



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:42 PM UTC

PDB ID : 7R43 / pdb_00007r43
EMDB ID : EMD-14261
Title : Bovine complex I in the presence of IM1761092, active class iii (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

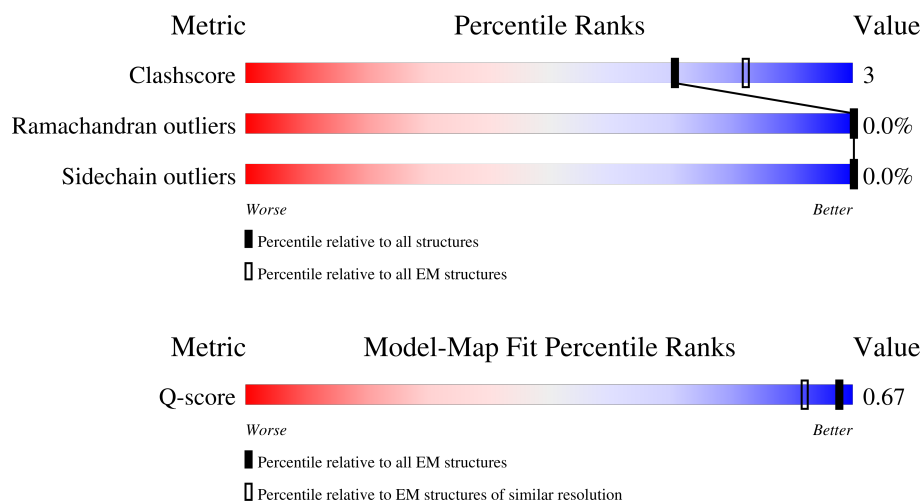
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



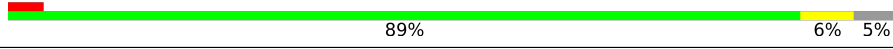
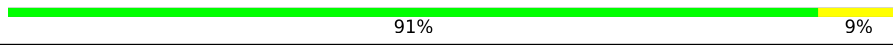
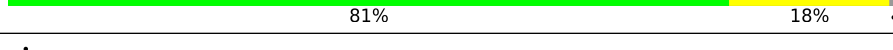
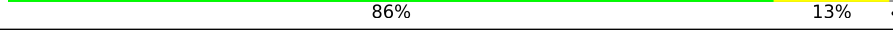
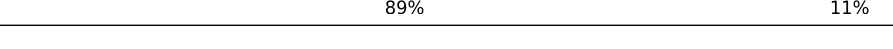
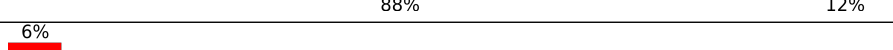
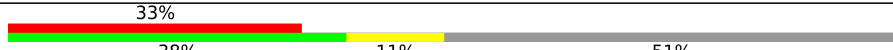
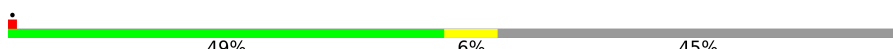
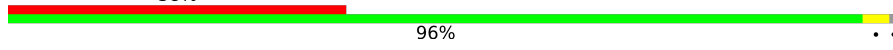
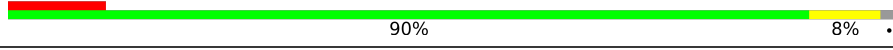
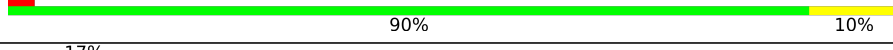
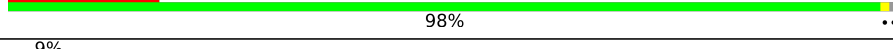
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	115	
2	B	216	
3	C	266	
4	D	463	

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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 68334 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	154	Total	C	N	O	S	0	0
			1230	786	220	210	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	431	Total	C	N	O	S	0	0
			3319	2091	593	615	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			739	483	111	130	15		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	601	Total	C	N	O	S	0	0
			4756	3166	729	818	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	341	Total	C	N	O	S	0	0
			2747	1777	486	479	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			693	447	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	112	Total	C	N	O	S	0	0
			934	613	157	161	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			819	518	156	139	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			451	296	79	75	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total	C	N	O	S	0	0
			824	529	137	154	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	106	Total	C	N	O	S	0	0
			912	600	157	154	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			580	381	95	103	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	114	Total	C	N	O	S	0	0
			960	617	168	175			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1443	904	266	265	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

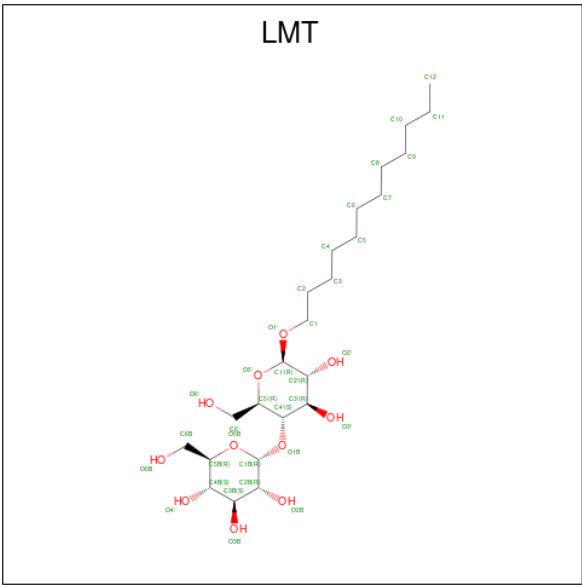
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



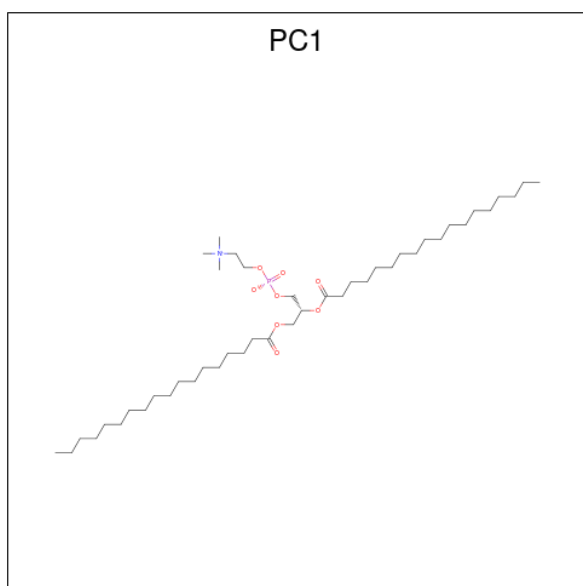
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	b	1	Total	C	O	0
			35	24	11	
45	f	1	Total	C	O	0
			35	24	11	

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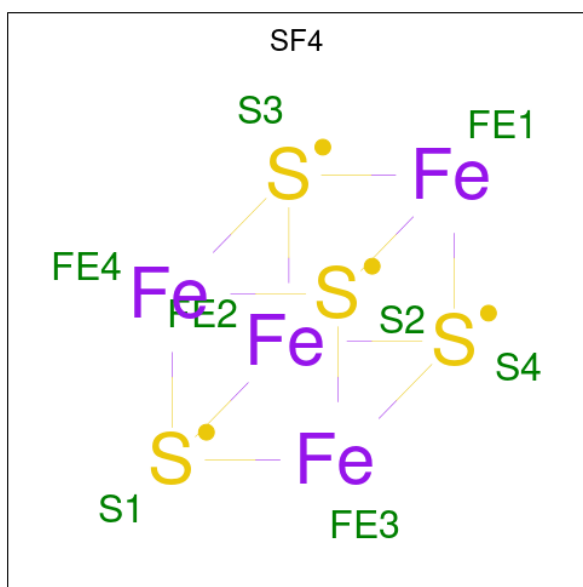
Mol	Chain	Residues	Atoms			AltConf
45	h	1	Total	C	O	0
			35	24	11	
45	j	1	Total	C	O	0
			35	24	11	
45	l	1	Total	C	O	0
			35	24	11	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



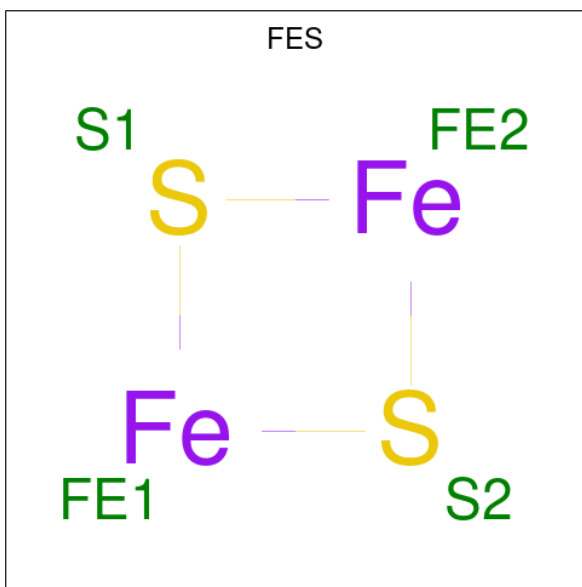
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			21	11	1	8	1	
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	P	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



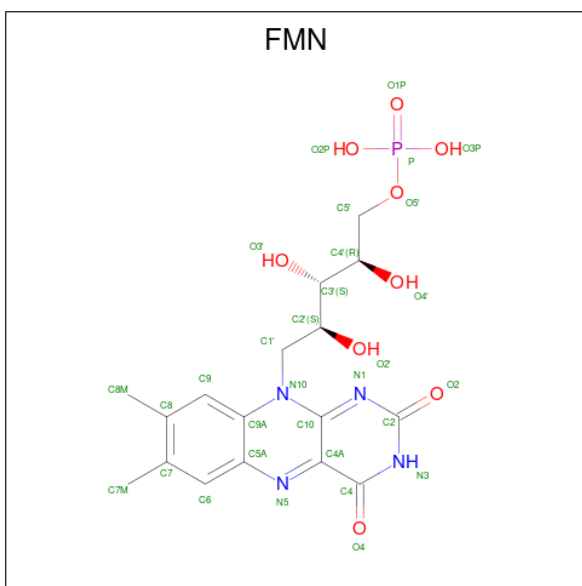
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total 4	Fe 2	S 2	0
48	G	1	Total 4	Fe 2	S 2	0

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

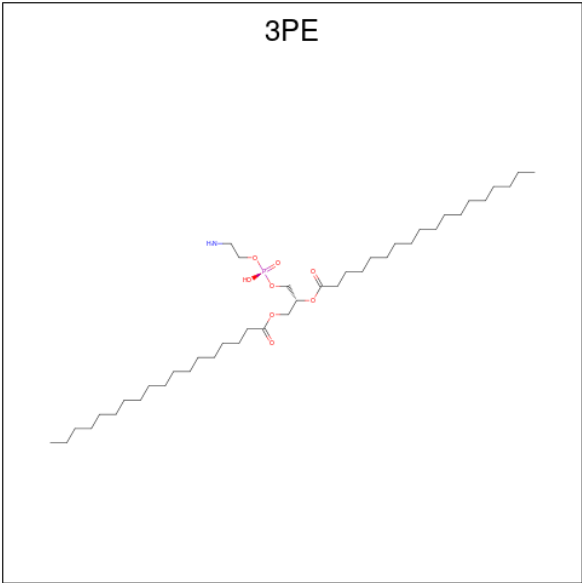


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



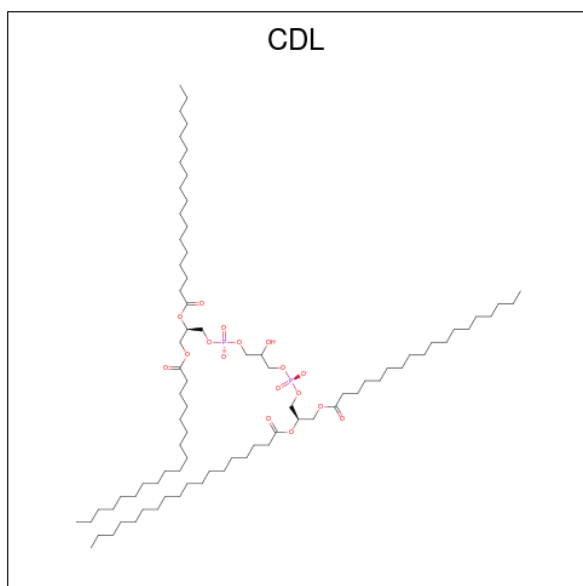
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
51	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
51	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

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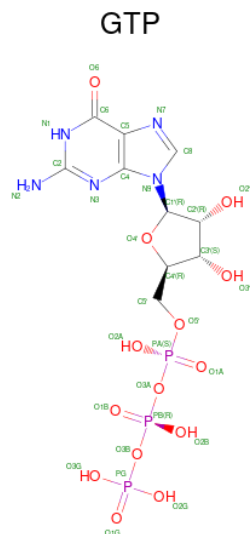
Mol	Chain	Residues	Atoms					AltConf
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			62	43	17	2	
52	K	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

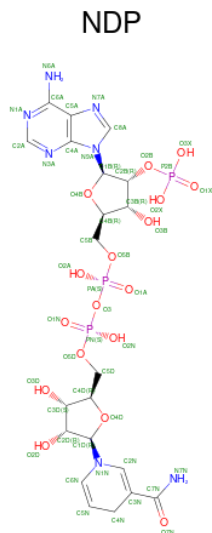


Mol	Chain	Residues	Atoms					AltConf
53	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

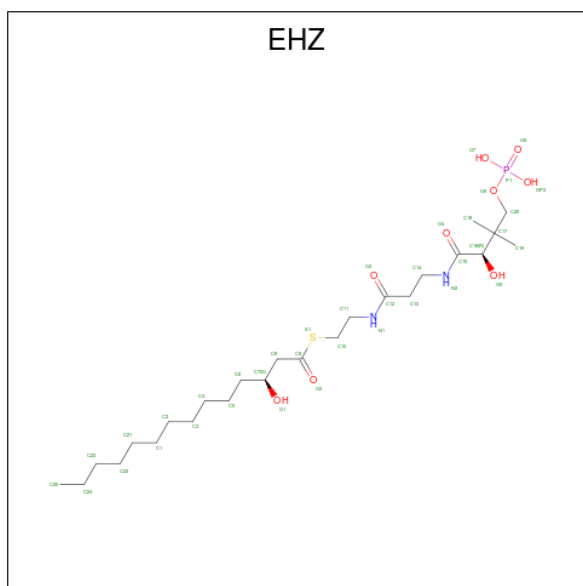


Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

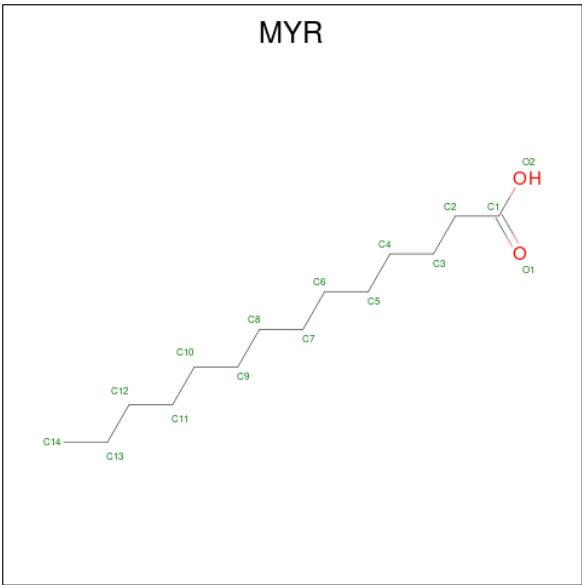
Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



Mol	Chain	Residues	Atoms						AltConf
57	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			AltConf
58	o	1	Total	C	O	0
			15	14	1	

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	A	12	Total	O	0
			12	12	
59	B	48	Total	O	0
			48	48	
59	C	66	Total	O	0
			66	66	
59	D	115	Total	O	0
			115	115	
59	E	5	Total	O	0
			5	5	
59	F	33	Total	O	0
			33	33	
59	G	135	Total	O	0
			135	135	
59	H	43	Total	O	0
			43	43	
59	I	79	Total	O	0
			79	79	
59	J	10	Total	O	0
			10	10	
59	K	9	Total	O	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
59	L	16	Total 16	O 16	0
59	M	28	Total 28	O 28	0
59	N	28	Total 28	O 28	0
59	O	13	Total 13	O 13	0
59	P	40	Total 40	O 40	0
59	Q	45	Total 45	O 45	0
59	R	19	Total 19	O 19	0
59	S	2	Total 2	O 2	0
59	V	6	Total 6	O 6	0
59	W	8	Total 8	O 8	0
59	X	13	Total 13	O 13	0
59	Y	1	Total 1	O 1	0
59	Z	11	Total 11	O 11	0
59	a	4	Total 4	O 4	0
59	b	4	Total 4	O 4	0
59	d	8	Total 8	O 8	0
59	e	5	Total 5	O 5	0
59	f	1	Total 1	O 1	0
59	g	1	Total 1	O 1	0
59	h	11	Total 11	O 11	0
59	j	2	Total 2	O 2	0

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Mol	Chain	Residues	Atoms		AltConf
59	l	8	Total 8	O 8	0
59	m	2	Total 2	O 2	0
59	n	5	Total 5	O 5	0
59	o	2	Total 2	O 2	0
59	p	9	Total 9	O 9	0
59	q	18	Total 18	O 18	0
59	r	20	Total 20	O 20	0

3 Residue-property plots [i](#)

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.

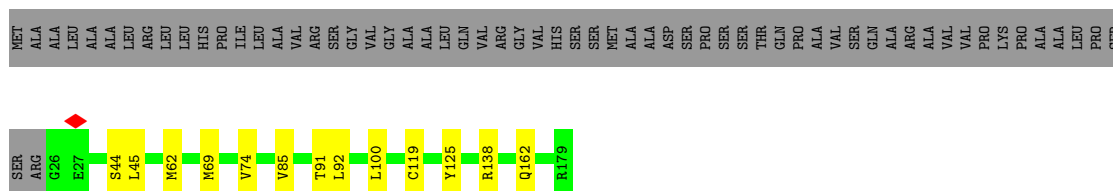
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



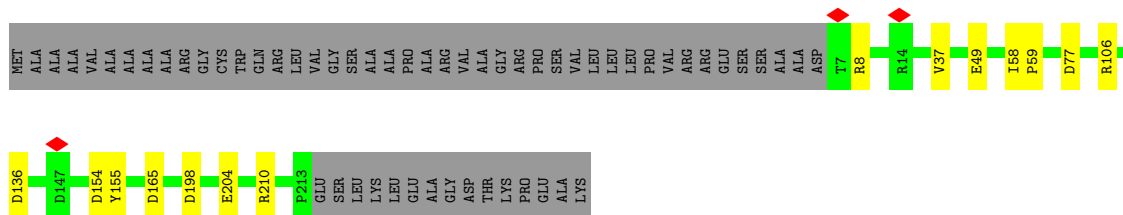
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



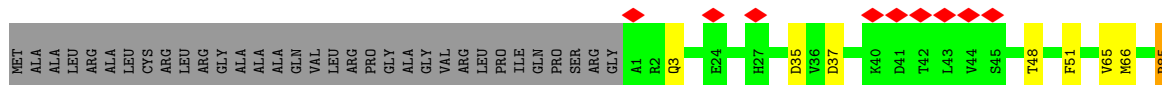
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



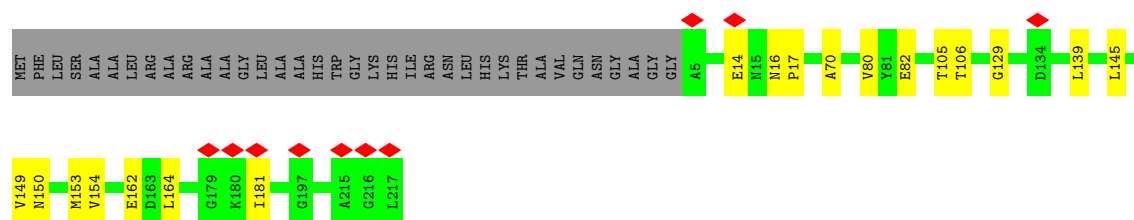
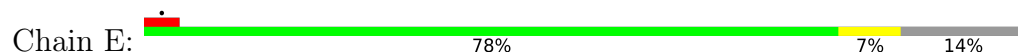
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

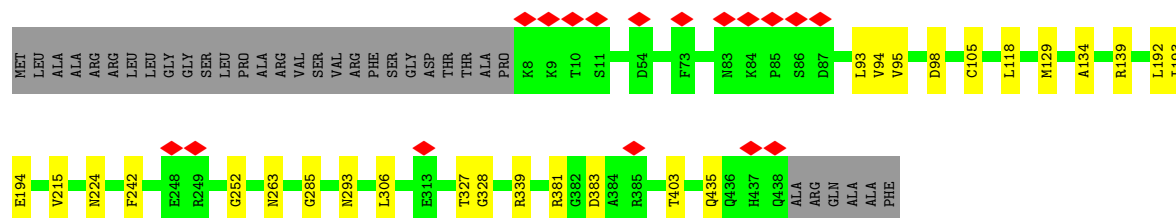
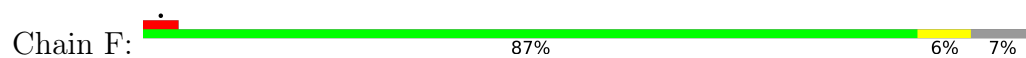




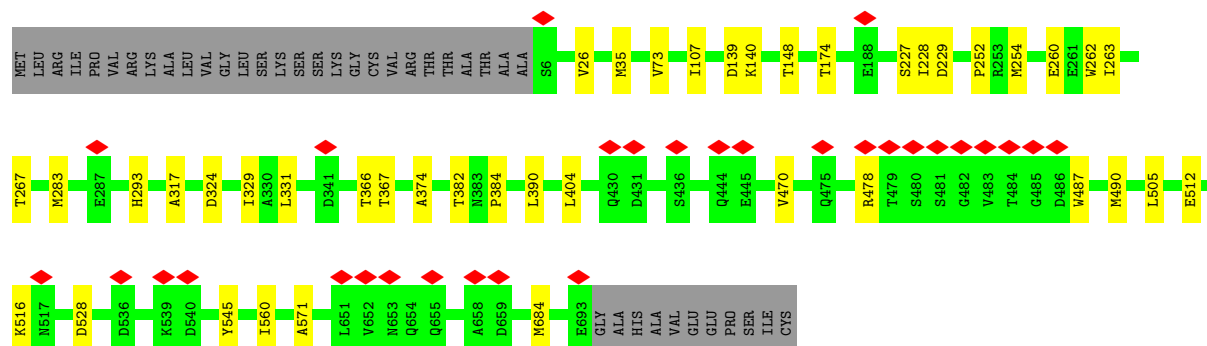
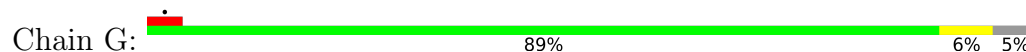
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



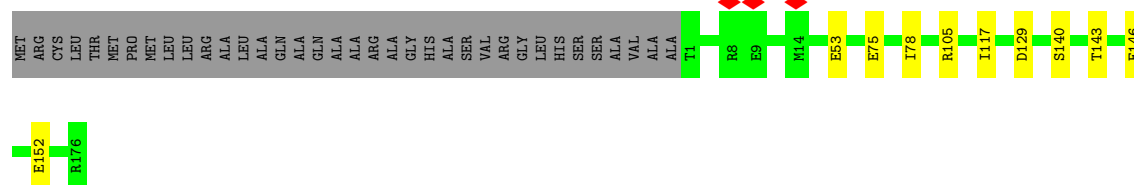
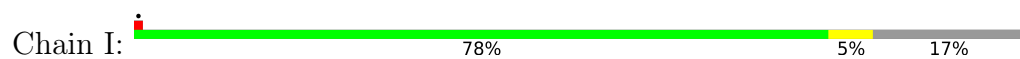
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



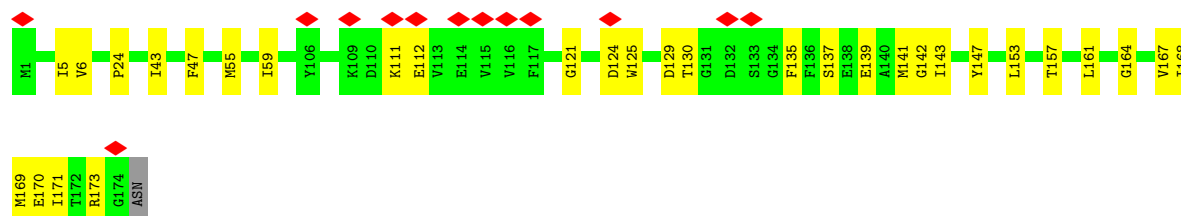
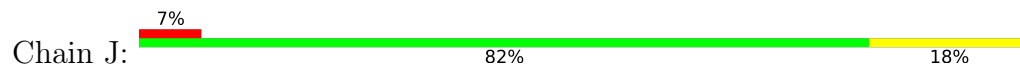
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



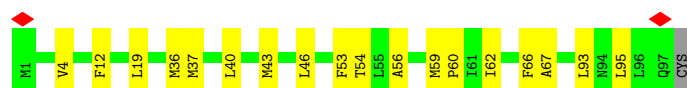
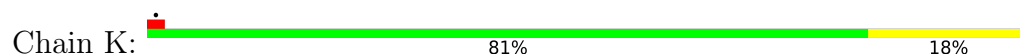
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



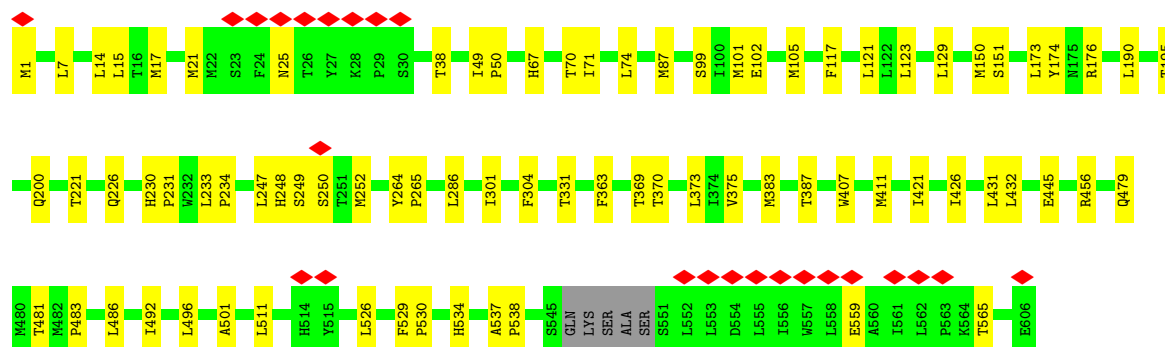
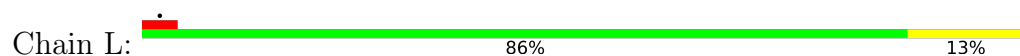
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



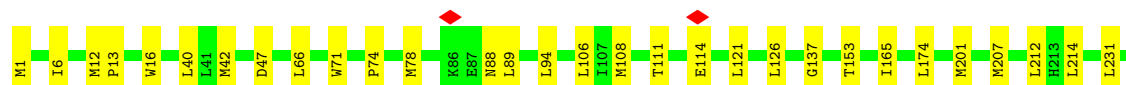
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

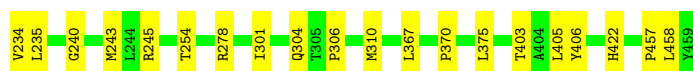


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4





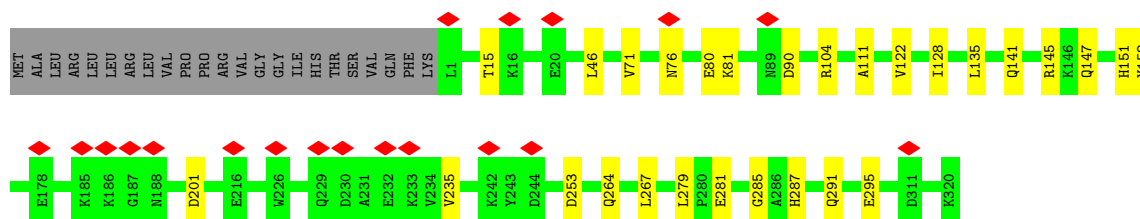
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 88% 12%



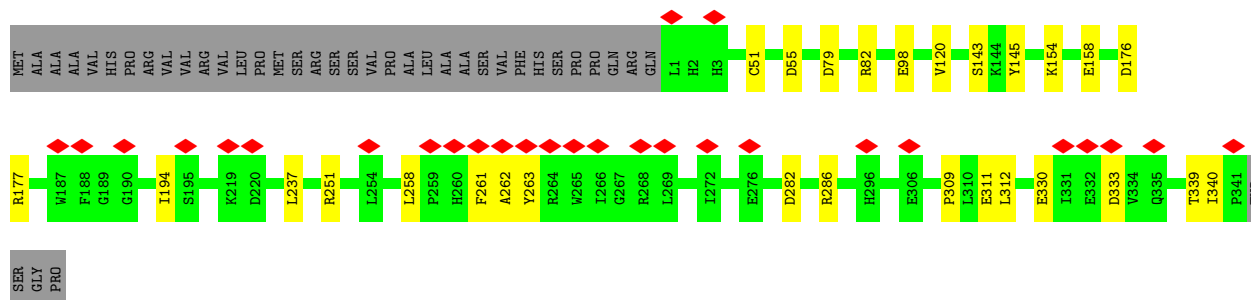
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 6% 85% 8% 7%



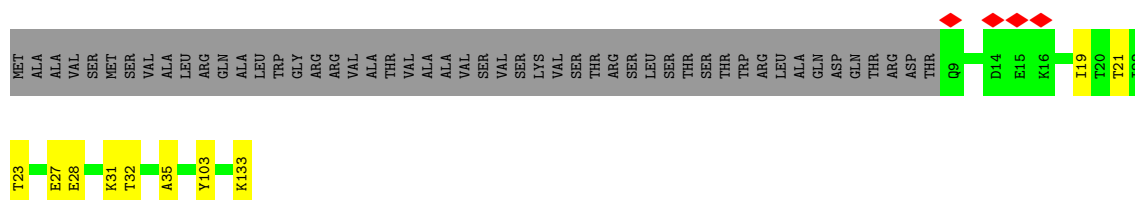
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 7% 82% 7% 10%

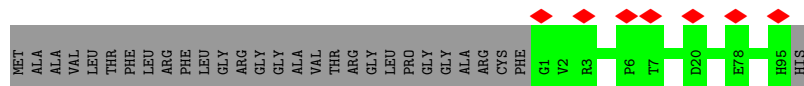
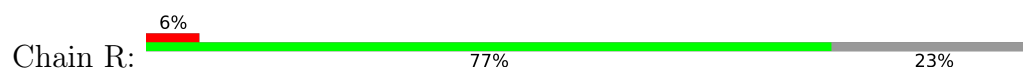


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

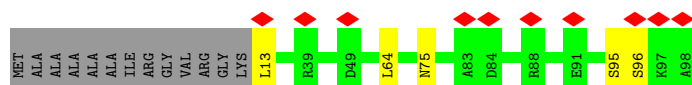
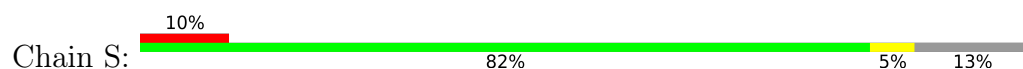
Chain Q: 66% 6% 29%



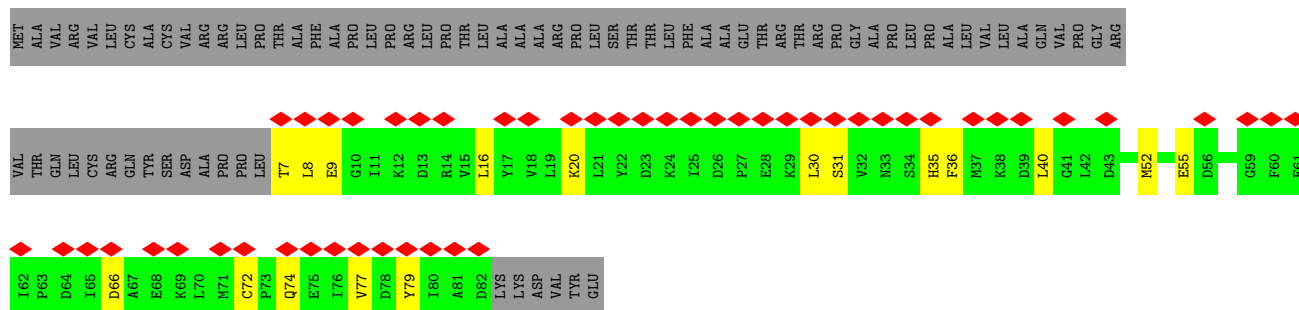
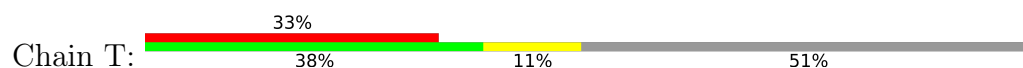
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



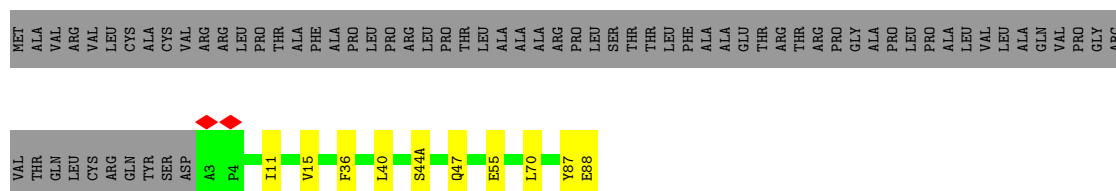
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein, mitochondrial



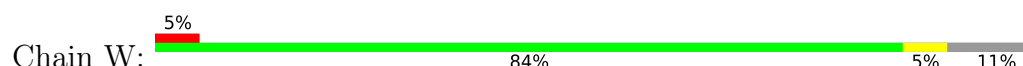
- Molecule 20: Acyl carrier protein, mitochondrial

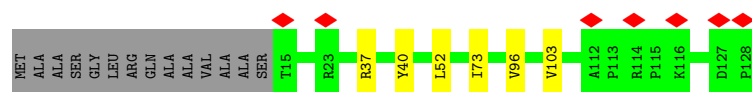


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

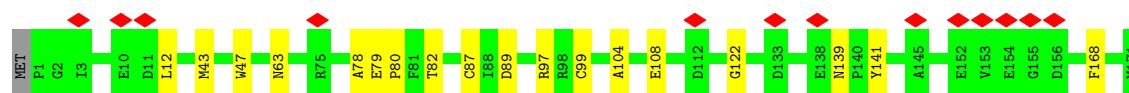
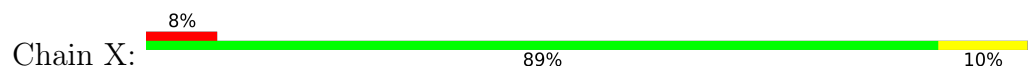


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

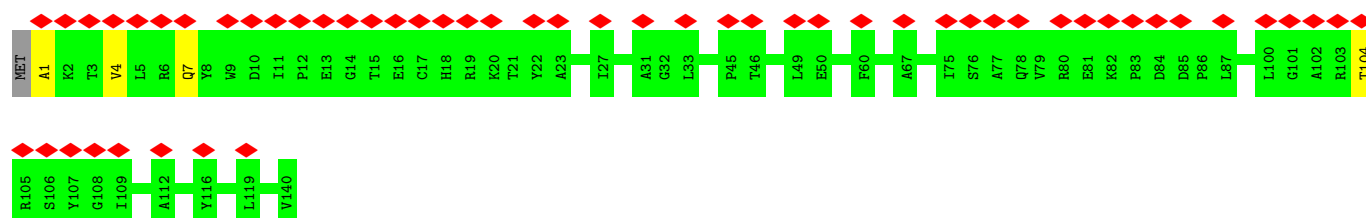
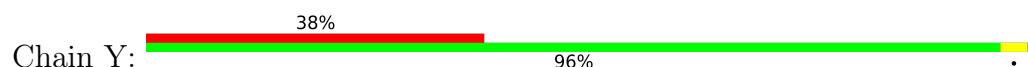




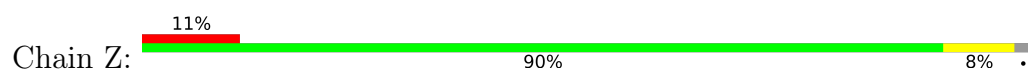
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



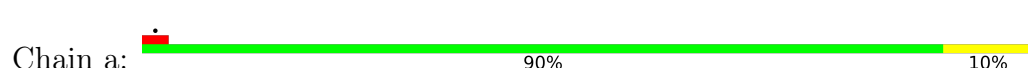
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



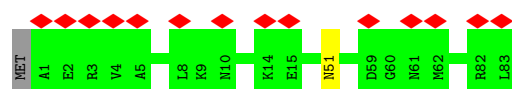
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

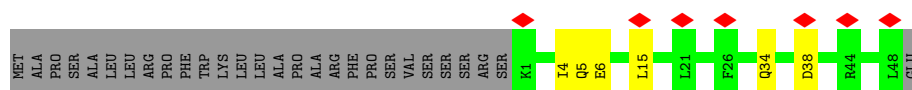


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

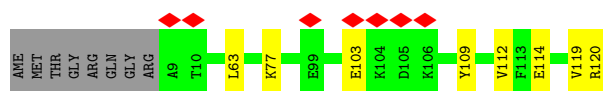
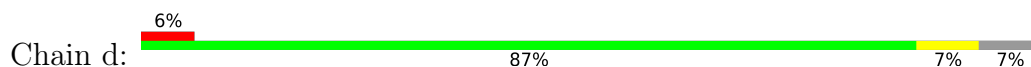


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

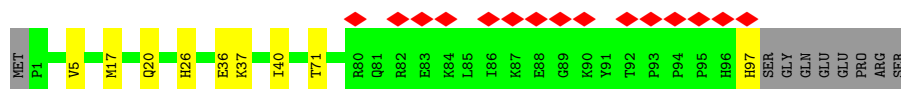
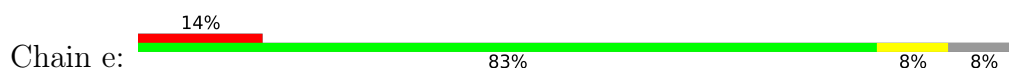




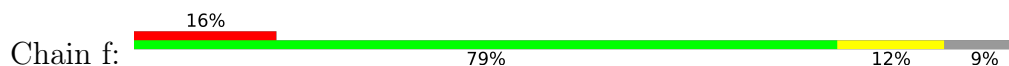
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



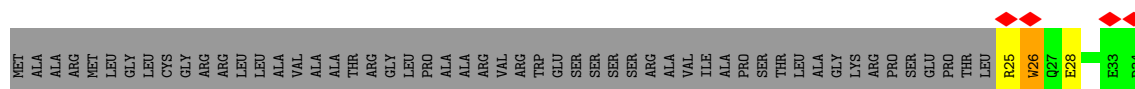
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



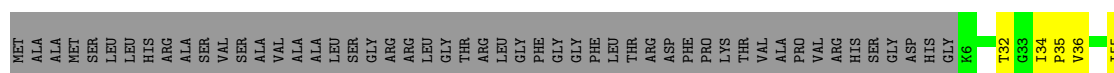
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



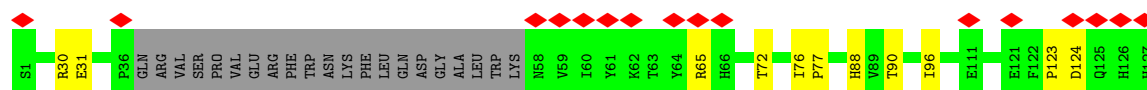
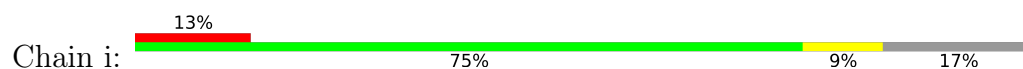
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



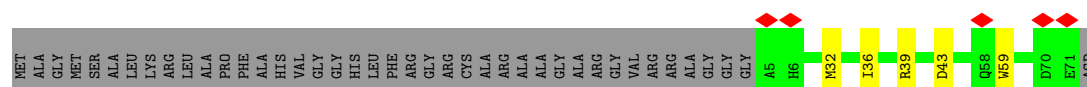
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



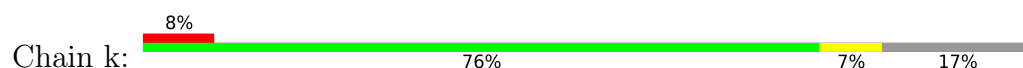
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



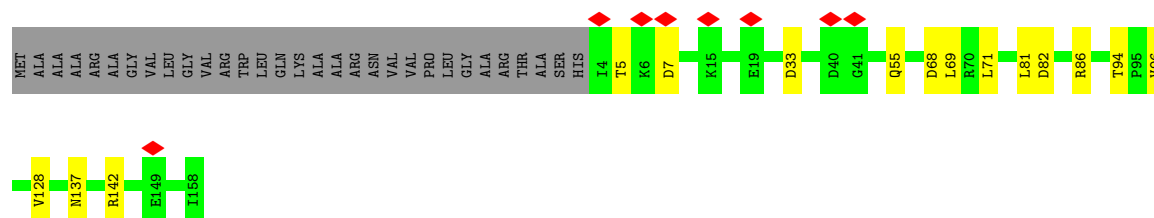
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



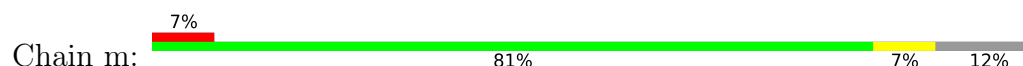
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

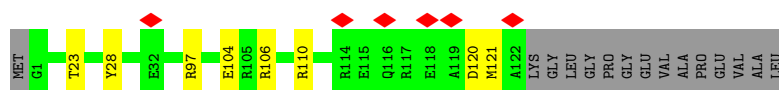


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  83% 6% 11%

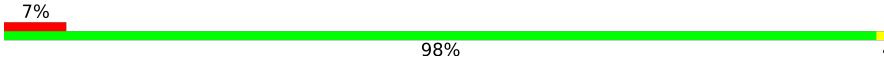


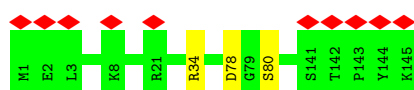
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  90% 7%



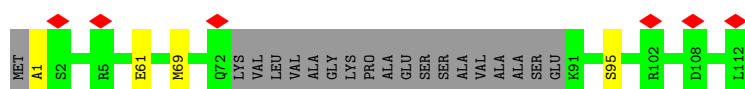
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  7% 98%



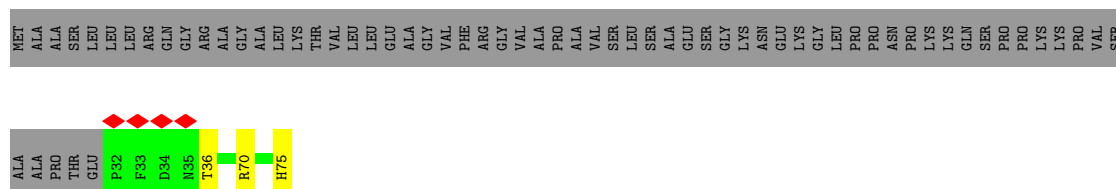
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  5% 80% 17%



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  38% 60%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27326	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	28.810	Depositor
Minimum map value	-11.274	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.033	Depositor
Recommended contour level	6	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, MYR, NDP, PC1, FME, GTP, SAC, LMT, FMN, FES, MG, SF4, 3PE, CDL, K, ZN, AYA, EHZ

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	0.23	0/936	0.30	0/1281
2	B	0.28	0/1261	0.40	0/1706
3	C	0.24	0/1772	0.31	0/2413
4	D	0.24	0/3537	0.31	0/4794
5	E	0.21	0/1695	0.32	0/2307
6	F	0.23	0/3393	0.31	0/4584
7	G	0.23	0/5367	0.32	0/7274
8	H	0.25	0/2571	0.32	0/3513
9	I	0.26	0/1445	0.34	0/1956
10	J	0.22	0/1362	0.30	0/1848
11	K	0.25	0/739	0.30	0/1000
12	L	0.25	0/4872	0.29	0/6630
13	M	0.25	0/3738	0.30	0/5097
14	N	0.24	0/2792	0.30	0/3800
15	O	0.22	0/2651	0.28	0/3587
16	P	0.22	0/2824	0.33	0/3831
17	Q	0.24	0/1039	0.30	0/1404
18	R	0.25	0/742	0.31	0/999
19	S	0.20	0/702	0.33	0/945
20	T	0.18	0/621	0.31	0/837
20	U	0.27	0/705	0.31	0/952
21	V	0.21	0/943	0.27	0/1277
22	W	0.22	0/995	0.29	0/1337
23	X	0.22	0/1439	0.32	0/1942
24	Y	0.16	0/1042	0.27	0/1414
25	Z	0.22	0/1181	0.29	0/1592
26	a	0.24	0/584	0.27	0/786
27	b	0.21	0/672	0.30	0/923
28	c	0.21	0/418	0.30	0/567
29	d	0.23	0/964	0.29	0/1305
30	e	0.23	0/840	0.33	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.22	0/464	0.35	0/626
32	g	0.24	0/850	0.29	0/1154
33	h	0.24	0/1188	0.29	0/1607
34	i	0.24	0/934	0.34	0/1271
35	j	0.25	0/607	0.28	0/833
36	k	0.24	0/672	0.28	0/906
37	l	0.26	0/1358	0.30	0/1858
38	m	0.24	0/983	0.30	0/1327
39	n	0.26	0/1545	0.30	0/2092
40	o	0.27	0/1073	0.32	0/1437
41	p	0.26	0/1476	0.29	0/1990
42	q	0.23	0/1250	0.31	0/1698
43	r	0.22	0/780	0.31	0/1056
44	s	0.19	0/383	0.26	0/518
All	All	0.24	0/67405	0.31	0/91397

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
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

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	921	0	952	13	0
2	B	1230	0	1238	14	0
3	C	1721	0	1675	12	0
4	D	3459	0	3404	27	0
5	E	1655	0	1661	12	0
6	F	3319	0	3274	17	0
7	G	5279	0	5301	27	0
8	H	2509	0	2621	23	0
9	I	1414	0	1370	11	0
10	J	1337	0	1346	25	0
11	K	739	0	780	26	0
12	L	4756	0	4905	50	0
13	M	3654	0	3852	41	0
14	N	2733	0	2912	37	0
15	O	2589	0	2566	22	0
16	P	2747	0	2766	19	0
17	Q	1016	0	1014	7	0
18	R	730	0	707	0	0
19	S	691	0	706	3	0
20	T	612	0	604	12	0
20	U	693	0	688	5	0
21	V	923	0	964	3	0
22	W	971	0	989	5	0
23	X	1402	0	1385	15	0
24	Y	1030	0	1039	2	0
25	Z	1152	0	1151	13	0
26	a	569	0	568	6	0
27	b	651	0	662	1	0
28	c	405	0	409	5	0
29	d	934	0	919	8	0
30	e	819	0	821	14	0
31	f	451	0	453	4	0
32	g	824	0	772	14	0
33	h	1154	0	1168	8	0
34	i	912	0	925	9	0
35	j	580	0	519	4	0
36	k	653	0	639	4	0
37	l	1304	0	1203	10	0
38	m	960	0	953	9	0
39	n	1492	0	1438	8	0
40	o	1048	0	1018	6	0
41	p	1443	0	1415	12	0
42	q	1209	0	1182	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	767	0	776	4	0
44	s	371	0	344	2	0
45	A	35	0	46	1	0
45	J	35	0	46	1	0
45	L	35	0	46	1	0
45	M	35	0	46	0	0
45	Y	35	0	46	0	0
45	b	35	0	46	0	0
45	f	35	0	46	0	0
45	h	35	0	46	2	0
45	j	35	0	46	1	0
45	l	35	0	46	1	0
46	A	21	0	18	1	0
46	B	35	0	44	0	0
46	M	49	0	75	0	0
46	P	54	0	88	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	H	78	0	112	1	0
51	I	51	0	82	0	0
51	L	94	0	142	1	0
51	M	97	0	151	1	0
51	Y	35	0	44	0	0
51	d	153	0	246	5	0
52	J	62	0	68	2	0
52	K	71	0	86	0	0
52	L	69	0	82	0	0
52	h	67	0	81	1	0
52	q	76	0	96	0	0
53	O	32	0	12	1	0
54	O	1	0	0	0	0
55	P	48	0	26	0	0
56	R	1	0	0	0	0
57	T	37	0	0	0	0
57	U	37	0	0	0	0
58	o	15	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	A	12	0	0	0	0
59	B	48	0	0	1	0
59	C	66	0	0	3	0
59	D	115	0	0	5	0
59	E	5	0	0	0	0
59	F	33	0	0	0	0
59	G	135	0	0	1	0
59	H	43	0	0	1	0
59	I	79	0	0	2	0
59	J	10	0	0	0	0
59	K	9	0	0	0	0
59	L	16	0	0	3	0
59	M	28	0	0	1	0
59	N	28	0	0	4	0
59	O	13	0	0	2	0
59	P	40	0	0	2	0
59	Q	45	0	0	0	0
59	R	19	0	0	0	0
59	S	2	0	0	0	0
59	V	6	0	0	0	0
59	W	8	0	0	0	0
59	X	13	0	0	1	0
59	Y	1	0	0	0	0
59	Z	11	0	0	0	0
59	a	4	0	0	1	0
59	b	4	0	0	0	0
59	d	8	0	0	1	0
59	e	5	0	0	0	0
59	f	1	0	0	0	0
59	g	1	0	0	0	0
59	h	11	0	0	0	0
59	j	2	0	0	0	0
59	l	8	0	0	1	0
59	m	2	0	0	0	0
59	n	5	0	0	1	0
59	o	2	0	0	0	0
59	p	9	0	0	1	0
59	q	18	0	0	0	0
59	r	20	0	0	1	0
All	All	68334	0	68013	471	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 3.

All (471) 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)
45:h:1002:LMT:O6B	41:p:58:ASN:OD1	1.90	0.90
25:Z:93:GLU:OE1	30:e:97:HIS:ND1	2.06	0.88
8:H:24:GLU:OE2	8:H:228:TYR:OH	1.93	0.84
23:X:139:ASN:OD1	59:X:201:HOH:O	1.94	0.84
7:G:478:ARG:NH1	7:G:487:TRP:O	2.10	0.84
4:D:3:GLN:NE2	13:M:137:GLY:O	2.11	0.84
43:r:95:SER:O	59:r:201:HOH:O	1.98	0.82
2:B:138:ARG:NH1	59:B:301:HOH:O	2.14	0.81
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.63	0.80
2:B:44:SER:OG	8:H:51:ASP:OD1	1.98	0.79
8:H:69:SER:OG	52:J:701:CDL:OB4	2.01	0.78
12:L:99:SER:OG	59:L:801:HOH:O	2.00	0.78
8:H:251:MET:O	59:H:501:HOH:O	2.01	0.78
15:O:128:ILE:O	59:O:501:HOH:O	2.02	0.77
12:L:102:GLU:OE2	12:L:456:ARG:NH2	2.18	0.77
40:o:23:THR:OG1	40:o:104:GLU:OE2	2.03	0.76
16:P:55:ASP:OD2	59:P:501:HOH:O	2.03	0.76
26:a:62:VAL:O	59:a:101:HOH:O	2.02	0.76
15:O:264:GLN:OE1	59:O:502:HOH:O	2.04	0.75
12:L:286:LEU:HD22	12:L:411:MET:SD	2.27	0.75
14:N:289:ASN:ND2	59:N:403:HOH:O	2.19	0.74
15:O:81:LYS:NZ	15:O:90:ASP:OD2	2.17	0.74
12:L:432:LEU:O	59:L:802:HOH:O	2.04	0.74
37:l:86:ARG:O	59:l:301:HOH:O	2.06	0.73
15:O:104:ARG:NH2	53:O:401:GTP:O6	2.22	0.73
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.22	0.73
39:n:174:ARG:NH1	59:n:201:HOH:O	2.22	0.72
12:L:479:GLN:NE2	12:L:481:THR:O	2.22	0.72
1:A:85:ASN:OD1	1:A:86:THR:N	2.23	0.72
12:L:559:GLU:O	12:L:565:THR:OG1	2.01	0.72
41:p:118:GLU:O	59:p:201:HOH:O	2.07	0.71
7:G:512:GLU:OE1	7:G:516:LYS:NZ	2.22	0.71
16:P:51:CYS:O	59:P:502:HOH:O	2.07	0.71
16:P:143:SER:OG	16:P:282:ASP:OD1	2.09	0.71
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.73	0.69
4:D:35:ASP:OD1	59:D:501:HOH:O	2.09	0.69
15:O:291:GLN:NE2	15:O:295:GLU:OE2	2.26	0.69
8:H:169:GLN:O	51:H:402:3PE:N	2.23	0.69
11:K:37:MET:SD	14:N:68:MET:HE1	2.33	0.68
16:P:311:GLU:OE1	16:P:311:GLU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.28	0.68
11:K:43:MET:HE1	14:N:72:MET:HE1	1.76	0.68
14:N:214:THR:HG22	14:N:218:MET:HE2	1.76	0.67
8:H:170:GLU:OE1	23:X:97:ARG:NH1	2.28	0.67
16:P:258:LEU:HD23	16:P:263:TYR:HD1	1.59	0.67
16:P:258:LEU:HD23	16:P:263:TYR:CD1	2.29	0.67
11:K:43:MET:CE	14:N:72:MET:HE1	2.25	0.66
14:N:174:GLN:OE1	59:N:401:HOH:O	2.11	0.66
2:B:45:LEU:HD22	2:B:85:VAL:CG2	2.26	0.66
4:D:210:ASP:OD2	59:D:502:HOH:O	2.13	0.66
7:G:366:THR:O	7:G:367:THR:OG1	2.13	0.66
1:A:71:LEU:O	10:J:147:TYR:OH	2.08	0.66
3:C:198:ASP:O	59:C:301:HOH:O	2.14	0.66
9:I:152:GLU:OE1	59:I:301:HOH:O	2.13	0.66
7:G:139:ASP:OD1	59:G:901:HOH:O	2.14	0.65
39:n:27:GLU:OE1	39:n:33:ARG:NH1	2.30	0.65
11:K:59:MET:HG2	14:N:27:LEU:HD22	1.78	0.65
13:M:245:ARG:NH1	59:M:701:HOH:O	2.29	0.65
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.78	0.64
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.26	0.64
13:M:214:LEU:HD13	38:m:76:TYR:CD1	2.31	0.64
42:q:78:ASP:OD1	42:q:80:SER:OG	2.12	0.64
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.80	0.64
14:N:308:THR:O	59:N:402:HOH:O	2.15	0.63
45:J:702:LMT:O5B	45:J:702:LMT:O3'	2.14	0.62
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.81	0.62
2:B:62:MET:HE3	2:B:69:MET:HE3	1.81	0.62
14:N:271:THR:HG22	14:N:276:ILE:HD13	1.82	0.61
14:N:68:MET:HE2	14:N:68:MET:HA	1.81	0.61
3:C:37:VAL:HG12	43:r:69:MET:CE	2.31	0.61
21:V:91:ARG:O	21:V:95:GLN:NE2	2.33	0.61
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.82	0.61
29:d:112:VAL:O	41:p:159:LYS:NZ	2.33	0.61
33:h:77:ARG:NH1	45:h:1002:LMT:O2'	2.33	0.61
7:G:470:VAL:HG12	7:G:490:MET:HE1	1.83	0.60
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.36	0.60
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.83	0.60
32:g:101:GLU:CG	32:g:107:ILE:HD11	2.31	0.60
5:E:105:THR:HG22	5:E:106:THR:H	1.68	0.59
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.83	0.59
7:G:684:MET:HA	7:G:684:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:86:MET:HE1	25:Z:125:TYR:CE2	2.37	0.59
16:P:154:LYS:O	16:P:158:GLU:OE1	2.21	0.59
1:A:44:MET:HE1	4:D:65:VAL:HG13	1.83	0.59
11:K:53:PHE:CE1	30:e:20:GLN:HA	2.38	0.59
26:a:59:ARG:NH2	26:a:61:TYR:OH	2.36	0.59
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.33	0.58
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.85	0.58
10:J:125:TRP:HB2	25:Z:137:THR:HG21	1.84	0.58
23:X:63:ASN:OD1	25:Z:81:ARG:NH2	2.35	0.58
11:K:53:PHE:CE2	11:K:56:ALA:HB2	2.40	0.57
44:s:70:ARG:NH1	44:s:75:HIS:O	2.37	0.57
4:D:385:ARG:NH1	59:D:512:HOH:O	2.36	0.57
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.85	0.57
15:O:15:THR:HG23	15:O:253:ASP:OD2	2.05	0.56
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.88	0.56
16:P:309:PRO:HD2	16:P:312:LEU:HD12	1.87	0.56
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.40	0.56
21:V:61:GLU:OE1	21:V:70:ARG:NH2	2.38	0.56
6:F:381:ARG:NH2	6:F:383:ASP:OD2	2.38	0.56
5:E:181:ILE:O	5:E:181:ILE:HG13	2.06	0.56
15:O:285:GLY:HA3	32:g:26:TRP:HZ3	1.70	0.56
19:S:95:SER:OG	19:S:96:SER:N	2.31	0.56
10:J:112:GLU:N	10:J:112:GLU:OE1	2.39	0.56
41:p:88:GLU:OE1	41:p:151:ALA:N	2.27	0.56
4:D:146:ARG:NH1	59:D:510:HOH:O	2.33	0.56
37:l:128:VAL:HG22	40:o:97:ARG:HB3	1.87	0.55
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.89	0.55
2:B:162:GLN:OE1	9:I:140:SER:OG	2.24	0.55
1:A:68:GLU:OE2	10:J:161:LEU:HD13	2.07	0.55
11:K:53:PHE:CD1	30:e:20:GLN:HB3	2.42	0.55
29:d:120:ARG:NH1	38:m:112:GLU:OE1	2.38	0.55
23:X:104:ALA:O	23:X:108:GLU:OE1	2.25	0.55
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.42	0.54
12:L:21:MET:O	12:L:25:ASN:N	2.40	0.54
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.89	0.54
20:T:7:THR:HG22	20:T:7:THR:O	2.07	0.54
12:L:383:MET:HE2	35:j:36:ILE:HD13	1.89	0.54
40:o:120:ASP:OD1	40:o:121:MET:N	2.41	0.54
29:d:114:GLU:OE2	59:d:1301:HOH:O	2.19	0.54
37:l:137:ASN:O	37:l:142:ARG:NH2	2.39	0.54
13:M:47:ASP:OD1	13:M:47:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.90	0.53
1:A:61:THR:HG21	1:A:105:GLU:OE2	2.08	0.53
12:L:14:LEU:HA	12:L:17:MET:HE2	1.90	0.53
20:T:30:LEU:HD12	20:T:31:SER:H	1.73	0.53
30:e:37:LYS:HG3	33:h:133:ILE:HD13	1.90	0.53
20:U:36:PHE:HD1	20:U:40:LEU:HD12	1.73	0.53
23:X:43:MET:HE3	23:X:47:TRP:CZ3	2.43	0.53
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.91	0.53
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.42	0.53
45:L:702:LMT:O3'	45:L:702:LMT:O2B	2.15	0.53
36:k:11:SER:O	36:k:13:MET:N	2.40	0.52
3:C:37:VAL:HG12	43:r:69:MET:HE1	1.91	0.52
3:C:136:ASP:OD1	59:C:302:HOH:O	2.19	0.52
10:J:157:THR:HG22	11:K:66:PHE:HE1	1.73	0.52
14:N:187:MET:HE3	14:N:187:MET:HA	1.91	0.52
34:i:90:THR:CG2	34:i:96:ILE:HD12	2.40	0.52
13:M:66:LEU:HD11	13:M:111:THR:HG23	1.90	0.52
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.91	0.52
4:D:371:LYS:HE2	4:D:424:VAL:HG23	1.91	0.52
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.91	0.52
7:G:26:VAL:HG22	7:G:73:VAL:HG12	1.92	0.52
35:j:39:ARG:NE	35:j:43:ASP:OD1	2.42	0.51
2:B:69:MET:HE2	2:B:74:VAL:HG12	1.92	0.51
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.92	0.51
15:O:80:GLU:N	15:O:80:GLU:OE1	2.43	0.51
10:J:111:LYS:O	10:J:121:GLY:N	2.39	0.51
1:A:51:PHE:CD1	8:H:133:LEU:HD13	2.46	0.51
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.43	0.51
51:d:1203:3PE:H2I2	51:d:1203:3PE:H3F2	1.92	0.51
31:f:7:VAL:HG12	31:f:9:ASP:H	1.76	0.51
38:m:75:ILE:HG22	38:m:76:TYR:CD1	2.46	0.51
6:F:263:ASN:ND2	6:F:285:GLY:O	2.39	0.51
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.92	0.51
12:L:123:LEU:HB2	12:L:150:MET:HE2	1.92	0.51
12:L:492:ILE:O	12:L:496:LEU:HD23	2.11	0.51
4:D:259:MET:HE2	4:D:421:GLN:HG2	1.93	0.51
13:M:370:PRO:HB3	13:M:375:LEU:HD22	1.93	0.51
20:T:30:LEU:HD12	20:T:31:SER:N	2.26	0.51
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.43	0.51
1:A:70:ALA:HA	10:J:55:MET:HE2	1.91	0.51
32:g:57:ASN:ND2	32:g:57:ASN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.38	0.51
13:M:304:GLN:O	29:d:119:VAL:HG11	2.10	0.51
29:d:63:LEU:HD23	51:d:1202:3PE:C31	2.41	0.51
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.92	0.50
4:D:37:ASP:OD2	11:K:95:LEU:HD13	2.11	0.50
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.12	0.50
39:n:12:GLN:NE2	39:n:16:LEU:HD11	2.26	0.50
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.92	0.50
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.47	0.50
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.93	0.50
52:h:1001:CDL:OB4	34:i:88:HIS:NE2	2.42	0.50
23:X:43:MET:HE3	23:X:47:TRP:HZ3	1.76	0.50
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.34	0.50
20:U:55:GLU:OE2	39:n:24:ARG:NH2	2.43	0.50
23:X:87:CYS:HG	23:X:99:CYS:HG	1.59	0.50
12:L:369:THR:OG1	12:L:445:GLU:OE1	2.29	0.50
28:c:34:GLN:NE2	28:c:38:ASP:OD2	2.45	0.49
11:K:37:MET:HE2	11:K:67:ALA:HB2	1.93	0.49
12:L:74:LEU:HD22	12:L:190:LEU:HD13	1.95	0.49
4:D:165:THR:OG1	8:H:275:ALA:O	2.25	0.49
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.47	0.49
3:C:165:ASP:OD2	59:C:303:HOH:O	2.20	0.49
32:g:25:ARG:O	32:g:26:TRP:HB3	2.12	0.49
6:F:306:LEU:C	6:F:306:LEU:HD12	2.37	0.49
28:c:4:ILE:HG23	28:c:5:GLN:OE1	2.13	0.49
4:D:51:PHE:HB2	4:D:66:MET:HE2	1.94	0.49
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.48	0.48
12:L:249:SER:OG	12:L:250:SER:N	2.45	0.48
13:M:40:LEU:HD22	33:h:79:PHE:HB3	1.94	0.48
11:K:19:LEU:CD2	11:K:36:MET:HE1	2.43	0.48
12:L:511:LEU:HD12	36:k:34:LYS:HE3	1.96	0.48
17:Q:21:THR:HG21	22:W:73:ILE:HD11	1.94	0.48
30:e:20:GLN:CG	30:e:36:GLU:OE1	2.62	0.48
12:L:264:TYR:N	12:L:265:PRO:CD	2.77	0.48
13:M:108:MET:HE1	51:d:1203:3PE:H3E2	1.95	0.48
4:D:322:GLU:OE1	4:D:322:GLU:N	2.36	0.48
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.96	0.48
36:k:23:ILE:O	36:k:26:THR:OG1	2.31	0.48
44:s:36:THR:O	44:s:36:THR:HG22	2.13	0.48
52:J:701:CDL:OA4	16:P:251:ARG:NH2	2.39	0.48
7:G:254:MET:HA	7:G:260:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:87:ILE:N	8:H:88:PRO:CD	2.77	0.47
12:L:71:ILE:HG23	13:M:310:MET:HE1	1.95	0.47
12:L:456:ARG:NH1	59:L:801:HOH:O	2.42	0.47
12:L:483:PRO:HD2	12:L:486:LEU:HD12	1.96	0.47
24:Y:4:VAL:O	24:Y:7:GLN:HG2	2.14	0.47
36:k:29:GLU:O	36:k:33:GLU:OE1	2.32	0.47
12:L:176:ARG:HH22	13:M:367:LEU:HD13	1.78	0.47
12:L:407:TRP:CH2	12:L:411:MET:HE3	2.49	0.47
23:X:122:GLY:N	25:Z:66:GLU:OE2	2.43	0.47
34:i:72:THR:HA	34:i:76:ILE:HD12	1.96	0.47
2:B:91:THR:HA	2:B:119:CYS:HB3	1.96	0.47
3:C:77:ASP:OD2	4:D:390:LYS:NZ	2.44	0.47
13:M:114:GLU:OE2	13:M:174:LEU:HB2	2.15	0.47
20:T:16:LEU:O	20:T:20:LYS:HG2	2.14	0.47
37:l:94:THR:OG1	37:l:96:VAL:O	2.28	0.47
38:m:22:TYR:O	38:m:23:ASP:C	2.57	0.47
13:M:114:GLU:HG2	23:X:168:PHE:HB3	1.97	0.47
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.97	0.47
7:G:528:ASP:OD2	7:G:545:TYR:OH	2.30	0.47
16:P:82:ARG:HG2	16:P:120:VAL:HG13	1.97	0.47
25:Z:120:MET:HE2	30:e:71:THR:HG21	1.96	0.47
11:K:53:PHE:CD1	30:e:20:GLN:HA	2.50	0.46
16:P:98:GLU:OE1	16:P:177:ARG:NE	2.41	0.46
16:P:237:LEU:HG	16:P:340:ILE:HD11	1.97	0.46
8:H:24:GLU:O	8:H:28:LEU:HD13	2.15	0.46
13:M:214:LEU:HD13	38:m:76:TYR:CE1	2.50	0.46
34:i:90:THR:HG22	34:i:96:ILE:HD12	1.97	0.46
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.14	0.46
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.47	0.46
15:O:285:GLY:HA3	32:g:26:TRP:CZ3	2.49	0.46
5:E:82:GLU:OE2	7:G:174:THR:N	2.48	0.46
13:M:306:PRO:HA	13:M:458:LEU:HD22	1.97	0.46
20:T:55:GLU:OE2	22:W:37:ARG:NH2	2.48	0.46
30:e:17:MET:O	30:e:17:MET:HG2	2.15	0.46
5:E:145:LEU:HD12	5:E:153:MET:SD	2.56	0.46
14:N:207:ILE:HD13	14:N:262:PRO:HD3	1.98	0.46
23:X:97:ARG:HD2	25:Z:60:LEU:HD13	1.98	0.46
11:K:40:LEU:HD21	14:N:72:MET:HE2	1.98	0.46
27:b:51:ASN:ND2	30:e:26:HIS:O	2.34	0.46
7:G:229:ASP:OD1	7:G:267:THR:HG23	2.16	0.46
12:L:331:THR:HB	12:L:387:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:375:VAL:HG22	35:j:32:MET:SD	2.56	0.46
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.97	0.46
16:P:330:GLU:N	16:P:333:ASP:OD1	2.49	0.46
20:T:74:GLN:O	20:T:77:VAL:HG22	2.15	0.46
2:B:62:MET:CE	2:B:69:MET:HE3	2.45	0.46
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.97	0.46
32:g:101:GLU:HG2	32:g:107:ILE:HD11	1.97	0.46
45:j:101:LMT:O6'	45:j:101:LMT:O5B	2.34	0.46
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.16	0.46
2:B:45:LEU:O	2:B:74:VAL:HA	2.16	0.45
2:B:125:TYR:HB2	9:I:117:ILE:HG21	1.97	0.45
16:P:339:THR:HG22	16:P:340:ILE:N	2.31	0.45
6:F:435:GLN:HA	6:F:435:GLN:NE2	2.31	0.45
7:G:283:MET:HE2	7:G:293:HIS:CD2	2.51	0.45
13:M:42:MET:HE1	32:g:77:VAL:HG22	1.98	0.45
3:C:8:ARG:NH2	43:r:61:GLU:OE2	2.39	0.45
13:M:201:MET:HE1	13:M:212:LEU:HD11	1.99	0.45
17:Q:27:GLU:OE1	17:Q:27:GLU:HA	2.17	0.45
5:E:105:THR:HG22	5:E:106:THR:N	2.30	0.45
9:I:143:THR:OG1	9:I:146:GLU:OE2	2.23	0.45
12:L:7:LEU:CD1	12:L:49:ILE:HG21	2.46	0.45
34:i:76:ILE:HB	34:i:77:PRO:HD3	1.98	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.45
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.51	0.45
3:C:210:ARG:NH1	7:G:35:MET:SD	2.90	0.45
8:H:236:ILE:HG23	8:H:259:PHE:CE2	2.51	0.45
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.30	0.45
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.99	0.45
14:N:100:MET:O	14:N:104:MET:HG3	2.16	0.45
15:O:147:GLN:OE1	15:O:147:GLN:N	2.46	0.45
15:O:287:HIS:HB2	32:g:28:GLU:OE2	2.17	0.45
10:J:129:ASP:OD1	10:J:130:THR:N	2.50	0.45
10:J:142:GLY:CA	11:K:54:THR:HG22	2.47	0.45
11:K:43:MET:HG2	14:N:75:ILE:HG21	1.99	0.45
12:L:174:TYR:OH	12:L:534:HIS:NE2	2.41	0.45
14:N:162:ILE:HD13	14:N:282:MET:HG2	1.99	0.45
14:N:337:LEU:HD23	51:d:1203:3PE:H391	1.98	0.45
19:S:13:LEU:HD12	19:S:13:LEU:O	2.17	0.45
19:S:64:LEU:O	19:S:75:ASN:HA	2.16	0.45
15:O:145:ARG:NH1	15:O:281:GLU:OE2	2.50	0.44
41:p:108:ARG:NH1	41:p:130:GLN:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HA	1:A:87:MET:SD	2.57	0.44
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.52	0.44
34:i:30:ARG:NH2	39:n:116:ASP:OD1	2.41	0.44
39:n:12:GLN:HE22	39:n:16:LEU:HD11	1.81	0.44
33:h:110:VAL:CG1	33:h:114:MET:HE3	2.47	0.44
38:m:124:PHE:HA	41:p:135:VAL:HG11	1.99	0.44
11:K:53:PHE:HE2	11:K:56:ALA:HB2	1.80	0.44
20:U:11:ILE:O	20:U:15:VAL:HG23	2.17	0.44
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.00	0.44
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.51	0.44
6:F:194:GLU:OE1	17:Q:133:LYS:NZ	2.42	0.44
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.44
14:N:236:LYS:HE2	15:O:267:LEU:HD13	2.00	0.44
51:d:1203:3PE:H2I2	51:d:1203:3PE:C3F	2.47	0.44
41:p:16:THR:HG23	41:p:16:THR:O	2.17	0.44
10:J:125:TRP:CB	25:Z:137:THR:HG21	2.48	0.44
10:J:153:LEU:O	10:J:157:THR:HG23	2.17	0.44
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.00	0.44
22:W:52:LEU:HD11	22:W:103:VAL:HG11	1.99	0.44
10:J:139:GLU:HG2	10:J:143:ILE:HD12	1.99	0.44
12:L:71:ILE:CG2	13:M:310:MET:HE1	2.48	0.44
13:M:74:PRO:O	13:M:78:MET:HG3	2.18	0.44
20:T:8:LEU:C	20:T:8:LEU:HD23	2.43	0.44
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.53	0.44
23:X:89:ASP:OD1	26:a:63:SER:OG	2.31	0.44
37:l:33:ASP:OD2	38:m:35:ARG:NE	2.50	0.44
6:F:403:THR:HB	47:F:502:SF4:S4	2.58	0.43
11:K:43:MET:HE3	14:N:72:MET:HE1	2.00	0.43
24:Y:104:THR:HG22	24:Y:104:THR:O	2.17	0.43
41:p:14:ARG:HG3	41:p:14:ARG:HH11	1.81	0.43
1:A:44:MET:HE3	4:D:48:THR:HG22	2.00	0.43
2:B:92:LEU:HD13	2:B:100:LEU:HD13	1.99	0.43
12:L:247:LEU:HD22	12:L:248:HIS:CD2	2.53	0.43
13:M:403:THR:HA	13:M:406:TYR:CE1	2.53	0.43
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.00	0.43
29:d:109:TYR:CE1	41:p:152:ARG:HD3	2.53	0.43
8:H:207:LEU:O	8:H:209:SER:N	2.51	0.43
25:Z:120:MET:HE2	30:e:71:THR:CG2	2.49	0.43
34:i:31:GLU:OE1	39:n:116:ASP:N	2.45	0.43
5:E:129:GLY:N	5:E:139:LEU:O	2.41	0.43
10:J:135:PHE:CD2	10:J:135:PHE:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:151:SER:OG	12:L:252:MET:SD	2.58	0.43
16:P:176:ASP:OD1	16:P:176:ASP:C	2.60	0.43
16:P:194:ILE:HD11	16:P:263:TYR:CD2	2.54	0.43
20:T:66:ASP:OD2	20:T:79:TYR:OH	2.30	0.43
29:d:103:GLU:OE1	29:d:103:GLU:N	2.50	0.43
12:L:230:HIS:N	12:L:231:PRO:HD3	2.34	0.43
14:N:269:GLU:OE1	59:N:404:HOH:O	2.21	0.43
4:D:241:ASP:OD2	4:D:290:ARG:NH2	2.52	0.43
10:J:5:ILE:HG23	10:J:6:VAL:N	2.33	0.43
15:O:151:HIS:HB2	15:O:279:LEU:HD11	2.00	0.43
10:J:164:GLY:O	10:J:168:ILE:HG23	2.19	0.43
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.01	0.43
13:M:207:MET:SD	13:M:240:GLY:N	2.92	0.43
14:N:261:MET:HG3	14:N:340:THR:HG23	2.00	0.43
10:J:47:PHE:CD1	11:K:46:LEU:HD22	2.53	0.42
51:M:603:3PE:H332	14:N:242:VAL:HG11	2.01	0.42
15:O:46:LEU:HD21	15:O:235:VAL:HG13	2.01	0.42
25:Z:86:MET:HE1	25:Z:125:TYR:CD2	2.54	0.42
33:h:34:ILE:HB	33:h:35:PRO:HD3	2.01	0.42
3:C:154:ASP:OD1	3:C:155:TYR:N	2.52	0.42
7:G:229:ASP:CG	7:G:267:THR:HG23	2.44	0.42
7:G:283:MET:HB2	7:G:560:ILE:HB	2.00	0.42
51:L:701:3PE:H272	13:M:405:LEU:HD13	2.00	0.42
33:h:87:TYR:OH	41:p:86:GLU:HG2	2.19	0.42
2:B:44:SER:O	8:H:54:LYS:HE2	2.19	0.42
5:E:70:ALA:HB2	5:E:80:VAL:HG21	2.01	0.42
8:H:232:ILE:HG21	26:a:16:LEU:HD21	2.01	0.42
12:L:87:MET:HA	12:L:87:MET:HE2	2.00	0.42
20:U:47:GLN:NE2	20:U:70:LEU:O	2.52	0.42
37:l:68:ASP:OD1	37:l:68:ASP:N	2.53	0.42
1:A:28:ASN:O	1:A:33:LYS:NZ	2.46	0.42
8:H:20:LEU:HD13	26:a:12:MET:HE1	2.00	0.42
12:L:173:LEU:HD12	13:M:405:LEU:HD21	2.01	0.42
32:g:101:GLU:HG3	32:g:107:ILE:HD11	2.00	0.42
3:C:204:GLU:OE1	3:C:210:ARG:NH1	2.50	0.42
12:L:363:PHE:CD2	12:L:370:THR:HG21	2.54	0.42
14:N:270:MET:CE	14:N:278:LEU:HD23	2.50	0.42
20:U:87:TYR:O	20:U:88:GLU:C	2.62	0.42
23:X:78:ALA:O	23:X:82:THR:OG1	2.31	0.42
33:h:55:ILE:HD12	41:p:66:GLU:OE1	2.19	0.42
4:D:261:ARG:NH2	4:D:303:GLU:OE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:374:ALA:O	7:G:404:LEU:HD13	2.20	0.42
8:H:255:TYR:CD1	8:H:255:TYR:C	2.98	0.42
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.01	0.42
13:M:457:PRO:O	32:g:84:ARG:NH2	2.53	0.42
17:Q:27:GLU:OE2	17:Q:31:LYS:NZ	2.49	0.42
20:T:9:GLU:OE1	20:T:9:GLU:HA	2.20	0.42
33:h:32:THR:O	33:h:36:VAL:HG23	2.20	0.42
5:E:149:VAL:HG13	6:F:105:CYS:SG	2.60	0.42
21:V:47:THR:O	21:V:51:THR:OG1	2.32	0.42
28:c:38:ASP:OD2	29:d:77:LYS:NZ	2.47	0.42
5:E:14:GLU:OE1	5:E:14:GLU:N	2.52	0.42
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.30	0.42
13:M:6:ILE:HD12	31:f:23:GLY:HA2	2.00	0.42
14:N:68:MET:HE2	14:N:68:MET:CA	2.47	0.42
17:Q:35:ALA:O	17:Q:103:TYR:HA	2.19	0.42
28:c:6:GLU:OE2	28:c:6:GLU:HA	2.20	0.42
30:e:20:GLN:HG2	30:e:36:GLU:OE1	2.20	0.42
2:B:100:LEU:C	2:B:100:LEU:HD23	2.45	0.42
3:C:49:GLU:OE2	3:C:106:ARG:NH2	2.46	0.42
4:D:417:ILE:HA	4:D:420:THR:HG22	2.01	0.42
9:I:75:GLU:O	9:I:105:ARG:NH1	2.53	0.42
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.50	0.42
25:Z:98:MET:HE3	25:Z:101:VAL:HG21	2.01	0.42
40:o:120:ASP:OD1	40:o:120:ASP:C	2.61	0.42
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.55	0.42
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.51	0.42
13:M:370:PRO:HB3	13:M:375:LEU:CD2	2.49	0.41
37:l:55:GLN:NE2	37:l:69:LEU:O	2.38	0.41
6:F:93:LEU:HD13	6:F:129:MET:HE1	2.01	0.41
7:G:227:SER:OG	7:G:228:ILE:N	2.51	0.41
11:K:93:LEU:HB3	14:N:54:GLU:HG3	2.01	0.41
13:M:306:PRO:O	13:M:310:MET:HG3	2.20	0.41
37:l:82:ASP:OD1	37:l:82:ASP:N	2.53	0.41
4:D:241:ASP:OD1	4:D:244:ILE:HD11	2.21	0.41
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.50	0.41
13:M:278:ARG:O	38:m:71:ARG:NH1	2.53	0.41
20:T:52:MET:HE1	22:W:40:TYR:CG	2.56	0.41
35:j:59:TRP:O	40:o:106:ARG:NH2	2.42	0.41
14:N:54:GLU:OE2	14:N:58:LYS:NZ	2.52	0.41
14:N:179:MET:HE2	14:N:215:MET:HB3	2.03	0.41
16:P:261:PHE:CG	16:P:262:ALA:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:MET:SD	4:D:111:MET:N	2.94	0.41
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.55	0.41
10:J:167:VAL:HG12	10:J:171:ILE:HD12	2.02	0.41
14:N:265:MET:HA	14:N:265:MET:HE2	2.02	0.41
22:W:96:VAL:HG12	22:W:96:VAL:O	2.20	0.41
11:K:59:MET:HB3	11:K:60:PRO:HD3	2.03	0.41
23:X:12:LEU:HD13	25:Z:85:GLN:HG3	2.02	0.41
41:p:14:ARG:HG3	41:p:14:ARG:NH1	2.36	0.41
6:F:293:ASN:O	6:F:339:ARG:N	2.54	0.41
7:G:329:ILE:HD13	7:G:505:LEU:HD22	2.02	0.41
16:P:79:ASP:OD1	16:P:82:ARG:NH1	2.54	0.41
4:D:123:GLU:OE1	4:D:138:ARG:NH2	2.54	0.41
9:I:75:GLU:OE2	59:I:302:HOH:O	2.22	0.41
10:J:43:ILE:HG22	11:K:46:LEU:HD21	2.02	0.41
12:L:15:LEU:HD12	12:L:129:LEU:HD12	2.02	0.41
13:M:12:MET:HB2	13:M:13:PRO:HD3	2.03	0.41
20:T:35:HIS:HA	20:T:72:CYS:SG	2.61	0.41
1:A:67:LEU:HD22	10:J:59:ILE:HD12	2.02	0.41
45:A:701:LMT:O5B	45:A:701:LMT:H3'	2.21	0.41
4:D:202:ASP:N	4:D:323:ILE:HD13	2.35	0.41
6:F:93:LEU:O	6:F:134:ALA:HA	2.21	0.41
7:G:382:THR:HG23	7:G:384:PRO:HD3	2.03	0.41
31:f:49:LYS:HB3	31:f:50:PRO:CD	2.51	0.41
45:l:201:LMT:C1B	45:l:201:LMT:H6'	2.34	0.41
46:A:702:PC1:O13	46:A:702:PC1:H132	2.21	0.41
5:E:16:ASN:HB2	5:E:17:PRO:HD2	2.02	0.41
7:G:252:PRO:HG3	7:G:263:ILE:HG12	2.04	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.03	0.41
13:M:88:ASN:OD1	13:M:89:LEU:N	2.53	0.41
34:i:123:PRO:O	34:i:124:ASP:HB2	2.21	0.41
4:D:300:ARG:NE	59:D:514:HOH:O	2.41	0.40
8:H:298:LEU:O	8:H:302:MET:HG3	2.21	0.40
10:J:47:PHE:CE1	11:K:46:LEU:HD22	2.56	0.40
10:J:137:SER:O	10:J:141:MET:HG2	2.21	0.40
13:M:106:LEU:HD13	13:M:234:VAL:HG11	2.03	0.40
14:N:342:MET:O	14:N:345:VAL:HG22	2.21	0.40
15:O:285:GLY:HA3	32:g:28:GLU:OE1	2.20	0.40
32:g:57:ASN:ND2	32:g:57:ASN:C	2.79	0.40
4:D:134:ALA:HB2	4:D:323:ILE:O	2.21	0.40
7:G:140:LYS:O	7:G:148:THR:OG1	2.29	0.40
12:L:101:MET:O	12:L:105:MET:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:301:ILE:CG2	12:L:426:ILE:HD11	2.51	0.40
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.03	0.40
13:M:16:TRP:HZ2	13:M:94:LEU:HD23	1.85	0.40
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.56	0.40
23:X:141:TYR:CZ	30:e:37:LYS:HE2	2.56	0.40
28:c:15:LEU:C	28:c:15:LEU:HD23	2.45	0.40
4:D:405:MET:HE2	4:D:417:ILE:HG23	2.04	0.40
13:M:254:THR:O	13:M:254:THR:HG22	2.21	0.40
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.04	0.40
11:K:40:LEU:CD2	14:N:72:MET:HE2	2.51	0.40
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.02	0.40
20:T:36:PHE:HD1	20:T:40:LEU:HD12	1.87	0.40
30:e:36:GLU:HG2	30:e:40:ILE:HD12	2.02	0.40
6:F:98:ASP:O	6:F:139:ARG:HD2	2.21	0.40
11:K:12:PHE:CG	14:N:72:MET:HE3	2.57	0.40
12:L:38:THR:HG21	34:i:65:ARG:HH12	1.87	0.40
14:N:22:ILE:HB	30:e:5:VAL:HG22	2.02	0.40
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.40
15:O:285:GLY:CA	32:g:26:TRP:HZ3	2.34	0.40
31:f:11:TRP:O	31:f:14:VAL:HG22	2.22	0.40
39:n:99:PRO:HB2	39:n:101:TRP:CD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	152/216 (70%)	146 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	413 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
6	F	429/464 (92%)	421 (98%)	8 (2%)	0	100	100
7	G	686/727 (94%)	665 (97%)	21 (3%)	0	100	100
8	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	172/175 (98%)	162 (94%)	9 (5%)	1 (1%)	21	32
11	K	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
12	L	597/606 (98%)	578 (97%)	19 (3%)	0	100	100
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	308 (97%)	10 (3%)	0	100	100
16	P	339/380 (89%)	332 (98%)	7 (2%)	0	100	100
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
19	S	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
20	U	84/156 (54%)	84 (100%)	0	0	100	100
21	V	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
25	Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	110/120 (92%)	108 (98%)	2 (2%)	0	100	100
30	e	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	47 (94%)	3 (6%)	0	100	100
32	g	96/154 (62%)	92 (96%)	3 (3%)	1 (1%)	12	20
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	102/127 (80%)	99 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
38	m	110/129 (85%)	107 (97%)	3 (3%)	0	100	100
39	n	170/179 (95%)	168 (99%)	2 (1%)	0	100	100
40	o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
41	p	169/176 (96%)	167 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8089/9212 (88%)	7881 (97%)	206 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	26	TRP
10	J	24	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	130/175 (74%)	130 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	84/85 (99%)	84 (100%)	0	100	100
12	L	527/533 (99%)	527 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	78 (100%)	0	100	100
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	78 (99%)	1 (1%)	61	80
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	88/96 (92%)	88 (100%)	0	100	100
31	f	49/54 (91%)	49 (100%)	0	100	100
32	g	89/131 (68%)	89 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	101/120 (84%)	101 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	63/76 (83%)	63 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	101/115 (88%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7138/7892 (90%)	7137 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	U	44(A)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	71	GLN
3	C	88	ASN
3	C	160	HIS
3	C	192	GLN
4	D	59	HIS
5	E	37	ASN
5	E	155	GLN
6	F	324	GLN
6	F	326	GLN
6	F	373	ASN
6	F	398	GLN
6	F	421	HIS
6	F	437	HIS
7	G	155	GLN
7	G	182	GLN
7	G	237	ASN
7	G	383	ASN
7	G	402	ASN
8	H	47	GLN
8	H	235	ASN
9	I	144	HIS
11	K	50	ASN
12	L	25	ASN

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Mol	Chain	Res	Type
12	L	56	HIS
13	M	82	HIS
13	M	138	ASN
13	M	175	ASN
13	M	184	GLN
13	M	366	ASN
13	M	399	ASN
15	O	114	HIS
15	O	288	GLN
16	P	250	HIS
17	Q	50	ASN
19	S	30	GLN
19	S	47	ASN
19	S	85	GLN
20	U	33	ASN
21	V	36	HIS
23	X	76	HIS
23	X	162	HIS
24	Y	88	ASN
28	c	9	HIS
29	d	88	HIS
31	f	30	ASN
31	f	51	ASN
32	g	36	ASN
35	j	6	HIS
35	j	58	GLN
37	l	56	GLN
37	l	87	ASN
37	l	126	GLN
37	l	137	ASN
42	q	5	GLN
42	q	54	GLN
42	q	112	ASN
44	s	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are 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$
1	FME	A	1	1	8,9,10	1.03	1 (12%)	8,9,11	0.86	0
12	FME	L	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.88	0
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.23	1 (16%)
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	1.03	0
34	SAC	i	1	34	7,8,9	1.09	0	7,9,11	0.88	0
4	2MR	D	85	4	10,12,13	2.74	4 (40%)	5,13,15	1.30	1 (20%)
10	FME	J	1	10	8,9,10	1.01	0	8,9,11	0.82	0
8	FME	H	1	8	8,9,10	0.99	0	8,9,11	0.94	0
13	FME	M	1	13	8,9,10	1.05	1 (12%)	8,9,11	0.89	0
11	FME	K	1	11	8,9,10	0.94	0	8,9,11	0.81	0
43	AYA	r	1	43	6,7,8	1.88	2 (33%)	6,8,10	1.32	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
24	AYA	Y	1	24	-	1/5/6/8	-
14	FME	N	1	14	-	3/7/9/11	-
34	SAC	i	1	34	-	3/7/8/10	-
4	2MR	D	85	4	-	1/10/13/15	-
10	FME	J	1	10	-	2/7/9/11	-
8	FME	H	1	8	-	2/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.41	1.44	1.33
4	D	85	2MR	CZ-NE	4.52	1.43	1.34
4	D	85	2MR	O-C	4.13	1.35	1.20
24	Y	1	AYA	CT-N	3.50	1.45	1.34
43	r	1	AYA	CT-N	3.37	1.45	1.34
13	M	1	FME	CA-N	-2.24	1.43	1.46
43	r	1	AYA	OT-CT	-2.17	1.18	1.23
1	A	1	FME	CA-N	-2.15	1.43	1.46
12	L	1	FME	CA-N	-2.14	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.10	1.42	1.46
24	Y	1	AYA	OT-CT	-2.03	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	NE-CZ-NH2	-2.69	117.01	119.48
43	r	1	AYA	CM-CT-N	2.37	120.04	116.12
24	Y	1	AYA	CM-CT-N	2.09	119.58	116.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
4	D	85	2MR	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	O-C-CA-CB
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
24	Y	1	AYA	O-C-CA-CB
34	i	1	SAC	O-C-CA-CB
8	H	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	CB-CA-N-C1A
10	J	1	FME	CB-CG-SD-CE
34	i	1	SAC	C-CA-N-C1A
8	H	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	LMT	A	701	-	36,36,36	1.26	3 (8%)	47,47,47	1.65	7 (14%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
53	GTP	O	401	54	33,34,34	3.24	16 (48%)	50,54,54	1.84	11 (22%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
49	FMN	F	501	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	6 (12%)
46	PC1	A	702	-	20,20,53	1.78	3 (15%)	24,27,61	1.18	1 (4%)
57	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	2.04	8 (22%)
46	PC1	M	604	-	48,48,53	1.01	3 (6%)	54,56,61	1.02	2 (3%)
46	PC1	P	401	-	53,53,53	0.94	3 (5%)	59,61,61	1.05	2 (3%)
52	CDL	q	201	-	75,75,99	1.01	7 (9%)	81,87,111	1.10	4 (4%)
51	3PE	L	701	-	48,48,50	0.90	3 (6%)	51,53,55	1.13	2 (3%)
58	MYR	o	201	40	13,14,15	0.97	0	12,13,15	0.56	0
47	SF4	G	801	7	0,12,12	-	-	-	-	-
55	NDP	P	402	-	51,52,52	2.20	4 (7%)	71,80,80	1.50	17 (23%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
51	3PE	Y	802	-	34,34,50	1.05	3 (8%)	37,39,55	1.18	2 (5%)
51	3PE	d	1201	-	50,50,50	0.85	4 (8%)	53,55,55	1.09	2 (3%)
51	3PE	d	1202	-	50,50,50	0.84	4 (8%)	53,55,55	1.11	4 (7%)
52	CDL	h	1001	-	66,66,99	1.07	7 (10%)	72,78,111	1.24	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	3PE	M	601	-	45,45,50	0.94	4 (8%)	48,50,55	0.99	2 (4%)
52	CDL	K	401	-	70,70,99	1.05	8 (11%)	76,82,111	1.06	4 (5%)
52	CDL	L	703	-	68,68,99	1.05	6 (8%)	74,80,111	1.11	4 (5%)
51	3PE	d	1203	-	50,50,50	0.87	4 (8%)	53,55,55	1.12	2 (3%)
45	LMT	L	702	-	36,36,36	1.15	2 (5%)	47,47,47	0.97	1 (2%)
51	3PE	L	704	-	44,44,50	0.93	4 (9%)	47,49,55	1.18	3 (6%)
45	LMT	h	1002	-	36,36,36	1.17	2 (5%)	47,47,47	0.93	1 (2%)
51	3PE	H	402	-	33,33,50	1.27	4 (12%)	34,37,55	1.23	2 (5%)
46	PC1	B	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.10	2 (5%)
51	3PE	M	603	-	50,50,50	0.87	3 (6%)	53,55,55	1.10	2 (3%)
45	LMT	f	1101	-	36,36,36	1.21	3 (8%)	47,47,47	0.92	0
45	LMT	l	201	-	36,36,36	1.22	3 (8%)	47,47,47	1.11	4 (8%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
45	LMT	J	702	-	36,36,36	1.24	3 (8%)	47,47,47	0.97	2 (4%)
57	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.52	5 (13%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
51	3PE	I	201	-	50,50,50	0.88	3 (6%)	53,55,55	1.07	2 (3%)
52	CDL	J	701	-	61,61,99	1.11	7 (11%)	67,73,111	1.30	5 (7%)
45	LMT	b	301	-	36,36,36	1.14	2 (5%)	47,47,47	1.02	3 (6%)
51	3PE	H	401	-	43,43,50	0.93	3 (6%)	46,48,55	1.09	2 (4%)
45	LMT	M	602	-	36,36,36	1.19	2 (5%)	47,47,47	0.84	1 (2%)
45	LMT	j	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.19	3 (6%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
45	LMT	Y	801	-	36,36,36	1.23	3 (8%)	47,47,47	1.12	4 (8%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-

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	LMT	A	701	-	-	13/21/61/61	0/2/2/2
53	GTP	O	401	54	-	7/22/38/38	0/3/3/3
47	SF4	B	201	2	-	-	0/6/5/5
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
48	FES	G	803	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	A	702	-	-	3/22/22/57	-
57	EHZ	T	101	20	-	12/42/44/45	-
46	PC1	M	604	-	-	19/52/52/57	-
46	PC1	P	401	-	-	20/57/57/57	-
52	CDL	q	201	-	-	23/86/86/110	-
51	3PE	L	701	-	-	18/52/52/54	-
58	MYR	o	201	40	-	9/12/12/13	-
47	SF4	G	801	7	-	-	0/6/5/5
55	NDP	P	402	-	-	4/34/77/77	0/5/5/5
47	SF4	G	802	7	-	-	0/6/5/5
51	3PE	Y	802	-	-	17/38/38/54	-
51	3PE	d	1201	-	-	27/54/54/54	-
51	3PE	d	1202	-	-	24/54/54/54	-
52	CDL	h	1001	-	-	35/77/77/110	-
51	3PE	M	601	-	-	16/49/49/54	-
52	CDL	K	401	-	-	31/81/81/110	-
52	CDL	L	703	-	-	34/79/79/110	-
51	3PE	d	1203	-	-	24/54/54/54	-
45	LMT	L	702	-	-	9/21/61/61	0/2/2/2
47	SF4	I	202	9	-	-	0/6/5/5
51	3PE	L	704	-	-	14/48/48/54	-
51	3PE	H	402	-	-	17/36/36/54	-
46	PC1	B	202	-	-	17/38/38/57	-
51	3PE	M	603	-	-	17/54/54/54	-
45	LMT	f	1101	-	-	9/21/61/61	0/2/2/2
45	LMT	l	201	-	-	8/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
45	LMT	J	702	-	-	7/21/61/61	0/2/2/2
57	EHZ	U	101	20	-	6/42/44/45	-
47	SF4	I	203	9	-	-	0/6/5/5
51	3PE	I	201	-	-	20/54/54/54	-
52	CDL	J	701	-	-	31/71/71/110	-
45	LMT	b	301	-	-	4/21/61/61	0/2/2/2
51	3PE	H	401	-	-	15/47/47/54	-
45	LMT	M	602	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	j	101	-	-	6/21/61/61	0/2/2/2
45	LMT	h	1002	-	-	6/21/61/61	0/2/2/2
45	LMT	Y	801	-	-	8/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	402	NDP	P2B-O2B	12.29	1.81	1.59
53	O	401	GTP	O6-C6	8.67	1.40	1.23
53	O	401	GTP	C5-N7	6.79	1.52	1.39
46	A	702	PC1	O21-C2	-5.01	1.40	1.46
57	T	101	EHZ	C12-N1	4.98	1.45	1.33
57	U	101	EHZ	C15-N2	4.95	1.45	1.33
57	U	101	EHZ	C12-N1	4.90	1.45	1.33
53	O	401	GTP	PB-O3A	4.80	1.64	1.59
53	O	401	GTP	C2-N1	4.79	1.49	1.37
57	T	101	EHZ	C15-N2	4.74	1.44	1.33
55	P	402	NDP	PA-O3	4.68	1.64	1.59
53	O	401	GTP	C2-N2	4.63	1.45	1.34
53	O	401	GTP	C2-N3	4.58	1.44	1.33
53	O	401	GTP	PA-O3A	4.55	1.64	1.59
53	O	401	GTP	C8-N9	-4.45	1.27	1.37
51	H	402	3PE	O21-C2	-4.42	1.40	1.46
53	O	401	GTP	PB-O3B	4.36	1.64	1.59
55	P	402	NDP	PN-O5D	4.03	1.75	1.59
45	J	702	LMT	O5B-C1B	3.72	1.51	1.41
53	O	401	GTP	C4-N9	-3.71	1.28	1.38
45	A	701	LMT	O5B-C1B	3.62	1.51	1.41
45	f	1101	LMT	O5B-C1B	3.48	1.50	1.41
45	l	201	LMT	O5B-C1B	3.45	1.50	1.41
45	l	201	LMT	O5'-C1'	3.40	1.50	1.41
45	A	701	LMT	O5'-C1'	3.34	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.34	1.50	1.41
45	Y	801	LMT	O5'-C1'	3.33	1.50	1.41
45	M	602	LMT	O5B-C1B	3.30	1.50	1.41
55	P	402	NDP	O2B-C2B	-3.27	1.32	1.44
45	b	301	LMT	O5B-C1B	3.23	1.50	1.41
45	Y	801	LMT	O5B-C1B	3.19	1.50	1.41
45	f	1101	LMT	O5'-C1'	3.16	1.50	1.41
46	A	702	PC1	O21-C21	3.15	1.40	1.33
45	L	702	LMT	O5B-C1B	3.15	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	H	402	3PE	O21-C21	3.15	1.40	1.33
45	j	101	LMT	O5B-C1B	3.14	1.49	1.41
45	J	702	LMT	O5'-C1'	3.12	1.49	1.41
45	M	602	LMT	O5'-C1'	3.06	1.49	1.41
49	F	501	FMN	C4A-N5	3.02	1.37	1.30
52	L	703	CDL	OA6-CA4	-2.99	1.39	1.46
45	j	101	LMT	O5'-C1'	2.96	1.49	1.41
51	L	701	3PE	O21-C2	-2.95	1.39	1.46
51	M	601	3PE	O21-C2	-2.95	1.39	1.46
51	H	401	3PE	O21-C2	-2.94	1.39	1.46
53	O	401	GTP	O4'-C1'	2.94	1.48	1.42
52	q	201	CDL	OA6-CA4	-2.93	1.39	1.46
45	b	301	LMT	O5'-C1'	2.92	1.49	1.41
52	J	701	CDL	OB6-CB4	-2.91	1.39	1.46
52	L	703	CDL	OB6-CB4	-2.91	1.39	1.46
52	K	401	CDL	OA6-CA4	-2.86	1.39	1.46
52	h	1001	CDL	OA6-CA4	-2.85	1.39	1.46
52	h	1001	CDL	OB6-CB4	-2.84	1.39	1.46
45	L	702	LMT	O5'-C1'	2.84	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.82	1.49	1.41
51	M	603	3PE	O21-C2	-2.81	1.40	1.46
46	M	604	PC1	O21-C2	-2.80	1.40	1.46
51	d	1203	3PE	O21-C2	-2.80	1.40	1.46
51	L	704	3PE	O21-C2	-2.79	1.40	1.46
52	K	401	CDL	OB6-CB4	-2.77	1.40	1.46
51	I	201	3PE	O21-C2	-2.74	1.40	1.46
51	Y	802	3PE	O21-C2	-2.74	1.40	1.46
46	P	401	PC1	O21-C2	-2.72	1.40	1.46
57	U	101	EHZ	O4-C15	-2.70	1.18	1.23
51	L	701	3PE	O31-C3	-2.68	1.39	1.45
52	q	201	CDL	OB6-CB4	-2.68	1.40	1.46
52	J	701	CDL	OB8-CB6	-2.64	1.39	1.45
53	O	401	GTP	C2'-C3'	-2.61	1.46	1.53
57	T	101	EHZ	O4-C15	-2.58	1.18	1.23
46	B	202	PC1	O21-C2	-2.55	1.40	1.46
52	q	201	CDL	OB8-CB7	2.53	1.40	1.33
51	d	1203	3PE	O31-C3	-2.50	1.39	1.45
52	J	701	CDL	OA6-CA5	2.49	1.40	1.35
52	K	401	CDL	OA8-CA6	-2.49	1.39	1.45
51	M	601	3PE	O31-C3	-2.48	1.39	1.45
51	H	402	3PE	O31-C31	2.47	1.40	1.33
53	O	401	GTP	PG-O3G	-2.43	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	T	101	EHZ	O3-C12	-2.43	1.18	1.23
52	J	701	CDL	OA8-CA7	2.42	1.40	1.33
51	Y	802	3PE	O31-C31	2.41	1.40	1.33
51	L	704	3PE	O31-C3	-2.40	1.39	1.45
51	d	1201	3PE	O31-C31	2.40	1.40	1.33
52	h	1001	CDL	OA8-CA7	2.40	1.40	1.33
52	L	703	CDL	OA8-CA7	2.40	1.40	1.33
51	M	603	3PE	O31-C3	-2.40	1.39	1.45
53	O	401	GTP	PG-O2G	-2.39	1.45	1.54
52	L	703	CDL	OB8-CB7	2.39	1.40	1.33
51	H	401	3PE	O31-C3	-2.38	1.39	1.45
57	U	101	EHZ	O3-C12	-2.36	1.18	1.23
52	K	401	CDL	OB8-CB7	2.36	1.40	1.33
51	d	1201	3PE	O21-C2	-2.36	1.41	1.46
52	q	201	CDL	OA8-CA7	2.35	1.40	1.33
51	I	201	3PE	O31-C3	-2.34	1.39	1.45
51	Y	802	3PE	O31-C3	-2.34	1.39	1.45
46	M	604	PC1	O31-C3	-2.33	1.40	1.45
46	B	202	PC1	O31-C31	2.31	1.40	1.33
51	d	1202	3PE	O21-C2	-2.31	1.41	1.46
52	h	1001	CDL	OB8-CB7	2.30	1.40	1.33
51	I	201	3PE	O31-C31	2.30	1.40	1.33
52	J	701	CDL	OA6-CA4	-2.29	1.41	1.46
51	M	603	3PE	O31-C31	2.28	1.40	1.33
51	M	601	3PE	O31-C31	2.27	1.40	1.33
52	K	401	CDL	OA8-CA7	2.27	1.40	1.33
46	M	604	PC1	O31-C31	2.27	1.40	1.33
45	Y	801	LMT	O5'-C5'	2.26	1.49	1.44
52	q	201	CDL	OA8-CA6	-2.26	1.40	1.45
52	h	1001	CDL	OB8-CB6	-2.25	1.40	1.45
52	K	401	CDL	OB8-CB6	-2.25	1.40	1.45
52	L	703	CDL	OB8-CB6	-2.24	1.40	1.45
46	P	401	PC1	O31-C31	2.24	1.39	1.33
51	d	1202	3PE	O31-C3	-2.24	1.40	1.45
51	H	401	3PE	O31-C31	2.23	1.39	1.33
45	J	702	LMT	O5B-C5B	2.23	1.49	1.44
46	B	202	PC1	O21-C21	2.23	1.40	1.34
52	J	701	CDL	OA8-CA6	-2.21	1.40	1.45
51	L	704	3PE	O31-C31	2.21	1.39	1.33
46	B	202	PC1	O31-C3	-2.20	1.40	1.45
46	A	702	PC1	O31-C3	-2.18	1.40	1.45
46	P	401	PC1	O31-C3	-2.18	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	703	CDL	OA8-CA6	-2.18	1.40	1.45
52	h	1001	CDL	OA8-CA6	-2.16	1.40	1.45
49	F	501	FMN	C10-N1	2.15	1.37	1.33
52	K	401	CDL	OB6-CB5	2.15	1.40	1.34
51	d	1201	3PE	O31-C3	-2.14	1.40	1.45
57	T	101	EHZ	C9-S1	2.13	1.81	1.76
45	f	1101	LMT	O5B-C5B	2.13	1.49	1.44
51	d	1201	3PE	O21-C21	2.12	1.40	1.34
51	L	701	3PE	O31-C31	2.11	1.39	1.33
51	d	1202	3PE	O31-C31	2.11	1.39	1.33
52	q	201	CDL	OB8-CB6	-2.10	1.40	1.45
45	l	201	LMT	O5B-C5B	2.07	1.49	1.44
51	M	601	3PE	O21-C21	2.07	1.40	1.34
51	d	1203	3PE	O21-C21	2.07	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.06	1.40	1.34
51	d	1203	3PE	O31-C31	2.05	1.39	1.33
51	H	402	3PE	O31-C3	-2.05	1.40	1.45
52	J	701	CDL	OB6-CB5	2.05	1.40	1.34
52	q	201	CDL	OB6-CB5	2.04	1.40	1.34
52	K	401	CDL	OA6-CA5	2.03	1.40	1.34
51	L	704	3PE	O21-C21	2.03	1.40	1.34
51	d	1202	3PE	O21-C21	2.03	1.40	1.34
45	A	701	LMT	O1B-C4'	2.02	1.49	1.43
57	U	101	EHZ	C9-S1	2.01	1.81	1.76
53	O	401	GTP	PA-O2A	-2.01	1.46	1.55
53	O	401	GTP	PB-O2B	-2.00	1.46	1.55

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	T	101	EHZ	C8-C9-S1	7.72	123.30	113.56
53	O	401	GTP	C8-N9-C4	7.43	119.96	106.03
57	U	101	EHZ	C8-C9-S1	5.97	121.10	113.56
45	A	701	LMT	C1-O1'-C1'	5.32	122.77	113.68
52	J	701	CDL	OA6-CA5-C11	5.08	120.15	111.09
51	H	402	3PE	O21-C21-O22	-4.78	119.57	125.70
46	A	702	PC1	O21-C21-O22	-4.67	119.70	125.70
52	J	701	CDL	OB6-CB5-C51	4.67	121.58	111.48
51	L	704	3PE	O21-C21-C22	4.54	121.30	111.48
46	P	401	PC1	O21-C21-C22	4.37	120.94	111.48
51	L	701	3PE	O21-C21-C22	4.36	120.91	111.48
52	h	1001	CDL	OB6-CB5-C51	4.36	120.91	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	202	PC1	O21-C21-C22	4.21	120.59	111.48
51	I	201	3PE	O21-C21-C22	4.18	120.52	111.48
52	h	1001	CDL	OA6-CA5-C11	4.11	120.37	111.48
51	d	1203	3PE	O21-C21-C22	4.07	120.28	111.48
51	Y	802	3PE	O21-C21-C22	4.01	120.17	111.48
51	d	1201	3PE	O21-C21-C22	3.97	120.06	111.48
52	q	201	CDL	OB6-CB5-C51	3.91	119.94	111.48
55	P	402	NDP	O2B-P2B-O1X	-3.82	95.73	109.33
52	K	401	CDL	OB6-CB5-C51	3.79	119.68	111.48
51	d	1202	3PE	O21-C21-C22	3.78	119.65	111.48
57	T	101	EHZ	C10-S1-C9	3.75	112.94	101.84
52	q	201	CDL	OA6-CA5-C11	3.74	119.58	111.48
51	H	401	3PE	O21-C21-C22	3.72	119.53	111.48
51	M	603	3PE	O21-C21-C22	3.71	119.51	111.48
46	M	604	PC1	O21-C21-C22	3.70	119.48	111.48
52	L	703	CDL	OB6-CB5-C51	3.70	119.48	111.48
52	L	703	CDL	OA6-CA5-C11	3.68	119.45	111.48
45	j	101	LMT	C3B-C4B-C5B	3.68	116.90	110.23
55	P	402	NDP	P2B-O2B-C2B	-3.65	113.68	123.43
45	A	701	LMT	O5B-C1B-C2B	3.62	117.81	110.37
45	A	701	LMT	O1'-C1'-C2'	3.58	113.70	108.27
52	K	401	CDL	OA6-CA5-C11	3.55	119.17	111.48
57	T	101	EHZ	O2-C9-S1	-3.54	118.18	122.68
45	A	701	LMT	O5B-C5B-C4B	3.48	115.96	109.70
45	A	701	LMT	C1B-O5B-C5B	3.46	120.47	113.72
55	P	402	NDP	O3-PA-O1A	-3.46	100.30	110.70
49	F	501	FMN	C4-N3-C2	-3.45	119.51	125.64
57	T	101	EHZ	O2-C9-C8	-3.31	118.53	123.74
53	O	401	GTP	C2-N1-C6	-3.21	119.29	125.11
51	d	1201	3PE	O31-C31-C32	3.16	121.47	111.83
57	T	101	EHZ	C13-C14-N2	-3.07	105.46	112.00
52	h	1001	CDL	OB8-CB7-C71	3.07	121.20	111.83
51	M	601	3PE	O21-C21-C22	3.07	118.11	111.48
51	M	603	3PE	O31-C31-C32	3.06	121.17	111.83
52	h	1001	CDL	OA8-CA7-C31	3.05	121.15	111.83
51	Y	802	3PE	O31-C31-C32	3.04	121.09	111.83
57	T	101	EHZ	C13-C12-N1	3.03	121.86	116.34
45	Y	801	LMT	C1'-O5'-C5'	2.97	119.51	113.72
49	F	501	FMN	C4A-C10-N10	2.95	120.70	116.48
45	j	101	LMT	C4B-C3B-C2B	2.95	116.00	110.83
46	M	604	PC1	O31-C31-C32	2.86	120.55	111.83
52	q	201	CDL	OA8-CA7-C31	2.85	120.54	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	K	401	CDL	OB8-CB7-C71	2.82	120.42	111.83
53	O	401	GTP	O2G-PG-O3B	2.80	114.04	104.64
55	P	402	NDP	PA-O5B-C5B	-2.80	105.29	121.35
51	H	401	3PE	O31-C31-C32	2.76	120.26	111.83
45	Y	801	LMT	O5'-C5'-C4'	2.76	115.43	109.72
51	L	701	3PE	O31-C31-C32	2.76	120.25	111.83
53	O	401	GTP	O3G-PG-O3B	2.73	113.78	104.64
55	P	402	NDP	O2N-PN-O3	2.72	114.64	107.27
52	L	703	CDL	OB8-CB7-C71	2.71	120.11	111.83
45	j	101	LMT	O5B-C5B-C4B	2.71	114.59	109.70
46	B	202	PC1	O31-C31-C32	2.70	120.08	111.83
57	U	101	EHZ	O2-C9-C8	-2.70	119.49	123.74
51	H	402	3PE	O31-C31-C32	2.69	120.03	111.83
52	q	201	CDL	OB8-CB7-C71	2.66	119.95	111.83
51	d	1202	3PE	O31-C31-C32	2.65	119.93	111.83
55	P	402	NDP	PN-O5D-C5D	-2.65	106.17	121.35
49	F	501	FMN	C4A-C4-N3	2.64	119.97	113.25
52	J	701	CDL	OB8-CB7-C71	2.63	119.87	111.83
53	O	401	GTP	C1'-N9-C8	-2.63	119.25	126.73
51	I	201	3PE	O31-C31-C32	2.62	119.84	111.83
45	A	701	LMT	C1B-C2B-C3B	2.62	115.52	110.01
46	P	401	PC1	O31-C31-C32	2.62	119.81	111.83
52	J	701	CDL	OA8-CA7-C31	2.61	119.80	111.83
52	L	703	CDL	OA8-CA7-C31	2.61	119.78	111.83
49	F	501	FMN	O4-C4-C4A	-2.60	119.67	126.53
51	M	601	3PE	O31-C31-C32	2.58	119.69	111.83
55	P	402	NDP	O3X-P2B-O2X	2.57	117.44	107.80
57	U	101	EHZ	O2-C9-S1	-2.57	119.41	122.68
45	l	201	LMT	C3B-C4B-C5B	2.56	114.88	110.23
45	l	201	LMT	O5B-C5B-C4B	2.56	114.31	109.70
53	O	401	GTP	O2A-PA-O1A	-2.54	100.63	112.44
53	O	401	GTP	C5-C6-N1	2.53	119.70	113.25
53	O	401	GTP	O2B-PB-O1B	-2.48	100.92	112.44
51	d	1203	3PE	O31-C31-C32	2.47	119.36	111.83
45	l	201	LMT	O5'-C1'-C2'	2.47	115.44	110.37
45	Y	801	LMT	C1B-O1B-C4'	-2.46	112.14	117.98
45	L	702	LMT	C1B-O5B-C5B	-2.46	108.92	113.72
55	P	402	NDP	N3A-C4A-N9A	2.45	131.33	127.17
51	L	704	3PE	O31-C31-C32	2.44	119.28	111.83
55	P	402	NDP	C2A-N1A-C6A	-2.44	114.73	118.73
57	U	101	EHZ	C10-S1-C9	2.39	108.92	101.84
45	Y	801	LMT	C3B-C4B-C5B	2.32	114.44	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	T	101	EHZ	C14-N2-C15	-2.32	118.38	122.55
55	P	402	NDP	O4B-C4B-C3B	2.32	109.75	105.15
53	O	401	GTP	O6-C6-C5	-2.31	120.44	126.53
53	O	401	GTP	C5-C4-N9	-2.28	101.58	105.66
51	d	1202	3PE	C3-C2-C1	-2.28	106.48	111.78
55	P	402	NDP	O2N-PN-O1N	2.27	123.03	112.44
45	b	301	LMT	C1B-C2B-C3B	2.26	114.77	110.01
52	K	401	CDL	OA8-CA7-C31	2.25	118.69	111.83
57	T	101	EHZ	C11-N1-C12	-2.24	118.66	122.82
55	P	402	NDP	C5A-C4A-N3A	-2.23	123.64	126.72
55	P	402	NDP	C2B-C1B-N9A	-2.23	110.09	113.75
55	P	402	NDP	O5D-PN-O1N	-2.22	100.13	108.94
55	P	402	NDP	O3X-P2B-O2B	-2.19	97.30	105.85
49	F	501	FMN	C10-C4A-N5	-2.19	120.33	124.81
45	M	602	LMT	O5'-C5'-C4'	2.17	114.20	109.72
51	d	1202	3PE	O21-C2-C3	2.14	116.03	108.34
45	A	701	LMT	C6B-C5B-C4B	-2.14	107.77	113.02
45	h	1002	LMT	C1B-O1B-C4'	-2.13	112.92	117.98
55	P	402	NDP	O7N-C7N-N7N	-2.13	118.12	122.89
55	P	402	NDP	O7N-C7N-C3N	2.13	124.90	120.90
45	b	301	LMT	C4B-C3B-C2B	2.12	114.56	110.83
51	L	704	3PE	C2-O21-C21	-2.12	112.71	117.80
57	U	101	EHZ	C16-C15-N2	2.12	120.50	116.48
45	b	301	LMT	C1B-O5B-C5B	-2.12	109.59	113.72
45	J	702	LMT	O5B-C5B-C4B	2.10	113.49	109.70
49	F	501	FMN	C4A-C10-N1	-2.09	119.47	124.59
45	J	702	LMT	O1B-C4'-C3'	2.03	112.38	107.23
45	l	201	LMT	C1B-O1B-C4'	-2.02	113.20	117.98
52	J	701	CDL	OB6-CB5-OB7	-2.01	119.01	123.70
53	O	401	GTP	N9-C8-N7	-2.01	109.68	113.40

There are no chirality outliers.

All (540) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	701	LMT	C2'-C1'-O1'-C1
45	A	701	LMT	O5'-C1'-O1'-C1
45	L	702	LMT	C2-C1-O1'-C1'
45	f	1101	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	O5'-C1'-O1'-C1
46	A	702	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	A	702	PC1	O22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	P	401	PC1	C1-O11-P-O14
46	P	401	PC1	C1-O11-P-O13
51	H	401	3PE	C1-O11-P-O14
51	H	402	3PE	C11-O13-P-O11
51	H	402	3PE	C11-O13-P-O12
51	H	402	3PE	C11-O13-P-O14
51	H	402	3PE	O13-C11-C12-N
51	H	402	3PE	C1-C2-O21-C21
51	H	402	3PE	O22-C21-O21-C2
51	I	201	3PE	C1-O11-P-O12
51	I	201	3PE	C1-O11-P-O13
51	I	201	3PE	C11-O13-P-O11
51	I	201	3PE	C11-O13-P-O14
51	I	201	3PE	O13-C11-C12-N
51	L	701	3PE	C22-C21-O21-C2
51	L	704	3PE	C11-O13-P-O11
51	L	704	3PE	C11-O13-P-O12
51	L	704	3PE	C11-O13-P-O14
51	L	704	3PE	O13-C11-C12-N
51	M	601	3PE	O13-C11-C12-N
51	M	603	3PE	C1-O11-P-O12
51	M	603	3PE	C1-O11-P-O13
51	M	603	3PE	C1-O11-P-O14
51	Y	802	3PE	C22-C21-O21-C2
51	d	1201	3PE	C11-O13-P-O11
51	d	1201	3PE	C11-O13-P-O12
51	d	1201	3PE	C11-O13-P-O14
51	d	1201	3PE	O13-C11-C12-N
51	d	1201	3PE	O32-C31-O31-C3
51	d	1201	3PE	C32-C31-O31-C3
51	d	1201	3PE	C22-C21-O21-C2
51	d	1202	3PE	C1-O11-P-O13
51	d	1202	3PE	C1-O11-P-O14
51	d	1202	3PE	C11-O13-P-O14
51	d	1202	3PE	O22-C21-O21-C2
51	d	1202	3PE	C22-C21-O21-C2
51	d	1203	3PE	C1-O11-P-O12
51	d	1203	3PE	C1-O11-P-O13
51	d	1203	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
51	d	1203	3PE	O22-C21-O21-C2
51	d	1203	3PE	C22-C21-O21-C2
52	J	701	CDL	CA2-OA2-PA1-OA4
52	J	701	CDL	CA2-OA2-PA1-OA5
52	J	701	CDL	CA3-OA5-PA1-OA2
52	J	701	CDL	CA3-OA5-PA1-OA4
52	J	701	CDL	C11-CA5-OA6-CA4
52	J	701	CDL	OB7-CB5-OB6-CB4
52	K	401	CDL	CB2-C1-CA2-OA2
52	K	401	CDL	CB2-OB2-PB2-OB3
52	K	401	CDL	CB2-OB2-PB2-OB4
52	K	401	CDL	CB2-OB2-PB2-OB5
52	L	703	CDL	CB2-C1-CA2-OA2
52	L	703	CDL	CA2-OA2-PA1-OA3
52	L	703	CDL	CA2-OA2-PA1-OA4
52	L	703	CDL	CA2-OA2-PA1-OA5
52	L	703	CDL	CA3-OA5-PA1-OA2
52	L	703	CDL	CA3-OA5-PA1-OA3
52	L	703	CDL	CB3-OB5-PB2-OB2
52	L	703	CDL	CB3-OB5-PB2-OB4
52	h	1001	CDL	O1-C1-CB2-OB2
52	h	1001	CDL	CA2-OA2-PA1-OA4
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CB2-OB2-PB2-OB4
52	h	1001	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	CB3-OB5-PB2-OB4
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	q	201	CDL	O1-C1-CA2-OA2
52	q	201	CDL	CB2-C1-CA2-OA2
52	q	201	CDL	CB2-OB2-PB2-OB4
52	q	201	CDL	CB2-OB2-PB2-OB5
53	O	401	GTP	C5'-O5'-PA-O3A
53	O	401	GTP	C5'-O5'-PA-O1A
57	T	101	EHZ	C11-C10-S1-C9
57	T	101	EHZ	C16-C17-C20-O6
57	T	101	EHZ	C18-C17-C20-O6
57	T	101	EHZ	C19-C17-C20-O6
57	T	101	EHZ	O2-C9-S1-C10
57	T	101	EHZ	C8-C9-S1-C10
57	U	101	EHZ	C5-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
58	o	201	MYR	O1-C1-C2-C3
52	J	701	CDL	OA7-CA5-OA6-CA4
45	J	702	LMT	O5B-C1B-O1B-C4'
51	H	401	3PE	O32-C31-O31-C3
51	H	402	3PE	O32-C31-O31-C3
51	M	603	3PE	O32-C31-O31-C3
51	Y	802	3PE	O32-C31-O31-C3
51	L	701	3PE	O22-C21-O21-C2
51	L	704	3PE	O22-C21-O21-C2
51	Y	802	3PE	O22-C21-O21-C2
52	L	703	CDL	OA7-CA5-OA6-CA4
52	q	201	CDL	OA7-CA5-OA6-CA4
45	l	201	LMT	C4'-C5'-C6'-O6'
51	H	401	3PE	C32-C31-O31-C3
51	H	402	3PE	C32-C31-O31-C3
51	Y	802	3PE	C32-C31-O31-C3
45	M	602	LMT	O5B-C5B-C6B-O6B
51	L	704	3PE	C22-C21-O21-C2
52	J	701	CDL	C51-CB5-OB6-CB4
52	L	703	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C51-CB5-OB6-CB4
52	q	201	CDL	C11-CA5-OA6-CA4
45	M	602	LMT	O5'-C5'-C6'-O6'
45	A	701	LMT	O5'-C5'-C6'-O6'
45	J	702	LMT	C3'-C4'-O1B-C1B
46	M	604	PC1	C32-C31-O31-C3
51	M	603	3PE	C32-C31-O31-C3
52	J	701	CDL	C31-CA7-OA8-CA6
52	K	401	CDL	C71-CB7-OB8-CB6
45	l	201	LMT	O5'-C5'-C6'-O6'
52	J	701	CDL	OA9-CA7-OA8-CA6
51	d	1201	3PE	O22-C21-O21-C2
45	A	701	LMT	C5'-C4'-O1B-C1B
52	J	701	CDL	O1-C1-CA2-OA2
46	B	202	PC1	C32-C31-O31-C3
51	L	701	3PE	C32-C31-O31-C3
52	K	401	CDL	OB9-CB7-OB8-CB6
45	j	101	LMT	C4'-C5'-C6'-O6'
52	K	401	CDL	C51-CB5-OB6-CB4
45	f	1101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
45	M	602	LMT	C4B-C5B-C6B-O6B
45	M	602	LMT	C4'-C5'-C6'-O6'
46	M	604	PC1	O32-C31-O31-C3
52	K	401	CDL	OB7-CB5-OB6-CB4
45	Y	801	LMT	O5B-C5B-C6B-O6B
45	Y	801	LMT	C4'-C5'-C6'-O6'
45	h	1002	LMT	C4'-C5'-C6'-O6'
46	B	202	PC1	O32-C31-O31-C3
45	A	701	LMT	C4'-C5'-C6'-O6'
45	L	702	LMT	O5'-C5'-C6'-O6'
51	L	701	3PE	O32-C31-O31-C3
45	h	1002	LMT	C2-C3-C4-C5
52	h	1001	CDL	CA2-C1-CB2-OB2
51	L	704	3PE	C32-C31-O31-C3
52	h	1001	CDL	C71-CB7-OB8-CB6
45	b	301	LMT	O5B-C5B-C6B-O6B
45	l	201	LMT	O5B-C5B-C6B-O6B
45	j	101	LMT	O5'-C5'-C6'-O6'
45	f	1101	LMT	C4'-C5'-C6'-O6'
52	h	1001	CDL	OB9-CB7-OB8-CB6
52	J	701	CDL	OB5-CB3-CB4-OB6
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	Y	801	LMT	C4B-C5B-C6B-O6B
51	H	401	3PE	C31-C32-C33-C34
52	K	401	CDL	CA5-C11-C12-C13
51	L	704	3PE	O32-C31-O31-C3
46	B	202	PC1	C21-C22-C23-C24
52	K	401	CDL	CB5-C51-C52-C53
52	L	703	CDL	CA5-C11-C12-C13
52	K	401	CDL	O1-C1-CA2-OA2
52	J	701	CDL	C71-CB7-OB8-CB6
45	Y	801	LMT	O5'-C5'-C6'-O6'
52	L	703	CDL	CA7-C31-C32-C33
52	h	1001	CDL	C31-CA7-OA8-CA6
45	b	301	LMT	C4B-C5B-C6B-O6B
51	I	201	3PE	C22-C21-O21-C2
51	I	201	3PE	O22-C21-O21-C2
45	f	1101	LMT	C3'-C4'-O1B-C1B
52	J	701	CDL	CB2-C1-CA2-OA2
45	L	702	LMT	O5B-C5B-C6B-O6B
45	l	201	LMT	O1'-C1-C2-C3
52	L	703	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	OA7-CA5-OA6-CA4
52	K	401	CDL	CB4-CB3-OB5-PB2
51	L	704	3PE	C21-C22-C23-C24
51	d	1202	3PE	C3-C2-O21-C21
52	h	1001	CDL	OA9-CA7-OA8-CA6
45	J	702	LMT	O5'-C5'-C6'-O6'
51	M	603	3PE	C3D-C3E-C3F-C3G
51	d	1203	3PE	C3C-C3D-C3E-C3F
51	d	1203	3PE	C22-C23-C24-C25
52	h	1001	CDL	C13-C14-C15-C16
52	h	1001	CDL	C31-C32-C33-C34
46	M	604	PC1	C27-C28-C29-C2A
51	L	704	3PE	C33-C34-C35-C36
51	M	601	3PE	C26-C27-C28-C29
52	J	701	CDL	C73-C74-C75-C76
45	j	101	LMT	C5-C6-C7-C8
46	P	401	PC1	C2C-C2D-C2E-C2F
52	J	701	CDL	C77-C78-C79-C80
51	L	701	3PE	C2D-C2E-C2F-C2G
46	P	401	PC1	C2A-C2B-C2C-C2D
46	M	604	PC1	C2B-C2C-C2D-C2E
51	M	603	3PE	C22-C21-O21-C2
45	j	101	LMT	C7-C8-C9-C10
51	d	1202	3PE	C24-C25-C26-C27
57	U	101	EHZ	C21-C1-C2-C3
52	L	703	CDL	O1-C1-CA2-OA2
45	f	1101	LMT	C5'-C4'-O1B-C1B
45	A	701	LMT	C11-C10-C9-C8
52	J	701	CDL	OB9-CB7-OB8-CB6
46	P	401	PC1	C25-C26-C27-C28
51	L	701	3PE	C23-C24-C25-C26
51	d	1203	3PE	C36-C37-C38-C39
52	L	703	CDL	OB9-CB7-OB8-CB6
51	L	701	3PE	C29-C2A-C2B-C2C
51	d	1201	3PE	C29-C2A-C2B-C2C
51	M	603	3PE	C35-C36-C37-C38
51	d	1202	3PE	C39-C3A-C3B-C3C
51	d	1202	3PE	C26-C27-C28-C29
46	M	604	PC1	C31-C32-C33-C34
46	B	202	PC1	C24-C25-C26-C27
46	M	604	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
51	M	603	3PE	C2D-C2E-C2F-C2G
51	d	1202	3PE	C23-C24-C25-C26
58	o	201	MYR	C3-C4-C5-C6
46	M	604	PC1	C23-C24-C25-C26
51	L	701	3PE	C3A-C3B-C3C-C3D
46	M	604	PC1	C33-C34-C35-C36
51	M	601	3PE	C35-C36-C37-C38
51	d	1203	3PE	C29-C2A-C2B-C2C
58	o	201	MYR	C10-C11-C12-C13
51	d	1203	3PE	C31-C32-C33-C34
46	M	604	PC1	C2-C1-O11-P
51	d	1201	3PE	C26-C27-C28-C29
46	M	604	PC1	C2D-C2E-C2F-C2G
51	M	603	3PE	C23-C24-C25-C26
52	q	201	CDL	C38-C39-C40-C41
52	L	703	CDL	C31-CA7-OA8-CA6
46	M	604	PC1	C37-C38-C39-C3A
45	A	701	LMT	C7-C8-C9-C10
51	H	402	3PE	C35-C36-C37-C38
51	I	201	3PE	C29-C2A-C2B-C2C
52	h	1001	CDL	C17-C18-C19-C20
46	B	202	PC1	C22-C21-O21-C2
51	M	601	3PE	C22-C21-O21-C2
45	M	602	LMT	C9-C10-C11-C12
45	J	702	LMT	C5'-C4'-O1B-C1B
51	M	603	3PE	O22-C21-O21-C2
52	L	703	CDL	C38-C39-C40-C41
58	o	201	MYR	C9-C10-C11-C12
46	P	401	PC1	C31-C32-C33-C34
51	L	701	3PE	C21-C22-C23-C24
45	Y	801	LMT	C3'-C4'-O1B-C1B
51	M	601	3PE	C39-C3A-C3B-C3C
45	Y	801	LMT	C5'-C4'-O1B-C1B
51	H	401	3PE	C3D-C3E-C3F-C3G
52	q	201	CDL	C58-C59-C60-C61
46	B	202	PC1	O22-C21-O21-C2
46	M	604	PC1	C34-C35-C36-C37
51	I	201	3PE	C33-C34-C35-C36
51	d	1203	3PE	C27-C28-C29-C2A
46	P	401	PC1	C21-C22-C23-C24
51	H	401	3PE	C21-C22-C23-C24
51	d	1201	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
52	J	701	CDL	C75-C76-C77-C78
45	f	1101	LMT	O1'-C1-C2-C3
52	h	1001	CDL	C16-C17-C18-C19
52	q	201	CDL	C52-C53-C54-C55
58	o	201	MYR	C6-C7-C8-C9
58	o	201	MYR	C5-C6-C7-C8
45	J	702	LMT	O1'-C1-C2-C3
51	Y	802	3PE	C37-C38-C39-C3A
52	q	201	CDL	C57-C58-C59-C60
52	h	1001	CDL	C14-C15-C16-C17
45	L	702	LMT	C5-C6-C7-C8
51	d	1201	3PE	C2E-C2F-C2G-C2H
52	J	701	CDL	C72-C73-C74-C75
45	Y	801	LMT	C1-C2-C3-C4
51	I	201	3PE	C3A-C3B-C3C-C3D
51	L	701	3PE	C25-C26-C27-C28
52	L	703	CDL	OA9-CA7-OA8-CA6
52	K	401	CDL	C52-C53-C54-C55
52	q	201	CDL	C51-C52-C53-C54
52	J	701	CDL	OB5-CB3-CB4-CB6
52	K	401	CDL	OB5-CB3-CB4-CB6
52	h	1001	CDL	OA5-CA3-CA4-CA6
57	U	101	EHZ	C5-C6-C7-C8
51	H	402	3PE	C3D-C3E-C3F-C3G
45	J	702	LMT	O5B-C5B-C6B-O6B
52	K	401	CDL	C11-CA5-OA6-CA4
52	q	201	CDL	C56-C57-C58-C59
52	K	401	CDL	C53-C54-C55-C56
51	M	603	3PE	C1-C2-C3-O31
51	d	1201	3PE	C1-C2-C3-O31
58	o	201	MYR	C11-C10-C9-C8
51	L	701	3PE	C33-C34-C35-C36
52	L	703	CDL	C34-C35-C36-C37
51	M	601	3PE	C33-C34-C35-C36
52	J	701	CDL	C78-C79-C80-C81
52	J	701	CDL	C51-C52-C53-C54
45	M	602	LMT	C5-C6-C7-C8
45	L	702	LMT	C4'-C5'-C6'-O6'
51	H	402	3PE	C34-C35-C36-C37
46	P	401	PC1	C2E-C2F-C2G-C2H
51	H	401	3PE	C27-C28-C29-C2A
51	L	701	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
45	L	702	LMT	O1'-C1-C2-C3
46	P	401	PC1	C26-C27-C28-C29
45	A	701	LMT	C3'-C4'-O1B-C1B
51	L	701	3PE	C2F-C2G-C2H-C2I
52	L	703	CDL	C54-C55-C56-C57
52	q	201	CDL	C71-C72-C73-C74
52	L	703	CDL	C60-C61-C62-C63
51	M	603	3PE	C3A-C3B-C3C-C3D
46	B	202	PC1	C33-C34-C35-C36
51	M	601	3PE	O22-C21-O21-C2
52	L	703	CDL	C71-C72-C73-C74
52	K	401	CDL	C40-C41-C42-C43
52	h	1001	CDL	C15-C16-C17-C18
45	A	701	LMT	C2-C1-O1'-C1'
45	Y	801	LMT	C2-C1-O1'-C1'
45	l	201	LMT	C2-C1-O1'-C1'
51	Y	802	3PE	C32-C33-C34-C35
57	T	101	EHZ	S1-C10-C11-N1
51	d	1203	3PE	C38-C39-C3A-C3B
45	L	702	LMT	C6-C7-C8-C9
45	M	602	LMT	C2'-C1'-O1'-C1
45	f	1101	LMT	C2'-C1'-O1'-C1
46	B	202	PC1	C32-C33-C34-C35
51	d	1201	3PE	C32-C33-C34-C35
46	P	401	PC1	O11-C1-C2-C3
51	Y	802	3PE	O11-C1-C2-C3
51	d	1201	3PE	O11-C1-C2-C3
52	h	1001	CDL	OB5-CB3-CB4-CB6
45	j	101	LMT	C3-C4-C5-C6
51	I	201	3PE	C36-C37-C38-C39
51	L	701	3PE	C28-C29-C2A-C2B
45	l	201	LMT	C4B-C5B-C6B-O6B
46	B	202	PC1	C1-C2-C3-O31
51	H	402	3PE	C1-C2-C3-O31
51	Y	802	3PE	C1-C2-C3-O31
52	L	703	CDL	CB3-CB4-CB6-OB8
51	H	402	3PE	C33-C34-C35-C36
51	M	601	3PE	C3A-C3B-C3C-C3D
52	h	1001	CDL	C52-C53-C54-C55
51	d	1202	3PE	C29-C2A-C2B-C2C
45	A	701	LMT	C4B-C5B-C6B-O6B
51	d	1202	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	K	401	CDL	OA7-CA5-OA6-CA4
51	Y	802	3PE	O11-C1-C2-O21
52	h	1001	CDL	OA5-CA3-CA4-OA6
51	L	704	3PE	C34-C35-C36-C37
51	d	1201	3PE	C34-C35-C36-C37
46	B	202	PC1	C2-C1-O11-P
51	d	1203	3PE	C32-C33-C34-C35
57	T	101	EHZ	O1-C7-C8-C9
51	M	601	3PE	O21-C21-C22-C23
46	B	202	PC1	O21-C2-C3-O31
46	M	604	PC1	O21-C2-C3-O31
51	H	402	3PE	O21-C2-C3-O31
51	M	603	3PE	O21-C2-C3-O31
51	Y	802	3PE	O21-C2-C3-O31
51	d	1202	3PE	C2C-C2D-C2E-C2F
51	H	402	3PE	C32-C33-C34-C35
51	d	1202	3PE	C21-C22-C23-C24
57	T	101	EHZ	C6-C7-C8-C9
51	L	704	3PE	C26-C27-C28-C29
51	d	1201	3PE	C3C-C3D-C3E-C3F
52	K	401	CDL	C15-C16-C17-C18
52	K	401	CDL	C35-C36-C37-C38
46	P	401	PC1	C33-C34-C35-C36
51	d	1202	3PE	C3C-C3D-C3E-C3F
58	o	201	MYR	C2-C3-C4-C5
53	O	401	GTP	PB-O3B-PG-O1G
51	Y	802	3PE	C23-C24-C25-C26
57	T	101	EHZ	C2-C3-C4-C5
52	J	701	CDL	CA3-CA4-OA6-CA5
51	Y	802	3PE	C34-C35-C36-C37
46	P	401	PC1	C32-C31-O31-C3
46	P	401	PC1	O11-C1-C2-O21
51	d	1201	3PE	O11-C1-C2-O21
52	h	1001	CDL	OB5-CB3-CB4-OB6
51	M	601	3PE	C12-C11-O13-P
51	d	1201	3PE	O21-C2-C3-O31
52	L	703	CDL	OB6-CB4-CB6-OB8
51	H	402	3PE	C3A-C3B-C3C-C3D
52	K	401	CDL	C11-C12-C13-C14
45	h	1002	LMT	C6-C7-C8-C9
52	q	201	CDL	C16-C17-C18-C19
46	B	202	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	O	401	GTP	PB-O3A-PA-O1A
52	L	703	CDL	C51-C52-C53-C54
51	I	201	3PE	C37-C38-C39-C3A
51	L	701	3PE	C32-C33-C34-C35
52	K	401	CDL	C16-C17-C18-C19
52	q	201	CDL	C11-C12-C13-C14
46	P	401	PC1	O32-C31-O31-C3
51	I	201	3PE	C25-C26-C27-C28
52	q	201	CDL	C59-C60-C61-C62
52	K	401	CDL	OB5-CB3-CB4-OB6
58	o	201	MYR	C11-C12-C13-C14
45	f	1101	LMT	C2-C3-C4-C5
51	I	201	3PE	C38-C39-C3A-C3B
55	P	402	NDP	O4D-C1D-N1N-C6N
52	L	703	CDL	C15-C16-C17-C18
51	I	201	3PE	C32-C31-O31-C3
51	H	401	3PE	C1-C2-C3-O31
51	M	601	3PE	C1-C2-C3-O31
45	A	701	LMT	O1'-C1-C2-C3
51	I	201	3PE	O32-C31-O31-C3
52	K	401	CDL	C37-C38-C39-C40
46	P	401	PC1	C11-O13-P-O14
46	P	401	PC1	C11-O13-P-O11
51	H	401	3PE	O13-C11-C12-N
51	I	201	3PE	C11-O13-P-O12
51	d	1201	3PE	C1-O11-P-O14
51	d	1202	3PE	O13-C11-C12-N
52	J	701	CDL	CB2-OB2-PB2-OB3
52	K	401	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CA3-OA5-PA1-OA3
51	H	402	3PE	C2-C1-O11-P
51	M	601	3PE	C32-C33-C34-C35
52	J	701	CDL	C31-C32-C33-C34
51	d	1201	3PE	C1-C2-O21-C21
51	d	1202	3PE	C2D-C2E-C2F-C2G
51	L	701	3PE	O11-C1-C2-C3
51	d	1203	3PE	C2A-C2B-C2C-C2D
52	L	703	CDL	C31-C32-C33-C34
46	P	401	PC1	O21-C21-C22-C23
45	M	602	LMT	O1'-C1-C2-C3
52	q	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
51	H	401	3PE	O21-C2-C3-O31
46	M	604	PC1	C1-C2-C3-O31
51	d	1202	3PE	C3E-C3F-C3G-C3H
52	L	703	CDL	C35-C36-C37-C38
51	d	1203	3PE	C39-C3A-C3B-C3C
46	M	604	PC1	C29-C2A-C2B-C2C
52	K	401	CDL	C1-CB2-OB2-PB2
52	L	703	CDL	C52-C53-C54-C55
51	H	401	3PE	C36-C37-C38-C39
51	Y	802	3PE	C35-C36-C37-C38
52	h	1001	CDL	OA6-CA4-CA6-OA8
51	Y	802	3PE	C39-C3A-C3B-C3C
45	b	301	LMT	O5'-C1'-O1'-C1
57	T	101	EHZ	C21-C22-C23-C24
51	M	603	3PE	C33-C34-C35-C36
46	B	202	PC1	C31-C32-C33-C34
51	d	1201	3PE	C37-C38-C39-C3A
57	U	101	EHZ	C2-C1-C21-C22
51	d	1203	3PE	C25-C26-C27-C28
52	q	201	CDL	C17-C18-C19-C20
51	M	603	3PE	C3B-C3C-C3D-C3E
52	h	1001	CDL	C73-C74-C75-C76
52	h	1001	CDL	CA6-CA4-OA6-CA5
52	J	701	CDL	C72-C71-CB7-OB8
45	L	702	LMT	C4B-C5B-C6B-O6B
51	d	1203	3PE	C3F-C3G-C3H-C3I
51	L	704	3PE	C2-C1-O11-P
51	Y	802	3PE	C2-C1-O11-P
46	M	604	PC1	C39-C3A-C3B-C3C
52	h	1001	CDL	C20-C21-C22-C23
46	M	604	PC1	C24-C25-C26-C27
51	M	603	3PE	C3F-C3G-C3H-C3I
51	M	601	3PE	O21-C2-C3-O31
52	q	201	CDL	OB6-CB4-CB6-OB8
46	P	401	PC1	C3B-C3C-C3D-C3E
55	P	402	NDP	O4D-C4D-C5D-O5D
51	L	701	3PE	C3D-C3E-C3F-C3G
51	d	1203	3PE	C2B-C2C-C2D-C2E
51	d	1201	3PE	C22-C23-C24-C25
52	L	703	CDL	C58-C59-C60-C61
52	q	201	CDL	CA4-CA3-OA5-PA1
52	q	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
51	d	1202	3PE	C27-C28-C29-C2A
45	A	701	LMT	O5B-C1B-O1B-C4'
52	q	201	CDL	C15-C16-C17-C18
52	L	703	CDL	CA2-C1-CB2-OB2
51	d	1202	3PE	C2E-C2F-C2G-C2H
46	A	702	PC1	O21-C2-C3-O31
52	K	401	CDL	OB6-CB4-CB6-OB8
49	F	501	FMN	C4'-C5'-O5'-P
52	J	701	CDL	CA4-CA3-OA5-PA1
51	M	601	3PE	C37-C38-C39-C3A
51	d	1201	3PE	C38-C39-C3A-C3B
52	J	701	CDL	CA7-C31-C32-C33
52	L	703	CDL	C12-C13-C14-C15
51	d	1203	3PE	C2D-C2E-C2F-C2G
45	b	301	LMT	C4-C5-C6-C7
52	q	201	CDL	C71-CB7-OB8-CB6
53	O	401	GTP	PB-O3B-PG-O2G
53	O	401	GTP	PB-O3B-PG-O3G
45	L	702	LMT	C1-C2-C3-C4
51	Y	802	3PE	C3B-C3C-C3D-C3E
45	h	1002	LMT	C11-C10-C9-C8
52	J	701	CDL	CA3-CA4-CA6-OA8
51	M	601	3PE	C2A-C2B-C2C-C2D
51	M	601	3PE	O22-C21-C22-C23
45	f	1101	LMT	C3-C4-C5-C6
52	K	401	CDL	C33-C34-C35-C36
46	M	604	PC1	C21-C22-C23-C24
51	d	1201	3PE	C3A-C3B-C3C-C3D
51	d	1203	3PE	O31-C31-C32-C33
46	M	604	PC1	C26-C27-C28-C29
51	d	1202	3PE	C3F-C3G-C3H-C3I
51	d	1202	3PE	C38-C39-C3A-C3B
51	d	1201	3PE	C35-C36-C37-C38
46	P	401	PC1	O31-C31-C32-C33
51	H	401	3PE	O21-C21-C22-C23
51	d	1203	3PE	C33-C34-C35-C36
45	h	1002	LMT	C7-C8-C9-C10
51	d	1202	3PE	C32-C33-C34-C35
52	K	401	CDL	C12-C11-CA5-OA6
51	d	1203	3PE	C3A-C3B-C3C-C3D
52	h	1001	CDL	C11-C12-C13-C14
51	H	401	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
55	P	402	NDP	O4B-C4B-C5B-O5B
55	P	402	NDP	C2B-O2B-P2B-O3X
52	L	703	CDL	C32-C31-CA7-OA8
57	T	101	EHZ	C2-C1-C21-C22
45	A	701	LMT	O5B-C5B-C6B-O6B
46	B	202	PC1	O21-C21-C22-C23
49	F	501	FMN	N10-C1'-C2'-O2'
51	d	1203	3PE	C3E-C3F-C3G-C3H
51	L	704	3PE	C38-C39-C3A-C3B
51	H	401	3PE	O22-C21-C22-C23
51	d	1202	3PE	C2A-C2B-C2C-C2D
45	J	702	LMT	C3-C4-C5-C6
51	H	401	3PE	C26-C27-C28-C29
52	L	703	CDL	C32-C31-CA7-OA9
51	Y	802	3PE	C36-C37-C38-C39
52	K	401	CDL	C12-C11-CA5-OA7
51	I	201	3PE	C39-C3A-C3B-C3C
51	I	201	3PE	C26-C27-C28-C29
51	d	1203	3PE	O32-C31-C32-C33
51	d	1201	3PE	C2-C1-O11-P
51	L	701	3PE	O21-C21-C22-C23
46	B	202	PC1	O22-C21-C22-C23
52	J	701	CDL	CA4-CA6-OA8-CA7
46	P	401	PC1	O32-C31-C32-C33
52	K	401	CDL	C72-C71-CB7-OB8
53	O	401	GTP	PG-O3B-PB-O2B
45	j	101	LMT	O1'-C1-C2-C3
51	I	201	3PE	C31-C32-C33-C34
52	J	701	CDL	C54-C55-C56-C57

There are no ring outliers.

17 monomers are involved in 22 short contacts:

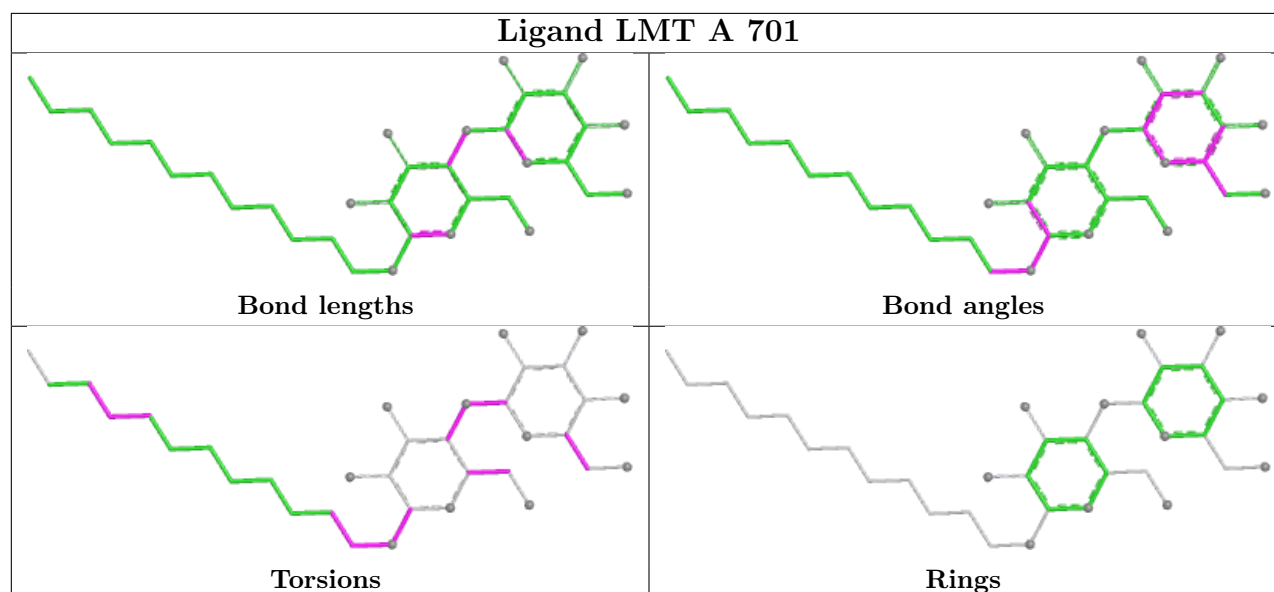
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	701	LMT	1	0
53	O	401	GTP	1	0
49	F	501	FMN	1	0
46	A	702	PC1	1	0
51	L	701	3PE	1	0
51	d	1202	3PE	1	0
52	h	1001	CDL	1	0
51	d	1203	3PE	4	0

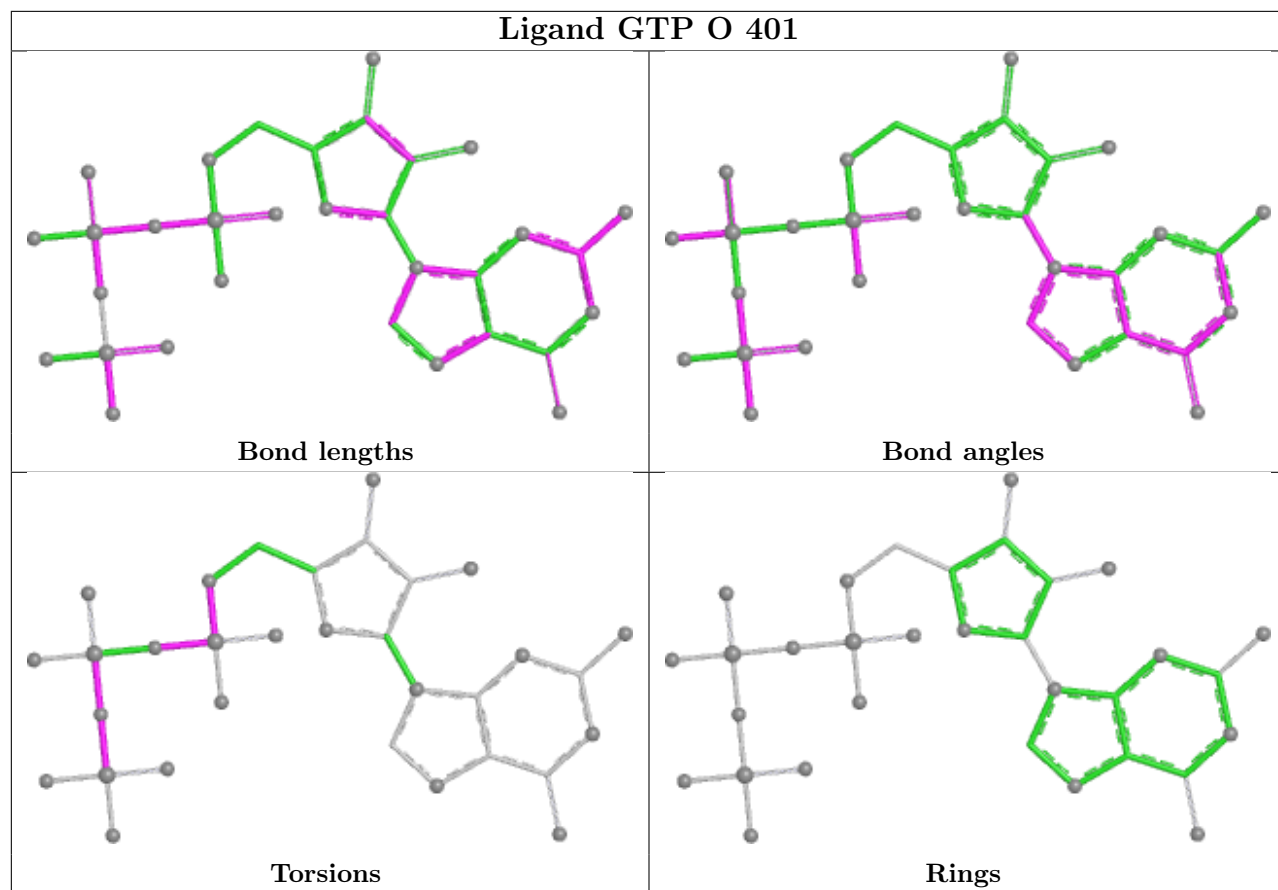
Continued on next page...

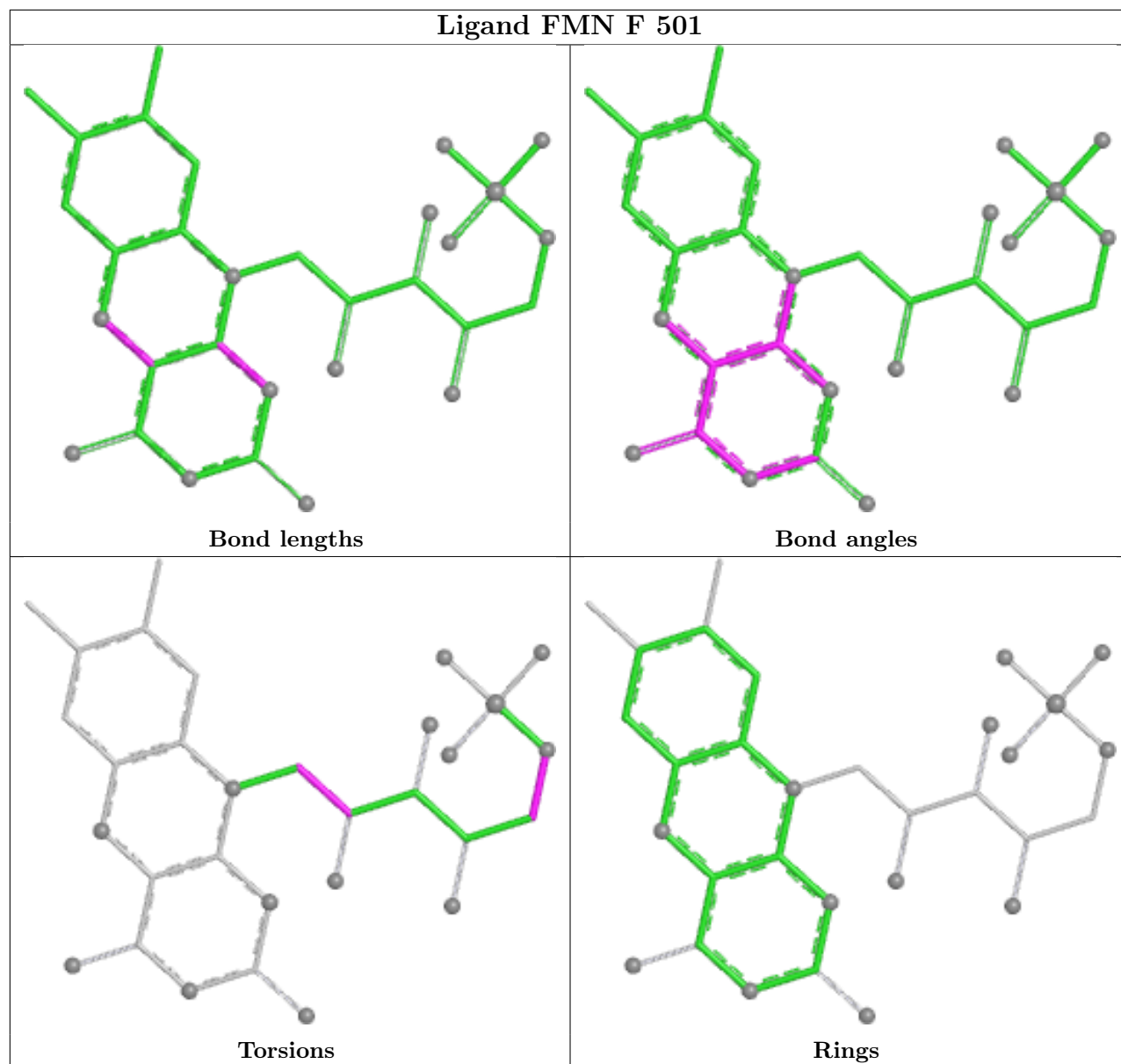
Continued from previous page...

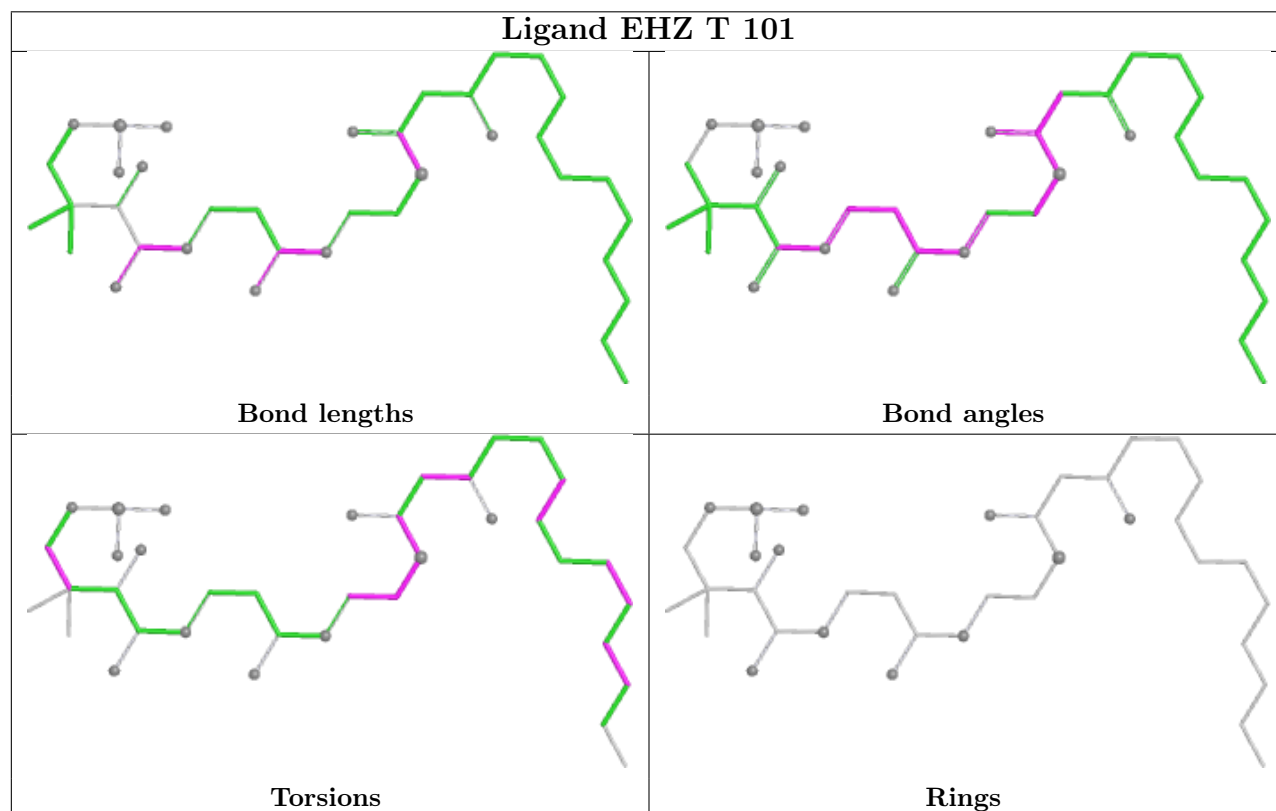
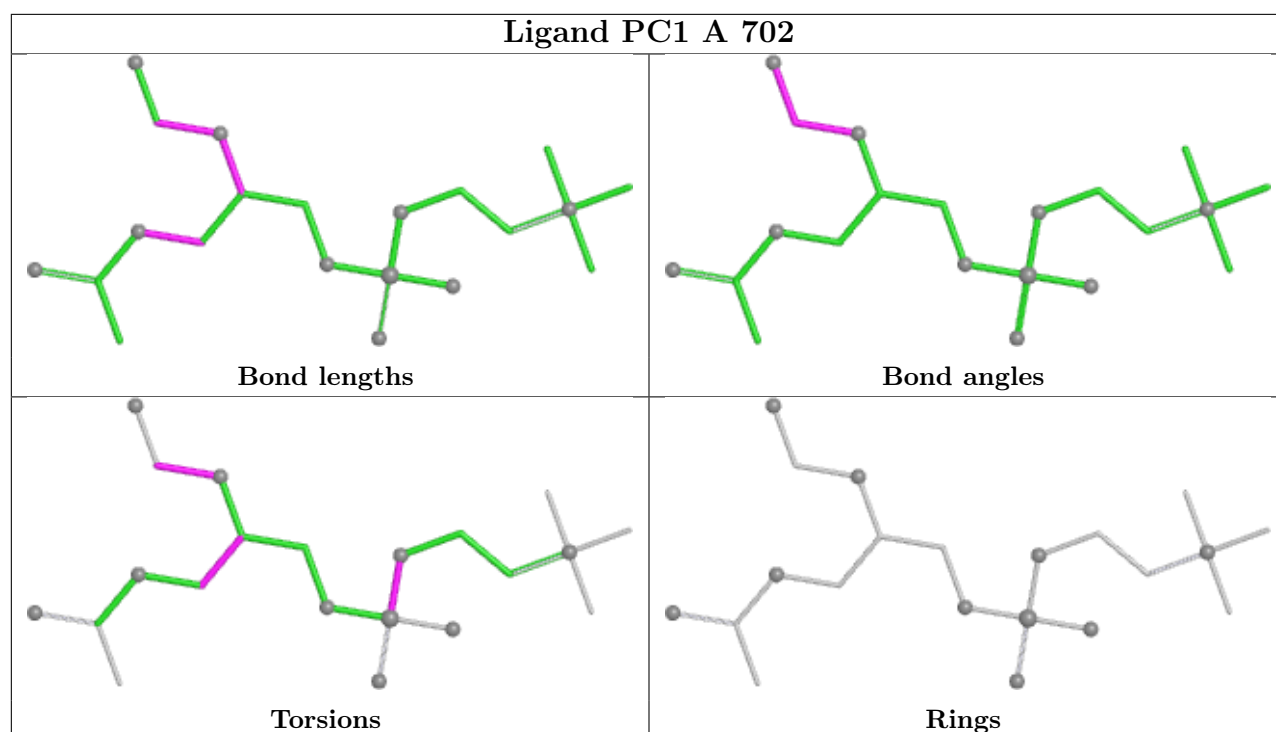
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	L	702	LMT	1	0
45	h	1002	LMT	2	0
51	H	402	3PE	1	0
51	M	603	3PE	1	0
45	l	201	LMT	1	0
45	J	702	LMT	1	0
52	J	701	CDL	2	0
45	j	101	LMT	1	0
47	F	502	SF4	1	0

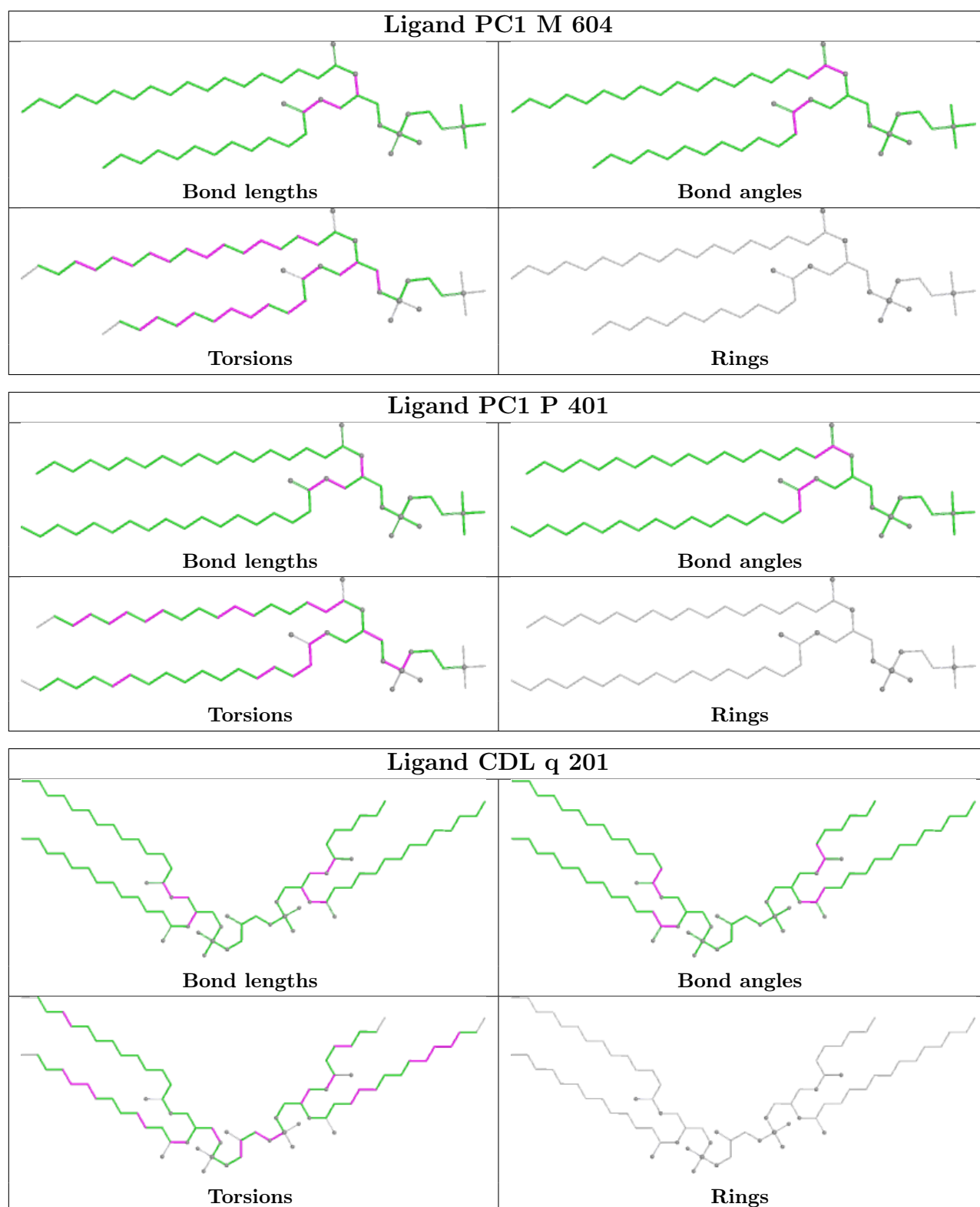
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

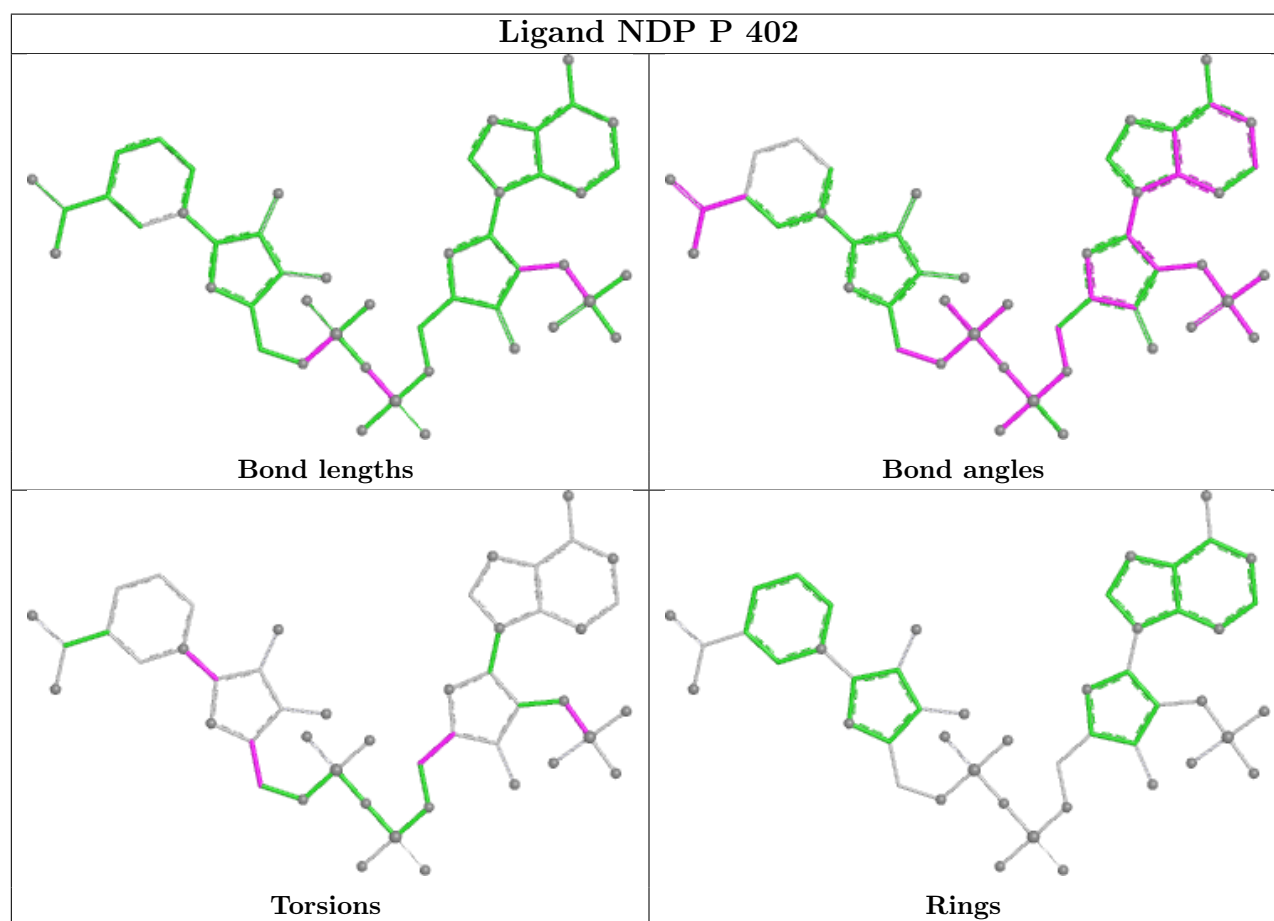
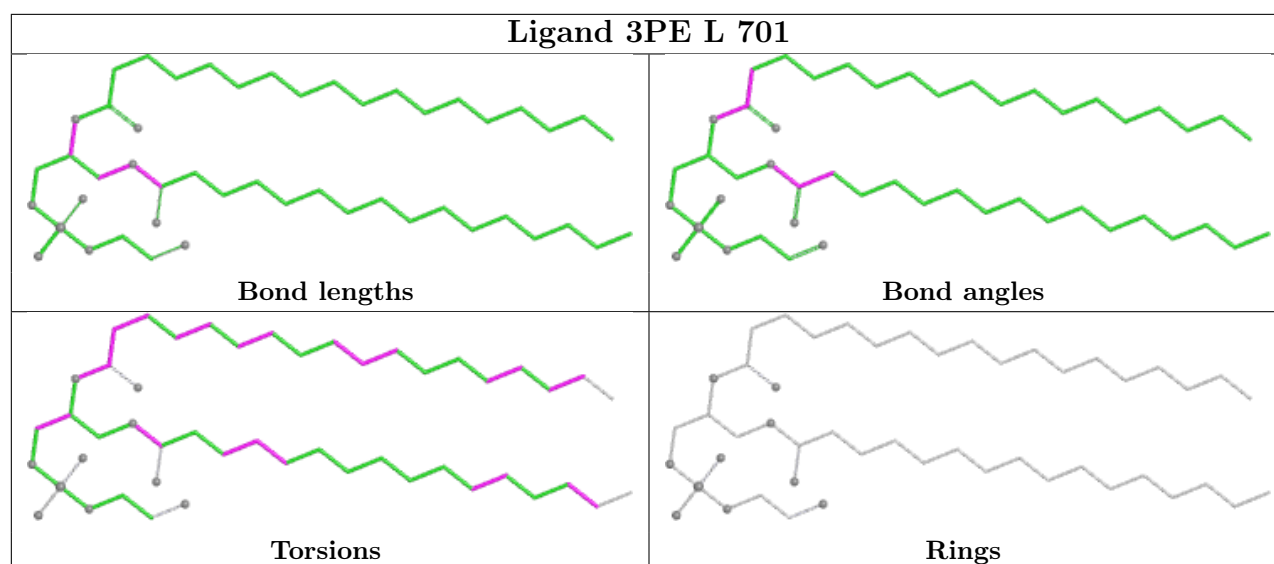


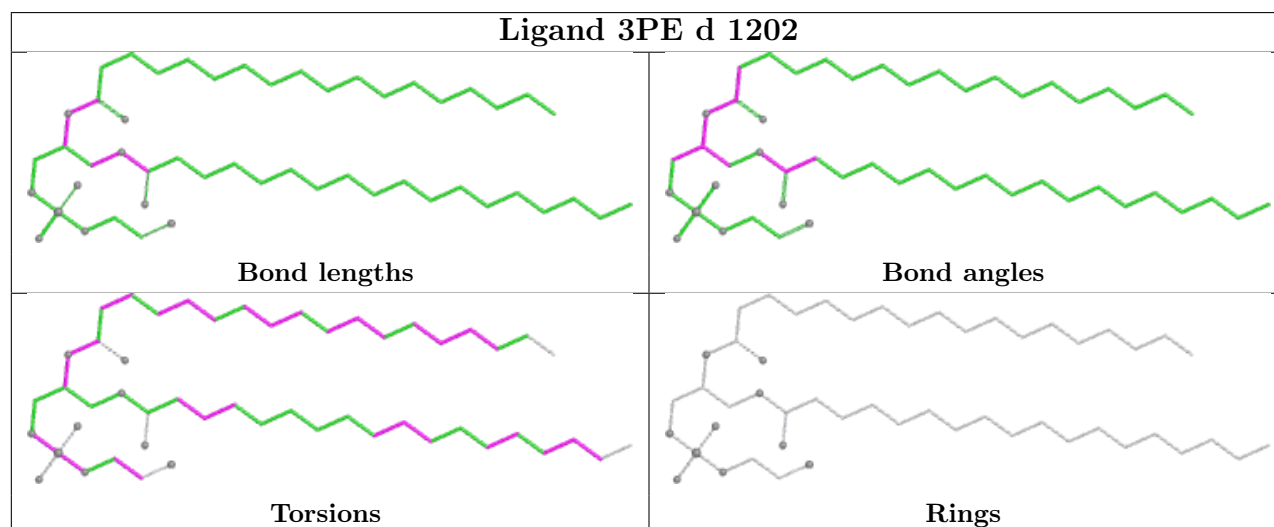
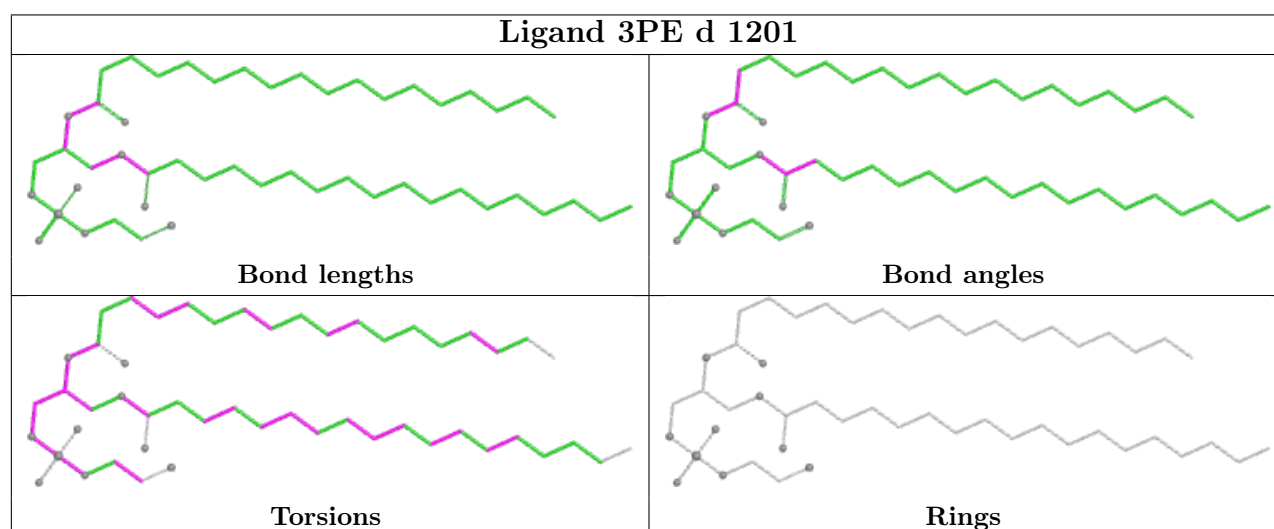
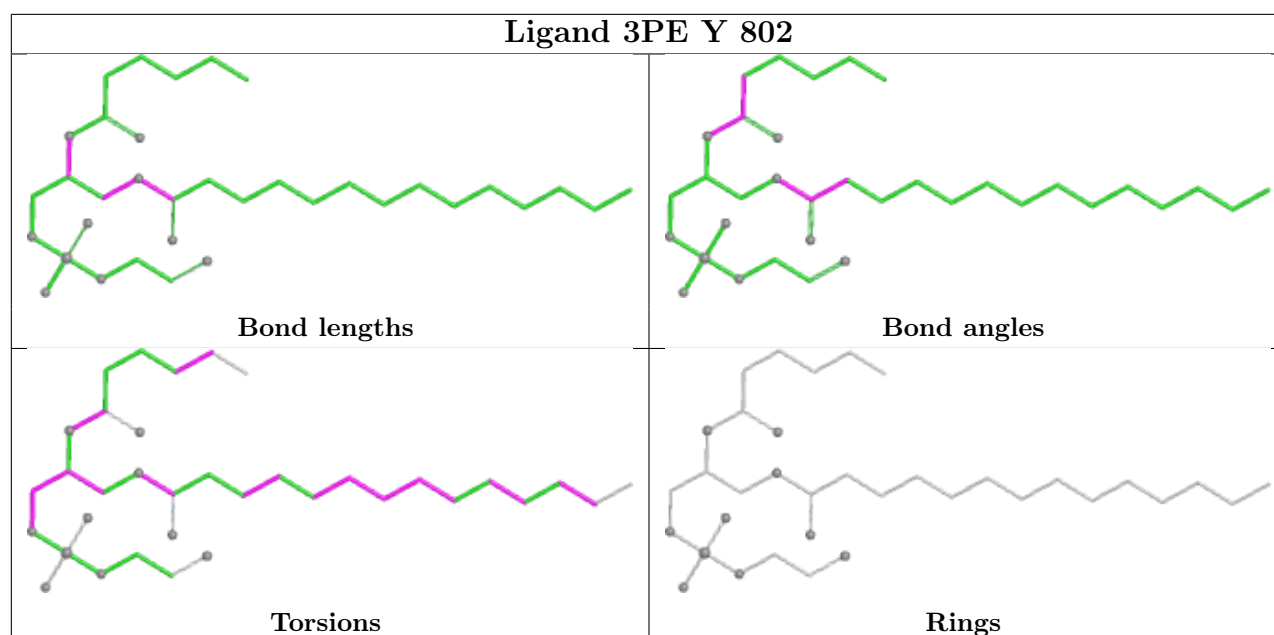


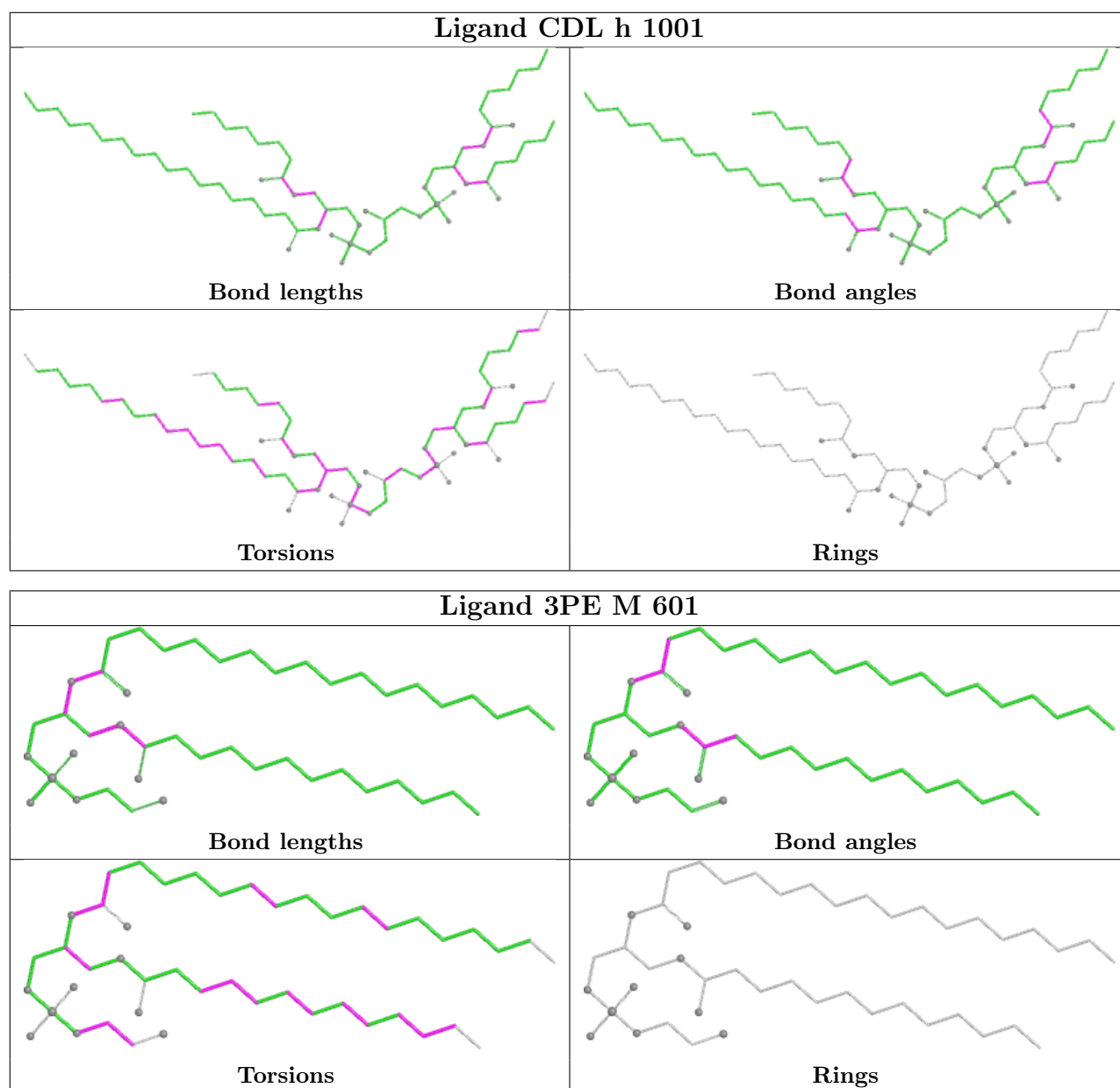


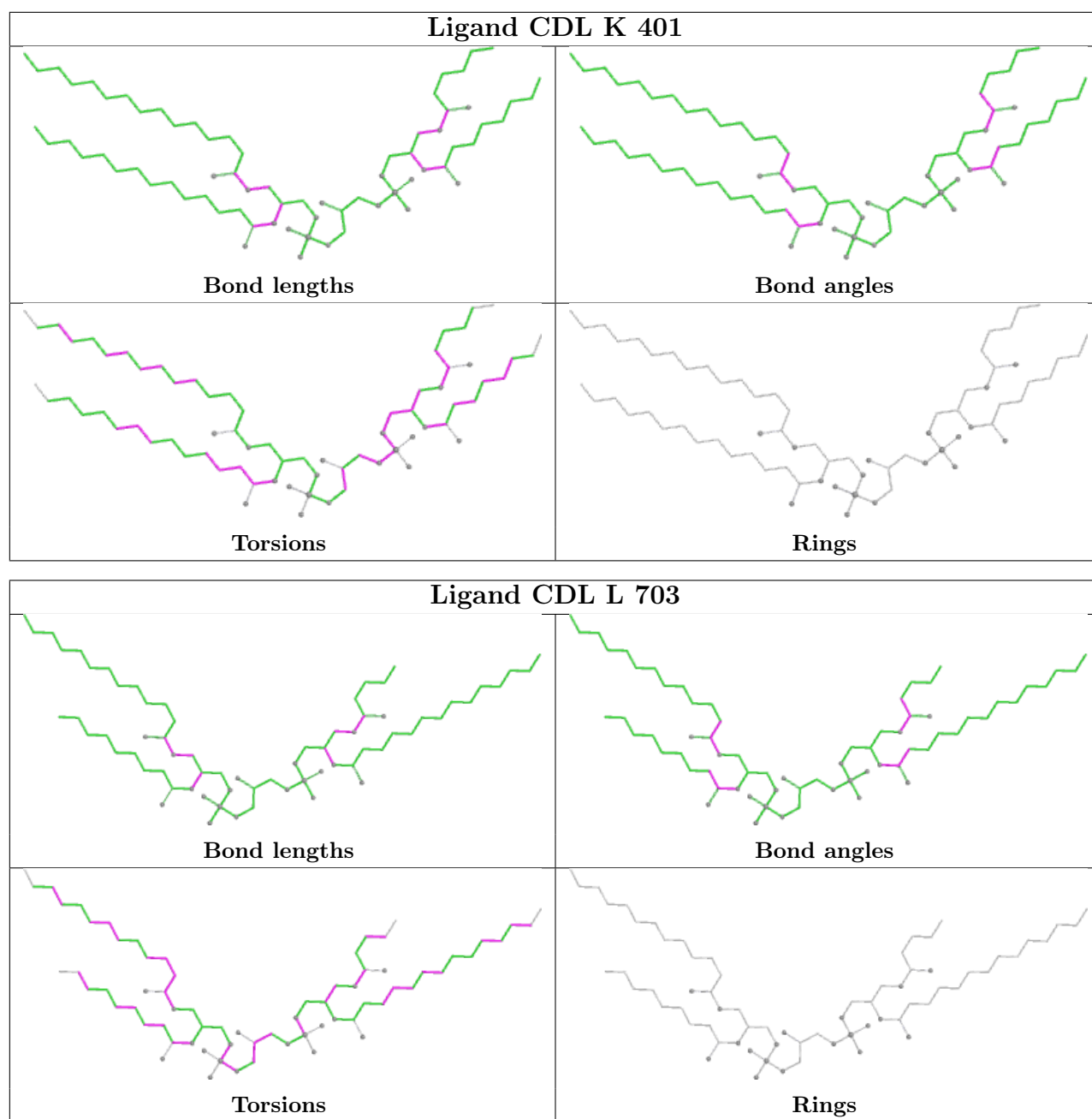


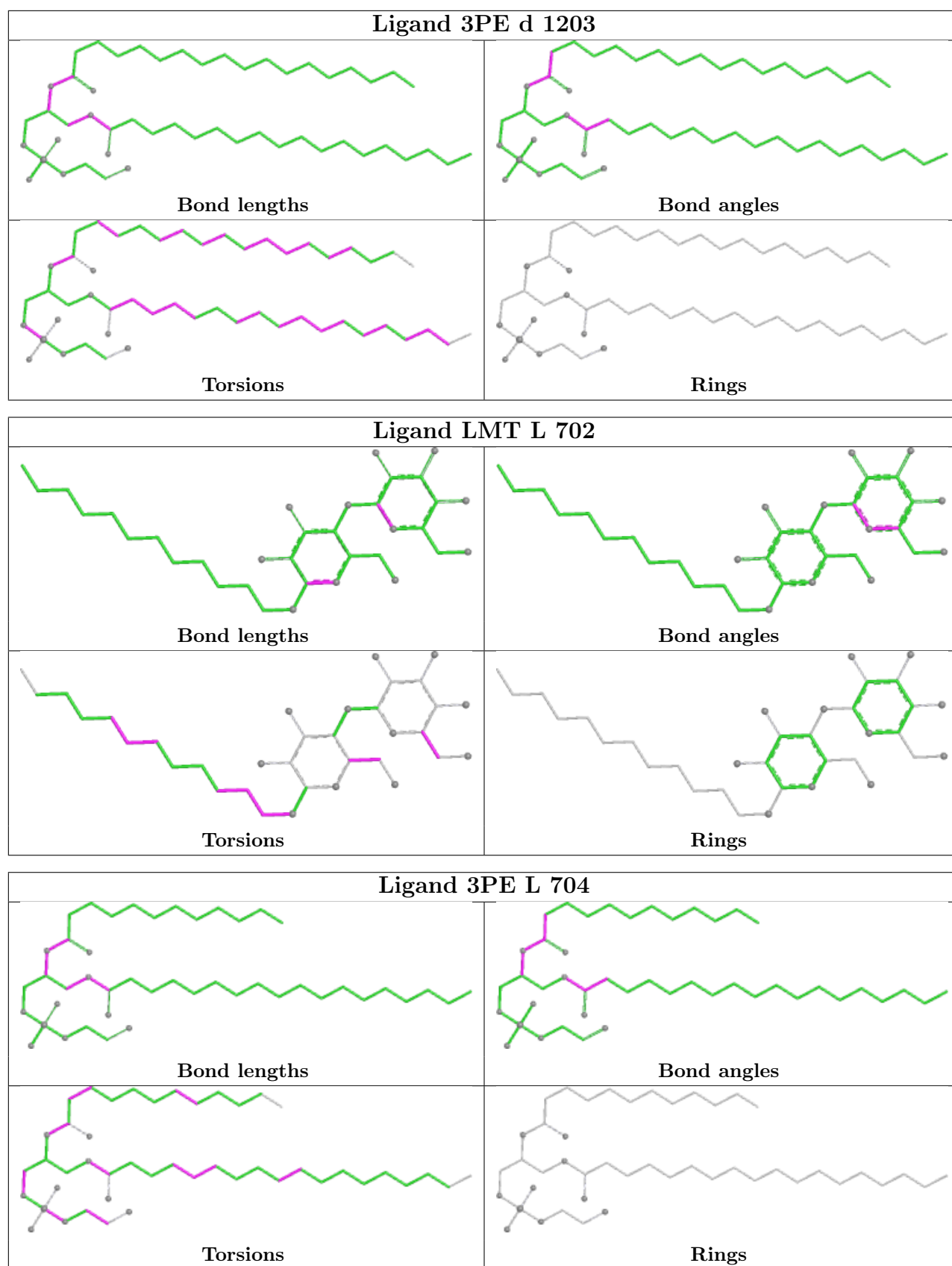


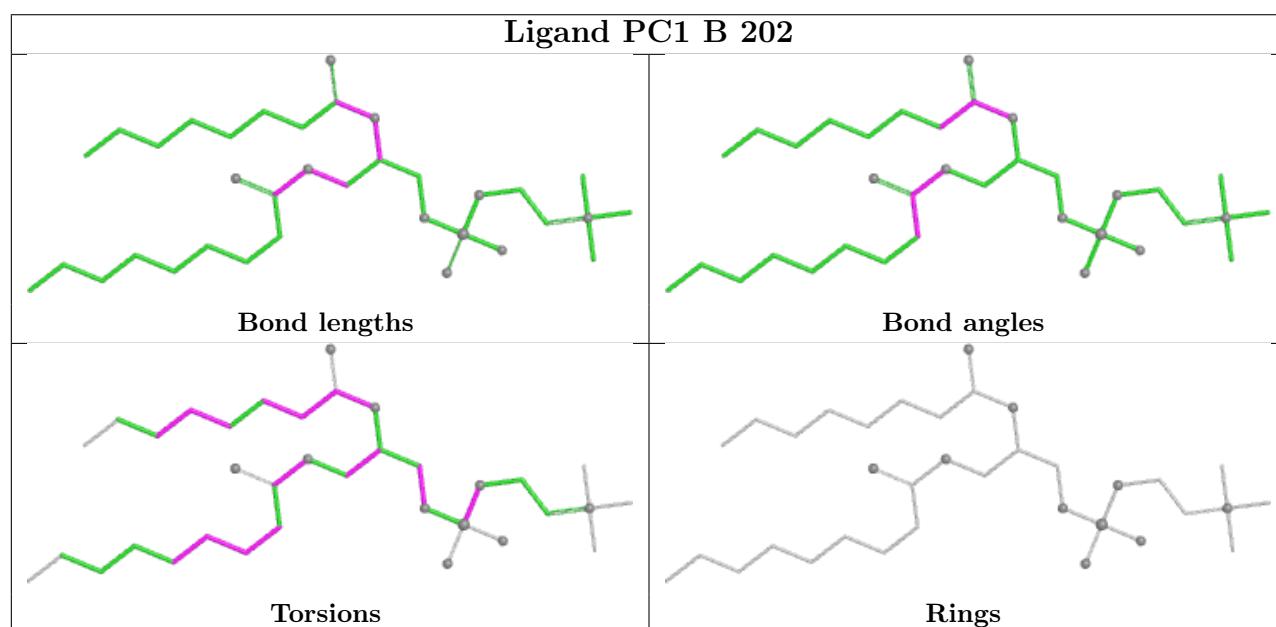
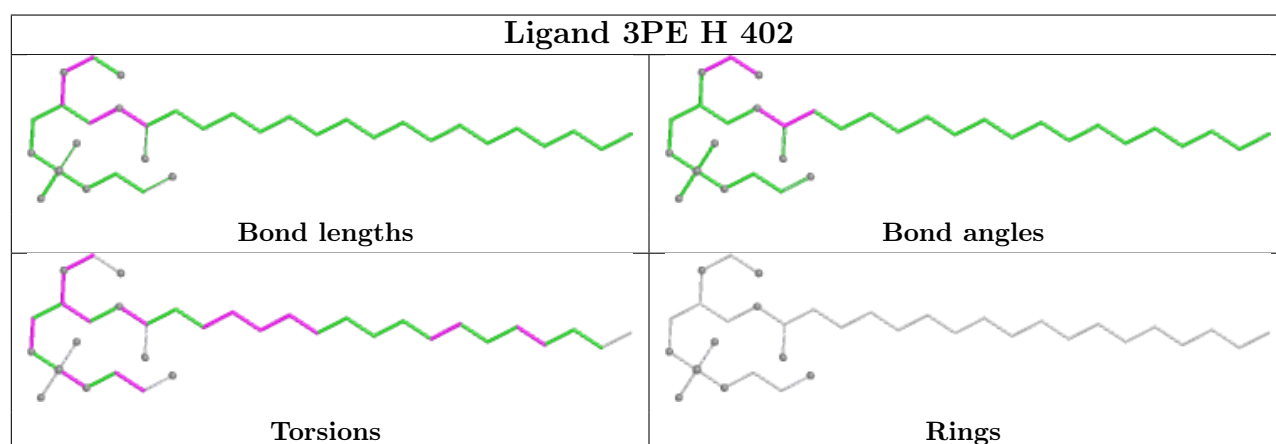
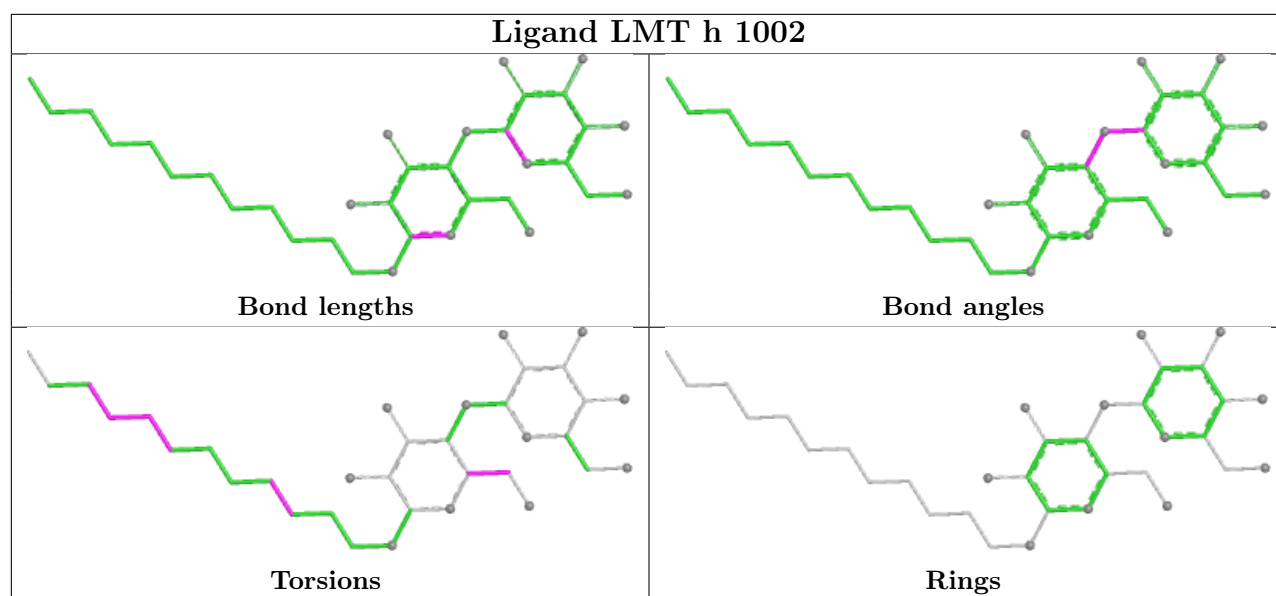


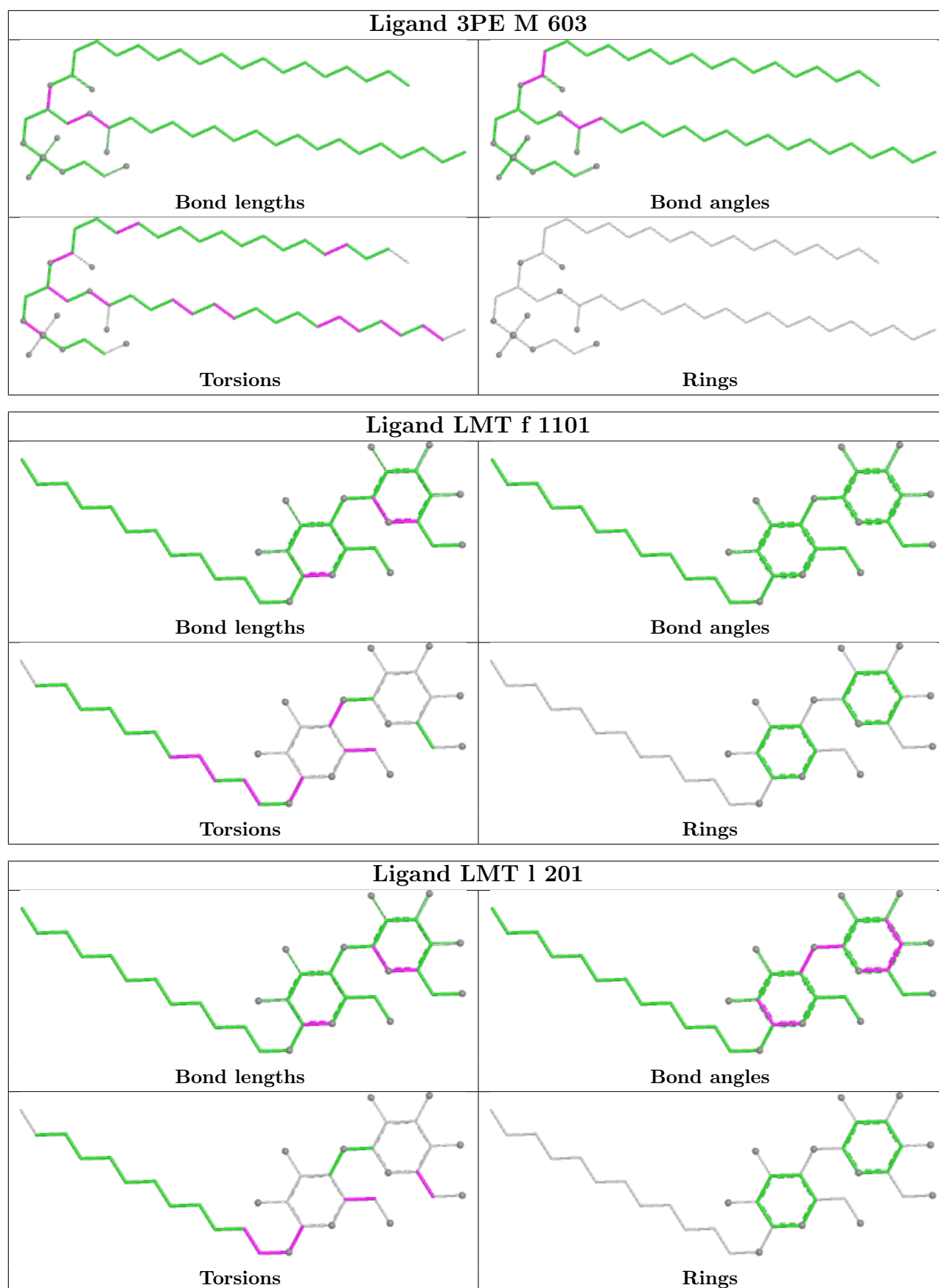


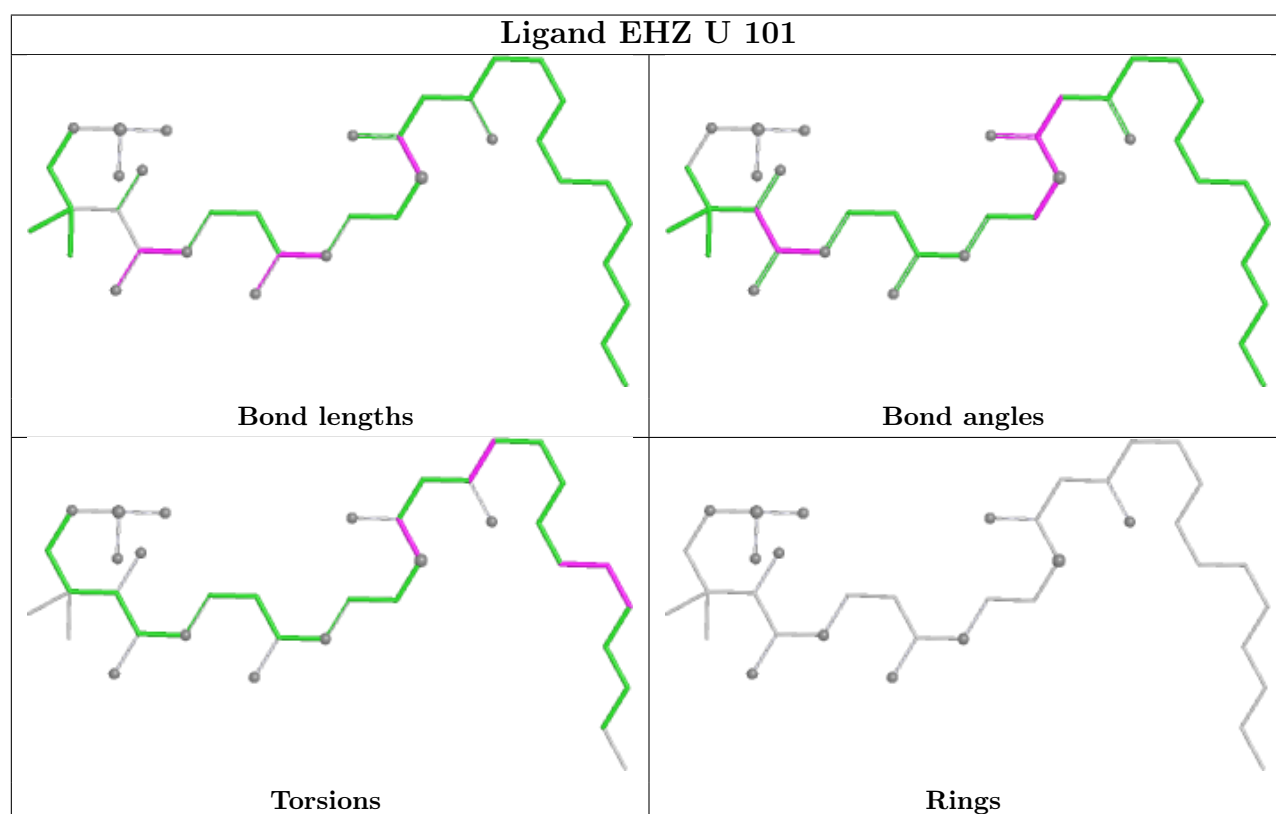
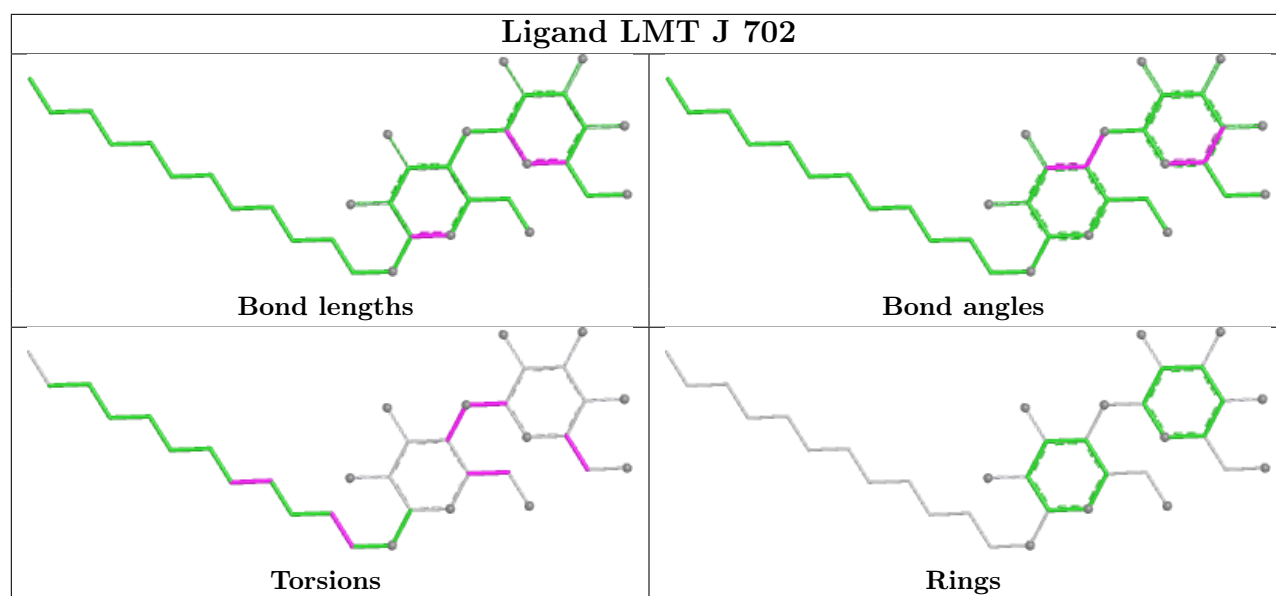


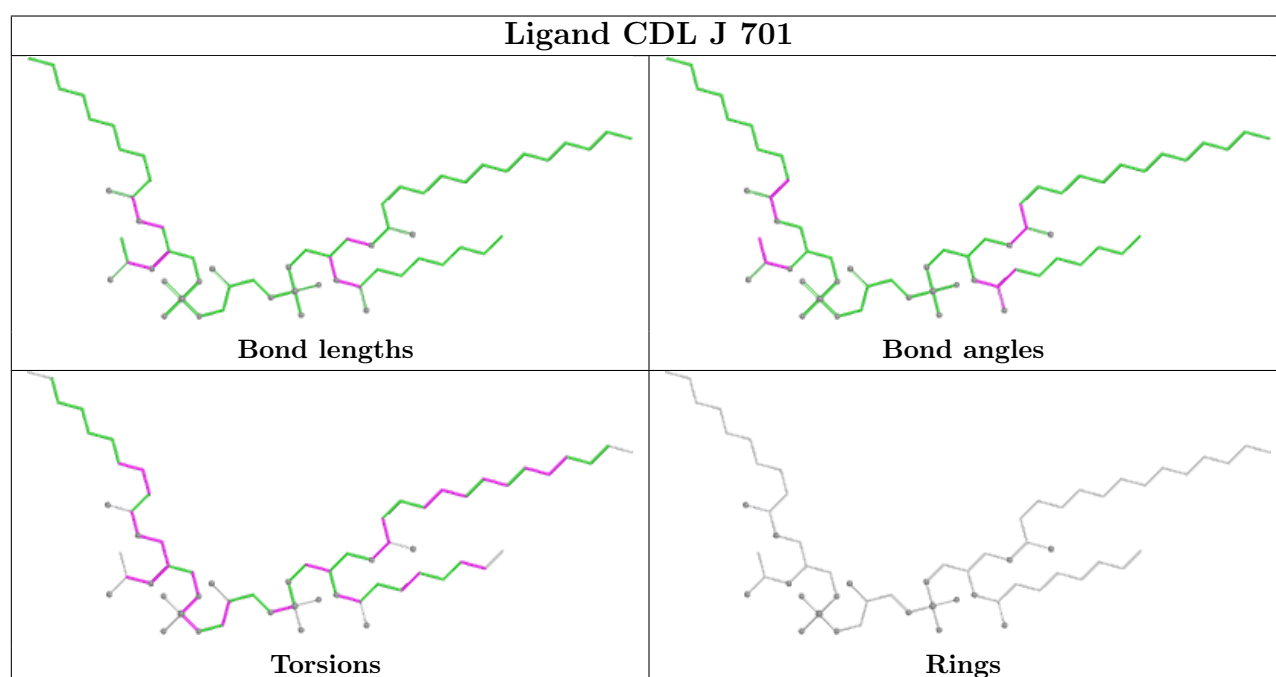
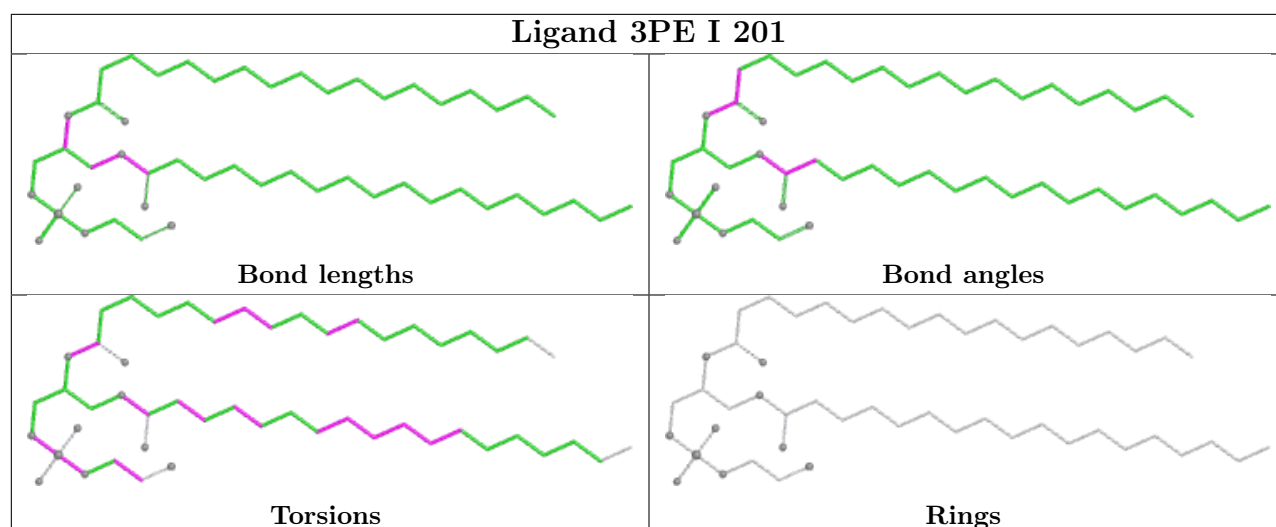


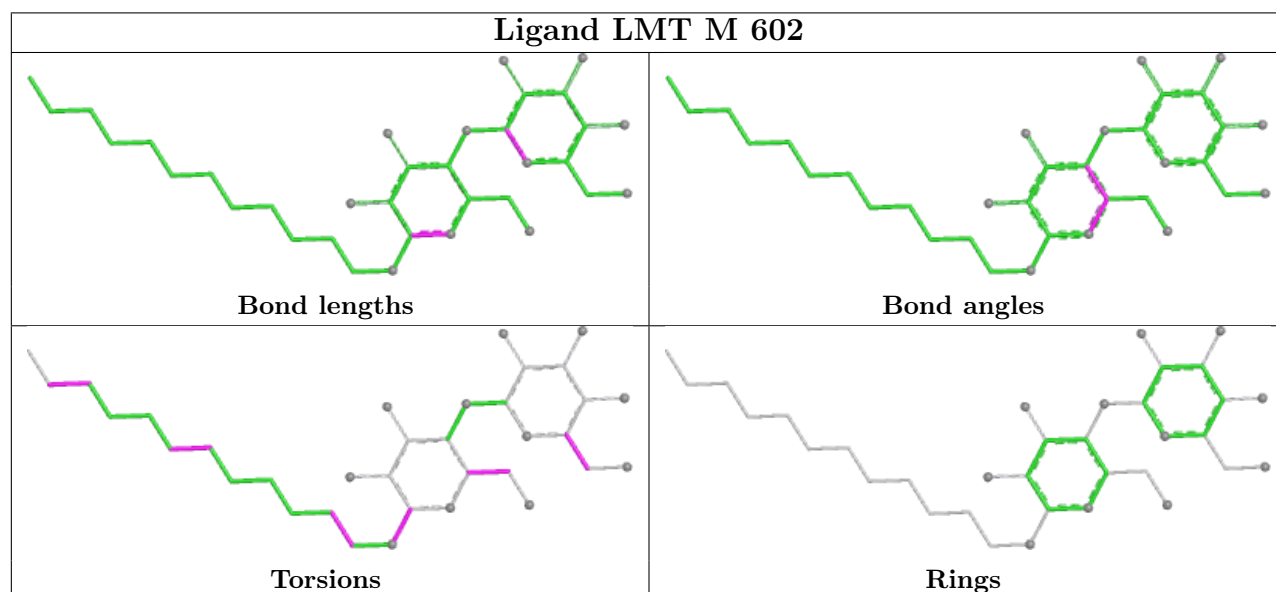
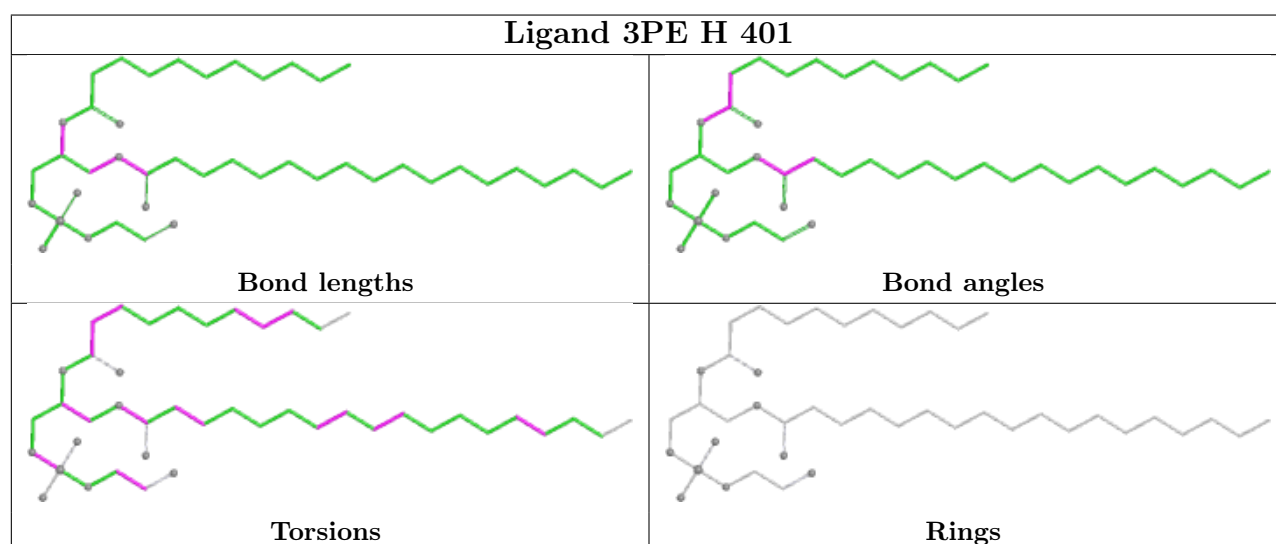
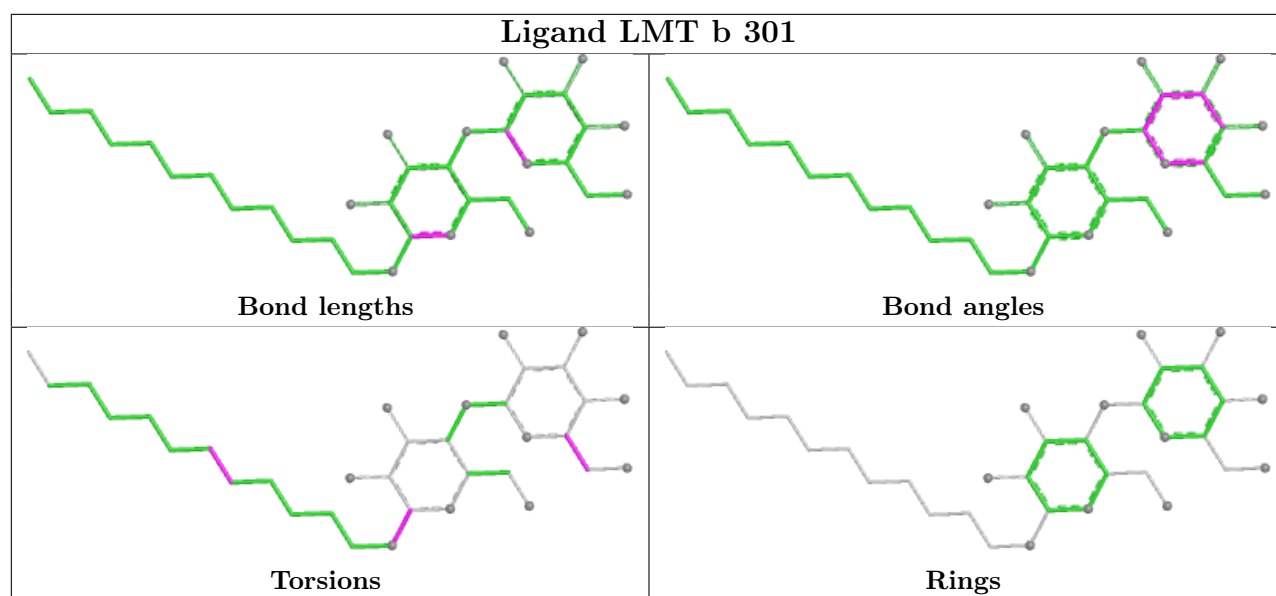


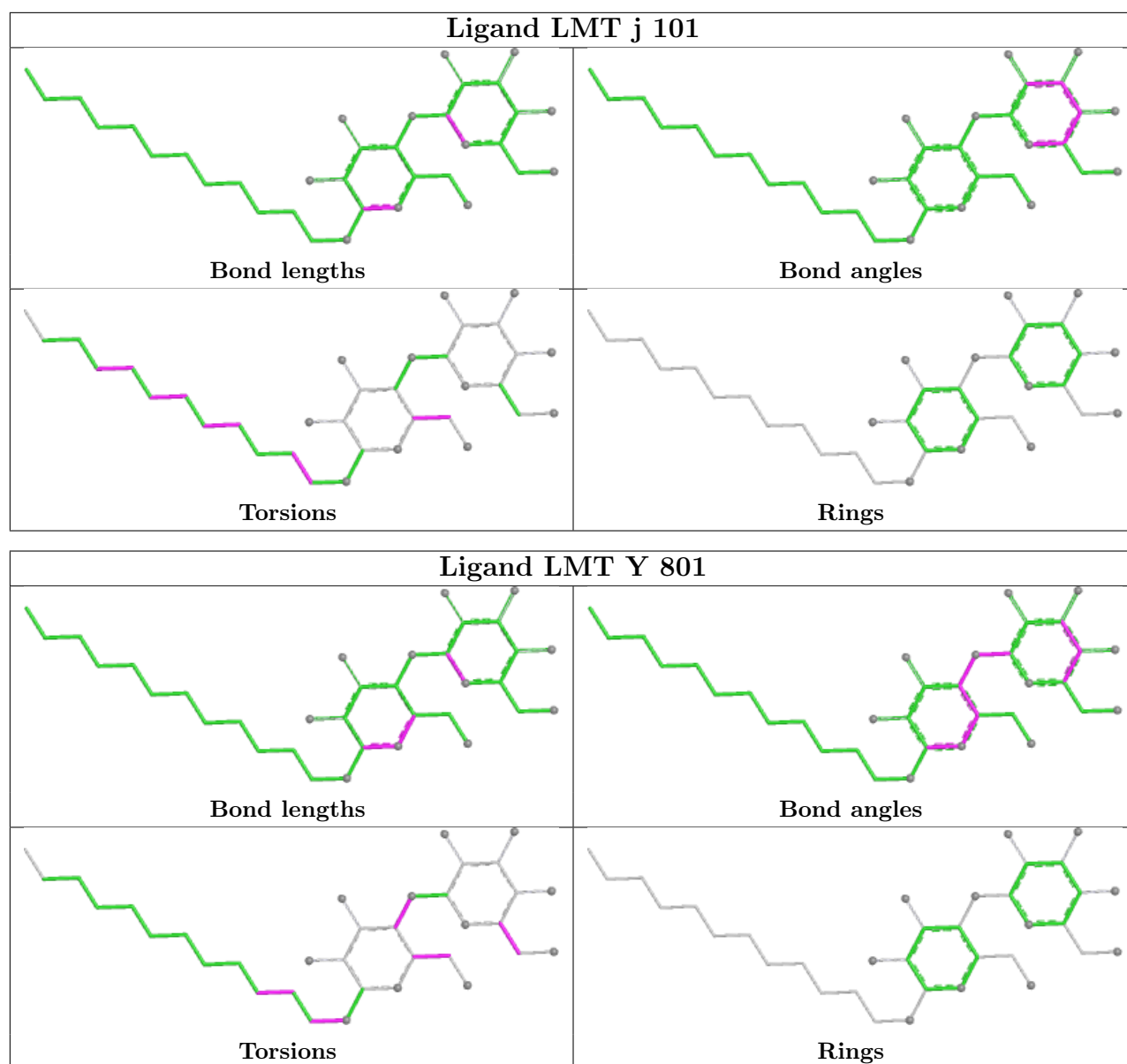












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

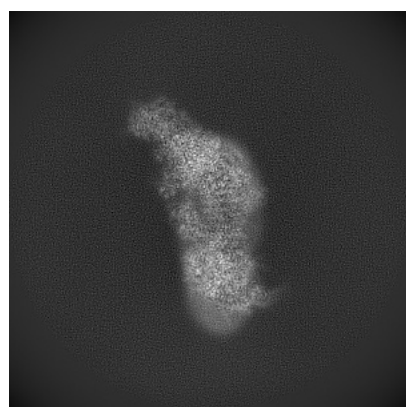
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14261. These allow visual inspection of the internal detail of the map and identification of artifacts.

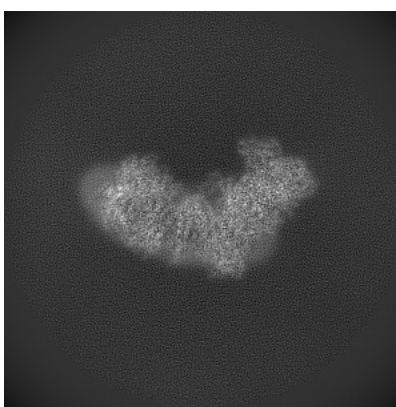
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

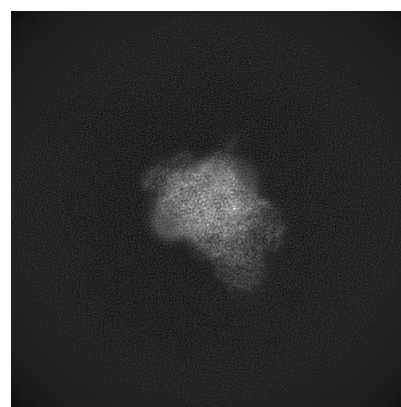
6.1.1 Primary map



X



Y

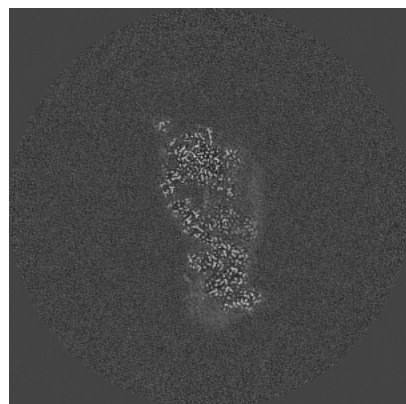


Z

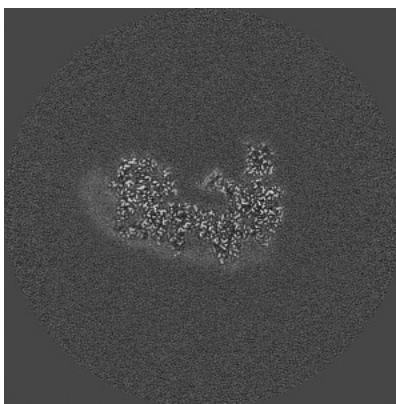
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

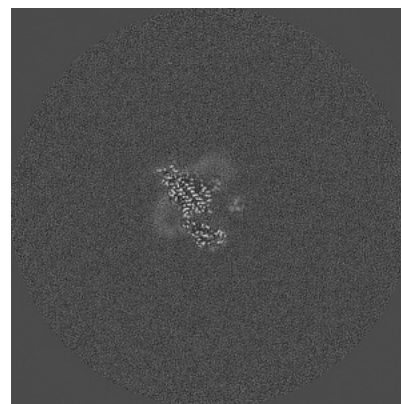
6.2.1 Primary map



X Index: 330



Y Index: 330

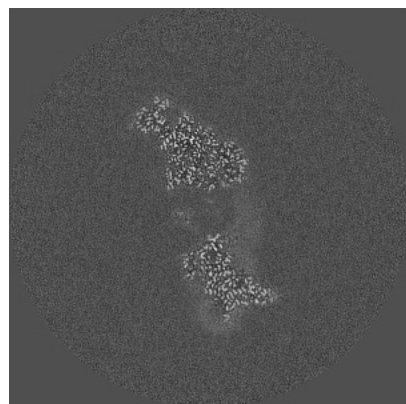


Z Index: 330

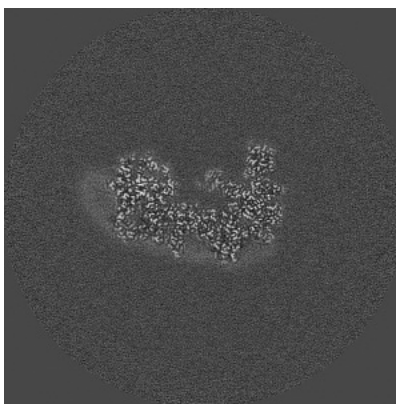
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

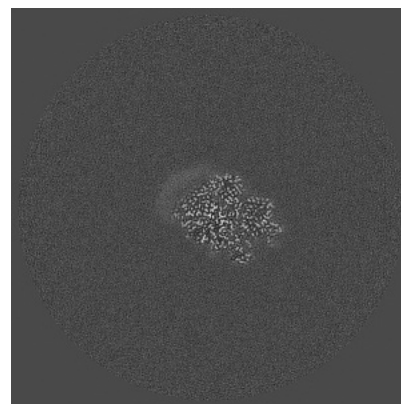
6.3.1 Primary map



X Index: 357



Y Index: 333

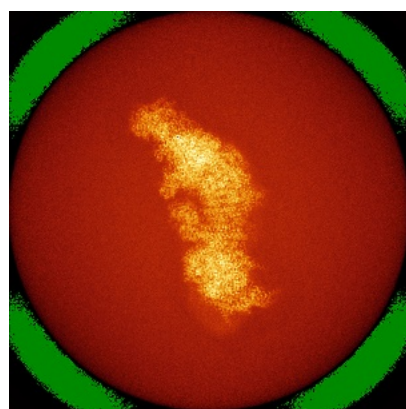


Z Index: 421

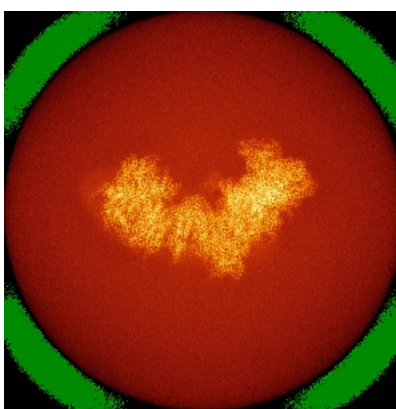
The images above show the largest variance slices of the map in three orthogonal directions.

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

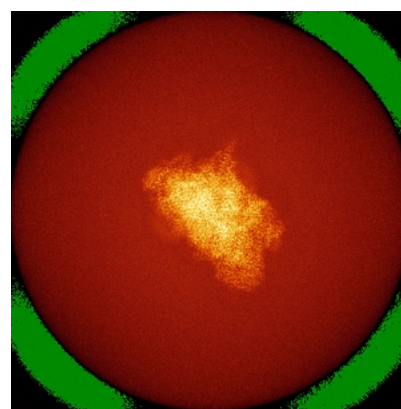
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

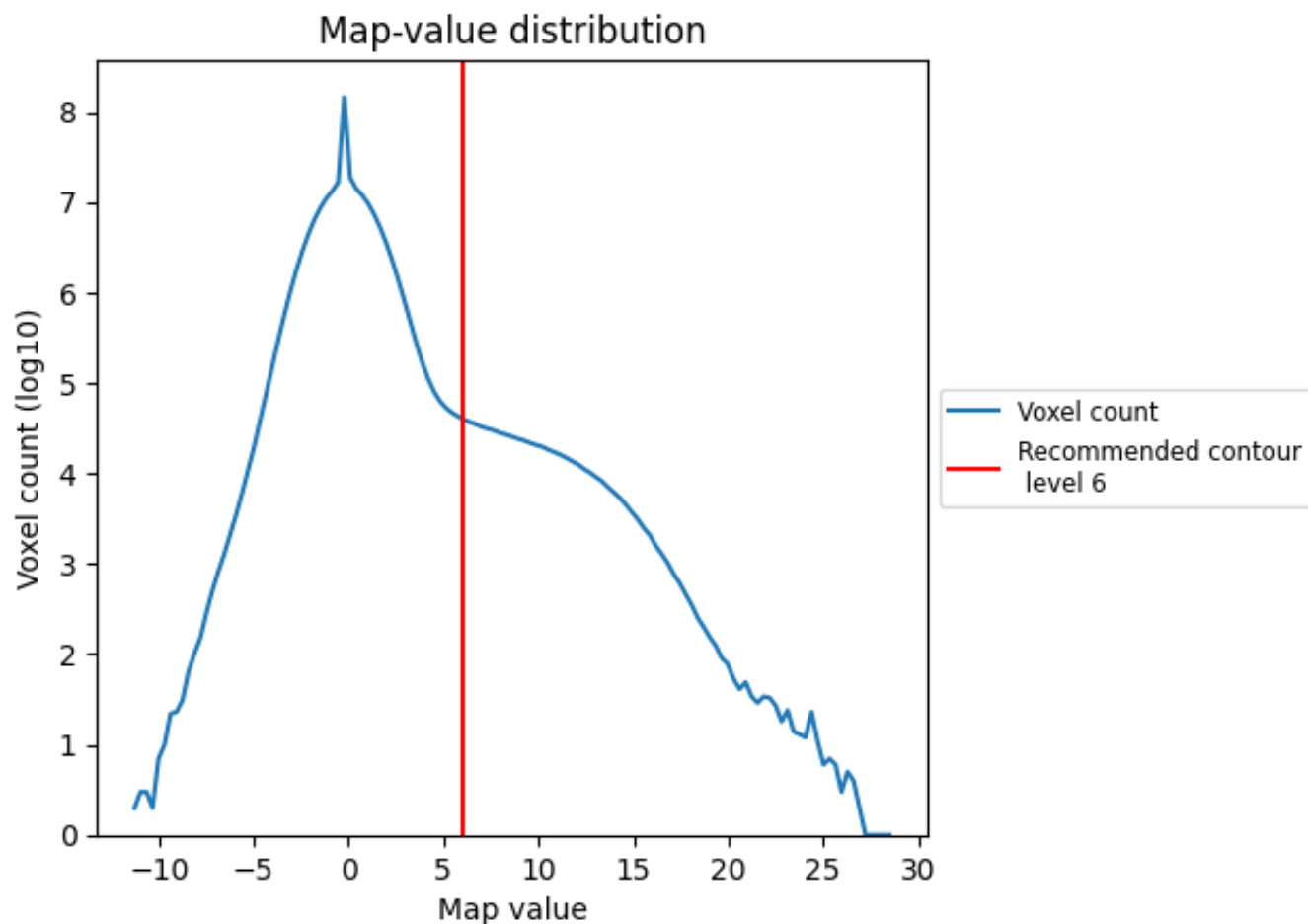
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

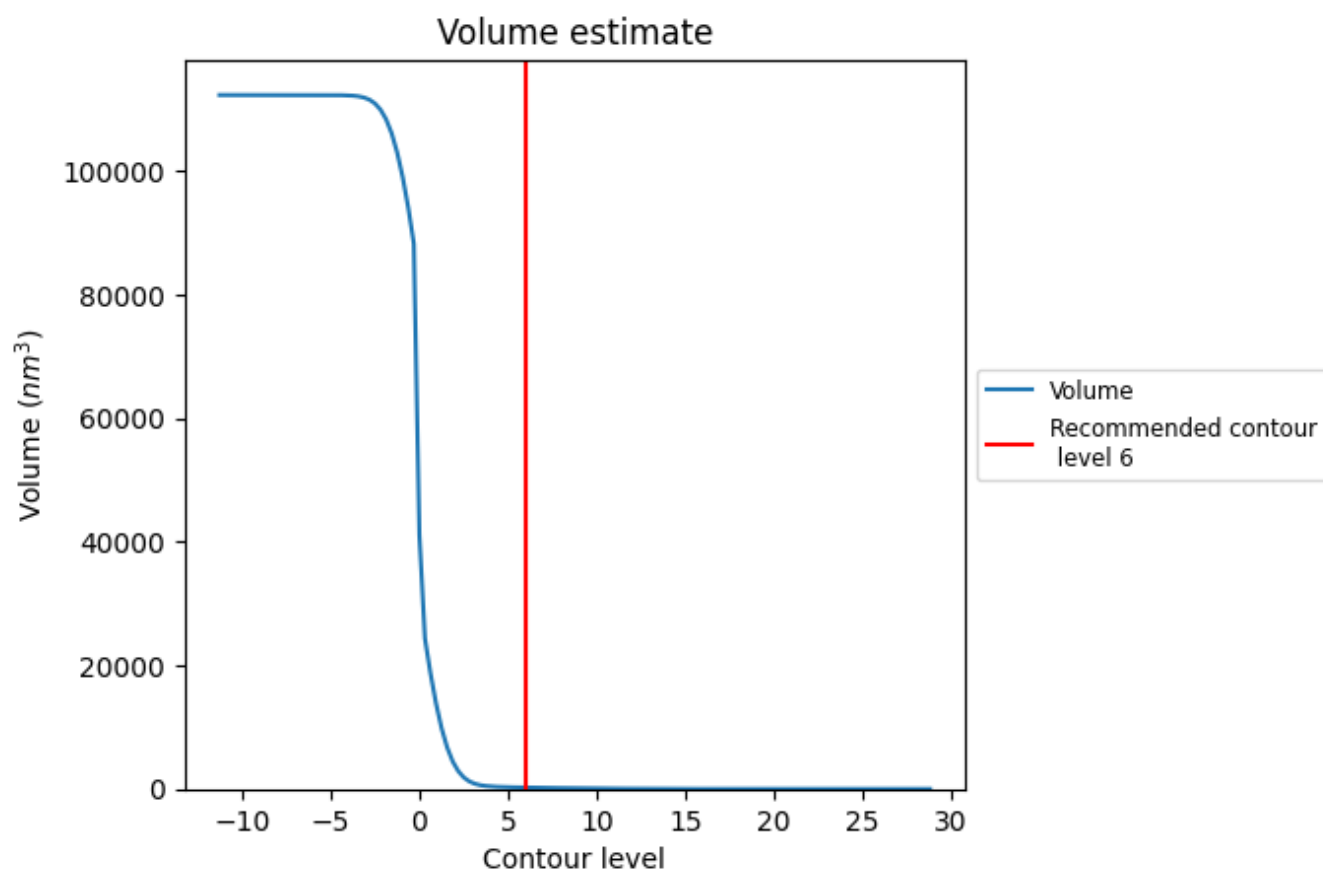
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

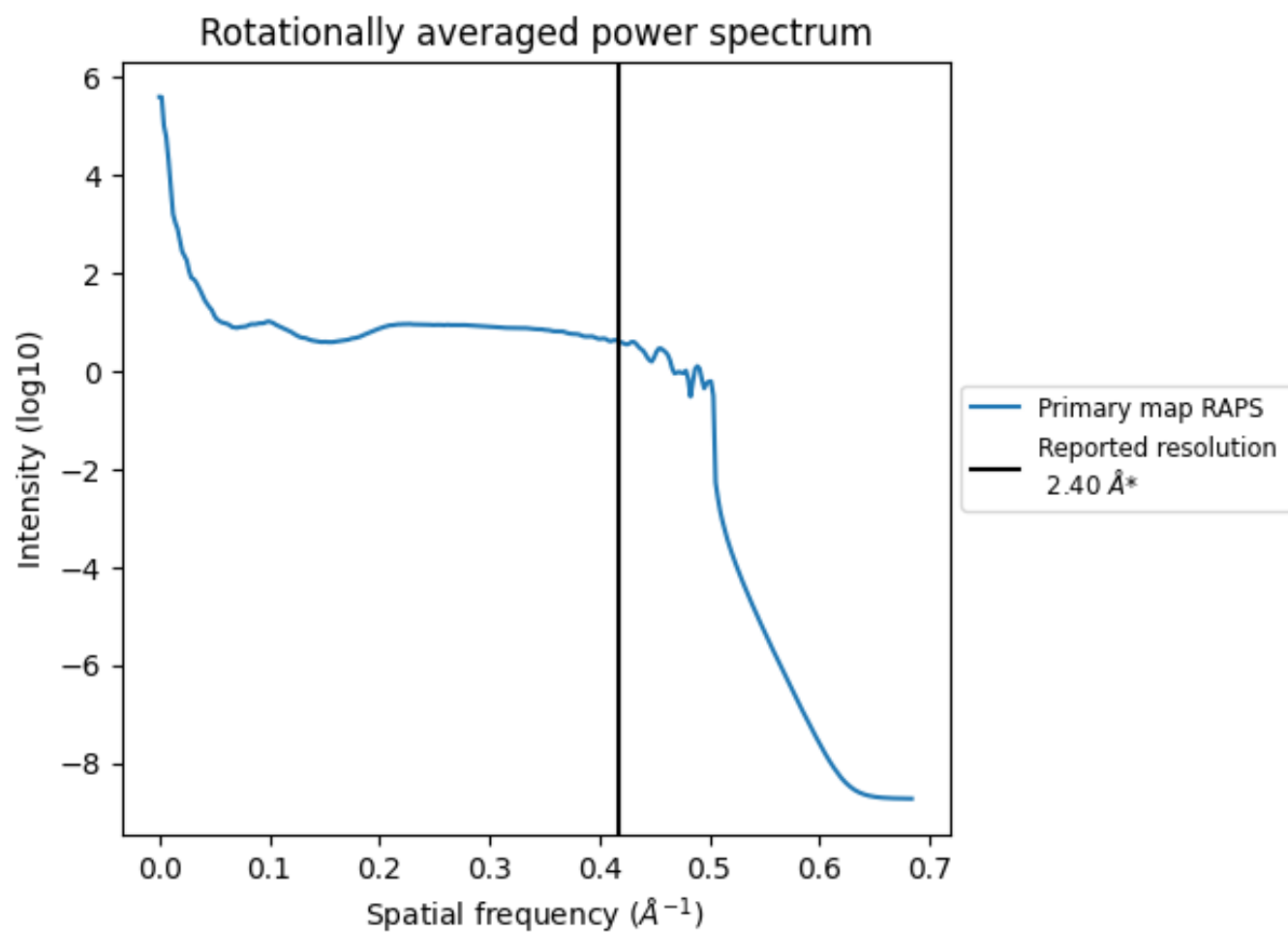
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 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 0.417 Å⁻¹

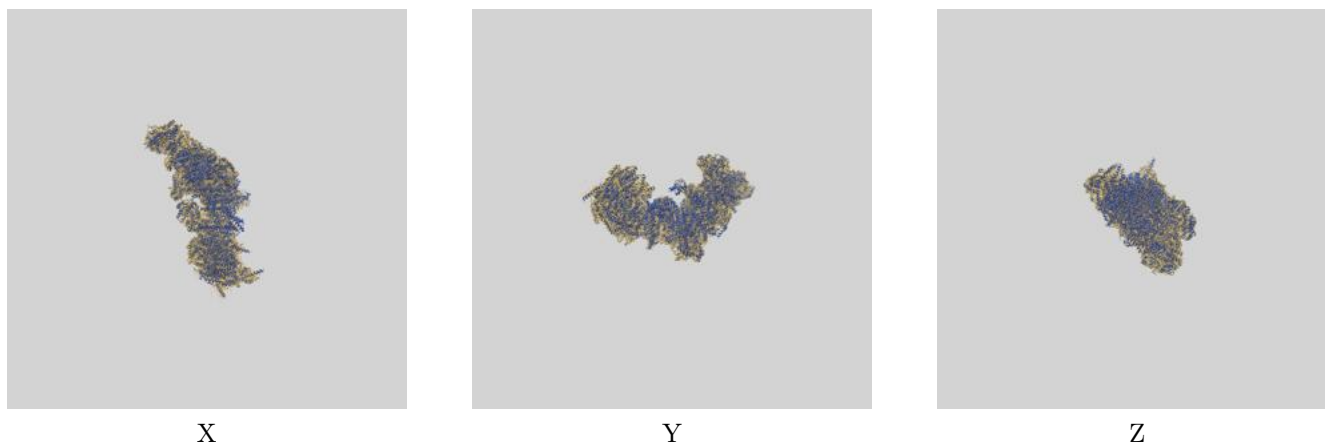
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

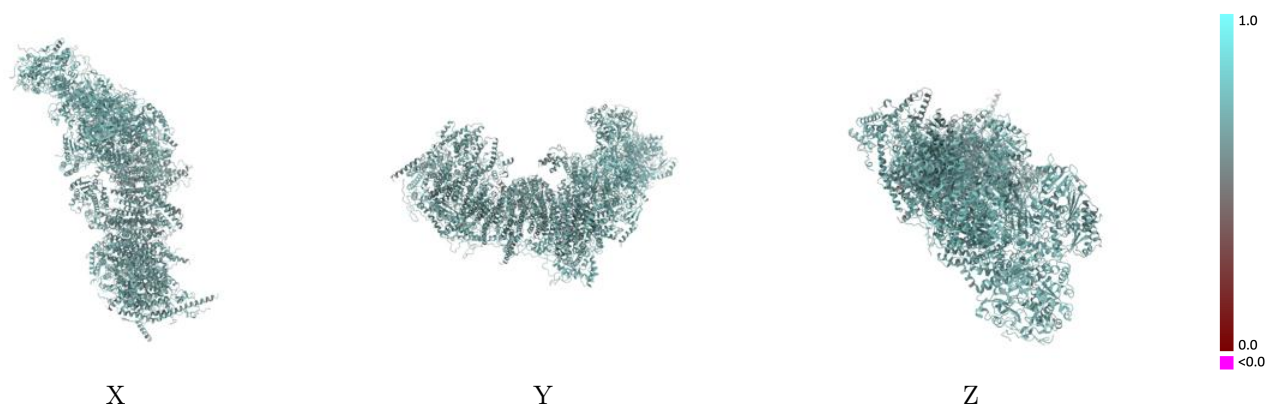
This section contains information regarding the fit between EMDB map EMD-14261 and PDB model 7R43. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



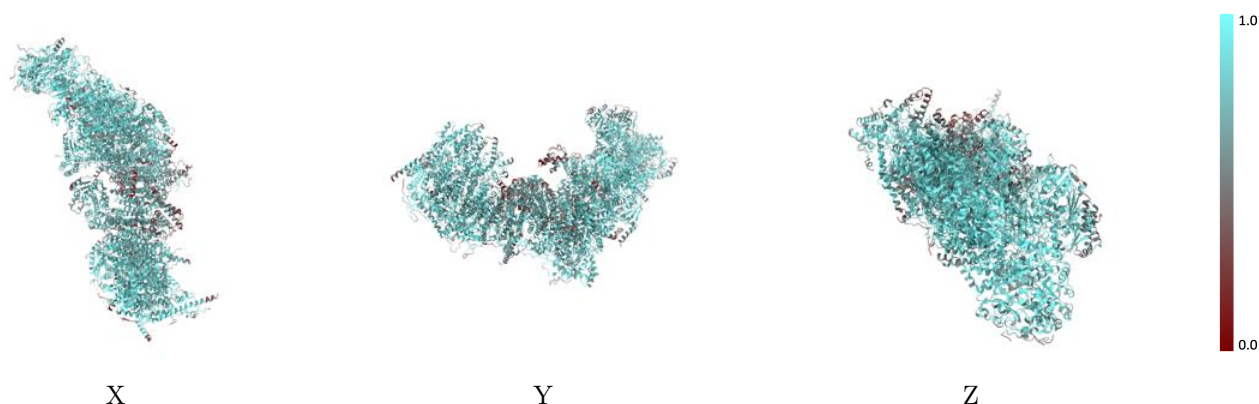
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



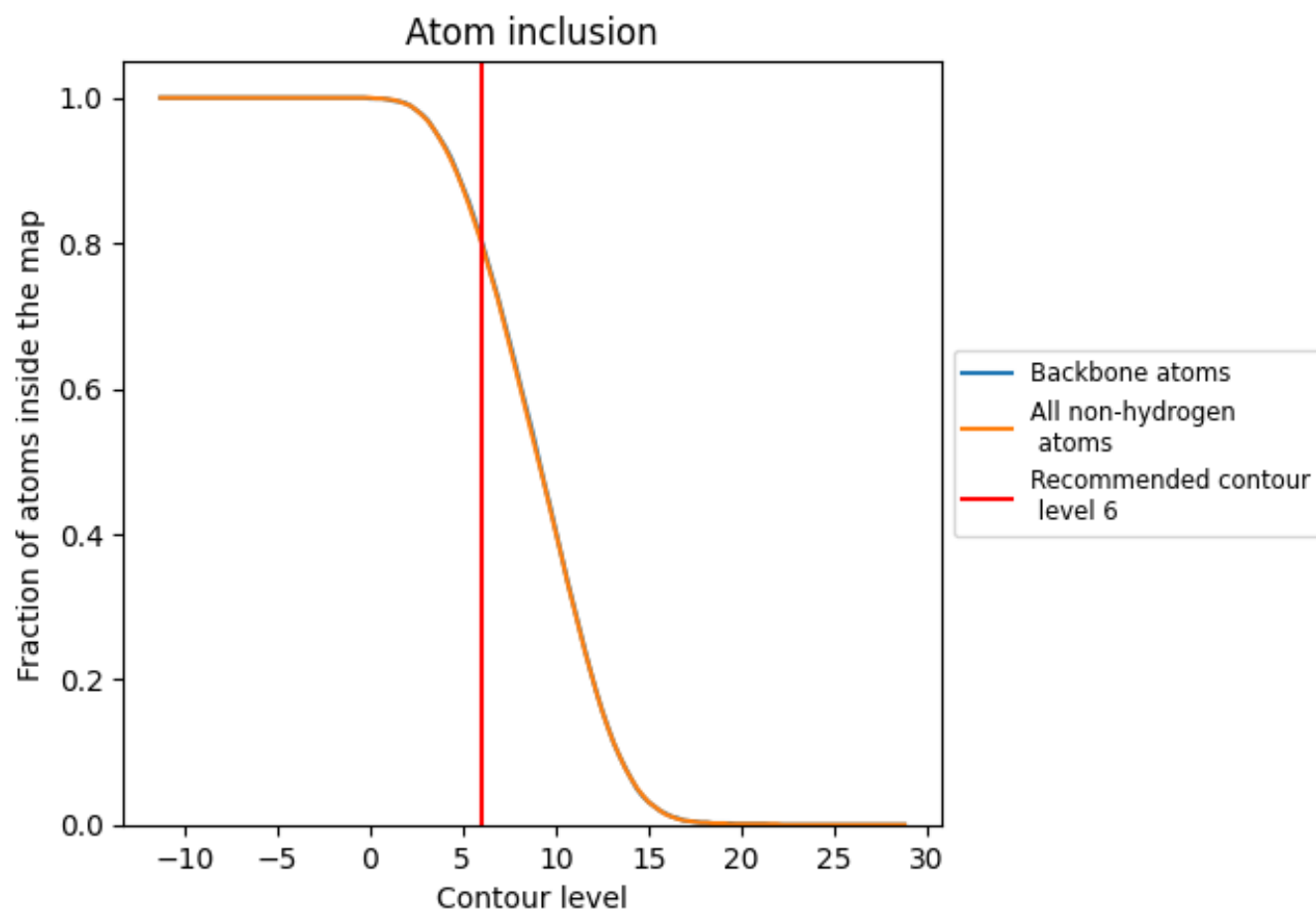
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.6700
A	 0.7900	 0.6770
B	 0.9150	 0.7130
C	 0.9100	 0.7120
D	 0.8960	 0.7090
E	 0.7780	 0.6640
F	 0.8300	 0.6770
G	 0.8400	 0.6880
H	 0.9010	 0.6960
I	 0.9200	 0.7150
J	 0.7570	 0.6660
K	 0.7970	 0.6830
L	 0.8240	 0.6530
M	 0.8750	 0.6800
N	 0.9030	 0.6940
O	 0.7610	 0.6550
P	 0.7760	 0.6730
Q	 0.8570	 0.7000
R	 0.8390	 0.6830
S	 0.6830	 0.6390
T	 0.3630	 0.5780
U	 0.8230	 0.6450
V	 0.7530	 0.6770
W	 0.7760	 0.6800
X	 0.7520	 0.6530
Y	 0.4500	 0.6130
Z	 0.7430	 0.6590
a	 0.8400	 0.6760
b	 0.6530	 0.6370
c	 0.6060	 0.6240
d	 0.7220	 0.6570
e	 0.6940	 0.6450
f	 0.6280	 0.6200
g	 0.7820	 0.6430
h	 0.7980	 0.6680



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Chain	Atom inclusion	Q-score
i	 0.7230	 0.6180
j	 0.7630	 0.6250
k	 0.7600	 0.6160
l	 0.8140	 0.6430
m	 0.7550	 0.6400
n	 0.8310	 0.6530
o	 0.8220	 0.6300
p	 0.8040	 0.6430
q	 0.7580	 0.6750
r	 0.7880	 0.6880
s	 0.7600	 0.6590