



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:19 AM UTC

PDB ID : 7R45 / pdb_00007r45
EMDB ID : EMD-14272
Title : Bovine complex I in the presence of IM1761092, deactive class i (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:

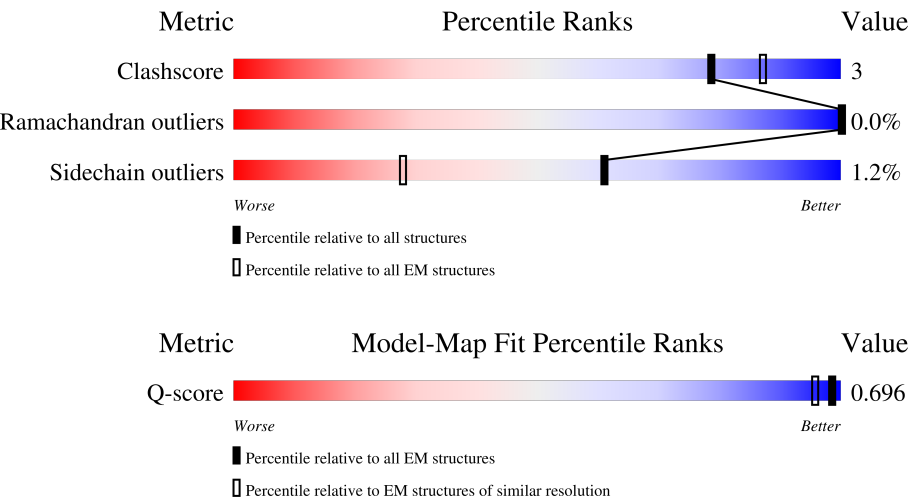
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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.



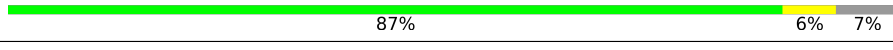
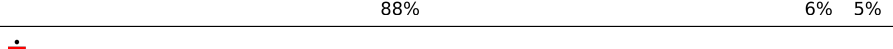
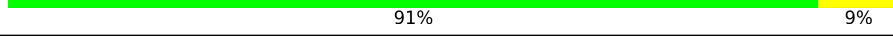
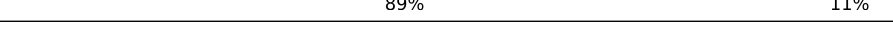
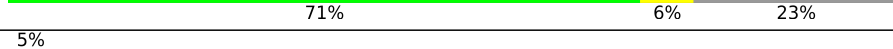
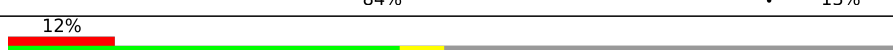
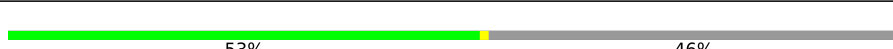
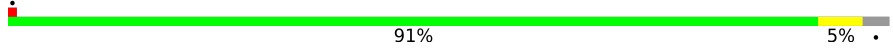
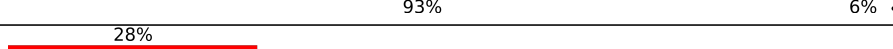
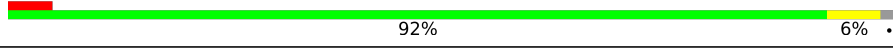
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	

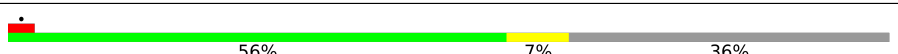
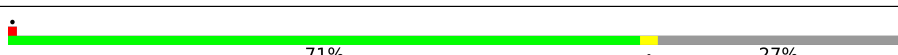
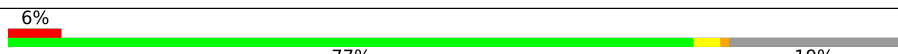
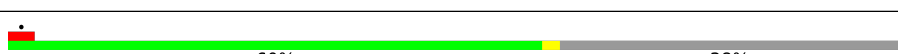
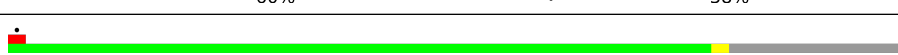
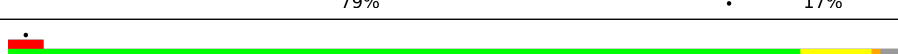
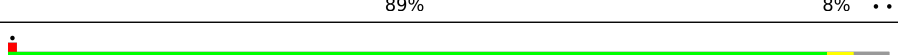
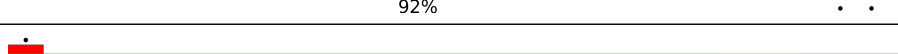
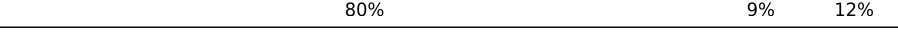
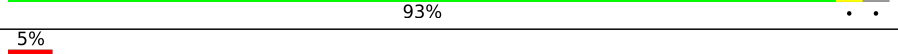
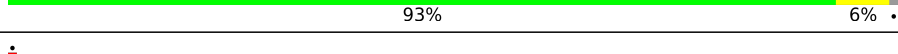
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	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 60 unique types of molecules in this entry. The entry contains 68195 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	101	Total	C	N	O	S	0	0
			814	555	118	136	5		

- 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	206	Total	C	N	O	S	0	0
			1714	1107	295	309	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	417	Total	C	N	O	S	0	0
			3363	2150	577	611	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	430	Total	C	N	O	S	0	0
			3310	2085	591	614	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	307	Total	C	N	O	S	0	0
			2425	1629	373	400	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	606	Total	C	N	O	S	0	0
			4786	3184	735	824	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	294	Total	C	N	O	S	0	0
			2342	1501	420	416	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	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	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	140	Total	C	N	O	S	0	0
			1146	737	200	200	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	69	Total	C	N	O	S	0	0
			561	361	103	92	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			646	422	108	114	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	95	Total	C	N	O	S	0	0
			799	506	150	137	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			444	291	78	74	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	103	Total	C	N	O	S	0	0
			884	584	149	150	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	79	Total	C	N	O	S	0	0
			638	418	107	111	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	126	Total	C	N	O		0	0
			1050	672	186	192			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1043	650	200	184	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1435	900	265	262	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

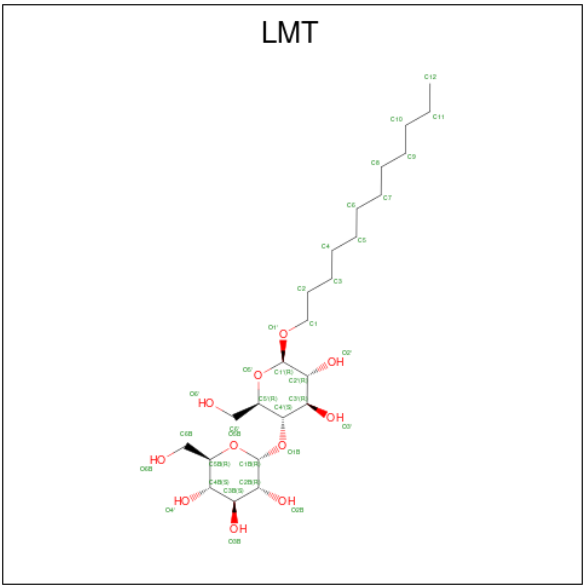
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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	43	Total	C	N	O	S	0	0
			364	228	65	70	1		

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



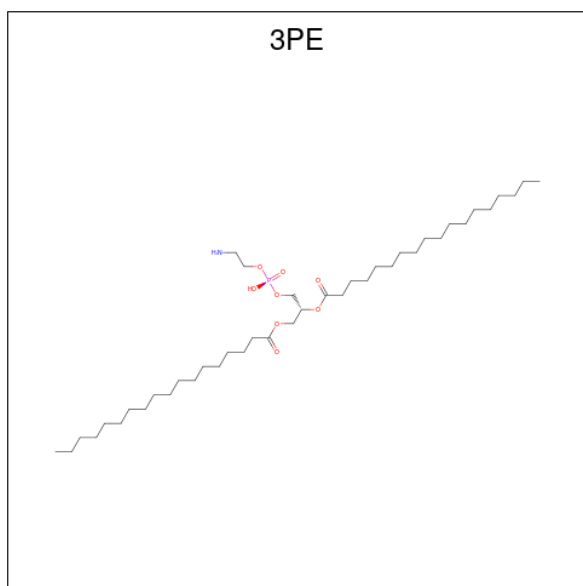
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	B	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	

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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



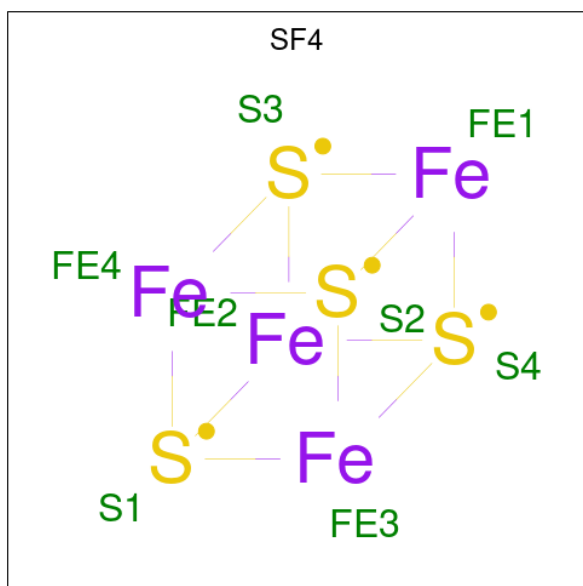
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	J	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	L	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	O	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	b	1	Total	C	N	O	P	0
			39	29	1	8	1	

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



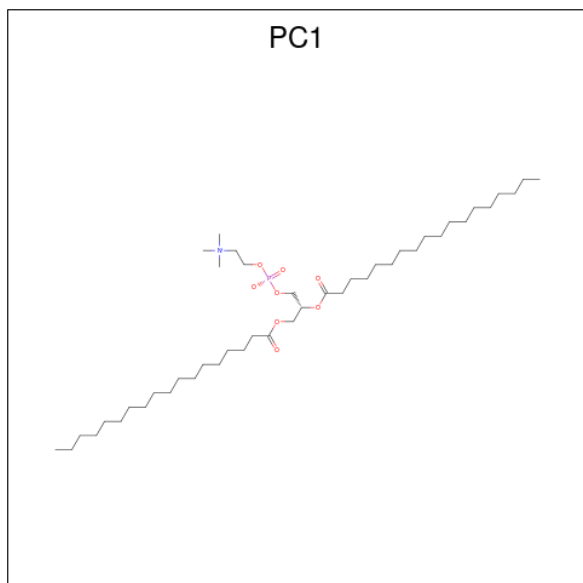
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	

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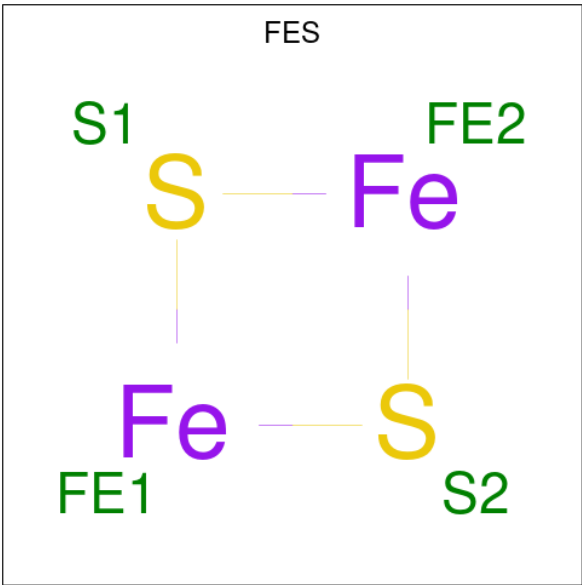
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



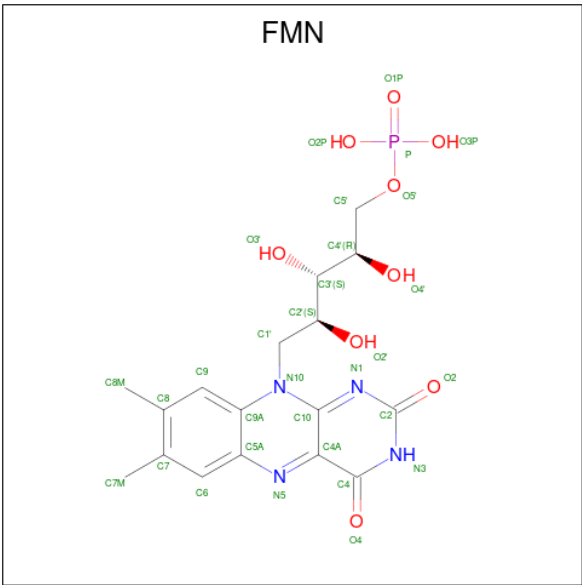
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	M	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

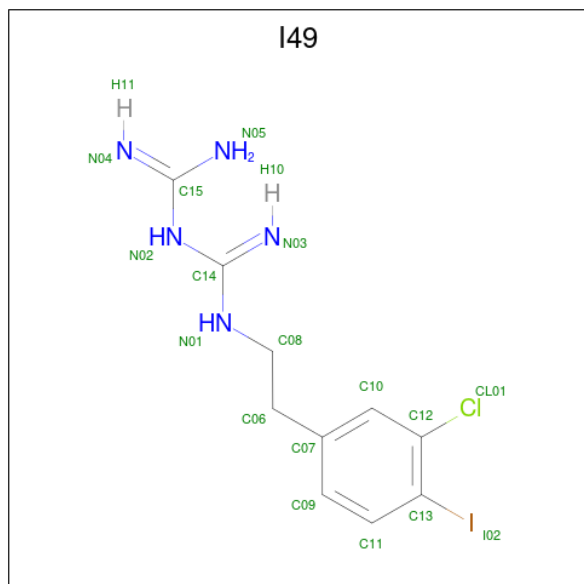


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

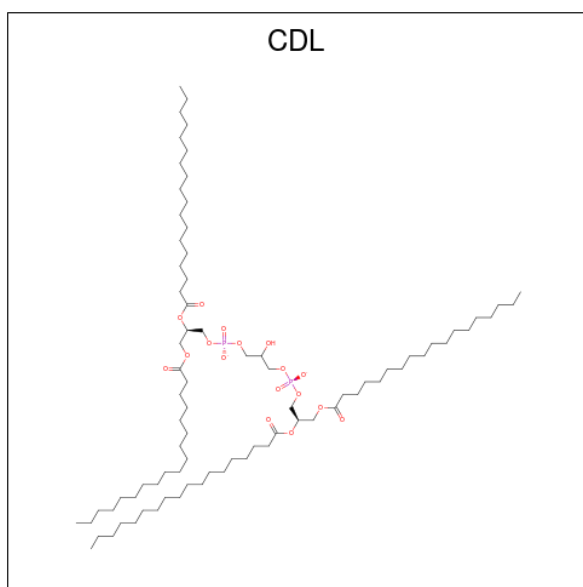
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- Molecule 52 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (CCD ID: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



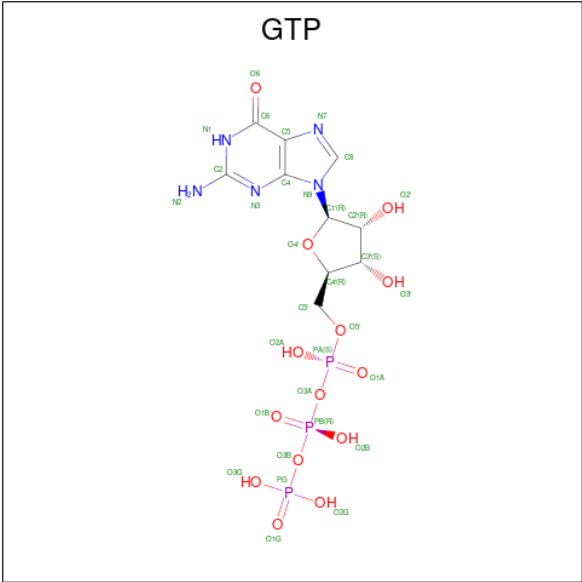
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	
52	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	K	1	Total	C	O	P	0
			67	48	17	2	
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	X	1	Total	C	O	P	0
			65	46	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

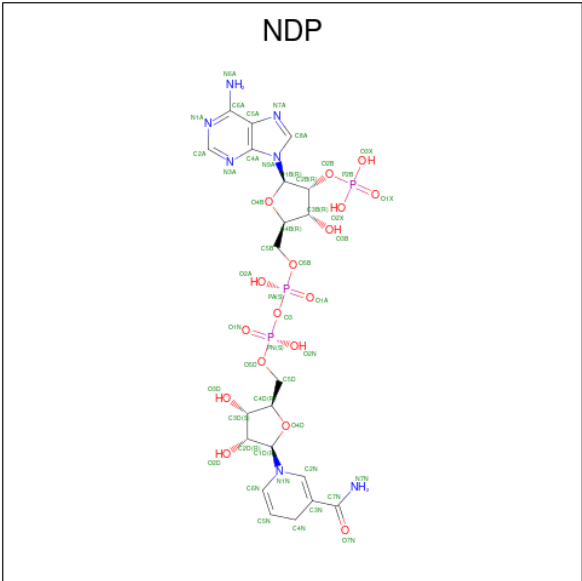


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

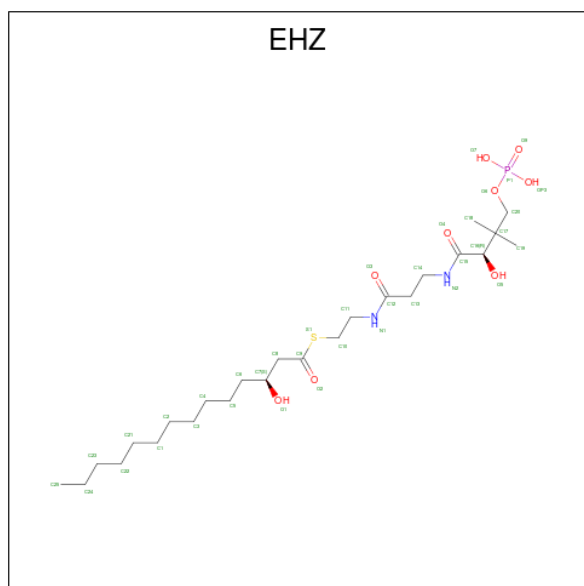


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

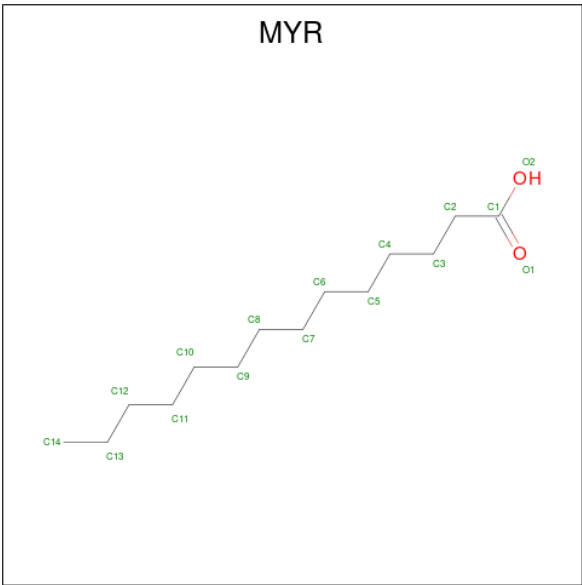
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 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
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	9	Total	O	0
			9	9	
60	B	53	Total	O	0
			53	53	
60	C	82	Total	O	0
			82	82	
60	D	150	Total	O	0
			150	150	
60	E	7	Total	O	0
			7	7	
60	F	55	Total	O	0
			55	55	
60	G	180	Total	O	0
			180	180	
60	H	39	Total	O	0
			39	39	
60	I	89	Total	O	0
			89	89	
60	J	8	Total	O	0
			8	8	
60	K	7	Total	O	0
			7	7	

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Mol	Chain	Residues	Atoms		AltConf
60	L	61	Total 61	O 61	0
60	M	63	Total 63	O 63	0
60	N	39	Total 39	O 39	0
60	O	11	Total 11	O 11	0
60	P	44	Total 44	O 44	0
60	Q	62	Total 62	O 62	0
60	R	31	Total 31	O 31	0
60	S	1	Total 1	O 1	0
60	T	1	Total 1	O 1	0
60	U	7	Total 7	O 7	0
60	V	10	Total 10	O 10	0
60	W	12	Total 12	O 12	0
60	X	23	Total 23	O 23	0
60	Y	2	Total 2	O 2	0
60	Z	18	Total 18	O 18	0
60	a	14	Total 14	O 14	0
60	b	5	Total 5	O 5	0
60	d	12	Total 12	O 12	0
60	e	13	Total 13	O 13	0
60	f	4	Total 4	O 4	0
60	g	17	Total 17	O 17	0

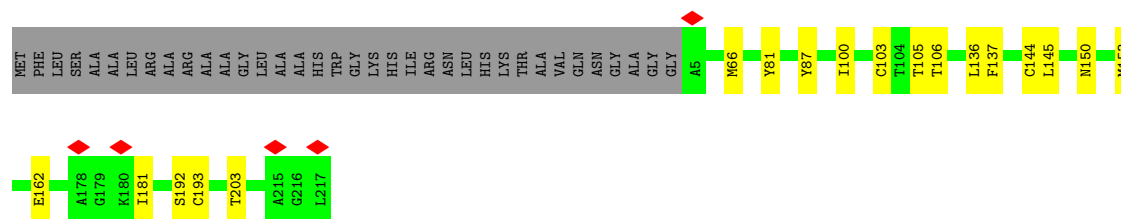
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Mol	Chain	Residues	Atoms		AltConf
60	h	18	Total 18	O 18	0
60	i	5	Total 5	O 5	0
60	j	3	Total 3	O 3	0
60	k	6	Total 6	O 6	0
60	l	28	Total 28	O 28	0
60	m	18	Total 18	O 18	0
60	n	29	Total 29	O 29	0
60	o	14	Total 14	O 14	0
60	p	25	Total 25	O 25	0
60	q	29	Total 29	O 29	0
60	r	27	Total 27	O 27	0
60	s	3	Total 3	O 3	0

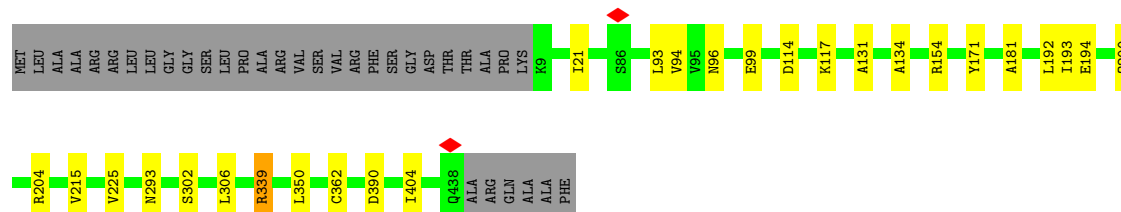
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  78% 7% 14%



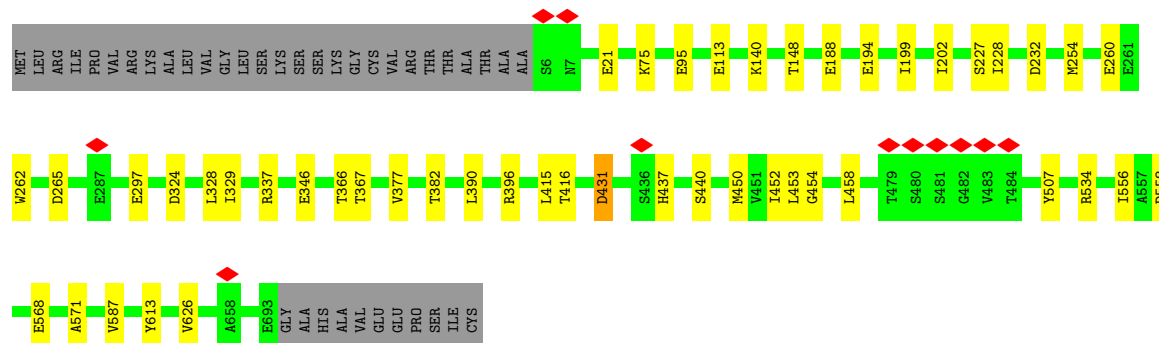
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  87% 6% 7%



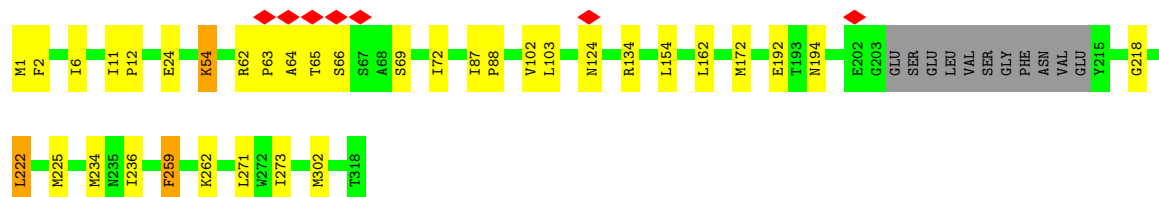
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  88% 6% 5%



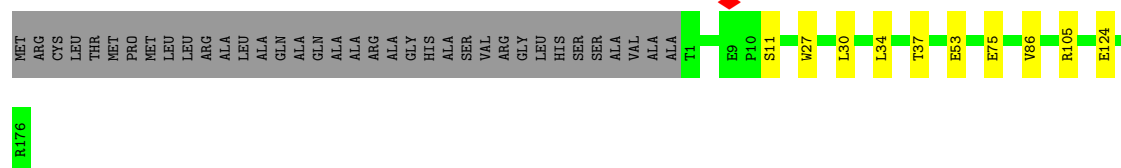
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  86% 10% 4%



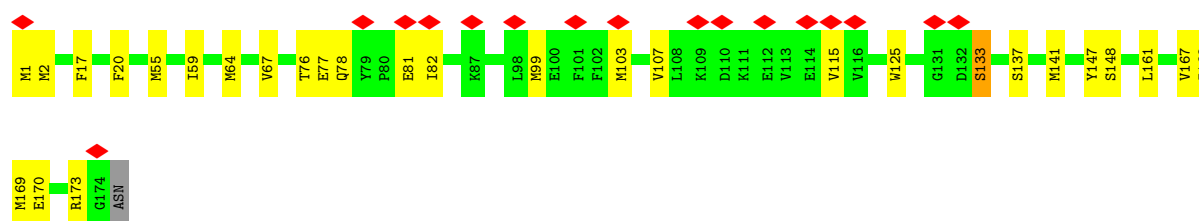
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  78% 5% 17%



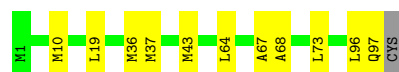
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  10% 83% 16% ..



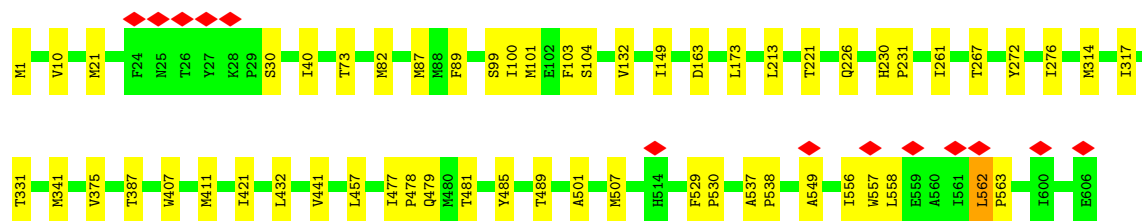
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  88% 11% .



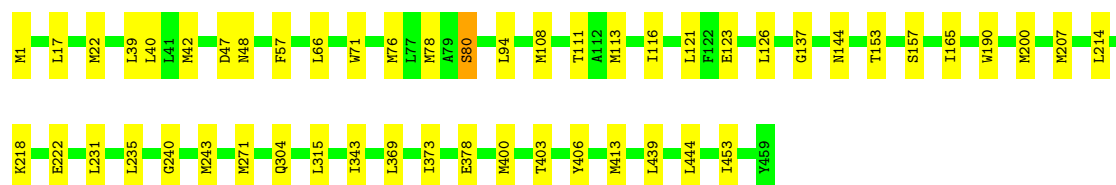
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  91% 9%

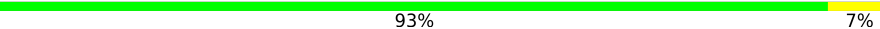


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  89% 11%



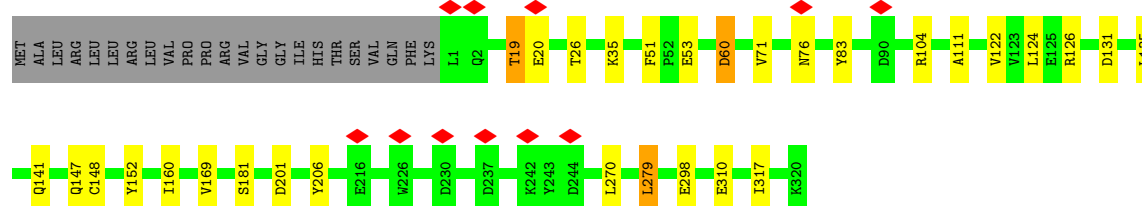
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  93% 7%



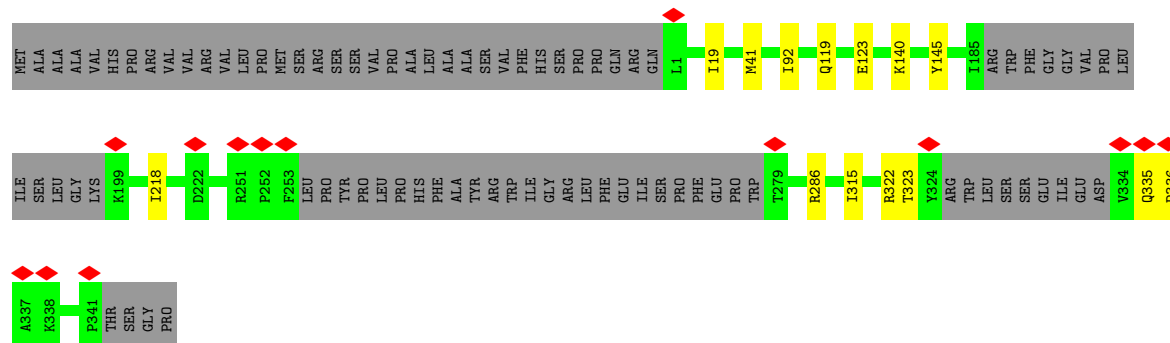
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  84% 8% 7%



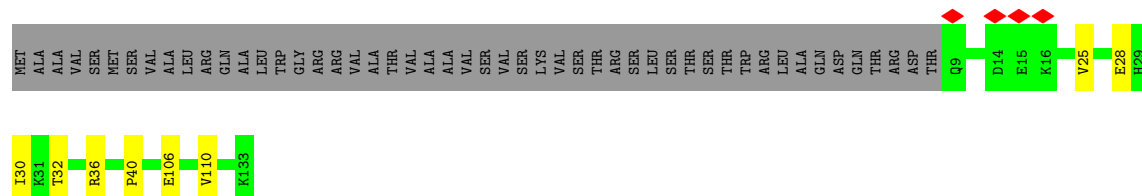
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  74% 23%



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

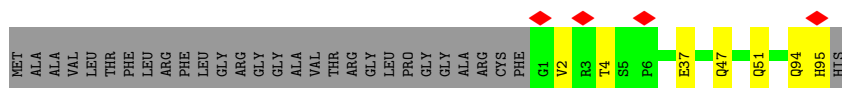
Chain Q:  67% 29% 5%



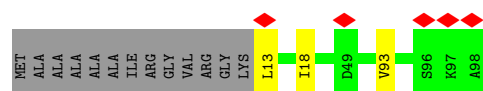
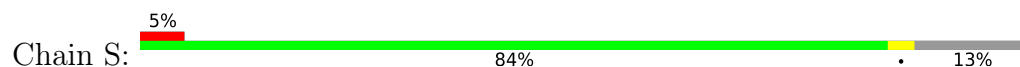
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  71% 23% 6%

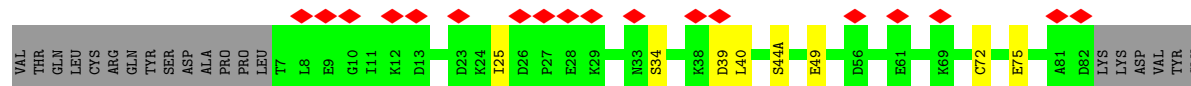
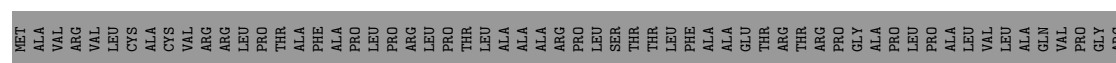
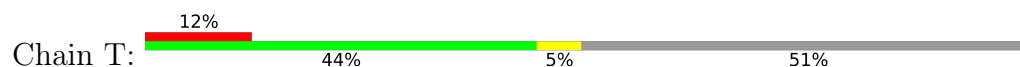




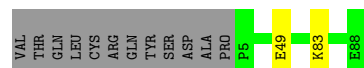
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein, mitochondrial



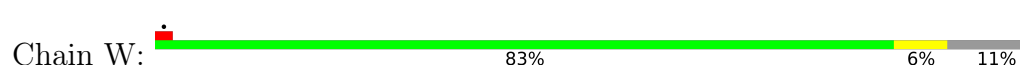
- Molecule 20: Acyl carrier protein, mitochondrial



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



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

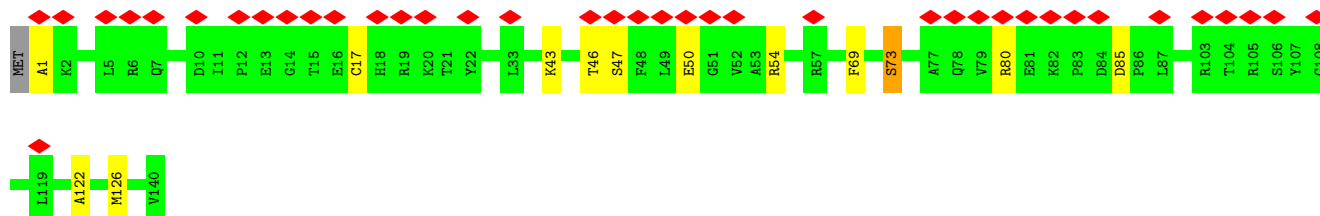
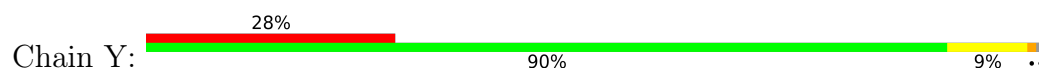


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

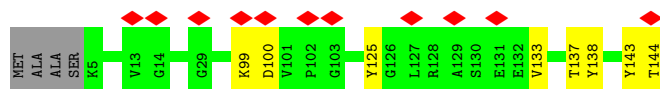
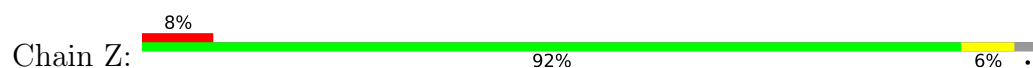




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



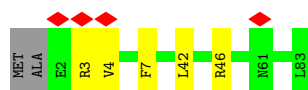
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



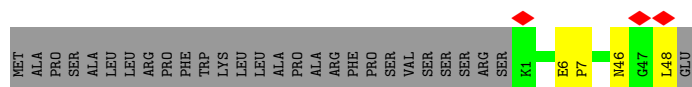
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



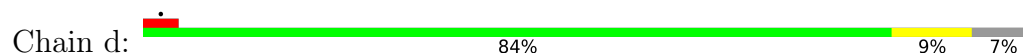
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

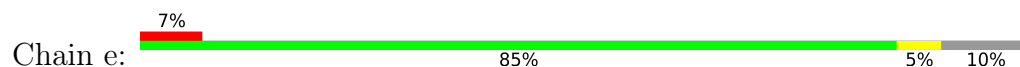


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

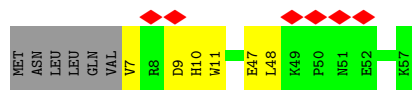
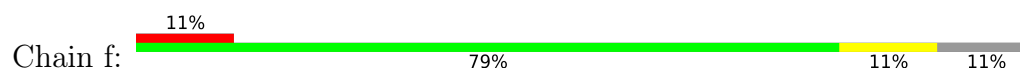




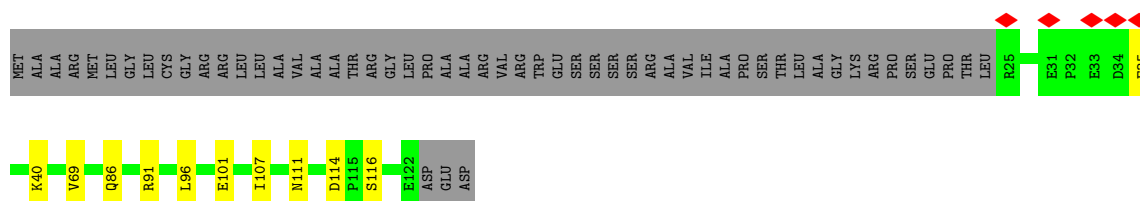
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



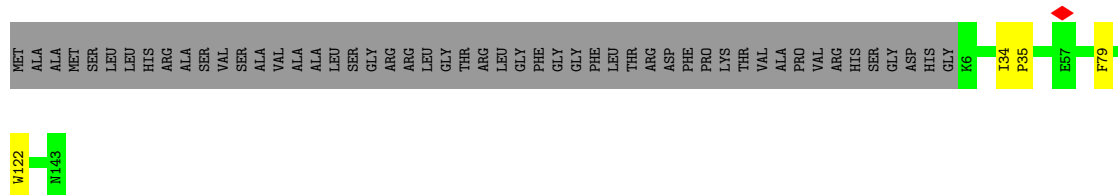
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



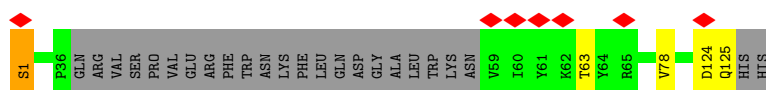
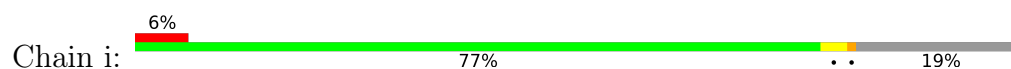
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

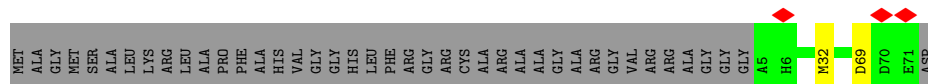


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



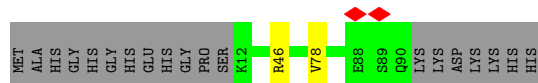
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j: 



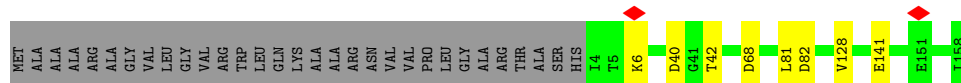
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k: 



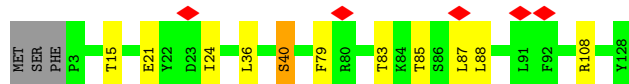
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l: 



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

Chain m: 



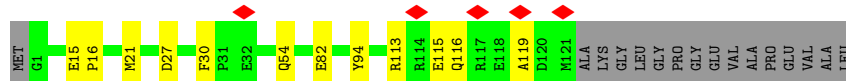
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 



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

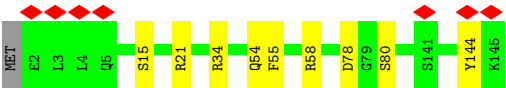
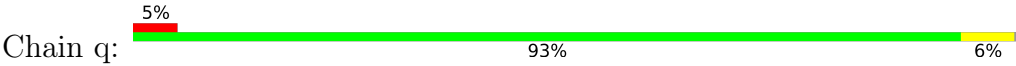
Chain o: 



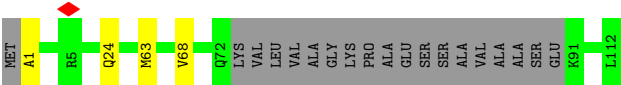
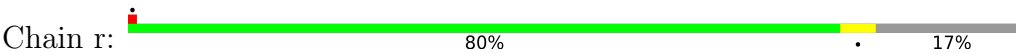
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



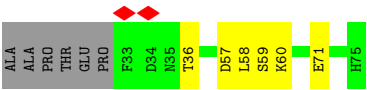
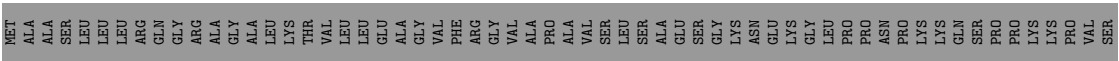
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68023	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	37.571	Depositor
Minimum map value	-16.074	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.063	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: MYR, FME, SAC, K, I49, SF4, 2MR, FES, NDP, MG, CDL, AYA, 3PE, GTP, EHZ, FMN, ZN, PC1, LMT

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	0.22	0/824	0.28	0/1128
2	B	0.28	0/1261	0.36	0/1706
3	C	0.25	0/1765	0.31	0/2403
4	D	0.25	0/3436	0.32	0/4652
5	E	0.22	0/1695	0.30	0/2307
6	F	0.23	0/3384	0.30	0/4573
7	G	0.24	0/5367	0.31	0/7274
8	H	0.26	0/2485	0.34	0/3395
9	I	0.26	0/1445	0.34	0/1956
10	J	0.21	0/1362	0.29	0/1848
11	K	0.23	0/739	0.27	0/1000
12	L	0.26	0/4903	0.30	0/6672
13	M	0.26	0/3738	0.30	0/5097
14	N	0.25	0/2792	0.31	0/3800
15	O	0.23	0/2651	0.28	0/3587
16	P	0.22	0/2395	0.31	0/3238
17	Q	0.24	0/1039	0.30	0/1404
18	R	0.24	0/742	0.29	0/999
19	S	0.21	0/702	0.32	0/945
20	T	0.18	0/621	0.28	0/837
20	U	0.29	0/692	0.28	0/932
21	V	0.21	0/931	0.26	0/1261
22	W	0.23	0/995	0.30	0/1337
23	X	0.23	0/1439	0.31	0/1942
24	Y	0.16	0/1042	0.26	0/1414
25	Z	0.22	0/1175	0.28	0/1584
26	a	0.25	0/576	0.31	0/775
27	b	0.21	0/667	0.30	0/916
28	c	0.21	0/418	0.27	0/567
29	d	0.23	0/964	0.30	0/1305
30	e	0.22	0/818	0.36	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.23	0/457	0.33	0/616
32	g	0.25	0/850	0.30	0/1154
33	h	0.25	0/1188	0.29	0/1607
34	i	0.27	0/904	0.32	0/1230
35	j	0.25	0/607	0.26	0/833
36	k	0.23	0/657	0.28	0/887
37	l	0.27	0/1358	0.30	0/1858
38	m	0.26	0/1076	0.30	0/1455
39	n	0.27	0/1540	0.30	0/2085
40	o	0.29	0/1068	0.33	0/1430
41	p	0.26	0/1468	0.29	0/1979
42	q	0.22	0/1242	0.33	0/1688
43	r	0.22	0/780	0.32	0/1056
44	s	0.21	0/375	0.27	0/507
All	All	0.24	0/66633	0.31	0/90332

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
34	i	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain
34	i	1	SAC	Mainchain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	814	0	858	11	0
2	B	1230	0	1238	8	0
3	C	1714	0	1668	4	0
4	D	3363	0	3306	19	0
5	E	1655	0	1661	11	0
6	F	3310	0	3261	16	0
7	G	5279	0	5301	33	0
8	H	2425	0	2545	25	0
9	I	1414	0	1370	8	0
10	J	1337	0	1346	27	0
11	K	739	0	780	16	0
12	L	4786	0	4933	37	0
13	M	3654	0	3852	37	0
14	N	2733	0	2912	21	0
15	O	2589	0	2566	18	0
16	P	2342	0	2371	7	0
17	Q	1016	0	1014	4	0
18	R	730	0	707	3	0
19	S	691	0	706	3	0
20	T	612	0	604	3	0
20	U	681	0	677	1	0
21	V	911	0	950	3	0
22	W	971	0	989	6	0
23	X	1402	0	1383	7	0
24	Y	1030	0	1041	7	0
25	Z	1146	0	1146	5	0
26	a	561	0	564	1	0
27	b	646	0	654	4	0
28	c	405	0	409	3	0
29	d	934	0	919	11	0
30	e	799	0	807	3	0
31	f	444	0	444	5	0
32	g	824	0	772	8	0
33	h	1154	0	1168	3	0
34	i	884	0	905	1	0
35	j	580	0	519	2	0
36	k	638	0	621	1	0
37	l	1304	0	1203	5	0
38	m	1050	0	1051	4	0
39	n	1487	0	1433	4	0
40	o	1043	0	1011	8	0
41	p	1435	0	1411	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	q	1201	0	1170	8	0
43	r	767	0	776	1	0
44	s	364	0	336	4	0
45	A	35	0	46	0	0
45	B	35	0	46	0	0
45	J	35	0	46	1	0
45	L	105	0	138	2	0
45	M	105	0	138	2	0
45	N	35	0	46	0	0
45	f	35	0	46	8	0
45	h	35	0	46	0	0
45	l	35	0	46	0	0
46	A	36	0	46	0	0
46	H	34	0	47	4	0
46	I	51	0	82	0	0
46	J	37	0	48	1	0
46	L	93	0	140	2	0
46	M	90	0	137	2	0
46	N	41	0	56	0	0
46	O	47	0	71	0	0
46	Y	35	0	44	0	0
46	b	39	0	52	0	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	B	35	0	44	0	0
48	M	41	0	59	1	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	H	17	0	0	3	0
52	N	17	0	0	2	0
53	K	67	0	78	0	0
53	L	100	0	156	4	0
53	X	65	0	76	0	0
53	d	65	0	77	0	0
53	h	67	0	81	1	0
53	q	76	0	96	0	0
54	O	32	0	12	4	0
55	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	P	48	0	26	0	0
57	R	1	0	0	0	0
58	T	37	0	0	0	0
58	U	37	0	0	0	0
59	o	15	0	27	0	0
60	A	9	0	0	0	0
60	B	53	0	0	1	0
60	C	82	0	0	1	0
60	D	150	0	0	5	0
60	E	7	0	0	0	0
60	F	55	0	0	3	0
60	G	180	0	0	6	0
60	H	39	0	0	0	0
60	I	89	0	0	1	0
60	J	8	0	0	0	0
60	K	7	0	0	0	0
60	L	61	0	0	5	0
60	M	63	0	0	0	0
60	N	39	0	0	0	0
60	O	11	0	0	0	0
60	P	44	0	0	0	0
60	Q	62	0	0	1	0
60	R	31	0	0	1	0
60	S	1	0	0	0	0
60	T	1	0	0	0	0
60	U	7	0	0	0	0
60	V	10	0	0	0	0
60	W	12	0	0	0	0
60	X	23	0	0	2	0
60	Y	2	0	0	0	0
60	Z	18	0	0	1	0
60	a	14	0	0	0	0
60	b	5	0	0	0	0
60	d	12	0	0	1	0
60	e	13	0	0	0	0
60	f	4	0	0	0	0
60	g	17	0	0	2	0
60	h	18	0	0	1	0
60	i	5	0	0	0	0
60	j	3	0	0	0	0
60	k	6	0	0	1	0
60	l	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	m	18	0	0	0	0
60	n	29	0	0	2	0
60	o	14	0	0	1	0
60	p	25	0	0	0	0
60	q	29	0	0	1	0
60	r	27	0	0	0	0
60	s	3	0	0	0	0
All	All	68195	0	67430	370	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 (370) 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)
10:J:64:MET:HE1	11:K:37:MET:HE1	1.41	1.00
45:L:702:LMT:H6B	45:L:706:LMT:H4O1	1.17	0.87
37:l:40:ASP:OD1	37:l:42:THR:OG1	1.91	0.86
12:L:479:GLN:NE2	12:L:481:THR:O	2.09	0.84
39:n:83:GLU:OE2	60:n:201:HOH:O	1.96	0.84
7:G:232:ASP:OD1	60:G:901:HOH:O	1.97	0.81
12:L:163:ASP:OD1	60:L:801:HOH:O	1.98	0.80
23:X:162:HIS:O	60:X:1801:HOH:O	1.98	0.80
20:T:49:GLU:OE2	22:W:64:ARG:NH1	2.15	0.79
14:N:196:TYR:O	52:N:503:I49:N04	2.16	0.78
11:K:43:MET:HE1	14:N:72:MET:HE1	1.64	0.78
33:h:122:TRP:O	60:h:1101:HOH:O	2.02	0.77
42:q:54:GLN:O	60:q:301:HOH:O	2.03	0.76
7:G:346:GLU:OE2	60:G:902:HOH:O	2.03	0.76
7:G:95:GLU:OE2	60:G:903:HOH:O	2.04	0.75
3:C:49:GLU:OE2	60:C:301:HOH:O	2.03	0.75
31:f:47:GLU:OE1	31:f:48:LEU:N	2.20	0.75
45:f:1901:LMT:O1'	45:f:1901:LMT:O6'	2.06	0.74
40:o:15:GLU:OE1	60:o:301:HOH:O	2.05	0.74
6:F:114:ASP:OD1	60:F:601:HOH:O	2.04	0.73
23:X:169:TRP:O	60:X:1802:HOH:O	2.05	0.73
7:G:265:ASP:OD2	60:G:904:HOH:O	2.05	0.73
42:q:78:ASP:OD1	42:q:80:SER:OG	2.06	0.73
32:g:114:ASP:OD1	32:g:116:SER:OG	2.05	0.73
18:R:2:VAL:HG21	18:R:37:GLU:OE1	1.87	0.73
4:D:88:GLU:OE2	60:D:501:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:113:GLU:OE2	60:G:905:HOH:O	2.07	0.72
16:P:335:GLN:NE2	16:P:336:PRO:O	2.22	0.72
12:L:478:PRO:O	60:L:805:HOH:O	2.08	0.72
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.72	0.71
24:Y:69:PHE:O	24:Y:73:SER:OG	2.08	0.71
12:L:432:LEU:O	60:L:804:HOH:O	2.06	0.71
2:B:138:ARG:NH1	60:B:301:HOH:O	2.23	0.70
8:H:225:MET:SD	52:H:602:I49:I02	3.19	0.70
24:Y:43:LYS:O	24:Y:54:ARG:NH2	2.24	0.70
29:d:117:HIS:O	60:d:301:HOH:O	2.08	0.70
31:f:10:HIS:CD2	45:f:1901:LMT:H2O2	2.09	0.69
7:G:396:ARG:NH1	7:G:416:THR:O	2.26	0.69
8:H:103:LEU:HD21	10:J:55:MET:HE3	1.75	0.69
10:J:64:MET:HE1	11:K:37:MET:CE	2.20	0.69
4:D:49:LEU:HD13	4:D:68:LEU:HD12	1.73	0.69
13:M:22:MET:HE3	45:f:1901:LMT:O5'	1.93	0.68
36:k:46:ARG:O	60:k:101:HOH:O	2.11	0.68
39:n:14:LYS:O	60:n:203:HOH:O	2.10	0.68
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.27	0.68
13:M:42:MET:HE1	13:M:453:ILE:HD12	1.74	0.68
15:O:53:GLU:OE2	15:O:126:ARG:NH2	2.27	0.68
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.27	0.67
24:Y:80:ARG:NH2	24:Y:85:ASP:OD1	2.28	0.67
7:G:260:GLU:OE2	60:G:906:HOH:O	2.13	0.67
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.77	0.67
11:K:43:MET:CE	14:N:72:MET:HE1	2.24	0.67
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.28	0.67
45:J:402:LMT:O6'	45:J:402:LMT:O2B	2.12	0.66
6:F:390:ASP:OD2	60:F:602:HOH:O	2.12	0.66
7:G:366:THR:O	7:G:367:THR:OG1	2.11	0.66
44:s:57:ASP:O	44:s:60:LYS:NZ	2.28	0.66
13:M:94:LEU:HD21	46:M:603:3PE:O32	1.96	0.66
17:Q:36:ARG:NH2	17:Q:106:GLU:OE2	2.29	0.66
17:Q:40:PRO:O	60:Q:201:HOH:O	2.12	0.66
11:K:43:MET:SD	14:N:72:MET:HE1	2.36	0.66
23:X:78:ALA:O	23:X:82:THR:OG1	2.13	0.65
10:J:133:SER:O	10:J:133:SER:OG	2.15	0.65
35:j:69:ASP:OD1	40:o:113:ARG:NH1	2.28	0.65
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.64
2:B:84:ASP:OD2	8:H:54:LYS:NZ	2.30	0.64
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.79	0.64
34:i:124:ASP:OD1	34:i:125:GLN:N	2.31	0.64
46:L:703:3PE:H372	53:L:704:CDL:H871	1.78	0.63
32:g:86:GLN:NE2	41:p:100:GLU:OE1	2.31	0.63
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.80	0.62
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.80	0.62
8:H:225:MET:HG3	52:H:602:I49:I02	2.69	0.62
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.82	0.62
12:L:21:MET:HE2	12:L:21:MET:HA	1.80	0.61
13:M:378:GLU:OE2	13:M:400:MET:HE2	2.01	0.61
13:M:373:ILE:HD11	13:M:444:LEU:HD12	1.82	0.61
7:G:431:ASP:OD1	7:G:431:ASP:N	2.33	0.60
31:f:10:HIS:CE1	45:f:1901:LMT:H2O2	2.18	0.60
1:A:3:LEU:HD21	46:J:401:3PE:H341	1.83	0.60
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.82	0.60
29:d:120:ARG:O	38:m:108:ARG:NH2	2.34	0.59
7:G:556:ILE:HG22	42:q:144:TYR:CE2	2.38	0.59
10:J:103:MET:HG2	10:J:115:VAL:HG21	1.85	0.59
8:H:65:THR:O	8:H:124:ASN:ND2	2.35	0.59
4:D:62:LEU:HD13	4:D:425:PHE:CZ	2.38	0.59
11:K:37:MET:HE2	11:K:67:ALA:CB	2.33	0.58
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.38	0.58
27:b:42:LEU:HD21	27:b:46:ARG:NH1	2.17	0.58
6:F:131:ALA:O	6:F:171:TYR:OH	2.12	0.58
4:D:71:GLU:OE2	8:H:134:ARG:NH1	2.36	0.58
2:B:48:MET:HE1	2:B:50:PHE:CD2	2.39	0.58
12:L:485:TYR:O	12:L:489:THR:OG1	2.21	0.57
13:M:78:MET:HE1	13:M:439:LEU:CD1	2.34	0.57
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.86	0.57
42:q:21:ARG:HH21	42:q:21:ARG:HG3	1.69	0.57
12:L:375:VAL:HG22	35:j:32:MET:SD	2.44	0.57
16:P:323:THR:HG23	16:P:323:THR:O	2.05	0.57
12:L:82:MET:HB3	12:L:87:MET:HE3	1.87	0.56
4:D:427:GLU:OE1	60:D:503:HOH:O	2.18	0.56
15:O:60:ASP:OD1	15:O:60:ASP:N	2.37	0.56
18:R:94:GLN:O	18:R:95:HIS:ND1	2.38	0.56
22:W:117:ASP:OD1	22:W:120:SER:OG	2.15	0.56
6:F:200:GLN:NE2	60:F:604:HOH:O	2.35	0.56
10:J:59:ILE:HB	11:K:64:LEU:HD21	1.88	0.56
12:L:558:LEU:HB3	13:M:214:LEU:HD21	1.88	0.56
15:O:35:LYS:NZ	54:O:1202:GTP:O3G	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:7:VAL:HG12	31:f:9:ASP:H	1.71	0.56
45:f:1901:LMT:H6'	45:f:1901:LMT:C1	2.19	0.56
15:O:310:GLU:HG3	15:O:317:ILE:HD12	1.88	0.56
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.39	0.55
29:d:10:THR:HG23	29:d:10:THR:O	2.07	0.55
40:o:115:GLU:O	40:o:119:ALA:N	2.31	0.55
9:I:75:GLU:O	9:I:105:ARG:NH1	2.38	0.55
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.88	0.55
4:D:228:MET:HE1	9:I:37:THR:HG23	1.87	0.55
10:J:103:MET:CG	10:J:115:VAL:HG21	2.37	0.55
11:K:37:MET:HE2	11:K:67:ALA:HB1	1.88	0.55
5:E:181:ILE:HG23	5:E:181:ILE:O	2.06	0.55
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.41	0.55
12:L:21:MET:HE2	12:L:21:MET:CA	2.37	0.55
13:M:78:MET:HE1	13:M:439:LEU:HD12	1.88	0.55
13:M:190:TRP:CE3	24:Y:126:MET:HE2	2.42	0.55
15:O:104:ARG:NH1	54:O:1202:GTP:O6	2.38	0.54
12:L:213:LEU:HD22	12:L:267:THR:HG22	1.89	0.54
25:Z:138:TYR:OH	60:Z:201:HOH:O	2.16	0.54
20:U:49:GLU:OE1	39:n:44:ARG:NH1	2.40	0.54
4:D:49:LEU:CD1	4:D:68:LEU:HD12	2.38	0.54
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.90	0.54
13:M:78:MET:HE3	60:g:207:HOH:O	2.05	0.54
10:J:1:FME:SD	10:J:2:MET:N	2.81	0.53
10:J:103:MET:SD	10:J:115:VAL:HG21	2.48	0.53
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.89	0.53
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.90	0.53
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.41	0.53
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.22	0.53
37:l:141:GLU:OE2	37:l:141:GLU:N	2.41	0.53
23:X:153:VAL:HG22	29:d:92:SER:HB3	1.91	0.53
8:H:103:LEU:HD21	10:J:55:MET:CE	2.39	0.53
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.91	0.53
7:G:140:LYS:O	7:G:148:THR:OG1	2.23	0.53
4:D:303:GLU:OE2	60:D:502:HOH:O	2.17	0.52
27:b:42:LEU:HD21	27:b:46:ARG:HH11	1.74	0.52
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.44	0.52
1:A:63:LEU:HB2	10:J:67:VAL:HG21	1.90	0.52
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.36	0.52
53:L:704:CDL:H872	53:h:1001:CDL:H242	1.91	0.52
30:e:58:GLU:N	30:e:58:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:THR:HG22	5:E:106:THR:H	1.75	0.51
10:J:141:MET:HA	10:J:141:MET:HE2	1.92	0.51
23:X:153:VAL:HG22	29:d:92:SER:CB	2.40	0.51
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.91	0.51
12:L:100:ILE:O	12:L:104:SER:OG	2.25	0.51
7:G:415:LEU:O	7:G:416:THR:OG1	2.23	0.51
10:J:64:MET:HE2	11:K:68:ALA:HA	1.92	0.51
13:M:373:ILE:HD11	13:M:444:LEU:CD1	2.41	0.51
14:N:70:LEU:HG	14:N:98:MET:HE2	1.93	0.51
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.93	0.51
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.92	0.50
5:E:192:SER:OG	5:E:193:CYS:N	2.38	0.50
12:L:226:GLN:HG3	12:L:314:MET:HE3	1.92	0.50
15:O:26:THR:CG2	15:O:169:VAL:HG22	2.42	0.50
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.93	0.50
8:H:273:ILE:HG13	46:H:601:3PE:H3I1	1.93	0.50
29:d:112:VAL:HG21	41:p:78:GLU:OE2	2.12	0.50
53:L:704:CDL:H622	53:L:704:CDL:H873	1.94	0.50
32:g:35:GLU:OE1	32:g:40:LYS:NZ	2.45	0.50
10:J:55:MET:HE2	10:J:55:MET:HA	1.93	0.50
11:K:96:LEU:HD13	14:N:117:GLU:O	2.12	0.50
8:H:192:GLU:HA	8:H:192:GLU:OE2	2.11	0.50
13:M:57:PHE:HB3	13:M:113:MET:HE3	1.94	0.50
2:B:59:MET:CE	2:B:69:MET:HE1	2.41	0.49
13:M:47:ASP:OD1	13:M:48:ASN:N	2.43	0.49
10:J:81:GLU:OE2	10:J:81:GLU:N	2.45	0.49
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.93	0.49
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.42	0.49
7:G:377:VAL:HG13	7:G:452:ILE:HD12	1.95	0.49
24:Y:50:GLU:HA	24:Y:50:GLU:OE2	2.13	0.49
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.47	0.49
15:O:83:TYR:OH	54:O:1202:GTP:O3'	1.95	0.49
12:L:261:ILE:HG13	12:L:317:ILE:HD11	1.95	0.49
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.94	0.49
14:N:218:MET:HE3	14:N:244:ILE:CG1	2.43	0.49
8:H:218:GLY:O	8:H:222:LEU:HD22	2.13	0.49
9:I:124:GLU:OE2	60:I:301:HOH:O	2.19	0.49
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.95	0.49
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.95	0.49
8:H:225:MET:CG	52:H:602:I49:I02	3.30	0.48
13:M:17:LEU:HD13	31:f:11:TRP:HH2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.95	0.48
13:M:22:MET:HE3	45:f:1901:LMT:C5'	2.43	0.48
8:H:72:ILE:HD13	8:H:72:ILE:N	2.29	0.48
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.95	0.48
19:S:13:LEU:O	19:S:13:LEU:HD23	2.13	0.48
13:M:304:GLN:O	29:d:119:VAL:HG11	2.13	0.48
18:R:47:GLN:NE2	60:R:301:HOH:O	2.29	0.48
29:d:13:PHE:O	29:d:78:ARG:NH1	2.47	0.48
7:G:328:LEU:O	7:G:507:TYR:OH	2.26	0.47
9:I:27:TRP:HB3	9:I:30:LEU:HD12	1.96	0.47
25:Z:99:LYS:NZ	25:Z:100:ASP:OD2	2.48	0.47
4:D:322:GLU:OE1	4:D:322:GLU:N	2.43	0.47
45:f:1901:LMT:H3O2	45:f:1901:LMT:H6B	1.63	0.47
22:W:104:MET:HE2	22:W:109:GLU:OE1	2.14	0.47
5:E:66:MET:HE2	5:E:81:TYR:CD1	2.50	0.47
6:F:21:ILE:HG22	6:F:117:LYS:HE2	1.96	0.47
13:M:123:GLU:OE2	13:M:157:SER:HB2	2.15	0.47
52:N:503:I49:I02	29:d:82:MET:HB3	2.85	0.47
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.50	0.47
32:g:96:LEU:HD12	41:p:97:VAL:HG11	1.97	0.47
39:n:27:GLU:OE1	39:n:33:ARG:NH1	2.40	0.47
3:C:208:ALA:HB1	43:r:63:MET:HE2	1.97	0.47
7:G:337:ARG:HG3	7:G:337:ARG:HH11	1.80	0.47
14:N:314:LYS:NZ	15:O:270:LEU:O	2.44	0.47
15:O:19:THR:OG1	15:O:20:GLU:N	2.47	0.47
15:O:83:TYR:OH	54:O:1202:GTP:O2'	2.28	0.47
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.97	0.46
11:K:37:MET:HB2	14:N:68:MET:HE1	1.98	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.46
23:X:154:GLU:HA	23:X:154:GLU:OE1	2.15	0.46
26:a:59:ARG:HH21	26:a:59:ARG:HG3	1.80	0.46
8:H:63:PRO:O	8:H:64:ALA:HB3	2.15	0.46
38:m:36:LEU:O	38:m:40:SER:OG	2.31	0.46
12:L:21:MET:HE2	12:L:21:MET:N	2.31	0.46
6:F:306:LEU:C	6:F:306:LEU:HD12	2.40	0.46
12:L:341:MET:SD	12:L:457:LEU:HD12	2.56	0.46
16:P:315:ILE:HD13	16:P:322:ARG:NH2	2.31	0.46
1:A:71:LEU:O	10:J:147:TYR:OH	2.22	0.46
10:J:115:VAL:O	10:J:115:VAL:HG12	2.15	0.46
13:M:39:LEU:HD12	45:M:605:LMT:H122	1.97	0.46
7:G:437:HIS:O	7:G:440:SER:OG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:450:MET:HE2	7:G:452:ILE:HD11	1.97	0.46
16:P:119:GLN:NE2	16:P:123:GLU:OE1	2.49	0.46
7:G:534:ARG:NH2	7:G:558:ASP:OD2	2.46	0.46
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.46
46:H:601:3PE:H3I2	9:I:34:LEU:HD13	1.98	0.46
2:B:48:MET:HE1	2:B:50:PHE:CE2	2.50	0.46
16:P:19:ILE:HD12	16:P:41:MET:HE3	1.98	0.46
14:N:207:ILE:HD13	14:N:262:PRO:HD3	1.97	0.45
38:m:21:GLU:O	38:m:24:ILE:HD11	2.17	0.45
12:L:556:ILE:HG22	12:L:557:TRP:N	2.30	0.45
14:N:218:MET:HE3	14:N:244:ILE:HG13	1.98	0.45
38:m:83:THR:HG22	38:m:87:LEU:HD12	1.98	0.45
4:D:228:MET:CE	9:I:37:THR:HG23	2.46	0.45
10:J:99:MET:HE2	11:K:10:MET:HE1	1.99	0.45
15:O:147:GLN:OE1	15:O:147:GLN:N	2.45	0.45
28:c:6:GLU:HA	28:c:6:GLU:OE1	2.17	0.45
28:c:6:GLU:OE1	28:c:7:PRO:HD2	2.17	0.45
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.52	0.45
27:b:3:ARG:O	27:b:7:PHE:N	2.45	0.45
1:A:82:ALA:O	27:b:42:LEU:HD23	2.17	0.45
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.46	0.45
4:D:284:ASP:OD1	60:D:504:HOH:O	2.21	0.44
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.99	0.44
12:L:549:ALA:HB2	13:M:271:MET:HE3	1.99	0.44
14:N:72:MET:HE2	14:N:76:ILE:HG13	1.98	0.44
30:e:88:GLU:HB3	30:e:90:LYS:NZ	2.32	0.44
14:N:89:LEU:HD12	14:N:95:SER:HA	1.99	0.44
4:D:117:ALA:HB2	4:D:367:ILE:HG12	1.99	0.44
12:L:562:LEU:CB	12:L:563:PRO:CD	2.95	0.44
29:d:99:GLU:CD	29:d:99:GLU:H	2.25	0.44
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.52	0.44
45:L:702:LMT:O6B	45:L:706:LMT:O4'	2.00	0.44
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.83	0.44
12:L:99:SER:OG	60:L:802:HOH:O	1.98	0.44
14:N:100:MET:O	14:N:104:MET:HG3	2.18	0.44
32:g:91:ARG:NH2	60:g:203:HOH:O	2.50	0.44
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.98	0.44
1:A:48:ARG:NH1	1:A:49:LEU:O	2.51	0.44
24:Y:122:ALA:O	24:Y:126:MET:HG3	2.18	0.43
13:M:343:ILE:HG13	13:M:413:MET:HE2	1.99	0.43
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	2.00	0.43
13:M:406:TYR:CD1	13:M:406:TYR:C	2.96	0.43
20:T:72:CYS:SG	20:T:75:GLU:HG3	2.58	0.43
4:D:3:GLN:NE2	13:M:137:GLY:O	2.46	0.43
5:E:145:LEU:HD12	5:E:153:MET:SD	2.59	0.43
11:K:37:MET:HE2	11:K:67:ALA:HB3	2.01	0.43
29:d:10:THR:HG21	30:e:7:LYS:HG3	2.00	0.43
44:s:71:GLU:OE1	44:s:71:GLU:HA	2.17	0.43
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.99	0.43
7:G:382:THR:HB	7:G:454:GLY:HA3	2.00	0.43
13:M:218:LYS:O	13:M:222:GLU:HG2	2.19	0.43
15:O:131:ASP:OD1	15:O:152:TYR:OH	2.35	0.43
7:G:199:ILE:HA	7:G:202:ILE:HG12	1.99	0.43
12:L:87:MET:HA	12:L:87:MET:HE2	2.00	0.43
13:M:126:LEU:HD21	13:M:153:THR:HG21	2.01	0.43
22:W:25:MET:HE1	22:W:79:VAL:HG21	2.00	0.43
22:W:104:MET:CE	22:W:109:GLU:OE1	2.66	0.43
28:c:46:ASN:HB2	28:c:48:LEU:HD12	2.01	0.43
13:M:207:MET:SD	13:M:240:GLY:N	2.92	0.42
12:L:40:ILE:HG13	12:L:101:MET:SD	2.59	0.42
5:E:87:TYR:HB3	6:F:181:ALA:O	2.19	0.42
13:M:190:TRP:NE1	45:M:602:LMT:O6'	2.46	0.42
3:C:51:CYS:HB3	21:V:111:TRP:CE2	2.54	0.42
8:H:262:LYS:NZ	46:H:601:3PE:O14	2.42	0.42
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.01	0.42
13:M:40:LEU:HD22	33:h:79:PHE:HB3	2.00	0.42
40:o:16:PRO:HB3	40:o:21:MET:HE2	2.01	0.42
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.01	0.42
15:O:148:CYS:HA	15:O:279:LEU:HD21	2.01	0.42
19:S:13:LEU:HD23	19:S:13:LEU:C	2.45	0.42
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.50	0.42
13:M:76:MET:O	13:M:80:SER:OG	2.26	0.42
13:M:200:MET:HE1	13:M:243:MET:HE3	2.01	0.42
42:q:21:ARG:HG3	42:q:21:ARG:NH2	2.34	0.42
4:D:385:ARG:NH1	60:D:525:HOH:O	2.47	0.42
6:F:154:ARG:HA	44:s:58:LEU:HD21	2.02	0.42
7:G:329:ILE:HD11	7:G:626:VAL:HG21	2.01	0.42
10:J:76:THR:O	10:J:78:GLN:NE2	2.52	0.42
12:L:73:THR:OG1	60:L:803:HOH:O	2.00	0.42
7:G:556:ILE:HG22	42:q:144:TYR:HE2	1.83	0.42
7:G:254:MET:HA	7:G:260:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:272:TYR:CZ	12:L:276:ILE:HD11	2.55	0.42
12:L:331:THR:HB	12:L:387:THR:HG22	2.02	0.42
1:A:108:GLN:HB2	10:J:169:MET:HE1	2.02	0.41
37:l:68:ASP:OD1	37:l:68:ASP:N	2.48	0.41
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.02	0.41
11:K:19:LEU:HD22	11:K:36:MET:HE2	2.02	0.41
12:L:477:ILE:HD11	40:o:54:GLN:HA	2.02	0.41
19:S:18:ILE:CD1	19:S:93:VAL:HG11	2.51	0.41
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.03	0.41
5:E:181:ILE:O	5:E:181:ILE:CG2	2.67	0.41
6:F:96:ASN:O	6:F:225:VAL:HG23	2.20	0.41
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.56	0.41
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	2.02	0.41
21:V:34:LEU:HD13	21:V:48:GLU:HG3	2.02	0.41
10:J:125:TRP:HB2	25:Z:137:THR:HG21	2.02	0.41
7:G:568:GLU:HA	7:G:587:VAL:O	2.21	0.41
8:H:102:VAL:HG22	8:H:162:LEU:HD23	2.02	0.41
14:N:146:PHE:HA	14:N:149:ILE:HD12	2.03	0.41
45:f:1901:LMT:O1'	45:f:1901:LMT:C6'	2.69	0.41
6:F:362:CYS:HB3	6:F:404:ILE:HD12	2.03	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.41
37:l:82:ASP:OD1	37:l:82:ASP:N	2.51	0.41
7:G:21:GLU:OE1	7:G:21:GLU:N	2.49	0.41
53:L:704:CDL:H672	48:M:604:PC1:H342	2.02	0.41
25:Z:143:TYR:O	25:Z:144:THR:C	2.63	0.41
44:s:36:THR:O	44:s:36:THR:HG22	2.21	0.41
2:B:59:MET:HE1	2:B:69:MET:HE1	2.03	0.41
8:H:273:ILE:CG1	46:H:601:3PE:H3I1	2.51	0.41
10:J:137:SER:O	10:J:141:MET:HG2	2.21	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.56	0.41
33:h:34:ILE:HB	33:h:35:PRO:HD3	2.03	0.41
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.56	0.41
40:o:82:GLU:OE1	40:o:82:GLU:N	2.52	0.41
7:G:227:SER:OG	7:G:228:ILE:N	2.53	0.41
7:G:337:ARG:HG3	7:G:337:ARG:NH1	2.36	0.41
11:K:37:MET:HG3	11:K:67:ALA:CB	2.51	0.41
12:L:173:LEU:HD11	46:L:701:3PE:H371	2.03	0.41
46:M:603:3PE:H332	14:N:242:VAL:HG11	2.02	0.41
2:B:91:THR:HA	2:B:119:CYS:HB3	2.01	0.40
5:E:103:CYS:SG	5:E:144:CYS:HA	2.61	0.40
6:F:293:ASN:O	6:F:339:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:236:ILE:HG23	8:H:259:PHE:CE2	2.55	0.40
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.57	0.40
8:H:172:MET:HE2	8:H:172:MET:HB3	1.95	0.40
1:A:49:LEU:O	1:A:51:PHE:N	2.49	0.40
2:B:45:LEU:O	2:B:74:VAL:HA	2.21	0.40
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.03	0.40
12:L:89:PHE:CE2	12:L:132:VAL:HG21	2.57	0.40
16:P:145:TYR:CD1	16:P:286:ARG:HD3	2.56	0.40
40:o:116:GLN:OE1	40:o:116:GLN:HA	2.22	0.40
7:G:194:GLU:OE1	7:G:194:GLU:N	2.47	0.40
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.03	0.40
20:T:25:ILE:HG12	20:T:40:LEU:HD22	2.03	0.40
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.57	0.40
5:E:100:ILE:HD11	5:E:137:PHE:HD1	1.86	0.40
6:F:93:LEU:O	6:F:134:ALA:HA	2.21	0.40
13:M:190:TRP:CD2	24:Y:126:MET:HE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
2	B	152/216 (70%)	145 (95%)	7 (5%)	0	100	100
3	C	204/266 (77%)	200 (98%)	4 (2%)	0	100	100
4	D	410/463 (89%)	401 (98%)	9 (2%)	0	100	100
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	428/464 (92%)	421 (98%)	7 (2%)	0	100	100
7	G	686/727 (94%)	669 (98%)	17 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	303/318 (95%)	291 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	159 (92%)	13 (8%)	0	100	100
11	K	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	583 (96%)	20 (3%)	1 (0%)	43	58
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	309 (97%)	9 (3%)	0	100	100
16	P	286/380 (75%)	281 (98%)	5 (2%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	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	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	110 (100%)	0	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	137 (99%)	1 (1%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
30	e	93/106 (88%)	91 (98%)	2 (2%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	96/154 (62%)	92 (96%)	4 (4%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	119/137 (87%)	115 (97%)	4 (3%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	39 (95%)	2 (5%)	0	100	100
All	All	7989/9212 (87%)	7805 (98%)	183 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

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	88/100 (88%)	87 (99%)	1 (1%)	65	82
2	B	130/175 (74%)	129 (99%)	1 (1%)	73	86
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	360/392 (92%)	356 (99%)	4 (1%)	65	82
5	E	183/205 (89%)	181 (99%)	2 (1%)	65	82
6	F	344/368 (94%)	342 (99%)	2 (1%)	78	89
7	G	578/608 (95%)	574 (99%)	4 (1%)	76	88
8	H	264/274 (96%)	256 (97%)	8 (3%)	36	58
9	I	151/175 (86%)	150 (99%)	1 (1%)	76	88
10	J	140/141 (99%)	135 (96%)	5 (4%)	31	52
11	K	84/85 (99%)	83 (99%)	1 (1%)	63	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	529/533 (99%)	525 (99%)	4 (1%)	73	86
13	M	412/412 (100%)	408 (99%)	4 (1%)	68	84
14	N	315/315 (100%)	314 (100%)	1 (0%)	86	93
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	64
16	P	253/327 (77%)	252 (100%)	1 (0%)	84	92
17	Q	112/153 (73%)	111 (99%)	1 (1%)	70	85
18	R	78/97 (80%)	76 (97%)	2 (3%)	40	63
19	S	76/82 (93%)	76 (100%)	0	100	100
20	T	70/135 (52%)	67 (96%)	3 (4%)	26	44
20	U	78/135 (58%)	77 (99%)	1 (1%)	61	80
21	V	100/102 (98%)	99 (99%)	1 (1%)	68	84
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	150 (97%)	4 (3%)	40	63
24	Y	101/102 (99%)	97 (96%)	4 (4%)	28	47
25	Z	119/121 (98%)	119 (100%)	0	100	100
26	a	58/59 (98%)	57 (98%)	1 (2%)	53	74
27	b	71/72 (99%)	70 (99%)	1 (1%)	59	79
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	99 (99%)	1 (1%)	68	84
30	e	86/96 (90%)	85 (99%)	1 (1%)	63	81
31	f	48/54 (89%)	48 (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	98/120 (82%)	96 (98%)	2 (2%)	48	70
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	60 (98%)	1 (2%)	55	76
37	l	139/159 (87%)	137 (99%)	2 (1%)	59	79
38	m	112/115 (97%)	107 (96%)	5 (4%)	24	42
39	n	156/161 (97%)	155 (99%)	1 (1%)	78	89
40	o	110/120 (92%)	108 (98%)	2 (2%)	51	73
41	p	154/157 (98%)	152 (99%)	2 (1%)	61	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	q	130/131 (99%)	129 (99%)	1 (1%)	73	86
43	r	84/97 (87%)	82 (98%)	2 (2%)	43	65
44	s	42/92 (46%)	41 (98%)	1 (2%)	43	65
All	All	7060/7892 (90%)	6975 (99%)	85 (1%)	61	81

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
2	B	54	CYS
4	D	76	CYS
4	D	341	SER
4	D	376	VAL
4	D	420	THR
5	E	136	LEU
5	E	203	THR
6	F	99	GLU
6	F	339	ARG
7	G	75	LYS
7	G	188	GLU
7	G	431	ASP
7	G	613	TYR
8	H	54	LYS
8	H	62	ARG
8	H	66	SER
8	H	69	SER
8	H	194	ASN
8	H	222	LEU
8	H	234	MET
8	H	259	PHE
9	I	11	SER
10	J	77	GLU
10	J	82	ILE
10	J	107	VAL
10	J	133	SER
10	J	148	SER
11	K	97	GLN
12	L	10	VAL
12	L	30	SER
12	L	441	VAL
12	L	507	MET

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Mol	Chain	Res	Type
13	M	80	SER
13	M	116	ILE
13	M	144	ASN
13	M	315	LEU
14	N	218	MET
15	O	19	THR
15	O	60	ASP
15	O	160	ILE
15	O	181	SER
15	O	206	TYR
15	O	279	LEU
15	O	298	GLU
16	P	140	LYS
17	Q	110	VAL
18	R	4	THR
18	R	51	GLN
20	T	34	SER
20	T	39	ASP
20	T	44(A)	SER
20	U	83	LYS
21	V	94	ILE
23	X	77	CYS
23	X	82	THR
23	X	99	CYS
23	X	143	SER
24	Y	17	CYS
24	Y	46	THR
24	Y	47	SER
24	Y	73	SER
26	a	30	SER
27	b	4	VAL
29	d	20	SER
30	e	92	THR
34	i	63	THR
34	i	78	VAL
36	k	78	VAL
37	l	6	LYS
37	l	81	LEU
38	m	15	THR
38	m	40	SER
38	m	79	PHE
38	m	85	THR

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Mol	Chain	Res	Type
38	m	88	LEU
39	n	140	GLN
40	o	27	ASP
40	o	30	PHE
41	p	134	VAL
41	p	171	GLU
42	q	15	SER
43	r	24	GLN
43	r	68	VAL
44	s	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	164	GLN
3	C	19	HIS
3	C	87	GLN
4	D	13	GLN
4	D	280	GLN
6	F	83	ASN
6	F	264	ASN
6	F	356	HIS
6	F	421	HIS
6	F	431	GLN
6	F	432	GLN
7	G	155	GLN
7	G	293	HIS
8	H	47	GLN
8	H	194	ASN
11	K	91	GLN
12	L	269	ASN
12	L	296	ASN
12	L	603	ASN
13	M	82	HIS
13	M	139	GLN
13	M	144	ASN
13	M	251	ASN
13	M	415	GLN
14	N	48	HIS
14	N	268	GLN
15	O	76	ASN
15	O	154	GLN

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Mol	Chain	Res	Type
15	O	190	HIS
15	O	271	ASN
16	P	8	HIS
16	P	119	GLN
19	S	85	GLN
23	X	76	HIS
24	Y	7	GLN
28	c	9	HIS
28	c	35	HIS
30	e	20	GLN
36	k	20	GLN
36	k	47	ASN
38	m	47	GLN
38	m	74	ASN
38	m	125	ASN
39	n	77	GLN
39	n	159	GLN
41	p	122	GLN
41	p	130	GLN

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	$\# Z > 2$
11	FME	K	1	11	8,9,10	0.94	0	8,9,11	0.92	0
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	1.00	1 (12%)
12	FME	L	1	12	8,9,10	0.95	0	8,9,11	0.98	1 (12%)
10	FME	J	1	10	8,9,10	0.94	0	8,9,11	0.86	0

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	0.94	0
34	SAC	i	1	34	7,8,9	1.88	1 (14%)	7,9,11	2.13	1 (14%)
8	FME	H	1	8	8,9,10	0.96	0	8,9,11	1.11	1 (12%)
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.44	1 (16%)
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.16	1 (16%)
13	FME	M	1	13	8,9,10	1.02	1 (12%)	8,9,11	1.06	1 (12%)
4	2MR	D	85	4	10,12,13	2.72	4 (40%)	5,13,15	1.15	1 (20%)

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.26	1.44	1.33
4	D	85	2MR	CZ-NE	4.63	1.44	1.34
34	i	1	SAC	O-C	4.31	1.36	1.20
4	D	85	2MR	O-C	4.05	1.35	1.20
24	Y	1	AYA	CT-N	3.54	1.45	1.34
43	r	1	AYA	CT-N	3.40	1.45	1.34
13	M	1	FME	CA-N	-2.15	1.43	1.46
1	A	1	FME	CA-N	-2.12	1.43	1.46
43	r	1	AYA	OT-CT	-2.09	1.18	1.23
4	D	85	2MR	CQ1-NH1	-2.05	1.42	1.46
24	Y	1	AYA	OT-CT	-2.05	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.79	112.44	124.77
43	r	1	AYA	CM-CT-N	2.49	120.25	116.12
13	M	1	FME	C-CA-N	2.31	113.95	109.50
8	H	1	FME	C-CA-N	2.30	113.93	109.50
4	D	85	2MR	NE-CZ-NH2	-2.28	117.39	119.48
14	N	1	FME	C-CA-N	2.16	113.67	109.50
24	Y	1	AYA	CM-CT-N	2.08	119.56	116.12
12	L	1	FME	C-CA-N	2.03	113.41	109.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
24	Y	1	AYA	O-C-CA-CB
34	i	1	SAC	C-CA-CB-OG
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
24	Y	1	AYA	C-CA-N-CT
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 3 are monoatomic - leaving 49 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	I49	N	503	-	15,17,17	0.88	1 (6%)	17,22,22	1.90	4 (23%)
46	3PE	Y	401	-	34,34,50	1.05	4 (11%)	37,39,55	1.17	2 (5%)
59	MYR	o	201	40	13,14,15	0.99	0	12,13,15	0.55	0
45	LMT	M	605	-	36,36,36	1.17	3 (8%)	47,47,47	0.97	2 (4%)
50	FMN	F	501	-	33,33,33	1.09	3 (9%)	48,50,50	1.28	6 (12%)
56	NDP	P	501	-	51,52,52	2.23	5 (9%)	71,80,80	1.49	15 (21%)
46	3PE	J	401	-	36,36,50	1.02	4 (11%)	39,41,55	1.13	2 (5%)
45	LMT	L	706	-	36,36,36	1.17	2 (5%)	47,47,47	0.93	1 (2%)
45	LMT	L	702	-	36,36,36	1.17	3 (8%)	47,47,47	1.14	4 (8%)
46	3PE	A	302	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
46	3PE	L	701	-	47,47,50	0.91	2 (4%)	50,52,55	1.04	2 (4%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
46	3PE	N	502	-	40,40,50	0.97	4 (10%)	43,45,55	1.17	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
45	LMT	A	301	-	36,36,36	1.22	4 (11%)	47,47,47	0.80	1 (2%)
48	PC1	B	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.10	2 (5%)
53	CDL	h	1001	-	66,66,99	1.07	6 (9%)	72,78,111	1.20	5 (6%)
58	EHZ	U	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.52	6 (16%)
53	CDL	L	704	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
45	LMT	M	602	-	36,36,36	1.16	3 (8%)	47,47,47	1.26	3 (6%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
47	SF4	G	802	7	0,12,12	-	-	-	-	-
53	CDL	q	201	-	75,75,99	1.00	7 (9%)	81,87,111	1.07	4 (4%)
48	PC1	M	604	-	40,40,53	1.10	4 (10%)	46,48,61	1.02	2 (4%)
52	I49	H	602	-	15,17,17	0.87	1 (6%)	17,22,22	1.92	5 (29%)
46	3PE	b	901	-	38,38,50	0.97	4 (10%)	41,43,55	1.12	2 (4%)
46	3PE	M	601	-	38,38,50	0.97	4 (10%)	41,43,55	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.11	4 (5%)
46	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.02	2 (3%)
45	LMT	J	402	-	36,36,36	1.21	3 (8%)	47,47,47	0.98	0
45	LMT	B	202	-	36,36,36	1.18	2 (5%)	47,47,47	0.87	1 (2%)
53	CDL	K	401	-	66,66,99	1.08	8 (12%)	72,78,111	1.07	4 (5%)
53	CDL	X	1701	-	64,64,99	1.02	6 (9%)	68,75,111	1.13	4 (5%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
45	LMT	M	606	-	36,36,36	1.28	5 (13%)	47,47,47	1.14	4 (8%)
54	GTP	O	1202	55	33,34,34	3.29	14 (42%)	50,54,54	1.89	14 (28%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
46	3PE	H	601	-	33,33,50	1.31	4 (12%)	34,37,55	1.14	2 (5%)
46	3PE	O	1201	-	46,46,50	0.92	4 (8%)	49,51,55	1.05	2 (4%)
46	3PE	M	603	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
45	LMT	L	705	-	36,36,36	1.16	3 (8%)	47,47,47	1.04	3 (6%)
45	LMT	h	1002	-	36,36,36	1.15	2 (5%)	47,47,47	1.12	4 (8%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
46	3PE	L	703	-	44,44,50	0.92	3 (6%)	47,49,55	1.17	2 (4%)
58	EHZ	T	101	20	31,36,37	1.55	5 (16%)	36,44,47	1.43	5 (13%)
45	LMT	l	201	-	36,36,36	1.18	3 (8%)	47,47,47	0.95	0
45	LMT	N	501	-	36,36,36	1.17	3 (8%)	47,47,47	0.90	1 (2%)
45	LMT	f	1901	-	36,36,36	1.18	2 (5%)	47,47,47	0.96	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	I49	N	503	-	-	3/10/10/10	0/1/1/1
46	3PE	Y	401	-	-	15/38/38/54	-
59	MYR	o	201	40	-	6/12/12/13	-
45	LMT	M	605	-	-	9/21/61/61	0/2/2/2
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
56	NDP	P	501	-	-	6/34/77/77	0/5/5/5
46	3PE	J	401	-	-	21/40/40/54	-
45	LMT	L	706	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	L	702	-	-	3/21/61/61	0/2/2/2
46	3PE	A	302	-	-	13/39/39/54	-
46	3PE	L	701	-	-	21/51/51/54	-
49	FES	E	301	5	-	-	0/1/1/1
46	3PE	N	502	-	-	21/44/44/54	-
47	SF4	B	201	2	-	-	0/6/5/5
45	LMT	A	301	-	-	10/21/61/61	0/2/2/2
48	PC1	B	203	-	-	12/38/38/57	-
53	CDL	h	1001	-	-	34/77/77/110	-
58	EHZ	U	101	20	-	8/42/44/45	-
53	CDL	L	704	-	-	42/110/110/110	-
45	LMT	M	602	-	-	5/21/61/61	0/2/2/2
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
53	CDL	q	201	-	-	35/86/86/110	-
48	PC1	M	604	-	-	14/44/44/57	-
52	I49	H	602	-	-	5/10/10/10	0/1/1/1
46	3PE	b	901	-	-	20/42/42/54	-
46	3PE	M	601	-	-	17/42/42/54	-
53	CDL	d	201	-	-	35/75/75/110	-
46	3PE	I	201	-	-	18/54/54/54	-
45	LMT	J	402	-	-	7/21/61/61	0/2/2/2
45	LMT	B	202	-	-	5/21/61/61	0/2/2/2
53	CDL	K	401	-	-	25/77/77/110	-
53	CDL	X	1701	-	-	35/74/74/110	-
49	FES	G	803	7	-	-	0/1/1/1
45	LMT	M	606	-	-	8/21/61/61	0/2/2/2
54	GTP	O	1202	55	-	5/22/38/38	0/3/3/3
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	H	601	-	-	14/36/36/54	-
46	3PE	O	1201	-	-	22/50/50/54	-
46	3PE	M	603	-	-	27/54/54/54	-
47	SF4	I	203	9	-	-	0/6/5/5
45	LMT	L	705	-	-	8/21/61/61	0/2/2/2
45	LMT	h	1002	-	-	3/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	L	703	-	-	20/48/48/54	-
58	EHZ	T	101	20	-	13/42/44/45	-
45	LMT	l	201	-	-	10/21/61/61	0/2/2/2
45	LMT	N	501	-	-	9/21/61/61	0/2/2/2
45	LMT	f	1901	-	-	12/21/61/61	0/2/2/2

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.95	1.82	1.59
54	O	1202	GTP	O6-C6	8.61	1.39	1.23
54	O	1202	GTP	C5-N7	6.68	1.52	1.39
54	O	1202	GTP	PA-O3A	5.14	1.65	1.59
54	O	1202	GTP	PB-O3A	5.07	1.65	1.59
54	O	1202	GTP	PB-O3B	5.01	1.64	1.59
58	U	101	EHZ	C15-N2	4.99	1.45	1.33
58	T	101	EHZ	C12-N1	4.86	1.44	1.33
58	U	101	EHZ	C12-N1	4.85	1.44	1.33
58	T	101	EHZ	C15-N2	4.84	1.45	1.33
54	O	1202	GTP	C2-N1	4.82	1.49	1.37
46	H	601	3PE	O21-C2	-4.81	1.40	1.46
54	O	1202	GTP	C2-N2	4.65	1.45	1.34
54	O	1202	GTP	C2-N3	4.59	1.44	1.33
54	O	1202	GTP	C8-N9	-4.40	1.27	1.37
54	O	1202	GTP	C4-N9	-3.81	1.28	1.38
45	M	606	LMT	O5'-C1'	3.57	1.51	1.41
45	J	402	LMT	O5B-C1B	3.52	1.50	1.41
56	P	501	NDP	PA-O3	3.51	1.63	1.59
45	N	501	LMT	O5B-C1B	3.45	1.50	1.41
45	M	605	LMT	O5B-C1B	3.44	1.50	1.41
45	f	1901	LMT	O5B-C1B	3.44	1.50	1.41
45	M	606	LMT	O5B-C1B	3.43	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.42	1.32	1.44
45	B	202	LMT	O5B-C1B	3.38	1.50	1.41
45	A	301	LMT	O5B-C1B	3.36	1.50	1.41
45	l	201	LMT	O5B-C1B	3.36	1.50	1.41
45	L	705	LMT	O5B-C1B	3.33	1.50	1.41
45	M	602	LMT	O5B-C1B	3.31	1.50	1.41
56	P	501	NDP	PN-O5D	3.26	1.72	1.59
50	F	501	FMN	C4A-N5	3.25	1.37	1.30
46	H	601	3PE	O21-C21	3.23	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	706	LMT	O5B-C1B	3.22	1.50	1.41
45	A	301	LMT	O5'-C1'	3.18	1.50	1.41
45	J	402	LMT	O5'-C1'	3.15	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.13	1.49	1.41
45	M	605	LMT	O5'-C1'	3.12	1.49	1.41
45	L	702	LMT	O5B-C1B	3.08	1.49	1.41
45	L	706	LMT	O5'-C1'	3.08	1.49	1.41
46	L	701	3PE	O21-C2	-3.06	1.39	1.46
53	h	1001	CDL	OA6-CA4	-2.98	1.39	1.46
45	l	201	LMT	O5'-C1'	2.98	1.49	1.41
45	f	1901	LMT	O5'-C1'	2.98	1.49	1.41
45	N	501	LMT	O5'-C1'	2.97	1.49	1.41
45	M	602	LMT	O5'-C1'	2.96	1.49	1.41
45	L	705	LMT	O5'-C1'	2.93	1.49	1.41
45	L	702	LMT	O5'-C1'	2.87	1.49	1.41
53	L	704	CDL	OB6-CB4	-2.83	1.39	1.46
46	L	703	3PE	O21-C2	-2.83	1.39	1.46
54	O	1202	GTP	O4'-C1'	2.83	1.48	1.42
45	B	202	LMT	O5'-C1'	2.83	1.49	1.41
53	q	201	CDL	OA6-CA4	-2.82	1.40	1.46
53	K	401	CDL	OA6-CA4	-2.82	1.40	1.46
53	X	1701	CDL	OA6-CA4	-2.81	1.40	1.46
46	O	1201	3PE	O21-C2	-2.80	1.40	1.46
53	h	1001	CDL	OB6-CB4	-2.78	1.40	1.46
45	h	1002	LMT	O5'-C1'	2.76	1.48	1.41
46	A	302	3PE	O21-C2	-2.74	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.74	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.73	1.40	1.46
46	M	603	3PE	O21-C2	-2.73	1.40	1.46
46	L	701	3PE	O31-C3	-2.73	1.39	1.45
53	X	1701	CDL	OB6-CB4	-2.72	1.40	1.46
48	M	604	PC1	O21-C2	-2.69	1.40	1.46
58	T	101	EHZ	O4-C15	-2.69	1.18	1.23
46	Y	401	3PE	O21-C2	-2.69	1.40	1.46
46	J	401	3PE	O21-C2	-2.68	1.40	1.46
46	I	201	3PE	O21-C2	-2.68	1.40	1.46
58	U	101	EHZ	O4-C15	-2.68	1.18	1.23
46	b	901	3PE	O21-C2	-2.68	1.40	1.46
46	N	502	3PE	O21-C2	-2.66	1.40	1.46
53	K	401	CDL	OB6-CB4	-2.66	1.40	1.46
48	B	203	PC1	O21-C2	-2.60	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.60	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	703	3PE	O31-C3	-2.59	1.39	1.45
46	I	201	3PE	O31-C3	-2.58	1.39	1.45
46	N	502	3PE	O31-C3	-2.56	1.39	1.45
52	N	503	I49	C15-N02	-2.52	1.31	1.36
53	L	704	CDL	OA6-CA4	-2.52	1.40	1.46
46	M	601	3PE	O21-C2	-2.51	1.40	1.46
53	h	1001	CDL	OB8-CB6	-2.50	1.39	1.45
53	K	401	CDL	OB8-CB7	2.49	1.40	1.33
58	U	101	EHZ	O3-C12	-2.47	1.18	1.23
53	L	704	CDL	OA8-CA7	2.46	1.40	1.33
54	O	1202	GTP	C2'-C3'	-2.45	1.46	1.53
48	M	604	PC1	O31-C3	-2.45	1.39	1.45
53	d	201	CDL	OB8-CB7	2.44	1.40	1.33
58	T	101	EHZ	O3-C12	-2.43	1.18	1.23
53	q	201	CDL	OB8-CB7	2.42	1.40	1.33
52	H	602	I49	C15-N02	-2.40	1.31	1.36
53	q	201	CDL	OA8-CA6	-2.40	1.39	1.45
53	X	1701	CDL	OB8-CB7	2.40	1.40	1.33
54	O	1202	GTP	PG-O2G	-2.39	1.45	1.54
46	J	401	3PE	O31-C31	2.38	1.40	1.33
46	Y	401	3PE	O31-C31	2.38	1.40	1.33
46	b	901	3PE	O31-C3	-2.38	1.39	1.45
46	A	302	3PE	O31-C31	2.36	1.40	1.33
46	O	1201	3PE	O31-C31	2.36	1.40	1.33
53	K	401	CDL	OA8-CA6	-2.35	1.39	1.45
54	O	1202	GTP	PG-O3G	-2.35	1.46	1.54
48	B	203	PC1	O31-C3	-2.35	1.39	1.45
53	L	704	CDL	OB8-CB6	-2.34	1.39	1.45
46	M	603	3PE	O31-C31	2.34	1.40	1.33
53	L	704	CDL	OB8-CB7	2.32	1.40	1.33
53	d	201	CDL	OA8-CA6	-2.30	1.40	1.45
53	q	201	CDL	OB8-CB6	-2.29	1.40	1.45
53	h	1001	CDL	OA8-CA7	2.28	1.40	1.33
46	M	603	3PE	O31-C3	-2.28	1.40	1.45
53	K	401	CDL	OA8-CA7	2.27	1.40	1.33
46	O	1201	3PE	O31-C3	-2.27	1.40	1.45
46	Y	401	3PE	O31-C3	-2.26	1.40	1.45
48	B	203	PC1	O21-C21	2.25	1.40	1.34
53	d	201	CDL	OA8-CA7	2.25	1.39	1.33
56	P	501	NDP	O5D-C5D	-2.25	1.36	1.44
48	M	604	PC1	O31-C31	2.24	1.39	1.33
53	h	1001	CDL	OA8-CA6	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	B	203	PC1	O31-C31	2.22	1.39	1.33
46	H	601	3PE	O31-C3	-2.21	1.40	1.45
53	L	704	CDL	OA6-CA5	2.20	1.40	1.34
46	M	601	3PE	O31-C3	-2.20	1.40	1.45
46	M	601	3PE	O31-C31	2.18	1.39	1.33
45	J	402	LMT	O5B-C5B	2.18	1.49	1.44
53	K	401	CDL	OB8-CB6	-2.18	1.40	1.45
46	I	201	3PE	O21-C21	2.18	1.40	1.34
46	A	302	3PE	O31-C3	-2.17	1.40	1.45
46	N	502	3PE	O31-C31	2.16	1.39	1.33
46	L	703	3PE	O31-C31	2.16	1.39	1.33
46	H	601	3PE	O31-C31	2.16	1.39	1.33
45	M	606	LMT	O5'-C5'	2.16	1.49	1.44
48	M	604	PC1	O21-C21	2.16	1.40	1.34
53	K	401	CDL	OB6-CB5	2.16	1.40	1.34
53	d	201	CDL	OB6-CB5	2.15	1.40	1.34
46	J	401	3PE	O31-C3	-2.15	1.40	1.45
58	U	101	EHZ	C9-S1	2.15	1.81	1.76
53	d	201	CDL	OA6-CA5	2.14	1.40	1.34
50	F	501	FMN	C10-N1	2.14	1.37	1.33
46	b	901	3PE	O31-C31	2.13	1.39	1.33
45	M	606	LMT	O1B-C4'	2.13	1.49	1.43
46	A	302	3PE	O21-C21	2.12	1.40	1.34
46	N	502	3PE	O21-C21	2.12	1.40	1.34
53	L	704	CDL	OA8-CA6	-2.12	1.40	1.45
53	L	704	CDL	OB6-CB5	2.12	1.40	1.34
53	K	401	CDL	OA6-CA5	2.11	1.40	1.34
45	L	702	LMT	O5B-C5B	2.11	1.49	1.44
53	h	1001	CDL	OB8-CB7	2.11	1.39	1.33
53	q	201	CDL	OA8-CA7	2.11	1.39	1.33
46	M	601	3PE	O21-C21	2.10	1.40	1.34
45	A	301	LMT	O1B-C4'	2.10	1.49	1.43
46	b	901	3PE	O21-C21	2.10	1.40	1.34
45	N	501	LMT	O5B-C5B	2.09	1.49	1.44
53	d	201	CDL	OB8-CB6	-2.09	1.40	1.45
45	A	301	LMT	O5'-C5'	2.08	1.49	1.44
53	X	1701	CDL	OB8-CB6	-2.07	1.40	1.45
53	q	201	CDL	OB6-CB5	2.07	1.40	1.34
46	J	401	3PE	O21-C21	2.06	1.40	1.34
58	T	101	EHZ	C9-S1	2.06	1.81	1.76
46	Y	401	3PE	O21-C21	2.06	1.40	1.34
53	X	1701	CDL	OB6-CB5	2.04	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	O	1201	3PE	O21-C21	2.04	1.40	1.34
50	F	501	FMN	C4A-C10	-2.04	1.38	1.44
46	I	201	3PE	O31-C31	2.04	1.39	1.33
45	M	606	LMT	O5B-C5B	2.02	1.49	1.44
46	M	603	3PE	O21-C21	2.02	1.40	1.34
45	M	602	LMT	O5B-C5B	2.02	1.49	1.44
45	M	605	LMT	O5B-C5B	2.02	1.49	1.44
53	X	1701	CDL	OA6-CA5	2.01	1.40	1.34
45	L	705	LMT	O5B-C5B	2.01	1.49	1.44
45	l	201	LMT	O5B-C5B	2.00	1.49	1.44

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	1202	GTP	C8-N9-C4	7.52	120.13	106.03
58	U	101	EHZ	C8-C9-S1	5.91	121.01	113.56
58	T	101	EHZ	C8-C9-S1	5.34	120.30	113.56
52	N	503	I49	N01-C14-N03	4.91	129.32	120.26
53	L	704	CDL	OA6-CA5-C11	4.50	121.21	111.48
53	h	1001	CDL	OB6-CB5-C51	4.45	121.10	111.48
53	d	201	CDL	OA6-CA5-C11	4.16	120.47	111.48
48	B	203	PC1	O21-C21-C22	4.14	120.44	111.48
53	X	1701	CDL	OB6-CB5-C51	4.12	120.39	111.48
46	A	302	3PE	O21-C21-C22	4.09	120.33	111.48
52	H	602	I49	N01-C14-N03	4.08	127.78	120.26
46	M	603	3PE	O21-C21-C22	4.03	120.20	111.48
46	M	601	3PE	O21-C21-C22	4.03	120.20	111.48
46	Y	401	3PE	O21-C21-C22	4.02	120.19	111.48
46	N	502	3PE	O21-C21-C22	4.01	120.17	111.48
46	H	601	3PE	O21-C21-O22	-4.01	120.55	125.70
53	X	1701	CDL	OA6-CA5-C11	4.00	120.13	111.48
46	O	1201	3PE	O21-C21-C22	3.93	119.98	111.48
48	M	604	PC1	O21-C21-C22	3.90	119.91	111.48
53	h	1001	CDL	OA6-CA5-C11	3.81	119.72	111.48
46	J	401	3PE	O21-C21-C22	3.75	119.60	111.48
53	q	201	CDL	OB6-CB5-C51	3.72	119.52	111.48
46	L	703	3PE	O21-C21-C22	3.70	119.48	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.69	96.17	109.33
45	M	602	LMT	C1'-C2'-C3'	3.64	117.66	110.01
53	K	401	CDL	OA6-CA5-C11	3.60	119.26	111.48
46	I	201	3PE	O21-C21-C22	3.59	119.25	111.48
46	L	701	3PE	O21-C21-C22	3.57	119.20	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	b	901	3PE	O21-C21-C22	3.55	119.17	111.48
53	K	401	CDL	OB6-CB5-C51	3.53	119.11	111.48
56	P	501	NDP	O3-PA-O1A	-3.50	100.16	110.70
56	P	501	NDP	P2B-O2B-C2B	-3.50	114.09	123.43
53	L	704	CDL	OB6-CB5-C51	3.49	119.03	111.48
50	F	501	FMN	C4-N3-C2	-3.48	119.46	125.64
45	L	705	LMT	C1B-O1B-C4'	-3.45	109.79	117.98
53	q	201	CDL	OA6-CA5-C11	3.45	118.94	111.48
45	h	1002	LMT	O5'-C5'-C4'	3.37	116.69	109.72
46	J	401	3PE	O31-C31-C32	3.22	121.67	111.83
54	O	1202	GTP	C2-N1-C6	-3.19	119.33	125.11
45	M	606	LMT	C1'-O5'-C5'	3.16	119.89	113.72
50	F	501	FMN	C4A-C10-N10	3.04	120.83	116.48
53	h	1001	CDL	OA8-CA7-C31	3.02	121.05	111.83
46	M	603	3PE	O31-C31-C32	3.02	121.05	111.83
46	Y	401	3PE	O31-C31-C32	2.97	120.89	111.83
54	O	1202	GTP	O3G-PG-O3B	2.97	114.59	104.64
45	L	702	LMT	O5B-C5B-C4B	2.95	115.02	109.70
58	U	101	EHZ	O2-C9-C8	-2.94	119.12	123.74
46	H	601	3PE	O31-C31-C32	2.93	120.76	111.83
53	q	201	CDL	OA8-CA7-C31	2.87	120.58	111.83
45	M	606	LMT	O1B-C4'-C5'	2.86	116.98	109.48
53	X	1701	CDL	OB8-CB7-C71	2.85	120.52	111.83
46	L	703	3PE	O31-C31-C32	2.84	120.51	111.83
52	H	602	I49	N05-C15-N04	-2.84	111.99	120.07
46	O	1201	3PE	O31-C31-C32	2.83	120.47	111.83
46	M	601	3PE	O31-C31-C32	2.83	120.46	111.83
46	A	302	3PE	O31-C31-C32	2.83	120.45	111.83
52	N	503	I49	N05-C15-N04	-2.83	112.03	120.07
50	F	501	FMN	C4A-C4-N3	2.82	120.43	113.25
56	P	501	NDP	PA-O5B-C5B	-2.81	105.23	121.35
53	d	201	CDL	OA8-CA7-C31	2.79	120.34	111.83
56	P	501	NDP	O2N-PN-O3	2.76	114.72	107.27
56	P	501	NDP	PN-O5D-C5D	-2.75	105.58	121.35
54	O	1202	GTP	O2G-PG-O3B	2.75	113.86	104.64
45	L	702	LMT	C3B-C4B-C5B	2.74	115.21	110.23
52	H	602	I49	N05-C15-N02	2.74	127.60	117.97
52	N	503	I49	N05-C15-N02	2.74	127.59	117.97
46	b	901	3PE	O31-C31-C32	2.73	120.17	111.83
45	M	602	LMT	C1B-O5B-C5B	-2.69	108.46	113.72
53	L	704	CDL	OA8-CA7-C31	2.69	120.03	111.83
53	d	201	CDL	OB8-CB7-C71	2.67	119.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	B	203	PC1	O31-C31-C32	2.67	119.97	111.83
53	h	1001	CDL	OB8-CB7-C71	2.65	119.92	111.83
58	T	101	EHZ	O2-C9-S1	-2.65	119.31	122.68
53	L	704	CDL	OB8-CB7-C71	2.64	119.89	111.83
52	H	602	I49	C08-N01-C14	-2.63	118.63	123.46
48	M	604	PC1	O31-C31-C32	2.61	119.80	111.83
53	d	201	CDL	OB6-CB5-C51	2.60	120.49	110.93
53	K	401	CDL	OB8-CB7-C71	2.59	119.73	111.83
54	O	1202	GTP	O2A-PA-O1A	-2.58	100.44	112.44
50	F	501	FMN	O4-C4-C4A	-2.56	119.78	126.53
45	M	606	LMT	O5'-C1'-C2'	2.56	115.62	110.37
58	U	101	EHZ	C16-C15-N2	2.55	121.32	116.48
56	P	501	NDP	O3X-P2B-O2X	2.52	117.25	107.80
46	N	502	3PE	O31-C31-C32	2.52	119.51	111.83
53	K	401	CDL	OA8-CA7-C31	2.51	119.50	111.83
54	O	1202	GTP	O2B-PB-O1B	-2.50	100.80	112.44
46	I	201	3PE	O31-C31-C32	2.50	119.46	111.83
54	O	1202	GTP	C5-C6-N1	2.50	119.61	113.25
54	O	1202	GTP	C2'-C3'-C4'	2.46	107.37	102.61
54	O	1202	GTP	C1'-N9-C8	-2.46	119.74	126.73
53	q	201	CDL	OB8-CB7-C71	2.45	119.32	111.83
50	F	501	FMN	C10-C4A-N5	-2.44	119.83	124.81
45	M	602	LMT	C2'-C3'-C4'	2.44	115.21	109.68
45	N	501	LMT	O1B-C4'-C3'	2.41	113.35	107.23
56	P	501	NDP	O5D-PN-O1N	-2.40	99.42	108.94
45	L	702	LMT	C1B-O1B-C4'	-2.37	112.36	117.98
45	h	1002	LMT	C1B-O1B-C4'	-2.37	112.36	117.98
46	L	701	3PE	O31-C31-C32	2.36	119.02	111.83
54	O	1202	GTP	C3'-C2'-C1'	2.35	105.90	101.46
56	P	501	NDP	O2N-PN-O1N	2.32	123.25	112.44
56	P	501	NDP	C2A-N1A-C6A	-2.32	114.93	118.73
54	O	1202	GTP	O6-C6-C5	-2.32	120.42	126.53
54	O	1202	GTP	C5-C4-N9	-2.31	101.52	105.66
45	B	202	LMT	O1'-C1'-C2'	2.29	111.75	108.27
56	P	501	NDP	O4B-C4B-C3B	2.29	109.70	105.15
45	L	705	LMT	C2'-C3'-C4'	2.25	114.79	109.68
52	N	503	I49	C09-C07-C10	2.25	121.65	118.55
58	T	101	EHZ	C13-C12-N1	2.23	120.41	116.34
45	L	702	LMT	C6B-C5B-C4B	-2.22	107.56	113.02
58	U	101	EHZ	O2-C9-S1	-2.21	119.87	122.68
56	P	501	NDP	N3A-C4A-N9A	2.21	130.92	127.17
56	P	501	NDP	C5B-C4B-C3B	-2.20	107.31	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	h	1002	LMT	C2'-C3'-C4'	2.17	114.61	109.68
45	A	301	LMT	O1B-C4'-C3'	2.17	112.73	107.23
45	f	1901	LMT	C1'-C2'-C3'	2.16	114.56	110.01
52	H	602	I49	C09-C07-C10	2.16	121.53	118.55
45	f	1901	LMT	C1B-O1B-C4'	-2.15	112.87	117.98
54	O	1202	GTP	C1'-N9-C4	-2.15	120.13	126.49
45	M	606	LMT	C3B-C4B-C5B	2.15	114.13	110.23
54	O	1202	GTP	N9-C8-N7	-2.14	109.43	113.40
45	h	1002	LMT	C3'-C4'-C5'	2.14	115.67	110.93
58	T	101	EHZ	O2-C9-C8	-2.13	120.39	123.74
56	P	501	NDP	O3X-P2B-O2B	-2.13	97.55	105.85
56	P	501	NDP	O7N-C7N-N7N	-2.11	118.16	122.89
45	L	705	LMT	C1'-C2'-C3'	2.11	114.44	110.01
50	F	501	FMN	C4A-C10-N1	-2.10	119.43	124.59
53	X	1701	CDL	CA4-OA6-CA5	-2.10	112.78	117.80
58	U	101	EHZ	C10-S1-C9	2.08	108.00	101.84
45	M	605	LMT	C1B-O1B-C4'	-2.08	113.04	117.98
45	L	706	LMT	C1B-O5B-C5B	-2.07	109.67	113.72
53	h	1001	CDL	OB6-CB5-OB7	-2.06	118.89	123.70
58	T	101	EHZ	C16-C15-N2	2.03	120.34	116.48
45	M	605	LMT	C2'-C3'-C4'	2.03	114.28	109.68
58	U	101	EHZ	C13-C12-N1	2.02	120.02	116.34
45	f	1901	LMT	C2'-C3'-C4'	2.02	114.26	109.68

There are no chirality outliers.

All (609) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	L	705	LMT	O5'-C1'-O1'-C1
45	M	606	LMT	C5'-C4'-O1B-C1B
46	A	302	3PE	O13-C11-C12-N
46	A	302	3PE	O22-C21-O21-C2
46	A	302	3PE	C22-C21-O21-C2
46	H	601	3PE	C1-O11-P-O14
46	H	601	3PE	C11-O13-P-O11
46	H	601	3PE	C11-O13-P-O12
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	O22-C21-O21-C2
46	I	201	3PE	C11-O13-P-O14
46	I	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	J	401	3PE	C1-O11-P-O14
46	J	401	3PE	C12-C11-O13-P
46	J	401	3PE	O13-C11-C12-N
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	O13-C11-C12-N
46	M	601	3PE	C1-O11-P-O13
46	M	601	3PE	C1-O11-P-O14
46	M	601	3PE	O13-C11-C12-N
46	M	603	3PE	C11-O13-P-O11
46	M	603	3PE	C11-O13-P-O12
46	N	502	3PE	C1-O11-P-O13
46	N	502	3PE	C1-O11-P-O14
46	N	502	3PE	C11-O13-P-O11
46	N	502	3PE	C11-O13-P-O14
46	N	502	3PE	O13-C11-C12-N
46	O	1201	3PE	C1-O11-P-O12
46	O	1201	3PE	C1-O11-P-O13
46	O	1201	3PE	C1-O11-P-O14
46	O	1201	3PE	C22-C21-O21-C2
46	Y	401	3PE	C22-C21-O21-C2
46	b	901	3PE	C11-O13-P-O12
46	b	901	3PE	O21-C2-C3-O31
48	B	203	PC1	C11-O13-P-O12
48	B	203	PC1	C11-O13-P-O14
48	B	203	PC1	C11-O13-P-O11
48	M	604	PC1	O21-C2-C3-O31
52	H	602	I49	N05-C15-N02-C14
52	N	503	I49	C07-C06-C08-N01
52	N	503	I49	N01-C14-N02-C15
52	N	503	I49	N03-C14-N02-C15
53	K	401	CDL	O1-C1-CB2-OB2
53	K	401	CDL	CB3-OB5-PB2-OB2
53	K	401	CDL	CB3-OB5-PB2-OB3
53	L	704	CDL	OA7-CA5-OA6-CA4
53	L	704	CDL	C11-CA5-OA6-CA4
53	X	1701	CDL	CA2-OA2-PA1-OA4
53	X	1701	CDL	CA3-OA5-PA1-OA2
53	X	1701	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	CA3-OA5-PA1-OA4
53	X	1701	CDL	OA9-CA7-OA8-CA6
53	X	1701	CDL	CB2-OB2-PB2-OB3
53	X	1701	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	OB9-CB7-OB8-CB6
53	d	201	CDL	CA2-OA2-PA1-OA3
53	d	201	CDL	CA2-OA2-PA1-OA5
53	d	201	CDL	CB3-OB5-PB2-OB2
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	h	1001	CDL	CA2-C1-CB2-OB2
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB3-OB5-PB2-OB2
53	h	1001	CDL	CB3-OB5-PB2-OB3
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	h	1001	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CB3-OB5-PB2-OB3
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
46	J	401	3PE	O32-C31-O31-C3
45	M	605	LMT	O5B-C1B-O1B-C4'
46	J	401	3PE	C32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	O	1201	3PE	O32-C31-O31-C3
46	Y	401	3PE	O32-C31-O31-C3
53	L	704	CDL	OA9-CA7-OA8-CA6
45	A	301	LMT	C3'-C4'-O1B-C1B
46	O	1201	3PE	O22-C21-O21-C2
46	M	603	3PE	C32-C31-O31-C3
46	O	1201	3PE	C32-C31-O31-C3
46	Y	401	3PE	C32-C31-O31-C3
53	L	704	CDL	C31-CA7-OA8-CA6
53	X	1701	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C51-CB5-OB6-CB4
45	N	501	LMT	C3'-C4'-O1B-C1B
45	J	402	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
46	L	703	3PE	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
46	Y	401	3PE	O22-C21-O21-C2
45	A	301	LMT	O5B-C5B-C6B-O6B
45	J	402	LMT	C2B-C1B-O1B-C4'
53	h	1001	CDL	O1-C1-CB2-OB2
48	B	203	PC1	C32-C31-O31-C3
45	L	706	LMT	O5'-C5'-C6'-O6'
45	M	606	LMT	O5B-C5B-C6B-O6B
45	N	501	LMT	O5'-C5'-C6'-O6'
45	f	1901	LMT	O5'-C5'-C6'-O6'
46	M	603	3PE	O32-C31-O31-C3
45	A	301	LMT	C4B-C5B-C6B-O6B
45	l	201	LMT	C4'-C5'-C6'-O6'
53	q	201	CDL	C11-CA5-OA6-CA4
45	B	202	LMT	C3'-C4'-O1B-C1B
45	M	605	LMT	O5B-C5B-C6B-O6B
45	N	501	LMT	C4'-C5'-C6'-O6'
45	J	402	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	C2-C3-C4-C5
48	M	604	PC1	C2-C1-O11-P
45	M	606	LMT	C4B-C5B-C6B-O6B
45	f	1901	LMT	C4'-C5'-C6'-O6'
45	M	606	LMT	O5B-C1B-O1B-C4'
45	M	606	LMT	C2B-C1B-O1B-C4'
53	d	201	CDL	OB9-CB7-OB8-CB6
45	N	501	LMT	O5'-C1'-O1'-C1
45	f	1901	LMT	O5'-C1'-O1'-C1
45	L	706	LMT	O5B-C5B-C6B-O6B
45	A	301	LMT	O5'-C5'-C6'-O6'
48	B	203	PC1	O32-C31-O31-C3
46	L	701	3PE	C22-C21-O21-C2
53	K	401	CDL	CA2-C1-CB2-OB2
46	N	502	3PE	C32-C31-O31-C3
48	M	604	PC1	C32-C31-O31-C3
53	h	1001	CDL	C31-CA7-OA8-CA6
45	M	602	LMT	O5B-C5B-C6B-O6B
45	L	706	LMT	C4'-C5'-C6'-O6'
45	f	1901	LMT	C2'-C1'-O1'-C1
46	L	701	3PE	C31-C32-C33-C34
45	l	201	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
48	M	604	PC1	O32-C31-O31-C3
46	A	302	3PE	O11-C1-C2-O21
45	f	1901	LMT	O5B-C1B-O1B-C4'
46	M	601	3PE	C21-C22-C23-C24
46	N	502	3PE	O32-C31-O31-C3
56	P	501	NDP	O4D-C4D-C5D-O5D
53	q	201	CDL	C71-CB7-OB8-CB6
45	L	705	LMT	O5'-C5'-C6'-O6'
53	q	201	CDL	OA7-CA5-OA6-CA4
45	M	605	LMT	C4B-C5B-C6B-O6B
45	L	702	LMT	O1'-C1-C2-C3
45	L	706	LMT	C4B-C5B-C6B-O6B
46	J	401	3PE	C31-C32-C33-C34
46	M	603	3PE	C21-C22-C23-C24
46	O	1201	3PE	C31-C32-C33-C34
46	Y	401	3PE	C31-C32-C33-C34
53	K	401	CDL	CA5-C11-C12-C13
45	J	402	LMT	C4'-C5'-C6'-O6'
46	A	302	3PE	C21-C22-C23-C24
53	h	1001	CDL	CB5-C51-C52-C53
53	h	1001	CDL	OA9-CA7-OA8-CA6
53	X	1701	CDL	O1-C1-CA2-OA2
53	d	201	CDL	C31-CA7-OA8-CA6
45	L	705	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	O22-C21-O21-C2
45	f	1901	LMT	O5B-C5B-C6B-O6B
53	h	1001	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	C31-CA7-OA8-CA6
46	L	703	3PE	C22-C21-O21-C2
53	L	704	CDL	CB5-C51-C52-C53
45	h	1002	LMT	C4B-C5B-C6B-O6B
46	L	703	3PE	O22-C21-O21-C2
53	X	1701	CDL	CB2-C1-CA2-OA2
53	q	201	CDL	OB9-CB7-OB8-CB6
53	X	1701	CDL	C11-CA5-OA6-CA4
53	d	201	CDL	C11-CA5-OA6-CA4
53	L	704	CDL	C83-C84-C85-C86
53	d	201	CDL	OA7-CA5-OA6-CA4
45	L	706	LMT	C2'-C1'-O1'-C1
53	d	201	CDL	O1-C1-CB2-OB2
53	d	201	CDL	OA9-CA7-OA8-CA6
59	o	201	MYR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	OA7-CA5-OA6-CA4
53	K	401	CDL	C11-CA5-OA6-CA4
45	N	501	LMT	C4B-C5B-C6B-O6B
53	q	201	CDL	OA9-CA7-OA8-CA6
46	M	603	3PE	C3A-C3B-C3C-C3D
53	L	704	CDL	C79-C80-C81-C82
53	h	1001	CDL	C12-C13-C14-C15
53	q	201	CDL	C56-C57-C58-C59
45	f	1901	LMT	C1-C2-C3-C4
45	J	402	LMT	C4-C5-C6-C7
46	b	901	3PE	C28-C29-C2A-C2B
53	L	704	CDL	C37-C38-C39-C40
53	X	1701	CDL	C11-C12-C13-C14
46	I	201	3PE	C2C-C2D-C2E-C2F
46	M	601	3PE	C28-C29-C2A-C2B
45	B	202	LMT	C3-C4-C5-C6
46	I	201	3PE	C3A-C3B-C3C-C3D
53	X	1701	CDL	C15-C16-C17-C18
53	X	1701	CDL	C55-C56-C57-C58
53	q	201	CDL	C51-C52-C53-C54
53	K	401	CDL	OA7-CA5-OA6-CA4
45	L	706	LMT	C2-C1-O1'-C1'
53	L	704	CDL	C53-C54-C55-C56
46	L	701	3PE	C2E-C2F-C2G-C2H
46	b	901	3PE	C27-C28-C29-C2A
58	T	101	EHZ	C5-C6-C7-C8
46	I	201	3PE	C21-C22-C23-C24
46	O	1201	3PE	C3B-C3C-C3D-C3E
53	h	1001	CDL	OB9-CB7-OB8-CB6
53	L	704	CDL	C74-C75-C76-C77
58	U	101	EHZ	C1-C2-C3-C4
53	X	1701	CDL	CB5-C51-C52-C53
53	d	201	CDL	CA2-C1-CB2-OB2
46	Y	401	3PE	C37-C38-C39-C3A
46	b	901	3PE	C24-C25-C26-C27
53	K	401	CDL	C38-C39-C40-C41
53	q	201	CDL	C37-C38-C39-C40
59	o	201	MYR	C10-C11-C12-C13
45	f	1901	LMT	C3-C4-C5-C6
53	h	1001	CDL	C32-C33-C34-C35
59	o	201	MYR	C7-C8-C9-C10
45	N	501	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
46	O	1201	3PE	C21-C22-C23-C24
45	L	706	LMT	C5-C6-C7-C8
53	L	704	CDL	C43-C44-C45-C46
52	H	602	I49	N04-C15-N02-C14
46	M	603	3PE	C2E-C2F-C2G-C2H
53	K	401	CDL	C40-C41-C42-C43
53	L	704	CDL	C60-C61-C62-C63
53	d	201	CDL	C33-C34-C35-C36
46	L	703	3PE	C25-C26-C27-C28
46	I	201	3PE	C33-C34-C35-C36
45	N	501	LMT	O5B-C5B-C6B-O6B
46	M	603	3PE	C39-C3A-C3B-C3C
46	J	401	3PE	C32-C33-C34-C35
46	L	703	3PE	C3C-C3D-C3E-C3F
46	M	603	3PE	C27-C28-C29-C2A
53	h	1001	CDL	C72-C73-C74-C75
53	L	704	CDL	C63-C64-C65-C66
59	o	201	MYR	C11-C10-C9-C8
46	L	703	3PE	C31-C32-C33-C34
58	U	101	EHZ	C3-C4-C5-C6
46	L	701	3PE	C29-C2A-C2B-C2C
45	l	201	LMT	O5B-C1B-O1B-C4'
46	N	502	3PE	C36-C37-C38-C39
46	L	701	3PE	C32-C31-O31-C3
46	I	201	3PE	C25-C26-C27-C28
53	K	401	CDL	C12-C13-C14-C15
58	T	101	EHZ	C5-C6-C7-O1
48	M	604	PC1	C2B-C2C-C2D-C2E
53	L	704	CDL	C38-C39-C40-C41
48	M	604	PC1	C2C-C2D-C2E-C2F
53	q	201	CDL	OB5-CB3-CB4-OB6
58	U	101	EHZ	C1-C21-C22-C23
53	L	704	CDL	CB7-C71-C72-C73
46	N	502	3PE	C22-C23-C24-C25
53	L	704	CDL	C17-C18-C19-C20
46	M	603	3PE	C3D-C3E-C3F-C3G
53	q	201	CDL	C58-C59-C60-C61
46	N	502	3PE	C27-C28-C29-C2A
46	b	901	3PE	C35-C36-C37-C38
48	M	604	PC1	C27-C28-C29-C2A
46	b	901	3PE	C23-C24-C25-C26
53	h	1001	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
45	h	1002	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	C51-CB5-OB6-CB4
58	T	101	EHZ	O4-C15-C16-O5
53	L	704	CDL	C58-C59-C60-C61
46	N	502	3PE	C24-C25-C26-C27
46	O	1201	3PE	C37-C38-C39-C3A
46	A	302	3PE	O11-C1-C2-C3
46	Y	401	3PE	O11-C1-C2-C3
46	N	502	3PE	C22-C21-O21-C2
53	K	401	CDL	C33-C34-C35-C36
46	L	701	3PE	C36-C37-C38-C39
53	q	201	CDL	C52-C53-C54-C55
46	O	1201	3PE	C1-C2-C3-O31
46	Y	401	3PE	C1-C2-C3-O31
46	b	901	3PE	C1-C2-C3-O31
48	B	203	PC1	C1-C2-C3-O31
53	K	401	CDL	C53-C54-C55-C56
46	I	201	3PE	C2B-C2C-C2D-C2E
46	N	502	3PE	C23-C24-C25-C26
46	L	701	3PE	C34-C35-C36-C37
53	q	201	CDL	C13-C14-C15-C16
59	o	201	MYR	C5-C6-C7-C8
53	X	1701	CDL	C74-C75-C76-C77
45	M	605	LMT	C2B-C1B-O1B-C4'
46	I	201	3PE	C32-C31-O31-C3
46	Y	401	3PE	C2-C1-O11-P
46	L	701	3PE	O32-C31-O31-C3
45	L	705	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	C51-C52-C53-C54
53	L	704	CDL	C16-C17-C18-C19
46	b	901	3PE	C32-C31-O31-C3
59	o	201	MYR	C9-C10-C11-C12
46	L	703	3PE	C37-C38-C39-C3A
45	L	706	LMT	O5'-C1'-O1'-C1
53	X	1701	CDL	C17-C18-C19-C20
48	B	203	PC1	C33-C34-C35-C36
46	A	302	3PE	C33-C34-C35-C36
53	L	704	CDL	C20-C21-C22-C23
45	A	301	LMT	C1-C2-C3-C4
53	h	1001	CDL	OB6-CB4-CB6-OB8
45	B	202	LMT	C5'-C4'-O1B-C1B
45	f	1901	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
53	K	401	CDL	C31-CA7-OA8-CA6
48	M	604	PC1	C32-C33-C34-C35
58	T	101	EHZ	O4-C15-C16-C17
45	M	602	LMT	C4B-C5B-C6B-O6B
53	L	704	CDL	C42-C43-C44-C45
45	J	402	LMT	C2-C1-O1'-C1'
45	M	602	LMT	C2-C1-O1'-C1'
56	P	501	NDP	C2B-O2B-P2B-O3X
53	K	401	CDL	CB4-CB3-OB5-PB2
46	M	603	3PE	C33-C34-C35-C36
46	L	703	3PE	C35-C36-C37-C38
53	L	704	CDL	C24-C25-C26-C27
53	q	201	CDL	C60-C61-C62-C63
46	L	703	3PE	O11-C1-C2-C3
46	M	601	3PE	O11-C1-C2-C3
53	d	201	CDL	OA5-CA3-CA4-CA6
46	Y	401	3PE	C23-C24-C25-C26
53	X	1701	CDL	C58-C59-C60-C61
45	f	1901	LMT	C5'-C4'-O1B-C1B
46	L	703	3PE	C29-C2A-C2B-C2C
58	T	101	EHZ	N2-C15-C16-C17
53	d	201	CDL	C76-C77-C78-C79
45	M	606	LMT	O5'-C5'-C6'-O6'
45	M	605	LMT	O5'-C1'-O1'-C1
46	I	201	3PE	O32-C31-O31-C3
46	L	701	3PE	C1-C2-C3-O31
48	M	604	PC1	C1-C2-C3-O31
53	h	1001	CDL	CB3-CB4-CB6-OB8
53	d	201	CDL	C31-C32-C33-C34
46	L	701	3PE	C37-C38-C39-C3A
45	l	201	LMT	C4-C5-C6-C7
53	d	201	CDL	CA5-C11-C12-C13
53	d	201	CDL	OB5-CB3-CB4-OB6
46	I	201	3PE	C27-C28-C29-C2A
53	L	704	CDL	C72-C73-C74-C75
46	J	401	3PE	O21-C2-C3-O31
46	L	701	3PE	O21-C2-C3-O31
46	M	601	3PE	O21-C2-C3-O31
46	Y	401	3PE	O21-C2-C3-O31
53	d	201	CDL	C77-C78-C79-C80
53	X	1701	CDL	C76-C77-C78-C79
53	d	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	b	901	3PE	O32-C31-O31-C3
53	h	1001	CDL	C15-C16-C17-C18
46	M	603	3PE	C31-C32-C33-C34
53	d	201	CDL	C38-C39-C40-C41
58	U	101	EHZ	C2-C3-C4-C5
46	L	701	3PE	C22-C23-C24-C25
58	T	101	EHZ	C6-C7-C8-C9
48	B	203	PC1	C25-C26-C27-C28
46	A	302	3PE	C23-C24-C25-C26
45	M	605	LMT	C2-C3-C4-C5
53	K	401	CDL	OB5-CB3-CB4-CB6
45	L	706	LMT	O1'-C1-C2-C3
48	M	604	PC1	C29-C2A-C2B-C2C
45	A	301	LMT	C2-C3-C4-C5
46	M	603	3PE	C36-C37-C38-C39
48	M	604	PC1	C2F-C2G-C2H-C2I
53	K	401	CDL	C36-C37-C38-C39
46	M	603	3PE	C22-C21-O21-C2
46	N	502	3PE	O22-C21-O21-C2
53	X	1701	CDL	OB7-CB5-OB6-CB4
52	H	602	I49	C07-C06-C08-N01
46	Y	401	3PE	C34-C35-C36-C37
53	L	704	CDL	C13-C14-C15-C16
46	M	603	3PE	C35-C36-C37-C38
53	X	1701	CDL	C56-C57-C58-C59
45	l	201	LMT	C1-C2-C3-C4
48	M	604	PC1	C23-C24-C25-C26
46	Y	401	3PE	C3B-C3C-C3D-C3E
53	K	401	CDL	OA9-CA7-OA8-CA6
46	L	703	3PE	C38-C39-C3A-C3B
46	O	1201	3PE	C36-C37-C38-C39
45	N	501	LMT	C5'-C4'-O1B-C1B
53	L	704	CDL	C71-CB7-OB8-CB6
46	L	703	3PE	O11-C1-C2-O21
46	b	901	3PE	O11-C1-C2-O21
53	K	401	CDL	OB5-CB3-CB4-OB6
53	L	704	CDL	OA5-CA3-CA4-OA6
53	X	1701	CDL	OA5-CA3-CA4-OA6
53	d	201	CDL	OA5-CA3-CA4-OA6
46	J	401	3PE	C27-C28-C29-C2A
46	J	401	3PE	C1-C2-C3-O31
46	M	601	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	CA3-CA4-CA6-OA8
58	U	101	EHZ	C22-C23-C24-C25
46	L	703	3PE	C39-C3A-C3B-C3C
46	M	601	3PE	C12-C11-O13-P
48	M	604	PC1	C2E-C2F-C2G-C2H
46	N	502	3PE	C33-C34-C35-C36
53	q	201	CDL	C15-C16-C17-C18
46	H	601	3PE	C36-C37-C38-C39
46	H	601	3PE	C33-C34-C35-C36
46	N	502	3PE	C32-C33-C34-C35
46	N	502	3PE	C26-C27-C28-C29
46	O	1201	3PE	C28-C29-C2A-C2B
53	L	704	CDL	OB9-CB7-OB8-CB6
53	q	201	CDL	C54-C55-C56-C57
45	f	1901	LMT	C2-C1-O1'-C1'
45	M	606	LMT	C4'-C5'-C6'-O6'
53	L	704	CDL	C11-C12-C13-C14
56	P	501	NDP	O4D-C1D-N1N-C6N
46	H	601	3PE	C3A-C3B-C3C-C3D
46	M	603	3PE	O11-C1-C2-C3
53	L	704	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	OB5-CB3-CB4-CB6
53	q	201	CDL	OB5-CB3-CB4-CB6
46	M	603	3PE	O22-C21-O21-C2
53	q	201	CDL	C35-C36-C37-C38
58	T	101	EHZ	C18-C17-C20-O6
45	L	706	LMT	C6-C7-C8-C9
53	X	1701	CDL	C19-C20-C21-C22
46	M	603	3PE	C2-C1-O11-P
53	K	401	CDL	C1-CB2-OB2-PB2
46	L	701	3PE	C2F-C2G-C2H-C2I
46	M	601	3PE	O11-C1-C2-O21
46	M	603	3PE	O11-C1-C2-O21
46	Y	401	3PE	O11-C1-C2-O21
46	L	701	3PE	C2A-C2B-C2C-C2D
53	d	201	CDL	C75-C76-C77-C78
52	H	602	I49	N01-C14-N02-C15
46	O	1201	3PE	O21-C2-C3-O31
48	B	203	PC1	O21-C2-C3-O31
53	h	1001	CDL	OA6-CA4-CA6-OA8
53	q	201	CDL	C16-C17-C18-C19
46	A	302	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
53	X	1701	CDL	CB3-CB4-CB6-OB8
53	q	201	CDL	CA5-C11-C12-C13
46	b	901	3PE	C2A-C2B-C2C-C2D
46	A	302	3PE	C27-C28-C29-C2A
45	f	1901	LMT	C4B-C5B-C6B-O6B
46	L	701	3PE	C26-C27-C28-C29
46	H	601	3PE	C11-O13-P-O14
46	J	401	3PE	C11-O13-P-O11
46	J	401	3PE	C11-O13-P-O12
46	J	401	3PE	C11-O13-P-O14
46	M	601	3PE	C1-O11-P-O12
46	N	502	3PE	C11-O13-P-O12
46	O	1201	3PE	O13-C11-C12-N
46	Y	401	3PE	C1-O11-P-O14
46	b	901	3PE	C11-O13-P-O11
46	b	901	3PE	C11-O13-P-O14
48	M	604	PC1	C11-O13-P-O12
53	K	401	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	CA2-OA2-PA1-OA3
53	X	1701	CDL	CA2-OA2-PA1-OA5
53	d	201	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CA2-OA2-PA1-OA3
53	q	201	CDL	CA2-OA2-PA1-OA5
54	O	1202	GTP	C5'-O5'-PA-O3A
54	O	1202	GTP	C5'-O5'-PA-O1A
54	O	1202	GTP	C5'-O5'-PA-O2A
53	h	1001	CDL	C71-C72-C73-C74
53	q	201	CDL	CA4-CA3-OA5-PA1
46	I	201	3PE	C35-C36-C37-C38
53	X	1701	CDL	C52-C53-C54-C55
46	O	1201	3PE	C3D-C3E-C3F-C3G
46	M	601	3PE	C3-C2-O21-C21
48	B	203	PC1	C36-C37-C38-C39
46	M	601	3PE	C25-C26-C27-C28
46	M	603	3PE	C2B-C2C-C2D-C2E
45	B	202	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	C3'-C4'-O1B-C1B
46	O	1201	3PE	C23-C24-C25-C26
46	M	601	3PE	C2A-C2B-C2C-C2D
53	K	401	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
53	L	704	CDL	C34-C35-C36-C37
46	L	701	3PE	C3A-C3B-C3C-C3D
53	L	704	CDL	C22-C23-C24-C25
56	P	501	NDP	C3D-C4D-C5D-O5D
46	I	201	3PE	C34-C35-C36-C37
53	L	704	CDL	C21-C22-C23-C24
46	I	201	3PE	C23-C24-C25-C26
46	O	1201	3PE	C22-C23-C24-C25
53	h	1001	CDL	C51-C52-C53-C54
53	h	1001	CDL	OA7-CA5-OA6-CA4
46	L	703	3PE	O21-C21-C22-C23
46	H	601	3PE	O11-C1-C2-O21
46	b	901	3PE	O11-C1-C2-C3
45	l	201	LMT	O1'-C1-C2-C3
46	I	201	3PE	C26-C27-C28-C29
46	M	603	3PE	C37-C38-C39-C3A
53	X	1701	CDL	C57-C58-C59-C60
46	L	701	3PE	C24-C25-C26-C27
53	q	201	CDL	C72-C73-C74-C75
53	L	704	CDL	CA4-CA3-OA5-PA1
45	l	201	LMT	C5'-C4'-O1B-C1B
45	B	202	LMT	O5B-C5B-C6B-O6B
45	J	402	LMT	C3-C4-C5-C6
46	L	701	3PE	C2B-C2C-C2D-C2E
45	A	301	LMT	C5'-C4'-O1B-C1B
46	L	703	3PE	C36-C37-C38-C39
45	L	705	LMT	C3-C4-C5-C6
53	L	704	CDL	C14-C15-C16-C17
45	l	201	LMT	C2B-C1B-O1B-C4'
46	I	201	3PE	C31-C32-C33-C34
53	K	401	CDL	CB7-C71-C72-C73
53	K	401	CDL	C35-C36-C37-C38
46	H	601	3PE	C3B-C3C-C3D-C3E
46	N	502	3PE	C2-C1-O11-P
50	F	501	FMN	C4'-C5'-O5'-P
53	L	704	CDL	C32-C33-C34-C35
46	A	302	3PE	O21-C2-C3-O31
53	L	704	CDL	OB6-CB4-CB6-OB8
45	M	605	LMT	O1'-C1-C2-C3
53	h	1001	CDL	C11-CA5-OA6-CA4
53	X	1701	CDL	C71-C72-C73-C74
46	L	703	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	C24-C25-C26-C27
46	M	601	3PE	C2E-C2F-C2G-C2H
45	L	705	LMT	C2'-C1'-O1'-C1
52	H	602	I49	N03-C14-N02-C15
45	L	702	LMT	C5-C6-C7-C8
53	K	401	CDL	O1-C1-CA2-OA2
45	L	706	LMT	C9-C10-C11-C12
46	J	401	3PE	C24-C25-C26-C27
53	h	1001	CDL	C31-C32-C33-C34
45	M	605	LMT	C9-C10-C11-C12
53	X	1701	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	OB6-CB4-CB6-OB8
53	d	201	CDL	C52-C51-CB5-OB6
45	N	501	LMT	C4-C5-C6-C7
45	M	605	LMT	C5-C6-C7-C8
53	q	201	CDL	C11-C12-C13-C14
46	J	401	3PE	C23-C24-C25-C26
53	q	201	CDL	C40-C41-C42-C43
46	H	601	3PE	C2-C1-O11-P
53	h	1001	CDL	C17-C18-C19-C20
53	d	201	CDL	CB3-CB4-CB6-OB8
45	L	705	LMT	C4-C5-C6-C7
53	d	201	CDL	C52-C51-CB5-OB7
53	L	704	CDL	C81-C82-C83-C84
45	M	602	LMT	C1-C2-C3-C4
53	L	704	CDL	C36-C37-C38-C39
53	L	704	CDL	C78-C79-C80-C81
53	X	1701	CDL	OA6-CA4-CA6-OA8
53	q	201	CDL	OB6-CB4-CB6-OB8
46	H	601	3PE	O11-C1-C2-C3
46	J	401	3PE	O11-C1-C2-C3
53	h	1001	CDL	C20-C21-C22-C23
46	J	401	3PE	C38-C39-C3A-C3B
53	L	704	CDL	C55-C56-C57-C58
53	q	201	CDL	C73-C74-C75-C76
54	O	1202	GTP	PA-O3A-PB-O1B
54	O	1202	GTP	PA-O3A-PB-O2B
56	P	501	NDP	PN-O3-PA-O1A
46	M	601	3PE	C22-C23-C24-C25
46	M	603	3PE	C22-C23-C24-C25
46	b	901	3PE	C22-C23-C24-C25
46	N	502	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	b	901	3PE	O31-C31-C32-C33
45	M	606	LMT	C5-C6-C7-C8
46	M	601	3PE	C32-C33-C34-C35
53	h	1001	CDL	C22-C23-C24-C25
53	K	401	CDL	C14-C15-C16-C17
46	L	701	3PE	C28-C29-C2A-C2B
46	M	603	3PE	O21-C21-C22-C23
48	B	203	PC1	O21-C21-C22-C23
46	L	703	3PE	C22-C23-C24-C25
46	b	901	3PE	O21-C21-C22-C23
46	H	601	3PE	C35-C36-C37-C38
46	J	401	3PE	O31-C31-C32-C33
53	d	201	CDL	C42-C43-C44-C45
50	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C19-C17-C20-O6
53	d	201	CDL	C73-C74-C75-C76
53	L	704	CDL	C52-C51-CB5-OB6
53	h	1001	CDL	C34-C35-C36-C37
46	A	302	3PE	O31-C31-C32-C33
46	O	1201	3PE	C2-C1-O11-P
56	P	501	NDP	C2B-O2B-P2B-O1X
45	L	702	LMT	C2-C3-C4-C5
45	l	201	LMT	C5-C6-C7-C8
46	N	502	3PE	O32-C31-C32-C33
46	b	901	3PE	O32-C31-C32-C33
45	M	602	LMT	C5'-C4'-O1B-C1B
58	T	101	EHZ	C21-C1-C2-C3
46	O	1201	3PE	C34-C35-C36-C37
46	J	401	3PE	O32-C31-C32-C33
48	B	203	PC1	O22-C21-C22-C23
46	L	703	3PE	C33-C34-C35-C36
46	J	401	3PE	C35-C36-C37-C38
45	L	705	LMT	C5-C6-C7-C8
53	q	201	CDL	C39-C40-C41-C42
58	T	101	EHZ	C16-C17-C20-O6
53	h	1001	CDL	OA5-CA3-CA4-CA6
46	I	201	3PE	C22-C23-C24-C25
46	M	603	3PE	O22-C21-C22-C23
46	O	1201	3PE	O21-C21-C22-C23
46	M	603	3PE	C23-C24-C25-C26
46	I	201	3PE	O31-C31-C32-C33
46	J	401	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	C32-C31-CA7-OA8
46	A	302	3PE	O32-C31-C32-C33
46	M	603	3PE	C26-C27-C28-C29
46	b	901	3PE	O22-C21-C22-C23
53	L	704	CDL	C52-C51-CB5-OB7
53	L	704	CDL	C64-C65-C66-C67
46	M	603	3PE	C3B-C3C-C3D-C3E

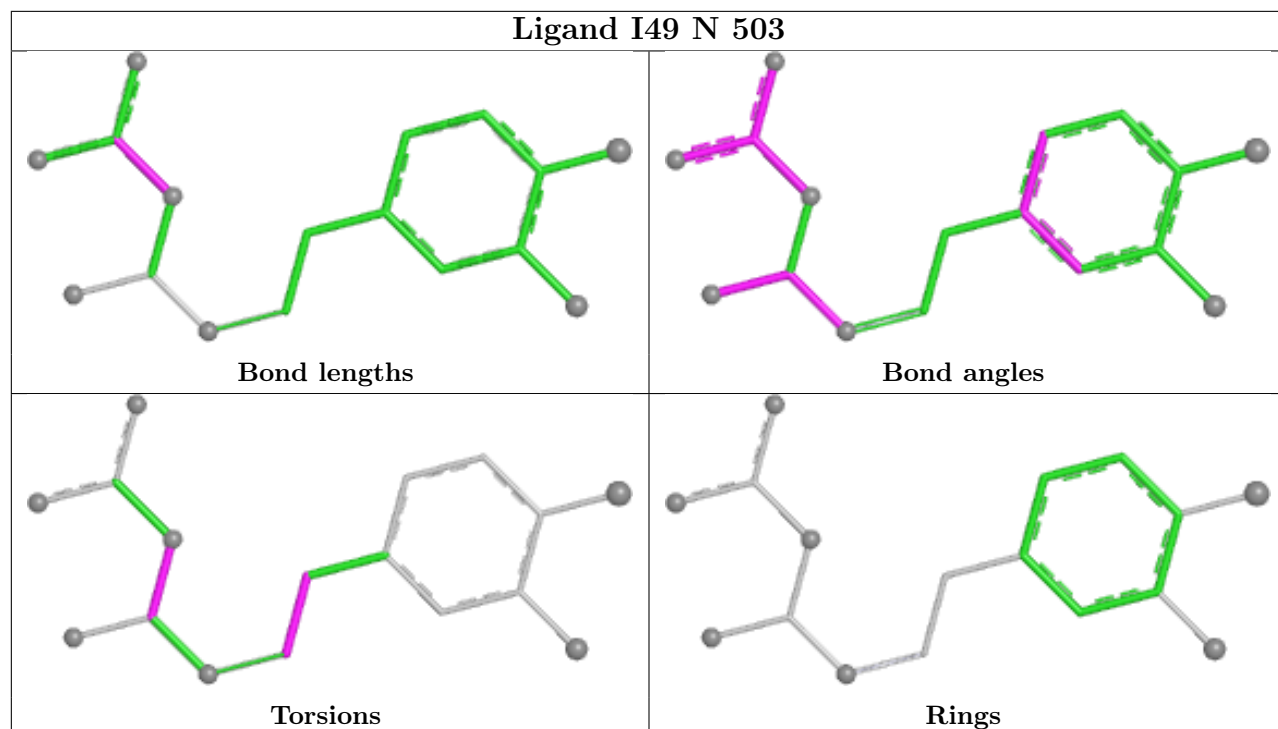
There are no ring outliers.

17 monomers are involved in 34 short contacts:

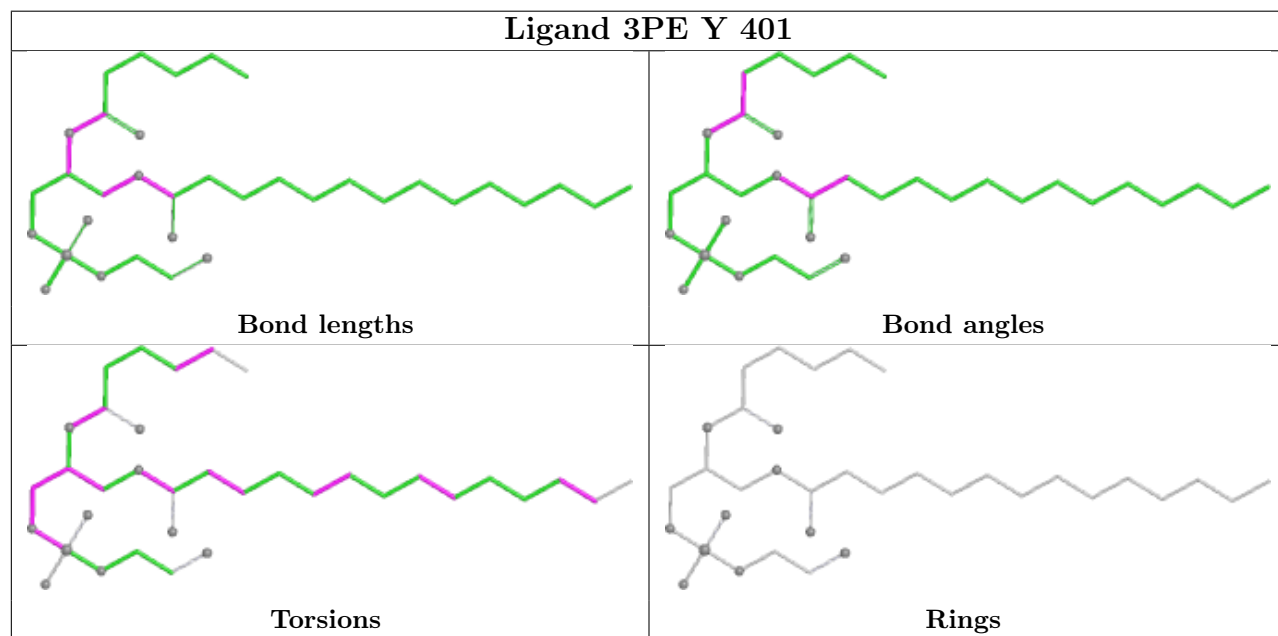
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	N	503	I49	2	0
45	M	605	LMT	1	0
46	J	401	3PE	1	0
45	L	706	LMT	2	0
45	L	702	LMT	2	0
46	L	701	3PE	1	0
53	h	1001	CDL	1	0
53	L	704	CDL	4	0
45	M	602	LMT	1	0
48	M	604	PC1	1	0
52	H	602	I49	3	0
45	J	402	LMT	1	0
54	O	1202	GTP	4	0
46	H	601	3PE	4	0
46	M	603	3PE	2	0
46	L	703	3PE	1	0
45	f	1901	LMT	8	0

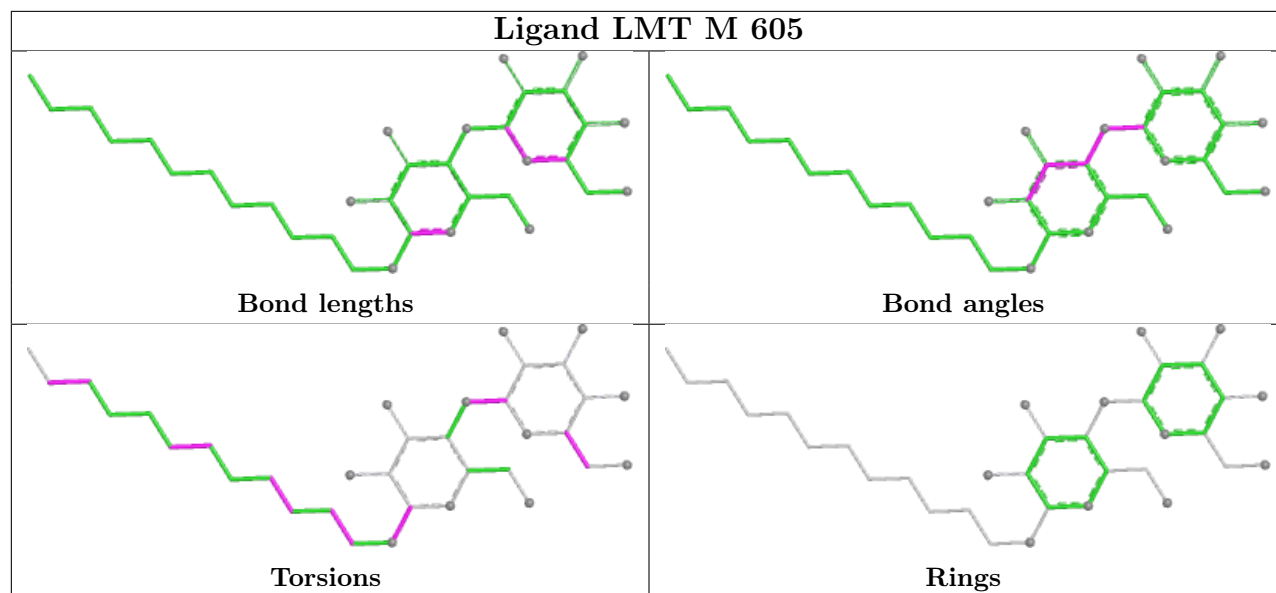
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

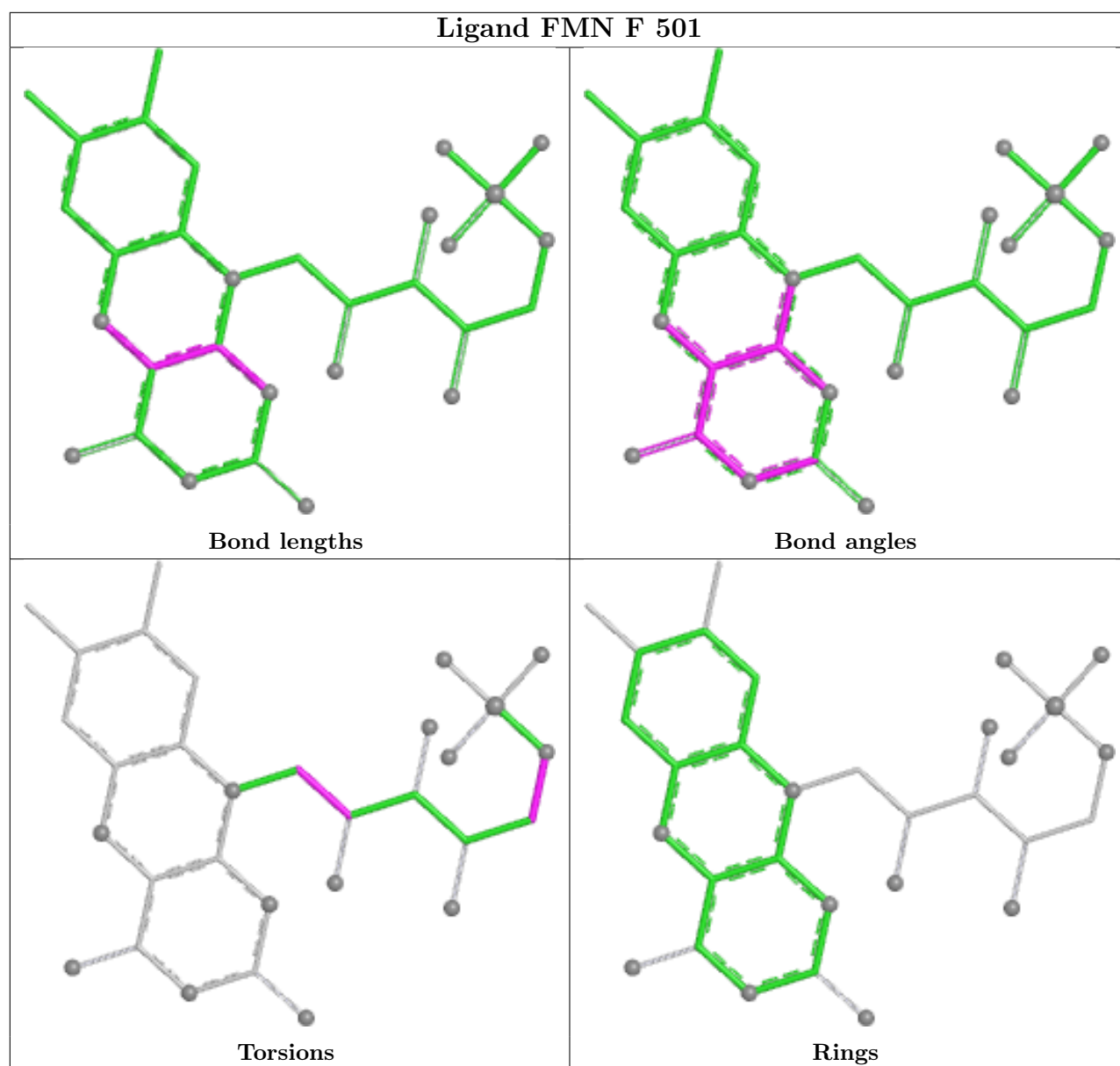
Ligand I49 N 503

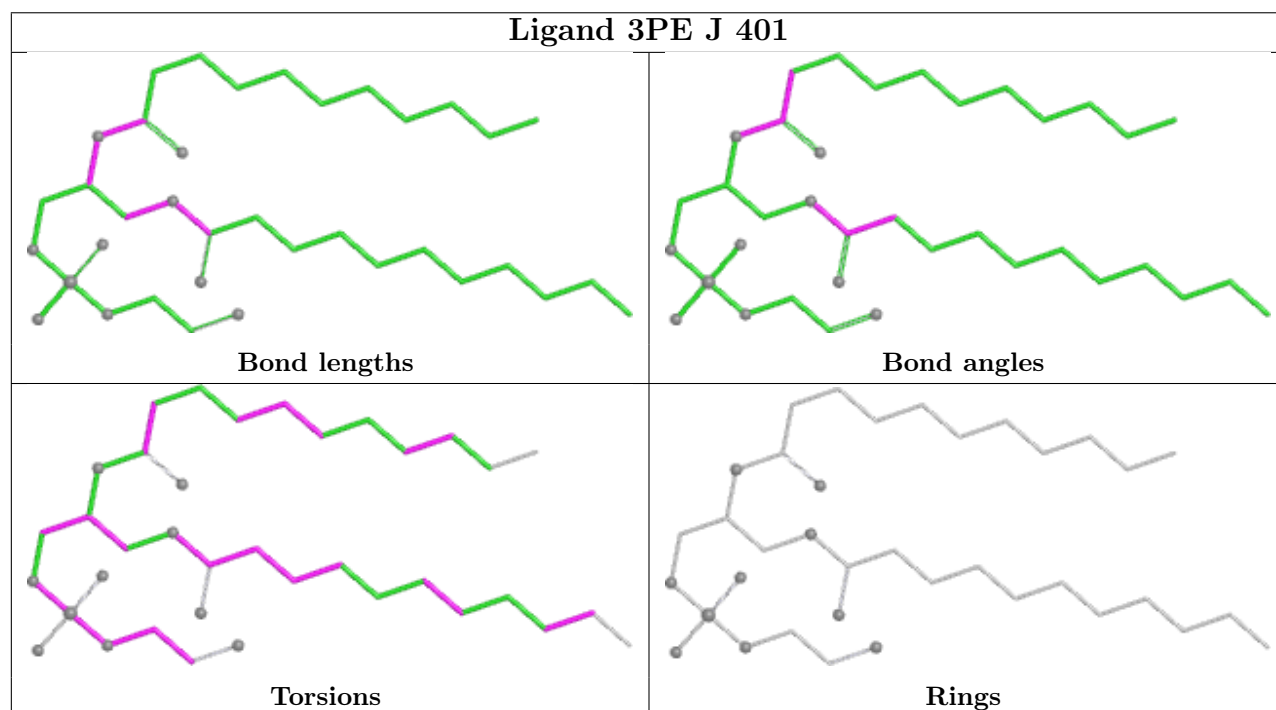
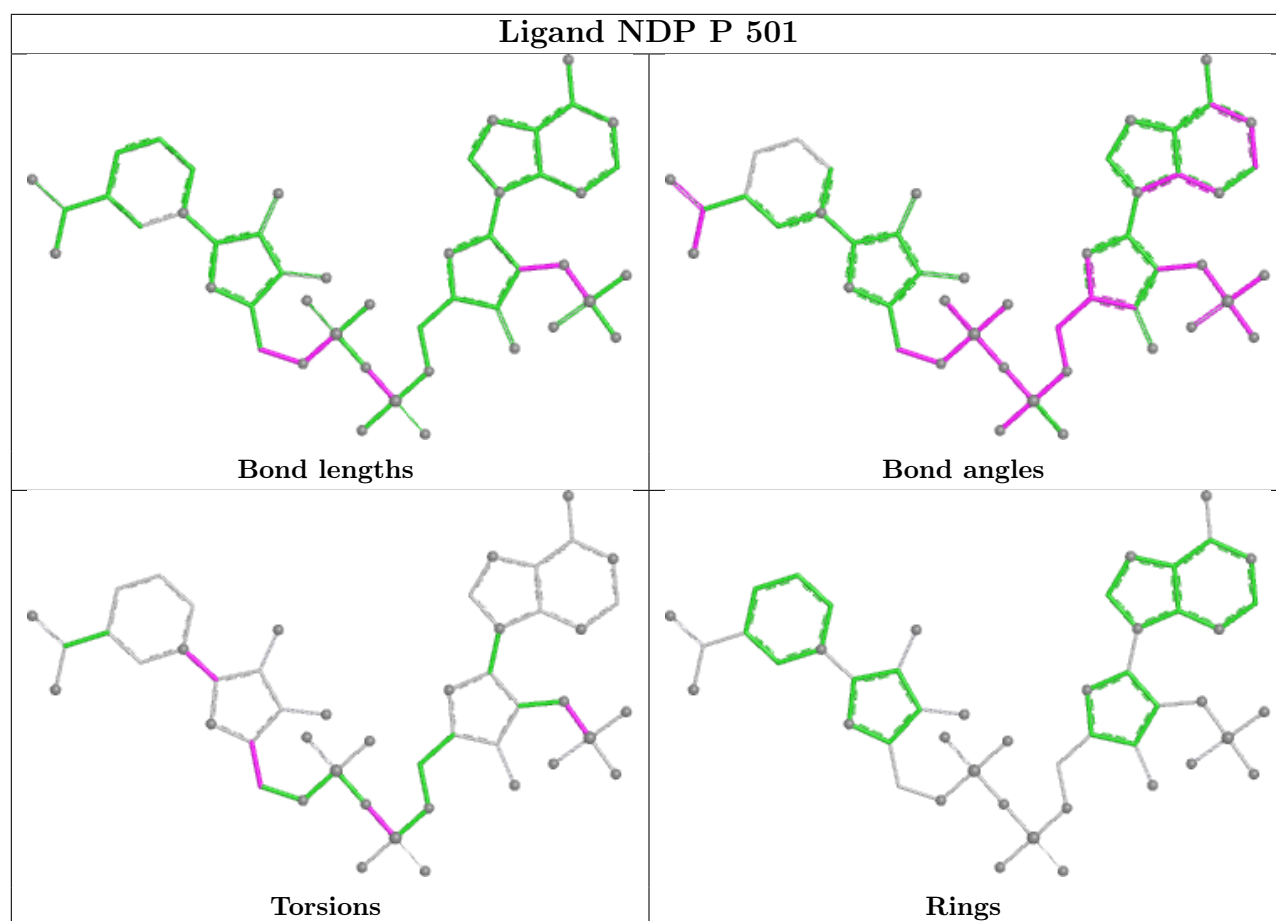


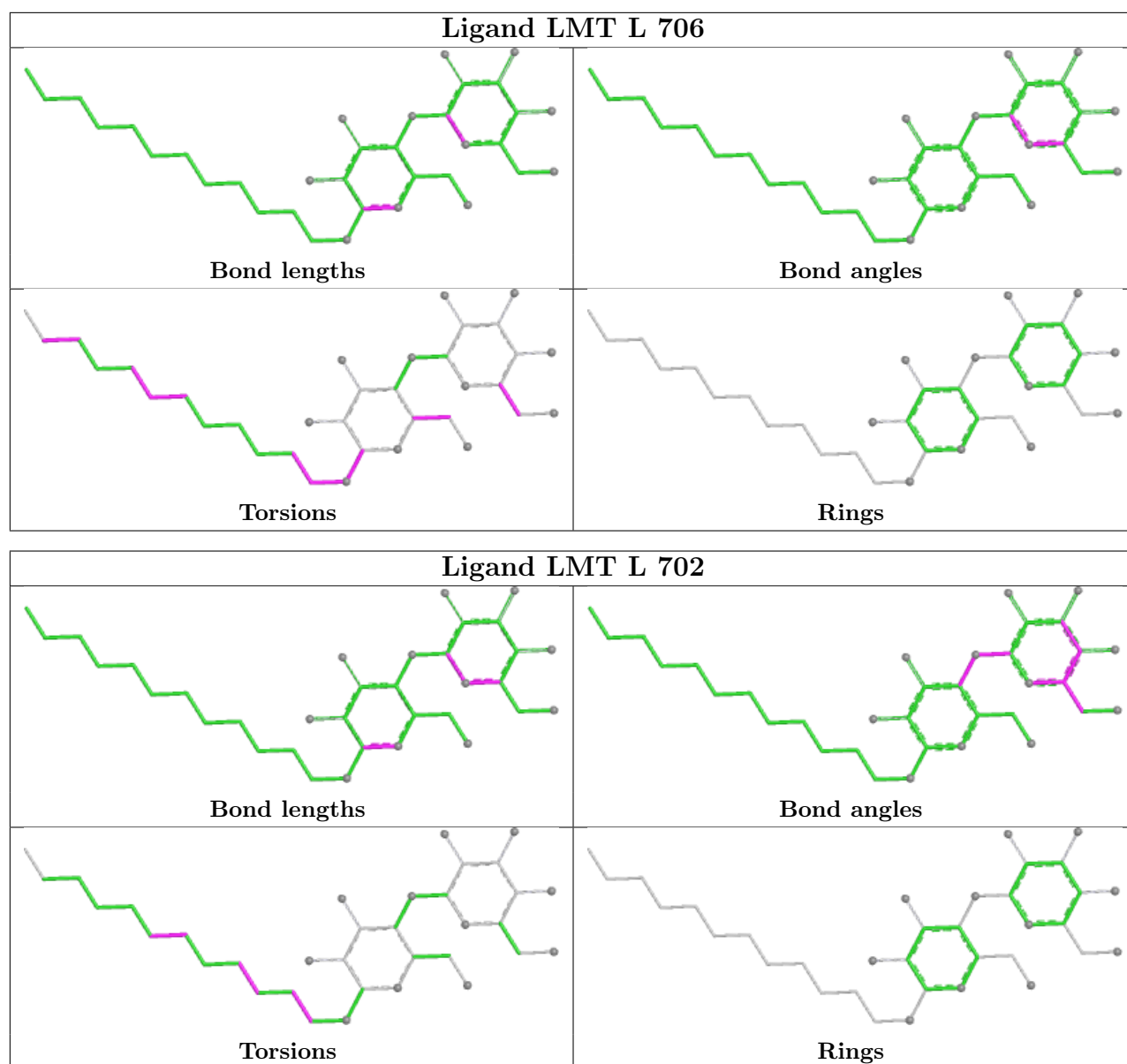
Ligand 3PE Y 401

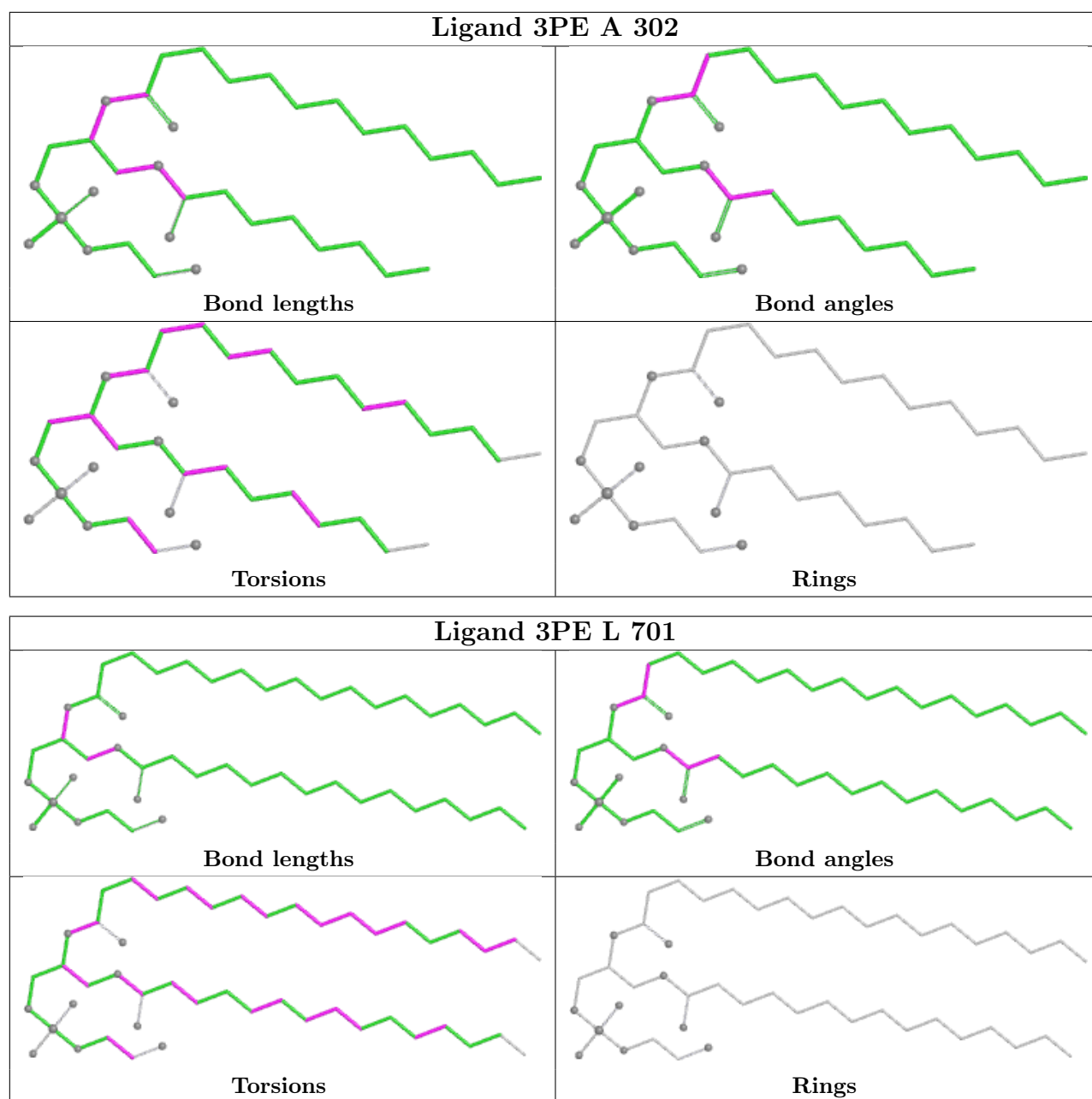


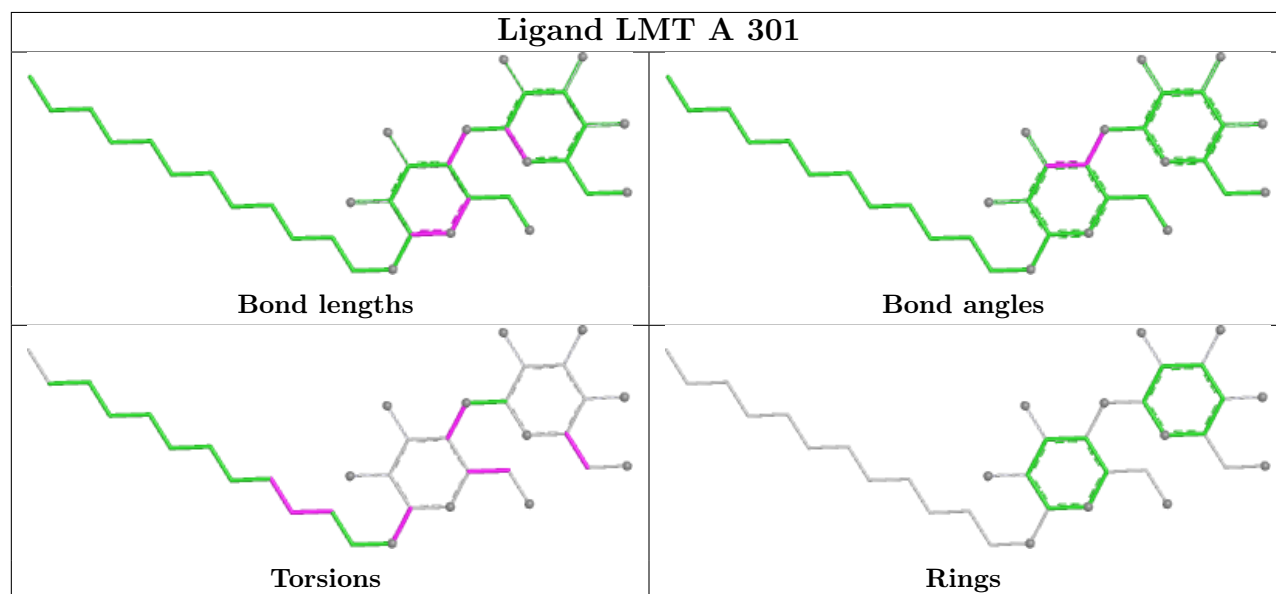
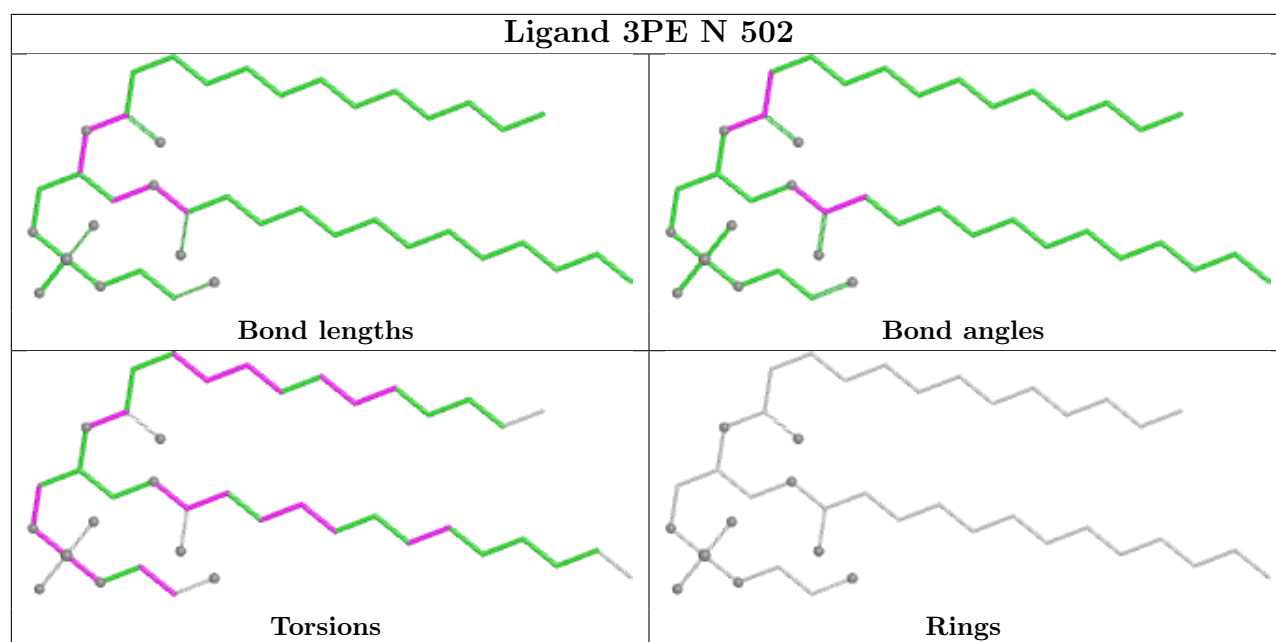


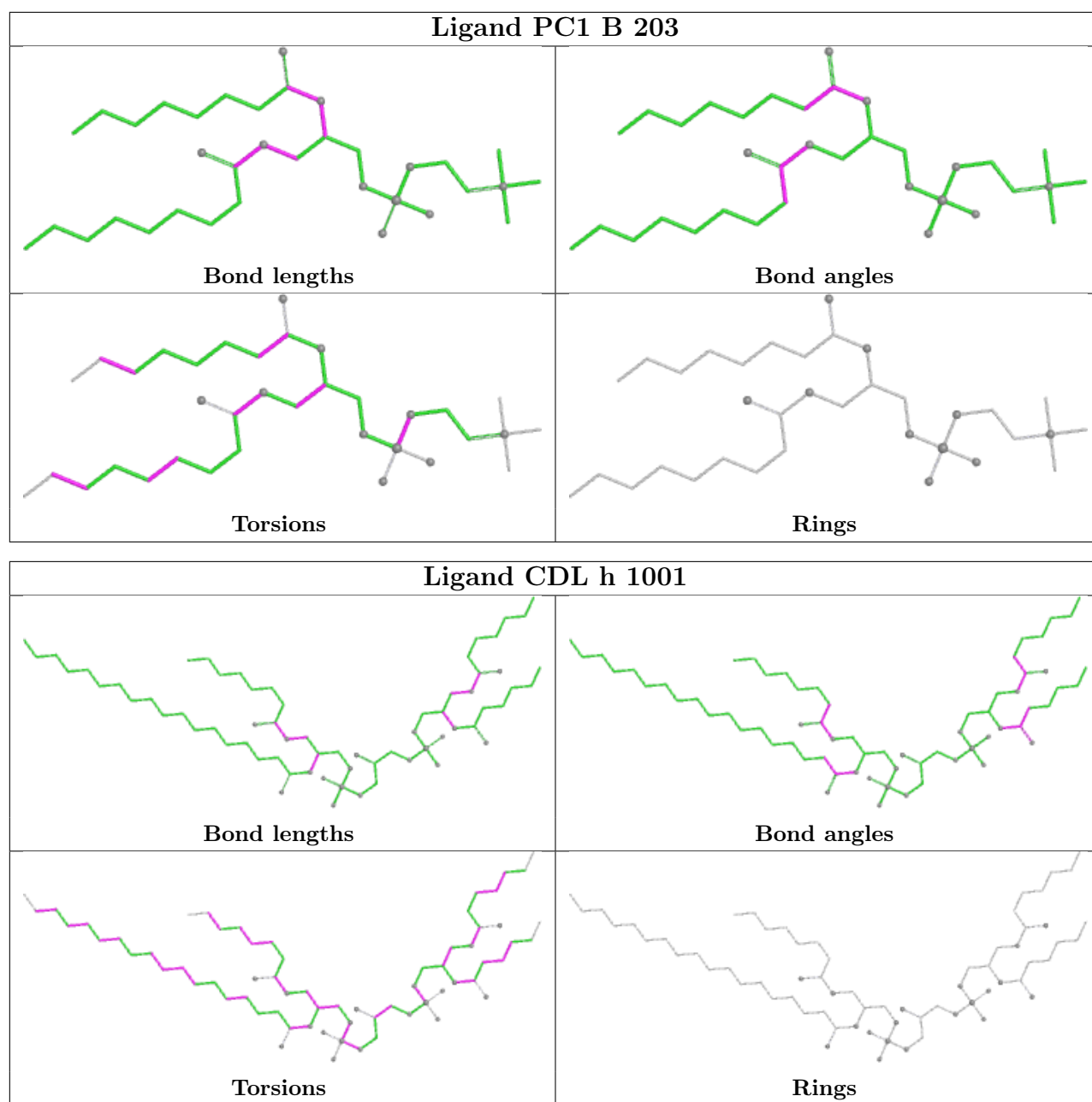


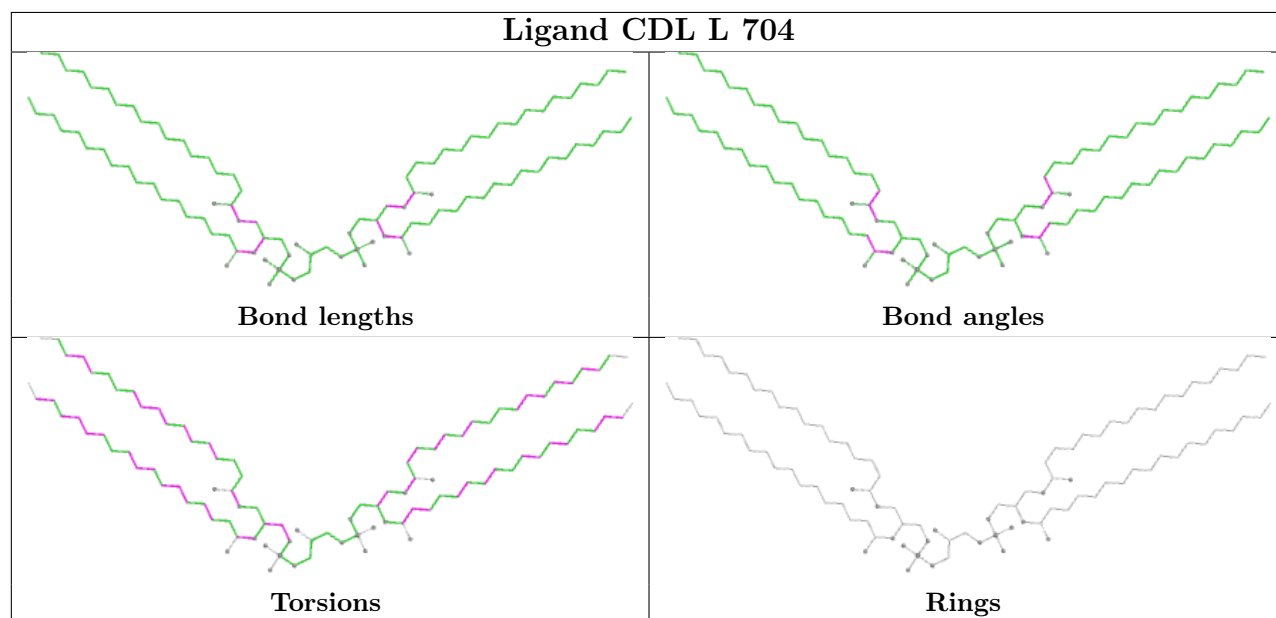
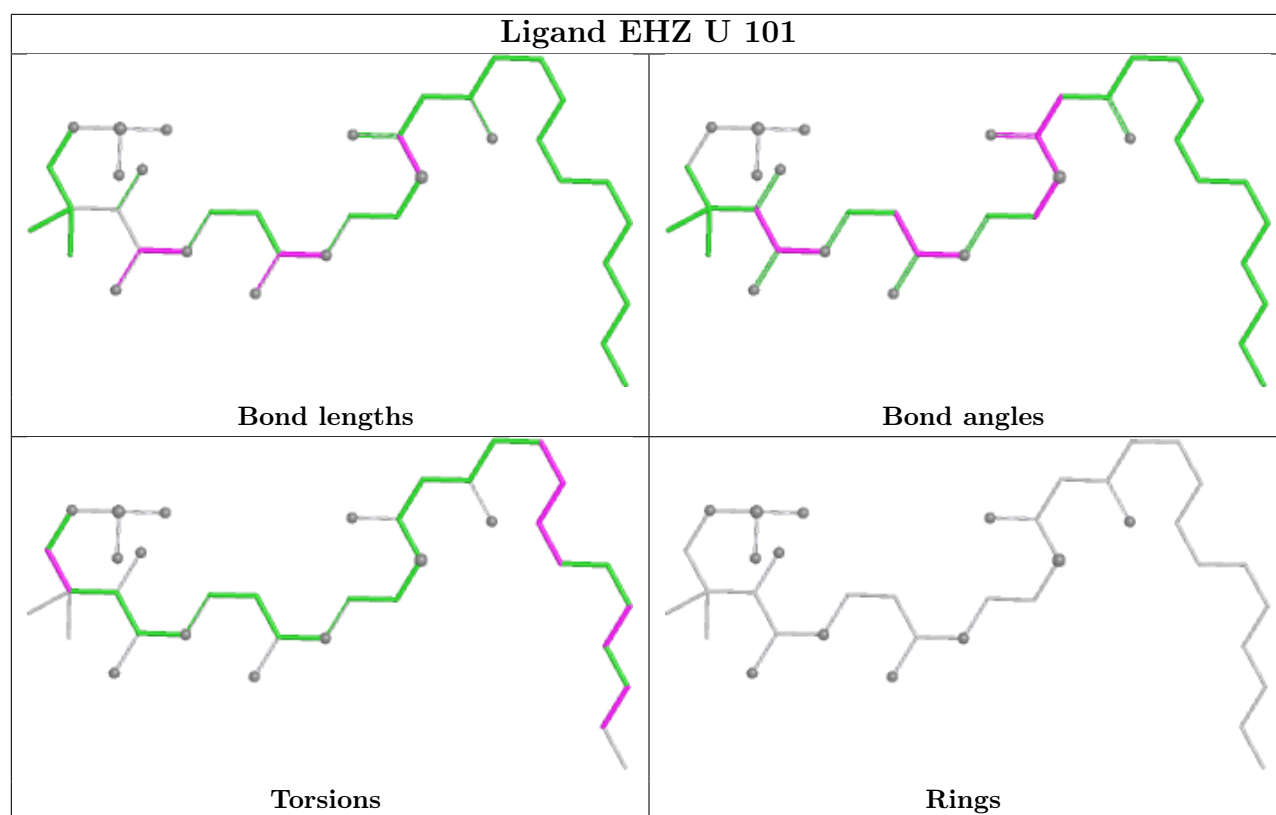


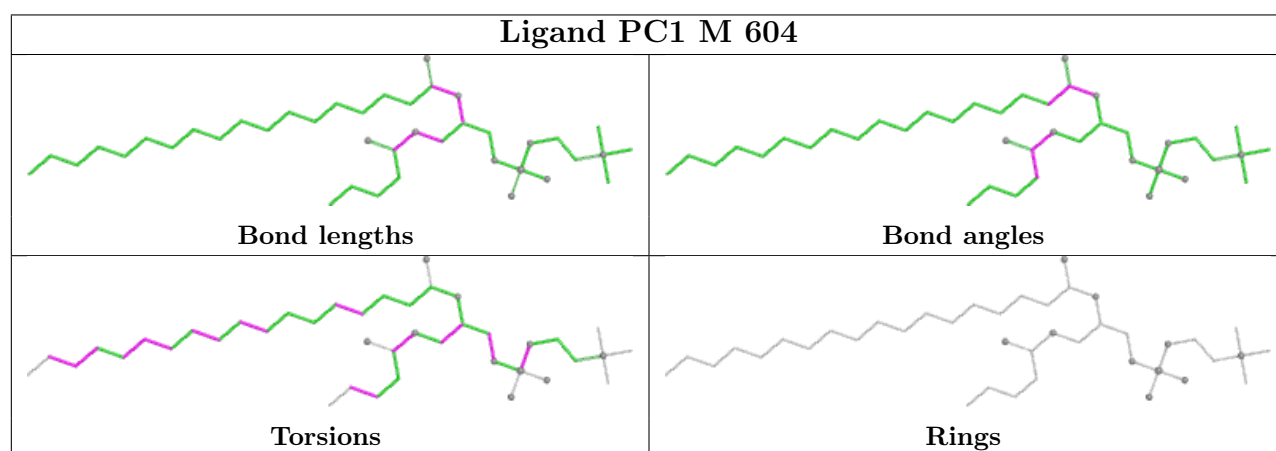
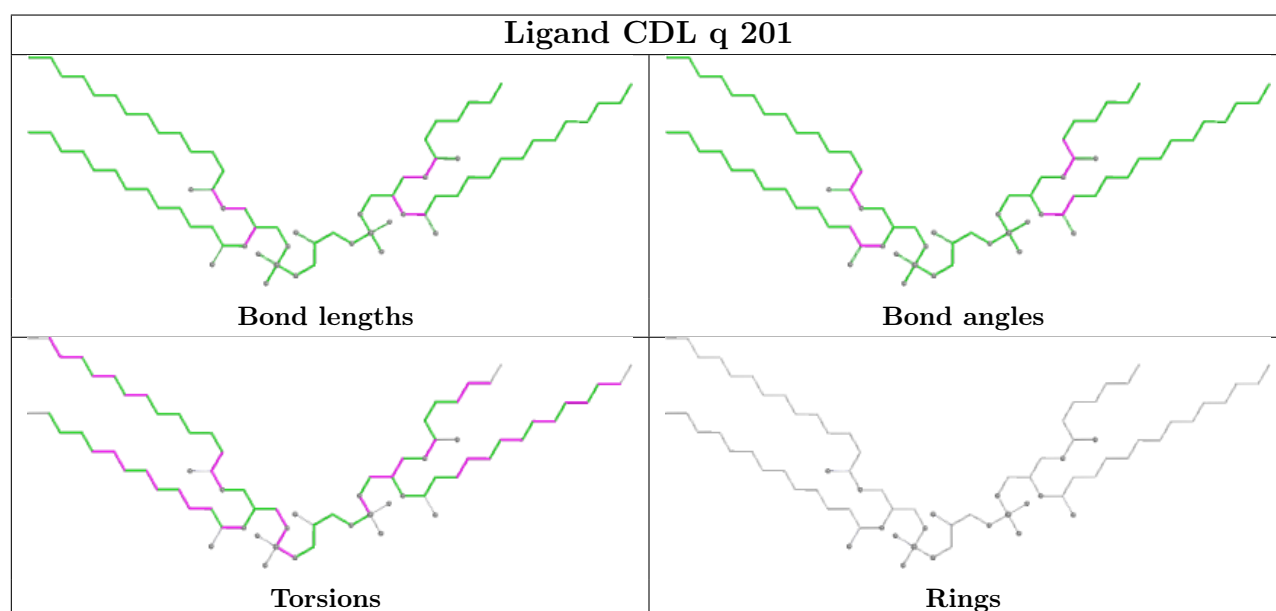
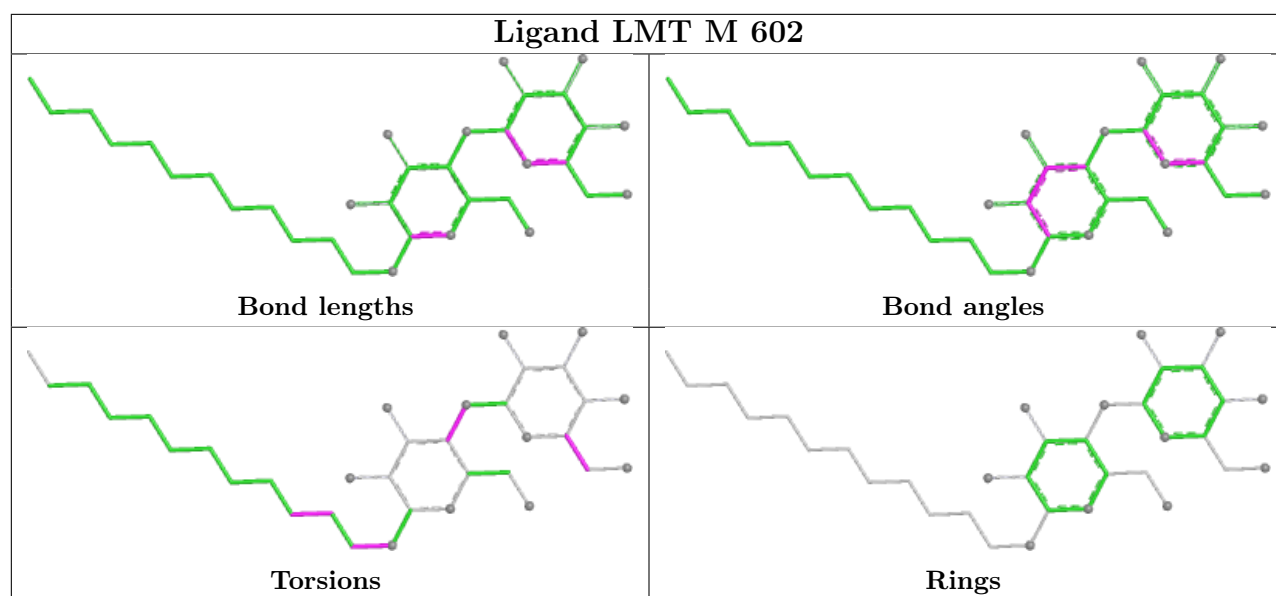




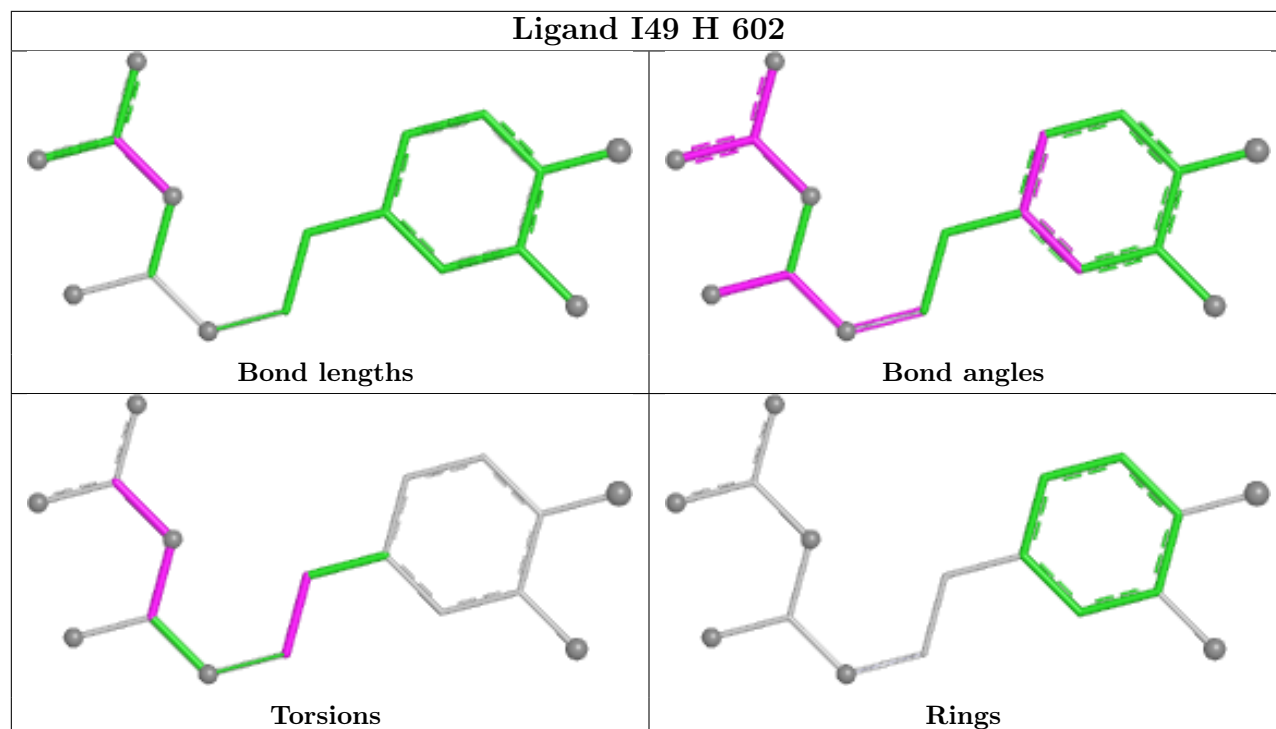




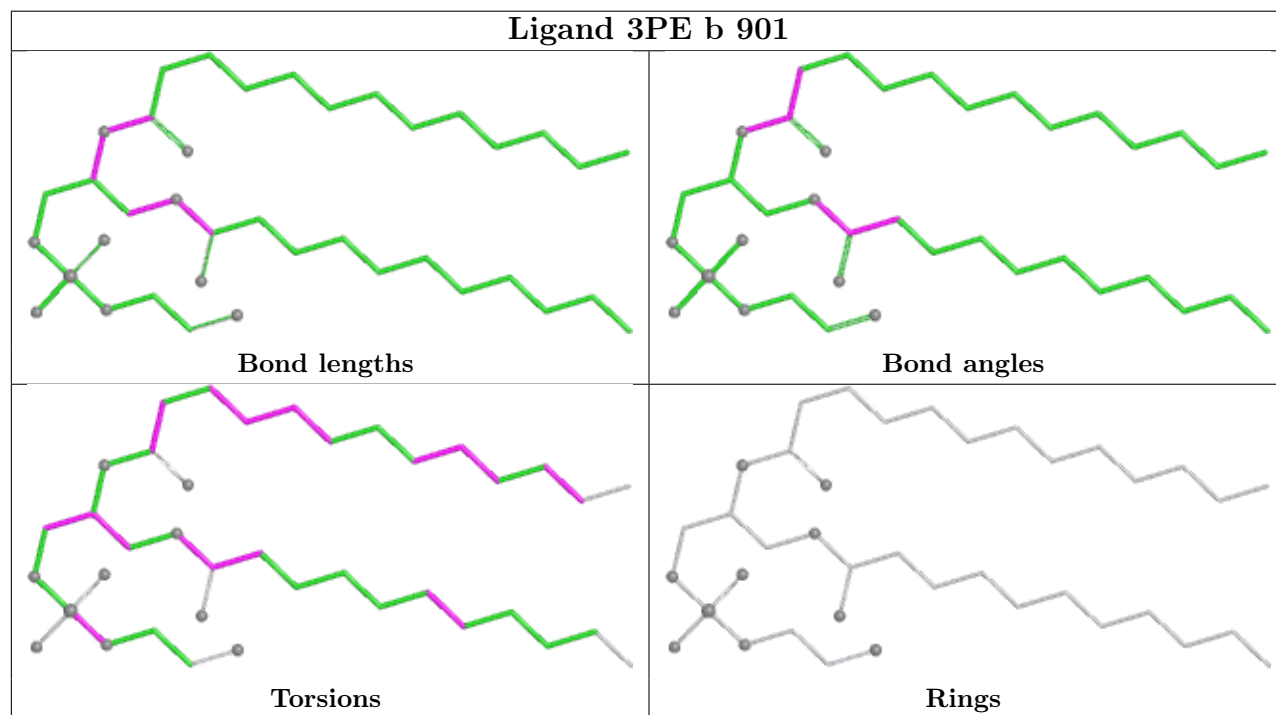


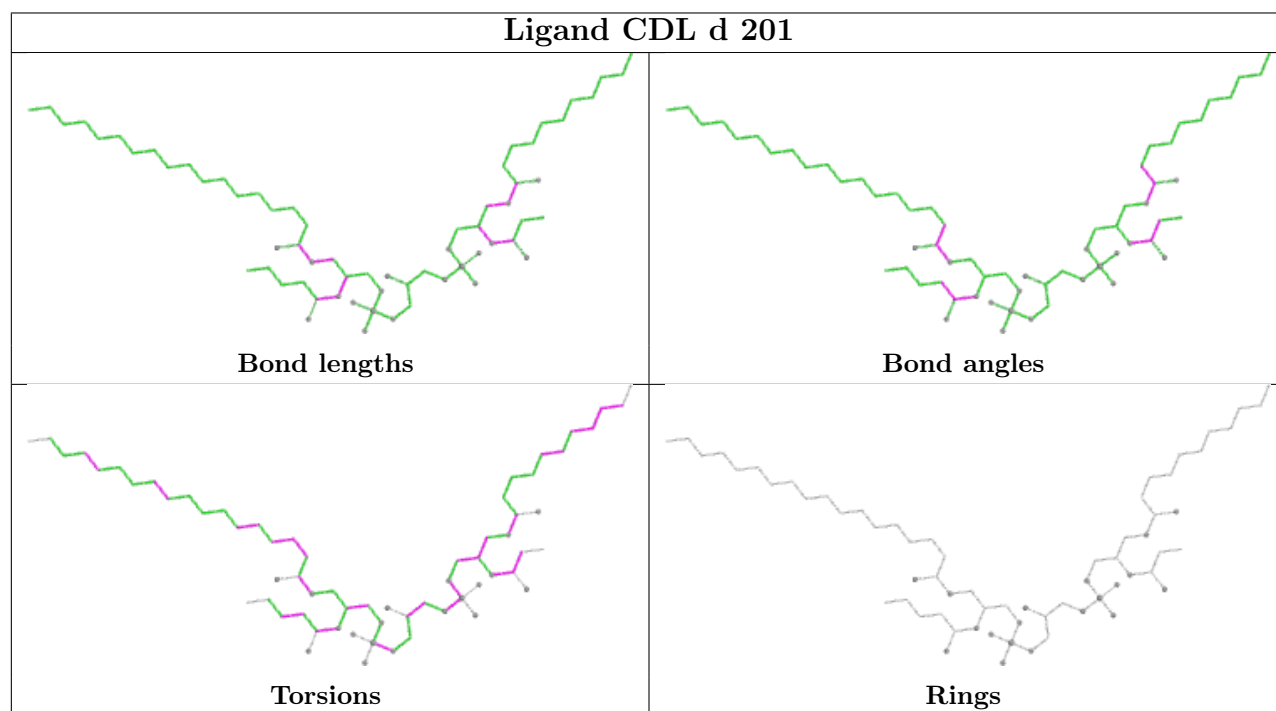
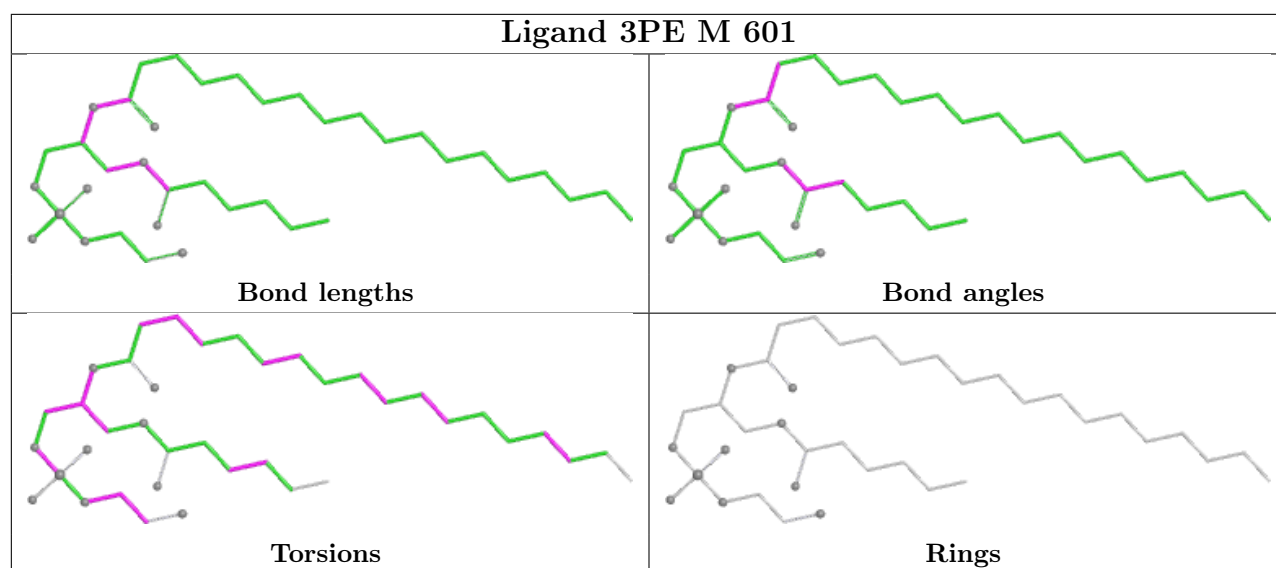


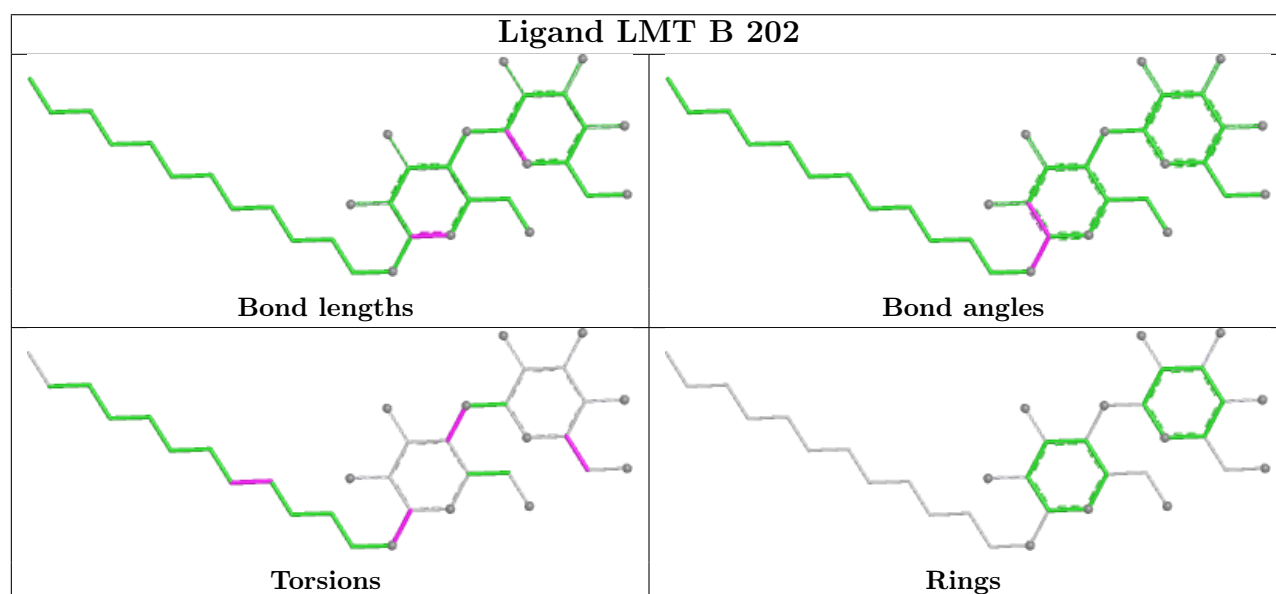
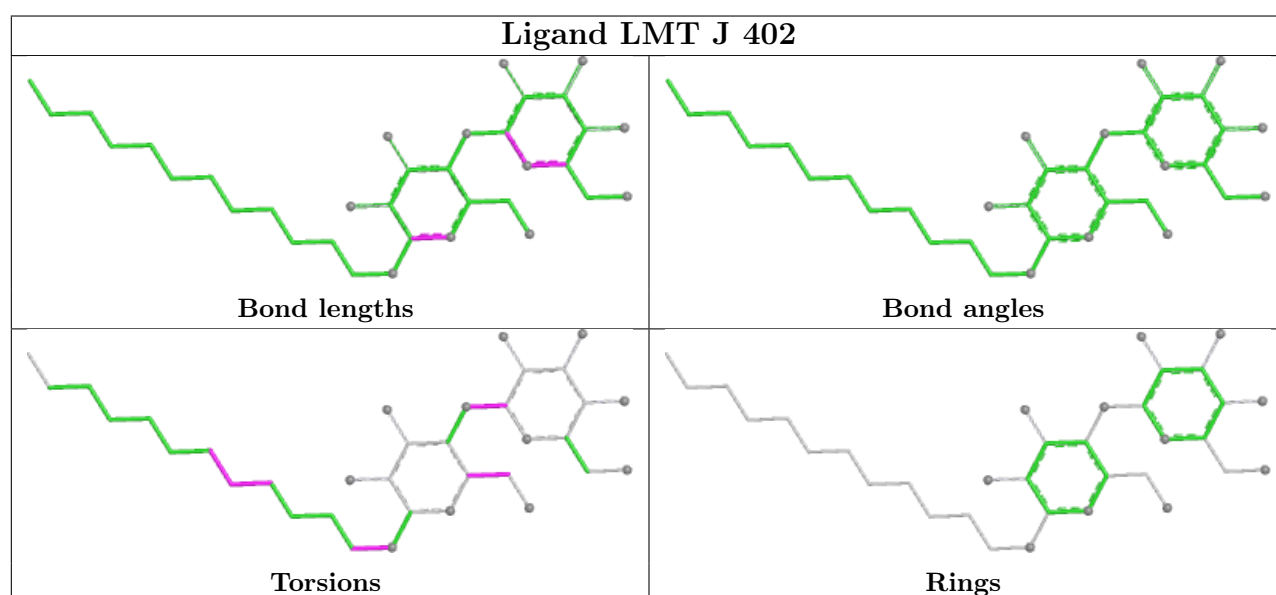
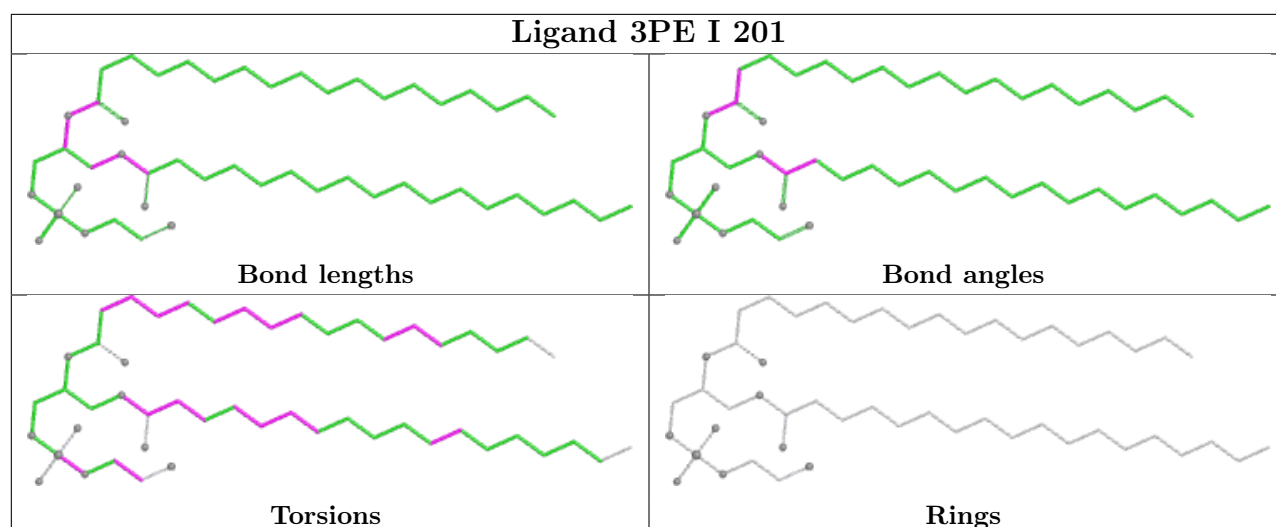
Ligand I49 H 602

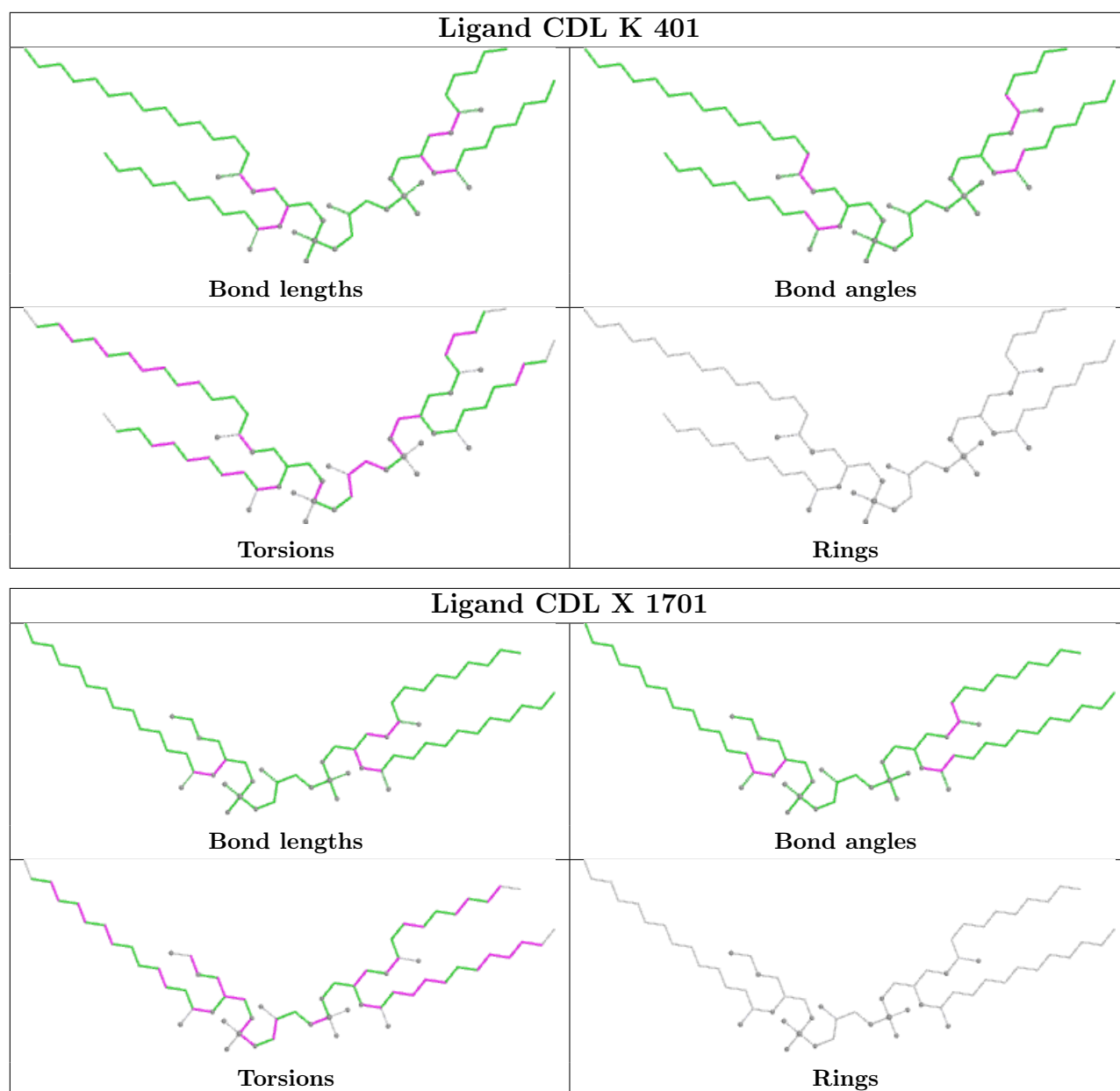


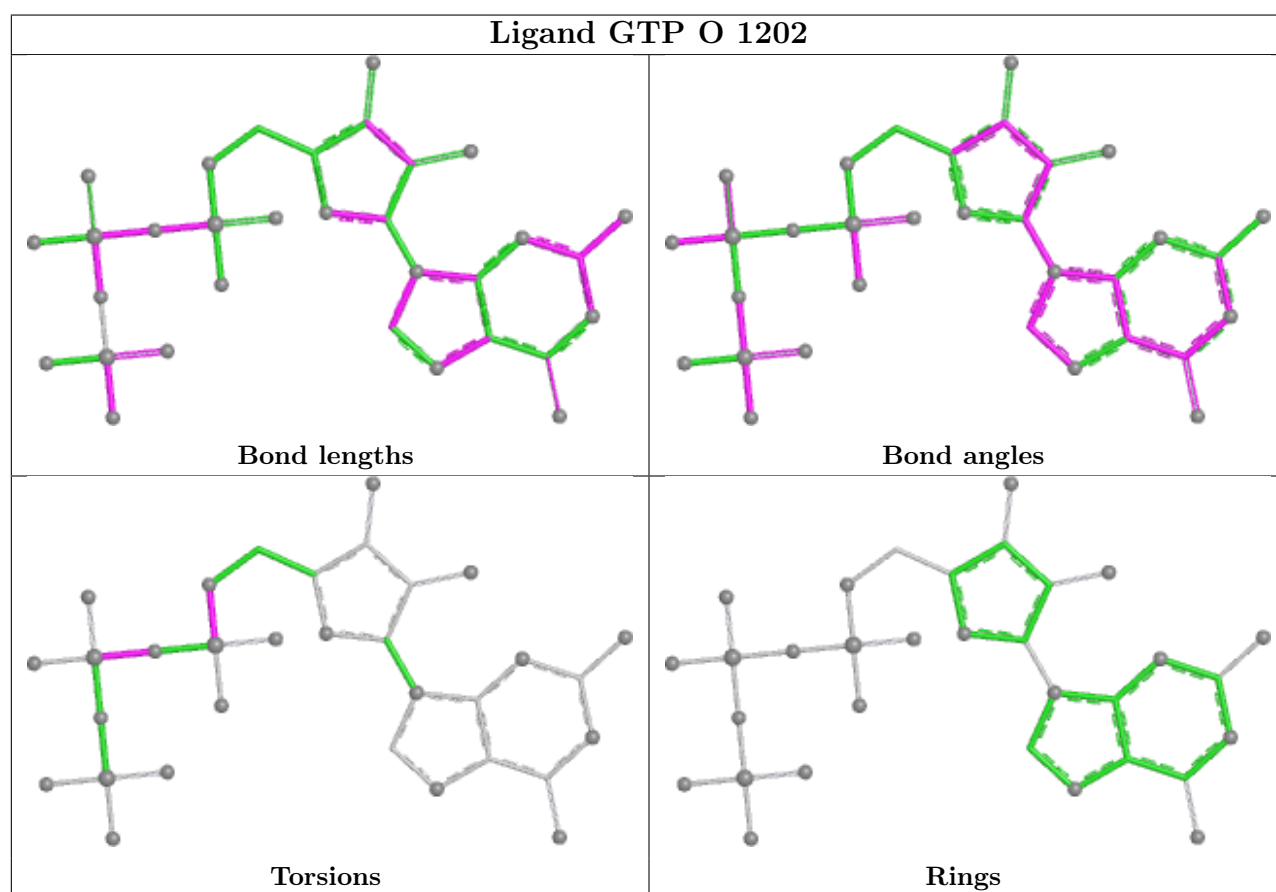
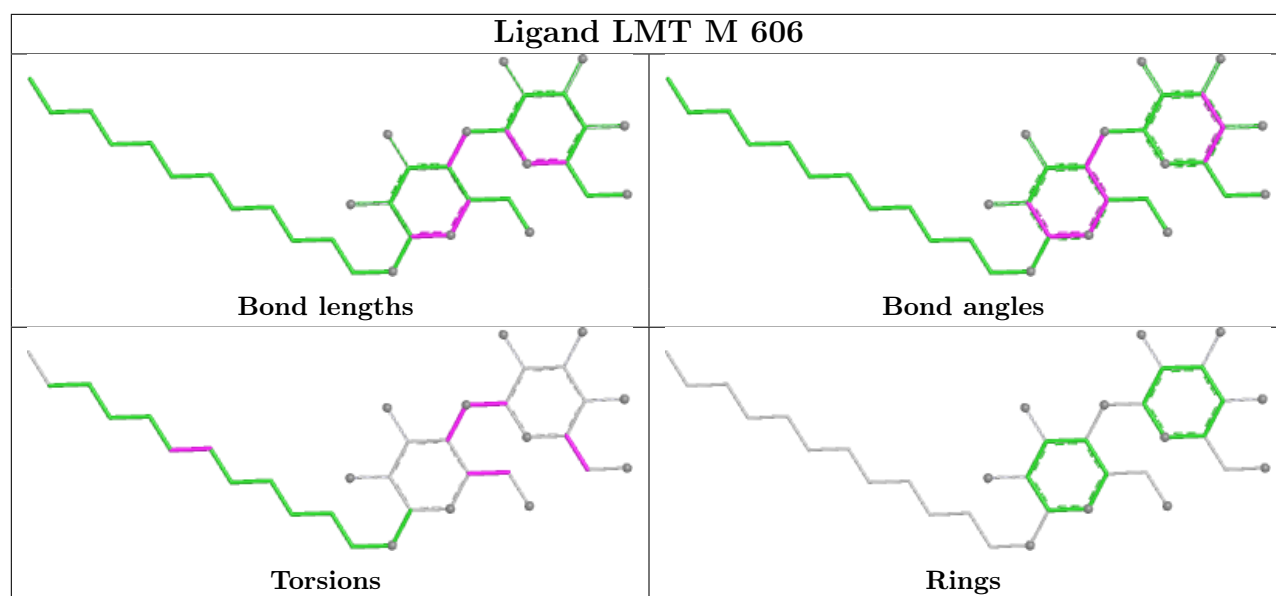
Ligand 3PE b 901

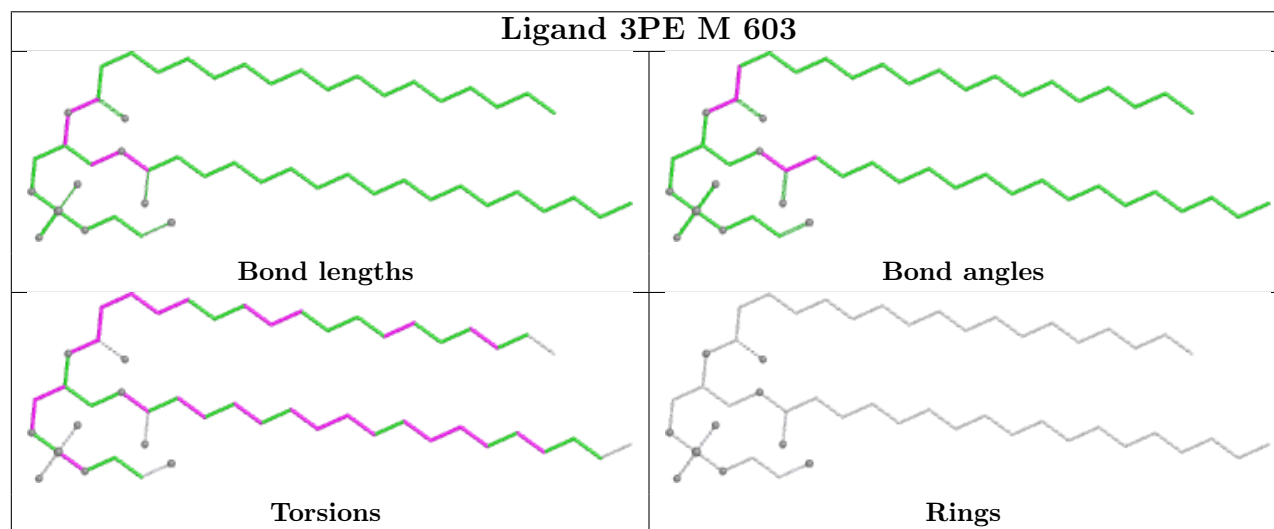
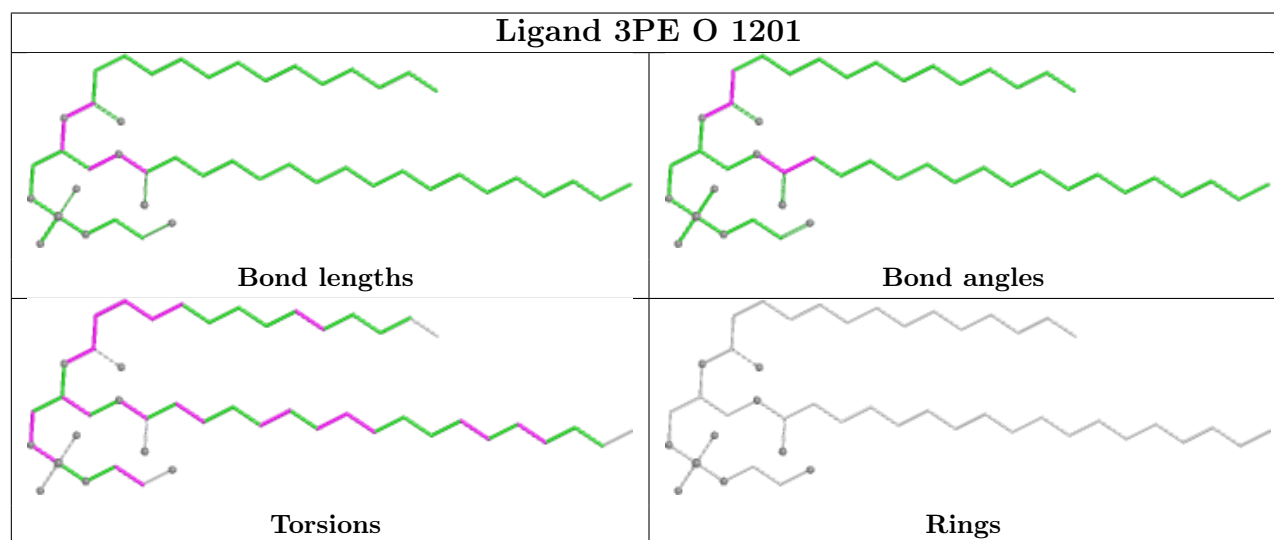
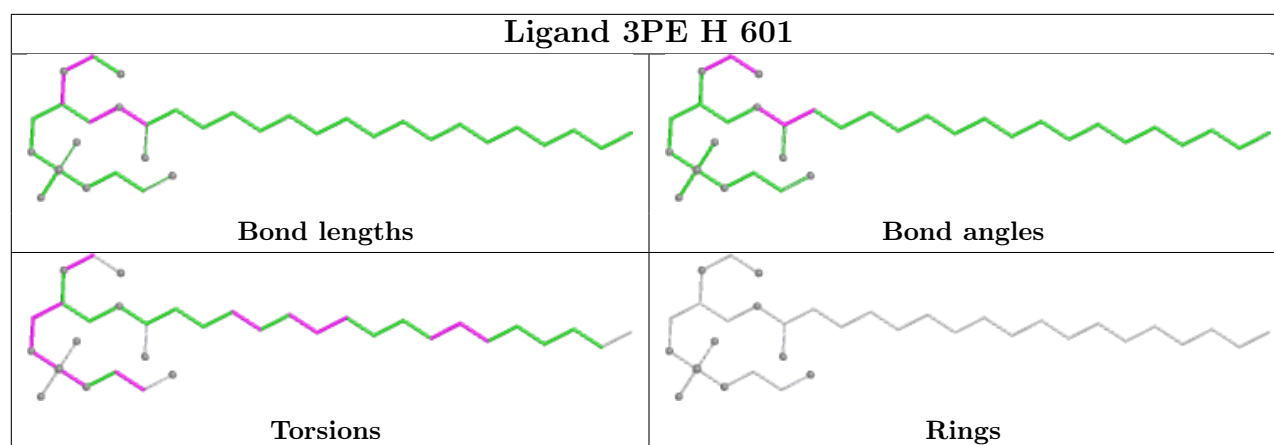


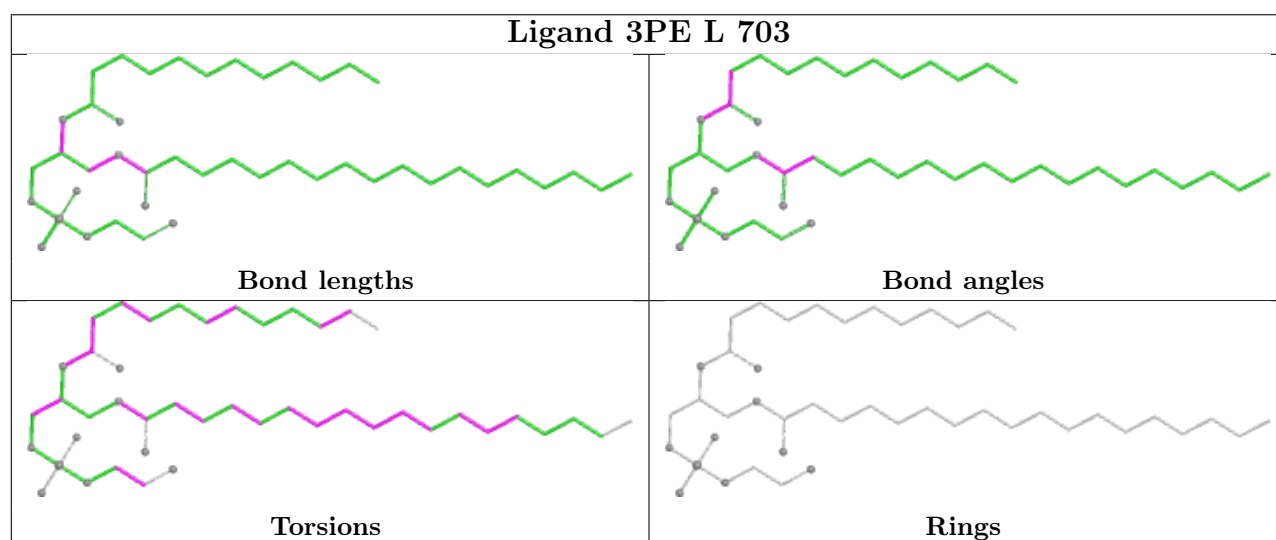
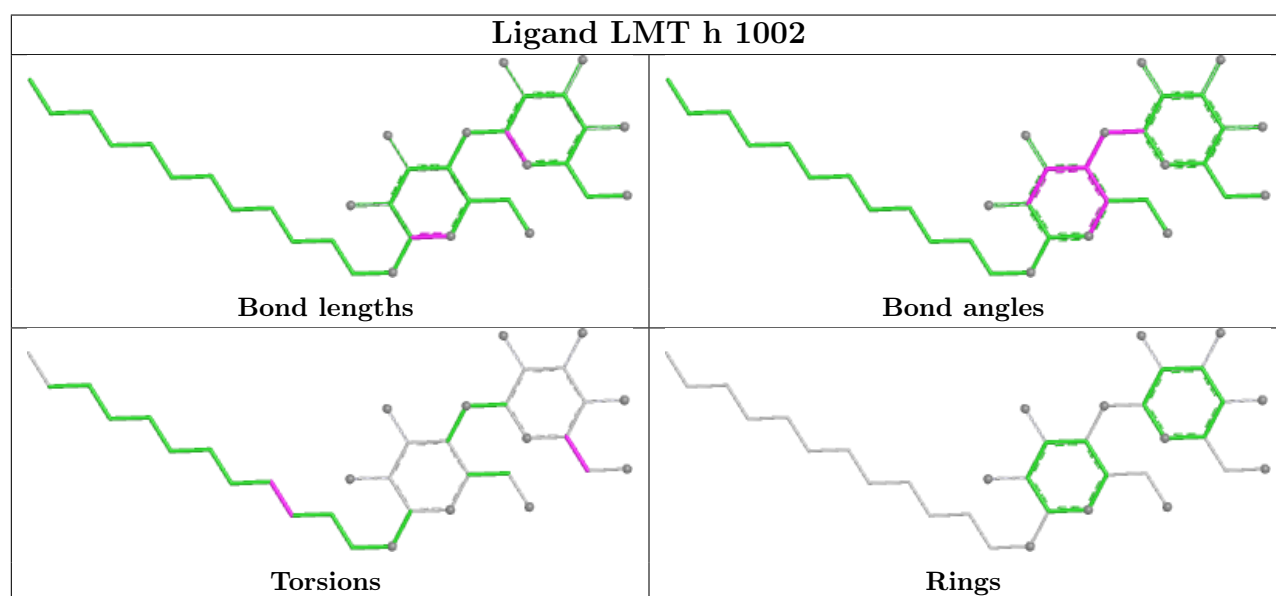
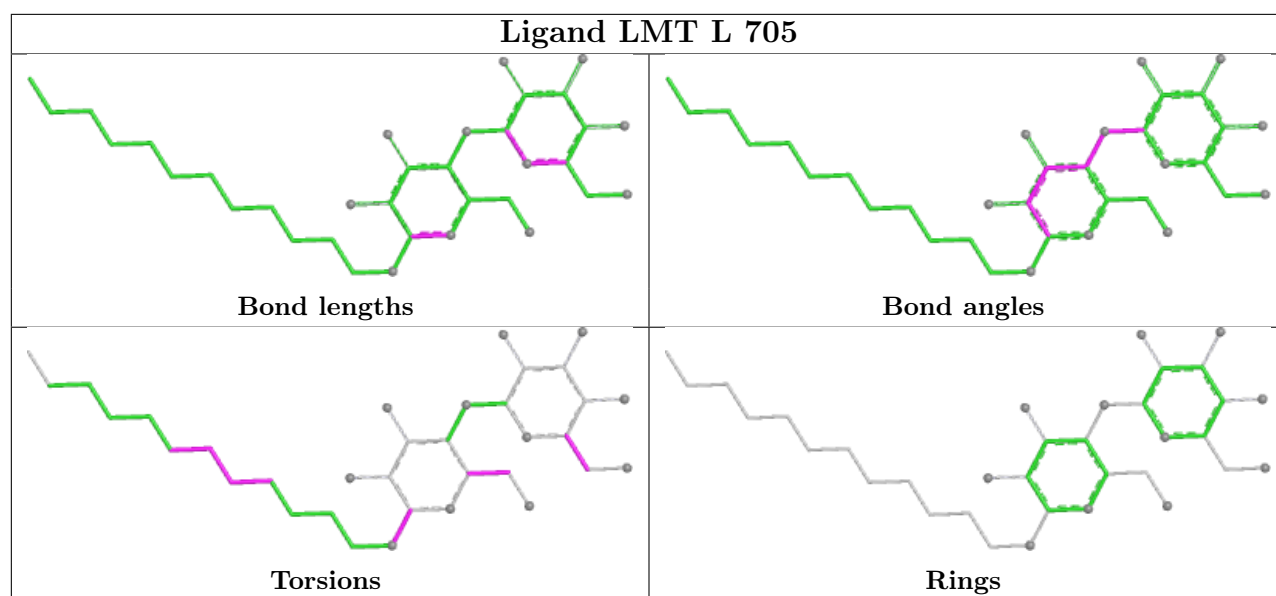


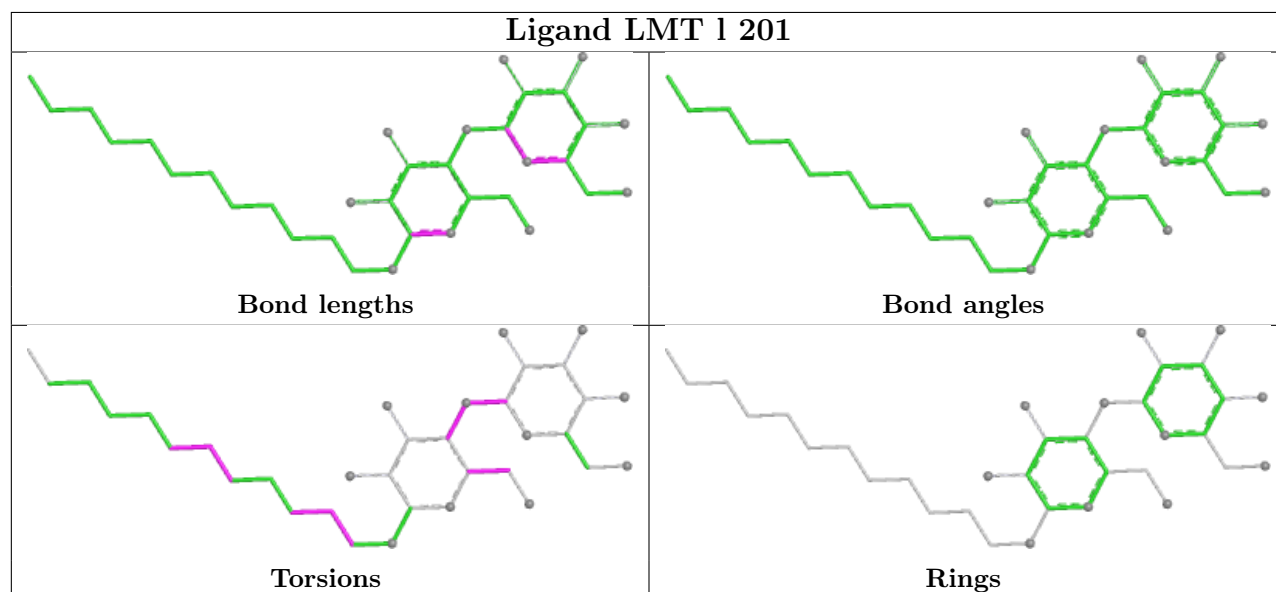
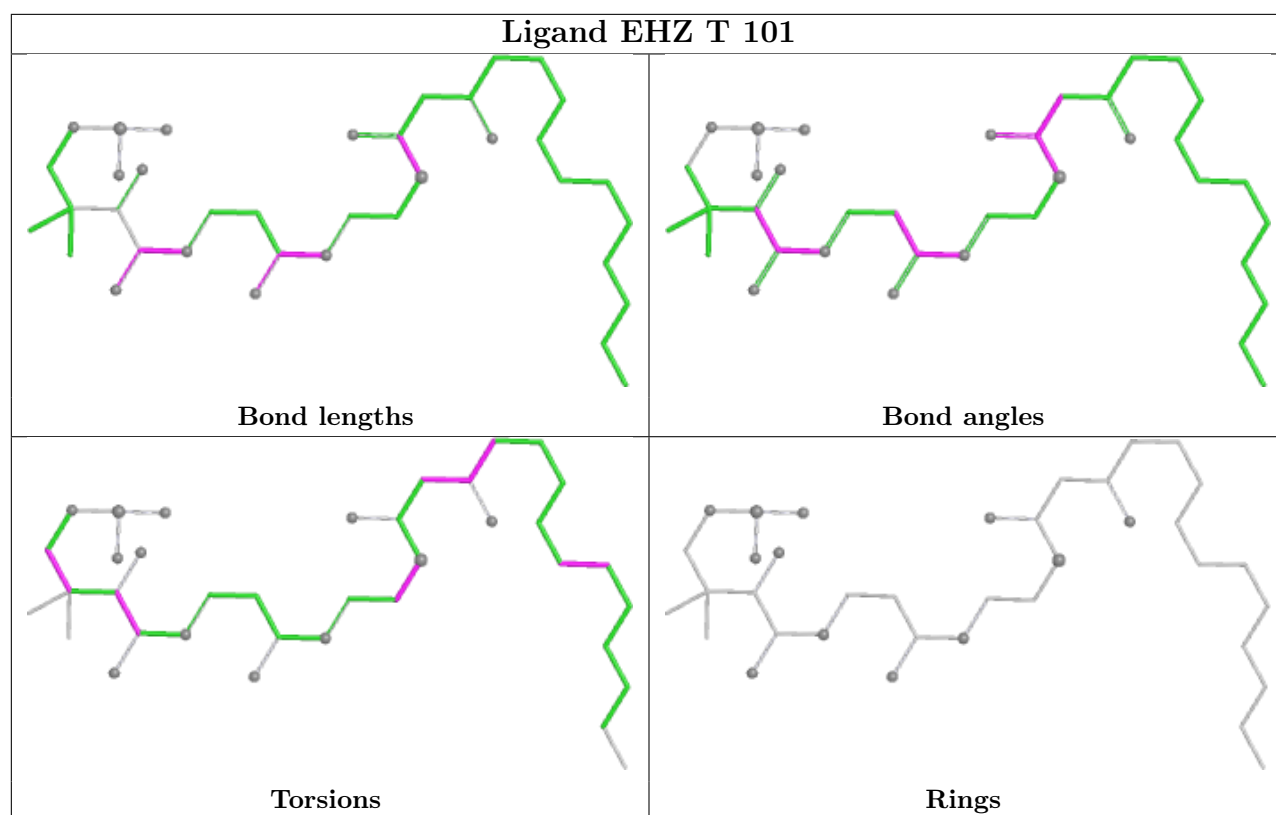


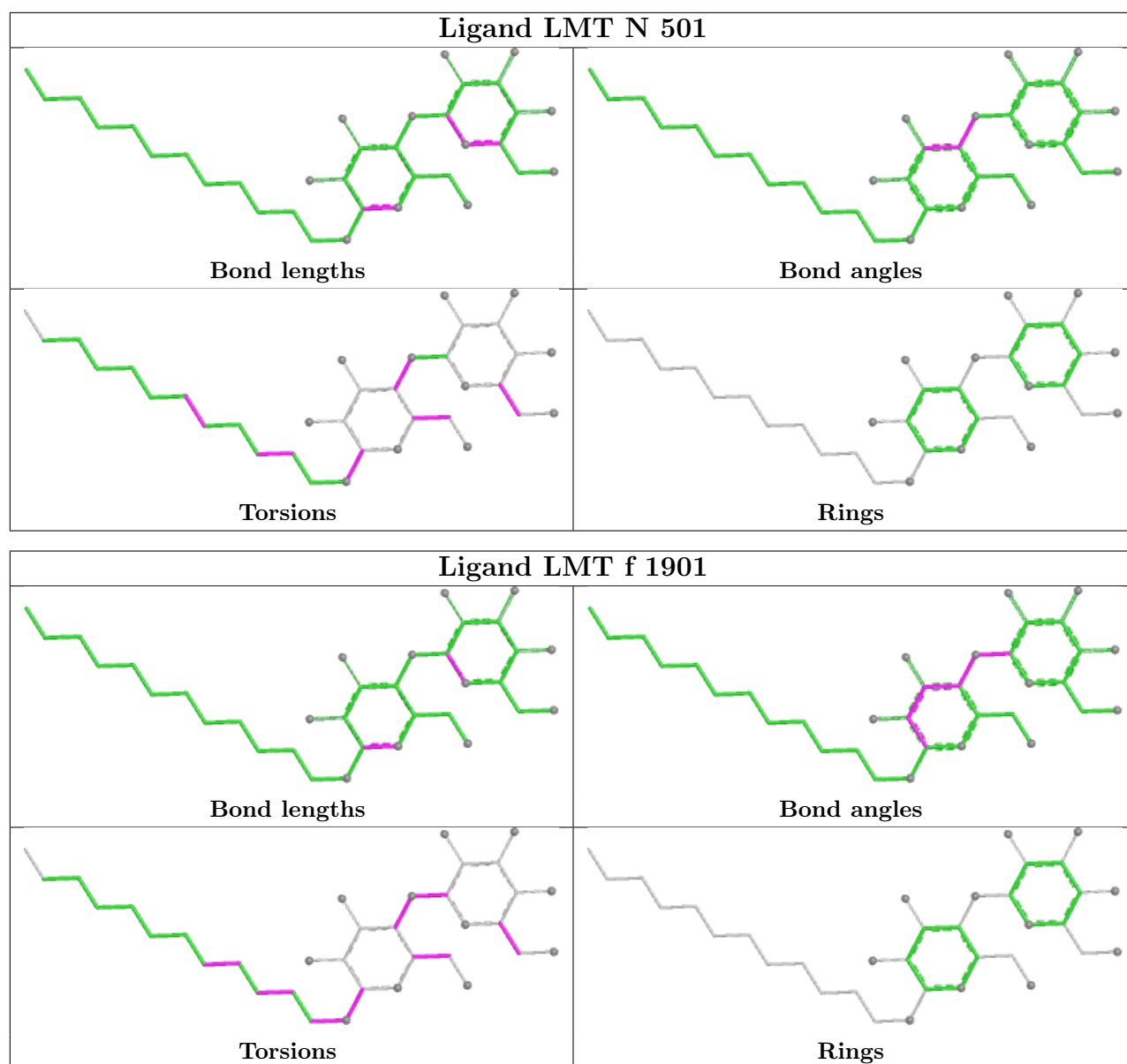












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

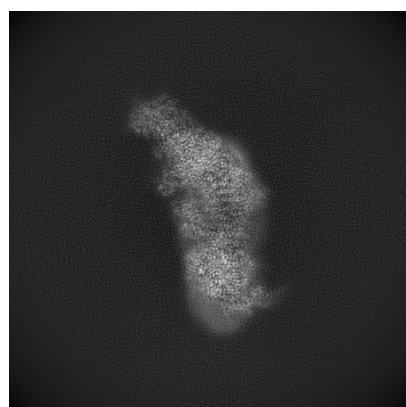
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14272. These allow visual inspection of the internal detail of the map and identification of artifacts.

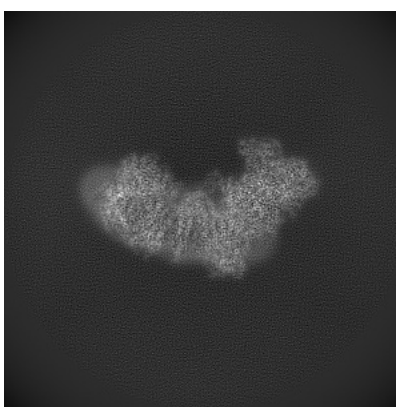
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

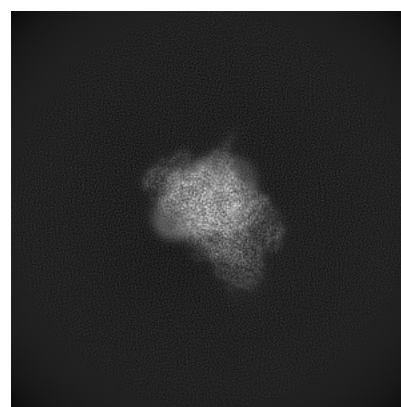
6.1.1 Primary map



X



Y

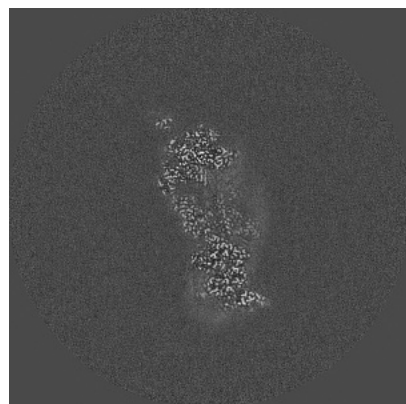


Z

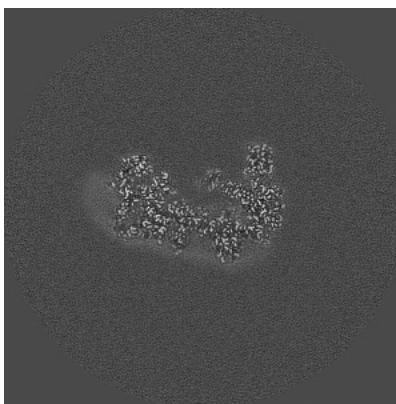
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

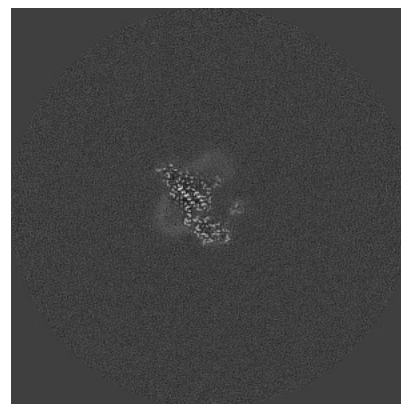
6.2.1 Primary map



X Index: 330



Y Index: 330

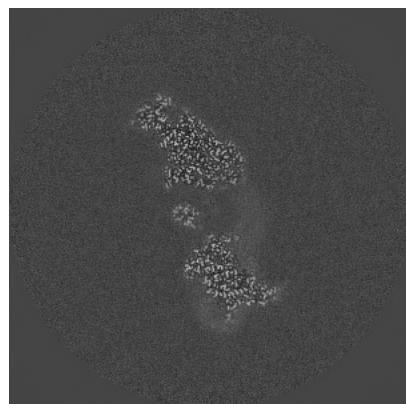


Z Index: 330

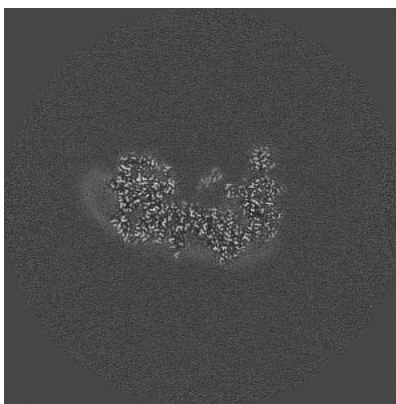
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

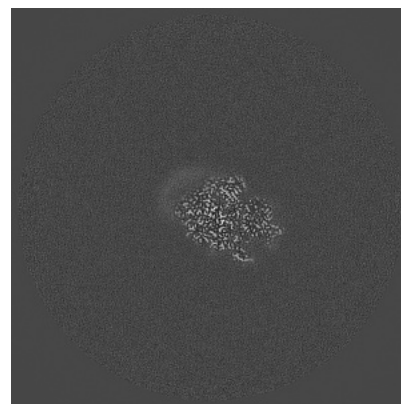
6.3.1 Primary map



X Index: 356



Y Index: 338

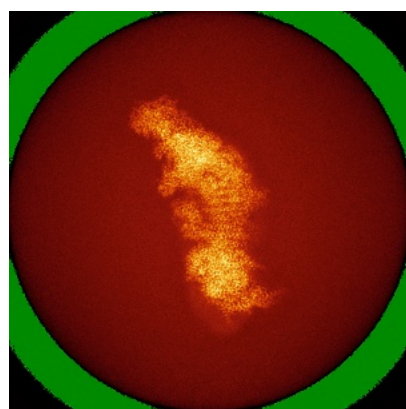


Z Index: 422

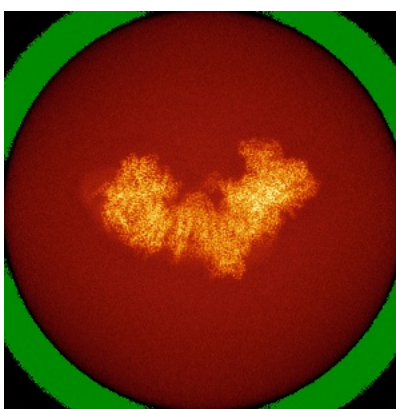
The images above show the largest variance slices of the map in three orthogonal directions.

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

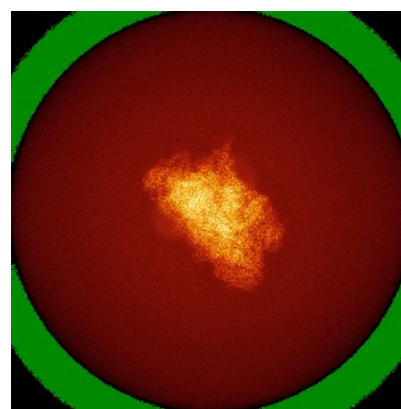
6.4.1 Primary map



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.

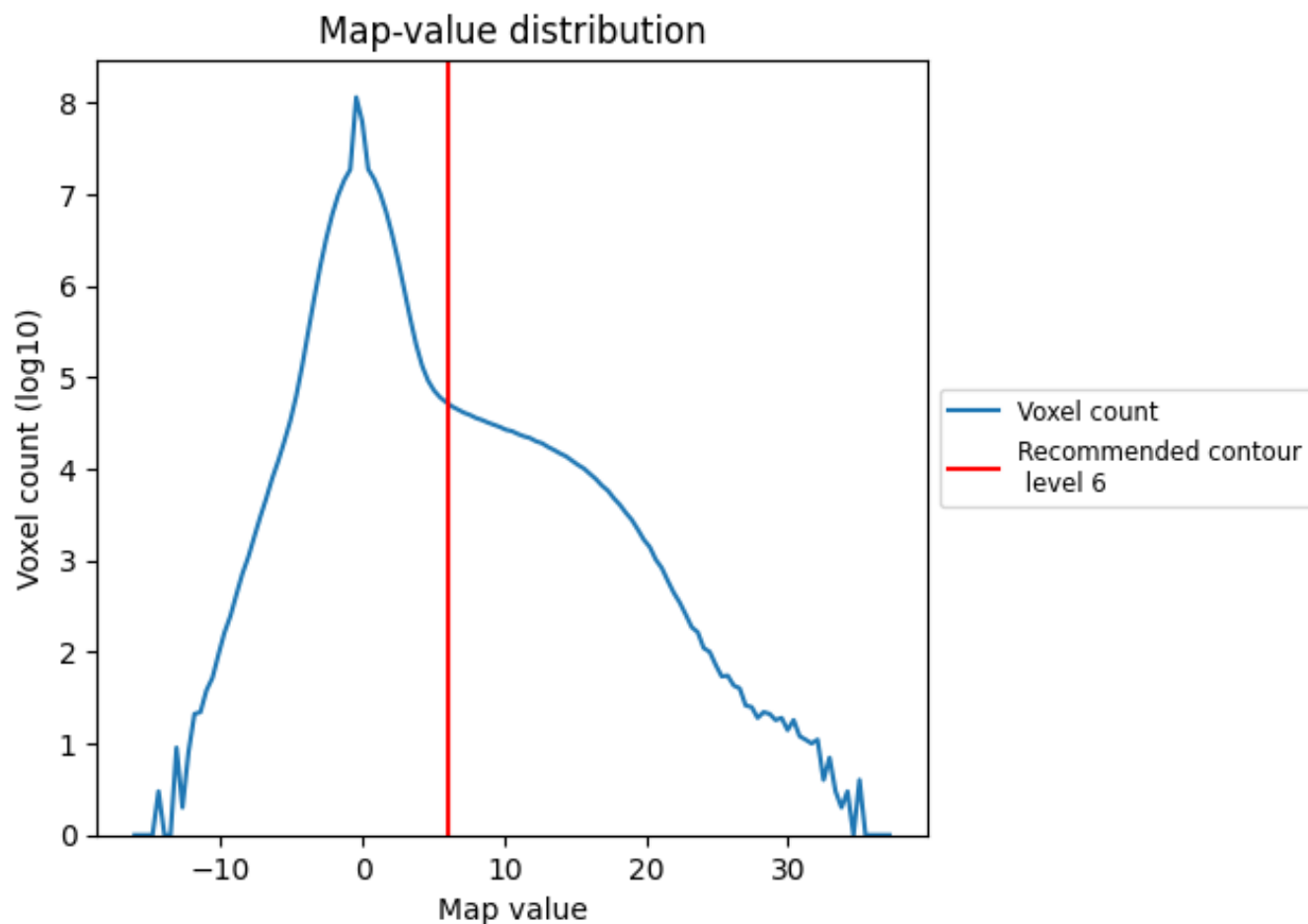
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

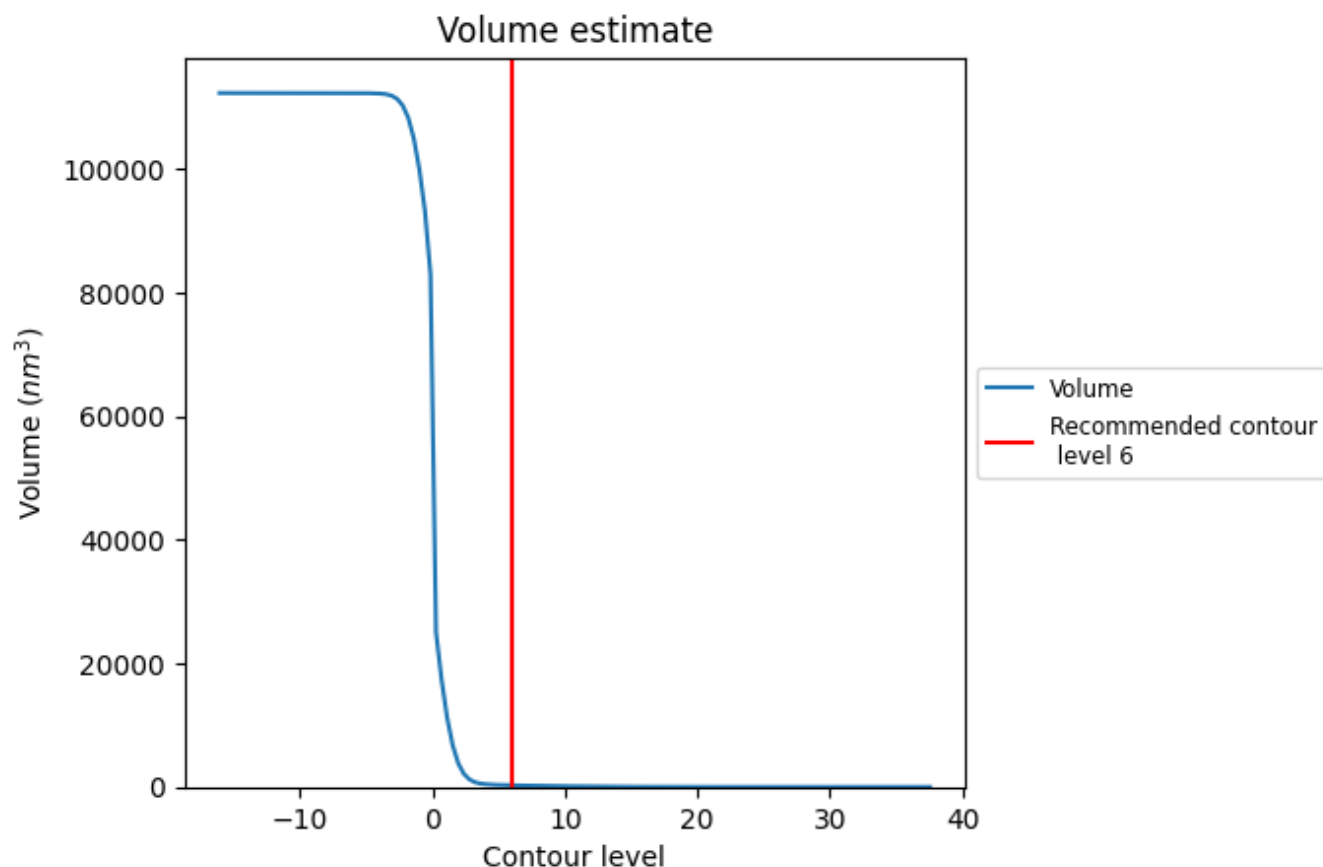
This section contains the results of statistical analysis of the map.

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.

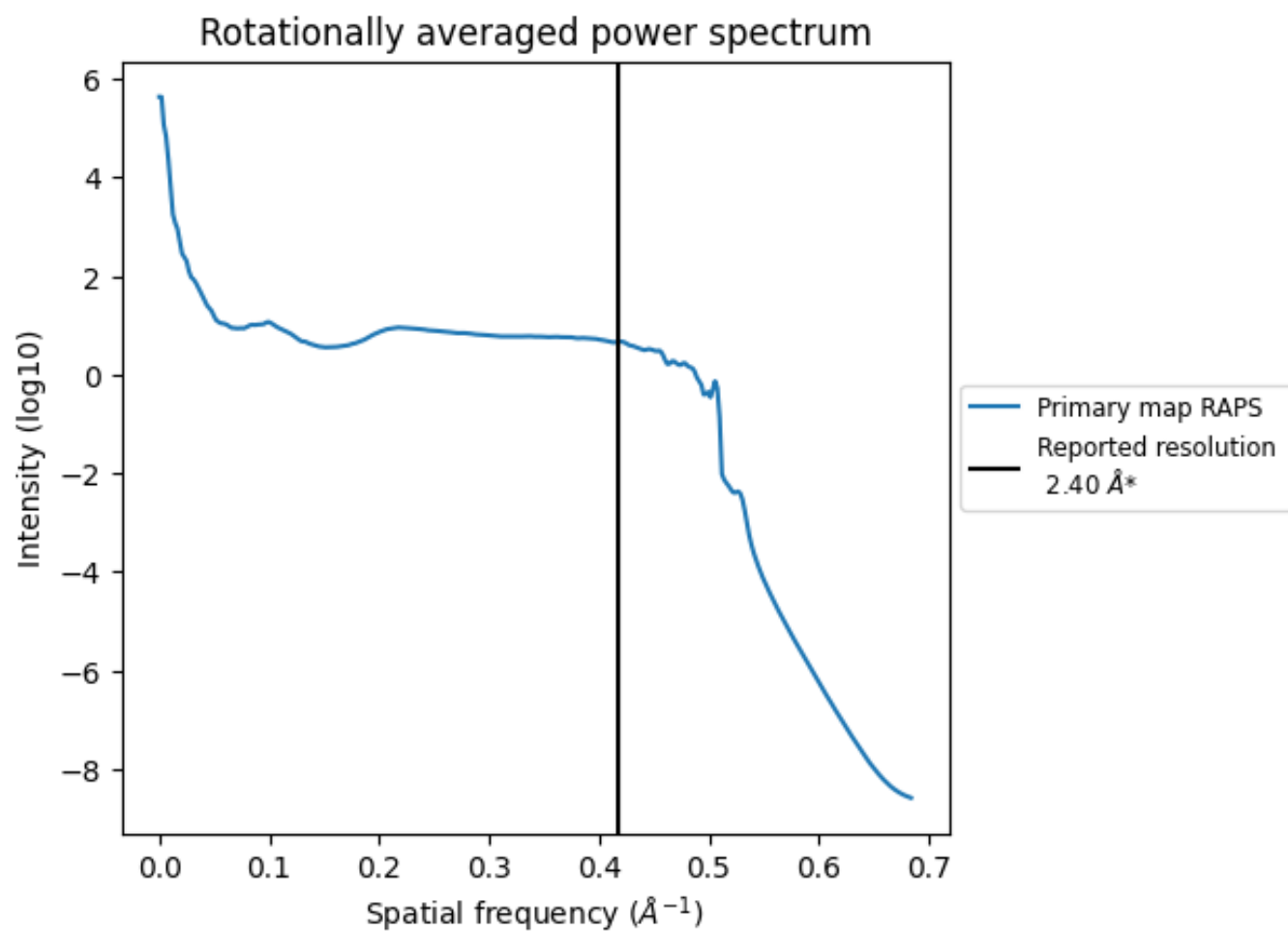
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 265 nm^3 ; this corresponds to an approximate mass of 240 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

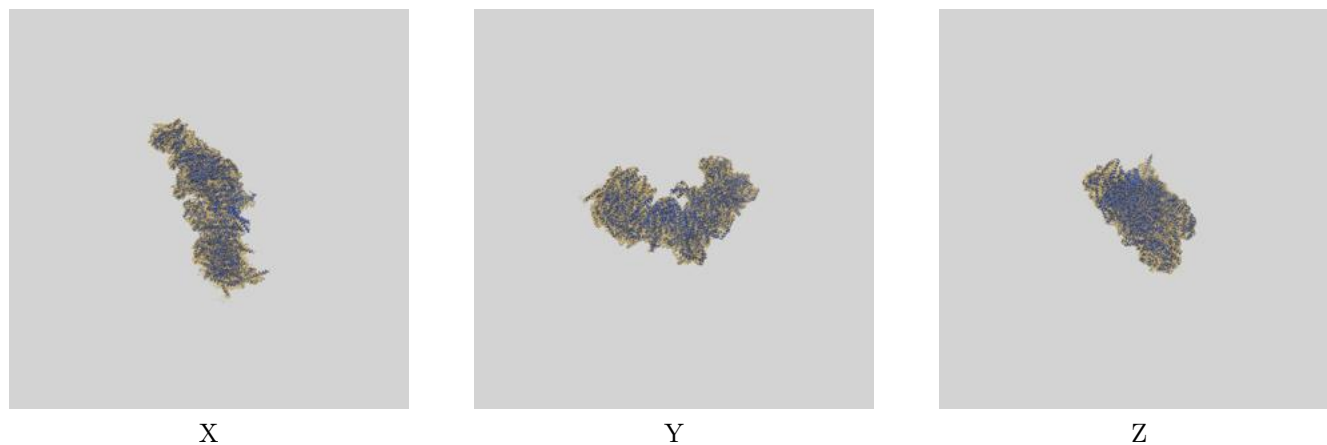
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

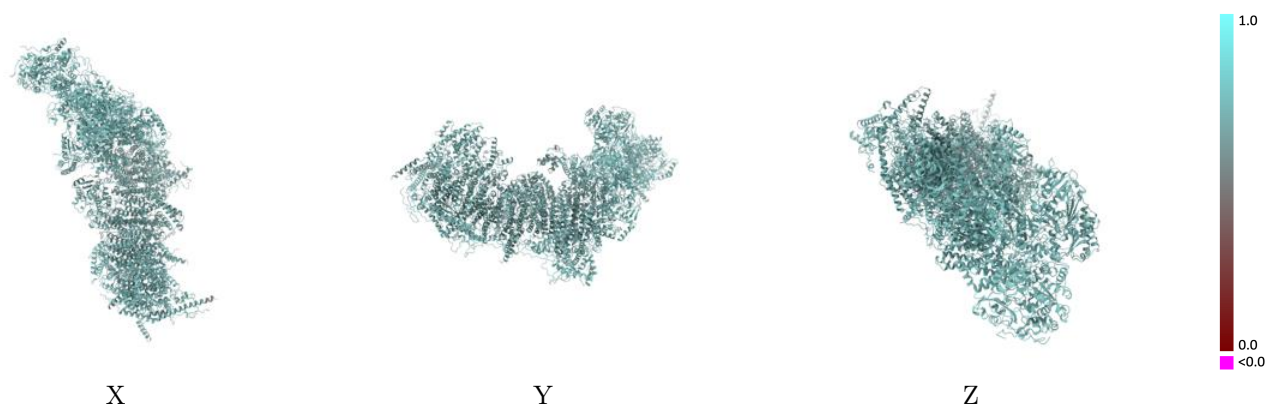
This section contains information regarding the fit between EMDB map EMD-14272 and PDB model 7R45. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



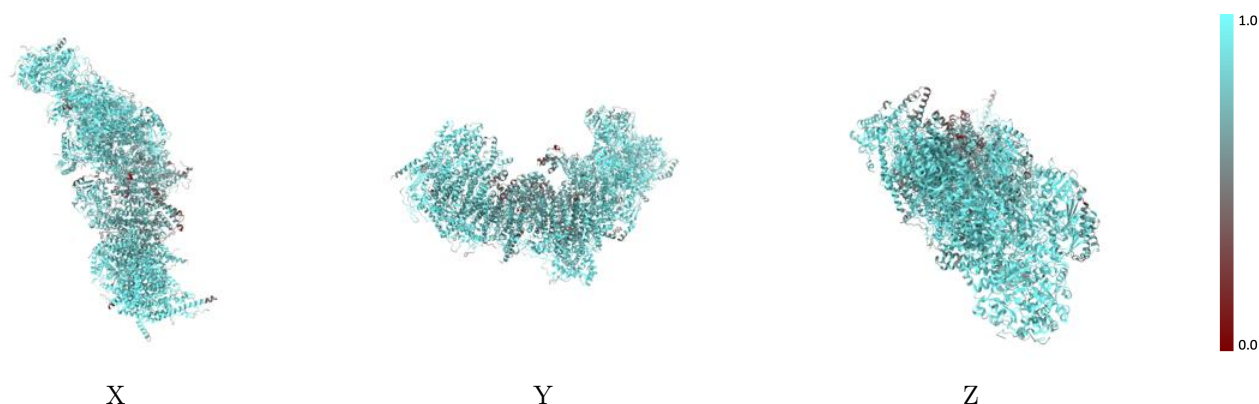
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



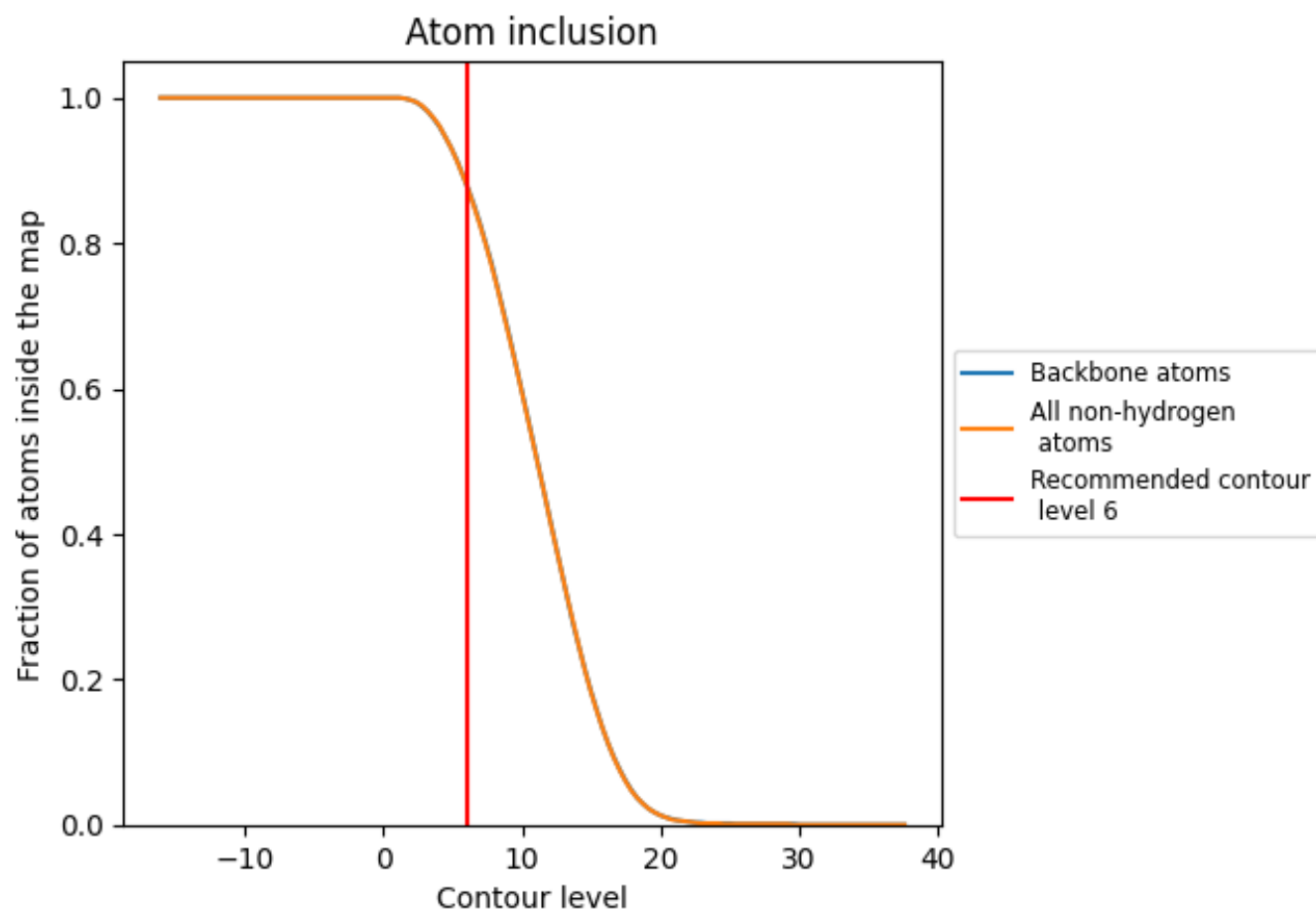
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 88% of all backbone atoms, 88% 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	 0.8800	 0.6960
A	 0.8240	 0.6800
B	 0.9260	 0.7230
C	 0.9600	 0.7340
D	 0.9260	 0.7280
E	 0.8750	 0.6910
F	 0.9220	 0.7050
G	 0.9070	 0.7120
H	 0.9280	 0.7010
I	 0.9490	 0.7370
J	 0.7900	 0.6740
K	 0.8820	 0.7000
L	 0.9030	 0.6870
M	 0.9450	 0.7060
N	 0.9430	 0.7130
O	 0.8370	 0.6710
P	 0.8470	 0.6950
Q	 0.9080	 0.7220
R	 0.8850	 0.7140
S	 0.8060	 0.6820
T	 0.5900	 0.6270
U	 0.9340	 0.6830
V	 0.8530	 0.7010
W	 0.8630	 0.7010
X	 0.8490	 0.6770
Y	 0.5420	 0.6420
Z	 0.8340	 0.6820
a	 0.9450	 0.6990
b	 0.8110	 0.6690
c	 0.7370	 0.6620
d	 0.8570	 0.6910
e	 0.8270	 0.6820
f	 0.7490	 0.6580
g	 0.8740	 0.6860
h	 0.9000	 0.6930



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Chain	Atom inclusion	Q-score
i	 0.8740	 0.6660
j	 0.8880	 0.6580
k	 0.8680	 0.6460
l	 0.9000	 0.6810
m	 0.8300	 0.6750
n	 0.9200	 0.6900
o	 0.8780	 0.6590
p	 0.9110	 0.6880
q	 0.8450	 0.7080
r	 0.8790	 0.7150
s	 0.8560	 0.6870