



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:01 PM UTC

PDB ID : 7R48 / pdb_00007r48
EMDB ID : EMD-14287
Title : Bovine complex I in the presence of IM1761092, deactive class iv (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.30 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:

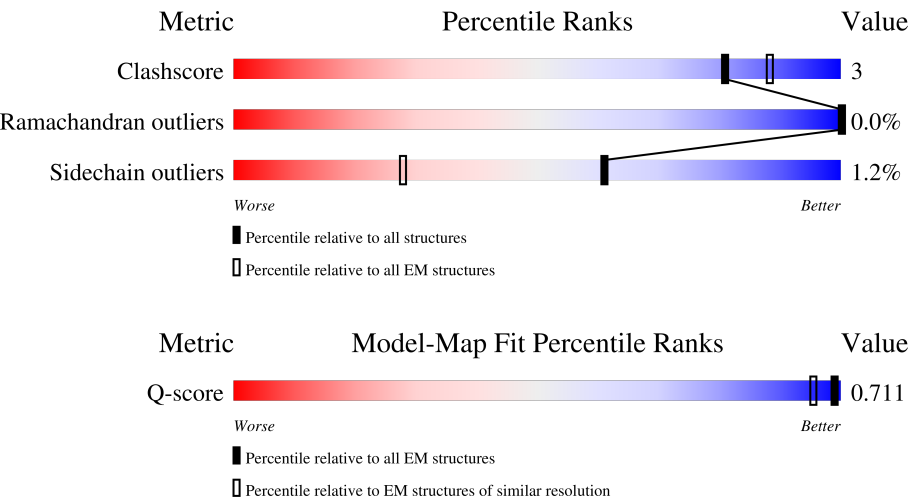
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.30 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.



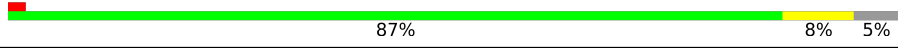
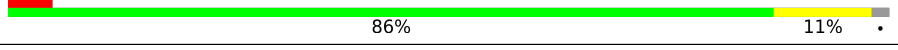
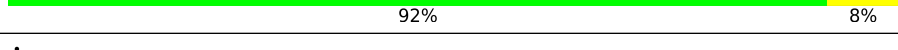
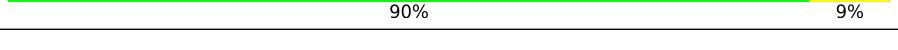
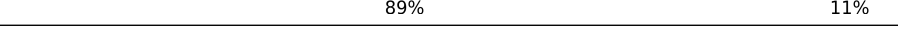
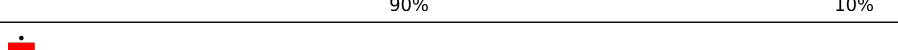
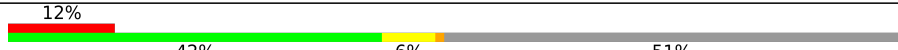
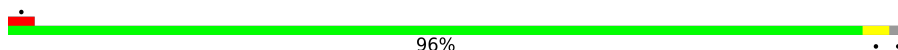
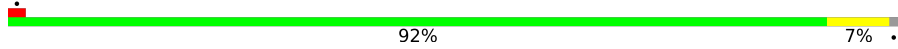
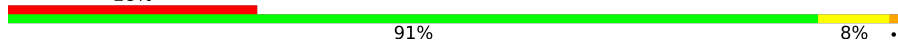
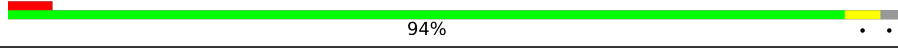
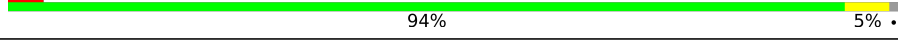
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	10% 72% 17% • 10%
2	B	216	• 68% • 28%

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	136	
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 69247 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	104	Total	C	N	O	S	0	0
			836	568	122	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	795	225	213	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	419	Total	C	N	O	S	0	0
			3373	2156	579	613	25		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	311	Total	C	N	O	S	0	0
			2457	1648	377	409	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	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- 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	295	Total	C	N	O	S	0	0
			2353	1507	424	417	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	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	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	104	Total	C	N	O	S	0	0
			892	588	151	152	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	S	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	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

- 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	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

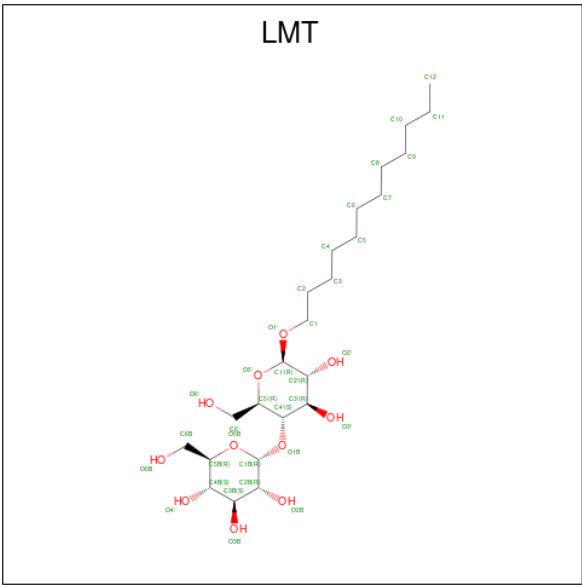
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

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



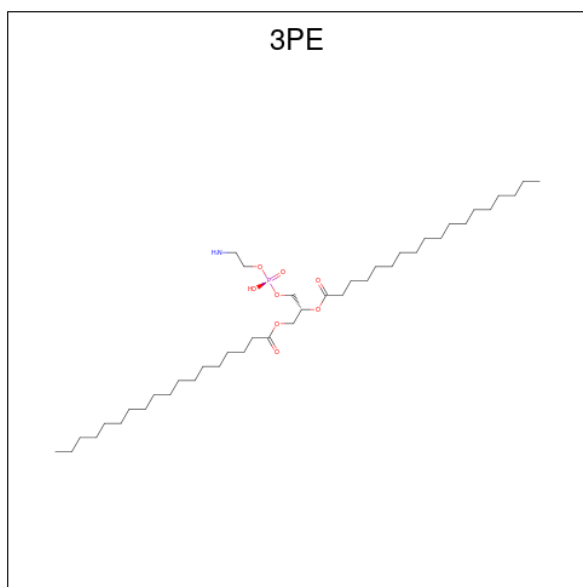
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	B	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
45	M	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	Y	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	k	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	

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



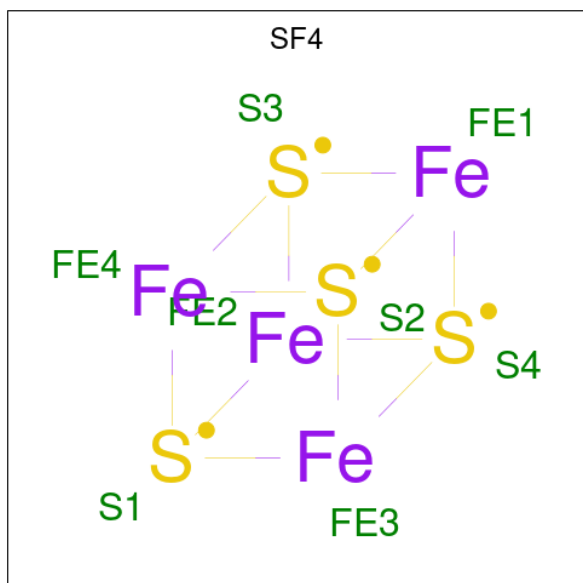
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	H	1	Total	C	N	O	P	0
			34	24	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	M	1	Total	C	N	O	P	0
			46	36	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	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	m	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



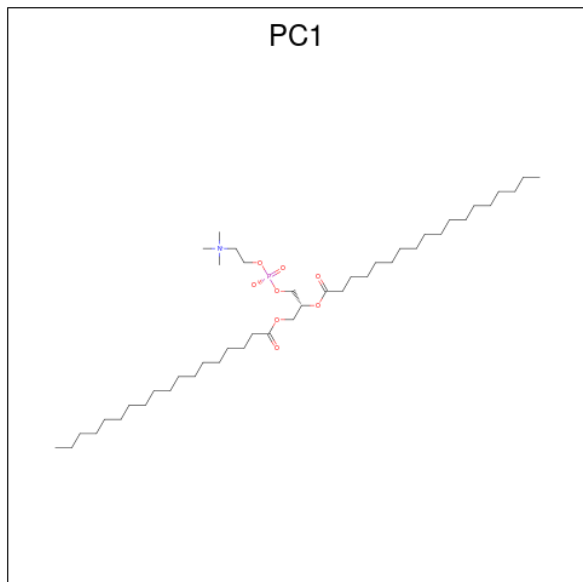
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

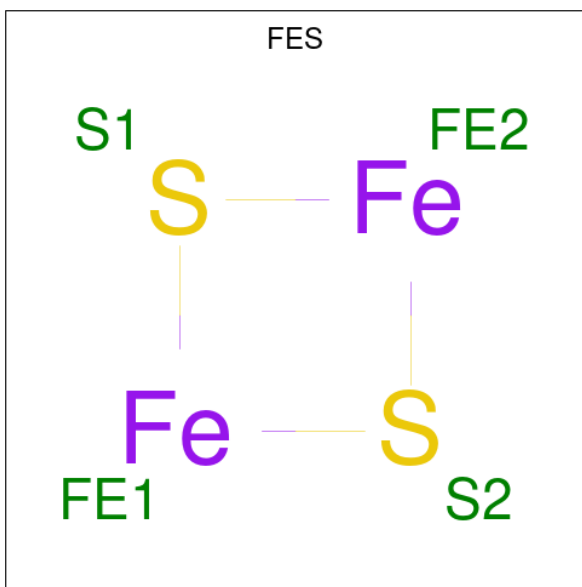
Mol	Chain	Residues	Atoms			AltConf
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



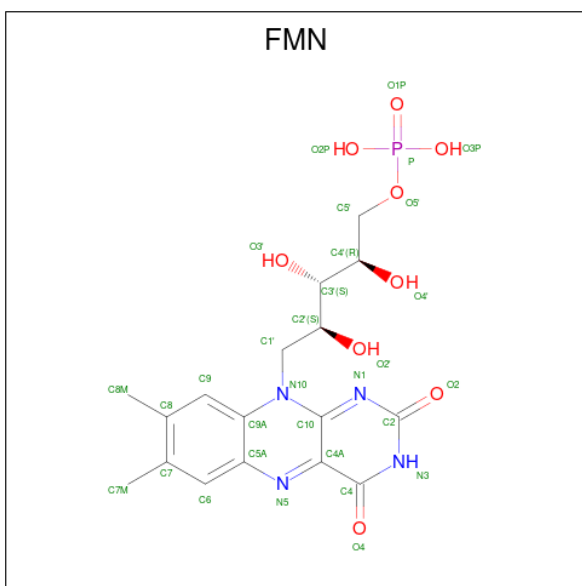
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	g	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



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

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

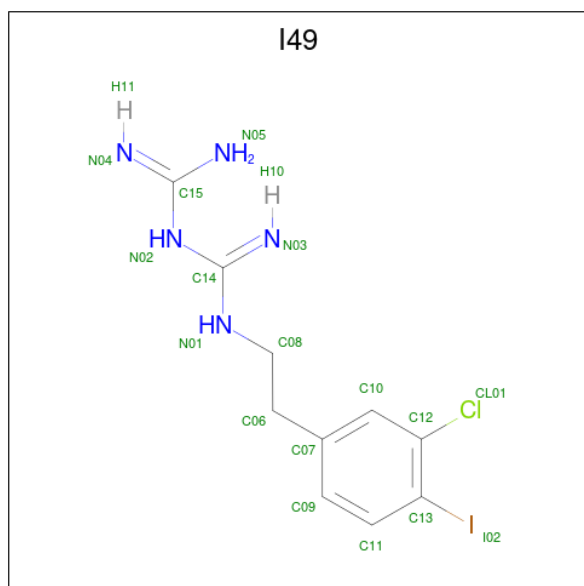


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total 31	C 17	N 4	O 9	P 1	0

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

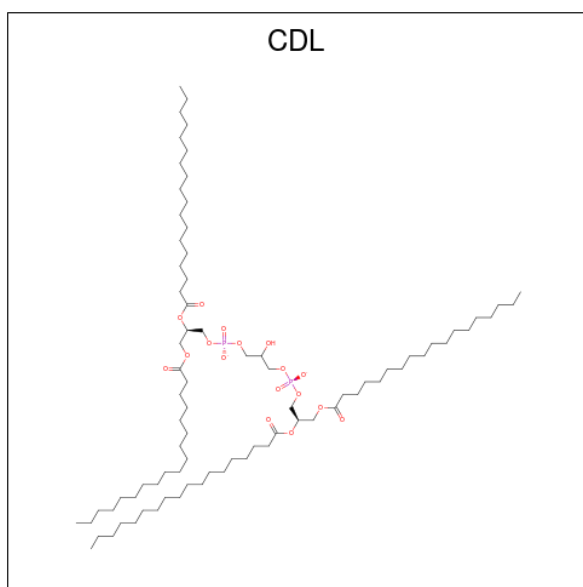
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- 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).



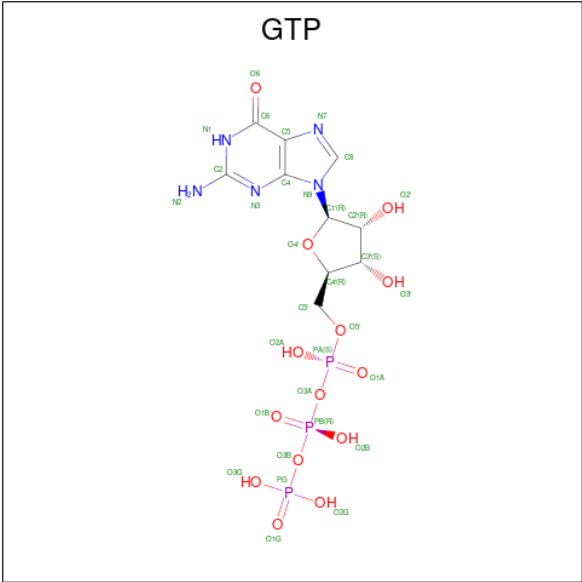
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	
52	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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



Mol	Chain	Residues	Atoms				AltConf
53	J	1	Total	C	O	P	0
			71	52	17	2	
53	L	1	Total	C	O	P	0
			69	50	17	2	
53	N	1	Total	C	O	P	0
			65	46	17	2	
53	d	1	Total	C	O	P	0
			73	54	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: $C_{10}H_{16}N_5O_{14}P_3$).

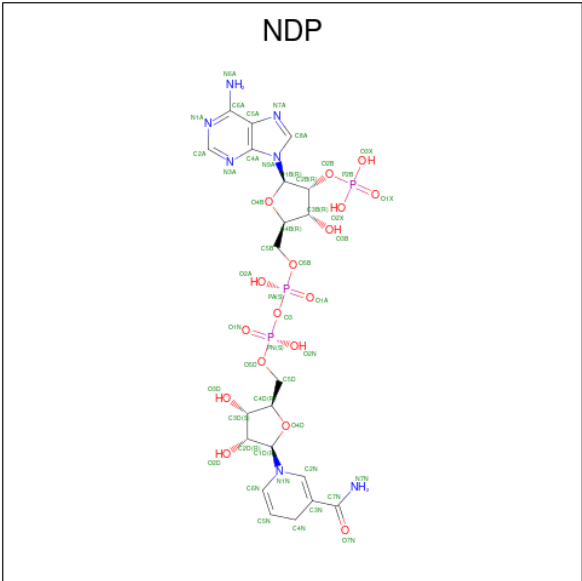


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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).

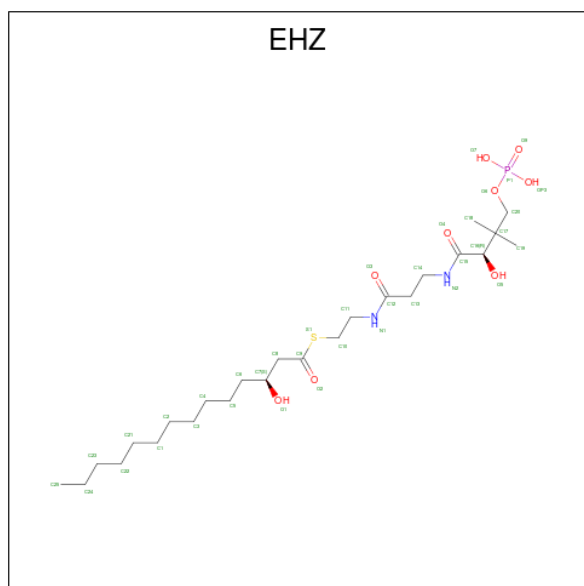


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

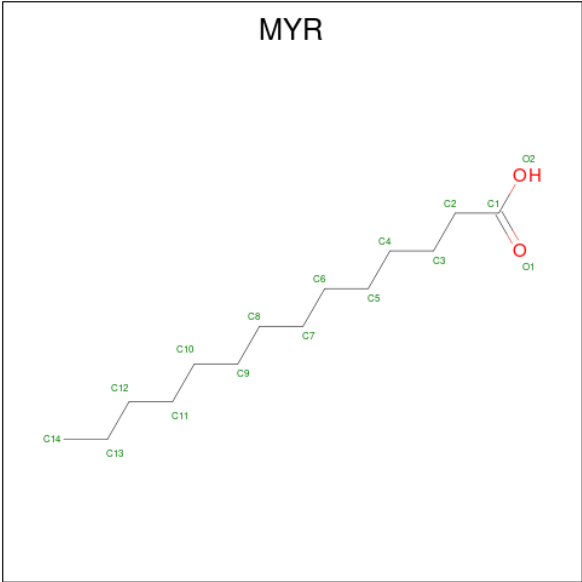
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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	15	Total	O	0
			15	15	
60	B	63	Total	O	0
			63	63	
60	C	113	Total	O	0
			113	113	
60	D	184	Total	O	0
			184	184	
60	E	38	Total	O	0
			38	38	
60	F	92	Total	O	0
			92	92	
60	G	248	Total	O	0
			248	248	
60	H	61	Total	O	0
			61	61	
60	I	111	Total	O	0
			111	111	
60	J	20	Total	O	0
			20	20	
60	K	14	Total	O	0
			14	14	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	L	100	Total 100	O 100	0
60	M	110	Total 110	O 110	0
60	N	61	Total 61	O 61	0
60	O	36	Total 36	O 36	0
60	P	67	Total 67	O 67	0
60	Q	98	Total 98	O 98	0
60	R	53	Total 53	O 53	0
60	S	3	Total 3	O 3	0
60	T	2	Total 2	O 2	0
60	U	22	Total 22	O 22	0
60	V	20	Total 20	O 20	0
60	W	26	Total 26	O 26	0
60	X	44	Total 44	O 44	0
60	Y	3	Total 3	O 3	0
60	Z	30	Total 30	O 30	0
60	a	22	Total 22	O 22	0
60	b	13	Total 13	O 13	0
60	d	16	Total 16	O 16	0
60	e	30	Total 30	O 30	0
60	f	10	Total 10	O 10	0
60	g	30	Total 30	O 30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	h	34	Total 34	O 34	0
60	i	19	Total 19	O 19	0
60	j	4	Total 4	O 4	0
60	k	17	Total 17	O 17	0
60	l	42	Total 42	O 42	0
60	m	26	Total 26	O 26	0
60	n	52	Total 52	O 52	0
60	o	35	Total 35	O 35	0
60	p	55	Total 55	O 55	0
60	q	41	Total 41	O 41	0
60	r	34	Total 34	O 34	0
60	s	10	Total 10	O 10	0

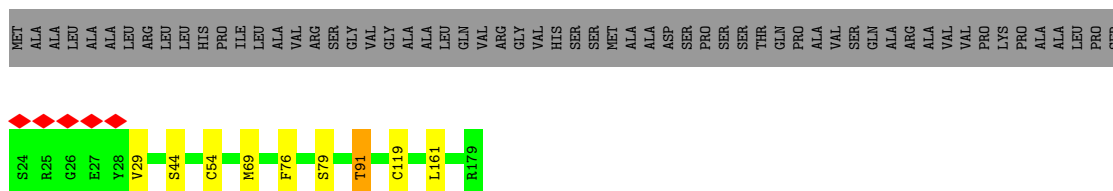
3 Residue-property plots [i](#)

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

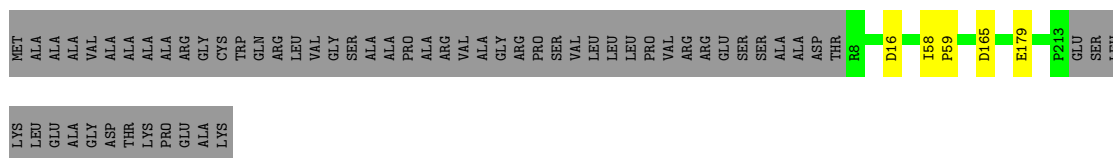
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



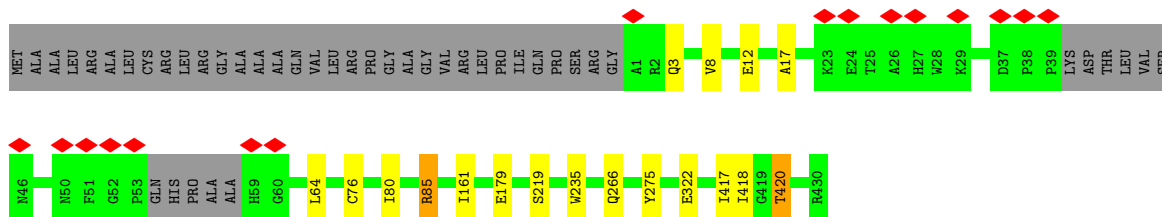
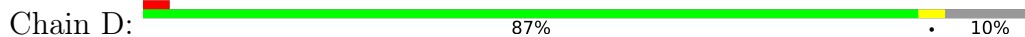
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

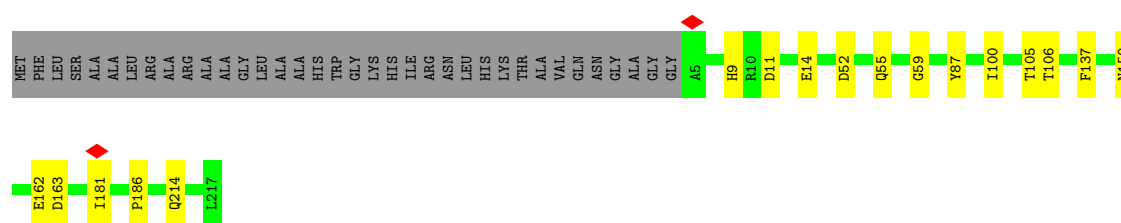


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



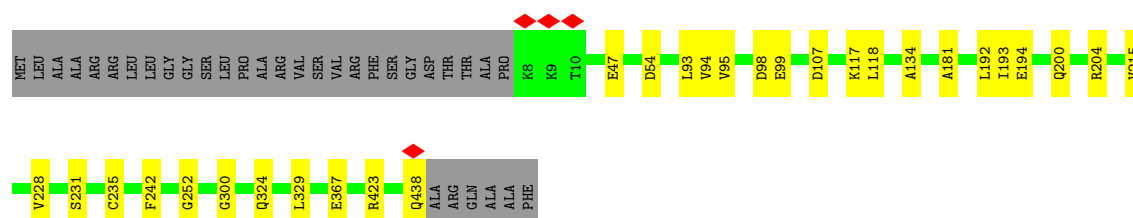
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  79% 7% 14%



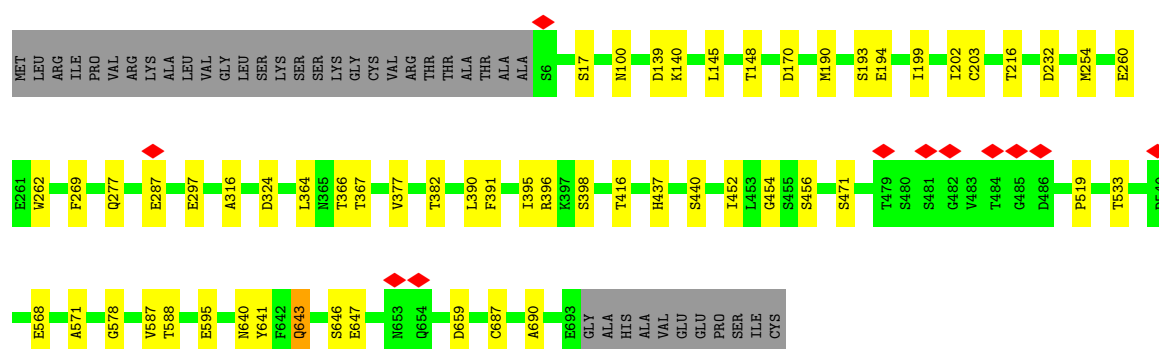
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  87% 6% 7%



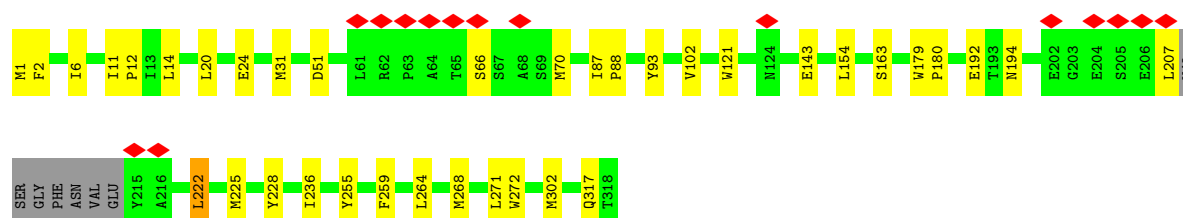
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  87% 8% 5%



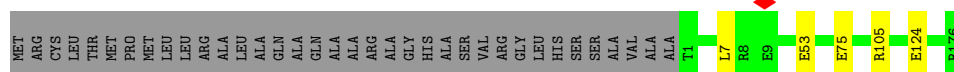
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  5% 86% 11%



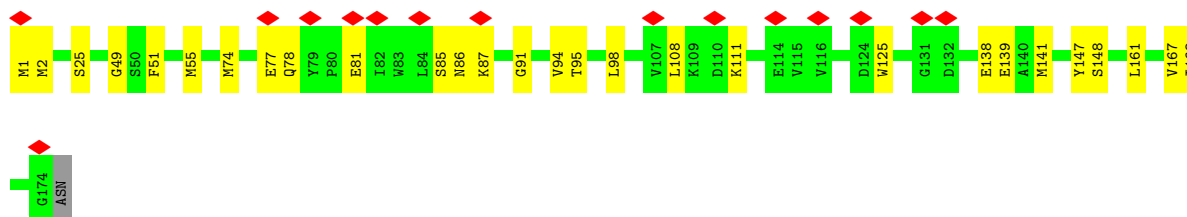
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  81% 17%

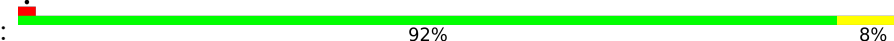


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  9% 83% 16%

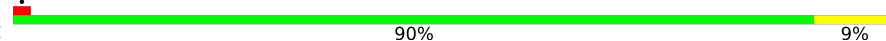


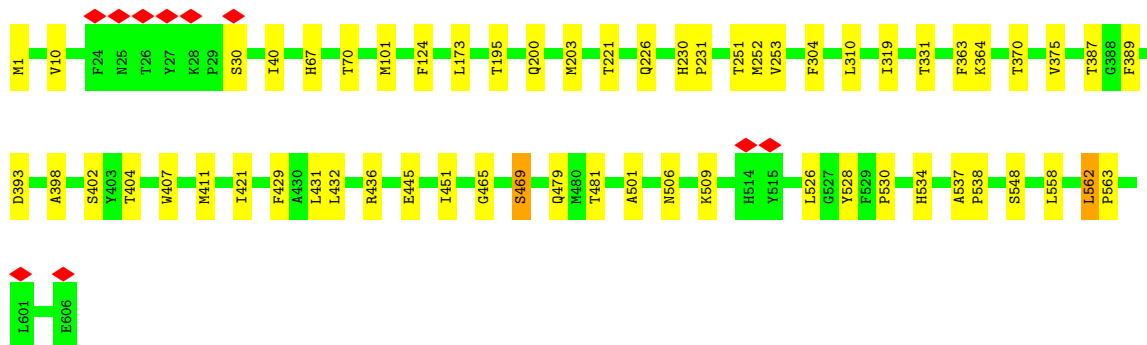
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  92% 8%

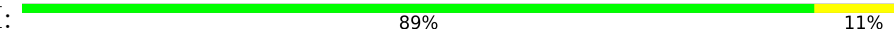


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  90% 9%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

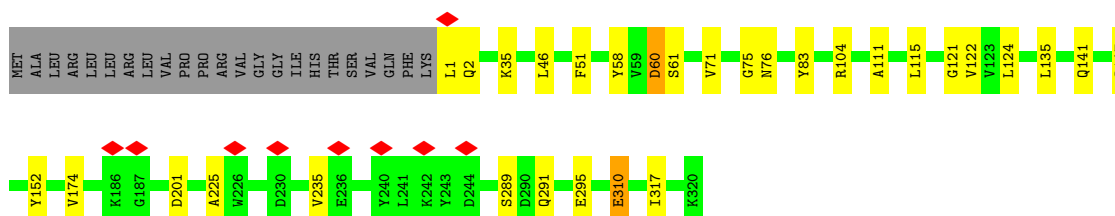
Chain M:  89% 11%



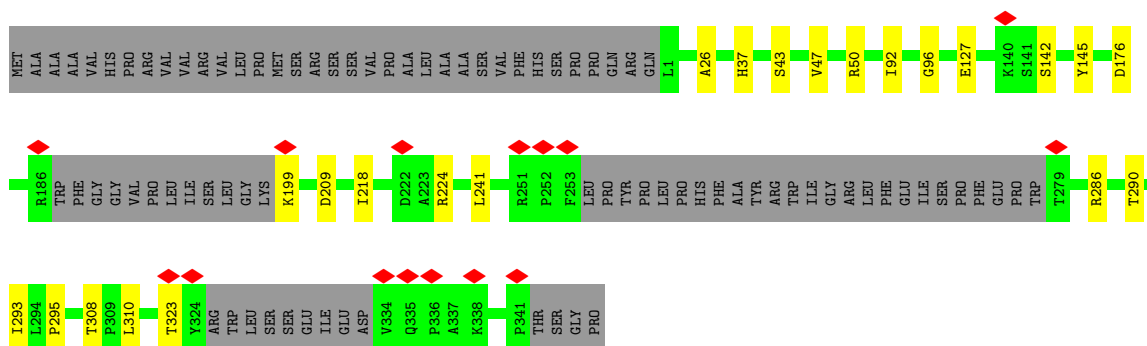
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

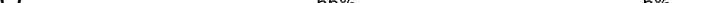
[illegible]

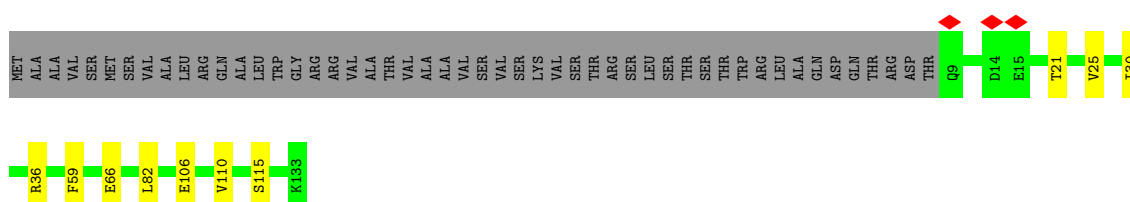
- Chain 0: 84% 8% 7%

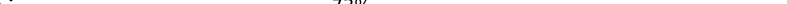


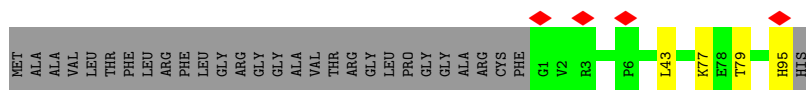
- Chain P:  72% 6% 22%



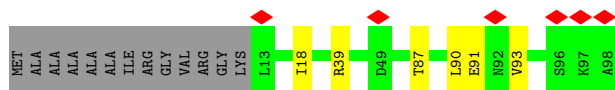
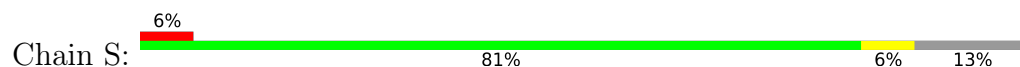
- Chain Q: 



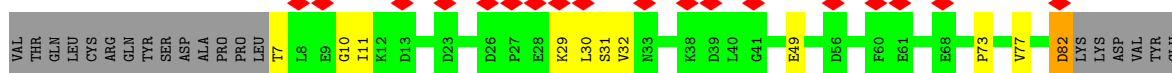
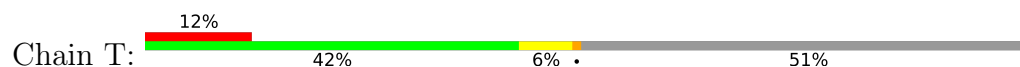
- Chain B:  73% 23%



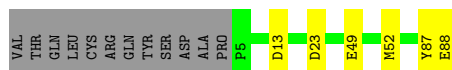
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



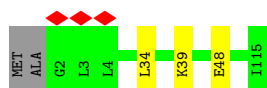
- Molecule 20: Acyl carrier protein, mitochondrial



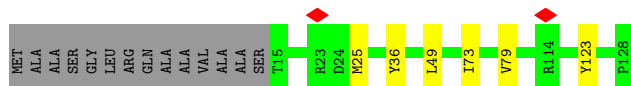
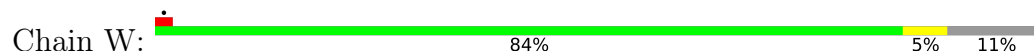
- Molecule 20: Acyl carrier protein, mitochondrial



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

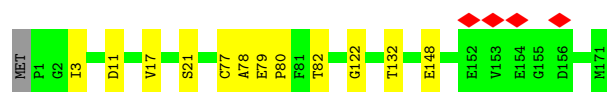


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

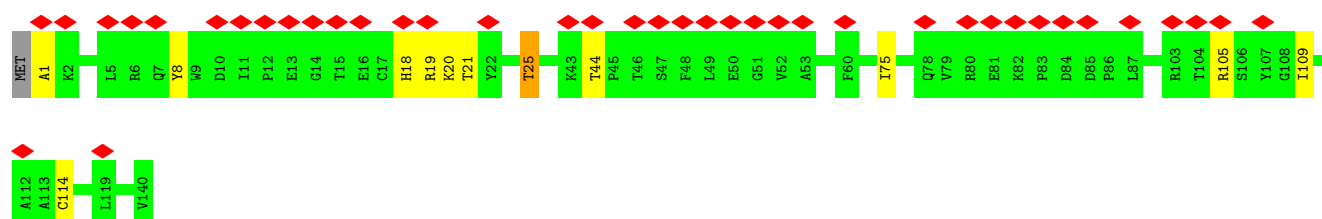
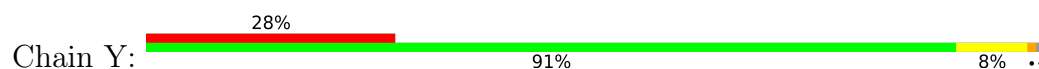


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

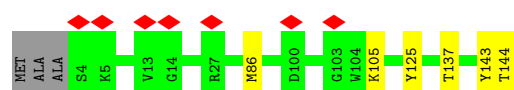




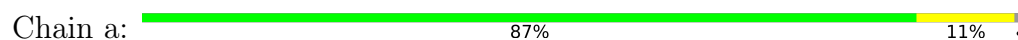
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



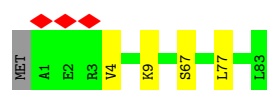
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



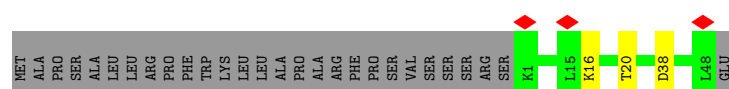
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



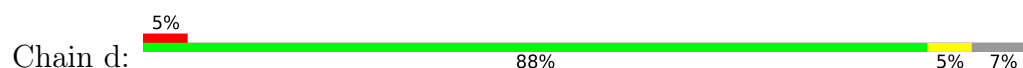
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

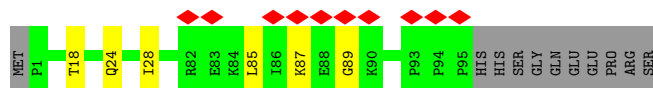
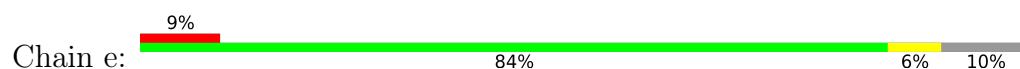


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

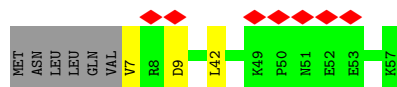
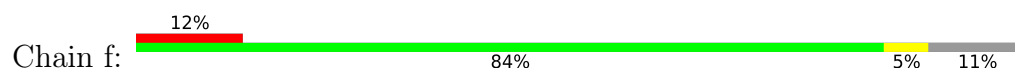




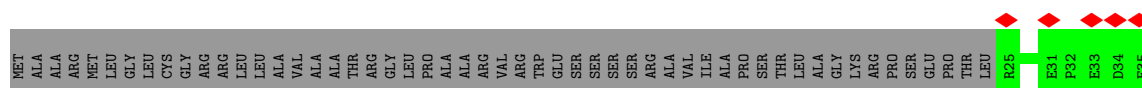
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



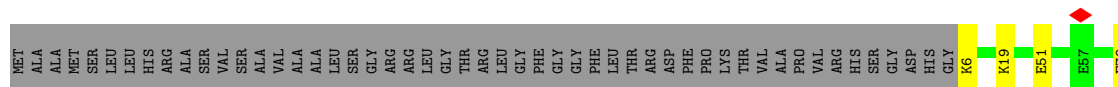
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



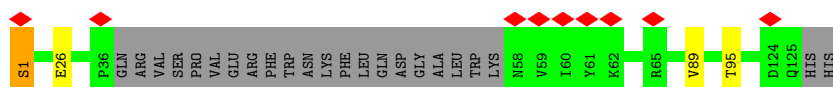
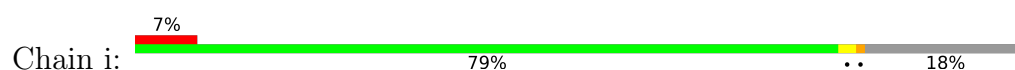
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

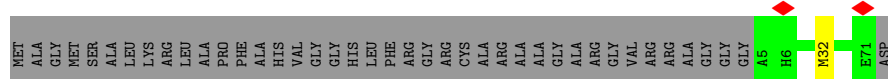


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



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

Chain j: 



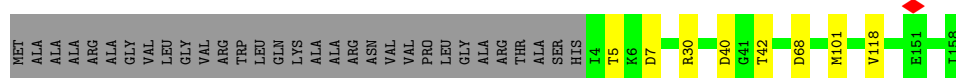
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

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: 



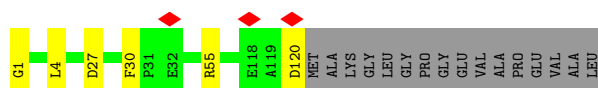
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 

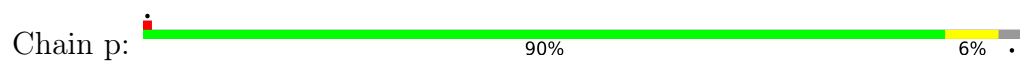


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 



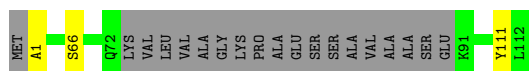
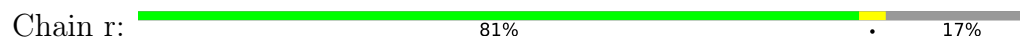
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



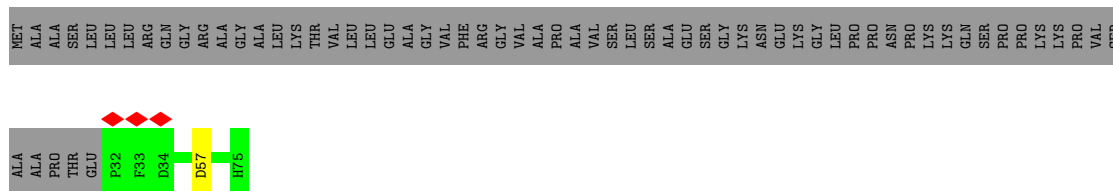
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	111066	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	44.750	Depositor
Minimum map value	-19.725	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.076	Depositor
Recommended contour level	6.5	Depositor
Map size ($\text{\AA}$)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: FMN, AYA, I49, MYR, FES, SAC, GTP, FME, NDP, K, 3PE, LMT, MG, PC1, 2MR, EHZ, ZN, SF4, CDL

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	0.24	0/846	0.30	0/1156
2	B	0.28	0/1278	0.36	0/1728
3	C	0.27	0/1765	0.34	0/2403
4	D	0.27	0/3446	0.34	0/4666
5	E	0.25	0/1695	0.30	0/2307
6	F	0.25	0/3393	0.30	0/4584
7	G	0.26	0/5367	0.33	0/7274
8	H	0.27	0/2517	0.35	0/3438
9	I	0.28	0/1445	0.36	0/1956
10	J	0.23	0/1362	0.30	0/1848
11	K	0.23	0/745	0.27	0/1008
12	L	0.28	0/4903	0.30	0/6672
13	M	0.28	0/3738	0.31	0/5097
14	N	0.26	0/2792	0.32	0/3800
15	O	0.25	0/2651	0.29	0/3587
16	P	0.24	0/2406	0.32	0/3252
17	Q	0.26	0/1039	0.32	0/1404
18	R	0.27	0/742	0.32	0/999
19	S	0.23	0/702	0.32	0/945
20	T	0.19	0/621	0.31	0/837
20	U	0.30	0/692	0.29	0/932
21	V	0.23	0/943	0.28	0/1277
22	W	0.24	0/995	0.29	0/1337
23	X	0.25	0/1439	0.31	0/1942
24	Y	0.17	0/1042	0.27	0/1414
25	Z	0.24	0/1181	0.29	0/1592
26	a	0.27	0/576	0.31	0/775
27	b	0.23	0/672	0.30	0/923
28	c	0.22	0/418	0.26	0/567
29	d	0.25	0/964	0.30	0/1305
30	e	0.23	0/818	0.33	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.24	0/457	0.34	0/616
32	g	0.26	0/850	0.29	0/1154
33	h	0.27	0/1188	0.30	0/1607
34	i	0.29	0/912	0.33	0/1241
35	j	0.28	0/607	0.27	0/833
36	k	0.27	0/657	0.28	0/887
37	l	0.30	0/1358	0.31	0/1858
38	m	0.30	0/1076	0.32	0/1455
39	n	0.29	0/1540	0.31	0/2085
40	o	0.31	0/1060	0.33	0/1420
41	p	0.29	0/1468	0.31	0/1979
42	q	0.23	0/1250	0.32	0/1698
43	r	0.24	0/780	0.33	0/1056
44	s	0.23	0/383	0.27	0/518
All	All	0.26	0/66779	0.31	0/90525

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	2
34	i	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	275	TYR	Peptide
4	D	85	2MR	Mainchain
34	i	1	SAC	Mainchain

5.2 Too-close contacts [i](#)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	836	0	880	16	0
2	B	1247	0	1256	3	0
3	C	1714	0	1668	4	0
4	D	3373	0	3316	10	0
5	E	1655	0	1661	10	0
6	F	3319	0	3274	18	0
7	G	5279	0	5301	37	0
8	H	2457	0	2573	26	0
9	I	1414	0	1370	4	0
10	J	1337	0	1346	23	0
11	K	745	0	785	7	0
12	L	4786	0	4933	37	0
13	M	3654	0	3852	34	0
14	N	2733	0	2912	24	0
15	O	2589	0	2566	17	0
16	P	2353	0	2384	12	0
17	Q	1016	0	1014	5	0
18	R	730	0	707	2	0
19	S	691	0	706	4	0
20	T	612	0	604	7	0
20	U	681	0	677	6	0
21	V	923	0	964	2	0
22	W	971	0	989	4	0
23	X	1402	0	1383	6	0
24	Y	1030	0	1041	4	0
25	Z	1152	0	1151	6	0
26	a	561	0	564	9	0
27	b	651	0	662	1	0
28	c	405	0	409	2	0
29	d	934	0	919	7	0
30	e	799	0	807	4	0
31	f	444	0	444	2	0
32	g	824	0	772	4	0
33	h	1154	0	1168	6	0
34	i	892	0	911	3	0
35	j	580	0	519	1	0
36	k	638	0	621	5	0
37	l	1304	0	1203	6	0
38	m	1050	0	1051	8	0
39	n	1487	0	1433	8	0
40	o	1035	0	1002	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	p	1435	0	1411	8	0
42	q	1209	0	1182	4	0
43	r	767	0	776	1	0
44	s	371	0	344	0	0
45	A	70	0	92	1	0
45	B	35	0	46	0	0
45	J	35	0	46	1	0
45	L	35	0	46	0	0
45	M	105	0	138	3	0
45	N	35	0	46	0	0
45	Y	35	0	46	0	0
45	f	35	0	46	0	0
45	h	35	0	46	0	0
45	k	35	0	46	1	0
45	l	35	0	46	0	0
45	m	35	0	46	0	0
46	A	48	0	73	0	0
46	H	78	0	112	0	0
46	I	51	0	82	0	0
46	L	123	0	174	1	0
46	M	97	0	151	2	0
46	N	41	0	56	0	0
46	Y	35	0	44	0	0
46	d	47	0	71	1	0
46	m	41	0	59	4	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	g	49	0	75	2	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	1	0
52	N	17	0	0	3	0
53	J	71	0	86	0	0
53	L	69	0	82	0	0
53	N	65	0	77	0	0
53	d	73	0	90	1	0
53	h	67	0	81	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	q	76	0	96	0	0
54	O	32	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	3	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	1	0
60	A	15	0	0	0	0
60	B	63	0	0	0	0
60	C	113	0	0	0	0
60	D	184	0	0	2	0
60	E	38	0	0	1	0
60	F	92	0	0	3	0
60	G	248	0	0	10	0
60	H	61	0	0	0	0
60	I	111	0	0	1	0
60	J	20	0	0	0	0
60	K	14	0	0	0	0
60	L	100	0	0	2	0
60	M	110	0	0	4	0
60	N	61	0	0	1	0
60	O	36	0	0	1	0
60	P	67	0	0	0	0
60	Q	98	0	0	0	0
60	R	53	0	0	1	0
60	S	3	0	0	0	0
60	T	2	0	0	0	0
60	U	22	0	0	1	0
60	V	20	0	0	0	0
60	W	26	0	0	0	0
60	X	44	0	0	0	0
60	Y	3	0	0	0	0
60	Z	30	0	0	0	0
60	a	22	0	0	1	0
60	b	13	0	0	0	0
60	d	16	0	0	0	0
60	e	30	0	0	1	0
60	f	10	0	0	0	0
60	g	30	0	0	3	0
60	h	34	0	0	0	0
60	i	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	j	4	0	0	0	0
60	k	17	0	0	1	0
60	l	42	0	0	0	0
60	m	26	0	0	1	0
60	n	52	0	0	1	0
60	o	35	0	0	1	0
60	p	55	0	0	1	0
60	q	41	0	0	0	0
60	r	34	0	0	0	0
60	s	10	0	0	0	0
All	All	69247	0	67738	353	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 (353) 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)
11:K:43:MET:HE1	14:N:72:MET:HE1	1.54	0.89
10:J:25:SER:OG	10:J:77:GLU:OE1	1.92	0.85
37:l:30:ARG:NH2	38:m:34:GLU:OE1	2.10	0.85
37:l:40:ASP:OD2	37:l:42:THR:OG1	1.96	0.83
20:T:29:LYS:O	20:T:29:LYS:NZ	2.11	0.82
37:l:5:THR:OG1	37:l:7:ASP:OD1	1.98	0.82
7:G:277:GLN:NE2	60:G:908:HOH:O	2.14	0.81
16:P:127:GLU:O	16:P:224:ARG:NH1	2.17	0.78
8:H:317:GLN:HE22	10:J:141:MET:HE1	1.49	0.77
12:L:479:GLN:NE2	12:L:481:THR:O	2.18	0.77
18:R:43:LEU:O	60:R:301:HOH:O	2.04	0.76
42:q:78:ASP:OD1	42:q:80:SER:OG	2.03	0.76
8:H:20:LEU:HD13	26:a:12:MET:HE1	1.68	0.76
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.69	0.75
9:I:124:GLU:OE2	60:I:301:HOH:O	2.04	0.75
5:E:52:ASP:OD1	60:E:401:HOH:O	2.04	0.75
17:Q:36:ARG:NH2	17:Q:106:GLU:OE2	2.20	0.74
7:G:170:ASP:OD2	60:G:901:HOH:O	2.06	0.74
32:g:101:GLU:OE2	60:g:1601:HOH:O	2.05	0.74
7:G:139:ASP:O	18:R:77:LYS:NZ	2.20	0.74
7:G:139:ASP:OD1	60:G:903:HOH:O	2.06	0.73
7:G:260:GLU:OE2	60:G:902:HOH:O	2.06	0.73
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:GLU:OE2	60:D:501:HOH:O	2.05	0.73
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.24	0.73
1:A:18:VAL:HG22	8:H:222:LEU:HD23	1.72	0.72
39:n:161:ASP:O	60:n:201:HOH:O	2.07	0.72
12:L:432:LEU:O	60:L:802:HOH:O	2.08	0.72
10:J:141:MET:HA	10:J:141:MET:HE2	1.72	0.71
7:G:232:ASP:O	60:G:904:HOH:O	2.07	0.71
7:G:232:ASP:OD1	60:G:905:HOH:O	2.08	0.71
46:L:704:3PE:N	48:g:1501:PC1:O14	2.18	0.71
32:g:77:VAL:O	60:g:1602:HOH:O	2.08	0.71
41:p:129:GLU:OE1	41:p:133:GLN:NE2	2.24	0.71
29:d:120:ARG:O	38:m:108:ARG:NH2	2.23	0.70
20:T:82:ASP:N	20:T:82:ASP:OD1	2.21	0.69
41:p:127:GLU:N	41:p:127:GLU:OE2	2.25	0.69
15:O:83:TYR:OH	54:O:401:GTP:O3'	2.06	0.69
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.75	0.69
13:M:382:VAL:HG22	13:M:396:MET:HE2	1.73	0.69
24:Y:21:THR:O	24:Y:25:THR:OG1	2.11	0.69
7:G:595:GLU:OE2	60:G:906:HOH:O	2.10	0.68
38:m:44:ARG:NH2	60:m:302:HOH:O	2.23	0.68
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.74	0.68
12:L:562:LEU:HD13	45:M:602:LMT:H121	1.76	0.67
15:O:104:ARG:NH2	60:O:502:HOH:O	2.27	0.67
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.76	0.66
4:D:266:GLN:OE1	60:D:502:HOH:O	2.12	0.66
31:f:7:VAL:HG12	31:f:9:ASP:H	1.60	0.66
10:J:1:FME:SD	10:J:2:MET:N	2.69	0.65
21:V:39:LYS:HE2	21:V:39:LYS:H	1.61	0.65
23:X:78:ALA:O	23:X:82:THR:OG1	2.11	0.65
2:B:69:MET:HE2	2:B:76:PHE:HA	1.79	0.64
5:E:214:GLN:NE2	6:F:235:CYS:O	2.32	0.63
12:L:558:LEU:HD21	46:m:202:3PE:H2G2	1.80	0.63
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.14	0.63
10:J:81:GLU:OE2	10:J:85:SER:OG	2.16	0.63
15:O:60:ASP:OD1	15:O:60:ASP:N	2.31	0.63
1:A:30:TYR:OH	56:P:501:NDP:O3X	2.15	0.63
14:N:337:LEU:HD23	53:d:1202:CDL:H601	1.79	0.62
15:O:35:LYS:N	54:O:401:GTP:O1G	2.32	0.62
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.29	0.62
23:X:3:ILE:HD11	25:Z:105:LYS:NZ	2.13	0.62
8:H:317:GLN:NE2	10:J:141:MET:HE1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.31	0.62
48:g:1501:PC1:O13	48:g:1501:PC1:H132	1.99	0.62
7:G:140:LYS:O	7:G:148:THR:OG1	2.18	0.62
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.35	0.61
20:U:23:ASP:OD2	36:k:41:ARG:NH2	2.31	0.61
12:L:562:LEU:HD13	45:M:602:LMT:C12	2.29	0.61
11:K:43:MET:CE	14:N:72:MET:HE1	2.28	0.61
15:O:291:GLN:NE2	15:O:295:GLU:OE1	2.34	0.61
20:T:30:LEU:HD12	20:T:31:SER:N	2.16	0.61
14:N:162:ILE:HD13	14:N:282:MET:HG2	1.84	0.59
20:U:49:GLU:OE1	39:n:44:ARG:NH1	2.36	0.59
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.35	0.59
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.37	0.59
6:F:99:GLU:OE1	6:F:107:ASP:N	2.36	0.58
14:N:344:SER:HB2	52:N:504:I49:I02	2.73	0.58
26:a:37:ARG:HG2	26:a:48:MET:HE2	1.85	0.58
12:L:375:VAL:HG22	35:j:32:MET:SD	2.43	0.58
13:M:382:VAL:HG22	13:M:396:MET:CE	2.34	0.57
13:M:333:ASN:ND2	60:M:704:HOH:O	2.31	0.57
46:m:202:3PE:C2E	46:m:202:3PE:H2I3	2.35	0.57
13:M:44:GLN:NE2	60:M:702:HOH:O	2.25	0.57
20:T:30:LEU:HD12	20:T:31:SER:H	1.67	0.57
23:X:3:ILE:HD11	25:Z:105:LYS:HZ2	1.68	0.57
45:k:101:LMT:O3'	45:k:101:LMT:O2B	2.23	0.56
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.87	0.56
15:O:46:LEU:HD21	15:O:235:VAL:HG13	1.88	0.56
12:L:398:ALA:O	12:L:402:SER:OG	2.14	0.56
6:F:228:VAL:O	6:F:231:SER:OG	2.24	0.56
13:M:342:MET:HE1	13:M:409:TYR:CE2	2.40	0.56
5:E:9:HIS:NE2	5:E:11:ASP:OD1	2.37	0.56
25:Z:143:TYR:CE2	26:a:48:MET:HE1	2.41	0.55
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.88	0.55
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.35	0.55
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.89	0.55
12:L:364:LYS:NZ	36:k:58:ASN:O	2.37	0.55
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.88	0.55
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.88	0.54
15:O:58:TYR:O	15:O:61:SER:OG	2.19	0.54
13:M:94:LEU:HD21	46:M:604:3PE:O32	2.08	0.54
10:J:125:TRP:HB2	25:Z:137:THR:HG21	1.89	0.54
30:e:24:GLN:O	60:e:201:HOH:O	2.18	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.90	0.53
10:J:141:MET:HE2	10:J:141:MET:CA	2.37	0.53
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.90	0.52
13:M:254:THR:HG21	13:M:304:GLN:HE21	1.74	0.52
45:M:603:LMT:O3'	45:M:603:LMT:O2B	2.23	0.52
26:a:37:ARG:NE	60:a:104:HOH:O	2.43	0.52
5:E:181:ILE:HG23	5:E:181:ILE:O	2.10	0.52
33:h:109:GLU:OE2	33:h:112:ARG:NH1	2.39	0.52
10:J:51:PHE:HB3	10:J:139:GLU:OE2	2.10	0.52
12:L:253:VAL:HB	12:L:310:LEU:HD11	1.91	0.52
12:L:363:PHE:CD1	12:L:370:THR:HG21	2.45	0.52
1:A:71:LEU:O	10:J:147:TYR:OH	2.25	0.51
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.91	0.51
13:M:47:ASP:OD1	13:M:48:ASN:N	2.43	0.51
6:F:200:GLN:NE2	60:F:603:HOH:O	2.30	0.51
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.92	0.51
12:L:558:LEU:HD11	46:m:202:3PE:H2I2	1.91	0.51
26:a:37:ARG:CG	26:a:48:MET:HE2	2.40	0.51
32:g:94:GLU:HG2	41:p:8:VAL:HG11	1.93	0.51
7:G:643:GLN:NE2	7:G:647:GLU:OE2	2.44	0.51
2:B:91:THR:HA	2:B:119:CYS:HB3	1.93	0.51
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.92	0.51
31:f:42:LEU:O	41:p:68:ARG:NH1	2.39	0.51
17:Q:59:PHE:CE2	17:Q:82:LEU:HD23	2.45	0.50
36:k:24:GLU:N	36:k:24:GLU:OE2	2.45	0.50
37:l:68:ASP:OD1	37:l:68:ASP:N	2.41	0.50
39:n:133:GLU:CD	39:n:133:GLU:H	2.19	0.50
15:O:147:GLN:N	15:O:147:GLN:OE1	2.43	0.50
20:T:49:GLU:OE2	22:W:36:TYR:OH	2.27	0.50
20:U:87:TYR:OH	34:i:26:GLU:OE1	2.26	0.50
10:J:138:GLU:HG2	30:e:28:ILE:HG21	1.93	0.50
37:l:118:VAL:HG12	59:o:201:MYR:H141	1.93	0.50
7:G:216:THR:O	60:G:909:HOH:O	2.20	0.50
16:P:323:THR:HG23	16:P:323:THR:O	2.12	0.50
10:J:91:GLY:O	10:J:95:THR:OG1	2.25	0.50
28:c:16:LYS:O	28:c:20:THR:OG1	2.22	0.50
46:m:202:3PE:H2I3	46:m:202:3PE:H2E2	1.93	0.50
12:L:251:THR:HG22	12:L:252:MET:N	2.26	0.50
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.47	0.49
26:a:1:MET:HE3	26:a:1:MET:HA	1.93	0.49
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.94	0.49
12:L:506:ASN:OD1	12:L:509:LYS:NZ	2.46	0.49
1:A:49:LEU:O	1:A:51:PHE:N	2.45	0.49
42:q:39:VAL:CG2	42:q:50:GLU:HG2	2.43	0.49
1:A:47:ALA:O	10:J:78:GLN:NE2	2.44	0.49
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.48	0.49
17:Q:25:VAL:HB	17:Q:30:ILE:HD11	1.94	0.49
13:M:378:GLU:O	13:M:382:VAL:HG23	2.12	0.49
14:N:196:TYR:O	52:N:504:I49:N04	2.46	0.49
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.94	0.48
34:i:89:VAL:O	34:i:95:THR:OG1	2.28	0.48
7:G:578:GLY:O	60:G:910:HOH:O	2.20	0.48
4:D:3:GLN:NE2	13:M:137:GLY:O	2.44	0.48
6:F:117:LYS:NZ	60:F:607:HOH:O	2.40	0.48
12:L:124:PHE:CE1	12:L:251:THR:HG21	2.48	0.48
14:N:174:GLN:OE1	60:N:601:HOH:O	2.20	0.48
6:F:438:GLN:N	6:F:438:GLN:OE1	2.47	0.48
9:I:75:GLU:O	9:I:105:ARG:NH1	2.46	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.96	0.48
33:h:6:LYS:HE2	34:i:26:GLU:OE1	2.13	0.48
5:E:55:GLN:O	5:E:59:GLY:N	2.41	0.48
8:H:70:MET:HE1	8:H:121:TRP:HB3	1.96	0.48
17:Q:21:THR:HG21	22:W:73:ILE:HD11	1.96	0.48
13:M:231:LEU:HD23	13:M:235:LEU:HD12	1.94	0.48
16:P:241:LEU:HD11	16:P:310:LEU:CD2	2.43	0.48
22:W:25:MET:HE1	22:W:79:VAL:HG21	1.95	0.48
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.38	0.48
14:N:347:GLU:HG3	52:N:504:I49:I02	2.84	0.48
16:P:209:ASP:OD2	16:P:308:THR:N	2.42	0.48
7:G:437:HIS:O	7:G:440:SER:OG	2.27	0.47
45:J:201:LMT:O1B	45:J:201:LMT:O4'	2.28	0.47
16:P:293:ILE:HG22	16:P:295:PRO:HD3	1.95	0.47
2:B:44:SER:OG	8:H:51:ASP:OD1	2.17	0.47
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.50	0.47
39:n:49:GLU:OE2	39:n:50:HIS:NE2	2.48	0.47
12:L:319:ILE:HG22	12:L:404:THR:HG21	1.97	0.47
12:L:465:GLY:O	12:L:469:SER:OG	2.30	0.47
40:o:27:ASP:OD1	40:o:27:ASP:N	2.46	0.47
12:L:389:PHE:N	60:L:816:HOH:O	2.48	0.47
14:N:249:LEU:HD22	14:N:254:LEU:HD12	1.96	0.47
5:E:87:TYR:HB3	6:F:181:ALA:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.95	0.46
16:P:96:GLY:O	56:P:501:NDP:H8A	2.15	0.46
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.96	0.46
25:Z:86:MET:HE1	25:Z:125:TYR:CE2	2.51	0.46
11:K:37:MET:HG3	11:K:67:ALA:CB	2.46	0.46
41:p:115:ARG:NH1	60:p:201:HOH:O	2.25	0.46
12:L:331:THR:HB	12:L:387:THR:HG22	1.98	0.46
12:L:445:GLU:O	12:L:451:ILE:HD11	2.16	0.46
13:M:40:LEU:HD22	33:h:79:PHE:HB3	1.98	0.46
20:T:7:THR:O	20:T:10:GLY:N	2.48	0.46
40:o:55:ARG:NH1	60:o:303:HOH:O	2.47	0.46
39:n:61:GLN:NE2	39:n:65:GLU:OE2	2.46	0.46
1:A:28:ASN:N	1:A:28:ASN:OD1	2.48	0.46
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.51	0.46
14:N:214:THR:HG22	14:N:218:MET:HE2	1.98	0.46
3:C:16:ASP:OD1	3:C:16:ASP:N	2.40	0.45
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.98	0.45
24:Y:8:TYR:O	24:Y:20:LYS:NZ	2.45	0.45
5:E:105:THR:HG22	5:E:106:THR:H	1.81	0.45
7:G:194:GLU:OE1	7:G:194:GLU:N	2.38	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.45
12:L:548:SER:HB3	38:m:92:PHE:CD2	2.51	0.45
7:G:202:ILE:C	7:G:202:ILE:HD12	2.41	0.45
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.50	0.45
13:M:296:LEU:CD2	13:M:396:MET:HE1	2.47	0.45
15:O:310:GLU:HG3	15:O:317:ILE:HD12	1.99	0.45
7:G:377:VAL:HG13	7:G:452:ILE:HD12	1.98	0.45
7:G:588:THR:OG1	60:G:907:HOH:O	2.10	0.45
7:G:640:ASN:CG	7:G:641:TYR:N	2.74	0.45
8:H:264:LEU:O	8:H:268:MET:HG2	2.16	0.45
29:d:106:LYS:HA	29:d:106:LYS:HE3	1.98	0.45
1:A:57:LEU:O	1:A:61:THR:OG1	2.21	0.45
12:L:562:LEU:CB	12:L:563:PRO:CD	2.95	0.45
13:M:42:MET:HE1	13:M:453:ILE:HD12	1.98	0.45
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.99	0.45
8:H:207:LEU:HD12	8:H:207:LEU:C	2.41	0.45
11:K:70:GLU:OE2	14:N:37:MET:HE1	2.17	0.45
13:M:205:VAL:HG22	13:M:212:LEU:HD13	1.98	0.45
7:G:254:MET:HA	7:G:260:GLU:O	2.17	0.45
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.99	0.45
36:k:15:LEU:O	60:k:201:HOH:O	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.57	0.45
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.98	0.45
10:J:125:TRP:CB	25:Z:137:THR:HG21	2.47	0.45
6:F:367:GLU:OE2	7:G:100:ASN:ND2	2.50	0.44
30:e:85:LEU:O	30:e:89:GLY:N	2.50	0.44
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.99	0.44
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.99	0.44
7:G:391:PHE:CE2	7:G:395:ILE:HD11	2.53	0.44
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.53	0.44
11:K:12:PHE:CD2	14:N:72:MET:HE3	2.52	0.44
6:F:47:GLU:OE1	6:F:47:GLU:N	2.49	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.00	0.44
7:G:190:MET:HE1	7:G:690:ALA:HB1	2.00	0.44
33:h:51:GLU:OE1	41:p:59:LYS:NZ	2.49	0.44
10:J:94:VAL:HG12	10:J:98:LEU:HD12	1.99	0.44
20:T:73:PRO:O	20:T:77:VAL:HG23	2.17	0.44
39:n:107:HIS:CD2	39:n:108:PRO:HD2	2.53	0.44
7:G:202:ILE:HD12	7:G:203:CYS:N	2.33	0.44
29:d:53:VAL:HG21	46:d:1201:3PE:H2	2.00	0.44
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.53	0.43
13:M:78:MET:HE3	60:g:1609:HOH:O	2.17	0.43
46:M:604:3PE:C33	14:N:242:VAL:HG11	2.48	0.43
14:N:237:THR:HG21	14:N:319:LEU:HD11	2.00	0.43
4:D:64:LEU:HD11	4:D:418:ILE:HD11	2.00	0.43
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.00	0.43
16:P:145:TYR:CD1	16:P:286:ARG:HD3	2.53	0.43
28:c:38:ASP:HB3	29:d:23:PRO:HG3	1.99	0.43
5:E:163:ASP:OD2	5:E:186:PRO:HB3	2.18	0.43
12:L:40:ILE:HG13	12:L:101:MET:SD	2.58	0.43
16:P:50:ARG:NH1	56:P:501:NDP:O2X	2.38	0.43
29:d:120:ARG:HD2	38:m:112:GLU:OE1	2.17	0.43
19:S:87:THR:O	19:S:91:GLU:HG3	2.18	0.43
33:h:19:LYS:HB3	33:h:19:LYS:NZ	2.33	0.43
6:F:98:ASP:O	6:F:99:GLU:C	2.61	0.43
21:V:34:LEU:HD13	21:V:48:GLU:HG3	2.00	0.43
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.01	0.43
10:J:108:LEU:O	10:J:111:LYS:NZ	2.26	0.43
14:N:309:ASN:OD1	15:O:75:GLY:HA3	2.19	0.43
1:A:70:ALA:HA	1:A:73:LEU:HD12	2.01	0.43
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.01	0.43
19:S:18:ILE:HD11	19:S:93:VAL:CG1	2.49	0.43
6:F:300:GLY:HA3	6:F:329:LEU:O	2.19	0.43
12:L:173:LEU:C	12:L:173:LEU:HD23	2.43	0.43
13:M:78:MET:HE1	13:M:439:LEU:HD12	2.01	0.43
7:G:366:THR:O	7:G:367:THR:OG1	2.26	0.43
8:H:179:TRP:N	8:H:180:PRO:CD	2.82	0.43
20:U:13:ASP:O	60:U:201:HOH:O	2.22	0.43
26:a:21:MET:SD	26:a:21:MET:C	3.02	0.43
38:m:112:GLU:OE1	38:m:112:GLU:HA	2.19	0.42
15:O:174:VAL:HG22	15:O:225:ALA:HB2	2.01	0.42
24:Y:18:HIS:ND1	24:Y:19:ARG:N	2.68	0.42
4:D:322:GLU:OE1	4:D:322:GLU:N	2.41	0.42
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.00	0.42
12:L:429:PHE:O	12:L:436:ARG:NH2	2.49	0.42
40:o:1:GLY:O	40:o:4:LEU:N	2.48	0.42
12:L:530:PRO:O	12:L:534:HIS:HB2	2.18	0.42
29:d:112:VAL:HG21	41:p:78:GLU:OE2	2.20	0.42
7:G:287:GLU:CD	7:G:287:GLU:H	2.28	0.42
12:L:124:PHE:CD1	12:L:251:THR:HG21	2.55	0.42
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.55	0.42
14:N:248:LEU:HD23	14:N:251:MET:CE	2.49	0.42
13:M:201:MET:O	13:M:205:VAL:HG23	2.19	0.42
3:C:165:ASP:HA	17:Q:82:LEU:HD11	2.01	0.42
3:C:179:GLU:OE2	16:P:37:HIS:NE2	2.32	0.42
6:F:93:LEU:O	6:F:134:ALA:HA	2.20	0.42
8:H:255:TYR:CD1	8:H:255:TYR:C	2.98	0.42
13:M:80:SER:OG	13:M:226:ALA:HB2	2.19	0.42
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.55	0.42
4:D:417:ILE:O	4:D:420:THR:HG22	2.19	0.42
13:M:459:TYR:OH	60:M:701:HOH:O	2.21	0.42
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.55	0.42
7:G:382:THR:HB	7:G:454:GLY:HA3	2.01	0.41
10:J:49:GLY:HA2	10:J:139:GLU:OE1	2.20	0.41
13:M:406:TYR:CD1	13:M:406:TYR:C	2.98	0.41
19:S:18:ILE:CD1	19:S:93:VAL:HG11	2.50	0.41
4:D:8:VAL:O	4:D:12:GLU:HG3	2.20	0.41
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.51	0.41
7:G:145:LEU:HD22	7:G:269:PHE:CD2	2.55	0.41
7:G:145:LEU:HD21	7:G:687:CYS:SG	2.60	0.41
7:G:640:ASN:CG	7:G:641:TYR:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.02	0.41
14:N:128:LEU:HD22	14:N:220:MET:HE1	2.03	0.41
20:U:88:GLU:OE1	33:h:6:LYS:NZ	2.53	0.41
12:L:203:MET:HG2	41:p:109:LEU:HD11	2.03	0.41
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.55	0.41
8:H:93:TYR:OH	26:a:35:GLU:OE1	2.35	0.41
19:S:18:ILE:HD11	19:S:93:VAL:HG11	2.01	0.41
7:G:316:ALA:HB3	7:G:519:PRO:HG3	2.03	0.41
8:H:2:PHE:HE2	8:H:6:ILE:HD11	1.77	0.41
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.02	0.41
15:O:71:VAL:HG22	15:O:76:ASN:HA	2.03	0.41
36:k:62:PHE:CE2	36:k:66:LEU:HD11	2.56	0.41
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.55	0.41
7:G:199:ILE:HA	7:G:202:ILE:HG13	2.02	0.41
7:G:396:ARG:NH1	7:G:416:THR:O	2.54	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.56	0.41
14:N:96:MET:O	14:N:100:MET:HG3	2.21	0.41
38:m:27:GLU:N	38:m:27:GLU:OE2	2.53	0.41
1:A:26:GLN:HB2	1:A:28:ASN:OD1	2.21	0.41
1:A:85:ASN:ND2	45:A:301:LMT:H2'	2.35	0.41
10:J:86:ASN:OD1	10:J:87:LYS:N	2.54	0.41
13:M:304:GLN:O	29:d:119:VAL:HG11	2.21	0.41
16:P:176:ASP:OD1	16:P:176:ASP:C	2.64	0.41
23:X:122:GLY:CA	27:b:77:LEU:HD12	2.51	0.41
8:H:225:MET:SD	52:H:403:I49:I02	3.49	0.41
12:L:528:TYR:CD1	37:l:101:MET:HG2	2.56	0.41
23:X:21:SER:OG	26:a:51:ASP:OD1	2.30	0.40
24:Y:105:ARG:NE	24:Y:105:ARG:HA	2.36	0.40
6:F:423:ARG:NH2	60:F:602:HOH:O	2.53	0.40
8:H:192:GLU:HA	8:H:192:GLU:OE2	2.20	0.40
9:I:7:LEU:HD23	43:r:111:TYR:HE2	1.86	0.40
13:M:76:MET:HE1	60:M:773:HOH:O	2.21	0.40
13:M:243:MET:HA	13:M:246:ILE:HG22	2.04	0.40
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.56	0.40
8:H:14:LEU:HD22	8:H:225:MET:HE3	2.03	0.40
13:M:379:LEU:O	13:M:383:MET:HG2	2.21	0.40
30:e:87:LYS:CA	30:e:87:LYS:HE2	2.50	0.40
8:H:143:GLU:HG3	8:H:192:GLU:OE1	2.22	0.40
12:L:421:ILE:HA	12:L:501:ALA:HB2	2.03	0.40
7:G:568:GLU:HA	7:G:587:VAL:O	2.22	0.40
14:N:146:PHE:N	14:N:147:PRO:CD	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:115:LEU:HD13	15:O:121:GLY:HA2	2.03	0.40
38:m:121:ASP:OD1	38:m:123:THR:OG1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	100/115 (87%)	98 (98%)	2 (2%)	0	100	100
2	B	154/216 (71%)	149 (97%)	5 (3%)	0	100	100
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	412/463 (89%)	400 (97%)	11 (3%)	1 (0%)	43	55
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	429/464 (92%)	422 (98%)	7 (2%)	0	100	100
7	G	686/727 (94%)	672 (98%)	14 (2%)	0	100	100
8	H	307/318 (96%)	294 (96%)	13 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	162 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
12	L	604/606 (100%)	583 (96%)	20 (3%)	1 (0%)	43	55
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
15	O	318/343 (93%)	314 (99%)	4 (1%)	0	100	100
16	P	287/380 (76%)	283 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	91 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	84/99 (85%)	80 (95%)	4 (5%)	0	100	100
20	T	74/156 (47%)	73 (99%)	1 (1%)	0	100	100
20	U	82/156 (53%)	81 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
25	Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	110 (100%)	0	0	100	100
30	e	93/106 (88%)	91 (98%)	2 (2%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	96/154 (62%)	93 (97%)	3 (3%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	100/127 (79%)	97 (97%)	3 (3%)	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%)	147 (96%)	6 (4%)	0	100	100
38	m	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	118/136 (87%)	113 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	167 (99%)	1 (1%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	88 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8009/9211 (87%)	7838 (98%)	169 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	80	ILE

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	90/100 (90%)	88 (98%)	2 (2%)	45	65
2	B	132/175 (75%)	127 (96%)	5 (4%)	29	44
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	360/392 (92%)	357 (99%)	3 (1%)	73	86
5	E	183/205 (89%)	182 (100%)	1 (0%)	81	90
6	F	345/368 (94%)	343 (99%)	2 (1%)	78	89
7	G	578/608 (95%)	568 (98%)	10 (2%)	53	72
8	H	268/274 (98%)	264 (98%)	4 (2%)	57	75
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	139 (99%)	1 (1%)	76	87
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	79
12	L	529/533 (99%)	525 (99%)	4 (1%)	73	86
13	M	412/412 (100%)	410 (100%)	2 (0%)	81	90
14	N	315/315 (100%)	314 (100%)	1 (0%)	86	93
15	O	283/303 (93%)	278 (98%)	5 (2%)	51	70
16	P	254/327 (78%)	250 (98%)	4 (2%)	55	73
17	Q	112/153 (73%)	109 (97%)	3 (3%)	39	58
18	R	78/97 (80%)	76 (97%)	2 (3%)	40	59
19	S	76/82 (93%)	74 (97%)	2 (3%)	40	59
20	T	70/135 (52%)	67 (96%)	3 (4%)	26	39
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	106 (99%)	1 (1%)	70	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	154/155 (99%)	149 (97%)	5 (3%)	34	51
24	Y	101/102 (99%)	96 (95%)	5 (5%)	22	33
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	86
26	a	58/59 (98%)	57 (98%)	1 (2%)	53	72
27	b	71/72 (99%)	68 (96%)	3 (4%)	26	40
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	85 (99%)	1 (1%)	63	79
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	89/131 (68%)	88 (99%)	1 (1%)	65	81
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	99/120 (82%)	99 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	61/76 (80%)	60 (98%)	1 (2%)	55	73
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	112/115 (97%)	110 (98%)	2 (2%)	51	70
39	n	156/161 (97%)	153 (98%)	3 (2%)	50	69
40	o	109/119 (92%)	107 (98%)	2 (2%)	51	70
41	p	154/157 (98%)	152 (99%)	2 (1%)	61	77
42	q	131/131 (100%)	128 (98%)	3 (2%)	44	63
43	r	84/97 (87%)	83 (99%)	1 (1%)	63	79
44	s	43/92 (47%)	42 (98%)	1 (2%)	44	63
All	All	7075/7891 (90%)	6987 (99%)	88 (1%)	61	79

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	85	ASN
2	B	29	VAL
2	B	54	CYS
2	B	79	SER
2	B	91	THR
2	B	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	76	CYS
4	D	219	SER
4	D	420	THR
5	E	14	GLU
6	F	54	ASP
6	F	324	GLN
7	G	17	SER
7	G	193	SER
7	G	364	LEU
7	G	398	SER
7	G	456	SER
7	G	471	SER
7	G	533	THR
7	G	643	GLN
7	G	646	SER
7	G	659	ASP
8	H	66	SER
8	H	163	SER
8	H	194	ASN
8	H	222	LEU
10	J	148	SER
11	K	46	LEU
12	L	10	VAL
12	L	30	SER
12	L	393	ASP
12	L	469	SER
13	M	72	LEU
13	M	116	ILE
14	N	67	SER
15	O	1	LEU
15	O	2	GLN
15	O	60	ASP
15	O	289	SER
15	O	310	GLU
16	P	43	SER
16	P	142	SER
16	P	199	LYS
16	P	290	THR
17	Q	66	GLU
17	Q	110	VAL
17	Q	115	SER
18	R	79	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	95	HIS
19	S	39	ARG
19	S	90	LEU
20	T	11	ILE
20	T	32	VAL
20	T	82	ASP
22	W	49	LEU
23	X	11	ASP
23	X	17	VAL
23	X	77	CYS
23	X	132	THR
23	X	148	GLU
24	Y	25	THR
24	Y	44	THR
24	Y	75	ILE
24	Y	109	ILE
24	Y	114	CYS
25	Z	144	THR
26	a	30	SER
27	b	4	VAL
27	b	9	LYS
27	b	67	SER
30	e	18	THR
32	g	122	GLU
36	k	58	ASN
38	m	8	SER
38	m	23	ASP
39	n	57	VAL
39	n	122	GLU
39	n	175	GLU
40	o	30	PHE
40	o	120	ASP
41	p	119	SER
41	p	134	VAL
42	q	4	LEU
42	q	15	SER
42	q	134	ILE
43	r	66	SER
44	s	57	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	88	ASN
4	D	217	ASN
5	E	42	HIS
6	F	83	ASN
6	F	148	ASN
6	F	224	ASN
6	F	421	HIS
6	F	437	HIS
7	G	581	GLN
7	G	653	ASN
8	H	47	GLN
9	I	144	HIS
9	I	170	GLN
12	L	135	ASN
12	L	194	ASN
12	L	199	GLN
12	L	200	GLN
12	L	269	ASN
12	L	296	ASN
12	L	471	ASN
12	L	546	GLN
12	L	603	ASN
13	M	180	GLN
13	M	251	ASN
13	M	338	HIS
13	M	415	GLN
14	N	48	HIS
14	N	144	GLN
14	N	268	GLN
14	N	289	ASN
15	O	271	ASN
15	O	288	GLN
16	P	119	GLN
16	P	243	GLN
18	R	94	GLN
20	T	33	ASN
21	V	82	GLN
21	V	95	GLN
23	X	76	HIS
24	Y	7	GLN
25	Z	112	HIS
28	c	5	GLN
28	c	34	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	c	46	ASN
29	d	97	HIS
30	e	20	GLN
32	g	86	GLN
35	j	6	HIS
36	k	58	ASN
38	m	125	ASN
39	n	77	GLN
40	o	42	GLN
40	o	49	GLN
40	o	53	GLN
41	p	120	HIS
41	p	122	GLN
42	q	13	GLN
42	q	112	ASN
44	s	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	FME	K	1	11	8,9,10	0.94	0	8,9,11	0.86	0
4	2MR	D	85	4	10,12,13	2.74	3 (30%)	5,13,15	1.31	1 (20%)
14	FME	N	1	14	8,9,10	1.02	0	8,9,11	0.83	0
34	SAC	i	1	34	7,8,9	1.94	1 (14%)	7,9,11	1.82	1 (14%)
1	FME	A	1	1	8,9,10	1.03	1 (12%)	8,9,11	0.93	0
24	AYA	Y	1	24	6,7,8	1.91	2 (33%)	6,8,10	1.26	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.29	1 (16%)
13	FME	M	1	13	8,9,10	1.05	1 (12%)	8,9,11	0.99	1 (12%)
8	FME	H	1	8	8,9,10	1.01	1 (12%)	8,9,11	0.84	0
12	FME	L	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.92	0
10	FME	J	1	10	8,9,10	0.97	0	8,9,11	0.88	0

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.33	1.44	1.33
4	D	85	2MR	CZ-NE	4.70	1.44	1.34
34	i	1	SAC	O-C	4.40	1.36	1.20
4	D	85	2MR	O-C	4.02	1.35	1.20
24	Y	1	AYA	CT-N	3.49	1.45	1.34
43	r	1	AYA	CT-N	3.35	1.45	1.34
13	M	1	FME	CA-N	-2.35	1.43	1.46
24	Y	1	AYA	OT-CT	-2.17	1.18	1.23
12	L	1	FME	CA-N	-2.15	1.43	1.46
1	A	1	FME	CA-N	-2.11	1.43	1.46
8	H	1	FME	CA-N	-2.08	1.43	1.46
43	r	1	AYA	OT-CT	-2.07	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-3.85	114.88	124.77
4	D	85	2MR	NE-CZ-NH2	-2.62	117.08	119.48
24	Y	1	AYA	CM-CT-N	2.32	119.97	116.12
43	r	1	AYA	CM-CT-N	2.23	119.81	116.12
13	M	1	FME	C-CA-N	2.10	113.55	109.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE
34	i	1	SAC	C-CA-N-C1A
10	J	1	FME	C-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	CB-CA-N-C1A
14	N	1	FME	C-CA-CB-CG

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 3 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
45	LMT	f	1801	-	36,36,36	1.15	3 (8%)	47,47,47	1.15	5 (10%)
46	3PE	A	302	-	47,47,50	0.88	4 (8%)	50,52,55	1.10	2 (4%)
53	CDL	q	201	-	75,75,99	1.01	8 (10%)	81,87,111	1.08	4 (4%)
56	NDP	P	501	-	51,52,52	2.21	7 (13%)	71,80,80	1.50	15 (21%)
53	CDL	d	1202	-	72,72,99	1.03	7 (9%)	78,84,111	1.23	5 (6%)
45	LMT	M	602	-	36,36,36	1.18	2 (5%)	47,47,47	0.95	0
48	PC1	B	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.19	2 (5%)
45	LMT	L	702	-	36,36,36	1.18	3 (8%)	47,47,47	0.91	2 (4%)
45	LMT	k	101	-	36,36,36	1.18	3 (8%)	47,47,47	0.85	0
46	3PE	d	1201	-	46,46,50	0.91	4 (8%)	49,51,55	1.13	2 (4%)
50	FMN	F	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.25	6 (12%)
46	3PE	L	704	-	44,44,50	0.92	3 (6%)	47,49,55	1.13	3 (6%)
53	CDL	N	503	-	64,64,99	1.09	8 (12%)	70,76,111	1.12	5 (7%)
53	CDL	L	703	-	68,68,99	1.05	6 (8%)	74,80,111	1.11	4 (5%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
58	EHZ	T	101	20	31,36,37	1.53	4 (12%)	36,44,47	1.32	4 (11%)
46	3PE	m	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.13	2 (4%)
46	3PE	L	705	-	28,28,50	1.14	4 (14%)	31,33,55	1.21	2 (6%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	LMT	l	201	-	36,36,36	1.22	3 (8%)	47,47,47	0.92	0
45	LMT	M	603	-	36,36,36	1.17	2 (5%)	47,47,47	1.31	6 (12%)
45	LMT	J	201	-	36,36,36	1.21	3 (8%)	47,47,47	0.96	1 (2%)
46	3PE	M	604	-	50,50,50	0.88	3 (6%)	53,55,55	1.14	2 (3%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
53	CDL	h	1001	-	66,66,99	1.07	7 (10%)	72,78,111	1.24	4 (5%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
45	LMT	Y	402	-	36,36,36	1.19	3 (8%)	47,47,47	1.03	1 (2%)
54	GTP	O	401	55	33,34,34	3.28	14 (42%)	50,54,54	1.89	14 (28%)
46	3PE	L	701	-	48,48,50	0.90	2 (4%)	51,53,55	1.00	2 (3%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	MYR	o	201	40	13,14,15	0.97	0	12,13,15	0.56	0
52	I49	N	504	-	15,17,17	0.88	1 (6%)	17,22,22	1.93	5 (29%)
46	3PE	N	502	-	40,40,50	0.96	4 (10%)	43,45,55	1.12	2 (4%)
53	CDL	J	202	-	70,70,99	1.04	8 (11%)	76,82,111	1.04	4 (5%)
45	LMT	N	501	-	36,36,36	1.15	3 (8%)	47,47,47	0.97	0
58	EHZ	U	101	20	31,36,37	1.53	5 (16%)	36,44,47	1.57	4 (11%)
45	LMT	h	1002	-	36,36,36	1.24	4 (11%)	47,47,47	1.20	3 (6%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
45	LMT	m	201	-	36,36,36	1.25	4 (11%)	47,47,47	1.33	5 (10%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
48	PC1	g	1501	-	48,48,53	1.02	3 (6%)	54,56,61	0.98	2 (3%)
52	I49	H	403	-	15,17,17	0.90	1 (6%)	17,22,22	1.92	4 (23%)
46	3PE	Y	401	-	34,34,50	1.05	4 (11%)	37,39,55	1.08	2 (5%)
45	LMT	B	202	-	36,36,36	1.19	2 (5%)	47,47,47	0.84	0
46	3PE	H	402	-	33,33,50	1.30	4 (12%)	34,37,55	1.13	2 (5%)
46	3PE	M	601	-	45,45,50	0.90	4 (8%)	48,50,55	1.16	2 (4%)
45	LMT	M	605	-	36,36,36	1.24	4 (11%)	47,47,47	1.01	2 (4%)
46	3PE	H	401	-	43,43,50	0.93	4 (9%)	46,48,55	1.12	2 (4%)
46	3PE	I	201	-	50,50,50	0.88	4 (8%)	53,55,55	0.96	2 (3%)
45	LMT	A	301	-	36,36,36	1.20	2 (5%)	47,47,47	0.95	1 (2%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
45	LMT	A	303	-	36,36,36	1.20	3 (8%)	47,47,47	1.06	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
45	LMT	f	1801	-	-	9/21/61/61	0/2/2/2
46	3PE	A	302	-	-	19/51/51/54	-
53	CDL	q	201	-	-	41/86/86/110	-
56	NDP	P	501	-	-	6/34/77/77	0/5/5/5
53	CDL	d	1202	-	-	35/83/83/110	-
45	LMT	M	602	-	-	11/21/61/61	0/2/2/2
48	PC1	B	203	-	-	12/38/38/57	-
45	LMT	L	702	-	-	2/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	k	101	-	-	5/21/61/61	0/2/2/2
46	3PE	d	1201	-	-	23/50/50/54	-
50	FMN	F	501	-	-	3/18/18/18	0/3/3/3
46	3PE	L	704	-	-	22/48/48/54	-
53	CDL	N	503	-	-	35/75/75/110	-
53	CDL	L	703	-	-	28/79/79/110	-
58	EHZ	T	101	20	-	12/42/44/45	-
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	m	202	-	-	20/44/44/54	-
46	3PE	L	705	-	-	13/32/32/54	-
49	FES	E	301	5	-	-	0/1/1/1
45	LMT	l	201	-	-	10/21/61/61	0/2/2/2
45	LMT	M	603	-	-	4/21/61/61	0/2/2/2
45	LMT	J	201	-	-	8/21/61/61	0/2/2/2
46	3PE	M	604	-	-	24/54/54/54	-
47	SF4	B	201	2	-	-	0/6/5/5
53	CDL	h	1001	-	-	29/77/77/110	-
49	FES	G	803	7	-	-	0/1/1/1
45	LMT	Y	402	-	-	12/21/61/61	0/2/2/2
54	GTP	O	401	55	-	5/22/38/38	0/3/3/3
46	3PE	L	701	-	-	24/52/52/54	-
59	MYR	o	201	40	-	6/12/12/13	-
47	SF4	I	202	9	-	-	0/6/5/5
52	I49	N	504	-	-	3/10/10/10	0/1/1/1
46	3PE	N	502	-	-	17/44/44/54	-
53	CDL	J	202	-	-	29/81/81/110	-
45	LMT	N	501	-	-	9/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	9/42/44/45	-
45	LMT	h	1002	-	-	4/21/61/61	0/2/2/2
47	SF4	G	801	7	-	-	0/6/5/5
45	LMT	m	201	-	-	8/21/61/61	0/2/2/2
47	SF4	I	203	9	-	-	0/6/5/5
48	PC1	g	1501	-	-	21/52/52/57	-
52	I49	H	403	-	-	8/10/10/10	0/1/1/1
46	3PE	Y	401	-	-	17/38/38/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	B	202	-	-	9/21/61/61	0/2/2/2
46	3PE	H	402	-	-	11/36/36/54	-
46	3PE	M	601	-	-	22/49/49/54	-
45	LMT	M	605	-	-	9/21/61/61	0/2/2/2
46	3PE	H	401	-	-	16/47/47/54	-
46	3PE	I	201	-	-	18/54/54/54	-
45	LMT	A	301	-	-	11/21/61/61	0/2/2/2
47	SF4	F	502	6	-	-	0/6/5/5
45	LMT	A	303	-	-	8/21/61/61	0/2/2/2

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.42	1.81	1.59
54	O	401	GTP	O6-C6	8.57	1.39	1.23
54	O	401	GTP	C5-N7	6.58	1.52	1.39
54	O	401	GTP	PA-O3A	5.23	1.65	1.59
54	O	401	GTP	PB-O3B	5.07	1.65	1.59
54	O	401	GTP	PB-O3A	4.94	1.64	1.59
58	U	101	EHZ	C15-N2	4.92	1.45	1.33
54	O	401	GTP	C2-N1	4.90	1.49	1.37
58	T	101	EHZ	C12-N1	4.80	1.44	1.33
58	T	101	EHZ	C15-N2	4.73	1.44	1.33
54	O	401	GTP	C2-N3	4.67	1.44	1.33
58	U	101	EHZ	C12-N1	4.66	1.44	1.33
54	O	401	GTP	C8-N9	-4.56	1.27	1.37
54	O	401	GTP	C2-N2	4.53	1.44	1.34
46	H	402	3PE	O21-C2	-4.49	1.40	1.46
56	P	501	NDP	PA-O3	4.41	1.64	1.59
54	O	401	GTP	C4-N9	-3.77	1.28	1.38
45	m	201	LMT	O5'-C1'	3.53	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.51	1.50	1.41
45	m	201	LMT	O5B-C1B	3.50	1.50	1.41
56	P	501	NDP	PN-O5D	3.50	1.73	1.59
45	Y	402	LMT	O5B-C1B	3.49	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.46	1.32	1.44
45	A	303	LMT	O5B-C1B	3.45	1.50	1.41
45	B	202	LMT	O5B-C1B	3.42	1.50	1.41
45	l	201	LMT	O5B-C1B	3.40	1.50	1.41
45	J	201	LMT	O5B-C1B	3.39	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	605	LMT	O5B-C1B	3.34	1.50	1.41
45	L	702	LMT	O5B-C1B	3.34	1.50	1.41
45	k	101	LMT	O5B-C1B	3.31	1.50	1.41
45	A	301	LMT	O5B-C1B	3.30	1.50	1.41
45	M	602	LMT	O5B-C1B	3.30	1.50	1.41
45	N	501	LMT	O5B-C1B	3.28	1.50	1.41
46	H	402	3PE	O21-C21	3.26	1.40	1.33
45	M	605	LMT	O5'-C1'	3.26	1.50	1.41
45	f	1801	LMT	O5B-C1B	3.25	1.50	1.41
45	h	1002	LMT	O5'-C1'	3.24	1.50	1.41
45	M	603	LMT	O5B-C1B	3.22	1.50	1.41
45	l	201	LMT	O5'-C1'	3.15	1.49	1.41
50	F	501	FMN	C4A-N5	3.14	1.37	1.30
45	k	101	LMT	O5'-C1'	3.11	1.49	1.41
45	Y	402	LMT	O5'-C1'	3.11	1.49	1.41
45	A	301	LMT	O5'-C1'	3.11	1.49	1.41
53	h	1001	CDL	OA6-CA4	-3.10	1.39	1.46
45	M	602	LMT	O5'-C1'	3.08	1.49	1.41
45	A	303	LMT	O5'-C1'	3.07	1.49	1.41
45	M	603	LMT	O5'-C1'	3.05	1.49	1.41
53	d	1202	CDL	OB6-CB4	-3.04	1.39	1.46
45	J	201	LMT	O5'-C1'	2.97	1.49	1.41
45	N	501	LMT	O5'-C1'	2.96	1.49	1.41
46	L	701	3PE	O21-C2	-2.93	1.39	1.46
53	L	703	CDL	OB6-CB4	-2.90	1.39	1.46
45	f	1801	LMT	O5'-C1'	2.88	1.49	1.41
53	d	1202	CDL	OA6-CA4	-2.87	1.39	1.46
45	L	702	LMT	O5'-C1'	2.86	1.49	1.41
48	g	1501	PC1	O21-C2	-2.86	1.39	1.46
45	B	202	LMT	O5'-C1'	2.86	1.49	1.41
46	L	704	3PE	O21-C2	-2.86	1.39	1.46
46	d	1201	3PE	O21-C2	-2.85	1.39	1.46
53	L	703	CDL	OA6-CA4	-2.84	1.39	1.46
54	O	401	GTP	O4'-C1'	2.83	1.48	1.42
46	I	201	3PE	O21-C2	-2.83	1.40	1.46
46	M	604	3PE	O21-C2	-2.82	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.82	1.40	1.46
53	N	503	CDL	OA6-CA4	-2.80	1.40	1.46
53	h	1001	CDL	OB6-CB4	-2.79	1.40	1.46
46	Y	401	3PE	O21-C2	-2.77	1.40	1.46
46	N	502	3PE	O21-C2	-2.75	1.40	1.46
53	q	201	CDL	OA6-CA4	-2.74	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	202	CDL	OA6-CA4	-2.73	1.40	1.46
46	L	701	3PE	O31-C3	-2.71	1.39	1.45
46	L	705	3PE	O21-C2	-2.70	1.40	1.46
53	N	503	CDL	OB6-CB4	-2.70	1.40	1.46
46	m	202	3PE	O21-C2	-2.68	1.40	1.46
58	T	101	EHZ	O4-C15	-2.64	1.18	1.23
46	I	201	3PE	O31-C3	-2.63	1.39	1.45
58	U	101	EHZ	O4-C15	-2.62	1.18	1.23
53	J	202	CDL	OB6-CB4	-2.58	1.40	1.46
46	H	401	3PE	O21-C2	-2.55	1.40	1.46
48	B	203	PC1	O21-C2	-2.53	1.40	1.46
53	h	1001	CDL	OB8-CB6	-2.53	1.39	1.45
58	T	101	EHZ	O3-C12	-2.52	1.18	1.23
53	N	503	CDL	OA8-CA6	-2.52	1.39	1.45
53	q	201	CDL	OA8-CA6	-2.50	1.39	1.45
58	U	101	EHZ	O3-C12	-2.48	1.18	1.23
46	Y	401	3PE	O31-C31	2.47	1.40	1.33
52	N	504	I49	C15-N02	-2.47	1.31	1.36
53	d	1202	CDL	OB8-CB7	2.47	1.40	1.33
53	N	503	CDL	OB8-CB7	2.46	1.40	1.33
52	H	403	I49	C15-N02	-2.45	1.31	1.36
46	L	704	3PE	O31-C3	-2.45	1.39	1.45
53	d	1202	CDL	OA8-CA7	2.44	1.40	1.33
53	J	202	CDL	OB8-CB7	2.44	1.40	1.33
46	A	302	3PE	O31-C31	2.42	1.40	1.33
46	L	705	3PE	O31-C3	-2.42	1.39	1.45
46	M	601	3PE	O21-C2	-2.42	1.40	1.46
54	O	401	GTP	PG-O2G	-2.41	1.45	1.54
46	M	604	3PE	O31-C3	-2.41	1.39	1.45
53	q	201	CDL	OB8-CB6	-2.40	1.39	1.45
46	N	502	3PE	O31-C3	-2.39	1.39	1.45
54	O	401	GTP	PG-O3G	-2.38	1.46	1.54
46	m	202	3PE	O31-C31	2.38	1.40	1.33
48	g	1501	PC1	O31-C31	2.37	1.40	1.33
46	M	604	3PE	O31-C31	2.37	1.40	1.33
53	L	703	CDL	OB8-CB7	2.37	1.40	1.33
46	A	302	3PE	O21-C2	-2.36	1.41	1.46
53	J	202	CDL	OA8-CA6	-2.35	1.39	1.45
53	q	201	CDL	OB8-CB7	2.35	1.40	1.33
48	g	1501	PC1	O31-C3	-2.34	1.39	1.45
53	h	1001	CDL	OA8-CA6	-2.33	1.40	1.45
53	L	703	CDL	OA8-CA7	2.32	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	503	CDL	OB8-CB6	-2.31	1.40	1.45
48	B	203	PC1	O31-C3	-2.31	1.40	1.45
48	B	203	PC1	O21-C21	2.29	1.40	1.34
46	m	202	3PE	O31-C3	-2.28	1.40	1.45
46	H	401	3PE	O31-C31	2.27	1.40	1.33
46	H	401	3PE	O31-C3	-2.27	1.40	1.45
54	O	401	GTP	C2'-C3'	-2.26	1.47	1.53
46	H	402	3PE	O31-C3	-2.26	1.40	1.45
46	H	402	3PE	O31-C31	2.25	1.39	1.33
46	d	1201	3PE	O31-C31	2.24	1.39	1.33
46	d	1201	3PE	O31-C3	-2.24	1.40	1.45
53	L	703	CDL	OA8-CA6	-2.24	1.40	1.45
46	N	502	3PE	O31-C31	2.23	1.39	1.33
46	L	704	3PE	O31-C31	2.23	1.39	1.33
53	d	1202	CDL	OB8-CB6	-2.23	1.40	1.45
45	m	201	LMT	O5B-C5B	2.22	1.49	1.44
53	J	202	CDL	OB6-CB5	2.22	1.40	1.34
46	A	302	3PE	O21-C21	2.22	1.40	1.34
53	J	202	CDL	OA8-CA7	2.20	1.39	1.33
46	M	601	3PE	O31-C3	-2.20	1.40	1.45
53	d	1202	CDL	OA8-CA6	-2.19	1.40	1.45
46	H	401	3PE	O21-C21	2.18	1.40	1.34
46	L	705	3PE	O31-C31	2.18	1.39	1.33
46	M	601	3PE	O31-C31	2.17	1.39	1.33
53	h	1001	CDL	OB8-CB7	2.15	1.39	1.33
45	M	605	LMT	O5'-C5'	2.15	1.49	1.44
48	B	203	PC1	O31-C31	2.15	1.39	1.33
46	M	601	3PE	O21-C21	2.15	1.40	1.34
46	m	202	3PE	O21-C21	2.14	1.40	1.34
45	h	1002	LMT	O5'-C5'	2.14	1.49	1.44
53	d	1202	CDL	OA6-CA5	2.14	1.40	1.34
53	q	201	CDL	OB6-CB5	2.13	1.40	1.34
45	l	201	LMT	O5B-C5B	2.13	1.49	1.44
53	N	503	CDL	OA6-CA5	2.13	1.40	1.34
53	L	703	CDL	OB8-CB6	-2.12	1.40	1.45
46	I	201	3PE	O31-C31	2.11	1.39	1.33
53	h	1001	CDL	OB6-CB5	2.11	1.40	1.34
53	J	202	CDL	OA6-CA5	2.11	1.40	1.34
45	J	201	LMT	O5B-C5B	2.10	1.49	1.44
45	M	605	LMT	O5B-C5B	2.10	1.49	1.44
45	L	702	LMT	O5B-C5B	2.09	1.49	1.44
45	f	1801	LMT	O5B-C5B	2.09	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	q	201	CDL	OA6-CA5	2.09	1.40	1.34
46	Y	401	3PE	O31-C3	-2.08	1.40	1.45
53	J	202	CDL	OB8-CB6	-2.08	1.40	1.45
46	A	302	3PE	O31-C3	-2.08	1.40	1.45
46	d	1201	3PE	O21-C21	2.07	1.40	1.34
53	N	503	CDL	OA8-CA7	2.07	1.39	1.33
56	P	501	NDP	O5D-C5D	-2.06	1.36	1.44
53	h	1001	CDL	OA8-CA7	2.06	1.39	1.33
46	L	705	3PE	O21-C21	2.05	1.40	1.34
46	I	201	3PE	O21-C21	2.05	1.40	1.34
45	A	303	LMT	O5'-C5'	2.05	1.49	1.44
53	q	201	CDL	OA8-CA7	2.05	1.39	1.33
50	F	501	FMN	C10-N1	2.04	1.37	1.33
45	Y	402	LMT	O5B-C5B	2.03	1.49	1.44
58	U	101	EHZ	C9-S1	2.02	1.81	1.76
45	m	201	LMT	O1B-C4'	2.02	1.49	1.43
45	N	501	LMT	O5B-C5B	2.02	1.49	1.44
45	h	1002	LMT	O5B-C5B	2.02	1.49	1.44
46	N	502	3PE	O21-C21	2.01	1.40	1.34
53	N	503	CDL	OB6-CB5	2.01	1.40	1.34
56	P	501	NDP	O2D-C2D	-2.01	1.38	1.43
46	Y	401	3PE	O21-C21	2.01	1.39	1.34
45	k	101	LMT	O5B-C5B	2.00	1.49	1.44
56	P	501	NDP	O5B-C5B	-2.00	1.37	1.44

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	GTP	C8-N9-C4	7.51	120.11	106.03
58	U	101	EHZ	C8-C9-S1	6.12	121.29	113.56
52	H	403	I49	N01-C14-N03	5.14	129.74	120.26
52	N	504	I49	N01-C14-N03	4.95	129.39	120.26
53	h	1001	CDL	OB6-CB5-C51	4.62	121.48	111.48
48	B	203	PC1	O21-C21-C22	4.47	121.15	111.48
58	T	101	EHZ	C8-C9-S1	4.36	119.06	113.56
46	L	705	3PE	O21-C21-C22	4.26	120.69	111.48
46	M	604	3PE	O21-C21-C22	4.23	120.63	111.48
46	L	704	3PE	O21-C21-C22	4.18	120.52	111.48
46	A	302	3PE	O21-C21-C22	4.12	120.39	111.48
46	d	1201	3PE	O21-C21-C22	4.11	120.38	111.48
46	N	502	3PE	O21-C21-C22	4.10	120.35	111.48
53	N	503	CDL	OA6-CA5-C11	4.08	120.32	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	d	1202	CDL	OB6-CB5-C51	4.07	120.28	111.48
45	M	603	LMT	C1'-C2'-C3'	4.02	118.46	110.01
46	H	401	3PE	O21-C21-C22	3.99	120.10	111.48
53	h	1001	CDL	OA6-CA5-C11	3.96	120.06	111.48
53	L	703	CDL	OB6-CB5-C51	3.89	119.90	111.48
56	P	501	NDP	P2B-O2B-C2B	-3.89	113.05	123.43
46	H	402	3PE	O21-C21-O22	-3.89	120.71	125.70
46	m	202	3PE	O21-C21-C22	3.88	119.88	111.48
45	m	201	LMT	O5'-C1'-C2'	3.87	118.33	110.37
53	q	201	CDL	OA6-CA5-C11	3.87	119.84	111.48
46	M	601	3PE	O21-C21-C22	3.84	119.79	111.48
53	q	201	CDL	OB6-CB5-C51	3.83	119.76	111.48
53	d	1202	CDL	OA6-CA5-C11	3.82	119.74	111.48
48	g	1501	PC1	O21-C21-C22	3.78	119.66	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.73	96.04	109.33
53	L	703	CDL	OA6-CA5-C11	3.72	119.53	111.48
46	L	701	3PE	O21-C21-C22	3.70	119.49	111.48
53	J	202	CDL	OA6-CA5-C11	3.59	119.24	111.48
50	F	501	FMN	C4-N3-C2	-3.47	119.47	125.64
45	m	201	LMT	C1'-C2'-C3'	3.47	117.30	110.01
56	P	501	NDP	O3-PA-O1A	-3.43	100.38	110.70
53	d	1202	CDL	OB8-CB7-C71	3.41	122.24	111.83
46	Y	401	3PE	O21-C21-C22	3.39	118.83	111.48
54	O	401	GTP	C2-N1-C6	-3.38	118.98	125.11
53	J	202	CDL	OB6-CB5-C51	3.35	118.72	111.48
45	m	201	LMT	O1B-C4'-C3'	3.27	115.55	107.23
46	I	201	3PE	O21-C21-C22	3.23	118.48	111.48
46	Y	401	3PE	O31-C31-C32	3.20	121.59	111.83
46	M	601	3PE	O31-C31-C32	3.17	121.51	111.83
53	d	1202	CDL	OA8-CA7-C31	3.17	121.51	111.83
46	H	401	3PE	O31-C31-C32	3.16	121.46	111.83
58	U	101	EHZ	O2-C9-C8	-3.08	118.89	123.74
48	B	203	PC1	O31-C31-C32	3.06	121.16	111.83
45	h	1002	LMT	O5'-C5'-C4'	3.03	115.98	109.72
45	h	1002	LMT	C1B-O1B-C4'	-3.02	110.83	117.98
46	M	604	3PE	O31-C31-C32	3.00	120.97	111.83
46	m	202	3PE	O31-C31-C32	2.98	120.92	111.83
45	f	1801	LMT	C1'-O5'-C5'	-2.97	107.92	113.72
54	O	401	GTP	O2G-PG-O3B	2.95	114.52	104.64
50	F	501	FMN	C4A-C10-N10	2.94	120.69	116.48
46	H	402	3PE	O31-C31-C32	2.93	120.77	111.83
53	h	1001	CDL	OB8-CB7-C71	2.88	120.62	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	302	3PE	O31-C31-C32	2.87	120.60	111.83
53	N	503	CDL	OB8-CB7-C71	2.85	120.51	111.83
56	P	501	NDP	PA-O5B-C5B	-2.83	105.15	121.35
53	h	1001	CDL	OA8-CA7-C31	2.83	120.45	111.83
52	N	504	I49	N05-C15-N02	2.82	127.87	117.97
52	N	504	I49	N05-C15-N04	-2.81	112.07	120.07
46	d	1201	3PE	O31-C31-C32	2.81	120.39	111.83
56	P	501	NDP	O2N-PN-O3	2.76	114.72	107.27
53	J	202	CDL	OB8-CB7-C71	2.75	120.23	111.83
45	M	603	LMT	C2'-C3'-C4'	2.75	115.92	109.68
53	q	201	CDL	OB8-CB7-C71	2.75	120.22	111.83
54	O	401	GTP	O3G-PG-O3B	2.75	113.85	104.64
50	F	501	FMN	C4A-C4-N3	2.68	120.08	113.25
52	H	403	I49	N05-C15-N04	-2.65	112.54	120.07
48	g	1501	PC1	O31-C31-C32	2.64	119.88	111.83
54	O	401	GTP	C1'-N9-C8	-2.63	119.27	126.73
56	P	501	NDP	PN-O5D-C5D	-2.62	106.33	121.35
45	J	201	LMT	O5'-C5'-C4'	2.60	115.10	109.72
46	L	705	3PE	O31-C31-C32	2.59	119.74	111.83
53	N	503	CDL	OB6-CB5-C51	2.58	120.42	110.93
46	L	704	3PE	O31-C31-C32	2.57	119.67	111.83
45	A	303	LMT	C1B-C2B-C3B	2.55	115.38	110.01
56	P	501	NDP	O3X-P2B-O2X	2.54	117.33	107.80
56	P	501	NDP	O4B-C4B-C3B	2.51	110.13	105.15
46	N	502	3PE	O31-C31-C32	2.50	119.47	111.83
45	f	1801	LMT	O5B-C5B-C4B	2.50	114.21	109.70
53	L	703	CDL	OB8-CB7-C71	2.50	119.45	111.83
45	A	303	LMT	O5'-C5'-C4'	2.49	114.87	109.72
54	O	401	GTP	C5-C6-N1	2.48	119.57	113.25
53	d	1202	CDL	CB4-OB6-CB5	-2.47	111.88	117.80
45	M	605	LMT	O5B-C5B-C4B	2.47	114.14	109.70
50	F	501	FMN	O4-C4-C4A	-2.46	120.03	126.53
50	F	501	FMN	C10-C4A-N5	-2.46	119.79	124.81
54	O	401	GTP	O2B-PB-O1B	-2.44	101.08	112.44
54	O	401	GTP	C2'-C3'-C4'	2.44	107.32	102.61
45	h	1002	LMT	C1'-O5'-C5'	2.44	118.48	113.72
53	L	703	CDL	OA8-CA7-C31	2.43	119.23	111.83
46	I	201	3PE	O31-C31-C32	2.42	119.21	111.83
54	O	401	GTP	O2A-PA-O1A	-2.41	101.23	112.44
53	N	503	CDL	OA8-CA7-C31	2.39	119.12	111.83
56	P	501	NDP	C2A-N1A-C6A	-2.39	114.81	118.73
45	m	201	LMT	O5B-C5B-C4B	2.38	113.99	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	L	701	3PE	O31-C31-C32	2.38	119.08	111.83
45	f	1801	LMT	C3B-C4B-C5B	2.38	114.54	110.23
53	J	202	CDL	OA8-CA7-C31	2.37	119.07	111.83
53	q	201	CDL	OA8-CA7-C31	2.36	119.02	111.83
45	m	201	LMT	C1'-O5'-C5'	2.35	118.31	113.72
45	M	605	LMT	C3B-C4B-C5B	2.34	114.48	110.23
54	O	401	GTP	O6-C6-C5	-2.34	120.36	126.53
52	H	403	I49	N02-C14-N01	-2.33	112.07	118.08
56	P	501	NDP	N3A-C4A-N9A	2.32	131.11	127.17
58	T	101	EHZ	O2-C9-S1	-2.32	119.74	122.68
45	f	1801	LMT	C1'-C2'-C3'	2.31	114.87	110.01
56	P	501	NDP	O5D-PN-O1N	-2.29	99.86	108.94
56	P	501	NDP	O2N-PN-O1N	2.29	123.08	112.44
56	P	501	NDP	C5B-C4B-C3B	-2.29	106.98	115.21
52	N	504	I49	C09-C07-C10	2.27	121.68	118.55
54	O	401	GTP	N9-C8-N7	-2.25	109.22	113.40
58	U	101	EHZ	O2-C9-S1	-2.25	119.82	122.68
58	T	101	EHZ	C13-C12-N1	2.25	120.44	116.34
56	P	501	NDP	O7N-C7N-N7N	-2.23	117.89	122.89
45	M	603	LMT	O2'-C2'-C3'	-2.22	105.15	110.38
54	O	401	GTP	C5-C4-N9	-2.21	101.69	105.66
45	A	301	LMT	O1B-C4'-C3'	2.20	112.83	107.23
45	f	1801	LMT	C2'-C3'-C4'	2.19	114.66	109.68
52	H	403	I49	C06-C07-C10	-2.19	116.86	120.54
45	L	702	LMT	O1'-C1'-C2'	2.19	111.60	108.27
53	N	503	CDL	CA4-OA6-CA5	-2.19	112.56	117.80
54	O	401	GTP	C3'-C2'-C1'	2.18	105.58	101.46
45	M	603	LMT	C1B-O5B-C5B	-2.15	109.51	113.72
45	L	702	LMT	C1B-O1B-C4'	-2.14	112.91	117.98
45	A	303	LMT	C1B-O1B-C4'	-2.12	112.95	117.98
52	N	504	I49	N02-C14-N01	-2.11	112.65	118.08
58	T	101	EHZ	C13-C14-N2	-2.10	107.53	112.00
45	Y	402	LMT	O1B-C4'-C3'	2.09	112.55	107.23
54	O	401	GTP	C4'-O4'-C1'	-2.09	104.85	109.47
56	P	501	NDP	C5A-C4A-N3A	-2.08	123.86	126.72
50	F	501	FMN	C4A-C10-N1	-2.07	119.53	124.59
58	U	101	EHZ	C13-C12-N1	2.05	120.08	116.34
45	M	603	LMT	O5'-C1'-C2'	2.03	114.55	110.37
45	M	603	LMT	C1B-O1B-C4'	-2.01	113.22	117.98
46	L	704	3PE	C2-O21-C21	-2.00	113.01	117.80

There are no chirality outliers.

All (647) 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	J	201	LMT	O5'-C1'-O1'-C1
45	J	201	LMT	C2-C1-O1'-C1'
45	M	602	LMT	C2'-C1'-O1'-C1
45	M	602	LMT	O5'-C1'-O1'-C1
45	M	602	LMT	C2-C1-O1'-C1'
45	Y	402	LMT	C2-C1-O1'-C1'
45	f	1801	LMT	O5'-C1'-O1'-C1
45	k	101	LMT	O5'-C1'-O1'-C1
46	A	302	3PE	O13-C11-C12-N
46	A	302	3PE	O21-C2-C3-O31
46	A	302	3PE	O22-C21-O21-C2
46	H	402	3PE	O13-C11-C12-N
46	H	402	3PE	C1-C2-O21-C21
46	H	402	3PE	O22-C21-O21-C2
46	I	201	3PE	C1-O11-P-O12
46	I	201	3PE	C1-O11-P-O13
46	I	201	3PE	C1-O11-P-O14
46	I	201	3PE	C11-O13-P-O11
46	I	201	3PE	C11-O13-P-O12
46	L	701	3PE	C1-O11-P-O13
46	L	701	3PE	C1-O11-P-O14
46	L	704	3PE	C11-O13-P-O11
46	L	704	3PE	C11-O13-P-O12
46	L	704	3PE	C11-O13-P-O14
46	L	704	3PE	O22-C21-O21-C2
46	L	704	3PE	C22-C21-O21-C2
46	L	705	3PE	C11-O13-P-O14
46	L	705	3PE	C22-C21-O21-C2
46	M	601	3PE	C1-O11-P-O12
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	604	3PE	O13-C11-C12-N
46	N	502	3PE	C11-O13-P-O11
46	N	502	3PE	C11-O13-P-O12
46	N	502	3PE	O13-C11-C12-N
46	N	502	3PE	O21-C2-C3-O31
46	d	1201	3PE	C1-O11-P-O12
46	d	1201	3PE	O13-C11-C12-N
46	d	1201	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	m	202	3PE	C1-O11-P-O12
46	m	202	3PE	C1-O11-P-O13
46	m	202	3PE	C1-O11-P-O14
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O13-C11-C12-N
46	m	202	3PE	C22-C21-O21-C2
48	g	1501	PC1	C11-O13-P-O12
48	g	1501	PC1	C11-O13-P-O14
48	g	1501	PC1	C11-O13-P-O11
48	g	1501	PC1	C1-O11-P-O12
48	g	1501	PC1	C1-O11-P-O14
48	g	1501	PC1	C1-O11-P-O13
48	g	1501	PC1	O13-C11-C12-N
52	H	403	I49	C07-C06-C08-N01
52	H	403	I49	N05-C15-N02-C14
52	N	504	I49	C07-C06-C08-N01
52	N	504	I49	N01-C14-N02-C15
52	N	504	I49	N03-C14-N02-C15
53	J	202	CDL	CB2-OB2-PB2-OB4
53	J	202	CDL	CB2-OB2-PB2-OB5
53	J	202	CDL	CB3-OB5-PB2-OB2
53	L	703	CDL	CB2-OB2-PB2-OB3
53	L	703	CDL	CB2-OB2-PB2-OB4
53	N	503	CDL	O1-C1-CA2-OA2
53	N	503	CDL	CA2-OA2-PA1-OA4
53	N	503	CDL	CA3-OA5-PA1-OA2
53	N	503	CDL	CA3-OA5-PA1-OA3
53	N	503	CDL	CA3-OA5-PA1-OA4
53	N	503	CDL	C11-CA5-OA6-CA4
53	N	503	CDL	CB3-OB5-PB2-OB2
53	N	503	CDL	CB3-OB5-PB2-OB4
53	N	503	CDL	OB7-CB5-OB6-CB4
53	d	1202	CDL	OA7-CA5-OA6-CA4
53	d	1202	CDL	C11-CA5-OA6-CA4
53	h	1001	CDL	CA2-C1-CB2-OB2
53	h	1001	CDL	CA2-OA2-PA1-OA3
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CB3-OB5-PB2-OB3
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA3
53	q	201	CDL	CA2-OA2-PA1-OA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CA3-OA5-PA1-OA4
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	CB3-OB5-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
58	T	101	EHZ	C5-C6-C7-C8
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
59	o	201	MYR	O1-C1-C2-C3
45	M	605	LMT	O5B-C1B-O1B-C4'
45	m	201	LMT	C3'-C4'-O1B-C1B
45	M	605	LMT	C2B-C1B-O1B-C4'
53	d	1202	CDL	OB9-CB7-OB8-CB6
45	m	201	LMT	O5B-C1B-O1B-C4'
53	L	703	CDL	CB4-CB6-OB8-CB7
53	d	1202	CDL	C71-CB7-OB8-CB6
46	H	401	3PE	O32-C31-O31-C3
46	L	704	3PE	O32-C31-O31-C3
46	L	705	3PE	O32-C31-O31-C3
46	M	604	3PE	O32-C31-O31-C3
46	Y	401	3PE	O32-C31-O31-C3
46	d	1201	3PE	O32-C31-O31-C3
53	d	1202	CDL	OA9-CA7-OA8-CA6
53	h	1001	CDL	OB9-CB7-OB8-CB6
45	m	201	LMT	C2B-C1B-O1B-C4'
46	L	705	3PE	O22-C21-O21-C2
46	d	1201	3PE	O22-C21-O21-C2
46	m	202	3PE	O22-C21-O21-C2
53	N	503	CDL	OA7-CA5-OA6-CA4
45	A	301	LMT	C3'-C4'-O1B-C1B
46	L	704	3PE	C32-C31-O31-C3
46	L	705	3PE	C32-C31-O31-C3
46	M	604	3PE	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	Y	401	3PE	C32-C31-O31-C3
46	d	1201	3PE	C32-C31-O31-C3
46	A	302	3PE	C22-C21-O21-C2
53	N	503	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	C51-CB5-OB6-CB4
46	H	401	3PE	C32-C31-O31-C3
53	L	703	CDL	C71-CB7-OB8-CB6
53	d	1202	CDL	C31-CA7-OA8-CA6
53	h	1001	CDL	C71-CB7-OB8-CB6
45	A	301	LMT	O5'-C5'-C6'-O6'
45	L	702	LMT	O5'-C5'-C6'-O6'
45	M	603	LMT	O5B-C5B-C6B-O6B
45	m	201	LMT	O5B-C5B-C6B-O6B
46	N	502	3PE	O32-C31-O31-C3
53	N	503	CDL	OB9-CB7-OB8-CB6
45	N	501	LMT	C3'-C4'-O1B-C1B
53	h	1001	CDL	O1-C1-CB2-OB2
53	N	503	CDL	C71-CB7-OB8-CB6
45	N	501	LMT	O5'-C5'-C6'-O6'
45	Y	402	LMT	O5B-C5B-C6B-O6B
45	M	603	LMT	C4B-C5B-C6B-O6B
45	l	201	LMT	C4'-C5'-C6'-O6'
46	N	502	3PE	C22-C21-O21-C2
45	M	605	LMT	C5'-C4'-O1B-C1B
45	A	301	LMT	O5B-C5B-C6B-O6B
45	B	202	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4B-C5B-C6B-O6B
45	A	301	LMT	C4'-C5'-C6'-O6'
45	m	201	LMT	C4B-C5B-C6B-O6B
46	N	502	3PE	C32-C31-O31-C3
45	M	602	LMT	O5'-C5'-C6'-O6'
45	L	702	LMT	C4'-C5'-C6'-O6'
53	L	703	CDL	OB9-CB7-OB8-CB6
45	A	303	LMT	O5'-C1'-O1'-C1
48	B	203	PC1	C32-C31-O31-C3
45	B	202	LMT	C3'-C4'-O1B-C1B
45	A	303	LMT	O5'-C5'-C6'-O6'
45	Y	402	LMT	O5'-C5'-C6'-O6'
45	Y	402	LMT	C4B-C5B-C6B-O6B
45	f	1801	LMT	C4'-C5'-C6'-O6'
53	q	201	CDL	C11-CA5-OA6-CA4
45	A	303	LMT	C4'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	402	LMT	C4'-C5'-C6'-O6'
48	B	203	PC1	O32-C31-O31-C3
48	g	1501	PC1	C32-C31-O31-C3
45	J	201	LMT	O5B-C5B-C6B-O6B
45	N	501	LMT	C4'-C5'-C6'-O6'
45	A	303	LMT	C2'-C1'-O1'-C1
53	N	503	CDL	O1-C1-CB2-OB2
53	q	201	CDL	O1-C1-CA2-OA2
45	l	201	LMT	O5'-C5'-C6'-O6'
45	J	201	LMT	C4'-C5'-C6'-O6'
58	T	101	EHZ	C5-C6-C7-O1
58	U	101	EHZ	C5-C6-C7-O1
45	J	201	LMT	O5'-C5'-C6'-O6'
45	f	1801	LMT	O5'-C5'-C6'-O6'
46	N	502	3PE	O22-C21-O21-C2
53	h	1001	CDL	C31-CA7-OA8-CA6
45	f	1801	LMT	O5B-C5B-C6B-O6B
46	m	202	3PE	C21-C22-C23-C24
53	q	201	CDL	OA7-CA5-OA6-CA4
45	M	602	LMT	C4'-C5'-C6'-O6'
46	I	201	3PE	C21-C22-C23-C24
46	L	701	3PE	C31-C32-C33-C34
46	M	604	3PE	C31-C32-C33-C34
53	J	202	CDL	CA5-C11-C12-C13
53	d	1202	CDL	CA5-C11-C12-C13
46	Y	401	3PE	C22-C21-O21-C2
46	H	402	3PE	C2-C1-O11-P
45	B	202	LMT	C4'-C5'-C6'-O6'
46	H	401	3PE	C31-C32-C33-C34
46	M	601	3PE	C21-C22-C23-C24
48	g	1501	PC1	O32-C31-O31-C3
45	h	1002	LMT	C2-C3-C4-C5
53	q	201	CDL	C31-CA7-OA8-CA6
46	L	701	3PE	C22-C21-O21-C2
53	h	1001	CDL	C11-CA5-OA6-CA4
45	f	1801	LMT	O5B-C1B-O1B-C4'
53	h	1001	CDL	CB5-C51-C52-C53
46	Y	401	3PE	O22-C21-O21-C2
53	h	1001	CDL	OA7-CA5-OA6-CA4
53	N	503	CDL	CB2-C1-CA2-OA2
53	h	1001	CDL	OA9-CA7-OA8-CA6
53	N	503	CDL	CA7-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	201	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	O22-C21-O21-C2
53	d	1202	CDL	O1-C1-CB2-OB2
48	B	203	PC1	C31-C32-C33-C34
53	J	202	CDL	OA7-CA5-OA6-CA4
45	B	202	LMT	O5'-C1'-O1'-C1
53	J	202	CDL	C11-CA5-OA6-CA4
46	L	705	3PE	C21-C22-C23-C24
45	k	101	LMT	O5'-C5'-C6'-O6'
53	q	201	CDL	OA9-CA7-OA8-CA6
45	M	605	LMT	C3'-C4'-O1B-C1B
48	g	1501	PC1	C2C-C2D-C2E-C2F
53	L	703	CDL	C55-C56-C57-C58
45	M	602	LMT	C5-C6-C7-C8
46	N	502	3PE	C29-C2A-C2B-C2C
46	H	402	3PE	C35-C36-C37-C38
46	L	701	3PE	C22-C23-C24-C25
46	d	1201	3PE	C33-C34-C35-C36
53	N	503	CDL	C33-C34-C35-C36
53	q	201	CDL	C59-C60-C61-C62
46	A	302	3PE	C2A-C2B-C2C-C2D
46	M	604	3PE	C3A-C3B-C3C-C3D
46	M	604	3PE	C22-C23-C24-C25
46	L	704	3PE	C21-C22-C23-C24
53	d	1202	CDL	CB7-C71-C72-C73
46	L	704	3PE	C3C-C3D-C3E-C3F
46	L	704	3PE	C25-C26-C27-C28
53	N	503	CDL	C73-C74-C75-C76
59	o	201	MYR	C2-C3-C4-C5
46	M	601	3PE	C37-C38-C39-C3A
53	q	201	CDL	C52-C53-C54-C55
53	q	201	CDL	C57-C58-C59-C60
46	d	1201	3PE	C21-C22-C23-C24
53	d	1202	CDL	C57-C58-C59-C60
53	d	1202	CDL	CA2-C1-CB2-OB2
53	q	201	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	CB3-CB4-CB6-OB8
46	I	201	3PE	C3A-C3B-C3C-C3D
46	N	502	3PE	C34-C35-C36-C37
53	h	1001	CDL	C20-C21-C22-C23
58	U	101	EHZ	C3-C4-C5-C6
53	q	201	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	I	201	3PE	C33-C34-C35-C36
46	m	202	3PE	C33-C34-C35-C36
48	g	1501	PC1	C29-C2A-C2B-C2C
53	N	503	CDL	C32-C33-C34-C35
59	o	201	MYR	C9-C10-C11-C12
46	L	704	3PE	C38-C39-C3A-C3B
46	L	705	3PE	C33-C34-C35-C36
45	Y	402	LMT	C3-C4-C5-C6
53	h	1001	CDL	C72-C73-C74-C75
48	g	1501	PC1	C2E-C2F-C2G-C2H
53	L	703	CDL	C51-CB5-OB6-CB4
45	h	1002	LMT	C4-C5-C6-C7
46	N	502	3PE	C33-C34-C35-C36
53	d	1202	CDL	C56-C57-C58-C59
46	Y	401	3PE	C37-C38-C39-C3A
53	N	503	CDL	C31-C32-C33-C34
53	L	703	CDL	C13-C14-C15-C16
46	A	302	3PE	C35-C36-C37-C38
46	A	302	3PE	C28-C29-C2A-C2B
46	H	401	3PE	C37-C38-C39-C3A
46	L	704	3PE	C32-C33-C34-C35
53	q	201	CDL	C11-C12-C13-C14
46	L	701	3PE	C32-C31-O31-C3
46	M	604	3PE	C2E-C2F-C2G-C2H
53	J	202	CDL	C12-C13-C14-C15
53	h	1001	CDL	C17-C18-C19-C20
45	m	201	LMT	C2'-C1'-O1'-C1
45	A	303	LMT	C6-C7-C8-C9
46	I	201	3PE	C2C-C2D-C2E-C2F
46	M	601	3PE	C39-C3A-C3B-C3C
46	M	604	3PE	C22-C21-O21-C2
53	d	1202	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	OB9-CB7-OB8-CB6
59	o	201	MYR	C11-C10-C9-C8
45	N	501	LMT	C1-C2-C3-C4
46	L	701	3PE	C29-C2A-C2B-C2C
46	M	604	3PE	C26-C27-C28-C29
53	d	1202	CDL	C11-C12-C13-C14
46	L	705	3PE	C31-C32-C33-C34
46	Y	401	3PE	C31-C32-C33-C34
46	L	705	3PE	C32-C33-C34-C35
46	d	1201	3PE	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	d	1202	CDL	C15-C16-C17-C18
53	L	703	CDL	C34-C35-C36-C37
53	q	201	CDL	OB5-CB3-CB4-OB6
48	g	1501	PC1	O21-C2-C3-O31
53	q	201	CDL	OB6-CB4-CB6-OB8
45	M	602	LMT	C4B-C5B-C6B-O6B
53	q	201	CDL	C31-C32-C33-C34
46	Y	401	3PE	C2-C1-O11-P
45	Y	402	LMT	C5'-C4'-O1B-C1B
45	B	202	LMT	C3-C4-C5-C6
45	Y	402	LMT	C2-C3-C4-C5
45	A	303	LMT	C11-C10-C9-C8
45	N	501	LMT	O5B-C5B-C6B-O6B
53	N	503	CDL	C76-C77-C78-C79
58	T	101	EHZ	O4-C15-C16-O5
53	J	202	CDL	C36-C37-C38-C39
53	h	1001	CDL	C12-C13-C14-C15
46	L	704	3PE	O11-C1-C2-C3
46	M	604	3PE	O22-C21-O21-C2
45	l	201	LMT	C4-C5-C6-C7
48	g	1501	PC1	C32-C33-C34-C35
58	U	101	EHZ	C1-C2-C3-C4
46	H	401	3PE	C3B-C3C-C3D-C3E
46	M	604	3PE	C2B-C2C-C2D-C2E
53	q	201	CDL	C37-C38-C39-C40
46	M	601	3PE	C22-C21-O21-C2
46	A	302	3PE	C2C-C2D-C2E-C2F
46	A	302	3PE	C3E-C3F-C3G-C3H
45	Y	402	LMT	C3'-C4'-O1B-C1B
53	L	703	CDL	OB7-CB5-OB6-CB4
53	h	1001	CDL	CA7-C31-C32-C33
46	L	701	3PE	C24-C25-C26-C27
48	g	1501	PC1	C26-C27-C28-C29
53	L	703	CDL	CA5-C11-C12-C13
46	L	701	3PE	O32-C31-O31-C3
46	H	401	3PE	C35-C36-C37-C38
50	F	501	FMN	C5'-O5'-P-O1P
46	M	604	3PE	C3D-C3E-C3F-C3G
46	A	302	3PE	C26-C27-C28-C29
46	A	302	3PE	C32-C31-O31-C3
46	A	302	3PE	C1-C2-O21-C21
46	L	701	3PE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C2A-C2B-C2C-C2D
53	h	1001	CDL	C71-C72-C73-C74
45	B	202	LMT	C5'-C4'-O1B-C1B
45	f	1801	LMT	C3'-C4'-O1B-C1B
45	l	201	LMT	C1-C2-C3-C4
45	f	1801	LMT	C5'-C4'-O1B-C1B
53	N	503	CDL	OA5-CA3-CA4-OA6
46	d	1201	3PE	C37-C38-C39-C3A
45	J	201	LMT	C4B-C5B-C6B-O6B
48	B	203	PC1	C32-C33-C34-C35
46	N	502	3PE	C23-C24-C25-C26
53	h	1001	CDL	C21-C22-C23-C24
53	q	201	CDL	C72-C73-C74-C75
46	I	201	3PE	C23-C24-C25-C26
53	d	1202	CDL	OB7-CB5-OB6-CB4
54	O	401	GTP	PG-O3B-PB-O1B
46	m	202	3PE	C35-C36-C37-C38
53	L	703	CDL	C57-C58-C59-C60
45	M	603	LMT	C2-C1-O1'-C1'
53	J	202	CDL	CB4-CB3-OB5-PB2
53	q	201	CDL	CA4-CA3-OA5-PA1
53	q	201	CDL	C51-C52-C53-C54
46	M	601	3PE	C31-C32-C33-C34
53	L	703	CDL	OB5-CB3-CB4-CB6
53	d	1202	CDL	OB5-CB3-CB4-CB6
46	L	701	3PE	C37-C38-C39-C3A
59	o	201	MYR	C11-C12-C13-C14
45	m	201	LMT	O5'-C5'-C6'-O6'
53	h	1001	CDL	C24-C25-C26-C27
46	A	302	3PE	C3C-C3D-C3E-C3F
46	I	201	3PE	C27-C28-C29-C2A
46	A	302	3PE	C1-C2-C3-O31
46	L	701	3PE	C1-C2-C3-O31
46	N	502	3PE	C1-C2-C3-O31
48	B	203	PC1	C1-C2-C3-O31
48	g	1501	PC1	C1-C2-C3-O31
46	m	202	3PE	C2A-C2B-C2C-C2D
45	M	602	LMT	O5B-C5B-C6B-O6B
59	o	201	MYR	C4-C5-C6-C7
46	A	302	3PE	O32-C31-O31-C3
45	N	501	LMT	C5'-C4'-O1B-C1B
46	L	704	3PE	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	L	703	CDL	OB5-CB3-CB4-OB6
46	L	701	3PE	C32-C33-C34-C35
58	T	101	EHZ	O1-C7-C8-C9
58	U	101	EHZ	O2-C9-S1-C10
45	l	201	LMT	C5'-C4'-O1B-C1B
46	L	701	3PE	C36-C37-C38-C39
46	H	402	3PE	C33-C34-C35-C36
53	N	503	CDL	C42-C43-C44-C45
53	h	1001	CDL	C16-C17-C18-C19
46	H	401	3PE	O21-C2-C3-O31
46	M	601	3PE	O21-C2-C3-O31
48	B	203	PC1	O21-C2-C3-O31
53	d	1202	CDL	OB6-CB4-CB6-OB8
53	d	1202	CDL	C72-C73-C74-C75
58	T	101	EHZ	C21-C22-C23-C24
46	Y	401	3PE	C21-C22-C23-C24
46	L	701	3PE	C2F-C2G-C2H-C2I
46	I	201	3PE	C32-C31-O31-C3
53	J	202	CDL	C31-CA7-OA8-CA6
45	l	201	LMT	C3'-C4'-O1B-C1B
46	H	402	3PE	C3C-C3D-C3E-C3F
46	L	701	3PE	C2B-C2C-C2D-C2E
53	L	703	CDL	C54-C55-C56-C57
52	H	403	I49	N03-C14-N02-C15
58	T	101	EHZ	C6-C7-C8-C9
53	h	1001	CDL	C73-C74-C75-C76
46	M	604	3PE	C39-C3A-C3B-C3C
58	U	101	EHZ	C8-C9-S1-C10
46	M	601	3PE	C28-C29-C2A-C2B
53	N	503	CDL	C75-C76-C77-C78
53	q	201	CDL	OB5-CB3-CB4-CB6
53	J	202	CDL	OA9-CA7-OA8-CA6
53	d	1202	CDL	C20-C21-C22-C23
46	d	1201	3PE	C31-C32-C33-C34
46	M	601	3PE	O22-C21-O21-C2
46	m	202	3PE	C2D-C2E-C2F-C2G
45	A	301	LMT	C1-C2-C3-C4
46	I	201	3PE	O32-C31-O31-C3
46	M	601	3PE	C3-C2-O21-C21
46	Y	401	3PE	C1-C2-C3-O31
53	d	1202	CDL	CA3-CA4-CA6-OA8
53	d	1202	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C12-C11-O13-P
46	M	604	3PE	C12-C11-O13-P
46	m	202	3PE	C12-C11-O13-P
45	l	201	LMT	C4B-C5B-C6B-O6B
46	L	701	3PE	O21-C2-C3-O31
46	Y	401	3PE	O21-C2-C3-O31
53	d	1202	CDL	OA6-CA4-CA6-OA8
46	I	201	3PE	C25-C26-C27-C28
53	J	202	CDL	C18-C19-C20-C21
53	h	1001	CDL	C32-C33-C34-C35
46	N	502	3PE	C32-C33-C34-C35
53	J	202	CDL	C14-C15-C16-C17
54	O	401	GTP	PB-O3A-PA-O1A
45	l	201	LMT	O1'-C1-C2-C3
46	A	302	3PE	C21-C22-C23-C24
45	B	202	LMT	C7-C8-C9-C10
48	g	1501	PC1	C37-C38-C39-C3A
53	J	202	CDL	C71-C72-C73-C74
46	H	401	3PE	C23-C24-C25-C26
46	m	202	3PE	C23-C24-C25-C26
46	Y	401	3PE	O11-C1-C2-C3
53	N	503	CDL	OA5-CA3-CA4-CA6
46	H	402	3PE	C37-C38-C39-C3A
45	Y	402	LMT	C1-C2-C3-C4
53	J	202	CDL	C52-C53-C54-C55
46	d	1201	3PE	C2-C1-O11-P
53	N	503	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	OB5-CB3-CB4-OB6
53	q	201	CDL	OA5-CA3-CA4-OA6
52	H	403	I49	C08-C06-C07-C10
46	L	701	3PE	C2E-C2F-C2G-C2H
46	M	601	3PE	C36-C37-C38-C39
53	q	201	CDL	C39-C40-C41-C42
45	N	501	LMT	C4-C5-C6-C7
52	H	403	I49	N01-C14-N02-C15
52	H	403	I49	C08-C06-C07-C09
46	L	705	3PE	O21-C2-C3-O31
46	d	1201	3PE	O21-C2-C3-O31
46	L	705	3PE	C1-C2-C3-O31
46	M	601	3PE	C1-C2-C3-O31
46	d	1201	3PE	C1-C2-C3-O31
53	J	202	CDL	CA3-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	402	3PE	C3D-C3E-C3F-C3G
46	L	701	3PE	C21-C22-C23-C24
53	J	202	CDL	C20-C21-C22-C23
46	M	604	3PE	C36-C37-C38-C39
45	M	603	LMT	C1-C2-C3-C4
45	M	602	LMT	C2-C3-C4-C5
53	d	1202	CDL	C54-C55-C56-C57
46	H	401	3PE	C1-O11-P-O14
46	H	401	3PE	O13-C11-C12-N
46	H	402	3PE	C11-O13-P-O14
46	L	701	3PE	C11-O13-P-O14
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C1-O11-P-O13
46	L	704	3PE	C1-O11-P-O14
46	L	705	3PE	C11-O13-P-O11
46	L	705	3PE	O13-C11-C12-N
46	M	604	3PE	C1-O11-P-O14
46	Y	401	3PE	C1-O11-P-O14
46	Y	401	3PE	O13-C11-C12-N
46	d	1201	3PE	C1-O11-P-O13
46	d	1201	3PE	C1-O11-P-O14
48	B	203	PC1	C11-O13-P-O14
48	B	203	PC1	C11-O13-P-O11
53	J	202	CDL	CA3-OA5-PA1-OA2
53	J	202	CDL	CA3-OA5-PA1-OA3
53	J	202	CDL	CA3-OA5-PA1-OA4
53	J	202	CDL	CB3-OB5-PB2-OB3
53	L	703	CDL	CA3-OA5-PA1-OA3
53	L	703	CDL	CB2-OB2-PB2-OB5
53	N	503	CDL	CA2-OA2-PA1-OA3
53	N	503	CDL	CA2-OA2-PA1-OA5
53	N	503	CDL	CB2-OB2-PB2-OB3
53	N	503	CDL	CB2-OB2-PB2-OB4
53	N	503	CDL	CB2-OB2-PB2-OB5
53	d	1202	CDL	CB2-OB2-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O2A
46	m	202	3PE	C27-C28-C29-C2A
53	d	1202	CDL	C53-C54-C55-C56
45	N	501	LMT	C3-C4-C5-C6
53	d	1202	CDL	CB4-CB3-OB5-PB2
53	q	201	CDL	C1-CA2-OA2-PA1
52	H	403	I49	N04-C15-N02-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	m	202	3PE	O11-C1-C2-C3
53	J	202	CDL	OB5-CB3-CB4-CB6
53	N	503	CDL	OB5-CB3-CB4-CB6
53	N	503	CDL	C38-C39-C40-C41
46	Y	401	3PE	O11-C1-C2-O21
46	m	202	3PE	O11-C1-C2-O21
45	A	301	LMT	O1'-C1-C2-C3
46	A	302	3PE	C2B-C2C-C2D-C2E
48	g	1501	PC1	C2B-C2C-C2D-C2E
53	J	202	CDL	C33-C34-C35-C36
53	q	201	CDL	C13-C14-C15-C16
48	g	1501	PC1	C2-C1-O11-P
48	g	1501	PC1	C2A-C2B-C2C-C2D
46	H	401	3PE	C24-C25-C26-C27
53	q	201	CDL	C15-C16-C17-C18
46	M	601	3PE	C25-C26-C27-C28
46	M	604	3PE	C37-C38-C39-C3A
46	H	401	3PE	C27-C28-C29-C2A
53	q	201	CDL	C35-C36-C37-C38
53	d	1202	CDL	C18-C19-C20-C21
46	H	401	3PE	C1-C2-C3-O31
58	T	101	EHZ	C21-C1-C2-C3
56	P	501	NDP	PN-O3-PA-O1A
53	d	1202	CDL	C52-C51-CB5-OB6
53	J	202	CDL	C16-C17-C18-C19
46	M	604	3PE	C33-C34-C35-C36
45	M	605	LMT	C5-C6-C7-C8
46	Y	401	3PE	C3B-C3C-C3D-C3E
45	M	605	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2-C1-O1'-C1'
46	N	502	3PE	C22-C23-C24-C25
45	A	301	LMT	C5'-C4'-O1B-C1B
46	M	604	3PE	O11-C1-C2-O21
53	N	503	CDL	C44-C45-C46-C47
46	H	402	3PE	C32-C33-C34-C35
46	M	601	3PE	C2E-C2F-C2G-C2H
46	H	401	3PE	C32-C33-C34-C35
53	L	703	CDL	C60-C61-C62-C63
53	J	202	CDL	C40-C41-C42-C43
56	P	501	NDP	O4D-C1D-N1N-C6N
53	J	202	CDL	C1-CB2-OB2-PB2
46	L	701	3PE	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	N	501	LMT	C11-C10-C9-C8
45	B	202	LMT	O5B-C5B-C6B-O6B
53	q	201	CDL	CB2-C1-CA2-OA2
53	d	1202	CDL	C19-C20-C21-C22
53	h	1001	CDL	C31-C32-C33-C34
45	M	605	LMT	C9-C10-C11-C12
46	L	704	3PE	C35-C36-C37-C38
53	L	703	CDL	C33-C34-C35-C36
46	M	604	3PE	C23-C24-C25-C26
46	d	1201	3PE	C3D-C3E-C3F-C3G
46	A	302	3PE	C2-C1-O11-P
53	q	201	CDL	OA5-CA3-CA4-CA6
45	M	602	LMT	O1'-C1-C2-C3
53	J	202	CDL	OA6-CA4-CA6-OA8
52	H	403	I49	C06-C08-N01-C14
46	L	704	3PE	C3B-C3C-C3D-C3E
53	L	703	CDL	OA7-CA5-OA6-CA4
53	L	703	CDL	CA2-C1-CB2-OB2
46	I	201	3PE	C32-C33-C34-C35
45	A	301	LMT	C2-C3-C4-C5
45	M	602	LMT	C6-C7-C8-C9
45	B	202	LMT	C5-C6-C7-C8
45	M	605	LMT	C7-C8-C9-C10
56	P	501	NDP	PN-O3-PA-O2A
48	B	203	PC1	C2-C1-O11-P
46	Y	401	3PE	C39-C3A-C3B-C3C
46	H	401	3PE	C38-C39-C3A-C3B
56	P	501	NDP	C2D-C1D-N1N-C6N
53	J	202	CDL	OB5-CB3-CB4-OB6
45	A	303	LMT	C2-C3-C4-C5
46	M	601	3PE	C26-C27-C28-C29
53	N	503	CDL	CA2-C1-CB2-OB2
46	M	601	3PE	O11-C1-C2-C3
46	d	1201	3PE	C38-C39-C3A-C3B
45	h	1002	LMT	C3-C4-C5-C6
53	d	1202	CDL	C75-C76-C77-C78
46	M	604	3PE	C3F-C3G-C3H-C3I
46	N	502	3PE	O31-C31-C32-C33
46	d	1201	3PE	C3A-C3B-C3C-C3D
46	A	302	3PE	C27-C28-C29-C2A
46	L	704	3PE	C28-C29-C2A-C2B
53	d	1202	CDL	CA7-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	I	201	3PE	C31-C32-C33-C34
53	h	1001	CDL	C22-C23-C24-C25
46	I	201	3PE	C37-C38-C39-C3A
45	J	201	LMT	C2B-C1B-O1B-C4'
46	H	401	3PE	C12-C11-O13-P
53	h	1001	CDL	C15-C16-C17-C18
46	M	601	3PE	C23-C24-C25-C26
45	J	201	LMT	O5B-C1B-O1B-C4'
46	Y	401	3PE	C22-C23-C24-C25
46	L	704	3PE	C29-C2A-C2B-C2C
45	l	201	LMT	O5B-C5B-C6B-O6B
46	m	202	3PE	O21-C21-C22-C23
46	d	1201	3PE	C34-C35-C36-C37
45	k	101	LMT	O5B-C1B-O1B-C4'
53	L	703	CDL	C11-CA5-OA6-CA4
45	l	201	LMT	O5B-C1B-O1B-C4'
46	L	701	3PE	O21-C21-C22-C23
45	f	1801	LMT	C4B-C5B-C6B-O6B
53	q	201	CDL	C52-C51-CB5-OB6
56	P	501	NDP	C2B-O2B-P2B-O3X
45	M	605	LMT	O5'-C5'-C6'-O6'
46	d	1201	3PE	O21-C21-C22-C23
53	L	703	CDL	C52-C51-CB5-OB6
53	q	201	CDL	C32-C31-CA7-OA8
53	J	202	CDL	O1-C1-CB2-OB2
46	d	1201	3PE	C35-C36-C37-C38
45	Y	402	LMT	O5'-C1'-O1'-C1
46	M	604	3PE	O21-C21-C22-C23
50	F	501	FMN	N10-C1'-C2'-O2'
45	k	101	LMT	C2B-C1B-O1B-C4'
46	M	604	3PE	C35-C36-C37-C38
46	I	201	3PE	C38-C39-C3A-C3B
53	L	703	CDL	O1-C1-CB2-OB2
46	L	704	3PE	O21-C21-C22-C23
48	g	1501	PC1	C23-C24-C25-C26
53	L	703	CDL	C35-C36-C37-C38
45	f	1801	LMT	C5-C6-C7-C8
46	m	202	3PE	O22-C21-C22-C23
45	A	303	LMT	C5'-C4'-O1B-C1B
46	N	502	3PE	C2-C1-O11-P
46	m	202	3PE	C24-C25-C26-C27
48	B	203	PC1	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	B	203	PC1	O21-C21-C22-C23
45	k	101	LMT	C4-C5-C6-C7
58	U	101	EHZ	C1-C21-C22-C23
46	L	701	3PE	O22-C21-C22-C23
53	q	201	CDL	C32-C31-CA7-OA9
53	d	1202	CDL	C12-C11-CA5-OA6
46	d	1201	3PE	O22-C21-C22-C23
53	L	703	CDL	CB3-CB4-CB6-OB8
50	F	501	FMN	C4'-C5'-O5'-P
53	L	703	CDL	C32-C31-CA7-OA8
46	M	604	3PE	O22-C21-C22-C23
45	Y	402	LMT	O1'-C1-C2-C3
53	q	201	CDL	C52-C51-CB5-OB7
48	B	203	PC1	O31-C31-C32-C33
53	d	1202	CDL	C32-C31-CA7-OA8
56	P	501	NDP	O4D-C4D-C5D-O5D
53	L	703	CDL	C52-C51-CB5-OB7

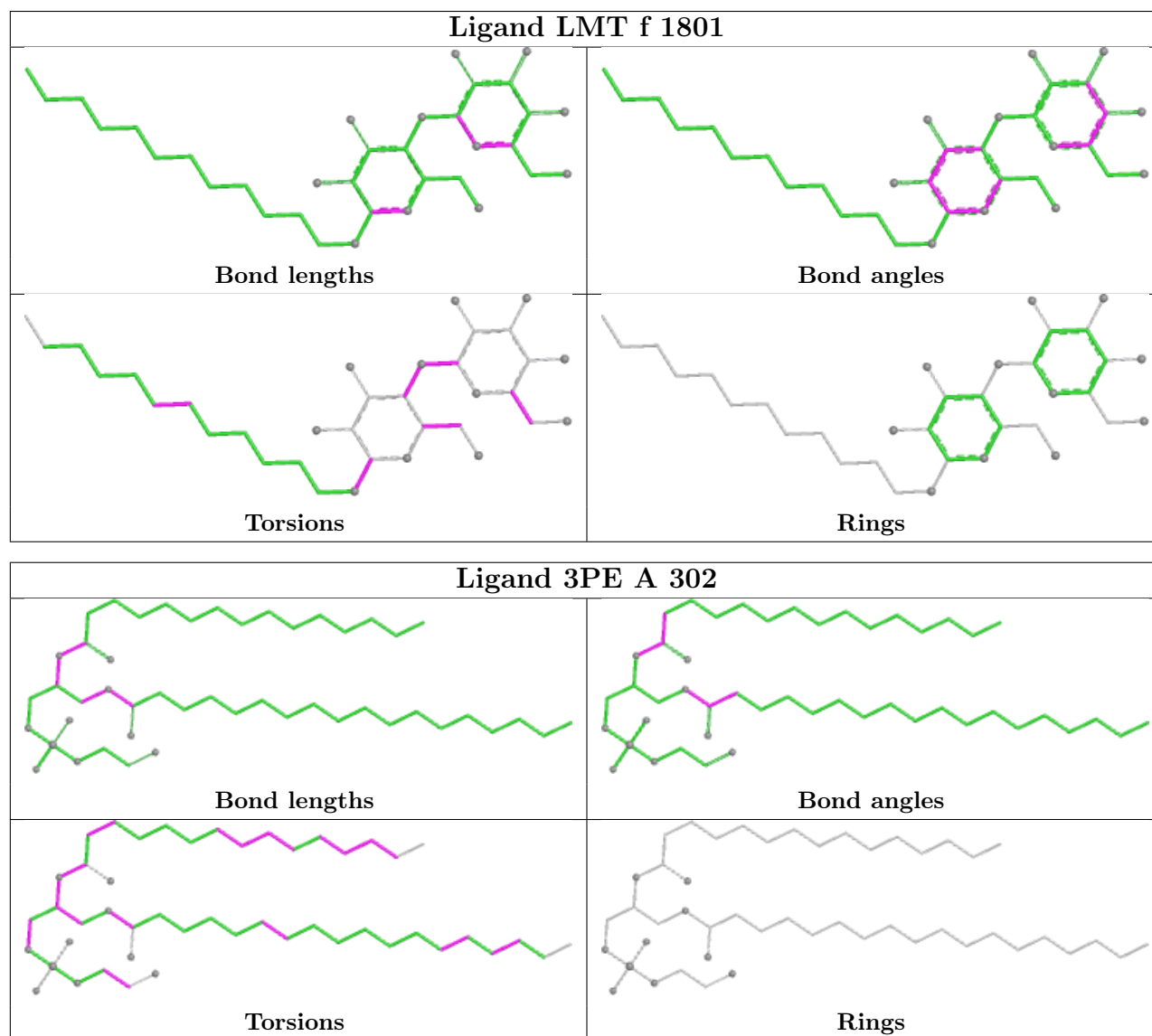
There are no ring outliers.

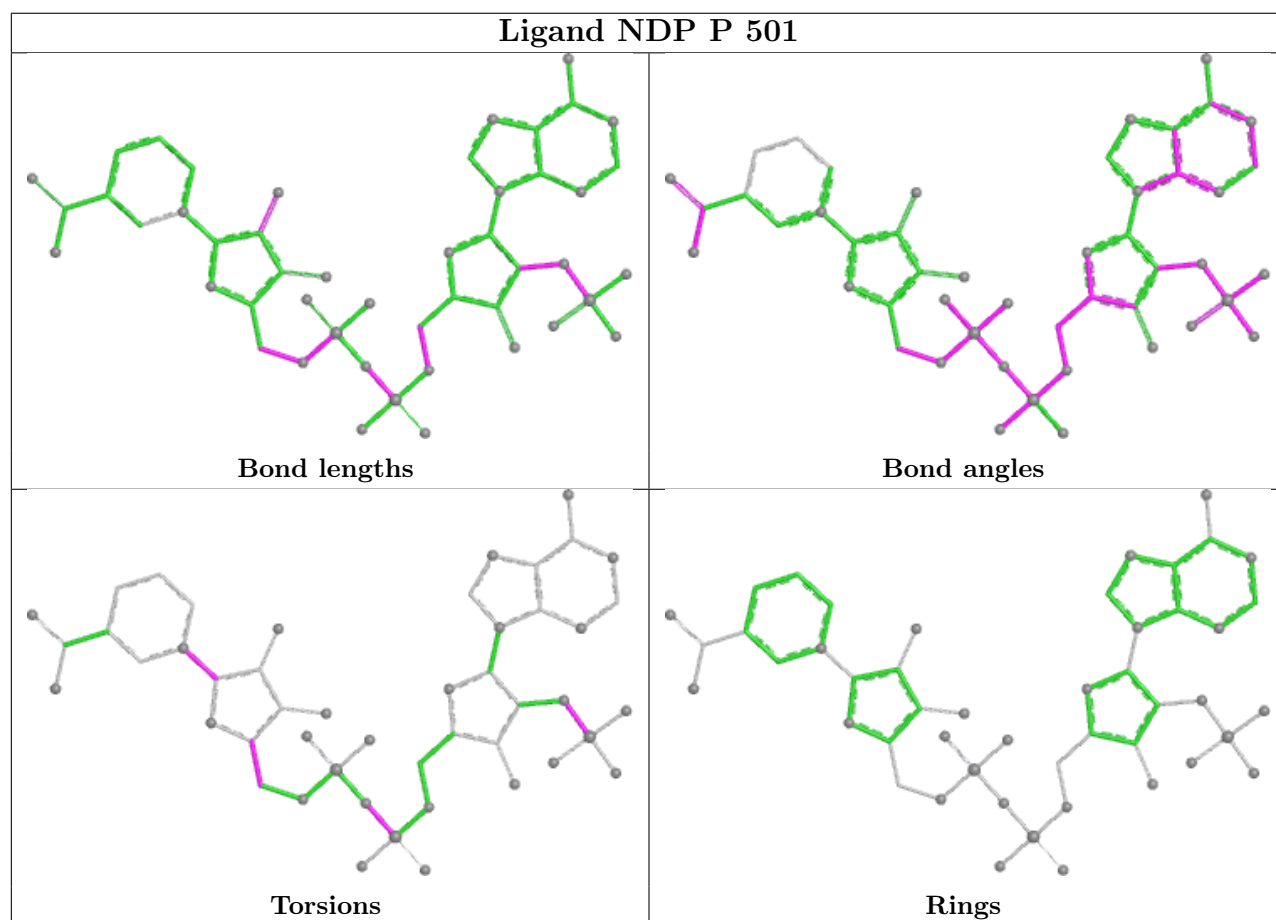
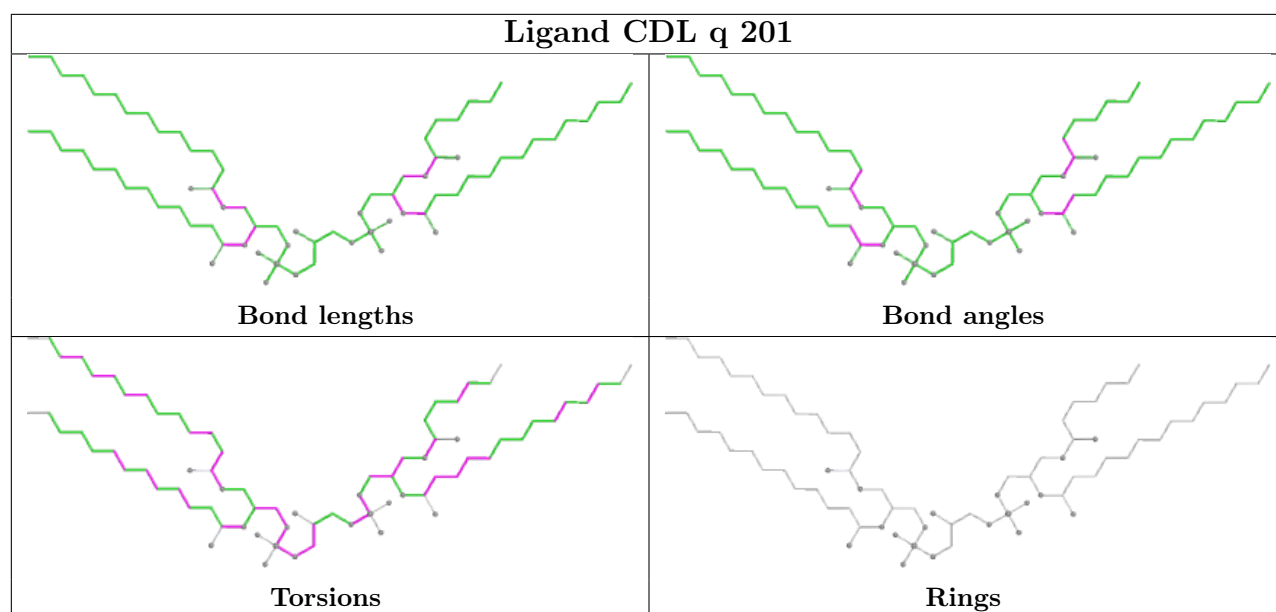
16 monomers are involved in 26 short contacts:

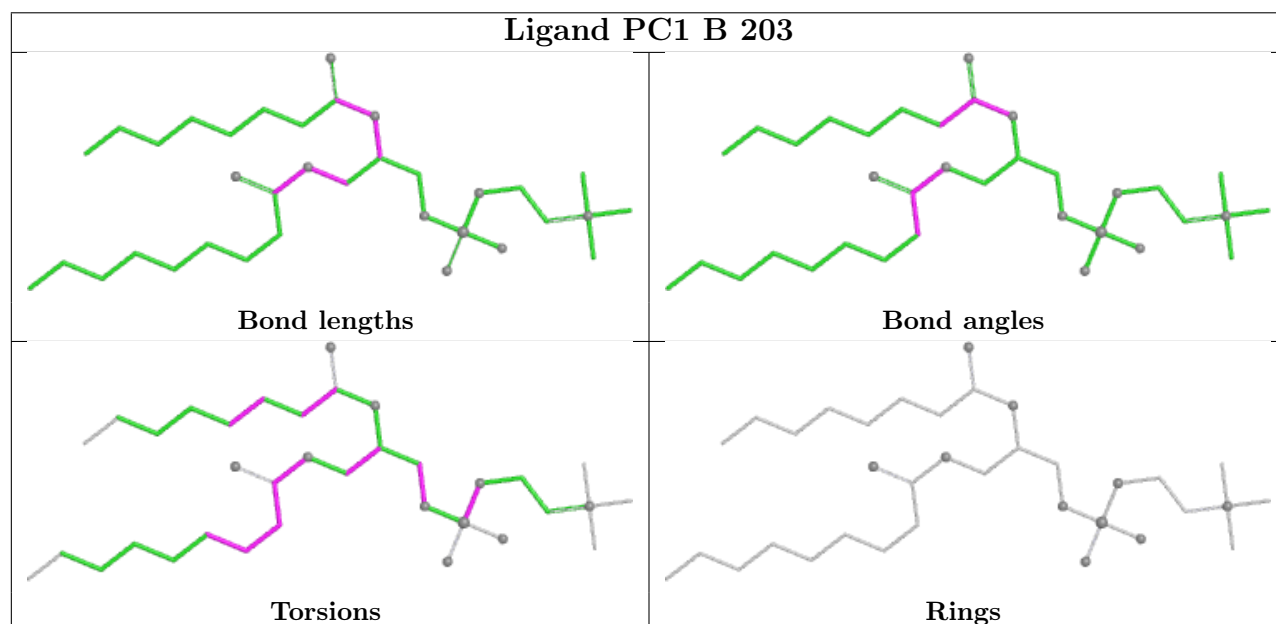
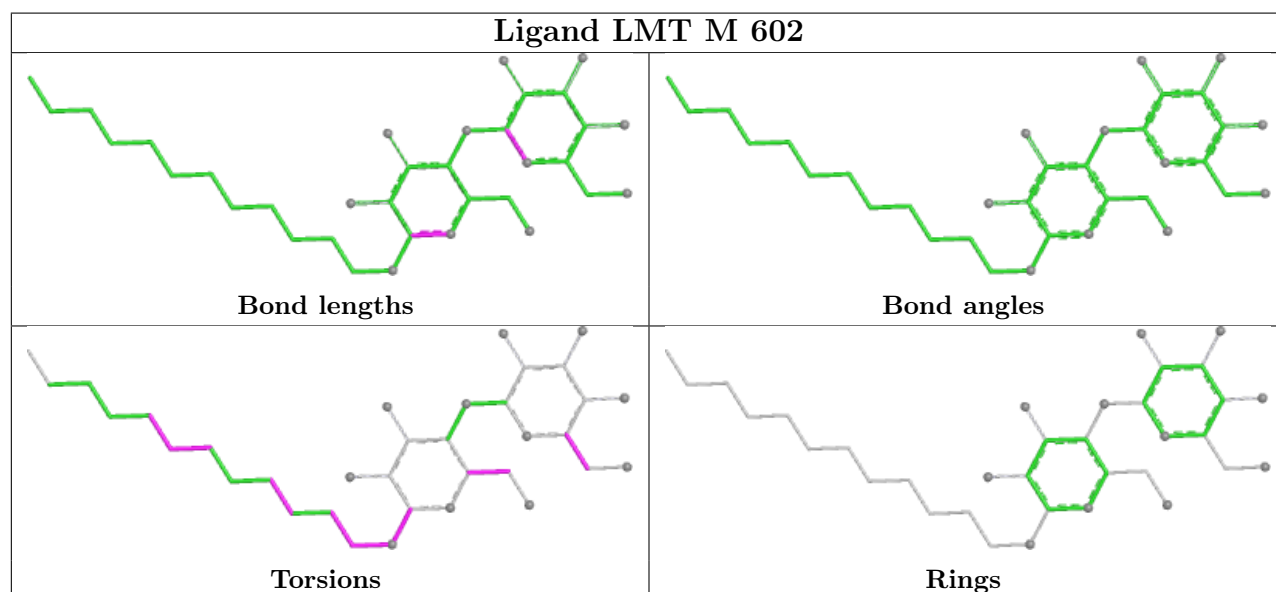
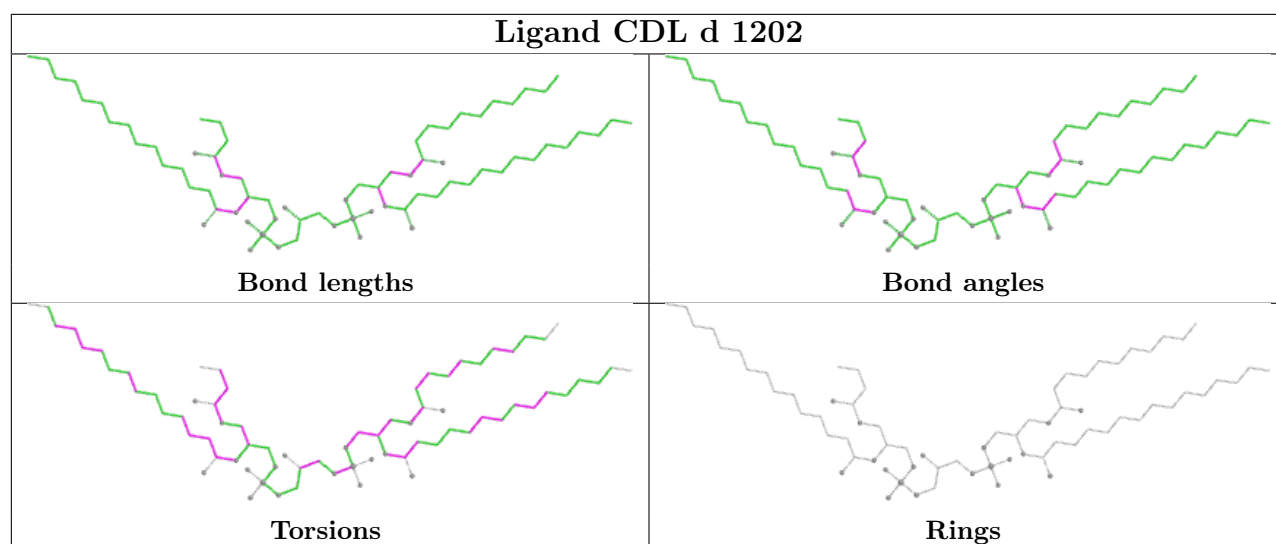
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	P	501	NDP	3	0
53	d	1202	CDL	1	0
45	M	602	LMT	2	0
45	k	101	LMT	1	0
46	d	1201	3PE	1	0
46	L	704	3PE	1	0
46	m	202	3PE	4	0
45	M	603	LMT	1	0
45	J	201	LMT	1	0
46	M	604	3PE	2	0
54	O	401	GTP	2	0
59	o	201	MYR	1	0
52	N	504	I49	3	0
48	g	1501	PC1	2	0
52	H	403	I49	1	0
45	A	301	LMT	1	0

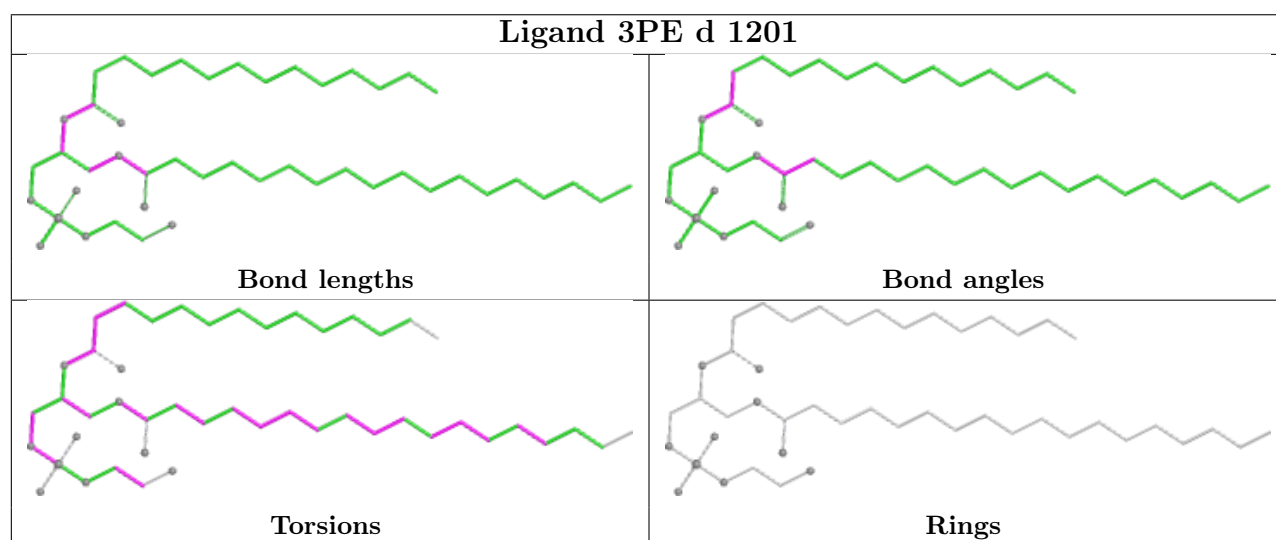
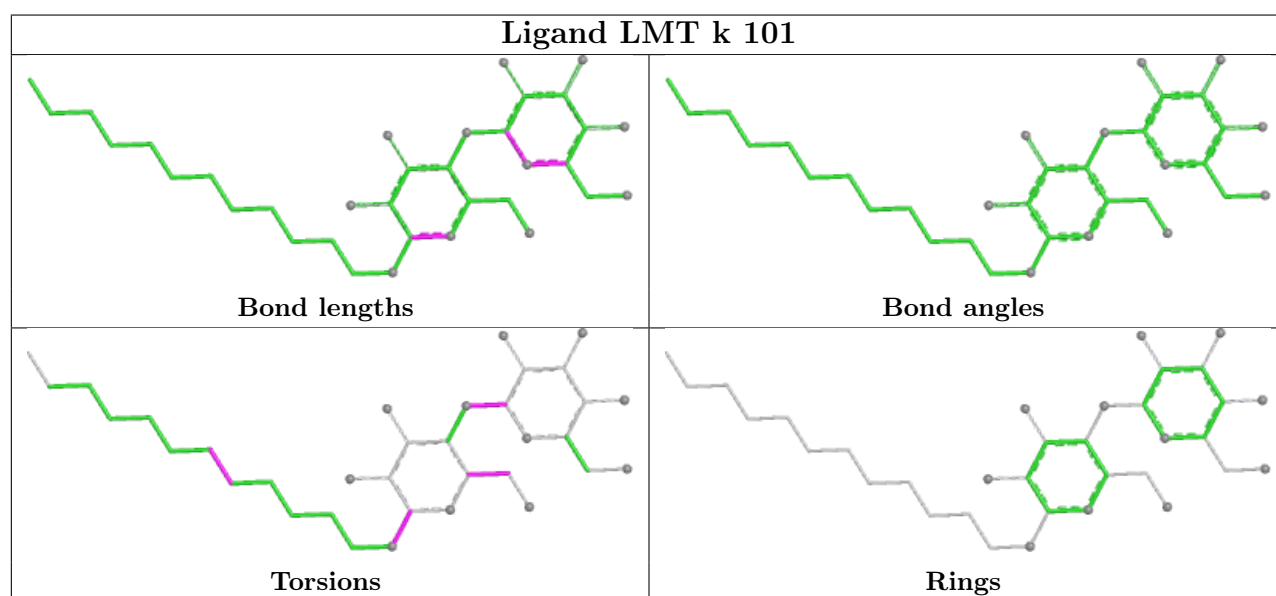
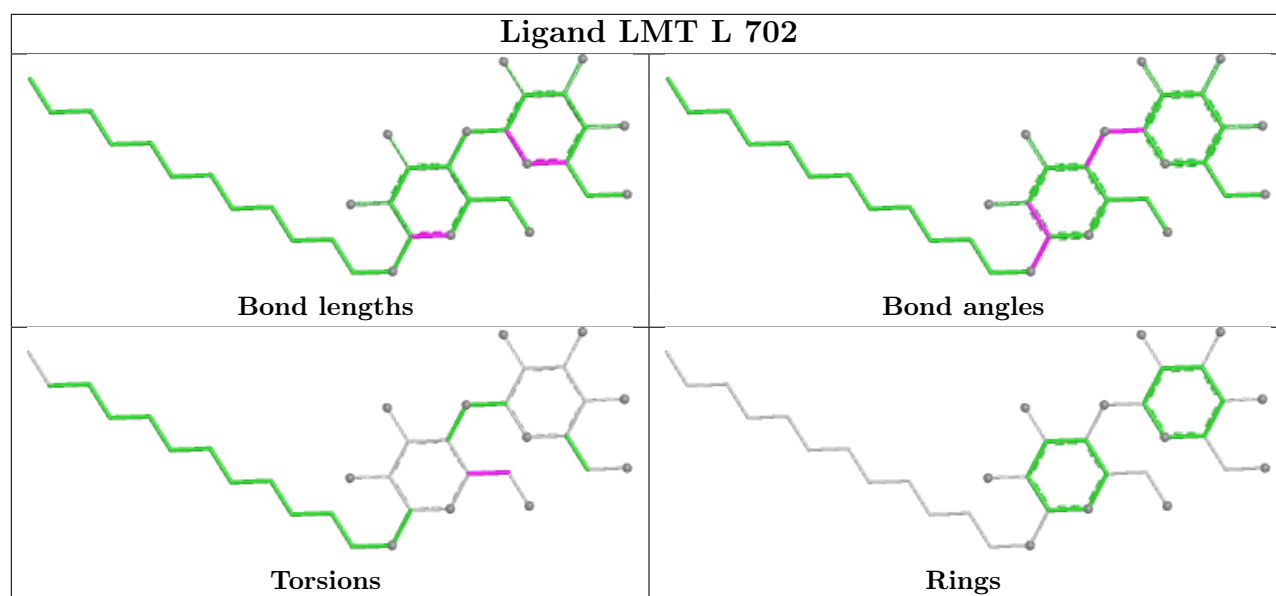
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

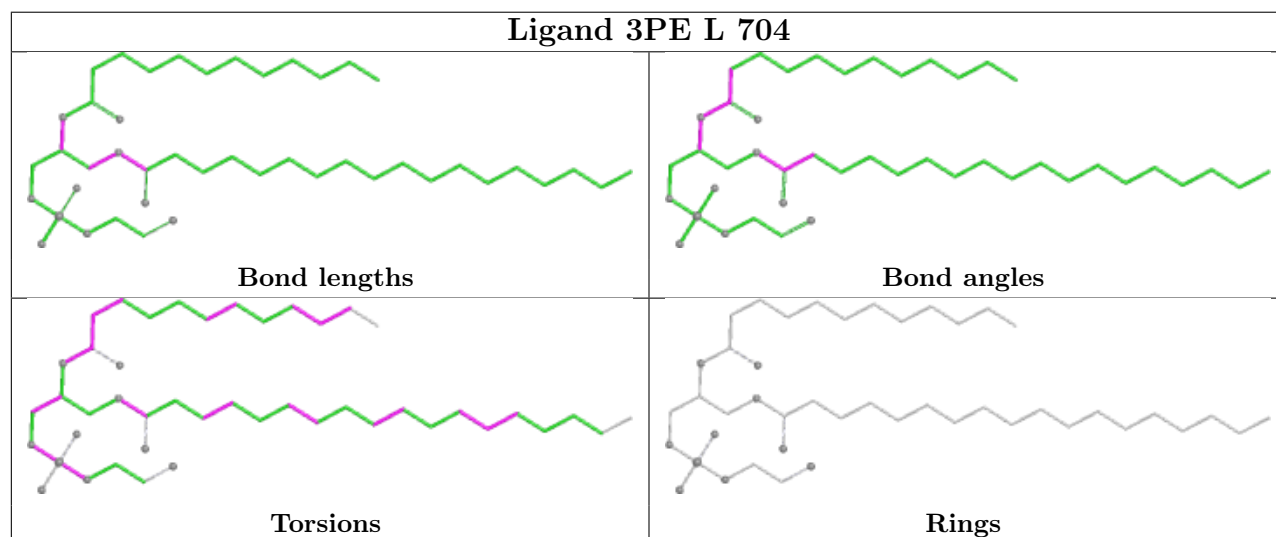
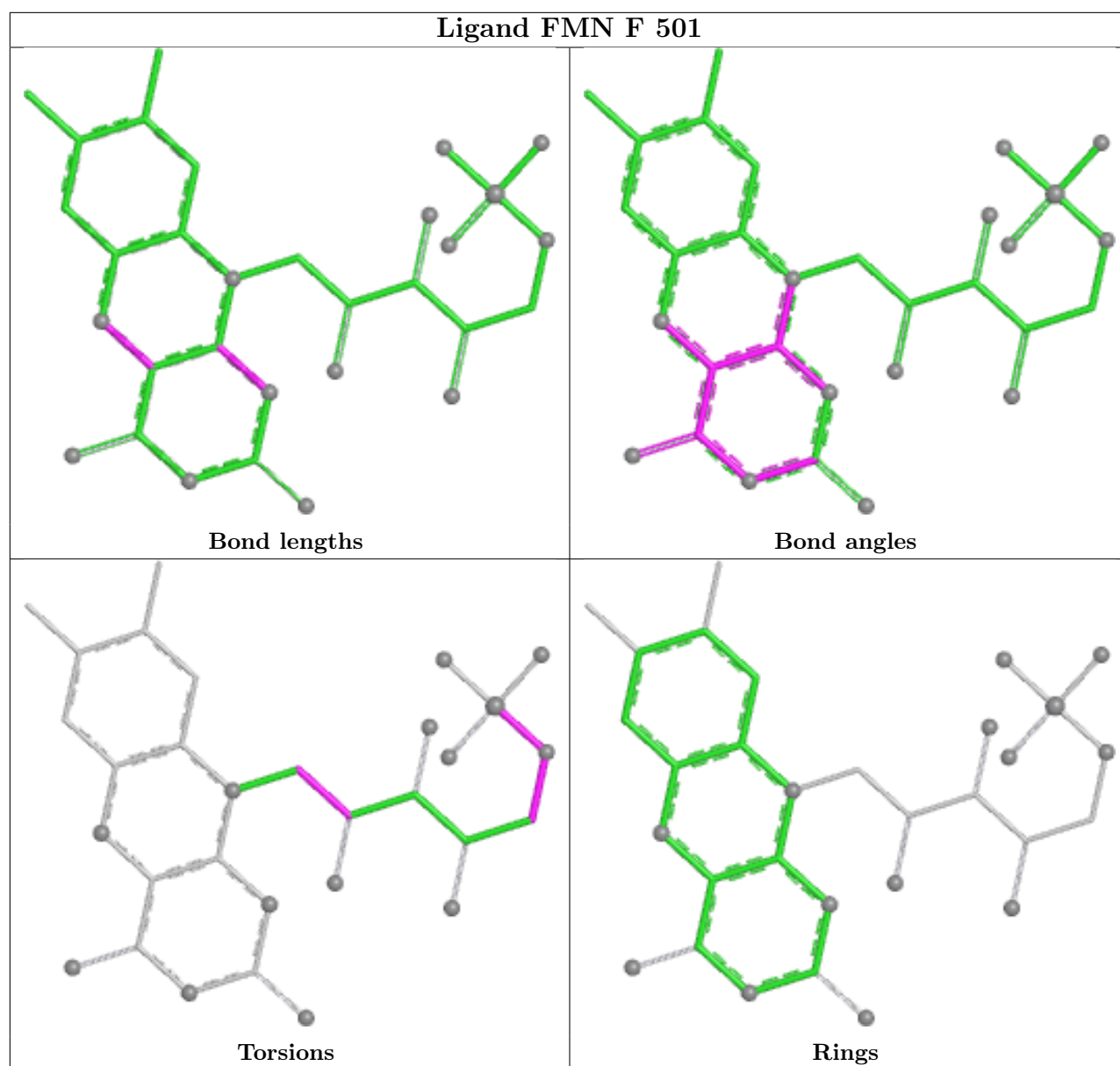
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

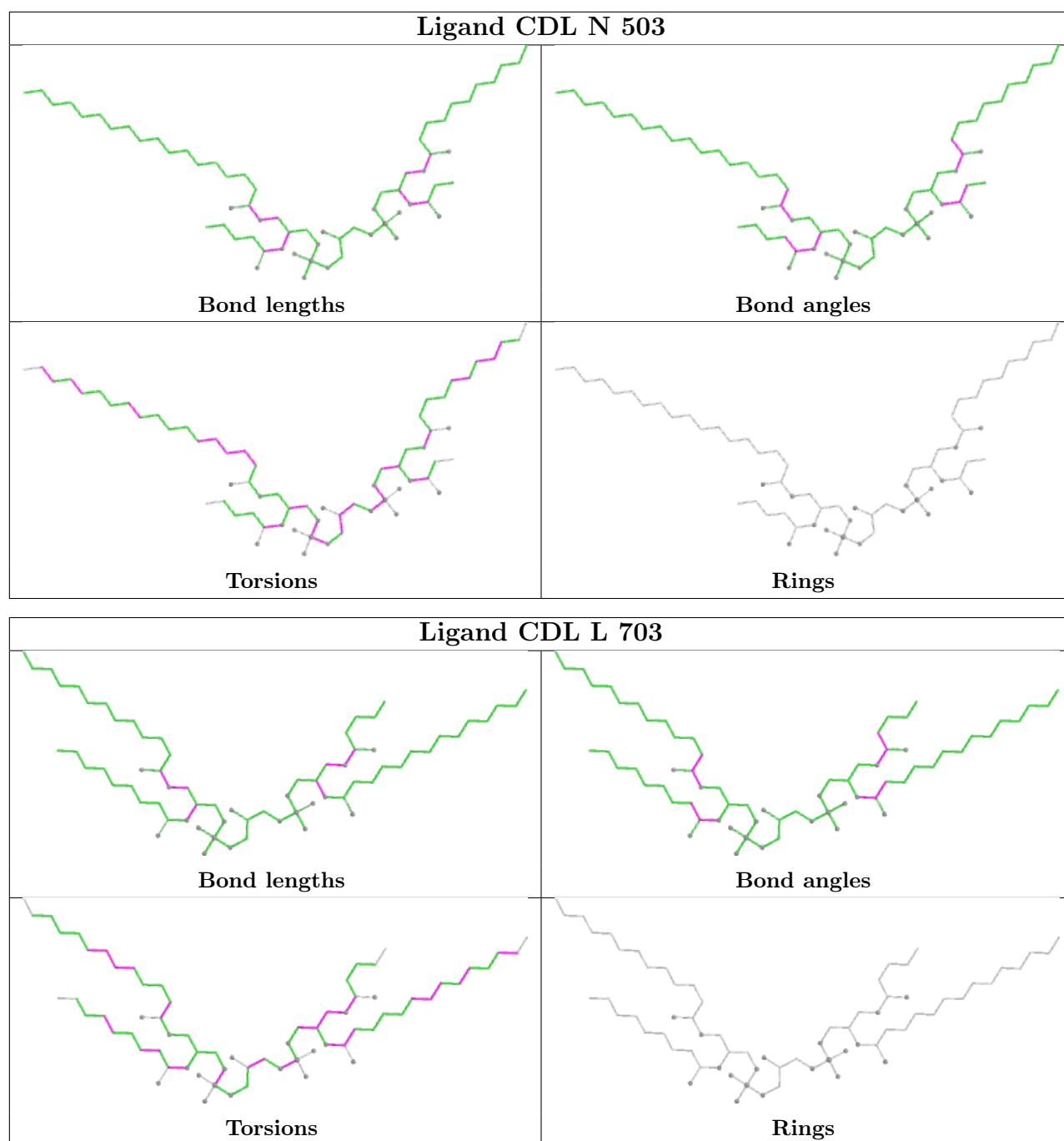


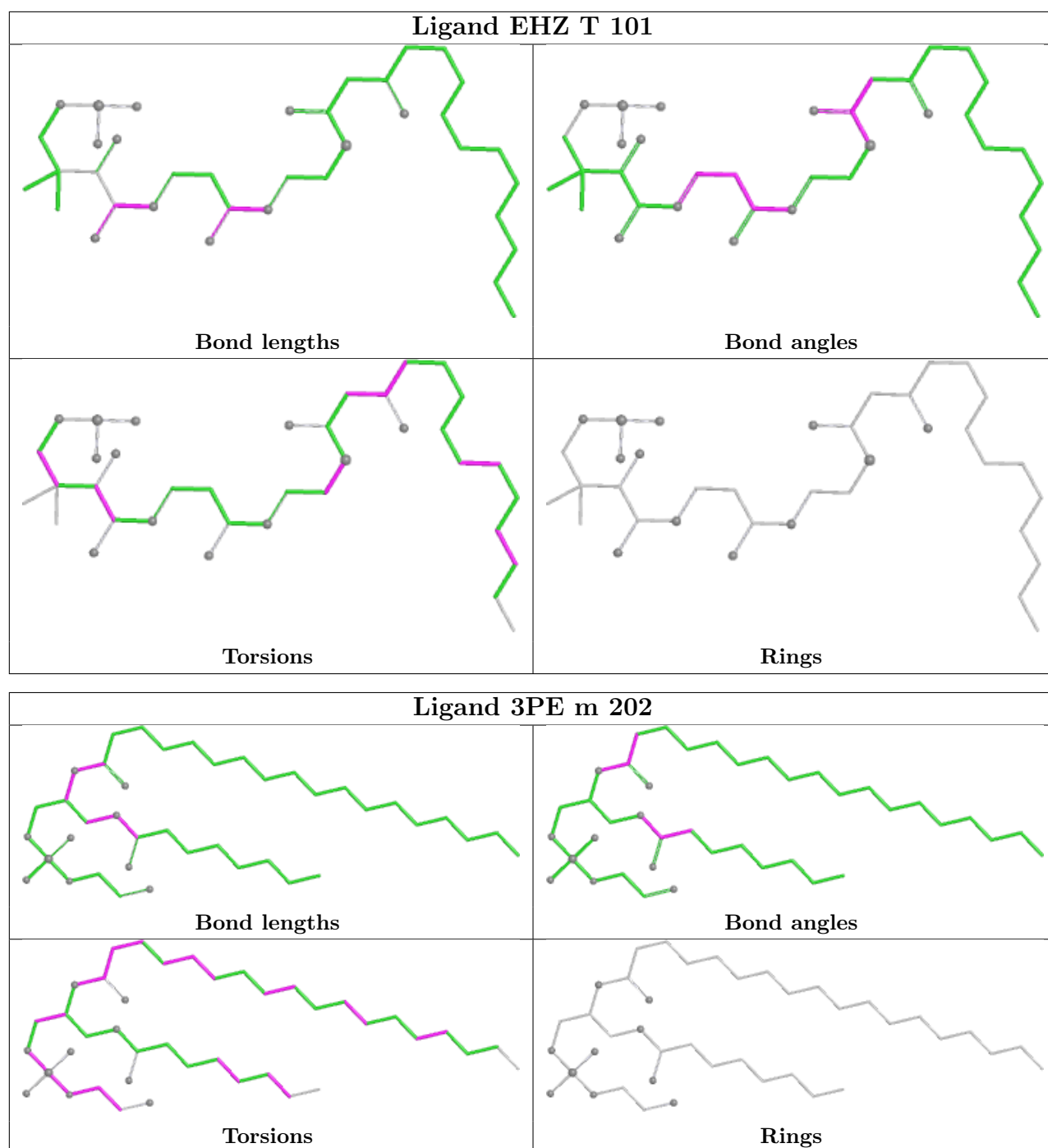


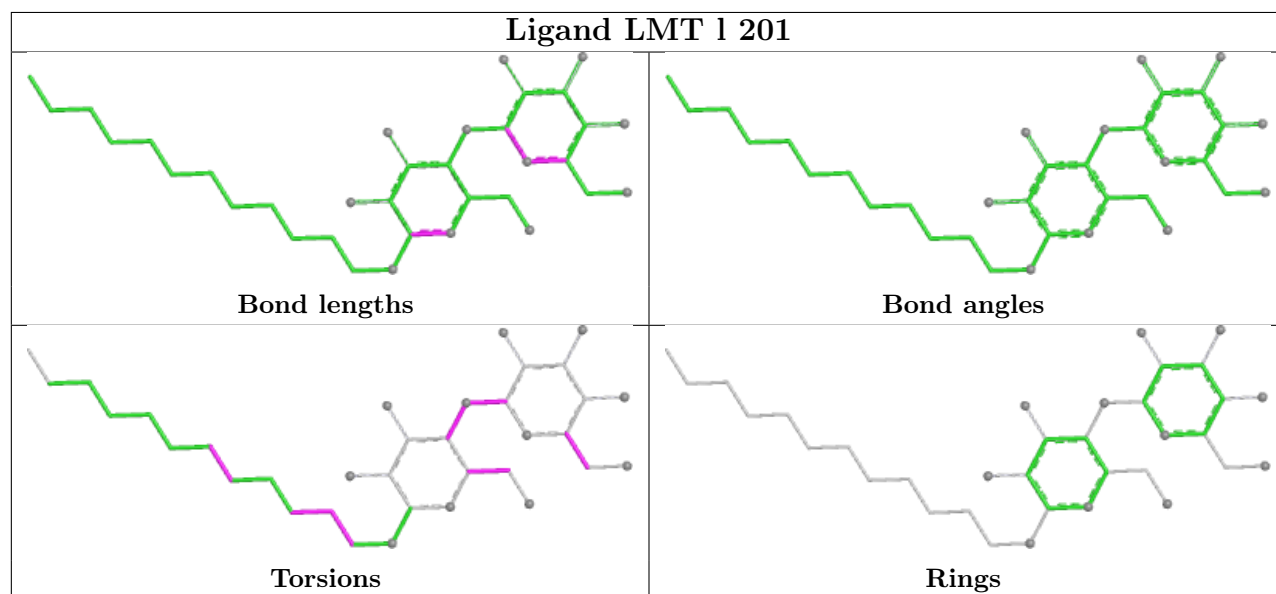
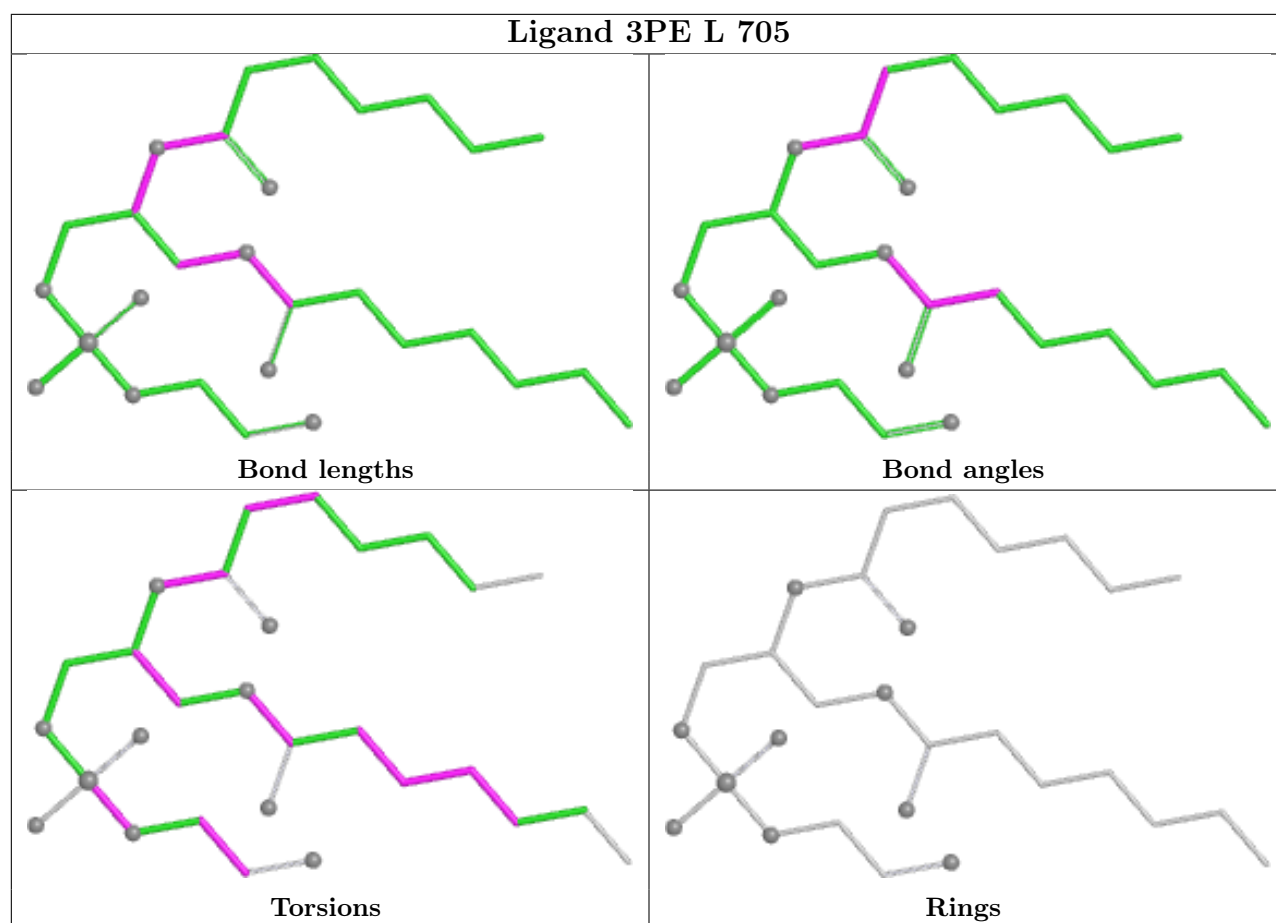


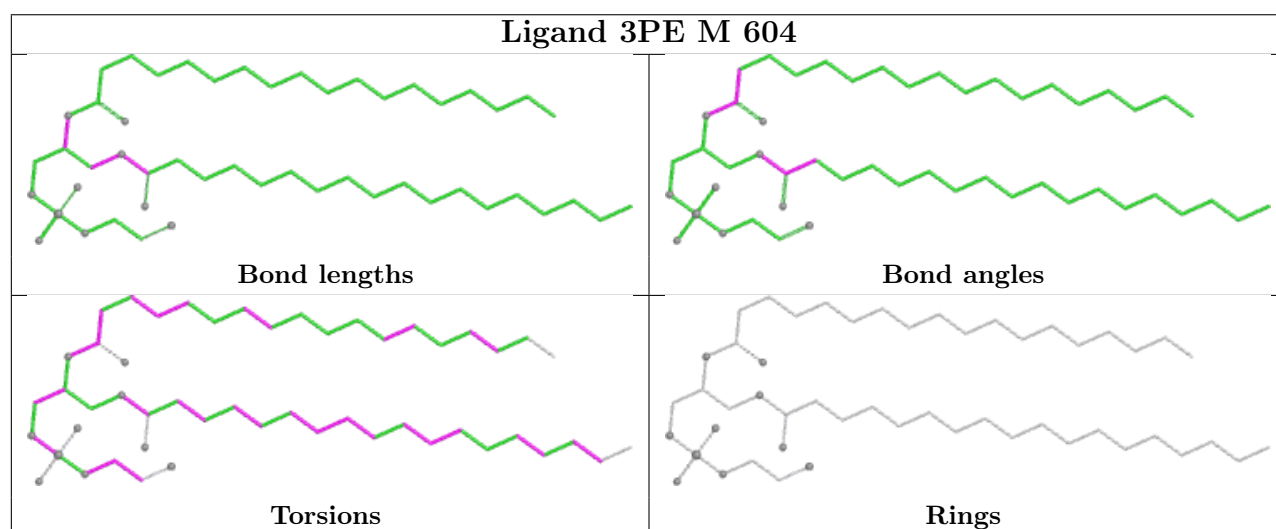
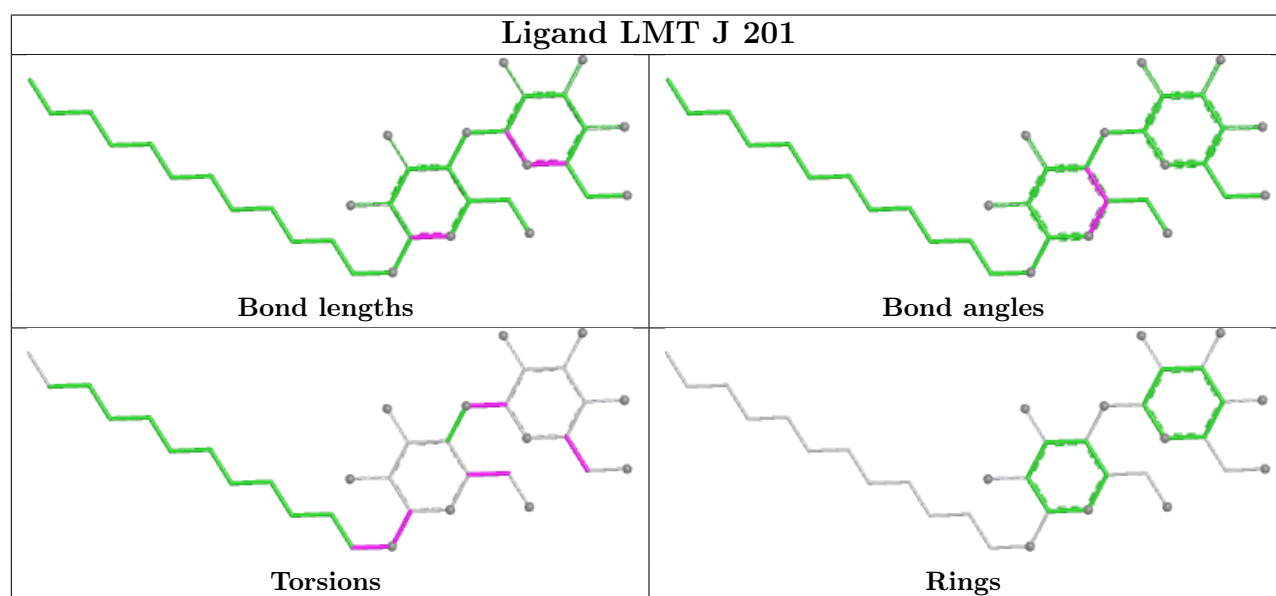
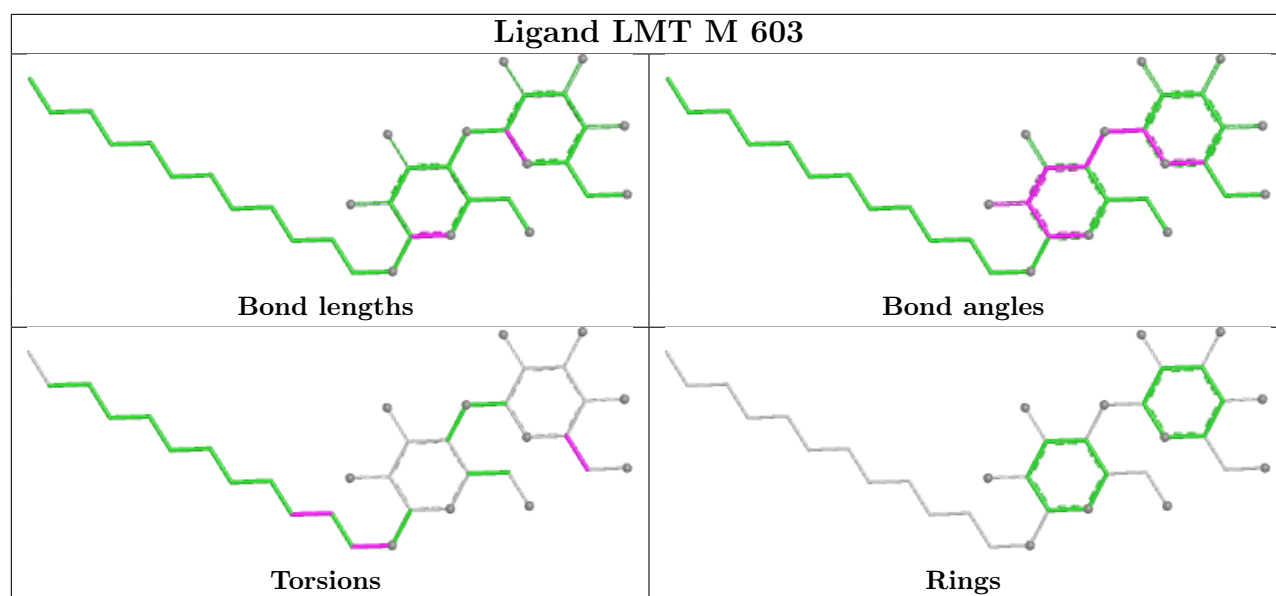


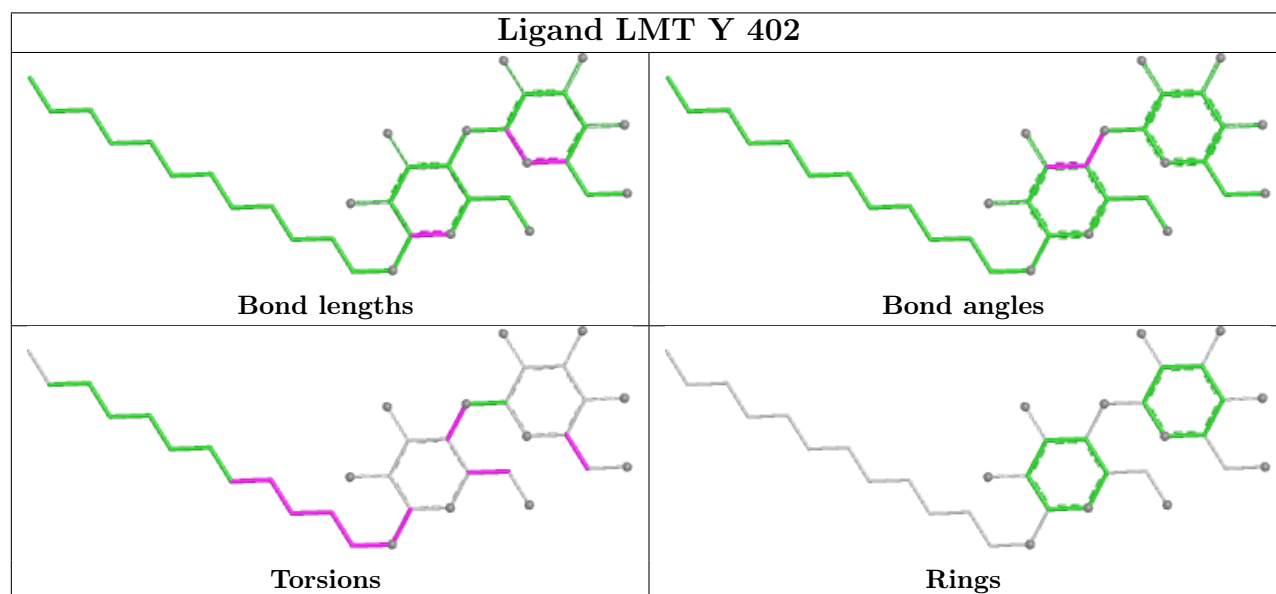
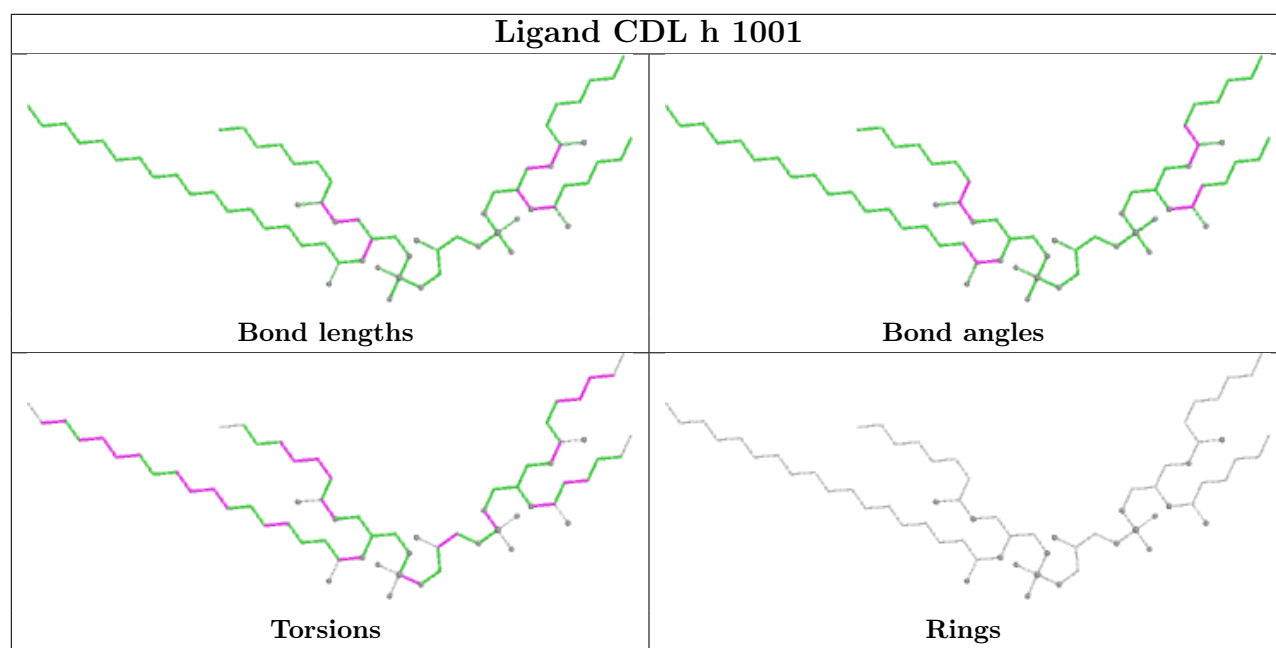


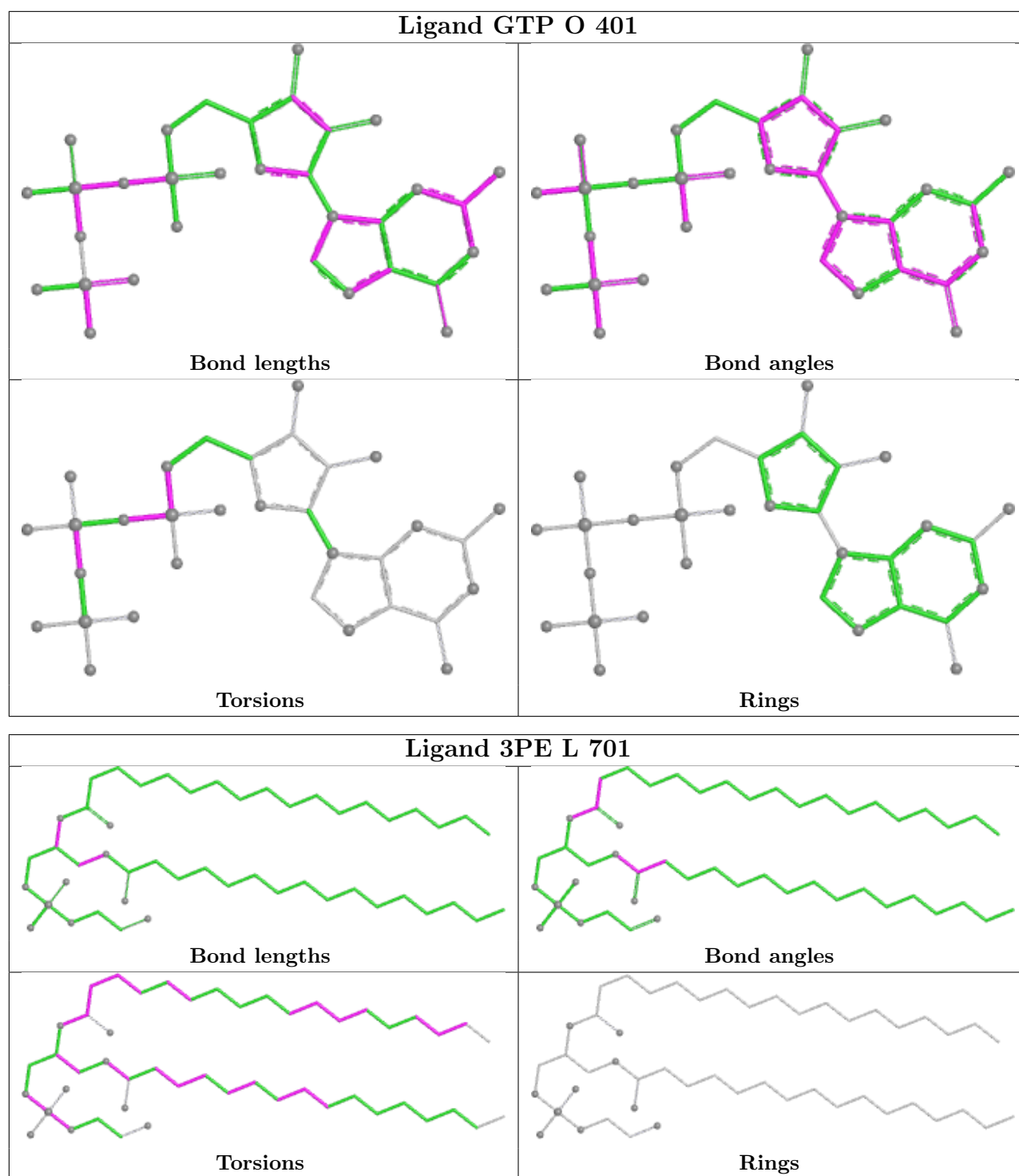


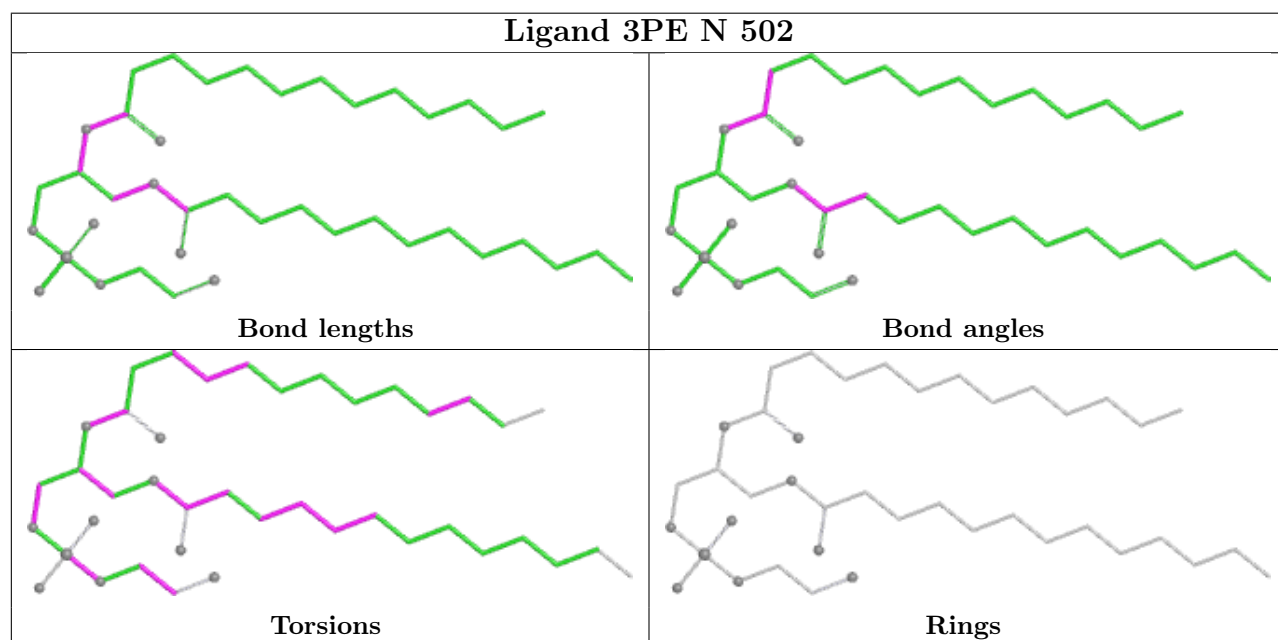
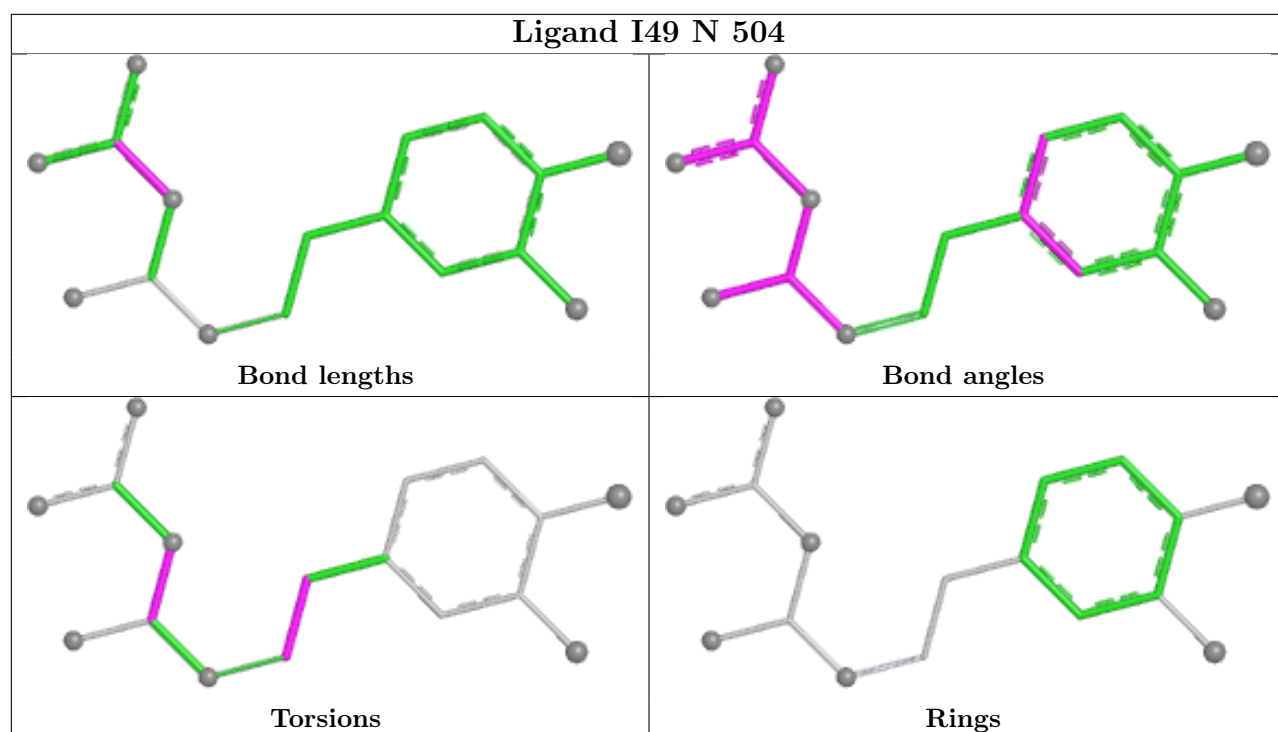


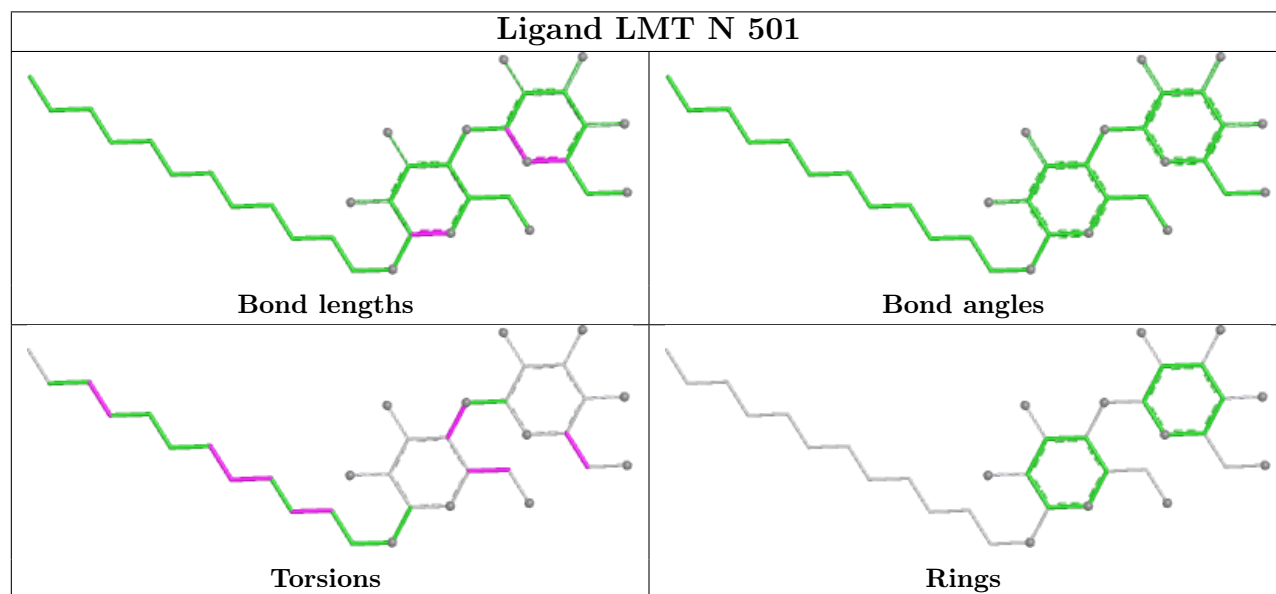
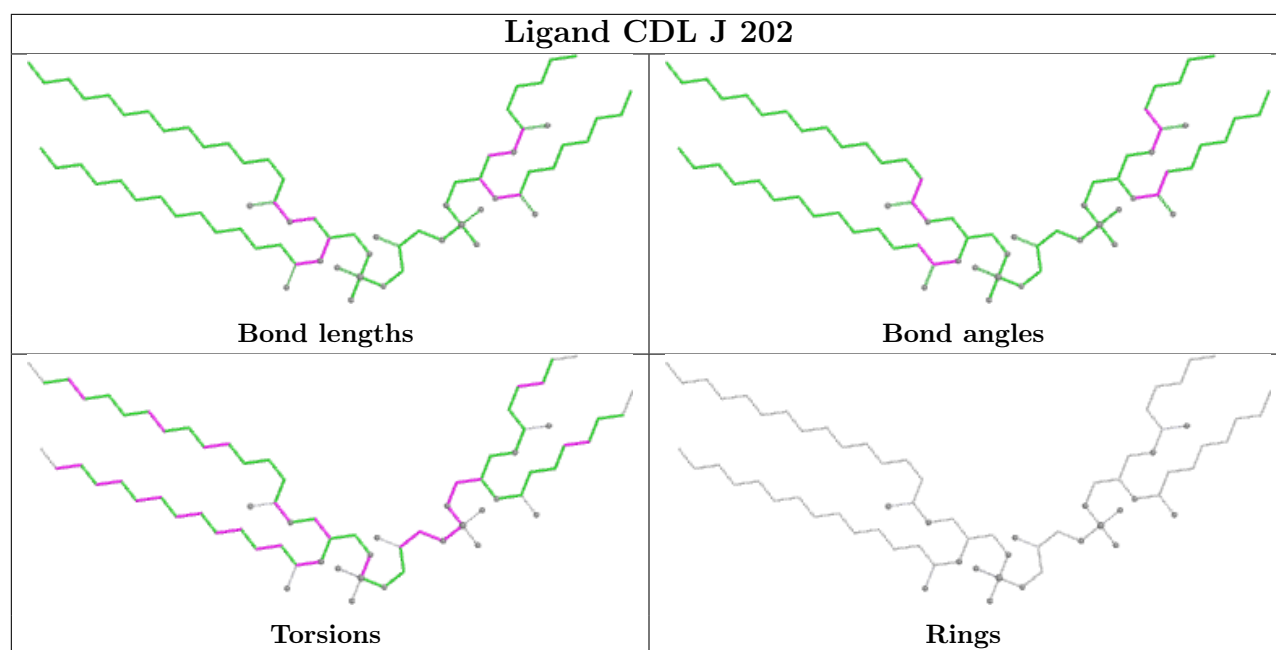


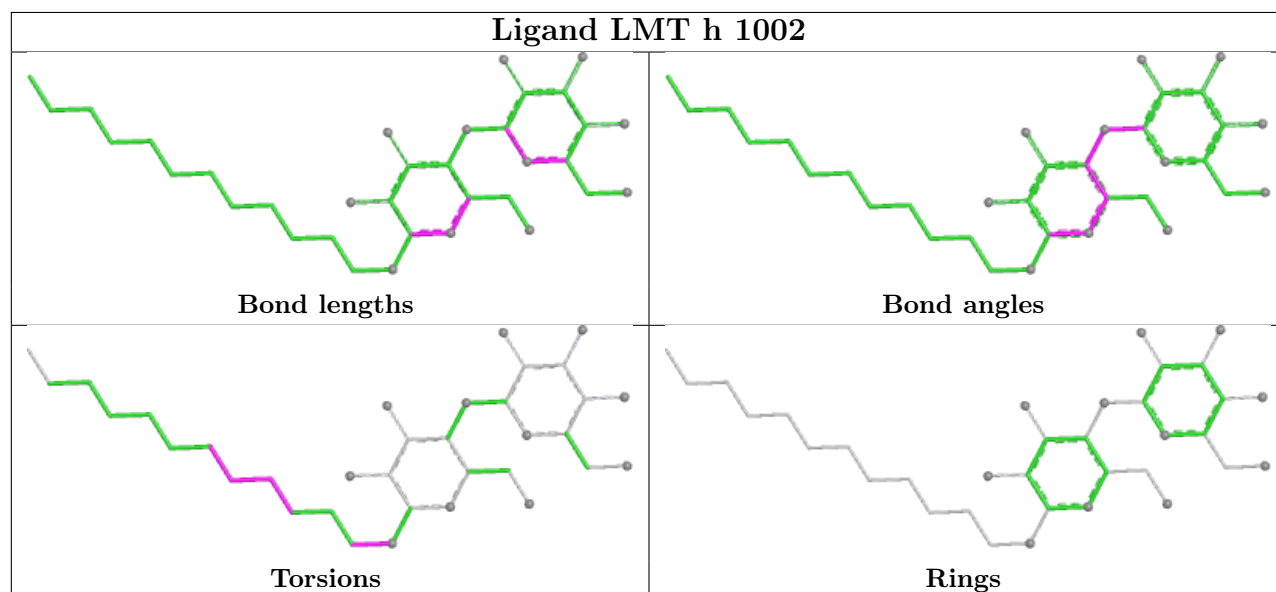
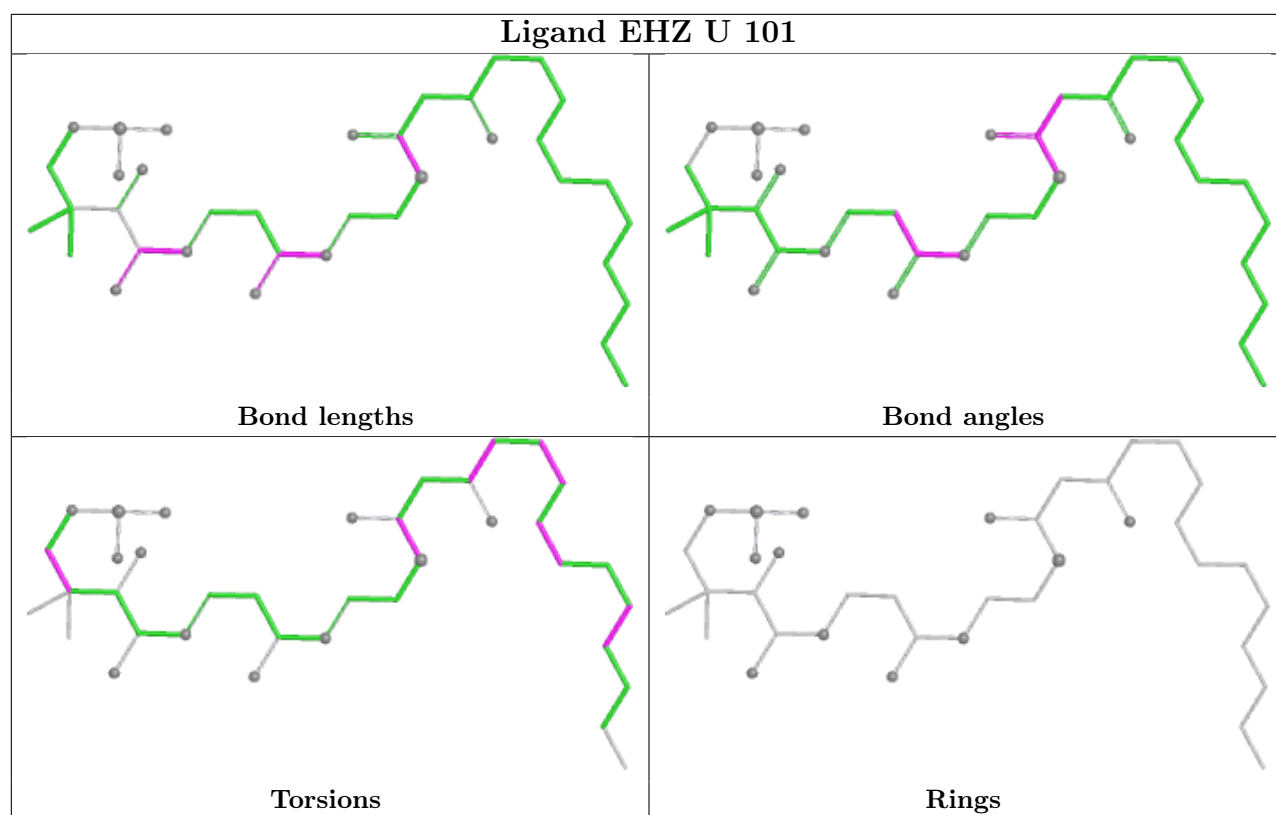


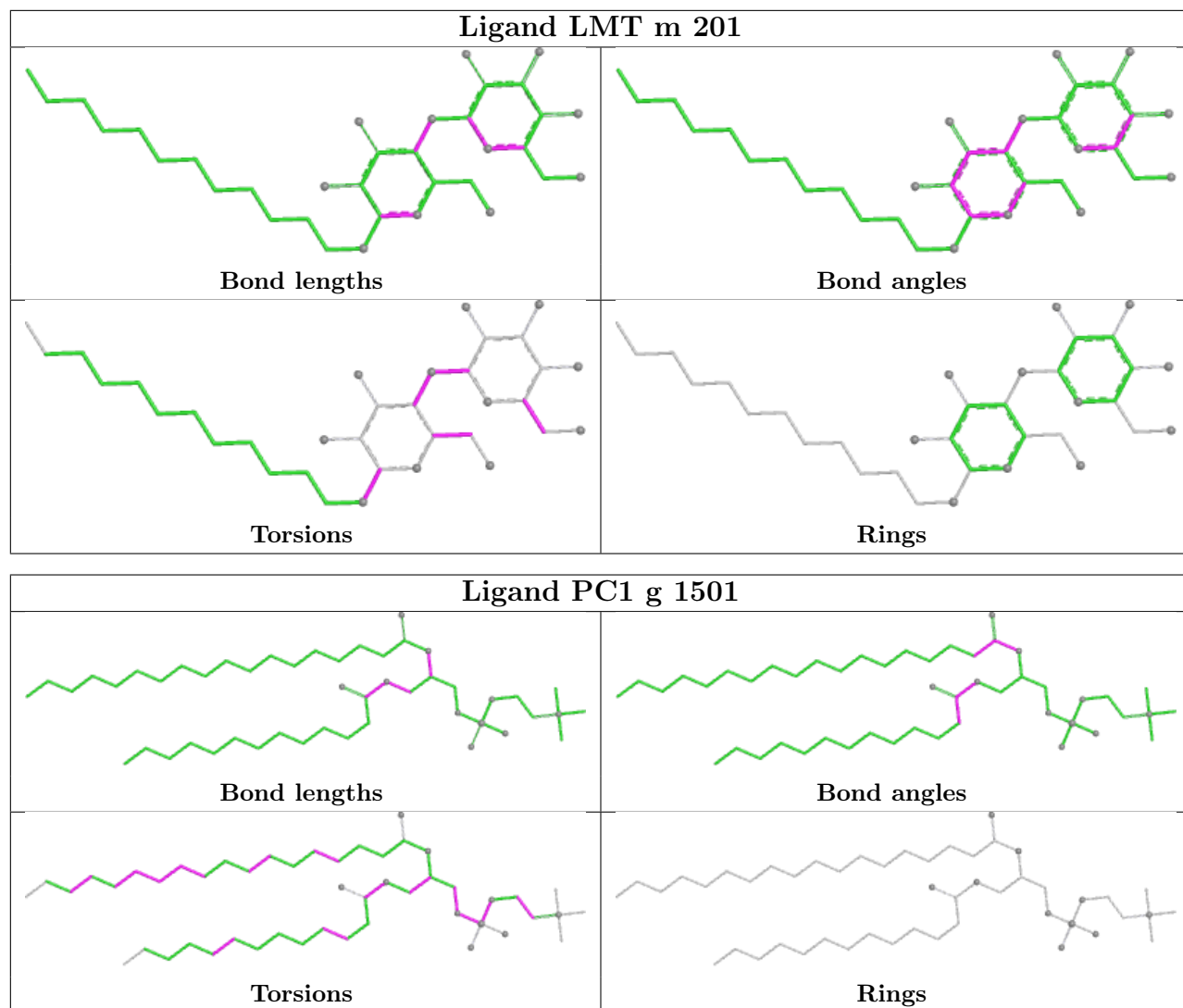




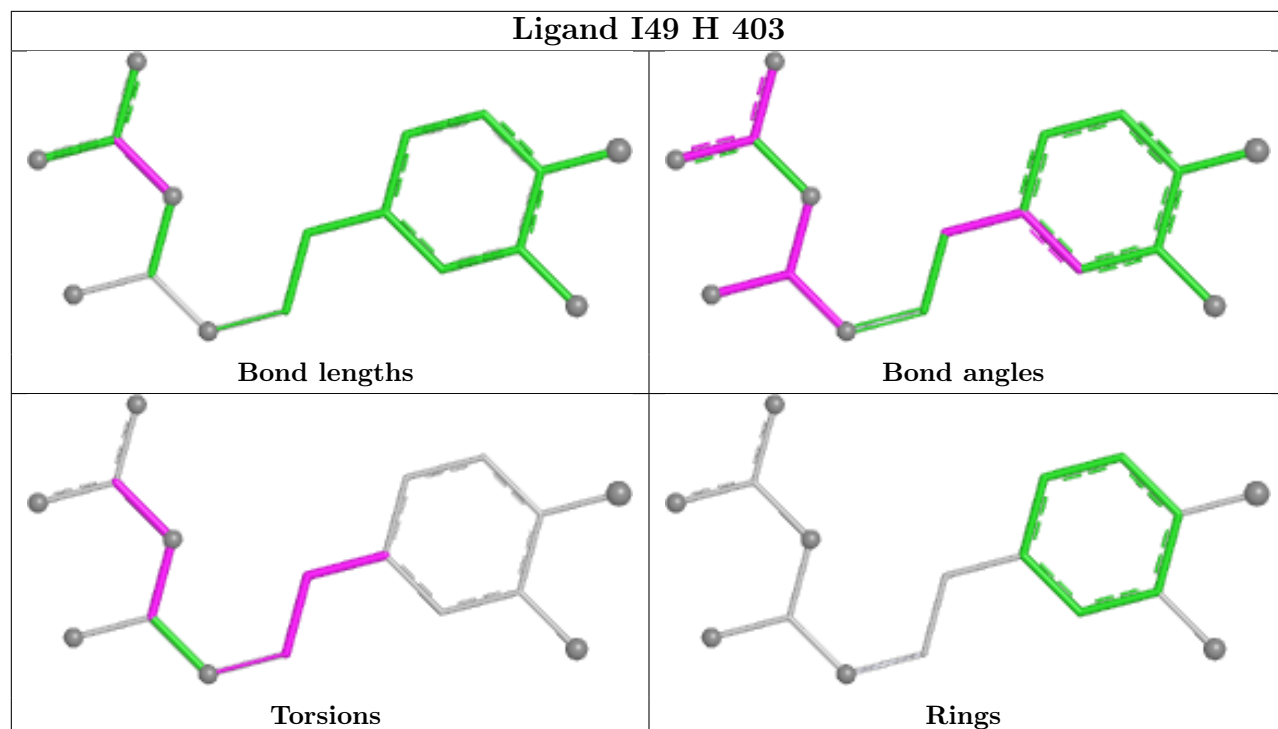




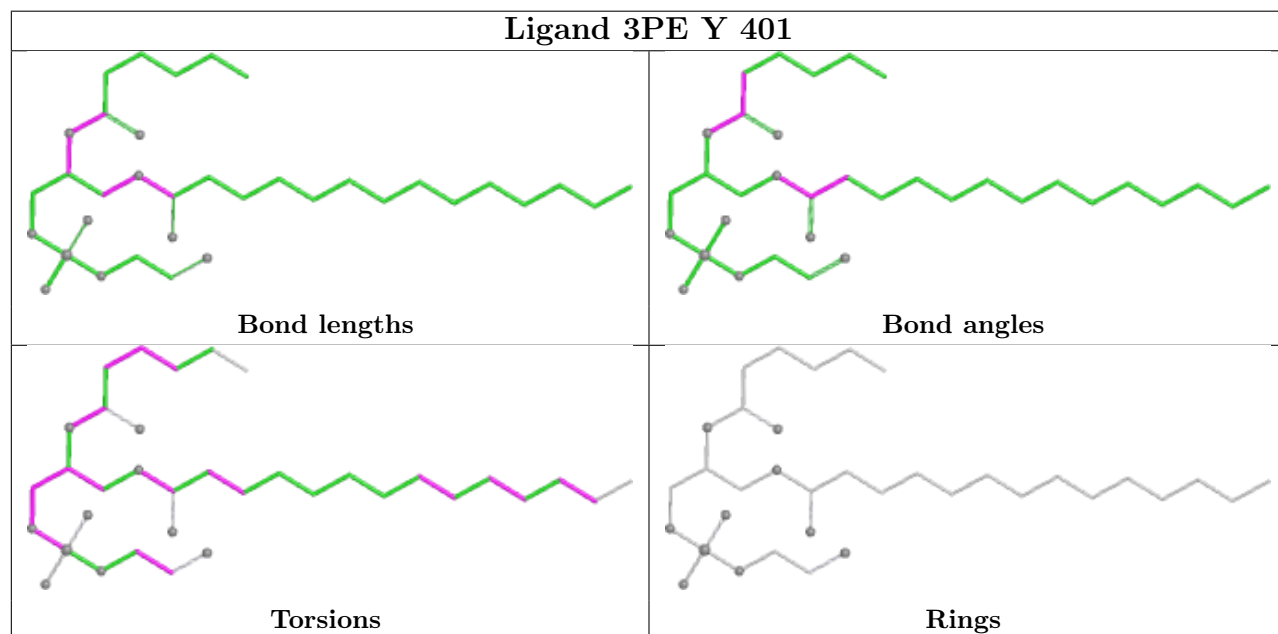


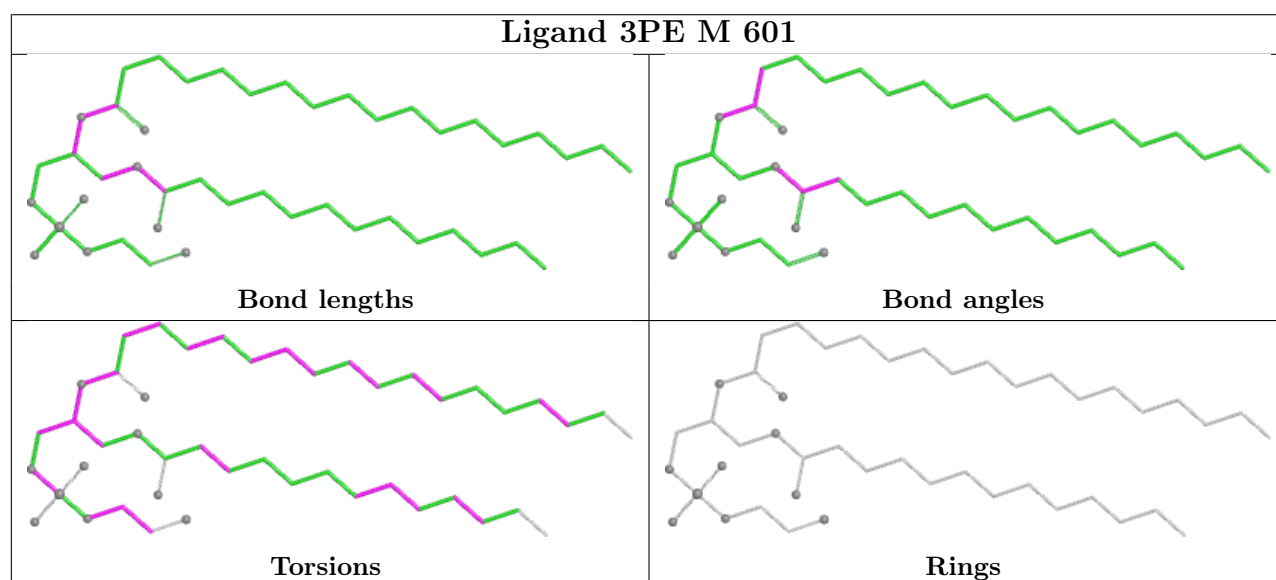
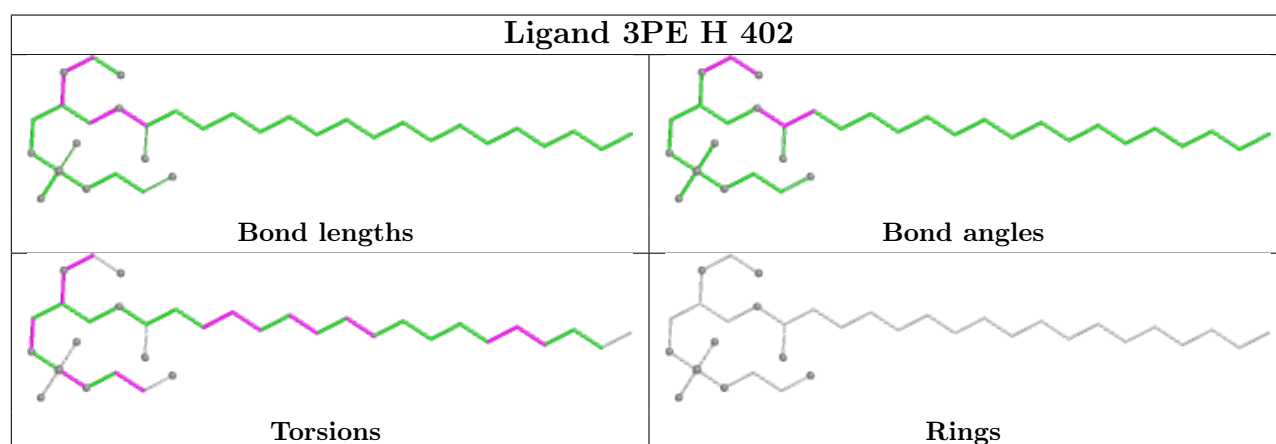
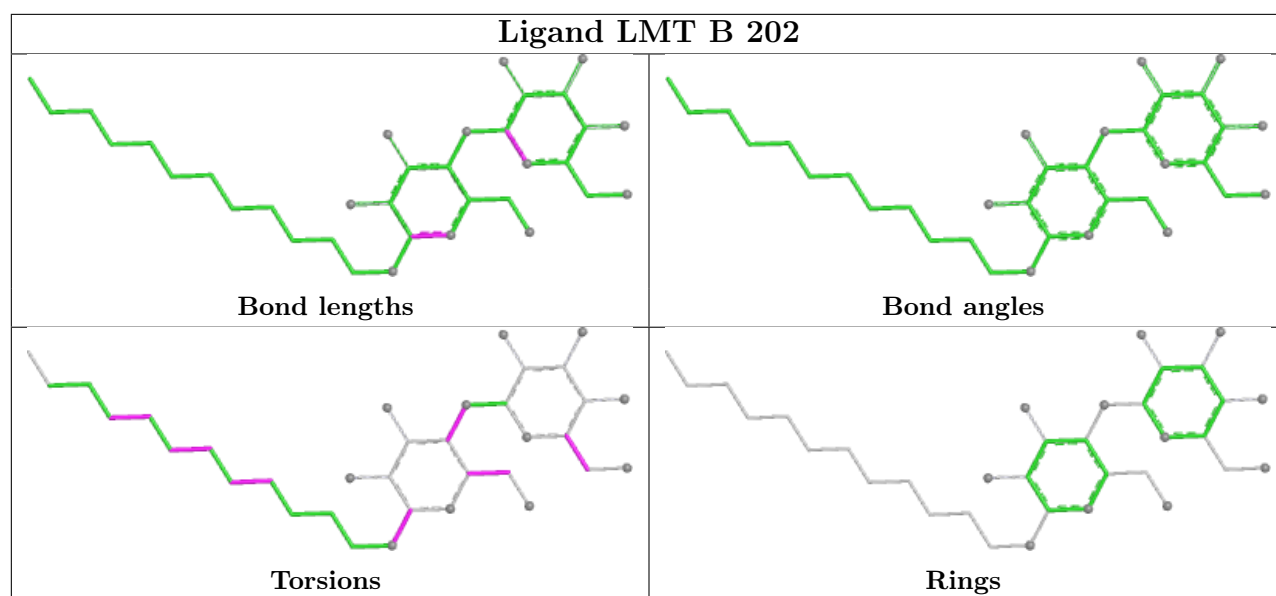


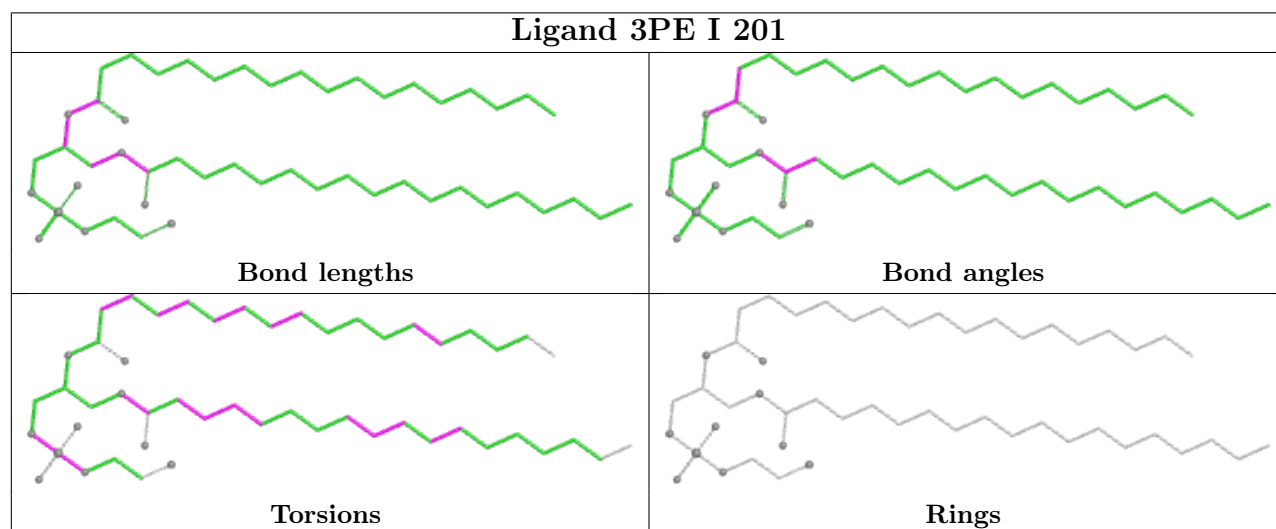
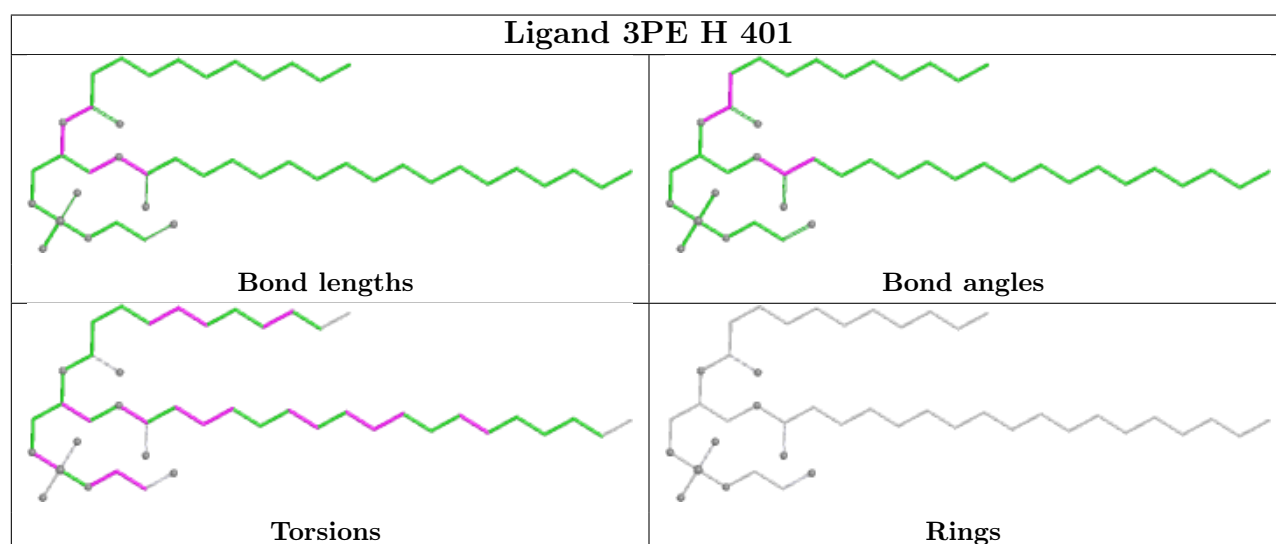
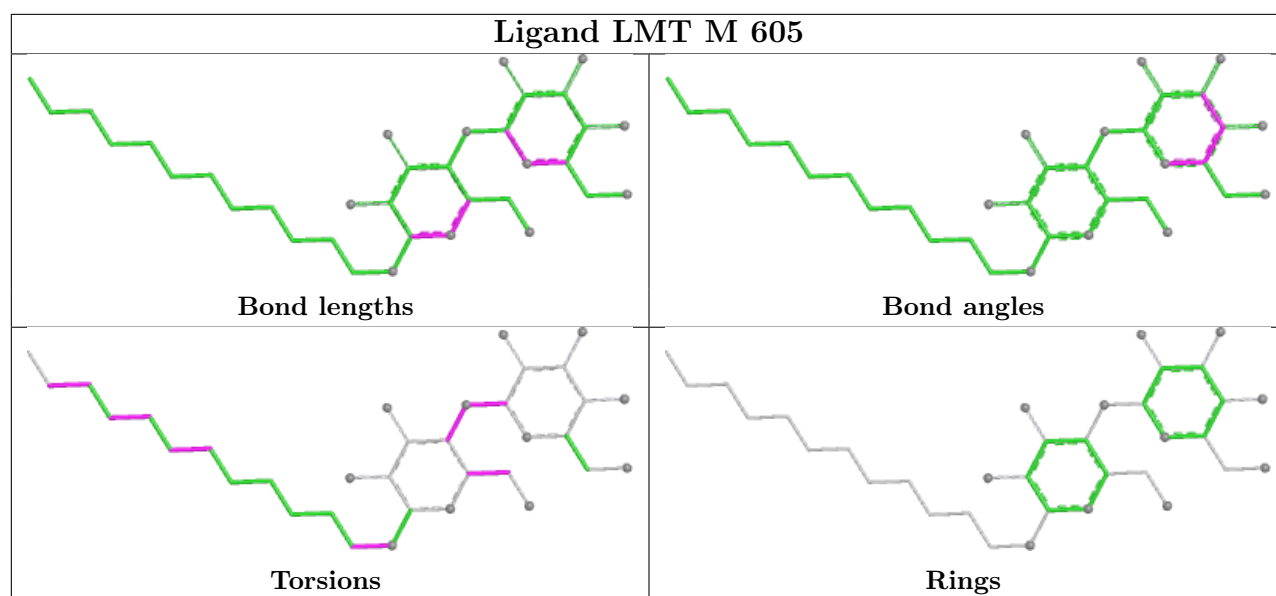
Ligand I49 H 403

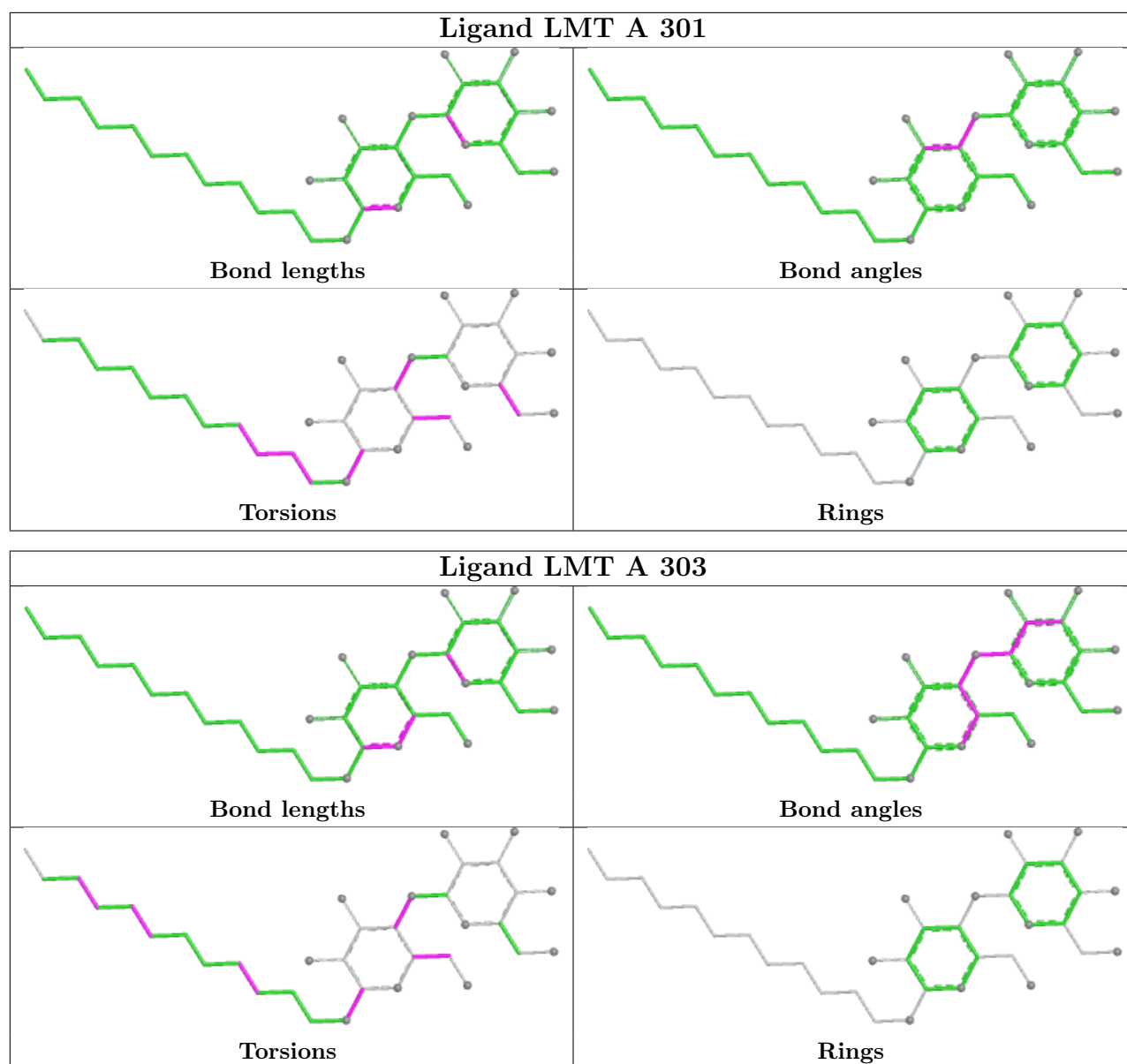


Ligand 3PE Y 401









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.

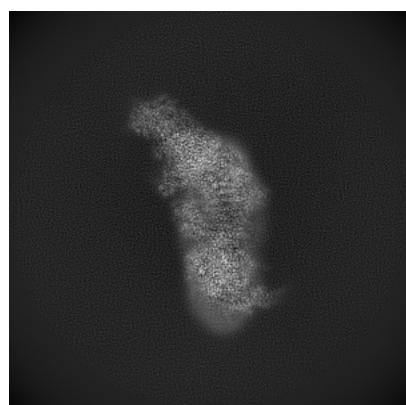
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14287. These allow visual inspection of the internal detail of the map and identification of artifacts.

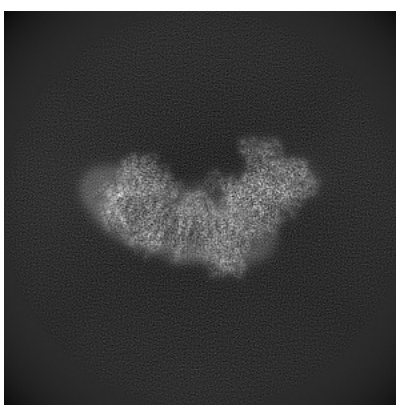
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

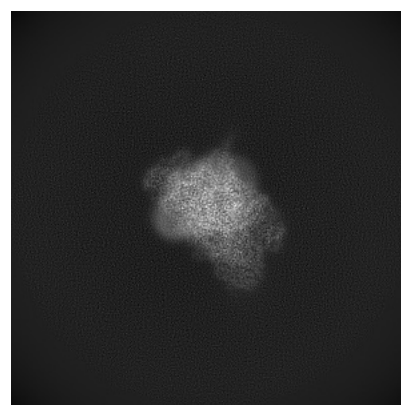
6.1.1 Primary map



X



Y

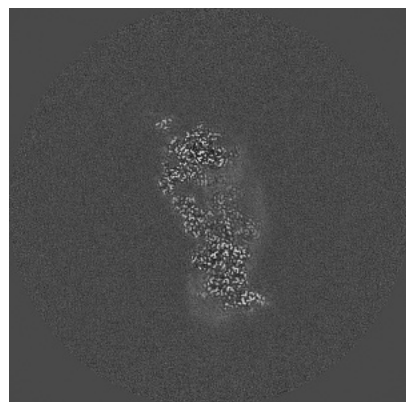


Z

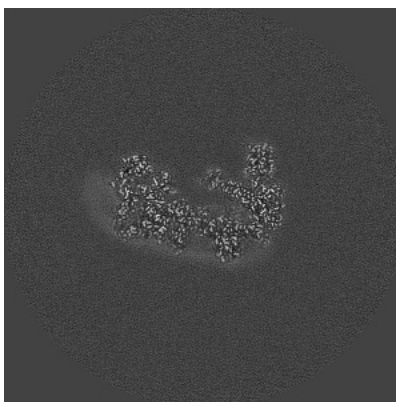
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

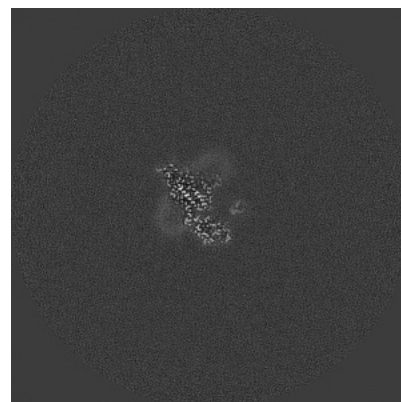
6.2.1 Primary map



X Index: 330



Y Index: 330

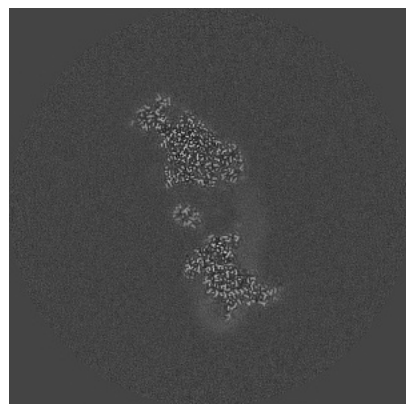


Z Index: 330

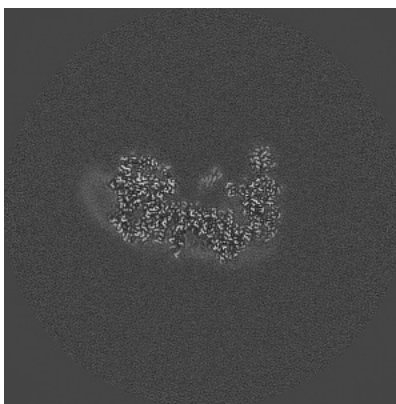
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

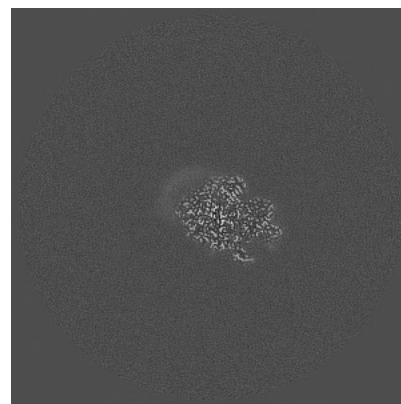
6.3.1 Primary map



X Index: 356



Y Index: 338

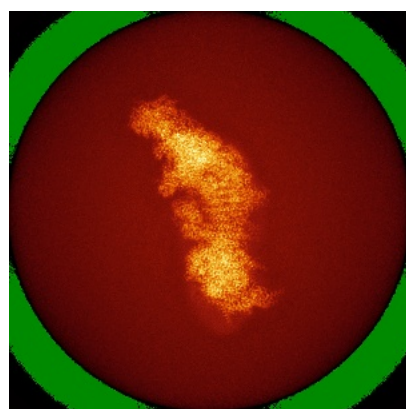


Z Index: 422

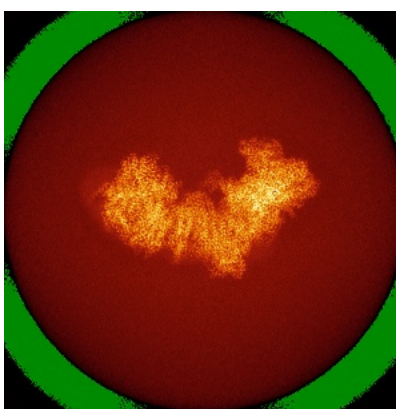
The images above show the largest variance slices of the map in three orthogonal directions.

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

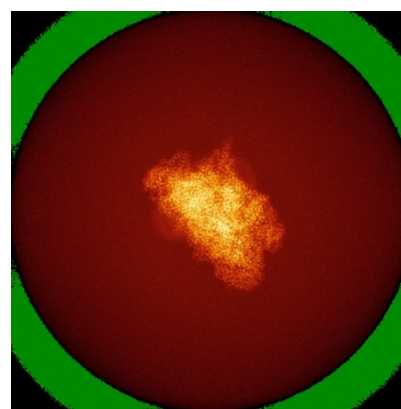
6.4.1 Primary map



X



Y

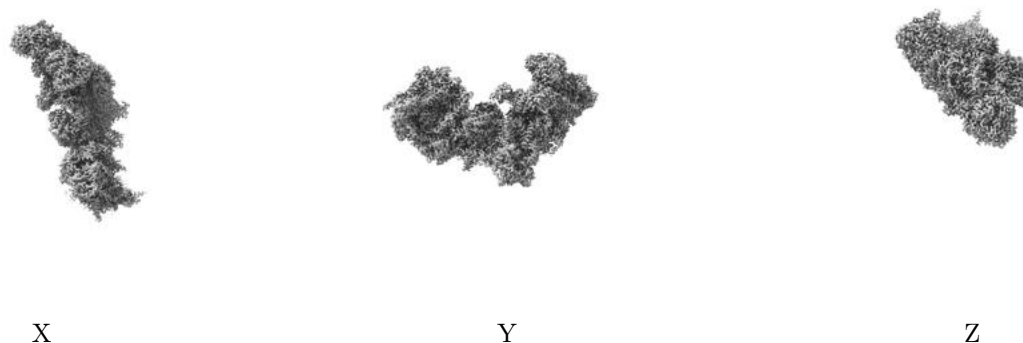


Z

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



The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

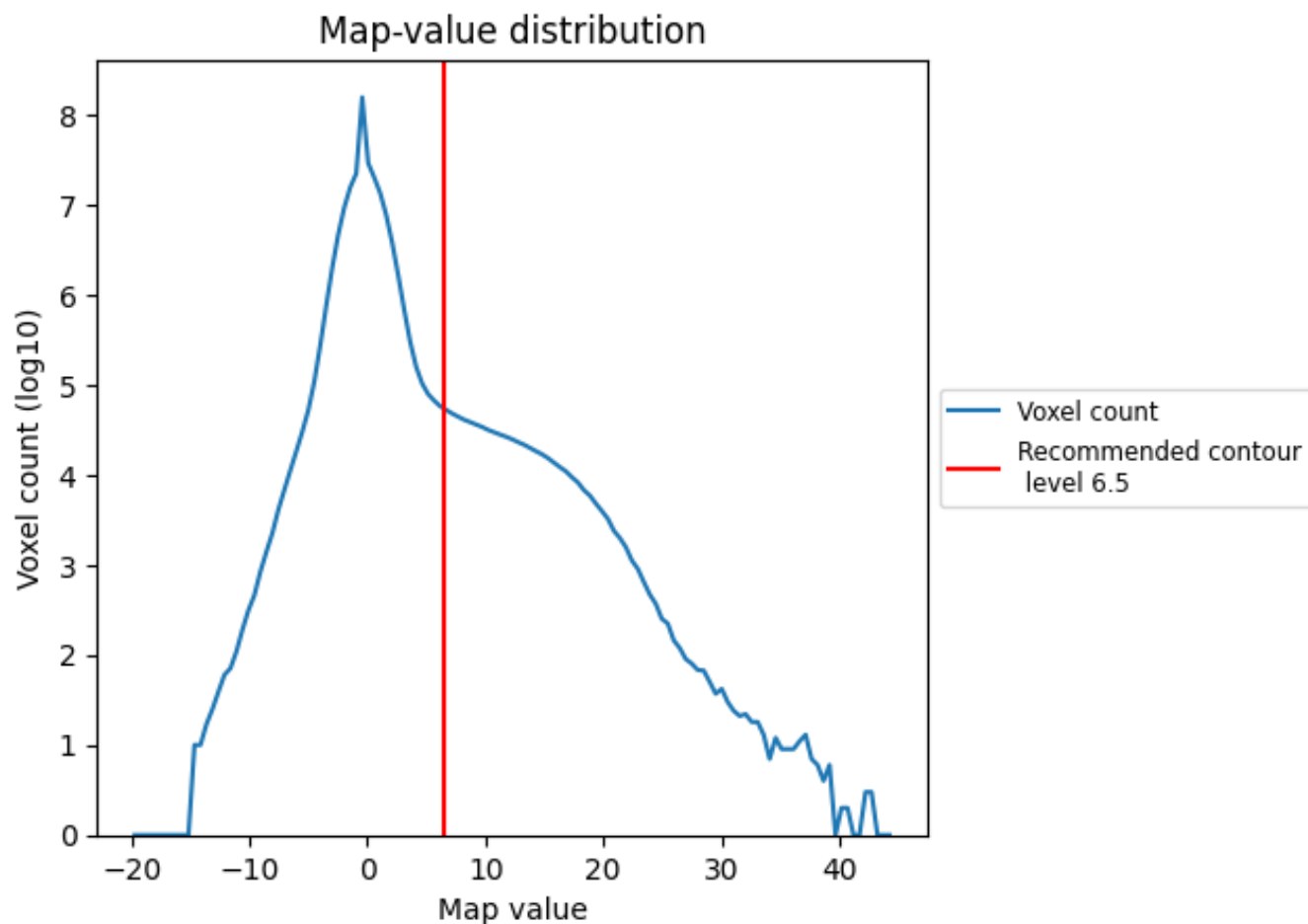
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

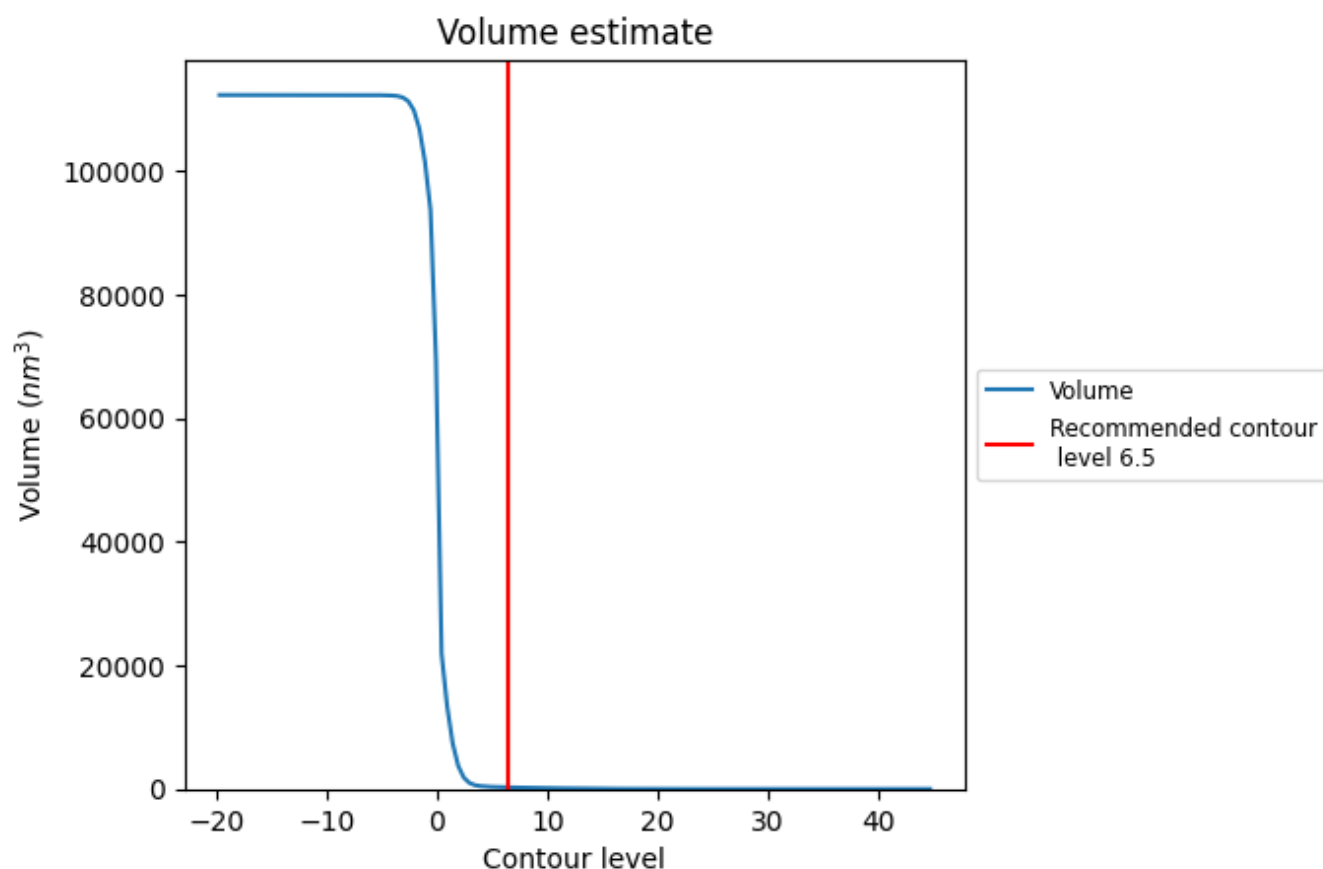
This section contains the results of statistical analysis of the map.

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.

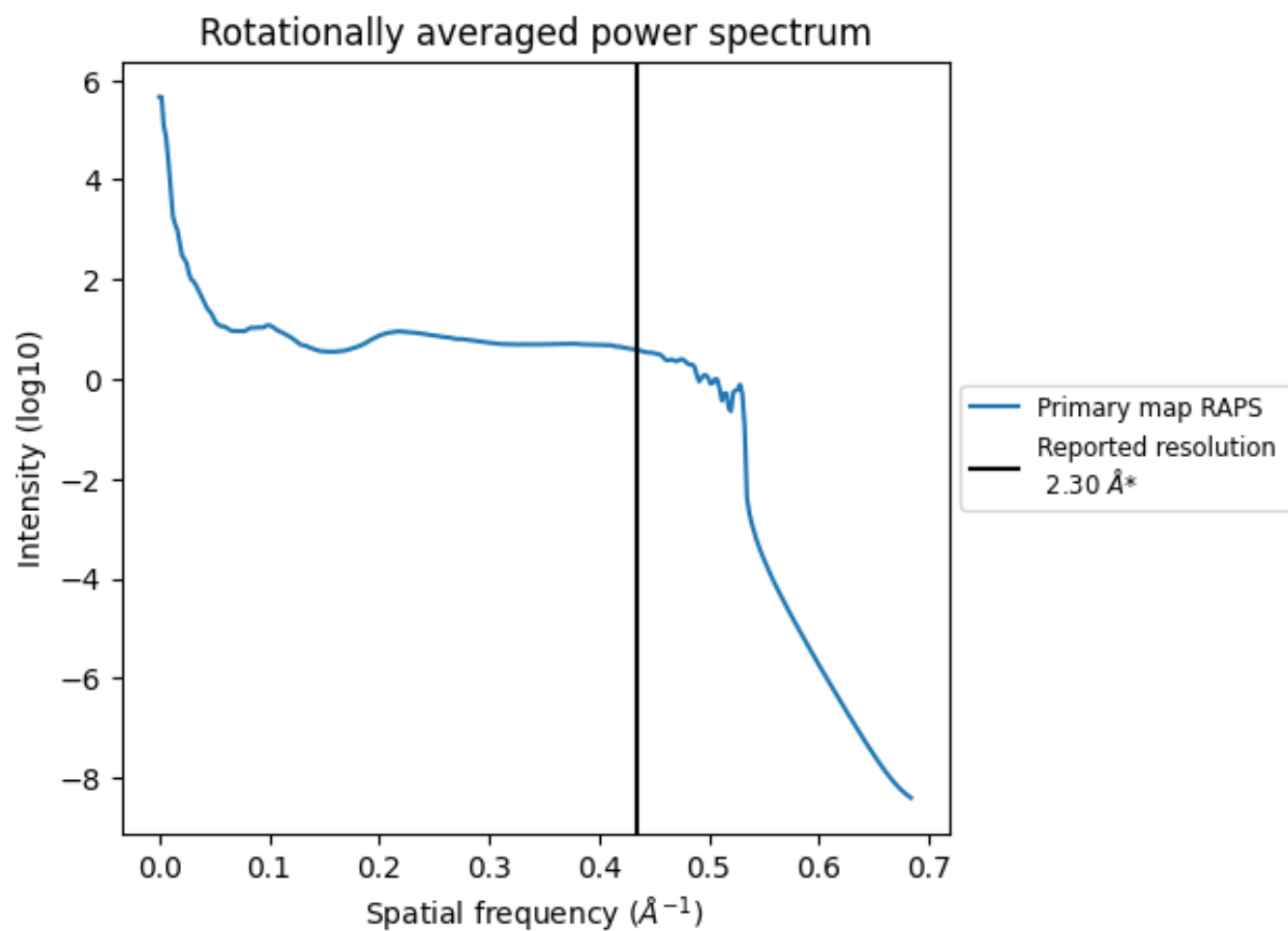
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm^3 ; this corresponds to an approximate mass of 232 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

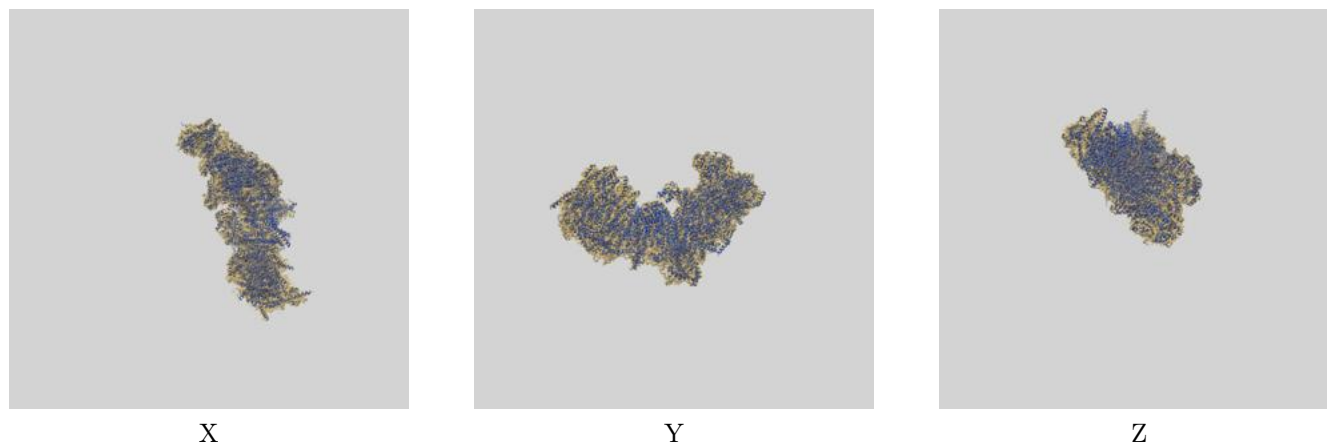
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

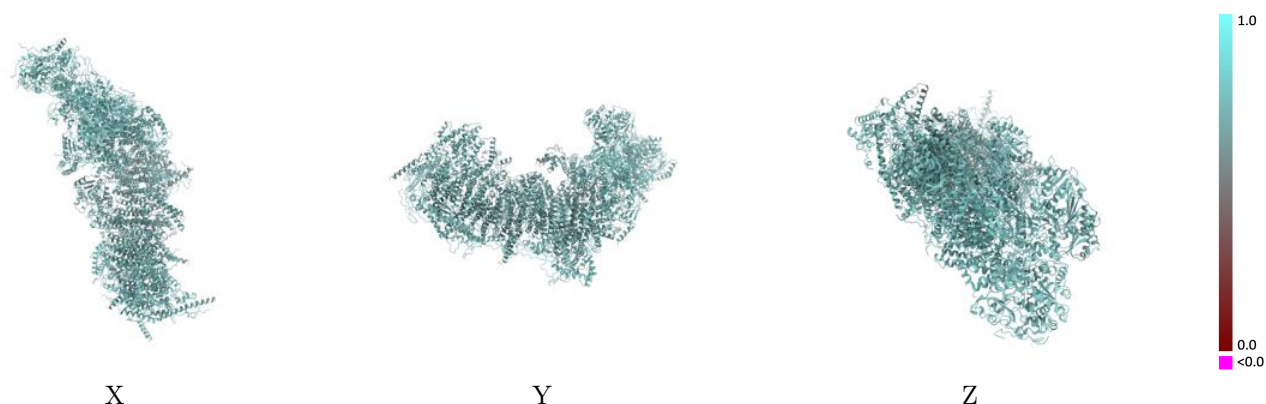
This section contains information regarding the fit between EMDB map EMD-14287 and PDB model 7R48. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



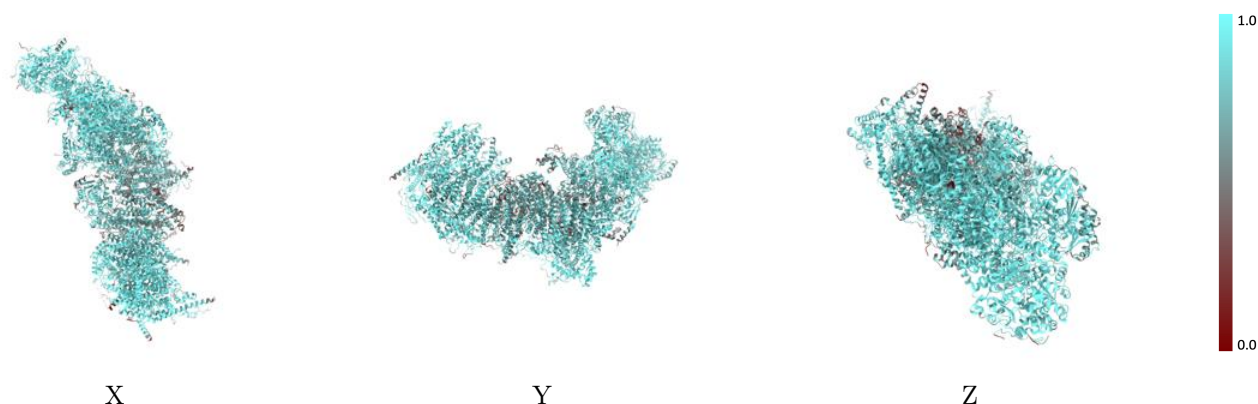
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



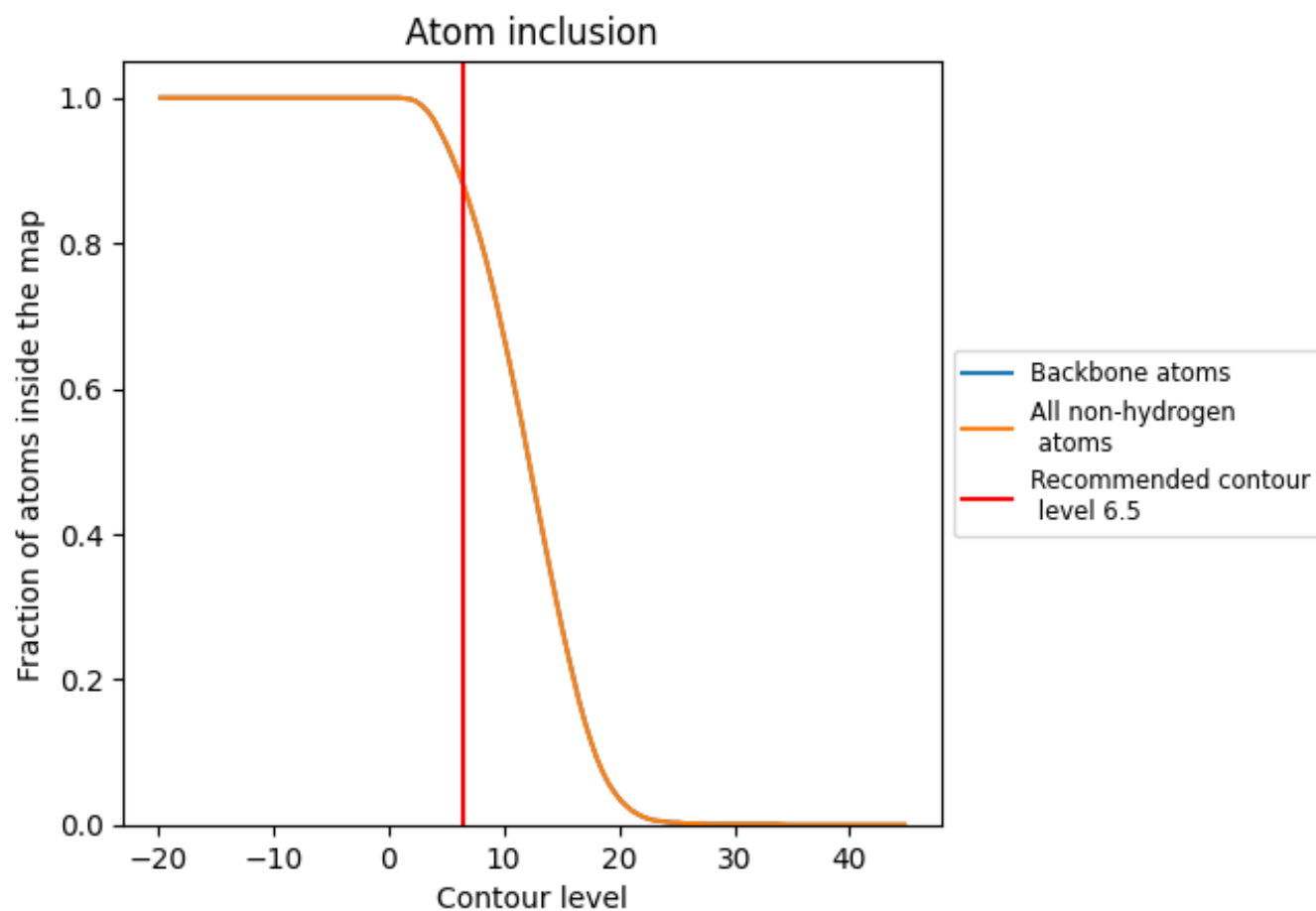
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.7110
A	 0.7480	 0.6800
B	 0.8890	 0.7340
C	 0.9630	 0.7490
D	 0.9240	 0.7420
E	 0.8860	 0.7050
F	 0.9230	 0.7190
G	 0.9150	 0.7270
H	 0.9070	 0.7160
I	 0.9660	 0.7530
J	 0.7850	 0.6910
K	 0.9430	 0.7280
L	 0.9220	 0.7060
M	 0.9460	 0.7230
N	 0.9380	 0.7260
O	 0.8540	 0.6910
P	 0.8510	 0.7070
Q	 0.9150	 0.7390
R	 0.8860	 0.7280
S	 0.8200	 0.6920
T	 0.6100	 0.6370
U	 0.9340	 0.7010
V	 0.8440	 0.7140
W	 0.8640	 0.7180
X	 0.8730	 0.6950
Y	 0.5510	 0.6600
Z	 0.8510	 0.7020
a	 0.9410	 0.7120
b	 0.8510	 0.6850
c	 0.7650	 0.6780
d	 0.8270	 0.6970
e	 0.8310	 0.6930
f	 0.7450	 0.6750
g	 0.8610	 0.6980
h	 0.8920	 0.7050



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8440	 0.6760
j	 0.8800	 0.6790
k	 0.8270	 0.6680
l	 0.9040	 0.7000
m	 0.8420	 0.6850
n	 0.9180	 0.7040
o	 0.8840	 0.6760
p	 0.9120	 0.7030
q	 0.8270	 0.7180
r	 0.8720	 0.7260
s	 0.8560	 0.6990