:H301	1.68	0.40
44:w:57:SER:O	44:w:156:GLY:HA3	2.21	0.40
2:B:156:GLY:O	2:B:160:GLU:HG2	2.21	0.40
9:J:236:VAL:HG11	9:J:270:ARG:HE	1.85	0.40
12:M:399:VAL:HG12	12:M:472:PRO:HA	2.03	0.40
16:Q:216:ARG:HH12	16:Q:243:ASP:CG	2.28	0.40
6:X:79:ILE:HD11	6:X:154:VAL:HG21	2.02	0.40
24:a:156:VAL:O	24:a:160:MET:HG3	2.20	0.40
25:b:69:ILE:O	25:b:73:THR:HG22	2.21	0.40
33:j:62:PHE:CD1	41:s:140:ILE:HB	2.56	0.40
35:l:153:LEU:HD23	35:l:153:LEU:HA	1.92	0.40
35:l:222:GLY:HA2	35:l:229:LEU:HD12	2.03	0.40
40:r:1:MET:HG2	40:r:111:THR:HG21	2.03	0.40
16:Q:234:GLN:O	16:Q:235:ASP:CB	2.69	0.40
26:c:169:GLU:HG2	43:v:56:ARG:NH1	2.37	0.40
29:f:70:LYS:HB2	29:f:70:LYS:HE3	1.85	0.40
32:i:342:ALA:HB3	48:i:402:PLX:H332	2.02	0.40
34:k:73:LEU:HA	36:m:168:ILE:HD11	2.03	0.40
35:l:331:MET:HE3	35:l:387:THR:O	2.21	0.40
41:s:195:ARG:HH11	41:s:231:ILE:HD13	1.87	0.40
43:v:45:GLU:H	43:v:45:GLU:HG2	1.61	0.40
2:B:99:GLY:N	2:B:169:GLU:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:143:SER:HA	16:Q:178:THR:HG22	2.04	0.40
32:i:335:LEU:HD21	53:r:503:CDL:H402	2.04	0.40
35:l:68:TRP:H	35:l:77:SER:HA	1.87	0.40
35:l:529:TYR:CZ	35:l:533:MET:HG3	2.56	0.40
40:r:346:ARG:O	40:r:419:TYR:HA	2.22	0.40
43:v:25:PHE:CD2	43:v:108:LEU:HB3	2.56	0.40
2:B:54:THR:HG21	21:W:33:TYR:CE1	2.56	0.40
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.56	0.40
8:I:42:PRO:HD3	21:W:6:VAL:HG13	2.03	0.40
8:I:74:LYS:HD2	8:I:74:LYS:HA	1.77	0.40
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.03	0.40
11:L:70:GLU:OE2	11:L:70:GLU:N	2.30	0.40
14:O:108:PRO:HA	14:O:109:PRO:HD3	2.00	0.40
32:i:49:ASN:O	32:i:53:THR:HG23	2.22	0.40
48:i:402:PLX:H312	48:i:402:PLX:H211	2.03	0.40
35:l:409:LEU:O	35:l:413:LEU:HG	2.22	0.40
36:m:55:MET:HE2	36:m:55:MET:HA	2.03	0.40
36:m:63:GLY:O	36:m:67:VAL:HG23	2.22	0.40
39:p:27:LEU:HD21	39:p:40:PHE:HB3	2.04	0.40
40:r:218:LYS:O	40:r:222:GLU:HG2	2.21	0.40
40:r:281:ASP:HB3	40:r:284:SER:HB2	2.04	0.40
41:s:113:VAL:HG22	41:s:136:VAL:HG22	2.02	0.40
43:v:49:ALA:HB2	43:v:64:ILE:HD11	2.03	0.40
44:w:93:TYR:OH	44:w:145:ASP:OD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.08	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	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	12.38	130.82	119.48
16	Q	118	2MR	CD-NE-CZ	4.50	131.82	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.25	130.62	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\# Z > 2$
45	SF4	M	802	12	0,12,12	-	-	-		
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.21	8 (16%)
48	PLX	a	202	-	51,51,51	1.22	4 (7%)	53,59,59	0.62	1 (1%)
51	FES	M	803	12	0,4,4	-	-	-		
51	FES	O	301	14	0,4,4	-	-	-		
53	CDL	V	201	-	70,70,99	1.25	8 (11%)	76,82,111	0.94	4 (5%)
55	PEE	l	704	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
48	PLX	C	302	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
53	CDL	r	503	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
48	PLX	i	402	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
55	PEE	l	703	-	45,45,50	1.25	6 (13%)	48,50,55	1.00	2 (4%)
53	CDL	l	702	-	99,99,99	1.12	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	C	301	16,3	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
50	NDP	J	401	-	51,52,52	4.30	25 (49%)	71,80,80	2.23	14 (19%)
56	UQ	s	402	-	28,28,63	3.32	9 (32%)	36,37,79	2.65	11 (30%)
53	CDL	a	201	-	90,90,99	1.16	8 (8%)	96,102,111	0.93	4 (4%)
55	PEE	j	201	-	46,46,50	1.23	6 (13%)	49,51,55	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
53	CDL	N	201	-	50,50,99	1.43	9 (18%)	56,62,111	1.14	4 (7%)
53	CDL	i	401	-	65,65,99	1.31	9 (13%)	71,77,111	1.03	4 (5%)
47	NAI	A	503	-	47,48,48	4.02	22 (46%)	64,73,73	1.68	11 (17%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
48	PLX	l	701	-	51,51,51	1.21	5 (9%)	53,59,59	0.60	1 (1%)
48	PLX	j	202	-	51,51,51	1.22	4 (7%)	53,59,59	0.62	1 (1%)
49	8Q1	G	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.58	6 (15%)
55	PEE	s	401	-	50,50,50	1.17	6 (12%)	53,55,55	1.02	2 (3%)
55	PEE	i	403	-	46,46,50	1.23	6 (13%)	49,51,55	1.01	2 (4%)
48	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.62	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
55	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
57	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.91	9 (20%)
49	8Q1	X	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.55	6 (15%)
55	PEE	m	201	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	M	802	12	-	-	0/6/5/5
46	FMN	A	502	-	-	2/18/18/18	0/3/3/3
48	PLX	a	202	-	-	21/55/55/55	-
53	CDL	V	201	-	-	50/81/81/110	-
55	PEE	l	704	-	-	21/49/49/54	-
51	FES	M	803	12	-	-	0/1/1/1
51	FES	O	301	14	-	-	0/1/1/1
48	PLX	C	302	-	-	25/55/55/55	-
53	CDL	r	503	-	-	63/110/110/110	-
48	PLX	i	402	-	-	24/55/55/55	-
55	PEE	l	703	-	-	23/49/49/54	-
53	CDL	l	702	-	-	59/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	C	301	16,3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	M	801	12	-	-	0/6/5/5
50	NDP	J	401	-	-	15/34/77/77	0/5/5/5
56	UQ	s	402	-	-	8/21/45/87	0/1/1/1
53	CDL	a	201	-	-	44/101/101/110	-
55	PEE	j	201	-	-	25/50/50/54	-
55	PEE	U	101	-	-	23/54/54/54	-
53	CDL	N	201	-	-	33/61/61/110	-
53	CDL	i	401	-	-	42/76/76/110	-
47	NAI	A	503	-	-	11/29/72/72	0/5/5/5
48	PLX	l	701	-	-	36/55/55/55	-
48	PLX	j	202	-	-	27/55/55/55	-
49	8Q1	G	201	-	-	20/41/41/41	-
45	SF4	A	501	1	-	-	0/6/5/5
55	PEE	s	401	-	-	26/54/54/54	-
55	PEE	i	403	-	-	24/50/50/54	-
48	PLX	r	502	-	-	28/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
55	PEE	r	501	-	-	29/54/54/54	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
49	8Q1	X	201	-	-	19/41/41/41	-
55	PEE	m	201	-	-	24/44/44/54	-

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-13.06	1.24	1.53
50	J	401	NDP	O4D-C4D	10.81	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.28	1.26	1.53
50	J	401	NDP	C3D-C4D	-9.93	1.27	1.53
56	s	402	UQ	C13-C14	9.60	1.55	1.33
47	A	503	NAI	O4B-C1B	9.38	1.63	1.42
56	s	402	UQ	C8-C9	9.29	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.86	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.26	1.26	1.45
50	J	401	NDP	O4B-C4B	-7.93	1.27	1.45
56	s	402	UQ	C18-C19	7.92	1.56	1.32
57	w	401	ADP	O4'-C4'	7.77	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.66	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C2N-C3N	7.51	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.36	1.30	1.53
50	J	401	NDP	C6N-C5N	7.27	1.55	1.33
47	A	503	NAI	O4D-C4D	7.03	1.60	1.45
50	J	401	NDP	PN-O3	6.75	1.66	1.59
57	w	401	ADP	PA-O3A	6.52	1.66	1.59
47	A	503	NAI	PA-O3	6.44	1.66	1.59
50	J	401	NDP	P2B-O2B	6.14	1.70	1.59
47	A	503	NAI	C2D-C3D	6.00	1.69	1.53
50	J	401	NDP	C6A-N6A	5.83	1.49	1.34
50	J	401	NDP	PA-O3	5.73	1.65	1.59
47	A	503	NAI	O4D-C1D	5.69	1.55	1.42
47	A	503	NAI	PN-O3	5.62	1.65	1.59
50	J	401	NDP	C3B-C4B	5.57	1.67	1.53
57	w	401	ADP	C6-N6	5.46	1.48	1.34
47	A	503	NAI	C7N-N7N	5.30	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.20	1.40	1.50
49	X	201	8Q1	C39-N41	5.17	1.45	1.33
49	G	201	8Q1	C34-N36	5.15	1.45	1.33
49	G	201	8Q1	C39-N41	5.12	1.45	1.33
49	X	201	8Q1	C34-N36	5.10	1.45	1.33
47	A	503	NAI	C6A-N6A	5.09	1.47	1.34
50	J	401	NDP	C6N-N1N	5.06	1.49	1.37
50	J	401	NDP	O4D-C1D	-5.02	1.30	1.42
50	J	401	NDP	O4B-C1B	4.69	1.52	1.42
50	J	401	NDP	C1B-N9A	-4.56	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.53	1.31	1.42
47	A	503	NAI	O2B-C2B	4.37	1.53	1.43
50	J	401	NDP	O2D-C2D	-3.90	1.33	1.43
50	J	401	NDP	C7N-N7N	3.85	1.44	1.33
55	l	703	PEE	C18-C19	3.83	1.53	1.31
55	j	201	PEE	C18-C19	3.83	1.53	1.31
55	r	501	PEE	C18-C19	3.82	1.53	1.31
55	l	704	PEE	C18-C19	3.81	1.53	1.31
55	s	401	PEE	C18-C19	3.81	1.53	1.31
55	i	403	PEE	C18-C19	3.80	1.53	1.31
55	U	101	PEE	C18-C19	3.80	1.53	1.31
55	m	201	PEE	C18-C19	3.80	1.53	1.31
55	l	703	PEE	C39-C38	3.75	1.53	1.31
55	r	501	PEE	C39-C38	3.74	1.52	1.31
55	U	101	PEE	C39-C38	3.73	1.52	1.31
55	j	201	PEE	C39-C38	3.73	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	i	403	PEE	C39-C38	3.73	1.52	1.31
55	l	704	PEE	C39-C38	3.73	1.52	1.31
55	s	401	PEE	C39-C38	3.72	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
53	V	201	CDL	OA8-CA7	3.51	1.43	1.33
53	l	702	CDL	OA8-CA7	3.50	1.43	1.33
46	A	502	FMN	C4A-N5	3.47	1.38	1.30
53	r	503	CDL	OA8-CA7	3.46	1.43	1.33
53	i	401	CDL	OA8-CA7	3.46	1.43	1.33
53	N	201	CDL	OA8-CA7	3.46	1.43	1.33
53	a	201	CDL	OA8-CA7	3.41	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.36	1.40	1.49
57	w	401	ADP	C8-N9	-3.31	1.31	1.37
57	w	401	ADP	O2'-C2'	-3.18	1.35	1.43
50	J	401	NDP	C8A-N9A	-3.11	1.32	1.37
53	l	702	CDL	OB6-CB5	3.10	1.43	1.34
53	i	401	CDL	OB6-CB5	3.09	1.43	1.34
53	i	401	CDL	OB8-CB7	3.05	1.42	1.33
53	a	201	CDL	OB8-CB7	3.04	1.42	1.33
53	a	201	CDL	OB6-CB5	3.03	1.42	1.34
53	r	503	CDL	OB6-CB5	3.02	1.42	1.34
50	J	401	NDP	C5A-N7A	-3.02	1.33	1.39
53	N	201	CDL	OB6-CB5	3.01	1.42	1.34
53	V	201	CDL	OB6-CB5	3.00	1.42	1.34
53	V	201	CDL	OB8-CB7	3.00	1.42	1.33
53	r	503	CDL	OA6-CA5	3.00	1.42	1.34
50	J	401	NDP	C7N-C3N	2.99	1.55	1.48
53	l	702	CDL	OB8-CB7	2.99	1.42	1.33
53	N	201	CDL	OB8-CB7	2.98	1.42	1.33
53	r	503	CDL	OB8-CB7	2.98	1.42	1.33
53	V	201	CDL	OA6-CA5	2.97	1.42	1.34
53	i	401	CDL	OA6-CA5	2.96	1.42	1.34
53	l	702	CDL	OA6-CA5	2.96	1.42	1.34
53	a	201	CDL	OA6-CA5	2.95	1.42	1.34
57	w	401	ADP	O3'-C3'	2.95	1.50	1.43
50	J	401	NDP	O3D-C3D	2.94	1.50	1.43
53	N	201	CDL	OA6-CA5	2.93	1.42	1.34
48	a	202	PLX	O6-C4	-2.92	1.40	1.44
48	C	302	PLX	O6-C4	-2.91	1.40	1.44
48	i	402	PLX	O6-C4	-2.82	1.41	1.44
48	l	701	PLX	O6-C4	-2.81	1.41	1.44
48	j	202	PLX	O6-C4	-2.71	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	C8A-N9A	-2.68	1.33	1.37
56	s	402	UQ	C6-C1	2.65	1.54	1.46
50	J	401	NDP	O2B-C2B	2.63	1.53	1.44
55	i	403	PEE	O2-C2	-2.57	1.40	1.46
55	s	401	PEE	O2-C2	-2.57	1.40	1.46
55	j	201	PEE	O2-C2	-2.57	1.40	1.46
53	V	201	CDL	OA6-CA4	-2.57	1.40	1.46
53	N	201	CDL	OA6-CA4	-2.56	1.40	1.46
53	a	201	CDL	OA6-CA4	-2.56	1.40	1.46
55	r	501	PEE	O2-C2	-2.56	1.40	1.46
53	l	702	CDL	OA6-CA4	-2.55	1.40	1.46
55	U	101	PEE	O2-C2	-2.54	1.40	1.46
46	A	502	FMN	C10-N1	2.54	1.38	1.33
53	r	503	CDL	OA6-CA4	-2.54	1.40	1.46
55	m	201	PEE	O2-C2	-2.53	1.40	1.46
55	l	703	PEE	O2-C2	-2.52	1.40	1.46
55	l	704	PEE	O2-C2	-2.51	1.40	1.46
47	A	503	NAI	PN-O5D	2.50	1.69	1.59
55	i	403	PEE	O3-C30	2.50	1.40	1.33
53	i	401	CDL	OA6-CA4	-2.50	1.40	1.46
55	U	101	PEE	O3-C30	2.48	1.40	1.33
55	l	704	PEE	O3-C30	2.47	1.40	1.33
55	r	501	PEE	O3-C30	2.46	1.40	1.33
55	j	201	PEE	O3-C30	2.46	1.40	1.33
55	m	201	PEE	O3-C30	2.46	1.40	1.33
48	r	502	PLX	C7-C6	2.45	1.55	1.50
47	A	503	NAI	C6N-C5N	2.45	1.40	1.33
49	G	201	8Q1	C1-S44	2.45	1.82	1.76
55	l	703	PEE	O3-C30	2.44	1.40	1.33
49	G	201	8Q1	C6-C1	2.43	1.53	1.50
49	X	201	8Q1	C1-S44	2.42	1.81	1.76
50	J	401	NDP	C2D-C3D	2.38	1.59	1.53
55	l	703	PEE	O2-C10	2.37	1.41	1.34
47	A	503	NAI	C5B-C4B	2.37	1.58	1.51
57	w	401	ADP	C5-N7	-2.37	1.34	1.39
48	j	202	PLX	C7-C6	2.36	1.55	1.50
48	i	402	PLX	C7-C6	2.36	1.55	1.50
48	l	701	PLX	C7-C6	2.36	1.55	1.50
47	A	503	NAI	O3B-C3B	-2.36	1.37	1.43
48	r	502	PLX	O6-C4	-2.35	1.41	1.44
48	a	202	PLX	C7-C6	2.35	1.55	1.50
49	X	201	8Q1	C6-C1	2.34	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	201	CDL	OB6-CB4	-2.34	1.41	1.46
49	G	201	8Q1	O35-C34	-2.34	1.18	1.23
48	C	302	PLX	C7-C6	2.34	1.55	1.50
55	m	201	PEE	O2-C10	2.32	1.40	1.34
55	j	201	PEE	O2-C10	2.32	1.40	1.34
55	l	704	PEE	O2-C10	2.32	1.40	1.34
55	s	401	PEE	O3-C30	2.31	1.40	1.33
55	U	101	PEE	O2-C10	2.30	1.40	1.34
49	X	201	8Q1	O35-C34	-2.29	1.19	1.23
55	i	403	PEE	O2-C10	2.28	1.40	1.34
53	V	201	CDL	PB2-OB2	2.28	1.68	1.59
53	i	401	CDL	PB2-OB2	2.27	1.68	1.59
49	G	201	8Q1	O40-C39	-2.27	1.18	1.23
55	r	501	PEE	O2-C10	2.26	1.40	1.34
53	V	201	CDL	OB6-CB4	-2.26	1.41	1.46
53	l	702	CDL	PB2-OB2	2.26	1.68	1.59
53	r	503	CDL	OB6-CB4	-2.26	1.41	1.46
55	s	401	PEE	O3-C3	-2.25	1.40	1.45
53	r	503	CDL	PB2-OB2	2.24	1.68	1.59
53	i	401	CDL	PB2-OB5	2.24	1.68	1.59
53	V	201	CDL	PB2-OB5	2.24	1.68	1.59
53	r	503	CDL	PB2-OB5	2.24	1.68	1.59
53	N	201	CDL	PB2-OB2	2.24	1.68	1.59
53	a	201	CDL	OB6-CB4	-2.23	1.41	1.46
53	i	401	CDL	OB6-CB4	-2.23	1.41	1.46
48	j	202	PLX	P1-O4	2.23	1.68	1.59
53	l	702	CDL	OB6-CB4	-2.22	1.41	1.46
50	J	401	NDP	PA-O5B	2.22	1.68	1.59
49	X	201	8Q1	O40-C39	-2.22	1.18	1.23
48	r	502	PLX	P1-O4	2.22	1.68	1.59
48	a	202	PLX	P1-O4	2.21	1.68	1.59
53	a	201	CDL	PB2-OB2	2.21	1.68	1.59
53	l	702	CDL	PB2-OB5	2.21	1.68	1.59
53	a	201	CDL	PB2-OB5	2.21	1.68	1.59
48	l	701	PLX	P1-O4	2.21	1.68	1.59
55	s	401	PEE	O2-C10	2.21	1.40	1.34
53	N	201	CDL	PB2-OB5	2.21	1.68	1.59
48	C	302	PLX	P1-O4	2.17	1.67	1.59
56	s	402	UQ	C7-C8	2.17	1.54	1.50
55	l	703	PEE	O3-C3	-2.16	1.40	1.45
56	s	402	UQ	O4-C4	-2.15	1.18	1.23
55	m	201	PEE	O3-C3	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	i	402	PLX	P1-O4	2.13	1.67	1.59
55	j	201	PEE	O3-C3	-2.12	1.40	1.45
55	U	101	PEE	O3-C3	-2.11	1.40	1.45
55	r	501	PEE	O3-C3	-2.11	1.40	1.45
48	l	701	PLX	P1-O1	2.09	1.67	1.59
50	J	401	NDP	O7N-C7N	-2.09	1.19	1.24
48	j	202	PLX	P1-O1	2.08	1.67	1.59
48	r	502	PLX	P1-O1	2.08	1.67	1.59
55	l	704	PEE	O3-C3	-2.08	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.08	1.35	1.39
48	a	202	PLX	P1-O1	2.08	1.67	1.59
56	s	402	UQ	O3-CM3	-2.06	1.40	1.45
48	C	302	PLX	P1-O1	2.06	1.67	1.59
55	i	403	PEE	O3-C3	-2.06	1.40	1.45
48	l	701	PLX	C1-C2	2.05	1.57	1.51
56	s	402	UQ	C5-C4	2.03	1.54	1.47
53	l	702	CDL	C11-CA5	2.03	1.56	1.50
53	i	401	CDL	C11-CA5	2.03	1.56	1.50
56	s	402	UQ	O1-C1	-2.02	1.18	1.23
48	r	502	PLX	C25-C24	2.02	1.55	1.50
48	i	402	PLX	P1-O1	2.01	1.67	1.59
53	N	201	CDL	C11-CA5	2.01	1.56	1.50

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	402	UQ	C7-C8-C9	-9.08	111.19	126.83
50	J	401	NDP	C1D-N1N-C2N	-7.39	108.96	121.14
50	J	401	NDP	C3N-C2N-N1N	-7.35	112.41	123.20
50	J	401	NDP	C6N-N1N-C2N	-6.77	112.08	119.32
56	s	402	UQ	C12-C13-C14	-6.22	113.39	127.62
49	G	201	8Q1	C6-C1-S44	5.87	120.39	113.40
49	X	201	8Q1	C6-C1-S44	5.77	120.28	113.40
50	J	401	NDP	C1D-N1N-C6N	-5.50	109.15	120.77
50	J	401	NDP	C5A-C4A-N3A	-5.49	119.16	126.72
57	w	401	ADP	C5-C4-N3	-5.45	119.22	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.42	119.26	126.72
57	w	401	ADP	N3-C2-N1	-4.58	121.64	128.58
47	A	503	NAI	N3A-C2A-N1A	-4.42	121.89	128.58
56	s	402	UQ	C10-C9-C8	-4.39	112.35	123.63
57	w	401	ADP	N3-C4-N9	4.33	134.53	127.17
55	s	401	PEE	O2-C10-C11	4.23	120.62	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	a	201	CDL	OA6-CA5-C11	4.18	120.53	111.48
50	J	401	NDP	N3A-C2A-N1A	-4.16	122.28	128.58
56	s	402	UQ	C17-C18-C19	-4.13	113.88	127.64
56	s	402	UQ	C15-C14-C13	-4.12	113.05	123.63
53	a	201	CDL	OB6-CB5-C51	4.07	120.29	111.48
53	i	401	CDL	OA6-CA5-C11	4.06	120.27	111.48
53	V	201	CDL	OB6-CB5-C51	4.05	120.24	111.48
56	s	402	UQ	C11-C9-C8	-4.04	112.10	121.17
53	l	702	CDL	OB6-CB5-C51	4.00	120.14	111.48
55	m	201	PEE	O2-C10-C11	3.99	120.12	111.48
53	i	401	CDL	OB6-CB5-C51	3.99	120.10	111.48
53	r	503	CDL	OB6-CB5-C51	3.96	120.06	111.48
50	J	401	NDP	N3A-C4A-N9A	3.94	133.87	127.17
55	i	403	PEE	O2-C10-C11	3.93	119.98	111.48
53	N	201	CDL	OA6-CA5-C11	3.92	119.97	111.48
55	U	101	PEE	O2-C10-C11	3.92	119.96	111.48
53	N	201	CDL	OB6-CB5-C51	3.90	119.93	111.48
55	r	501	PEE	O2-C10-C11	3.90	119.91	111.48
53	r	503	CDL	OA6-CA5-C11	3.87	119.84	111.48
47	A	503	NAI	N3A-C4A-N9A	3.86	133.73	127.17
55	l	704	PEE	O2-C10-C11	3.85	119.81	111.48
53	l	702	CDL	OA6-CA5-C11	3.84	119.79	111.48
55	l	703	PEE	O2-C10-C11	3.83	119.77	111.48
55	j	201	PEE	O2-C10-C11	3.82	119.74	111.48
47	A	503	NAI	C2A-N3A-C4A	3.67	120.78	111.83
50	J	401	NDP	C2A-N3A-C4A	3.57	120.56	111.83
57	w	401	ADP	C2-N3-C4	3.57	120.54	111.83
56	s	402	UQ	C16-C14-C13	-3.52	113.27	121.17
57	w	401	ADP	N9-C8-N7	-3.51	108.96	113.94
49	G	201	8Q1	O4-C1-C6	-3.49	119.95	123.98
49	X	201	8Q1	O4-C1-C6	-3.44	120.01	123.98
49	G	201	8Q1	C37-C38-C39	3.42	118.09	112.39
47	A	503	NAI	C4A-C5A-N7A	-3.42	106.67	110.58
47	A	503	NAI	C5A-N7A-C8A	3.40	108.80	103.45
47	A	503	NAI	C3D-C2D-C1D	3.34	107.79	101.46
47	A	503	NAI	N9A-C8A-N7A	-3.32	109.22	113.94
57	w	401	ADP	C4-N9-C8	3.23	109.13	105.74
56	s	402	UQ	C21-C19-C18	-3.20	113.06	122.66
46	A	502	FMN	C4-N3-C2	-3.19	119.97	125.64
57	w	401	ADP	C5-N7-C8	3.15	108.39	103.45
50	J	401	NDP	C4A-C5A-N7A	-3.12	107.01	110.58
50	J	401	NDP	N9A-C8A-N7A	-3.10	109.53	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	401	NDP	C5A-N7A-C8A	3.01	108.18	103.45
55	s	401	PEE	O3-C30-C31	2.95	120.82	111.83
56	s	402	UQ	C20-C19-C18	-2.92	113.91	122.66
57	w	401	ADP	C4-C5-N7	-2.90	107.27	110.58
49	X	201	8Q1	C37-C38-C39	2.86	117.15	112.39
47	A	503	NAI	C2D-C3D-C4D	2.80	108.02	102.61
56	s	402	UQ	CM5-C5-C6	-2.79	119.86	124.45
50	J	401	NDP	C2B-C3B-C4B	2.76	107.94	101.99
53	V	201	CDL	OA8-CA7-C31	2.76	120.24	111.83
55	l	703	PEE	O3-C30-C31	2.76	120.24	111.83
55	r	501	PEE	O3-C30-C31	2.76	120.24	111.83
56	s	402	UQ	C7-C6-C5	-2.75	120.17	124.89
53	N	201	CDL	OB8-CB7-C71	2.75	120.20	111.83
55	i	403	PEE	O3-C30-C31	2.73	120.16	111.83
53	r	503	CDL	OA8-CA7-C31	2.72	120.12	111.83
55	l	704	PEE	O3-C30-C31	2.70	120.07	111.83
55	U	101	PEE	O3-C30-C31	2.70	120.07	111.83
53	l	702	CDL	OB8-CB7-C71	2.69	120.05	111.83
53	a	201	CDL	OB8-CB7-C71	2.69	120.02	111.83
53	i	401	CDL	OB8-CB7-C71	2.67	119.99	111.83
53	N	201	CDL	OA8-CA7-C31	2.66	119.96	111.83
53	i	401	CDL	OA8-CA7-C31	2.66	119.96	111.83
53	a	201	CDL	OA8-CA7-C31	2.64	119.89	111.83
53	V	201	CDL	OB8-CB7-C71	2.62	119.83	111.83
53	l	702	CDL	OA8-CA7-C31	2.62	119.82	111.83
46	A	502	FMN	C4A-C4-N3	2.62	119.92	113.25
55	j	201	PEE	O3-C30-C31	2.62	119.82	111.83
55	m	201	PEE	O3-C30-C31	2.60	119.77	111.83
48	l	701	PLX	C1A-N1-C1	2.60	120.23	109.91
53	r	503	CDL	OB8-CB7-C71	2.59	119.72	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.58	103.76	109.47
46	A	502	FMN	O4-C4-C4A	-2.52	119.89	126.53
48	i	402	PLX	C1A-N1-C1	2.51	119.90	109.91
48	a	202	PLX	C1A-N1-C1	2.49	119.83	109.91
46	A	502	FMN	C4A-C10-N10	2.47	120.02	116.48
48	j	202	PLX	C1A-N1-C1	2.46	119.67	109.91
49	G	201	8Q1	C43-S44-C1	2.45	109.10	101.84
53	V	201	CDL	OA6-CA5-C11	2.45	119.94	110.93
48	r	502	PLX	C1A-N1-C1	2.45	119.65	109.91
50	J	401	NDP	C4A-N9A-C8A	2.44	108.30	105.74
47	A	503	NAI	C4A-N9A-C8A	2.43	108.29	105.74
49	G	201	8Q1	O4-C1-S44	-2.38	119.65	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	X	201	8Q1	O4-C1-S44	-2.34	119.71	122.68
49	X	201	8Q1	C43-S44-C1	2.32	108.69	101.84
46	A	502	FMN	C5A-C9A-N10	2.30	120.05	117.97
46	A	502	FMN	C10-C4A-N5	-2.28	120.16	124.81
48	C	302	PLX	C1A-N1-C1	2.25	118.84	109.91
49	G	201	8Q1	C38-C39-N41	2.24	120.42	116.34
46	A	502	FMN	C9A-C5A-N5	-2.22	120.09	122.45
50	J	401	NDP	C2B-C1B-N9A	-2.22	110.10	113.75
57	w	401	ADP	C4'-O4'-C1'	-2.17	104.66	109.47
49	X	201	8Q1	C38-C39-N41	2.15	120.27	116.34
46	A	502	FMN	C4A-C10-N1	-2.06	119.53	124.59

There are no chirality outliers.

All (726) 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'
48	C	302	PLX	O7-C6-C7-C8
48	C	302	PLX	C3-O4-P1-O1
48	C	302	PLX	N1-C1-C2-O1
48	C	302	PLX	O9-C24-C25-C26
48	a	202	PLX	O7-C6-C7-C8
48	i	402	PLX	O7-C6-C7-C8
48	i	402	PLX	O7-C6-O6-C4
48	j	202	PLX	O7-C6-C7-C8
48	j	202	PLX	O7-C6-O6-C4
48	j	202	PLX	C3-O4-P1-O1
48	j	202	PLX	C3-O4-P1-O3
48	l	701	PLX	O7-C6-O6-C4
48	l	701	PLX	C3-O4-P1-O1
48	l	701	PLX	C3-O4-P1-O3
48	l	701	PLX	O9-C24-O8-C5
48	l	701	PLX	O9-C24-C25-C26
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C2-O1-P1-O2
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43

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Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	O27-C28-C29-C30
49	G	201	8Q1	O27-C28-C29-C31
49	G	201	8Q1	O27-C28-C29-C32
49	G	201	8Q1	N41-C42-C43-S44
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C42-C43-S44-C1
49	X	201	8Q1	C28-O27-P24-O3
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	J	401	NDP	C2N-C3N-C7N-N7N
53	N	201	CDL	O1-C1-CA2-OA2
53	N	201	CDL	CB2-C1-CA2-OA2
53	N	201	CDL	CA2-OA2-PA1-OA3
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA2-OA2-PA1-OA5
53	N	201	CDL	CA3-OA5-PA1-OA3
53	N	201	CDL	CB2-OB2-PB2-OB3
53	N	201	CDL	CB2-OB2-PB2-OB4
53	N	201	CDL	CB2-OB2-PB2-OB5
53	N	201	CDL	CB3-OB5-PB2-OB2
53	N	201	CDL	CB3-OB5-PB2-OB3
53	N	201	CDL	C51-CB5-OB6-CB4
53	V	201	CDL	CB2-C1-CA2-OA2
53	V	201	CDL	CA2-OA2-PA1-OA3
53	V	201	CDL	CA2-OA2-PA1-OA4
53	V	201	CDL	CA2-OA2-PA1-OA5
53	V	201	CDL	CA3-OA5-PA1-OA3
53	V	201	CDL	OA9-CA7-OA8-CA6
53	V	201	CDL	C31-CA7-OA8-CA6
53	V	201	CDL	CB2-OB2-PB2-OB3
53	V	201	CDL	CB2-OB2-PB2-OB5
53	V	201	CDL	CB3-OB5-PB2-OB2
53	V	201	CDL	CB3-OB5-PB2-OB3
53	V	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CA3-OA5-PA1-OA4
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB2-OB2-PB2-OB4
53	a	201	CDL	CB2-OB2-PB2-OB5
53	i	401	CDL	CA3-OA5-PA1-OA2
53	i	401	CDL	CA3-OA5-PA1-OA3
53	i	401	CDL	CA3-OA5-PA1-OA4
53	i	401	CDL	CB2-OB2-PB2-OB3
53	i	401	CDL	CB2-OB2-PB2-OB4
53	i	401	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	CA2-OA2-PA1-OA4
53	l	702	CDL	CA2-OA2-PA1-OA5
53	l	702	CDL	CA3-OA5-PA1-OA2
53	l	702	CDL	CA3-OA5-PA1-OA3
53	l	702	CDL	CA3-OA5-PA1-OA4
53	l	702	CDL	OA6-CA4-CA6-OA8
53	l	702	CDL	CB2-OB2-PB2-OB4
53	l	702	CDL	CB2-OB2-PB2-OB5
53	l	702	CDL	OB6-CB4-CB6-OB8
53	r	503	CDL	CA2-OA2-PA1-OA3
53	r	503	CDL	CA2-OA2-PA1-OA4
53	r	503	CDL	CA2-OA2-PA1-OA5
53	r	503	CDL	CA3-OA5-PA1-OA2
53	r	503	CDL	CA3-OA5-PA1-OA3
53	r	503	CDL	CA3-OA5-PA1-OA4
53	r	503	CDL	OA6-CA4-CA6-OA8
53	r	503	CDL	CB3-OB5-PB2-OB2
53	r	503	CDL	CB3-OB5-PB2-OB3
55	U	101	PEE	C1-O3P-P-O1P
55	U	101	PEE	C1-O3P-P-O4P
55	i	403	PEE	C11-C10-O2-C2
55	j	201	PEE	C1-O3P-P-O1P
55	j	201	PEE	C1-O3P-P-O4P
55	l	703	PEE	C4-O4P-P-O3P
55	l	703	PEE	C4-O4P-P-O1P
55	l	704	PEE	O4P-C4-C5-N
55	m	201	PEE	C11-C10-O2-C2
55	m	201	PEE	O4-C10-O2-C2
55	m	201	PEE	C1-O3P-P-O2P
55	m	201	PEE	C1-O3P-P-O1P
55	m	201	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
55	m	201	PEE	C4-O4P-P-O3P
55	m	201	PEE	C4-O4P-P-O1P
55	r	501	PEE	C1-O3P-P-O2P
55	r	501	PEE	C1-O3P-P-O1P
55	r	501	PEE	C1-O3P-P-O4P
55	r	501	PEE	C4-O4P-P-O3P
55	r	501	PEE	C4-O4P-P-O2P
55	r	501	PEE	C4-O4P-P-O1P
55	s	401	PEE	C1-O3P-P-O2P
55	s	401	PEE	C1-O3P-P-O1P
55	s	401	PEE	C1-O3P-P-O4P
55	s	401	PEE	C4-O4P-P-O3P
55	s	401	PEE	C4-O4P-P-O2P
55	s	401	PEE	C4-O4P-P-O1P
56	s	402	UQ	C7-C8-C9-C11
57	w	401	ADP	C5'-O5'-PA-O2A
56	s	402	UQ	C17-C18-C19-C21
53	i	401	CDL	C31-CA7-OA8-CA6
53	i	401	CDL	OA9-CA7-OA8-CA6
53	N	201	CDL	OB7-CB5-OB6-CB4
55	i	403	PEE	O4-C10-O2-C2
55	j	201	PEE	O4-C10-O2-C2
55	j	201	PEE	C11-C10-O2-C2
56	s	402	UQ	C7-C8-C9-C10
55	l	704	PEE	C37-C38-C39-C40
55	s	401	PEE	C17-C18-C19-C20
55	s	401	PEE	C37-C38-C39-C40
53	r	503	CDL	OB9-CB7-OB8-CB6
55	l	704	PEE	O5-C30-O3-C3
48	C	302	PLX	C28-C29-C30-C31
53	V	201	CDL	O1-C1-CA2-OA2
53	a	201	CDL	O1-C1-CB2-OB2
53	l	702	CDL	O1-C1-CB2-OB2
53	r	503	CDL	C71-CB7-OB8-CB6
55	l	704	PEE	C31-C30-O3-C3
53	r	503	CDL	C51-CB5-OB6-CB4
55	U	101	PEE	C11-C10-O2-C2
55	l	703	PEE	C11-C10-O2-C2
53	l	702	CDL	C71-CB7-OB8-CB6
55	m	201	PEE	C31-C30-O3-C3
56	s	402	UQ	C12-C11-C9-C10
53	r	503	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
56	s	402	UQ	C9-C11-C12-C13
56	s	402	UQ	C14-C16-C17-C18
48	r	502	PLX	C9-C10-C11-C12
53	l	702	CDL	OB9-CB7-OB8-CB6
55	i	403	PEE	C31-C30-O3-C3
55	U	101	PEE	C17-C18-C19-C20
55	r	501	PEE	C17-C18-C19-C20
48	r	502	PLX	C30-C31-C32-C33
53	a	201	CDL	C34-C35-C36-C37
53	l	702	CDL	C11-C12-C13-C14
53	l	702	CDL	C59-C60-C61-C62
55	m	201	PEE	O5-C30-O3-C3
55	l	703	PEE	O4-C10-O2-C2
53	V	201	CDL	CA2-C1-CB2-OB2
53	a	201	CDL	CA2-C1-CB2-OB2
53	r	503	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	C71-CB7-OB8-CB6
55	l	703	PEE	C31-C30-O3-C3
48	j	202	PLX	C28-C29-C30-C31
48	i	402	PLX	C7-C8-C9-C10
48	l	701	PLX	C12-C13-C14-C15
53	i	401	CDL	O1-C1-CA2-OA2
55	s	401	PEE	C12-C13-C14-C15
55	l	703	PEE	O5-C30-O3-C3
53	r	503	CDL	C74-C75-C76-C77
55	U	101	PEE	O4-C10-O2-C2
53	N	201	CDL	OA5-CA3-CA4-OA6
53	a	201	CDL	OA5-CA3-CA4-OA6
55	l	703	PEE	O3P-C1-C2-O2
53	i	401	CDL	C71-CB7-OB8-CB6
50	J	401	NDP	C2D-C1D-N1N-C6N
55	i	403	PEE	C10-C11-C12-C13
48	j	202	PLX	C15-C16-C17-C18
53	l	702	CDL	C71-C72-C73-C74
53	a	201	CDL	C31-C32-C33-C34
48	l	701	PLX	C2-C1-N1-C1A
53	a	201	CDL	CA7-C31-C32-C33
53	i	401	CDL	CB5-C51-C52-C53
53	l	702	CDL	CB5-C51-C52-C53
53	l	702	CDL	CB7-C71-C72-C73
53	l	702	CDL	C35-C36-C37-C38
53	r	503	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	OB9-CB7-OB8-CB6
55	i	403	PEE	O5-C30-O3-C3
53	V	201	CDL	O1-C1-CB2-OB2
53	a	201	CDL	O1-C1-CA2-OA2
53	r	503	CDL	O1-C1-CA2-OA2
53	i	401	CDL	OB9-CB7-OB8-CB6
56	s	402	UQ	C13-C14-C16-C17
53	N	201	CDL	CB5-C51-C52-C53
53	i	401	CDL	CB7-C71-C72-C73
53	r	503	CDL	CB5-C51-C52-C53
48	a	202	PLX	C29-C30-C31-C32
55	r	501	PEE	C10-C11-C12-C13
53	V	201	CDL	C74-C75-C76-C77
53	i	401	CDL	C14-C15-C16-C17
53	a	201	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CB2-C1-CA2-OA2
53	l	702	CDL	CA2-C1-CB2-OB2
48	l	701	PLX	C2-C1-N1-C1C
50	J	401	NDP	O4B-C4B-C5B-O5B
48	i	402	PLX	O8-C24-C25-C26
48	l	701	PLX	O8-C24-C25-C26
55	s	401	PEE	C11-C10-O2-C2
55	s	401	PEE	O4-C10-O2-C2
53	V	201	CDL	C60-C61-C62-C63
53	r	503	CDL	OB6-CB4-CB6-OB8
55	m	201	PEE	C13-C14-C15-C16
48	r	502	PLX	C16-C17-C18-C19
53	a	201	CDL	C35-C36-C37-C38
53	r	503	CDL	C71-C72-C73-C74
48	i	402	PLX	C11-C10-C9-C8
48	j	202	PLX	C10-C11-C12-C13
53	V	201	CDL	C56-C57-C58-C59
53	N	201	CDL	CA7-C31-C32-C33
53	a	201	CDL	C32-C33-C34-C35
53	l	702	CDL	C40-C41-C42-C43
48	i	402	PLX	O9-C24-C25-C26
48	l	701	PLX	C25-C26-C27-C28
53	i	401	CDL	C37-C38-C39-C40
53	r	503	CDL	C56-C57-C58-C59
48	i	402	PLX	C32-C33-C34-C35
53	V	201	CDL	C54-C55-C56-C57
53	i	401	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
55	r	501	PEE	C31-C32-C33-C34
48	j	202	PLX	C7-C8-C9-C10
53	r	503	CDL	C73-C74-C75-C76
48	i	402	PLX	C33-C34-C35-C36
53	a	201	CDL	C73-C74-C75-C76
53	l	702	CDL	C54-C55-C56-C57
48	a	202	PLX	C28-C29-C30-C31
48	i	402	PLX	C27-C28-C29-C30
48	r	502	PLX	C12-C13-C14-C15
47	A	503	NAI	C3D-C4D-C5D-O5D
48	a	202	PLX	C10-C11-C12-C13
48	l	701	PLX	C14-C15-C16-C17
53	a	201	CDL	C11-C12-C13-C14
53	i	401	CDL	C71-C72-C73-C74
53	l	702	CDL	C73-C74-C75-C76
48	a	202	PLX	C33-C34-C35-C36
48	l	701	PLX	C29-C30-C31-C32
53	l	702	CDL	C75-C76-C77-C78
48	i	402	PLX	C30-C31-C32-C33
53	V	201	CDL	C52-C53-C54-C55
53	V	201	CDL	C71-CB7-OB8-CB6
55	l	704	PEE	C1-C2-C3-O3
48	a	202	PLX	C14-C15-C16-C17
48	i	402	PLX	C9-C10-C11-C12
48	j	202	PLX	C27-C28-C29-C30
48	l	701	PLX	C10-C11-C12-C13
48	r	502	PLX	C7-C8-C9-C10
53	l	702	CDL	C60-C61-C62-C63
53	r	503	CDL	C75-C76-C77-C78
53	i	401	CDL	CA7-C31-C32-C33
53	r	503	CDL	CA7-C31-C32-C33
48	r	502	PLX	C28-C29-C30-C31
53	a	201	CDL	C37-C38-C39-C40
53	l	702	CDL	C55-C56-C57-C58
55	l	704	PEE	C33-C34-C35-C36
55	r	501	PEE	C12-C13-C14-C15
48	C	302	PLX	C7-C8-C9-C10
48	C	302	PLX	C25-C26-C27-C28
55	i	403	PEE	C12-C13-C14-C15
55	r	501	PEE	C20-C21-C22-C23
55	s	401	PEE	C14-C15-C16-C17
48	i	402	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
48	l	701	PLX	C28-C29-C30-C31
53	l	702	CDL	C39-C40-C41-C42
48	l	701	PLX	C33-C34-C35-C36
53	a	201	CDL	C17-C18-C19-C20
53	a	201	CDL	C52-C53-C54-C55
53	i	401	CDL	C34-C35-C36-C37
53	l	702	CDL	C63-C64-C65-C66
53	r	503	CDL	CA5-C11-C12-C13
53	V	201	CDL	C11-CA5-OA6-CA4
55	s	401	PEE	C15-C16-C17-C18
53	V	201	CDL	C62-C63-C64-C65
55	s	401	PEE	C21-C22-C23-C24
48	r	502	PLX	C15-C16-C17-C18
53	a	201	CDL	C75-C76-C77-C78
53	r	503	CDL	C78-C79-C80-C81
53	V	201	CDL	OB9-CB7-OB8-CB6
53	a	201	CDL	C16-C17-C18-C19
48	j	202	PLX	C13-C14-C15-C16
53	r	503	CDL	C41-C42-C43-C44
53	l	702	CDL	C37-C38-C39-C40
53	V	201	CDL	C75-C76-C77-C78
55	j	201	PEE	C32-C33-C34-C35
48	i	402	PLX	C25-C26-C27-C28
55	m	201	PEE	C11-C12-C13-C14
48	l	701	PLX	C13-C14-C15-C16
53	l	702	CDL	C52-C53-C54-C55
48	C	302	PLX	C9-C10-C11-C12
48	l	701	PLX	C27-C28-C29-C30
53	N	201	CDL	C11-C12-C13-C14
53	V	201	CDL	C51-CB5-OB6-CB4
55	r	501	PEE	C11-C10-O2-C2
53	N	201	CDL	CB7-C71-C72-C73
53	r	503	CDL	C43-C44-C45-C46
53	i	401	CDL	C11-C12-C13-C14
55	l	703	PEE	C37-C38-C39-C40
48	l	701	PLX	C2-C1-N1-C1B
53	r	503	CDL	C59-C60-C61-C62
55	j	201	PEE	C42-C43-C44-C45
53	a	201	CDL	C22-C23-C24-C25
55	l	704	PEE	C31-C32-C33-C34
48	i	402	PLX	C28-C29-C30-C31
53	r	503	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
48	C	302	PLX	C16-C17-C18-C19
48	r	502	PLX	C27-C28-C29-C30
48	r	502	PLX	C10-C11-C12-C13
53	V	201	CDL	OB6-CB4-CB6-OB8
55	i	403	PEE	C35-C36-C37-C38
53	V	201	CDL	C55-C56-C57-C58
55	l	703	PEE	C31-C32-C33-C34
55	r	501	PEE	C40-C41-C42-C43
55	U	101	PEE	C36-C37-C38-C39
53	r	503	CDL	C82-C83-C84-C85
55	l	703	PEE	C13-C14-C15-C16
53	r	503	CDL	C51-C52-C53-C54
55	r	501	PEE	O4-C10-O2-C2
48	a	202	PLX	C31-C32-C33-C34
48	j	202	PLX	C14-C15-C16-C17
49	G	201	8Q1	C11-C12-C13-C14
55	U	101	PEE	C34-C35-C36-C37
55	s	401	PEE	C31-C30-O3-C3
53	i	401	CDL	C35-C36-C37-C38
53	l	702	CDL	C56-C57-C58-C59
55	l	704	PEE	C21-C22-C23-C24
55	j	201	PEE	C37-C38-C39-C40
55	r	501	PEE	C13-C14-C15-C16
53	i	401	CDL	C52-C53-C54-C55
55	l	703	PEE	C19-C20-C21-C22
55	r	501	PEE	C39-C40-C41-C42
53	i	401	CDL	C32-C33-C34-C35
55	l	704	PEE	C14-C15-C16-C17
53	V	201	CDL	OB5-CB3-CB4-CB6
55	l	703	PEE	O3P-C1-C2-C3
48	r	502	PLX	C13-C14-C15-C16
48	i	402	PLX	C14-C15-C16-C17
53	r	503	CDL	C42-C43-C44-C45
48	C	302	PLX	C33-C34-C35-C36
53	r	503	CDL	C35-C36-C37-C38
53	r	503	CDL	C17-C18-C19-C20
55	U	101	PEE	C31-C30-O3-C3
55	j	201	PEE	C31-C30-O3-C3
55	r	501	PEE	C36-C37-C38-C39
55	U	101	PEE	C23-C24-C25-C26
53	V	201	CDL	OA7-CA5-OA6-CA4
53	V	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	V	201	CDL	C84-C85-C86-C87
48	C	302	PLX	C14-C15-C16-C17
48	a	202	PLX	C3-C4-C5-O8
48	l	701	PLX	C3-C4-C5-O8
48	r	502	PLX	C3-C4-C5-O8
53	N	201	CDL	CA3-CA4-CA6-OA8
53	l	702	CDL	CB3-CB4-CB6-OB8
53	r	503	CDL	CB3-CB4-CB6-OB8
55	j	201	PEE	C1-C2-C3-O3
53	r	503	CDL	C62-C63-C64-C65
55	i	403	PEE	C19-C20-C21-C22
55	s	401	PEE	C39-C40-C41-C42
48	a	202	PLX	C26-C27-C28-C29
49	X	201	8Q1	C9-C10-C11-C12
53	l	702	CDL	O1-C1-CA2-OA2
48	j	202	PLX	C12-C13-C14-C15
53	i	401	CDL	C13-C14-C15-C16
55	s	401	PEE	C42-C43-C44-C45
55	s	401	PEE	O5-C30-O3-C3
49	G	201	8Q1	C28-O27-P24-O3
48	i	402	PLX	C12-C13-C14-C15
53	r	503	CDL	C60-C61-C62-C63
55	j	201	PEE	O5-C30-O3-C3
48	a	202	PLX	C11-C12-C13-C14
55	i	403	PEE	C21-C22-C23-C24
53	r	503	CDL	OB5-CB3-CB4-OB6
48	a	202	PLX	C7-C8-C9-C10
53	a	201	CDL	C71-C72-C73-C74
48	C	302	PLX	C27-C28-C29-C30
53	l	702	CDL	C58-C59-C60-C61
53	l	702	CDL	C72-C73-C74-C75
55	U	101	PEE	O5-C30-O3-C3
53	a	201	CDL	CB5-C51-C52-C53
53	V	201	CDL	OA6-CA4-CA6-OA8
53	i	401	CDL	OB6-CB4-CB6-OB8
53	V	201	CDL	C64-C65-C66-C67
48	j	202	PLX	C9-C10-C11-C12
48	a	202	PLX	C11-C10-C9-C8
55	l	703	PEE	C14-C15-C16-C17
53	l	702	CDL	C64-C65-C66-C67
55	j	201	PEE	C15-C16-C17-C18
53	N	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
53	i	401	CDL	C74-C75-C76-C77
53	r	503	CDL	C55-C56-C57-C58
55	i	403	PEE	C34-C35-C36-C37
55	r	501	PEE	C31-C30-O3-C3
48	a	202	PLX	C19-C20-C21-C22
49	G	201	8Q1	C7-C8-C9-C10
55	s	401	PEE	C22-C23-C24-C25
53	V	201	CDL	C59-C60-C61-C62
48	C	302	PLX	C26-C27-C28-C29
55	r	501	PEE	C41-C42-C43-C44
53	r	503	CDL	C64-C65-C66-C67
53	N	201	CDL	OA5-CA3-CA4-CA6
53	N	201	CDL	OB5-CB3-CB4-CB6
53	a	201	CDL	OA5-CA3-CA4-CA6
48	C	302	PLX	C11-C12-C13-C14
55	s	401	PEE	C34-C35-C36-C37
48	C	302	PLX	C30-C31-C32-C33
48	r	502	PLX	C14-C15-C16-C17
55	l	704	PEE	C24-C25-C26-C27
48	l	701	PLX	C7-C8-C9-C10
55	U	101	PEE	C19-C20-C21-C22
48	i	402	PLX	C3-C4-C5-O8
48	j	202	PLX	C3-C4-C5-O8
53	V	201	CDL	CB3-CB4-CB6-OB8
55	i	403	PEE	C1-C2-C3-O3
55	i	403	PEE	C24-C25-C26-C27
48	r	502	PLX	C31-C32-C33-C34
55	U	101	PEE	C44-C45-C46-C47
49	G	201	8Q1	C12-C13-C14-C15
48	l	701	PLX	C16-C17-C18-C19
48	l	701	PLX	C9-C10-C11-C12
53	r	503	CDL	C15-C16-C17-C18
48	i	402	PLX	O4-C3-C4-O6
53	N	201	CDL	OB5-CB3-CB4-OB6
53	V	201	CDL	OB5-CB3-CB4-OB6
48	C	302	PLX	C31-C32-C33-C34
49	X	201	8Q1	O4-C1-S44-C43
48	j	202	PLX	C31-C32-C33-C34
48	l	701	PLX	C31-C32-C33-C34
48	i	402	PLX	O6-C4-C5-O8
48	j	202	PLX	O6-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
53	N	201	CDL	OA6-CA4-CA6-OA8
55	i	403	PEE	O2-C2-C3-O3
55	j	201	PEE	O2-C2-C3-O3
55	r	501	PEE	O2-C2-C3-O3
50	J	401	NDP	C3B-C4B-C5B-O5B
48	j	202	PLX	C30-C31-C32-C33
48	C	302	PLX	O8-C24-C25-C26
48	a	202	PLX	O6-C6-C7-C8
53	i	401	CDL	C15-C16-C17-C18
55	r	501	PEE	C30-C31-C32-C33
48	l	701	PLX	C15-C16-C17-C18
55	m	201	PEE	C19-C20-C21-C22
55	s	401	PEE	C19-C20-C21-C22
55	r	501	PEE	C24-C25-C26-C27
53	r	503	CDL	C81-C82-C83-C84
55	l	704	PEE	C18-C19-C20-C21
49	X	201	8Q1	C11-C12-C13-C14
48	a	202	PLX	C30-C31-C32-C33
53	a	201	CDL	C15-C16-C17-C18
48	i	402	PLX	O4-C3-C4-C5
53	r	503	CDL	OB5-CB3-CB4-CB6
48	r	502	PLX	C33-C34-C35-C36
48	l	701	PLX	C11-C12-C13-C14
55	i	403	PEE	C22-C23-C24-C25
55	m	201	PEE	O3-C30-C31-C32
53	N	201	CDL	OB9-CB7-OB8-CB6
55	r	501	PEE	O5-C30-O3-C3
48	a	202	PLX	C9-C10-C11-C12
53	l	702	CDL	C32-C33-C34-C35
55	l	704	PEE	C15-C16-C17-C18
48	j	202	PLX	C33-C34-C35-C36
53	i	401	CDL	C75-C76-C77-C78
48	C	302	PLX	C18-C19-C20-C21
48	C	302	PLX	O4-C3-C4-O6
48	j	202	PLX	O4-C3-C4-O6
53	l	702	CDL	OA5-CA3-CA4-OA6
53	r	503	CDL	CA3-CA4-CA6-OA8
55	r	501	PEE	C1-C2-C3-O3
55	j	201	PEE	C30-C31-C32-C33
55	i	403	PEE	C16-C17-C18-C19
48	a	202	PLX	O6-C4-C5-O8
53	V	201	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
53	V	201	CDL	C82-C83-C84-C85
53	V	201	CDL	C53-C54-C55-C56
53	l	702	CDL	C17-C18-C19-C20
47	A	503	NAI	O4D-C4D-C5D-O5D
53	r	503	CDL	C31-CA7-OA8-CA6
55	i	403	PEE	C2-C1-O3P-P
53	r	503	CDL	C76-C77-C78-C79
53	N	201	CDL	O1-C1-CB2-OB2
53	l	702	CDL	C12-C13-C14-C15
48	C	302	PLX	C11-C10-C9-C8
55	l	703	PEE	C32-C33-C34-C35
55	U	101	PEE	C37-C38-C39-C40
53	a	201	CDL	C11-CA5-OA6-CA4
48	j	202	PLX	C25-C24-O8-C5
48	j	202	PLX	O4-C3-C4-C5
53	l	702	CDL	OA5-CA3-CA4-CA6
49	G	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	O27-C28-C29-C30
55	j	201	PEE	C13-C14-C15-C16
55	r	501	PEE	C11-C12-C13-C14
55	m	201	PEE	C23-C24-C25-C26
53	a	201	CDL	C60-C61-C62-C63
49	G	201	8Q1	C42-C43-S44-C1
48	C	302	PLX	O6-C6-C7-C8
55	U	101	PEE	C32-C33-C34-C35
53	r	503	CDL	OA9-CA7-OA8-CA6
50	J	401	NDP	C2N-C3N-C7N-O7N
48	l	701	PLX	O6-C4-C5-O8
55	l	704	PEE	O2-C2-C3-O3
53	V	201	CDL	CA3-CA4-CA6-OA8
53	i	401	CDL	CB3-CB4-CB6-OB8
53	l	702	CDL	CA3-CA4-CA6-OA8
55	l	703	PEE	C36-C37-C38-C39
55	U	101	PEE	C21-C22-C23-C24
53	a	201	CDL	C76-C77-C78-C79
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C5B-O5B-PA-O3
48	C	302	PLX	C3-O4-P1-O3
48	i	402	PLX	C3-O4-P1-O2
48	l	701	PLX	C3-O4-P1-O2
48	l	701	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
48	l	701	PLX	C2-O1-P1-O2
48	l	701	PLX	C2-O1-P1-O3
48	r	502	PLX	C2-O1-P1-O4
48	r	502	PLX	C2-O1-P1-O3
50	J	401	NDP	C5B-O5B-PA-O1A
50	J	401	NDP	C5B-O5B-PA-O2A
50	J	401	NDP	C5B-O5B-PA-O3
53	N	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	CA2-OA2-PA1-OA5
53	l	702	CDL	CA2-OA2-PA1-OA3
53	l	702	CDL	CB2-OB2-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB2
53	l	702	CDL	CB3-OB5-PB2-OB3
53	l	702	CDL	CB3-OB5-PB2-OB4
53	r	503	CDL	CB2-OB2-PB2-OB3
53	r	503	CDL	CB2-OB2-PB2-OB4
53	r	503	CDL	CB2-OB2-PB2-OB5
55	U	101	PEE	C1-O3P-P-O2P
55	i	403	PEE	C1-O3P-P-O1P
55	j	201	PEE	C1-O3P-P-O2P
55	l	703	PEE	C4-O4P-P-O2P
55	l	704	PEE	C1-O3P-P-O1P
55	m	201	PEE	C4-O4P-P-O2P
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O3A
53	r	503	CDL	C20-C21-C22-C23
48	l	701	PLX	C30-C31-C32-C33
53	r	503	CDL	CB4-CB3-OB5-PB2
53	i	401	CDL	C12-C13-C14-C15
55	i	403	PEE	C31-C32-C33-C34
55	m	201	PEE	C31-C32-C33-C34
48	l	701	PLX	C24-C25-C26-C27
55	l	703	PEE	C30-C31-C32-C33
47	A	503	NAI	C2D-C1D-N1N-C2N
55	m	201	PEE	C3-C2-O2-C10
53	l	702	CDL	C62-C63-C64-C65
53	r	503	CDL	C11-C12-C13-C14
53	i	401	CDL	C36-C37-C38-C39
55	l	704	PEE	C12-C13-C14-C15
48	C	302	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	C44-C45-C46-C47
55	U	101	PEE	C38-C39-C40-C41
55	s	401	PEE	C23-C24-C25-C26
53	a	201	CDL	OA7-CA5-OA6-CA4
55	l	704	PEE	O4-C10-O2-C2
55	i	403	PEE	C14-C15-C16-C17
55	l	703	PEE	C11-C12-C13-C14
48	i	402	PLX	C13-C14-C15-C16
55	j	201	PEE	C33-C34-C35-C36
55	l	704	PEE	C11-C10-O2-C2
53	V	201	CDL	CB7-C71-C72-C73
55	m	201	PEE	C24-C25-C26-C27
53	l	702	CDL	C33-C34-C35-C36
55	j	201	PEE	C39-C40-C41-C42
49	G	201	8Q1	C30-C29-C32-O33
53	r	503	CDL	C31-C32-C33-C34
55	i	403	PEE	C38-C39-C40-C41
55	l	704	PEE	C38-C39-C40-C41
50	J	401	NDP	C2B-O2B-P2B-O3X
53	V	201	CDL	C12-C11-CA5-OA6
55	j	201	PEE	C20-C21-C22-C23
53	N	201	CDL	C31-CA7-OA8-CA6
53	N	201	CDL	C52-C53-C54-C55
47	A	503	NAI	O4D-C1D-N1N-C2N
55	m	201	PEE	C18-C19-C20-C21
55	r	501	PEE	C38-C39-C40-C41
53	l	702	CDL	C15-C16-C17-C18
53	V	201	CDL	C79-C80-C81-C82
48	r	502	PLX	C29-C30-C31-C32
55	j	201	PEE	C18-C19-C20-C21
55	s	401	PEE	C18-C19-C20-C21
53	N	201	CDL	OA9-CA7-OA8-CA6
53	V	201	CDL	C12-C11-CA5-OA7
48	l	701	PLX	C36-C37-C38-C39
53	V	201	CDL	CA7-C31-C32-C33
55	l	704	PEE	C16-C17-C18-C19
48	C	302	PLX	C15-C16-C17-C18
55	l	703	PEE	C39-C40-C41-C42
55	l	704	PEE	C39-C40-C41-C42
48	j	202	PLX	C34-C35-C36-C37
49	X	201	8Q1	O33-C32-C34-N36
53	a	201	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
48	j	202	PLX	C16-C17-C18-C19
53	l	702	CDL	C82-C83-C84-C85
55	l	703	PEE	C3-C2-O2-C10
48	l	701	PLX	C26-C27-C28-C29
48	C	302	PLX	C17-C18-C19-C20
53	a	201	CDL	C53-C54-C55-C56
53	r	503	CDL	C83-C84-C85-C86
55	s	401	PEE	C2-C1-O3P-P
53	l	702	CDL	C34-C35-C36-C37
55	s	401	PEE	C36-C37-C38-C39
55	l	703	PEE	O2-C2-C3-O3
47	A	503	NAI	C2N-C3N-C7N-N7N
50	J	401	NDP	O4D-C4D-C5D-O5D
53	r	503	CDL	C14-C15-C16-C17
49	G	201	8Q1	C6-C7-C8-C9
55	r	501	PEE	C18-C19-C20-C21
48	r	502	PLX	O8-C24-C25-C26
55	i	403	PEE	C32-C33-C34-C35
48	i	402	PLX	C16-C17-C18-C19
53	i	401	CDL	C72-C73-C74-C75
53	a	201	CDL	C38-C39-C40-C41
50	J	401	NDP	PN-O3-PA-O1A
50	J	401	NDP	PN-O3-PA-O2A
53	a	201	CDL	C74-C75-C76-C77
55	U	101	PEE	C22-C23-C24-C25
49	G	201	8Q1	C1-C6-C7-C8
48	l	701	PLX	C32-C33-C34-C35
53	l	702	CDL	C44-C45-C46-C47
55	m	201	PEE	C22-C23-C24-C25
55	l	703	PEE	C16-C17-C18-C19
55	i	403	PEE	C17-C18-C19-C20
55	U	101	PEE	C24-C25-C26-C27
55	j	201	PEE	C38-C39-C40-C41
53	l	702	CDL	C43-C44-C45-C46
53	a	201	CDL	C33-C34-C35-C36
48	r	502	PLX	C4-C5-O8-C24
49	G	201	8Q1	C28-O27-P24-O1
55	i	403	PEE	C36-C37-C38-C39
55	j	201	PEE	C36-C37-C38-C39
55	m	201	PEE	C16-C17-C18-C19
53	r	503	CDL	C33-C34-C35-C36
53	V	201	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
53	a	201	CDL	C41-C42-C43-C44
55	s	401	PEE	C43-C44-C45-C46
53	N	201	CDL	C71-C72-C73-C74
47	A	503	NAI	C2D-C1D-N1N-C6N
48	l	701	PLX	C19-C20-C21-C22
53	i	401	CDL	CA4-CA3-OA5-PA1
48	j	202	PLX	C19-C20-C21-C22
55	l	704	PEE	C11-C12-C13-C14
53	V	201	CDL	C83-C84-C85-C86
53	i	401	CDL	CA3-CA4-CA6-OA8
55	l	703	PEE	C1-C2-C3-O3
55	j	201	PEE	C11-C12-C13-C14
55	r	501	PEE	C33-C34-C35-C36
49	G	201	8Q1	C31-C29-C32-C34
53	l	702	CDL	C76-C77-C78-C79
55	j	201	PEE	C44-C45-C46-C47
53	i	401	CDL	OA6-CA4-CA6-OA8
55	j	201	PEE	O3-C30-C31-C32
53	i	401	CDL	OA5-CA3-CA4-CA6
48	i	402	PLX	C7-C6-O6-C4
48	j	202	PLX	C7-C6-O6-C4
48	a	202	PLX	C27-C28-C29-C30
53	i	401	CDL	C52-C51-CB5-OB6
55	U	101	PEE	O2-C10-C11-C12
55	i	403	PEE	C18-C19-C20-C21
53	l	702	CDL	C14-C15-C16-C17
55	m	201	PEE	C15-C16-C17-C18
49	G	201	8Q1	C31-C29-C32-O33
53	i	401	CDL	C31-C32-C33-C34
55	m	201	PEE	C33-C34-C35-C36
55	r	501	PEE	C22-C23-C24-C25
53	l	702	CDL	C12-C11-CA5-OA6
53	r	503	CDL	C54-C55-C56-C57
48	a	202	PLX	C18-C19-C20-C21
49	X	201	8Q1	C7-C8-C9-C10
53	V	201	CDL	C32-C31-CA7-OA8
50	J	401	NDP	C2B-O2B-P2B-O2X
53	r	503	CDL	C52-C51-CB5-OB6
48	a	202	PLX	C13-C14-C15-C16
49	G	201	8Q1	C29-C28-O27-P24
53	N	201	CDL	C12-C11-CA5-OA6
53	l	702	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
55	m	201	PEE	O5-C30-C31-C32
49	X	201	8Q1	O27-C28-C29-C31
49	G	201	8Q1	C11-C10-C9-C8
47	A	503	NAI	O4B-C4B-C5B-O5B
56	s	402	UQ	C12-C13-C14-C16
53	r	503	CDL	C72-C73-C74-C75
57	w	401	ADP	C4'-C5'-O5'-PA
47	A	503	NAI	O4D-C1D-N1N-C6N
50	J	401	NDP	O4D-C1D-N1N-C6N
50	J	401	NDP	C2B-O2B-P2B-O1X
53	l	702	CDL	C12-C11-CA5-OA7
53	i	401	CDL	OA5-CA3-CA4-OA6
55	U	101	PEE	O4-C10-C11-C12
48	r	502	PLX	C11-C12-C13-C14
55	j	201	PEE	O5-C30-C31-C32
48	a	202	PLX	C6-C7-C8-C9
53	i	401	CDL	C52-C51-CB5-OB7
55	U	101	PEE	C40-C41-C42-C43
53	r	503	CDL	C80-C81-C82-C83
48	j	202	PLX	C29-C30-C31-C32
48	j	202	PLX	C4-C5-O8-C24
53	r	503	CDL	C44-C45-C46-C47
53	l	702	CDL	C52-C51-CB5-OB6
53	V	201	CDL	C32-C31-CA7-OA9
55	U	101	PEE	C16-C17-C18-C19
53	N	201	CDL	C12-C11-CA5-OA7
53	a	201	CDL	C72-C71-CB7-OB8
53	a	201	CDL	C72-C71-CB7-OB9

There are no ring outliers.

25 monomers are involved in 86 short contacts:

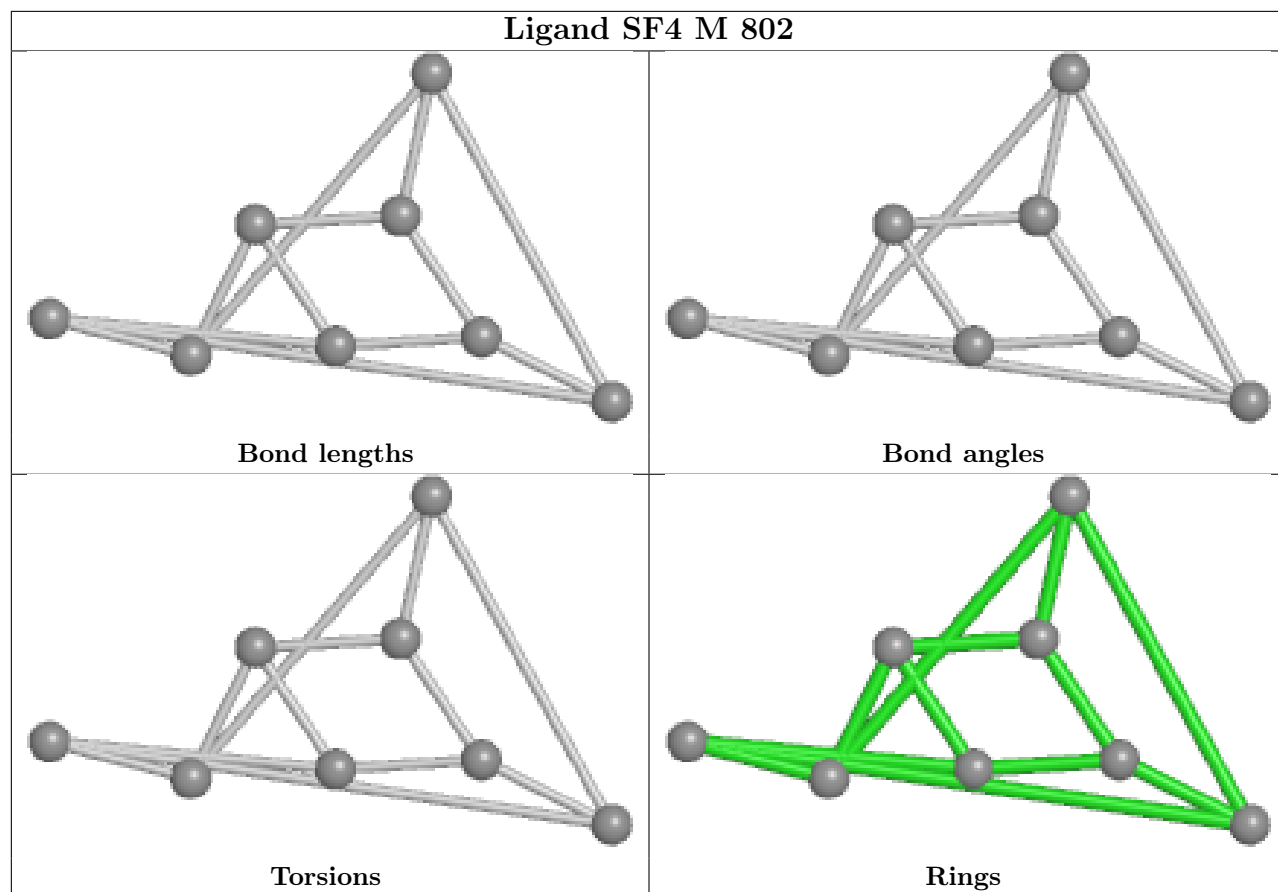
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	6	0
48	a	202	PLX	1	0
53	V	201	CDL	7	0
55	l	704	PEE	2	0
48	C	302	PLX	4	0
53	r	503	CDL	7	0
48	i	402	PLX	4	0
55	l	703	PEE	2	0
53	l	702	CDL	5	0

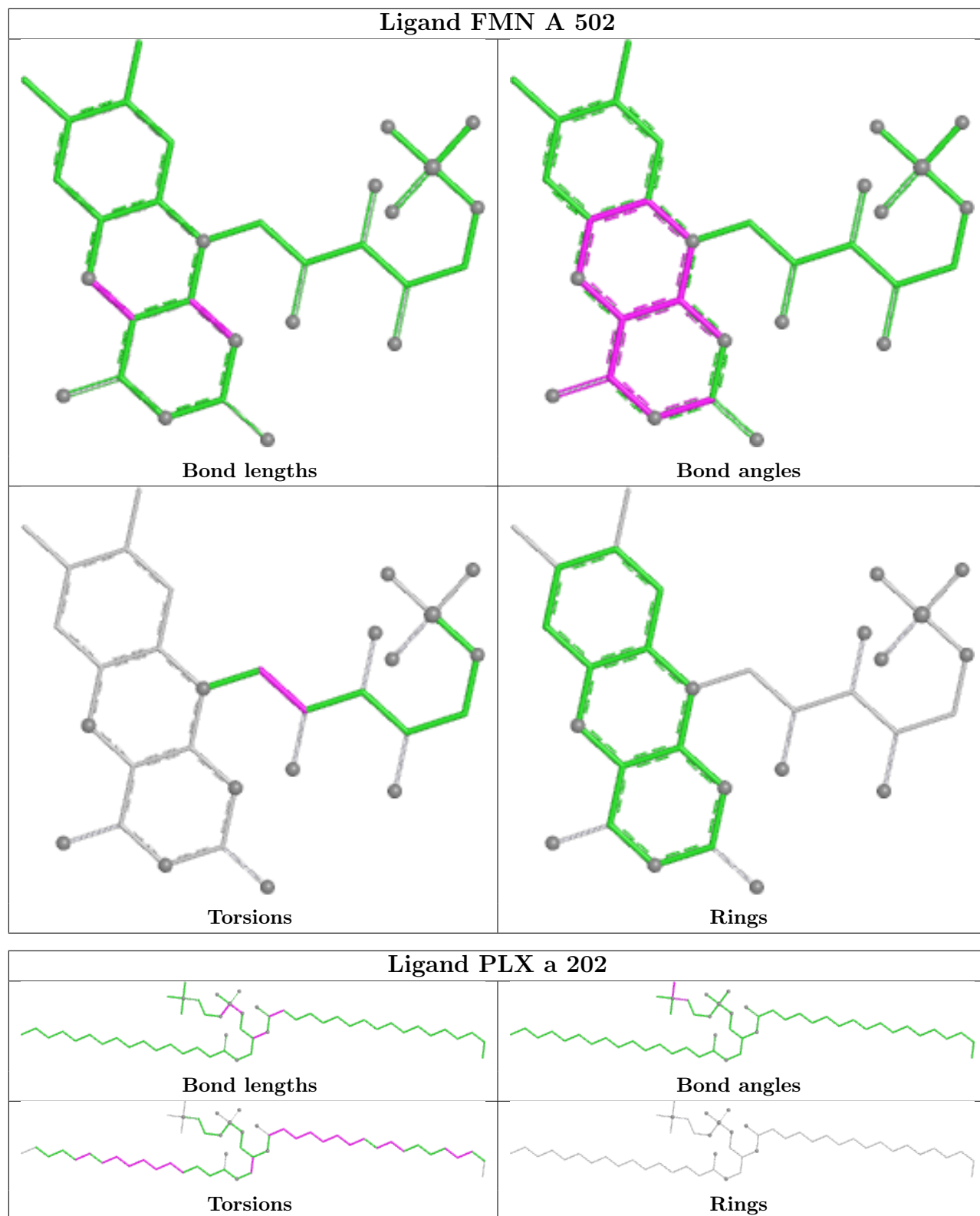
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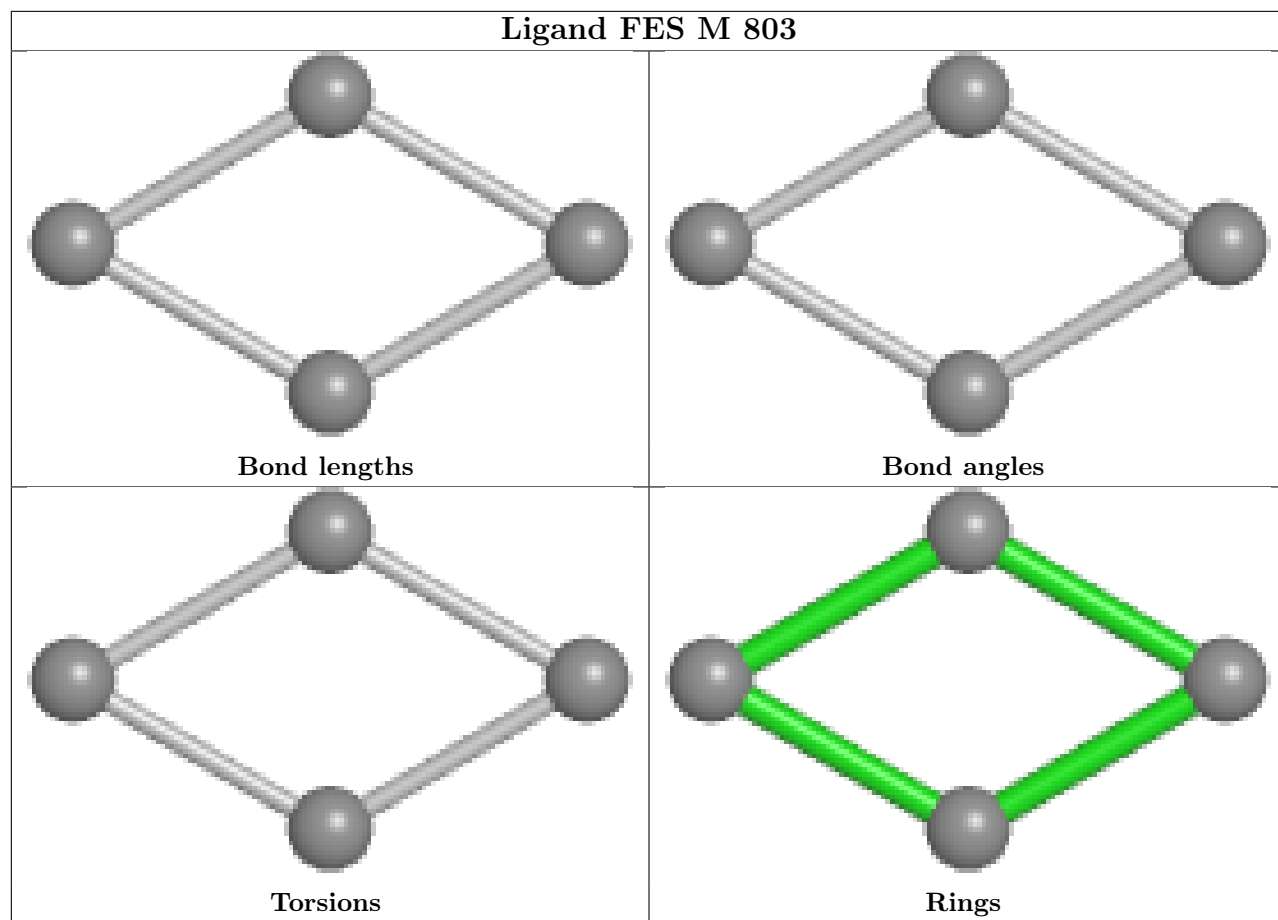
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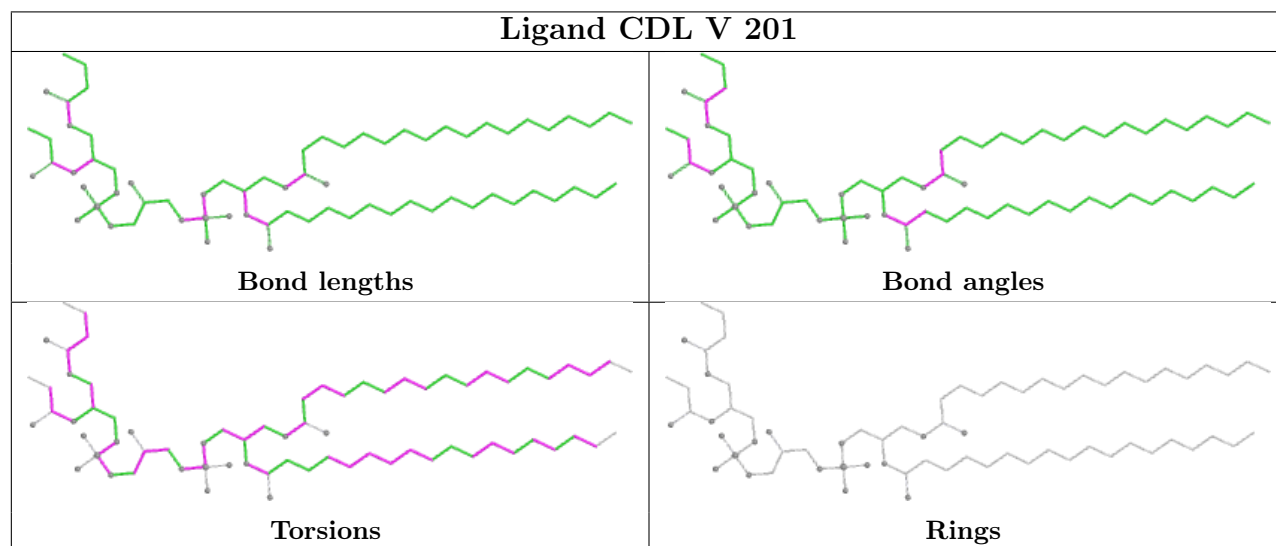
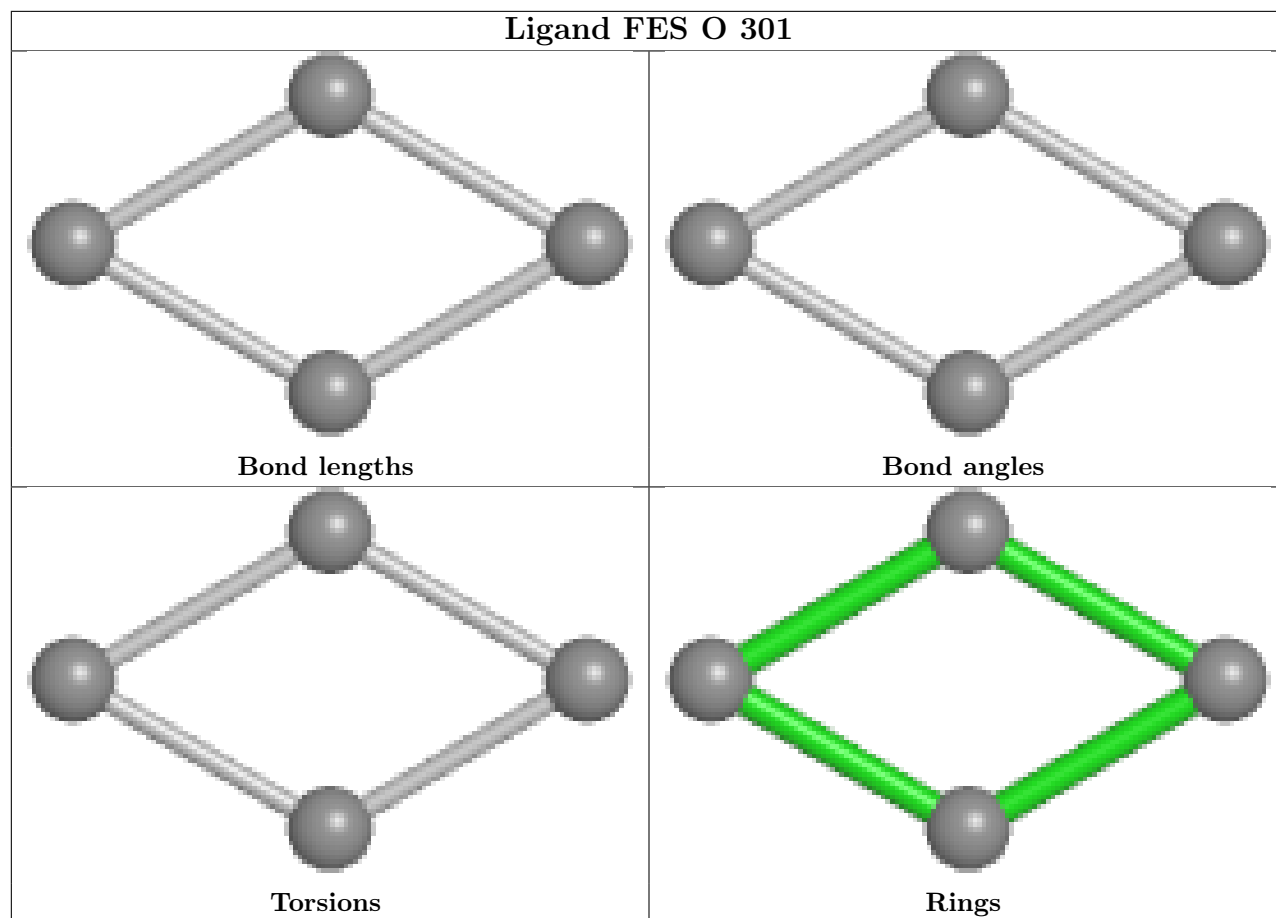
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	J	401	NDP	1	0
56	s	402	UQ	2	0
53	a	201	CDL	4	0
55	j	201	PEE	2	0
55	U	101	PEE	5	0
53	i	401	CDL	2	0
47	A	503	NAI	2	0
45	A	501	SF4	1	0
48	l	701	PLX	5	0
48	j	202	PLX	3	0
55	s	401	PEE	8	0
55	i	403	PEE	5	0
48	r	502	PLX	2	0
55	r	501	PEE	2	0
57	w	401	ADP	2	0
49	X	201	8Q1	6	0

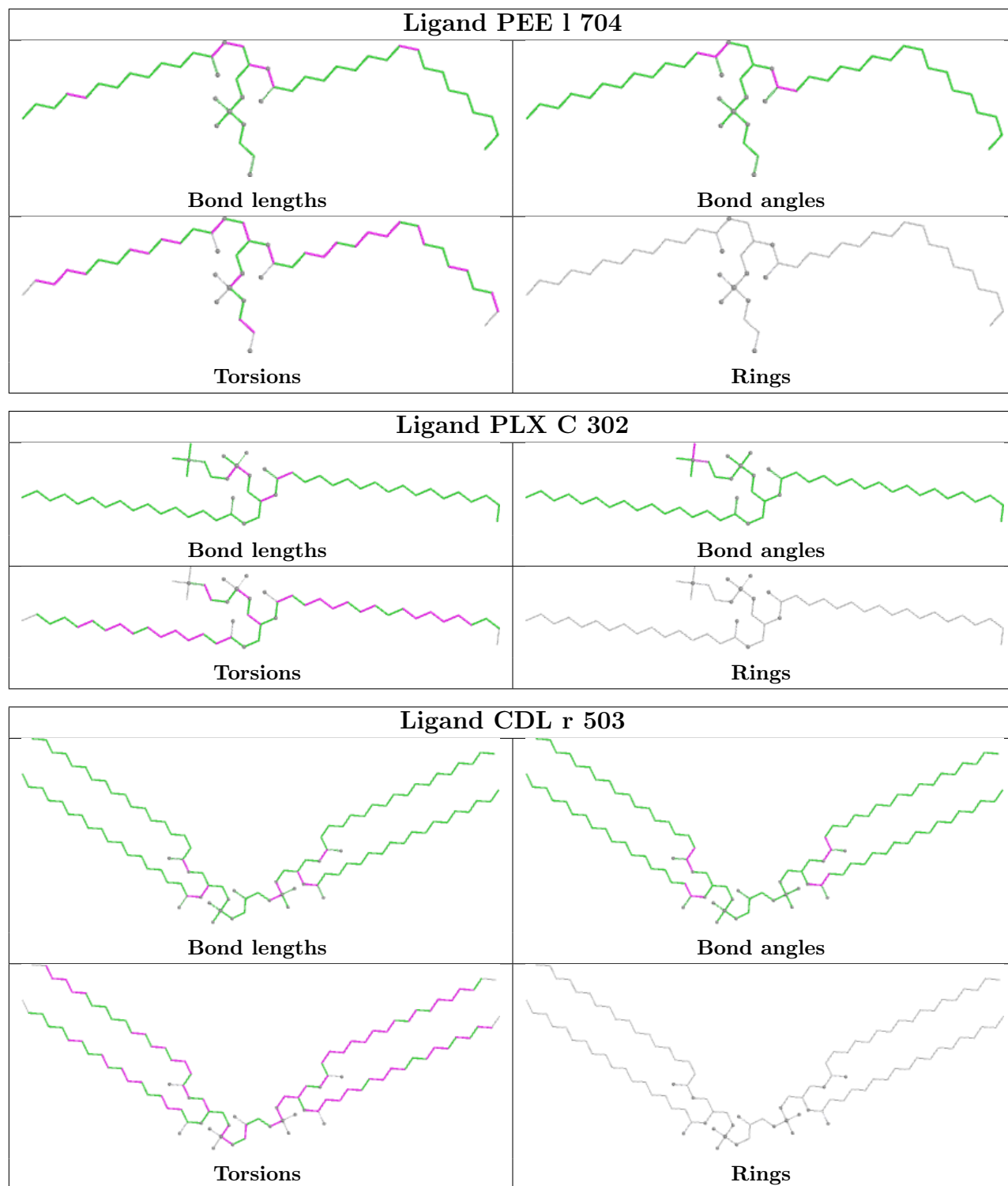
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

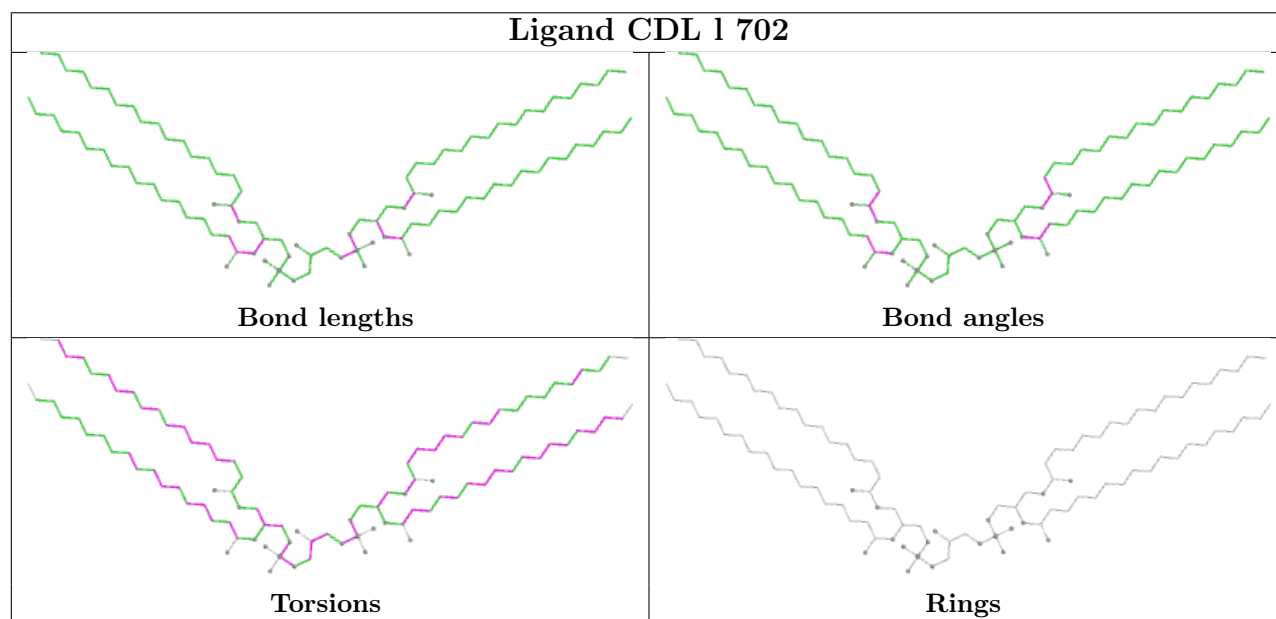
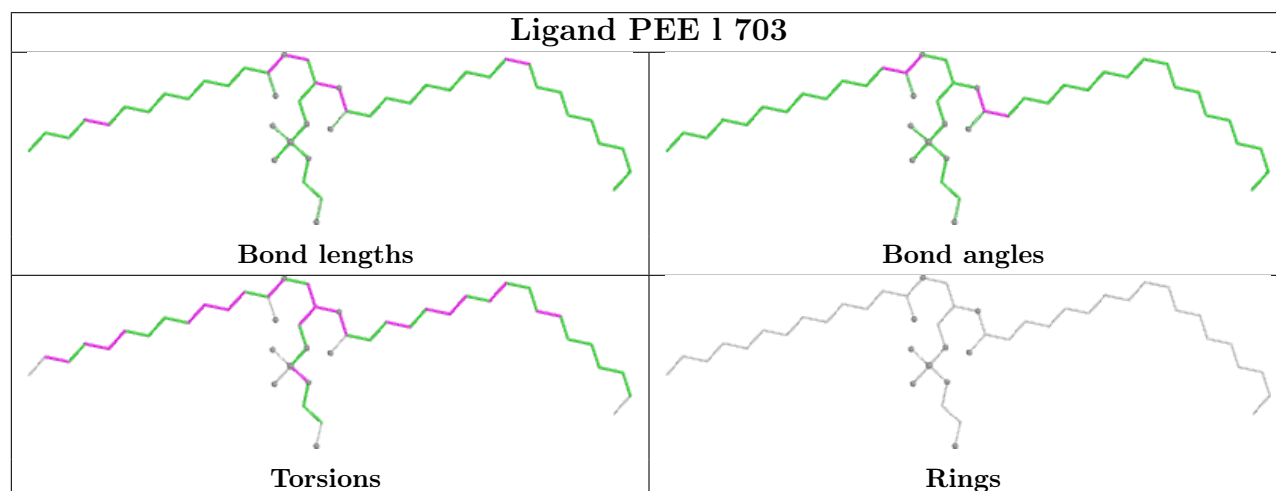
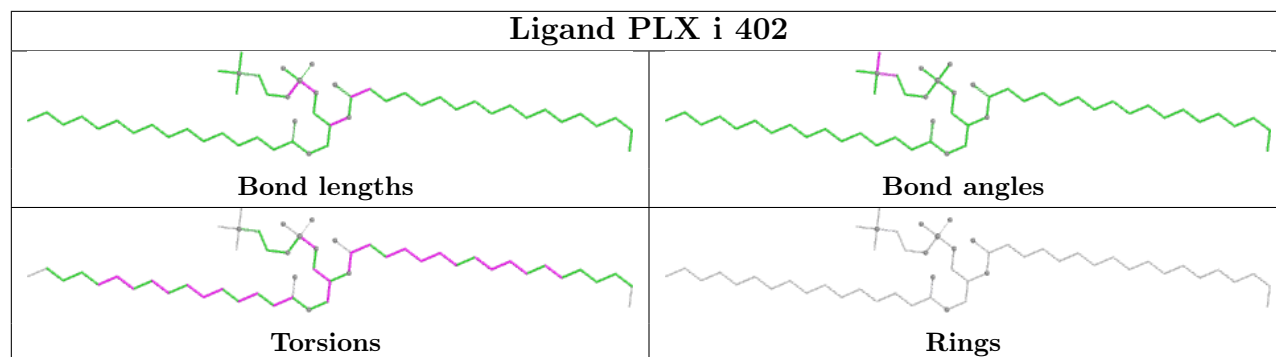


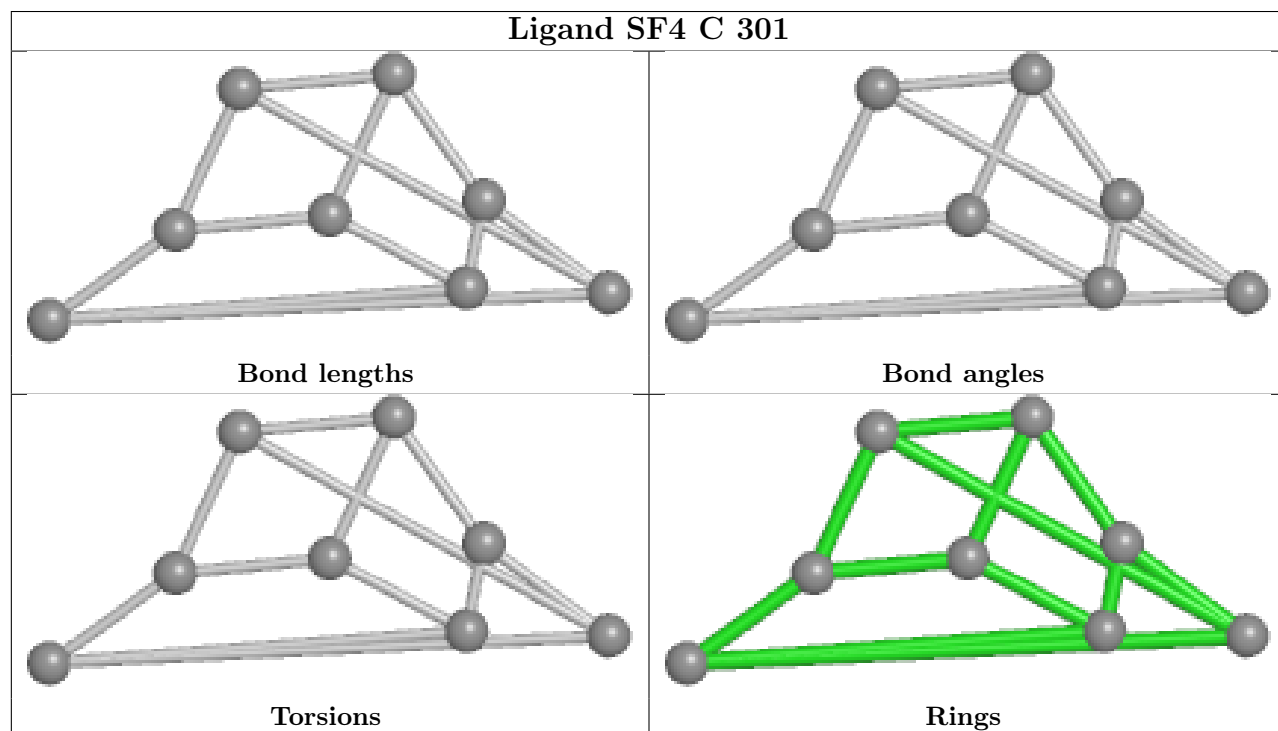
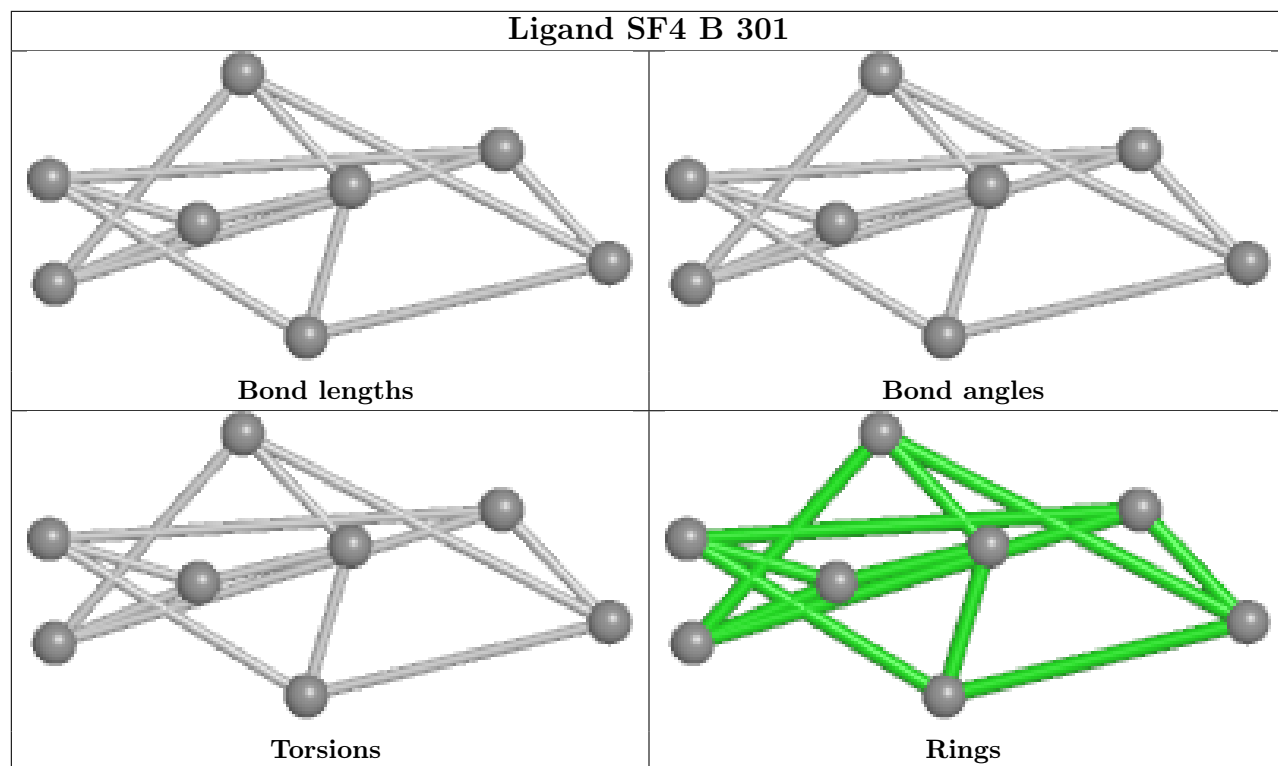


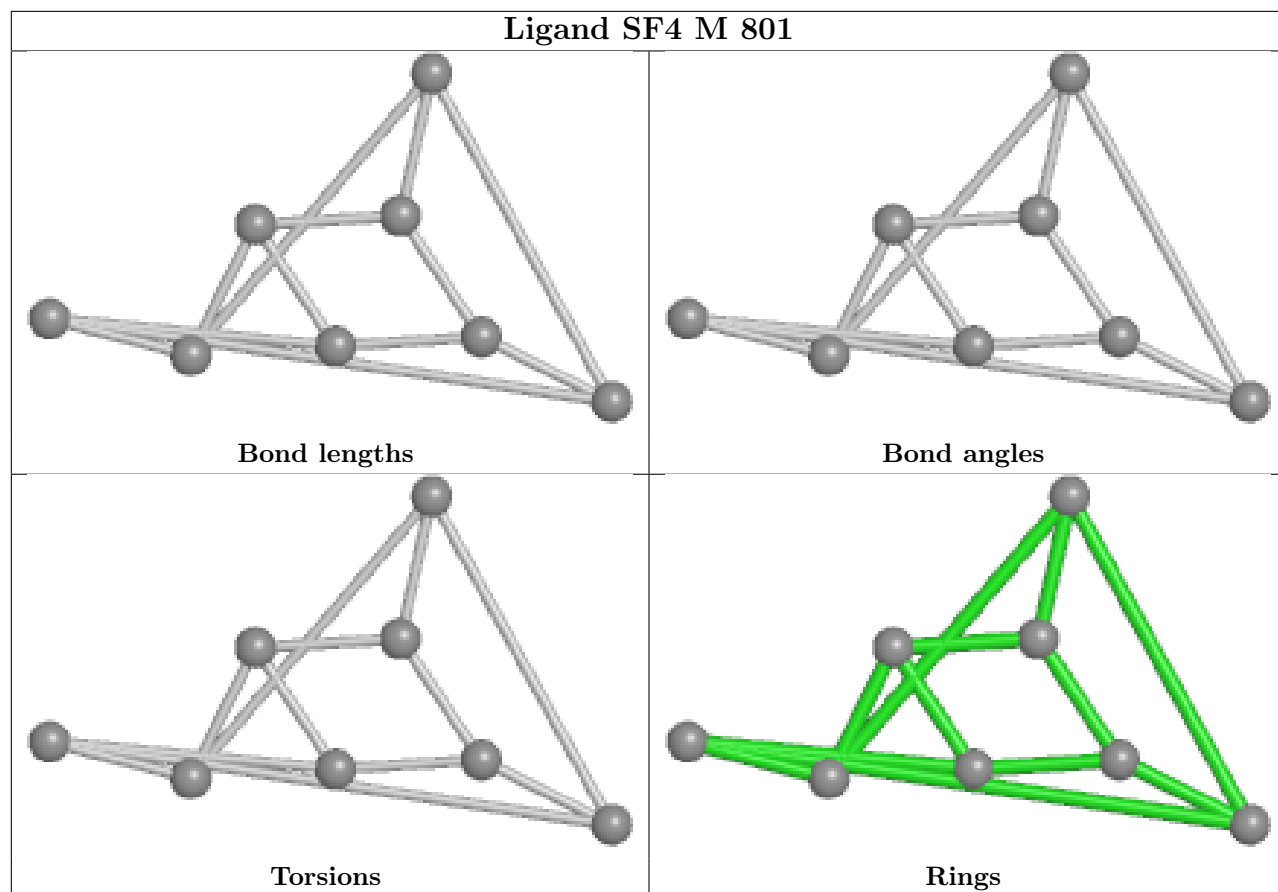




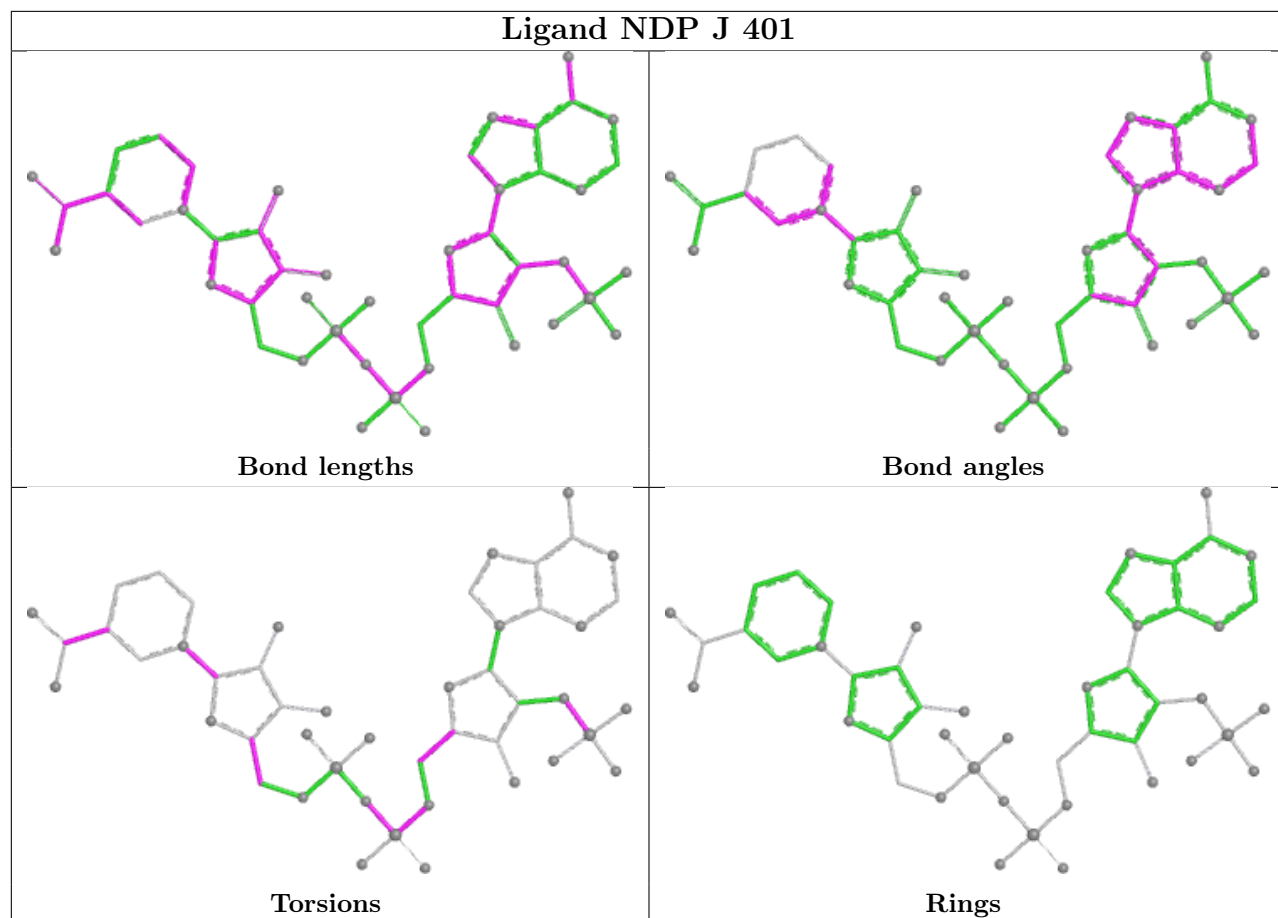




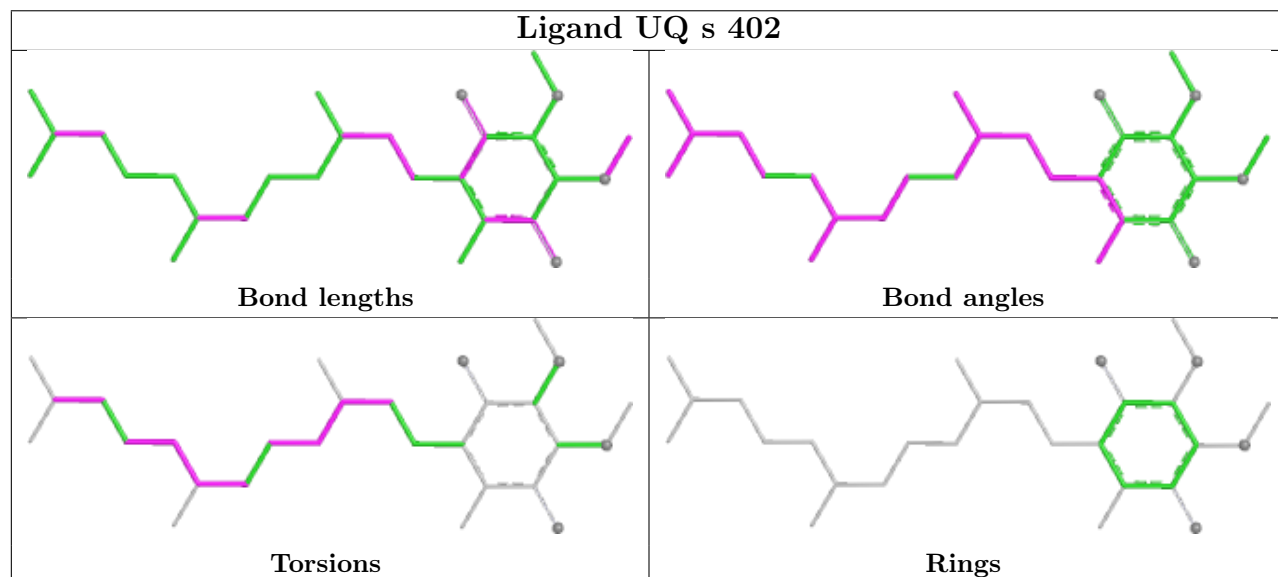


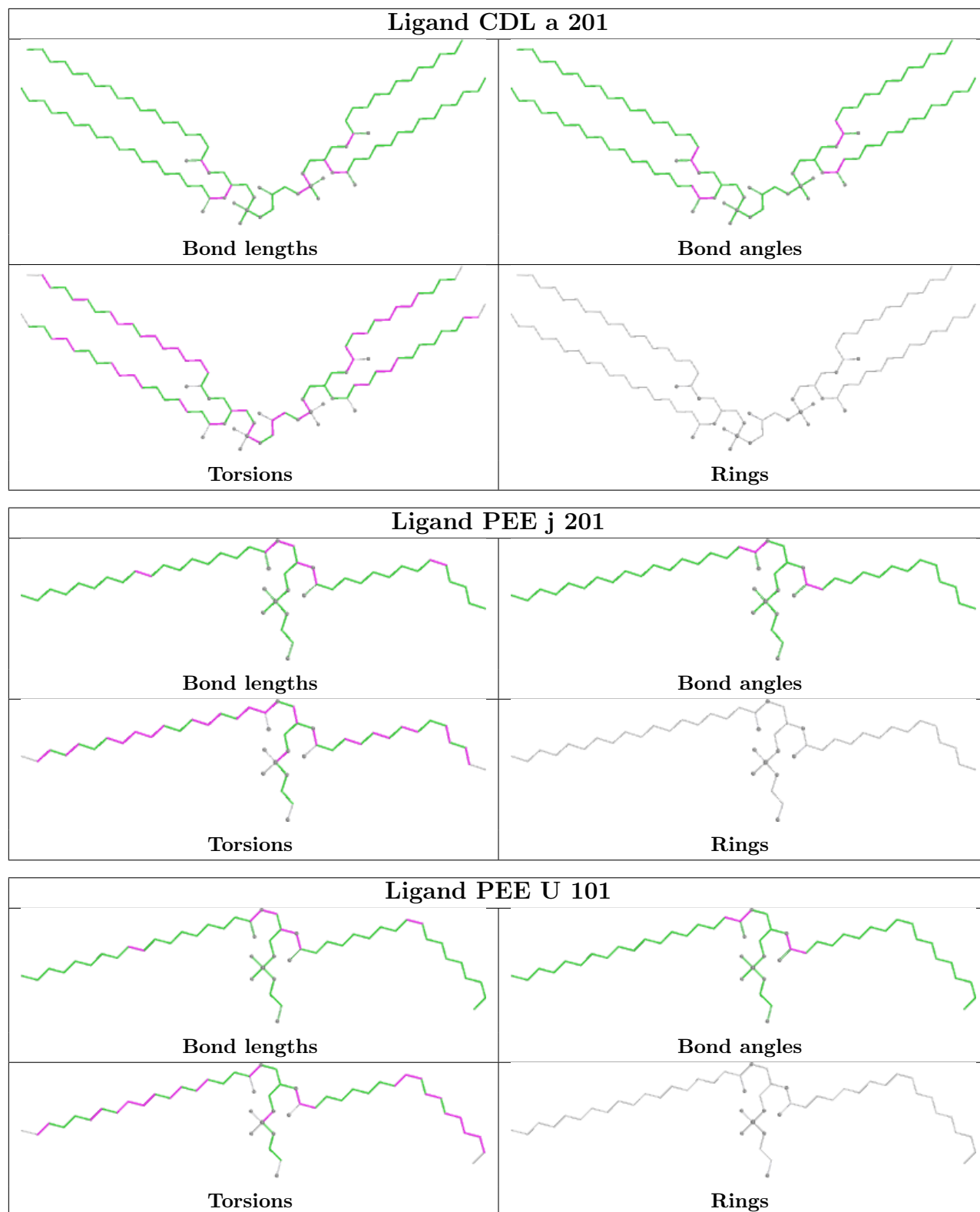


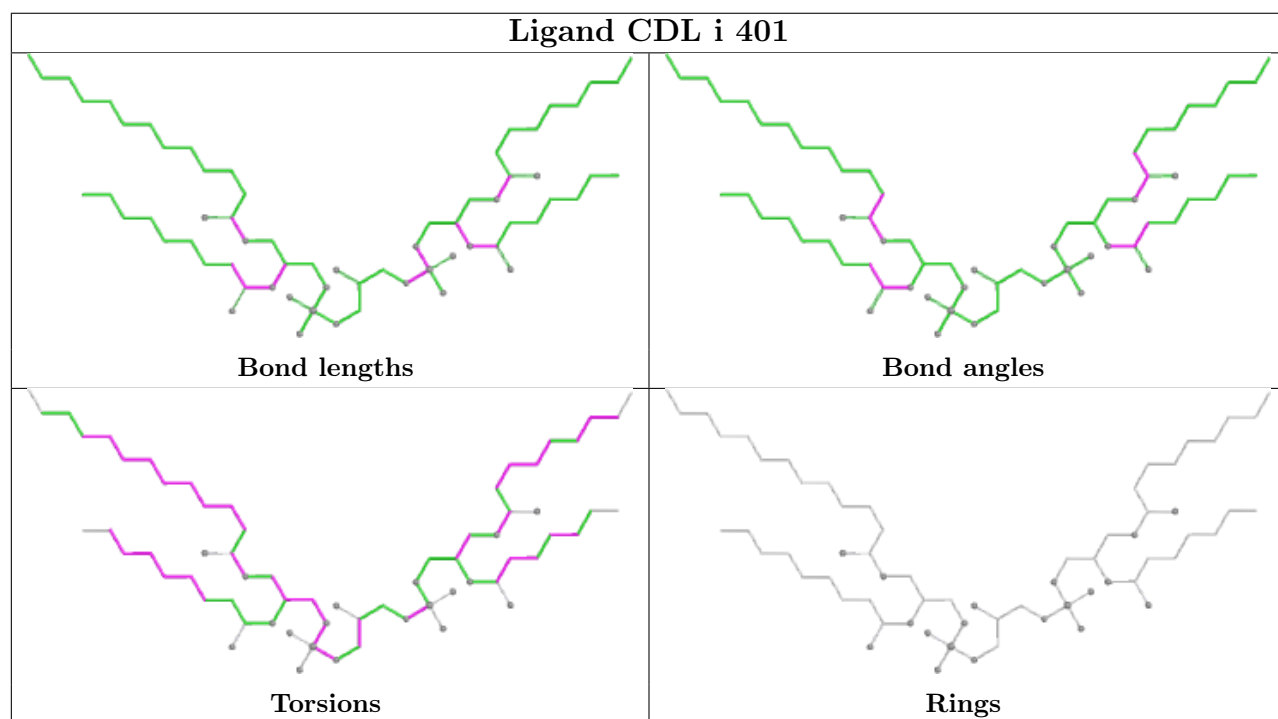
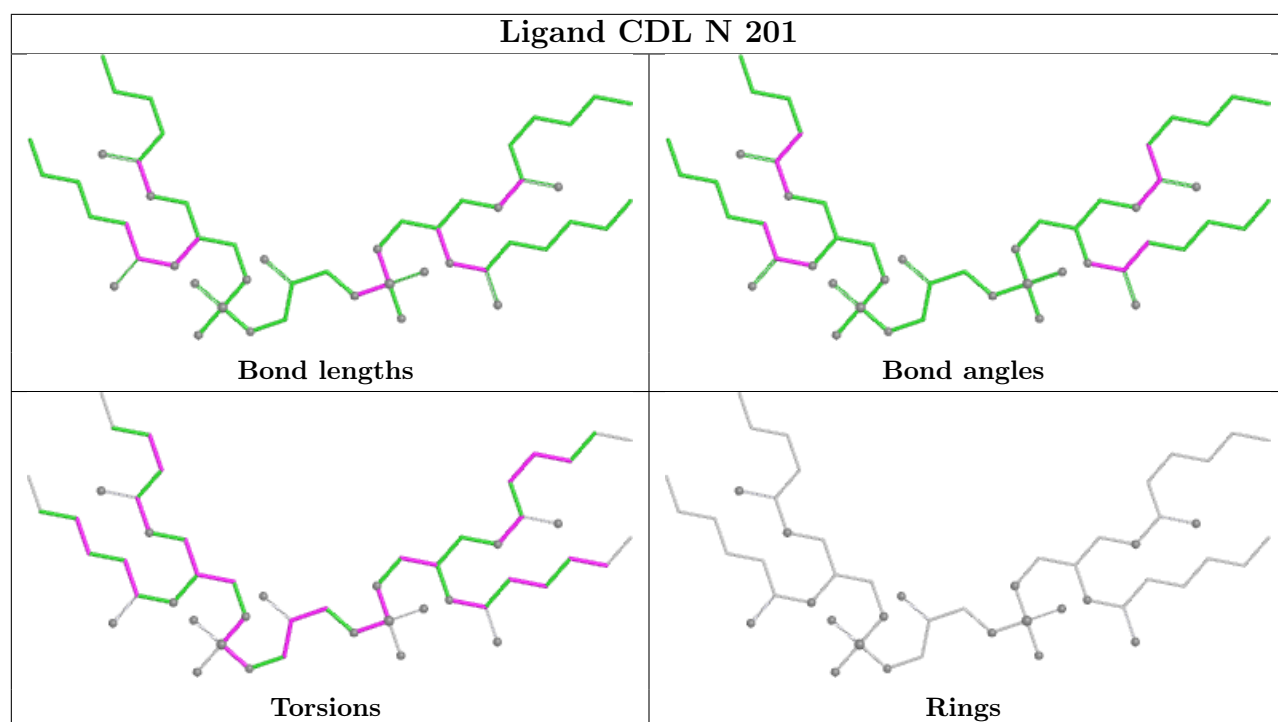
Ligand NDP J 401



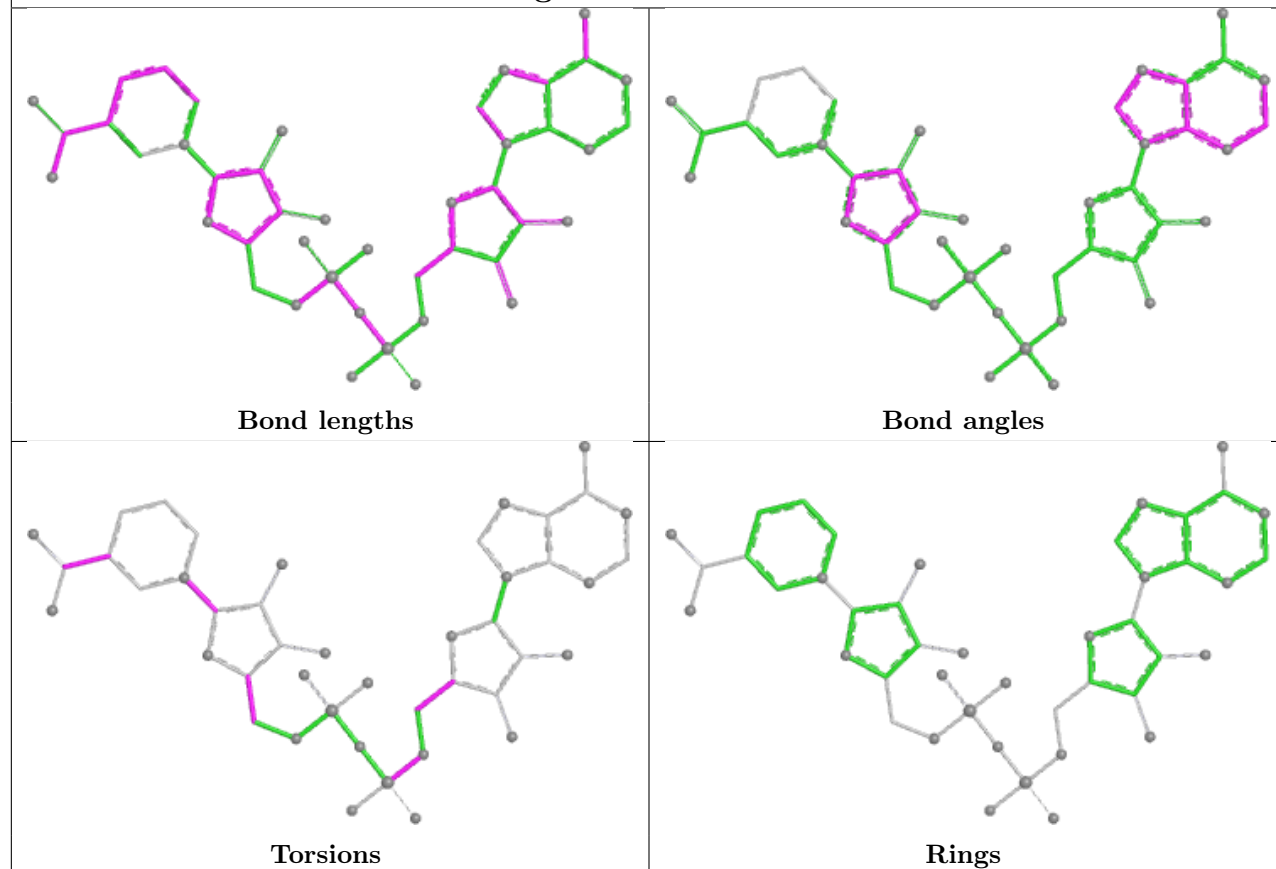
Ligand UQ s 402



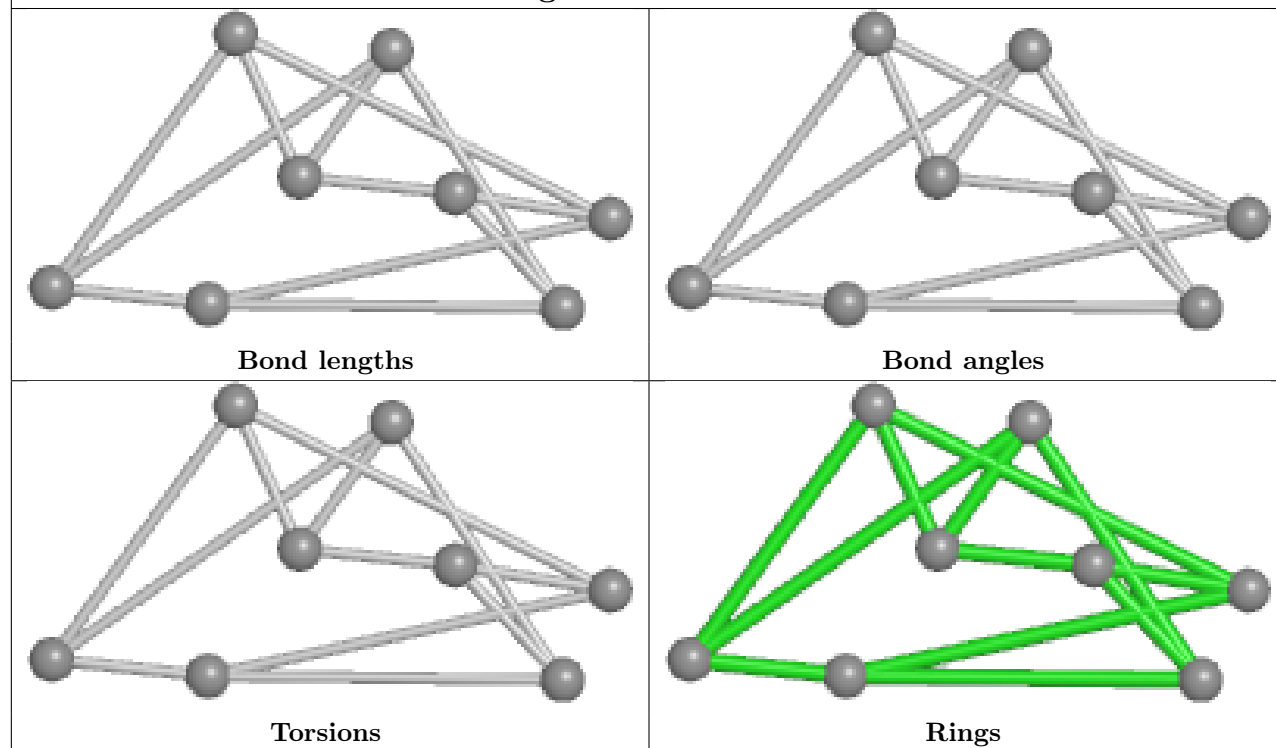


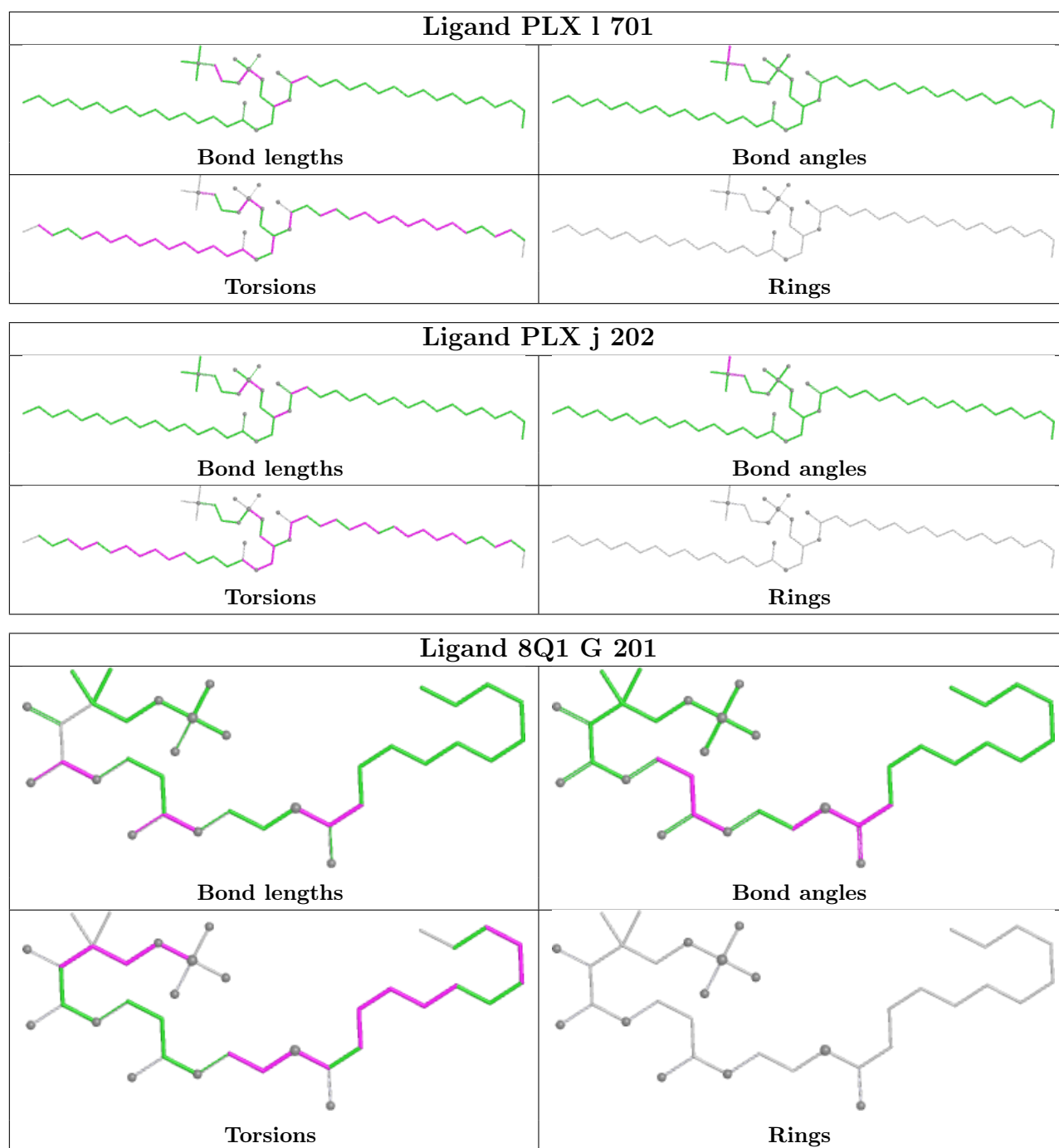


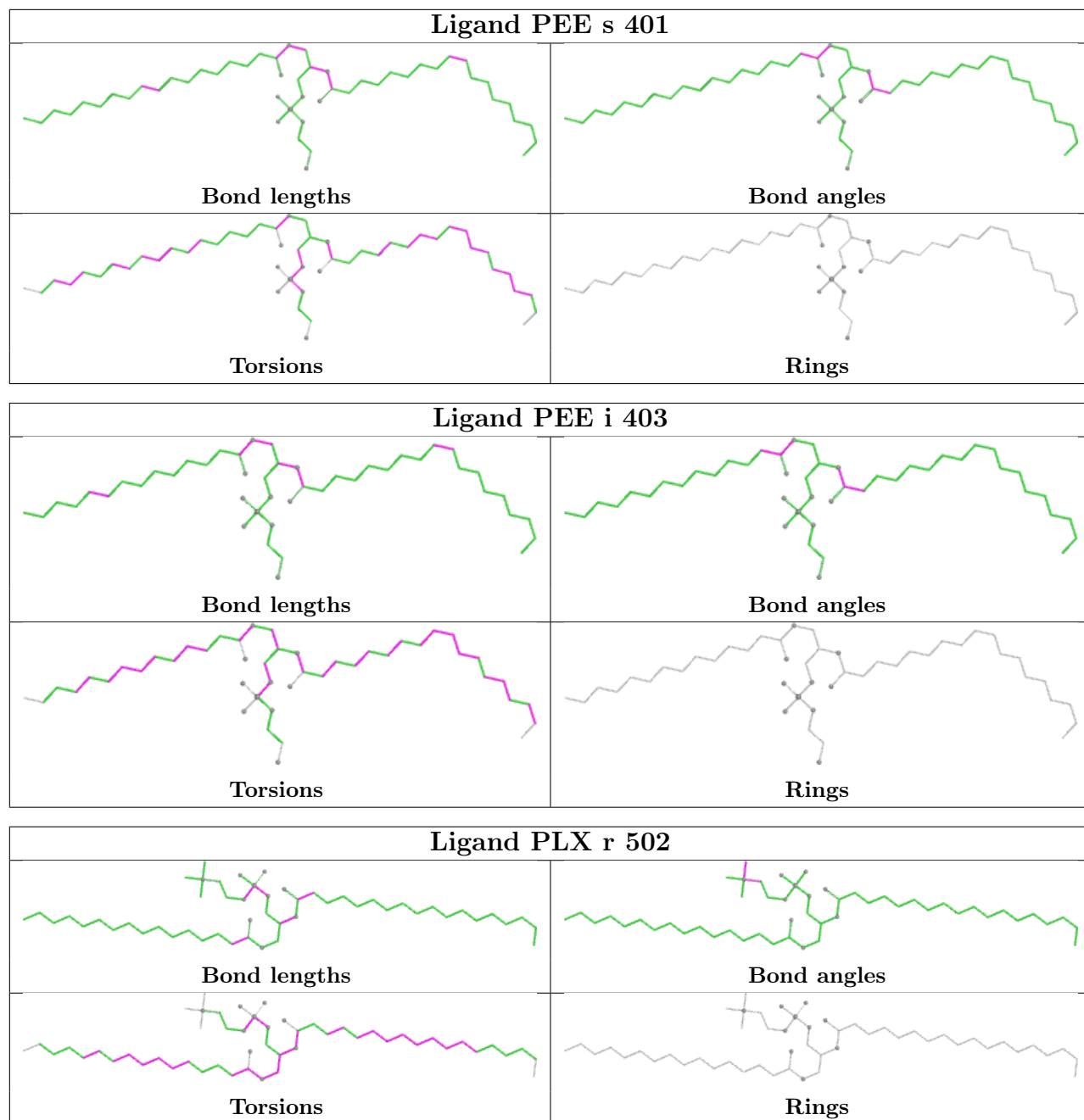
Ligand NAI A 503

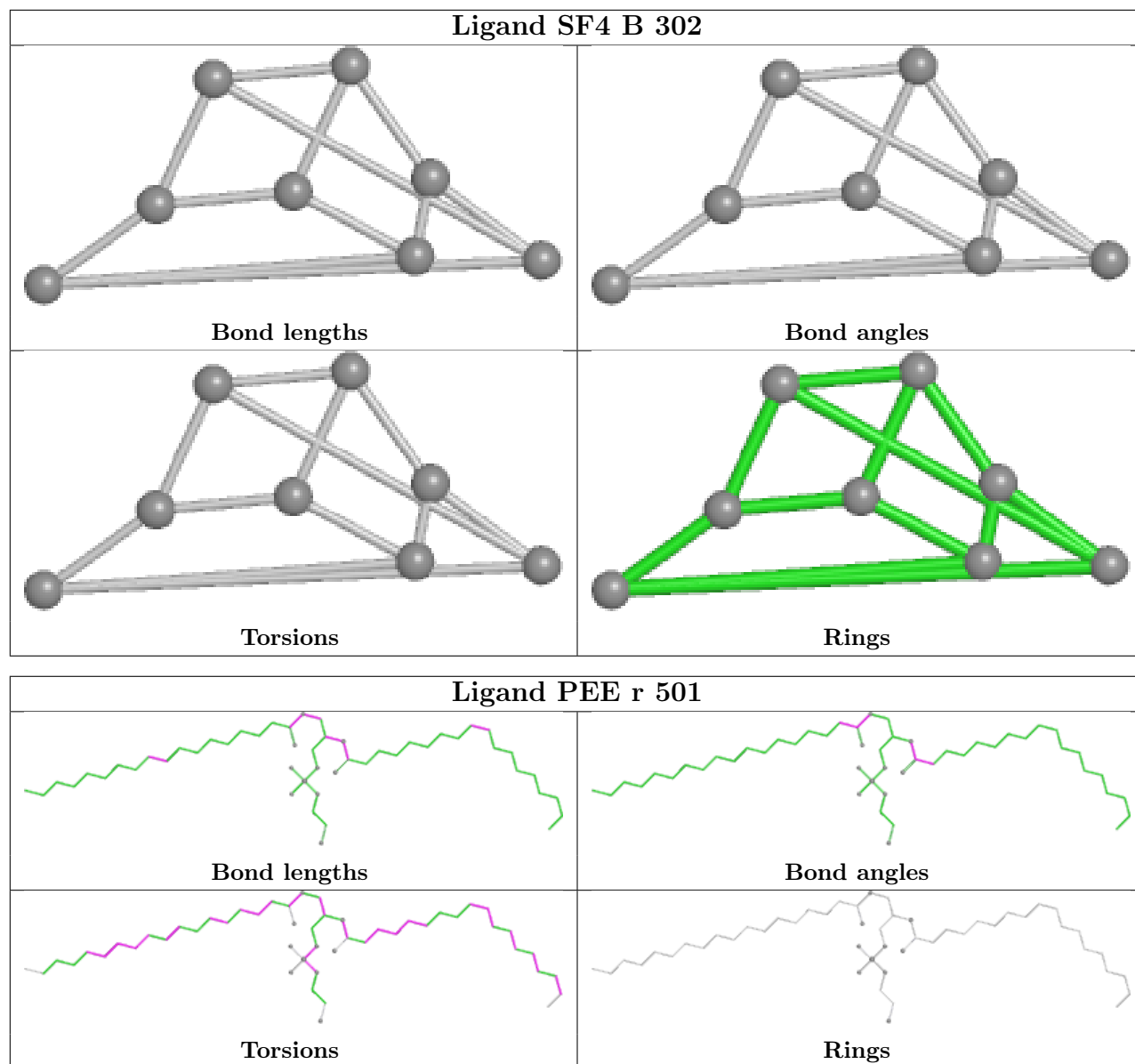


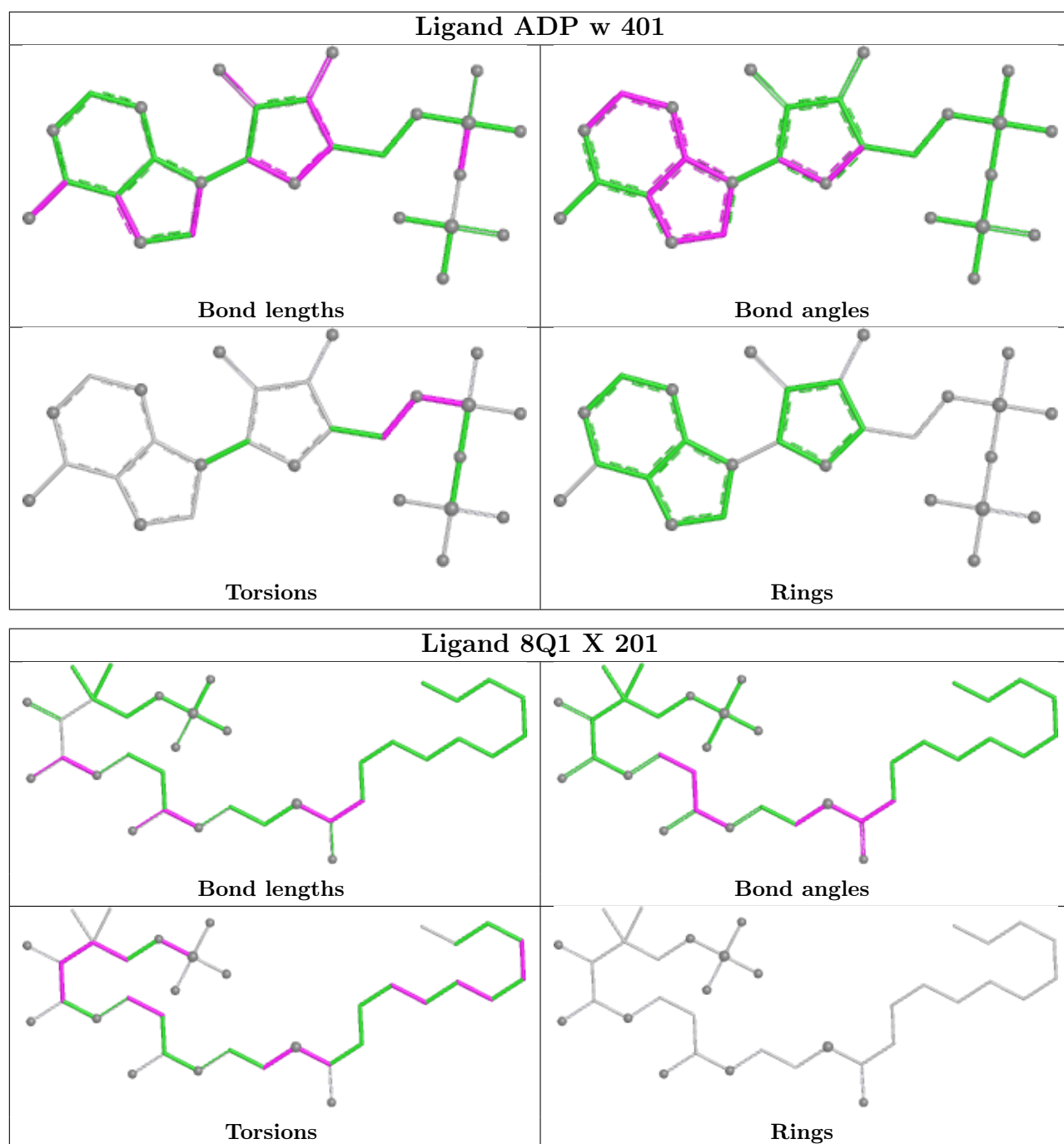
Ligand SF4 A 501

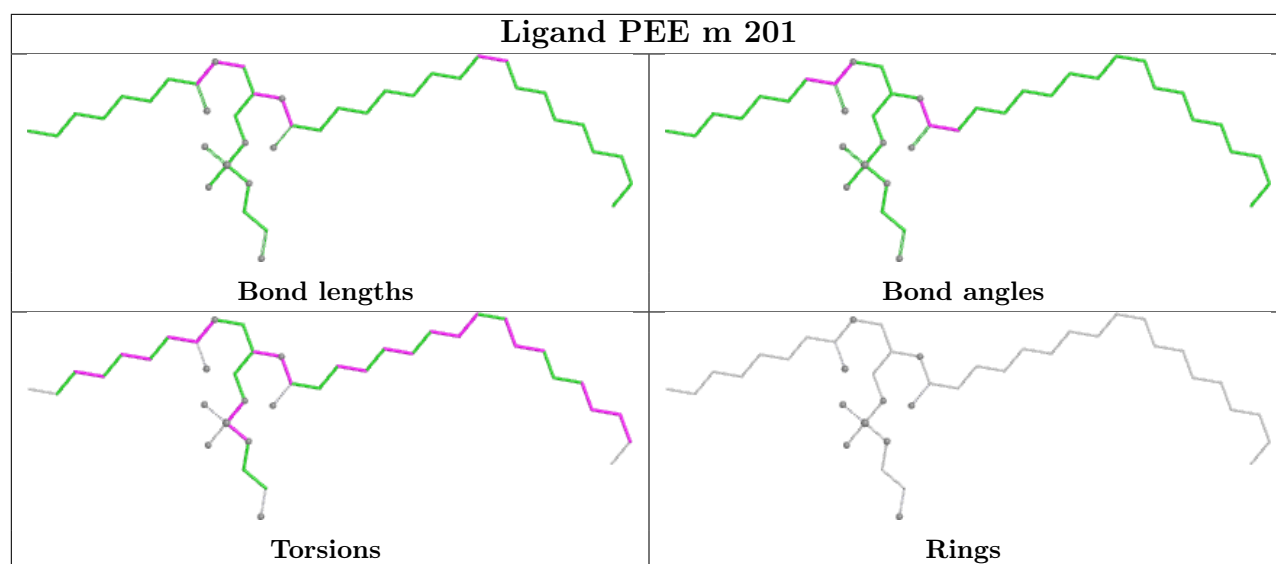












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

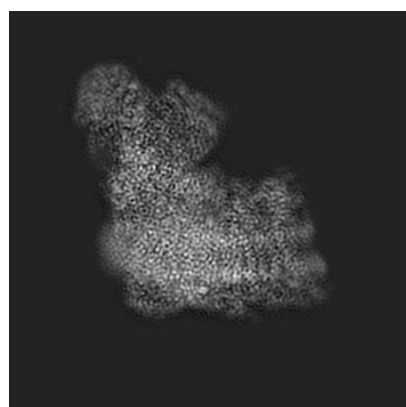
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32305. These allow visual inspection of the internal detail of the map and identification of artifacts.

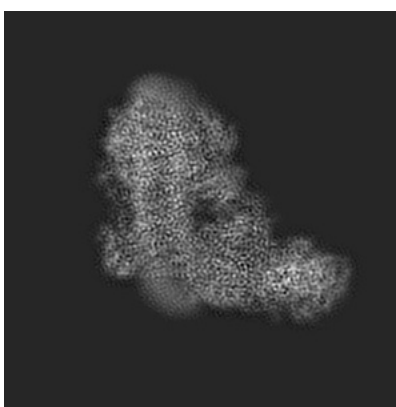
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

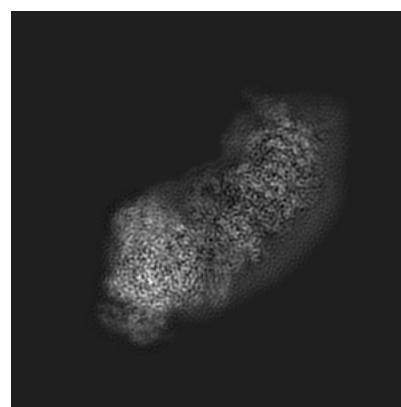
6.1.1 Primary map



X



Y

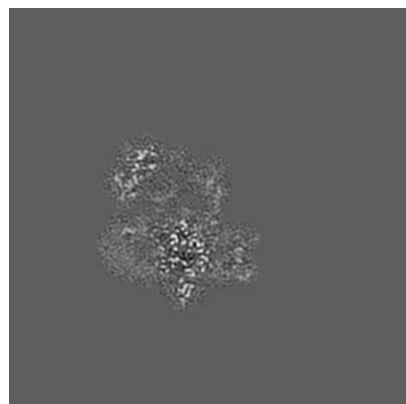


Z

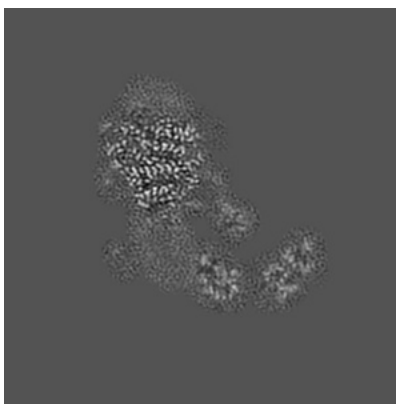
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

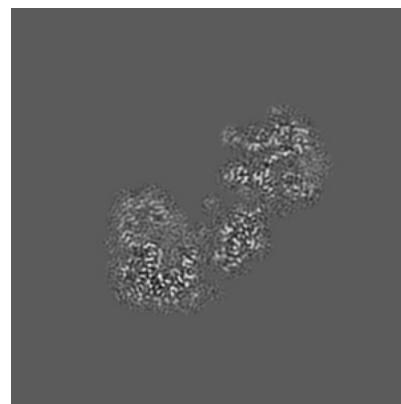
6.2.1 Primary map



X Index: 152



Y Index: 152

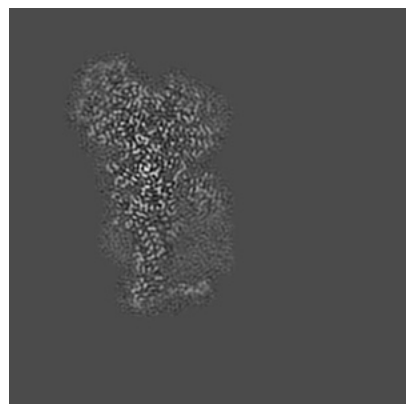


Z Index: 152

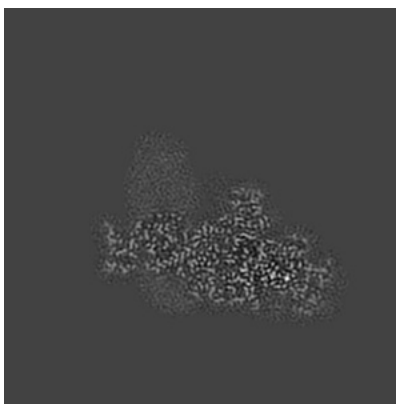
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

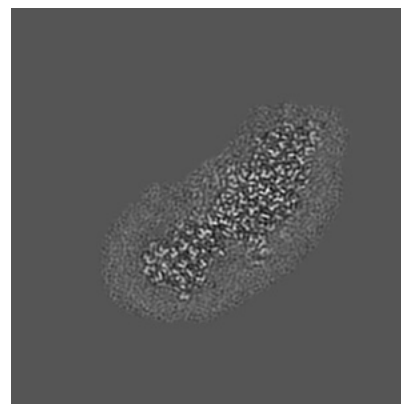
6.3.1 Primary map



X Index: 105



Y Index: 99

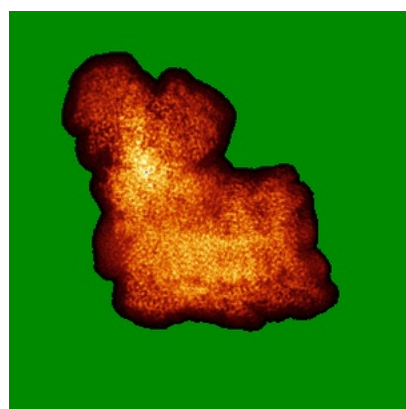


Z Index: 127

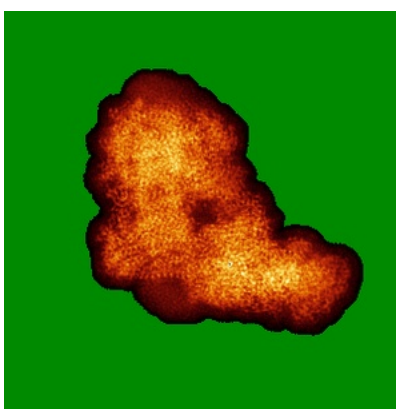
The images above show the largest variance slices of the map in three orthogonal directions.

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

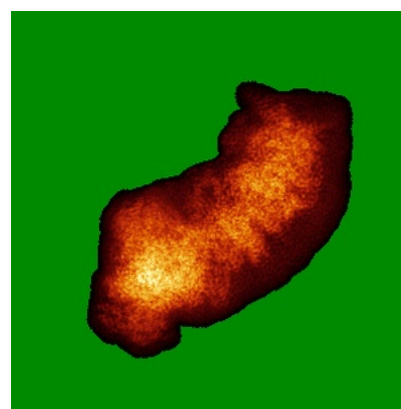
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

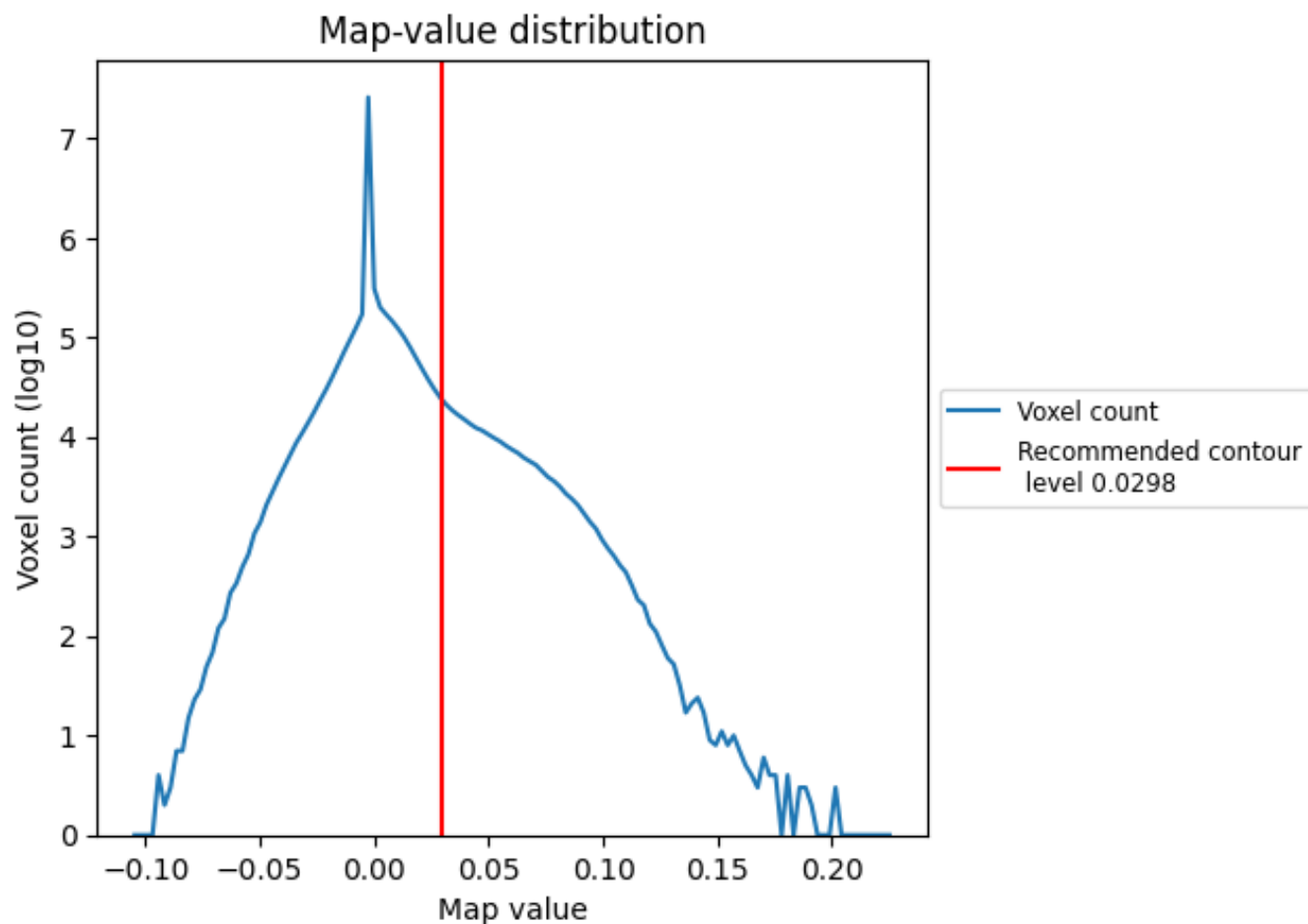
6.6 Mask visualisation

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

7 Map analysis [i](#)

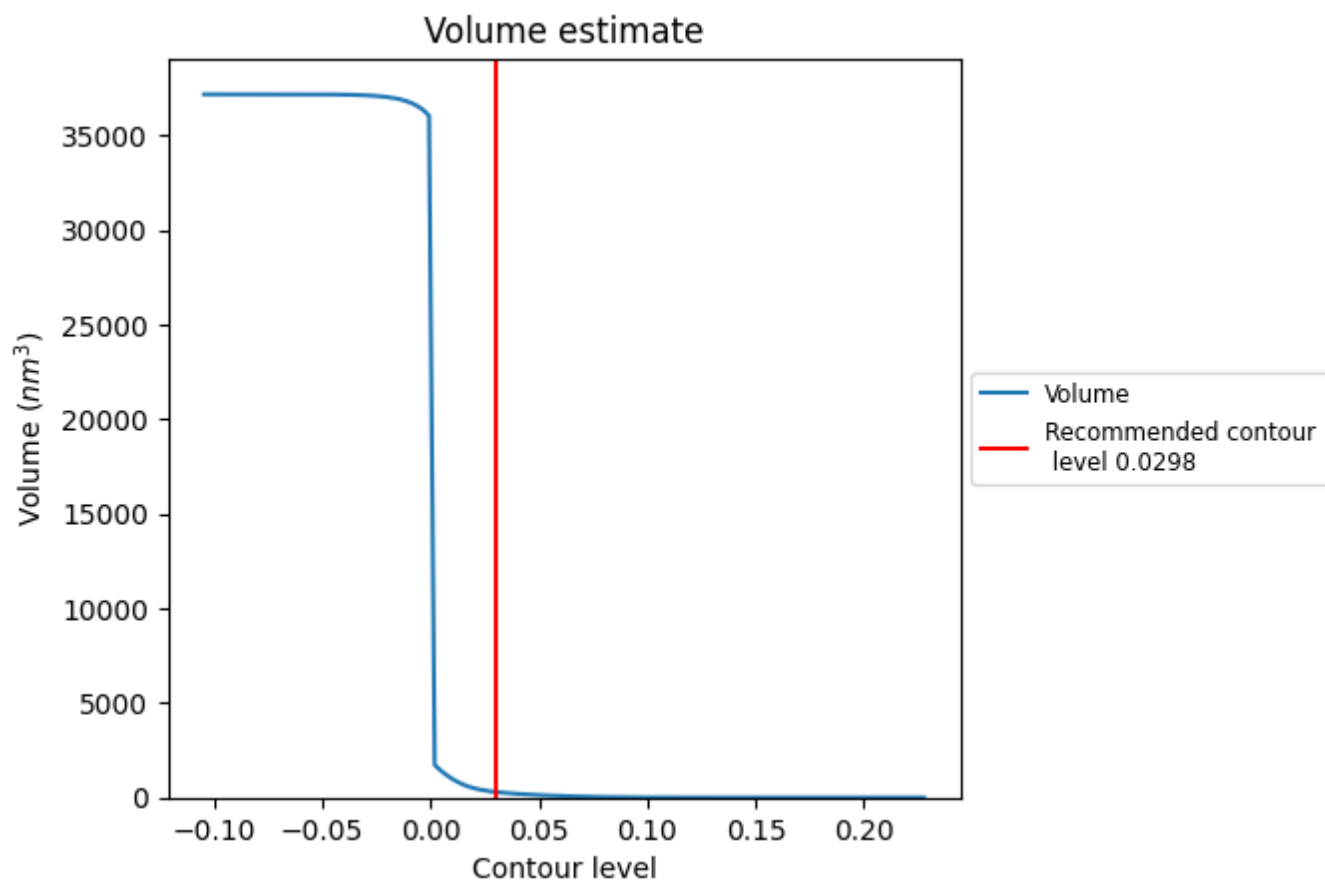
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

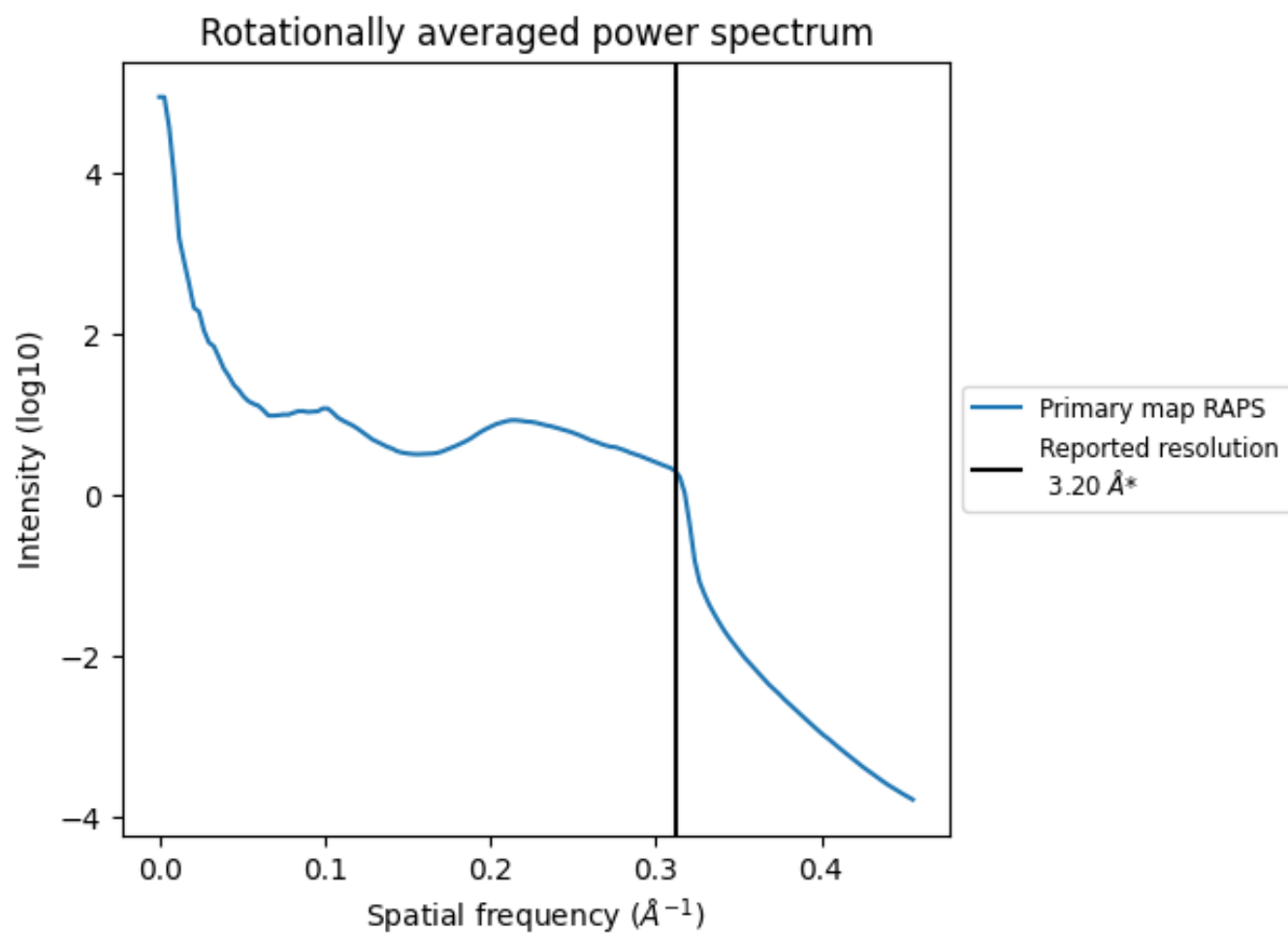
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 269 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 0.312 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

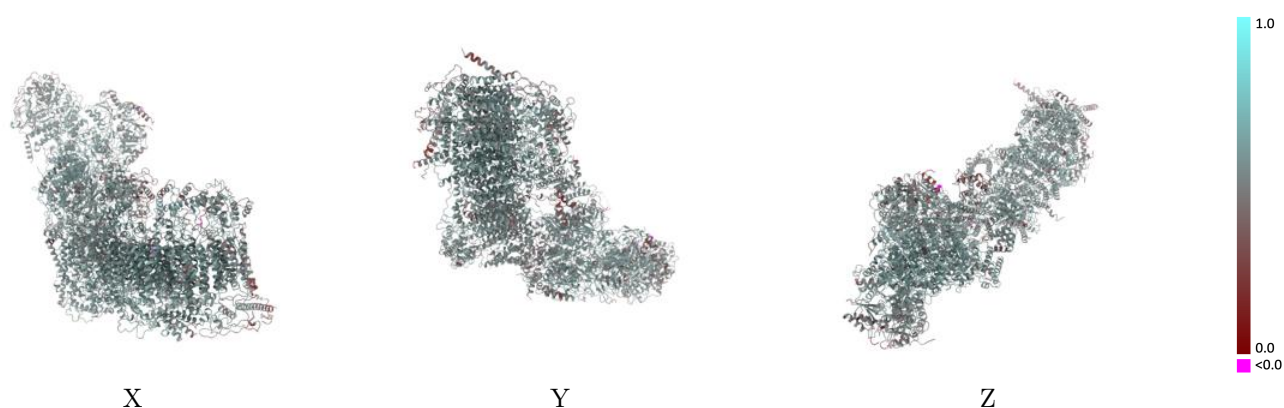
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32305 and PDB model 7W4J. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

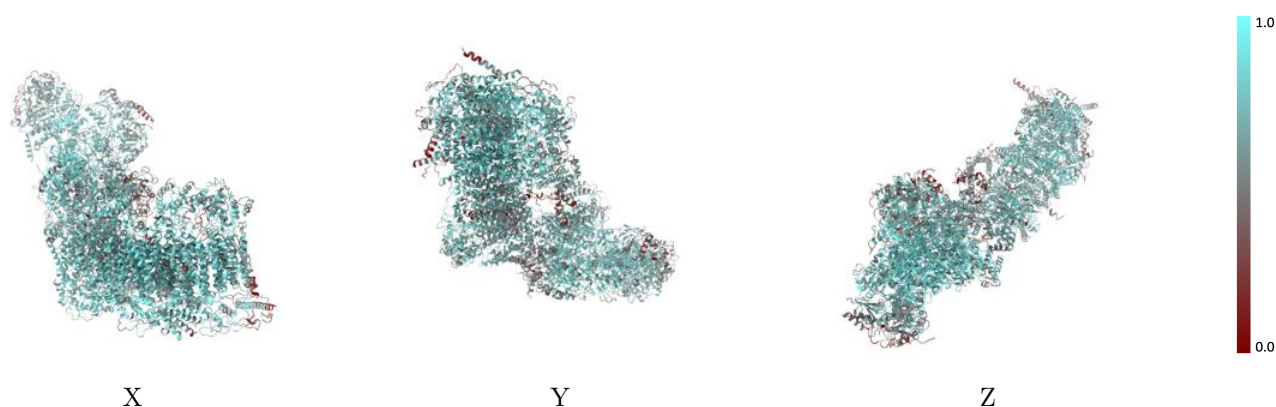
This section was not generated.

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



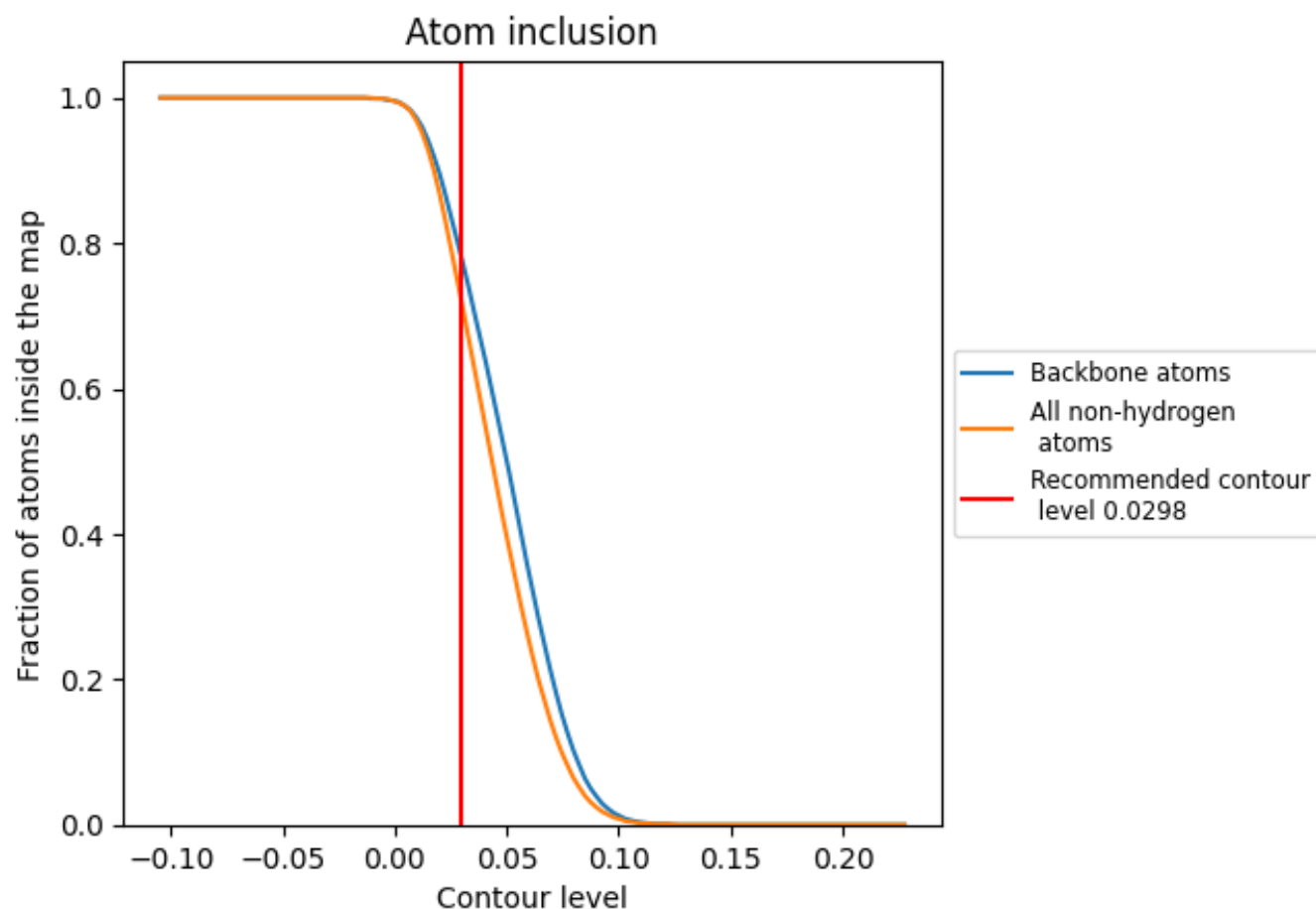
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0298).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.0298) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.5480
A	 0.6350	 0.5250
B	 0.8670	 0.5980
C	 0.8340	 0.5910
E	 0.6780	 0.5380
F	 0.5270	 0.4500
G	 0.3770	 0.3990
H	 0.6770	 0.5350
I	 0.7350	 0.5610
J	 0.6240	 0.5190
K	 0.5440	 0.4960
L	 0.7720	 0.5750
M	 0.7420	 0.5570
N	 0.7430	 0.5720
O	 0.5930	 0.5050
P	 0.8450	 0.5980
Q	 0.8270	 0.5910
S	 0.7900	 0.5640
T	 0.7230	 0.5590
U	 0.7150	 0.5310
V	 0.4780	 0.4920
W	 0.7610	 0.5580
X	 0.6450	 0.5100
Y	 0.5910	 0.4690
Z	 0.5270	 0.4350
a	 0.7440	 0.5700
b	 0.6430	 0.4970
c	 0.7370	 0.5540
d	 0.7140	 0.5400
e	 0.6690	 0.5320
f	 0.6410	 0.5130
g	 0.8000	 0.5760
h	 0.7280	 0.5560
i	 0.8060	 0.5820
j	 0.6030	 0.5210



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Chain	Atom inclusion	Q-score
k	 0.6940	 0.5560
l	 0.7560	 0.5620
m	 0.6580	 0.5320
n	 0.6100	 0.5260
o	 0.7250	 0.5580
p	 0.7290	 0.5370
r	 0.8130	 0.5820
s	 0.7710	 0.5590
u	 0.7460	 0.5510
v	 0.5940	 0.4880
w	 0.6840	 0.5340