



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:27 PM UTC

PDB ID : 7R47 / pdb_00007r47
EMDB ID : EMD-14282
Title : Bovine complex I in the presence of IM1761092, deactive class iii (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:

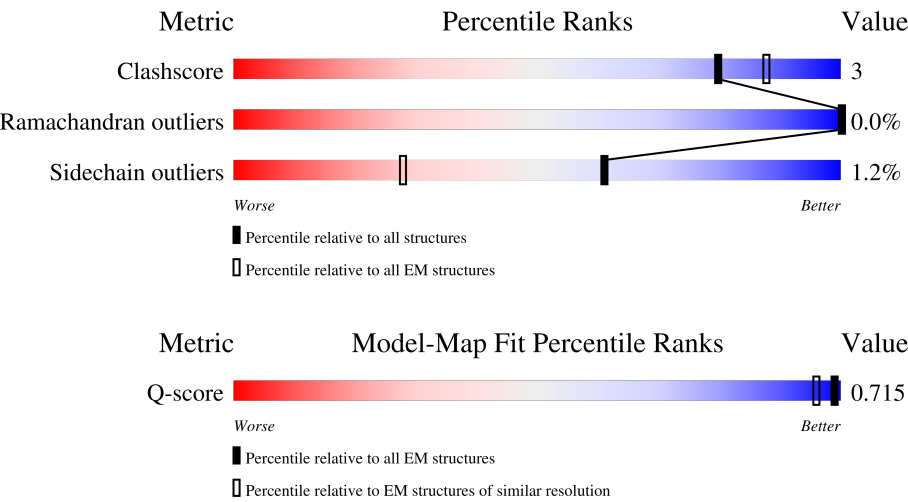
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



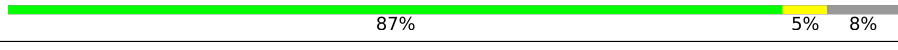
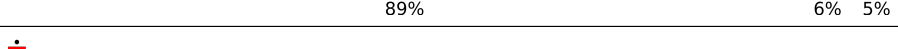
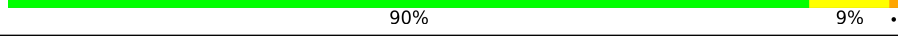
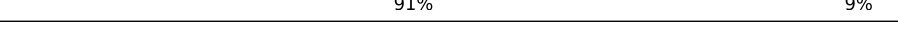
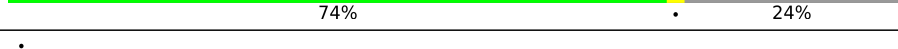
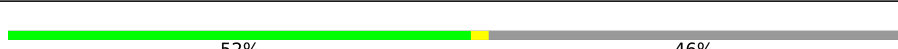
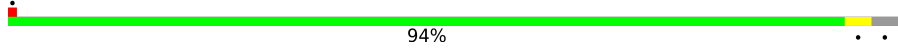
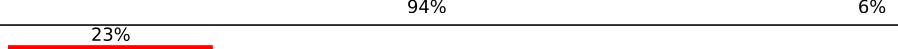
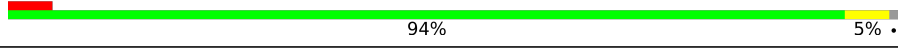
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	7% 73%12%13%
2	B	216	67%29%
3	C	266	74%23%
4	D	463	85%10%

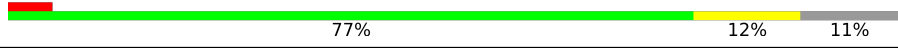
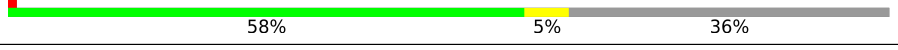
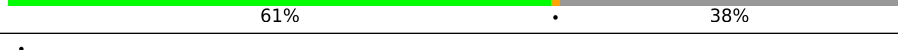
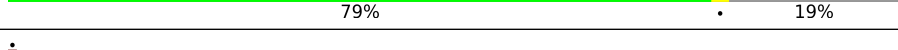
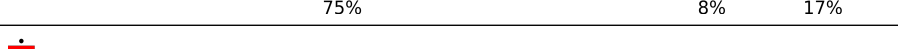
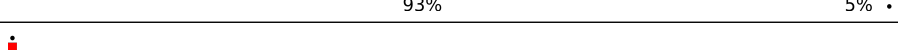
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 68578 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	100	Total	C	N	O	S	0	0
			808	552	117	134	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1714	1107	295	309	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	415	Total	C	N	O	S	0	0
			3347	2138	575	609	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	212	Total	C	N	O	S	0	0
			1650	1054	276	310	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3301	2080	589	612	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	307	Total	C	N	O	S	0	0
			2422	1625	370	404	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
			4784	3181	736	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	290	Total	C	N	O	S	0	0
			2309	1478	416	410	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	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	85	Total	C	N	O	S	0	0
			683	428	128	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	140	Total	C	N	O	S	0	0
			1146	737	200	200	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	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	111	Total	C	N	O	S	0	0
			929	610	156	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	95	Total	C	N	O	S	0	0
			799	506	150	137	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			444	291	78	74	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	103	Total	C	N	O	S	0	0
			884	584	149	150	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	79	Total	C	N	O	S	0	0
			638	418	107	111	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	N	O	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	121	Total	C	N	O	S	0	0
			1043	650	200	184	9		

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

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

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

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

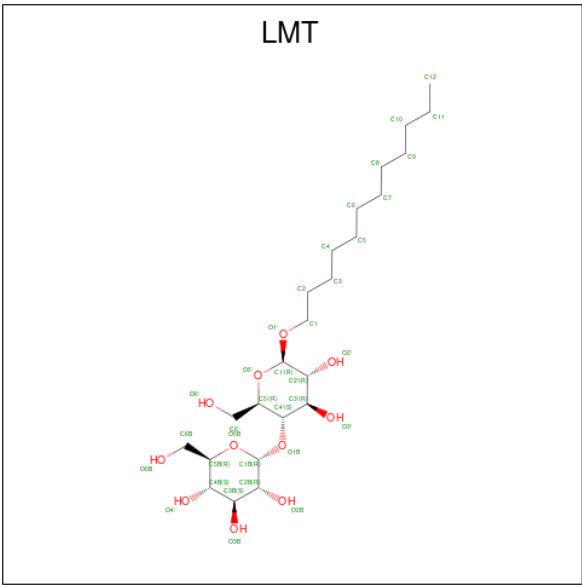
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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



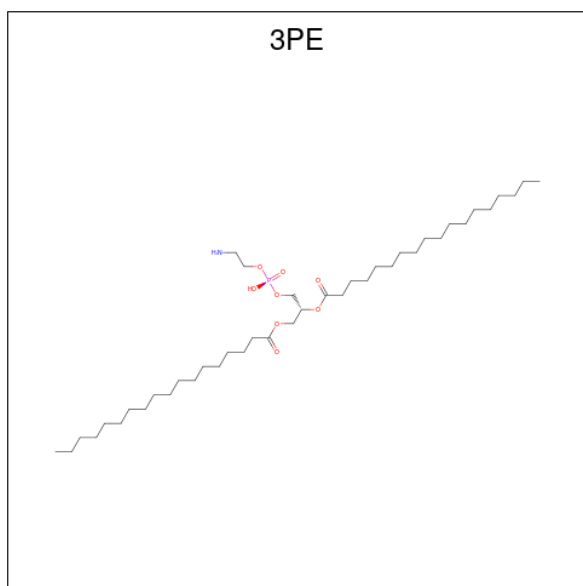
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	B	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	d	1	Total	C	O	0
			35	24	11	

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

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



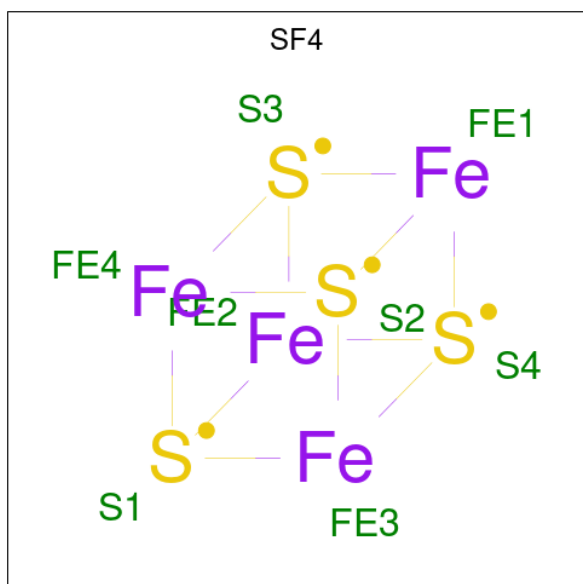
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	M	1	Total	C	N	O	P	0
			49	39	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	b	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	d	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



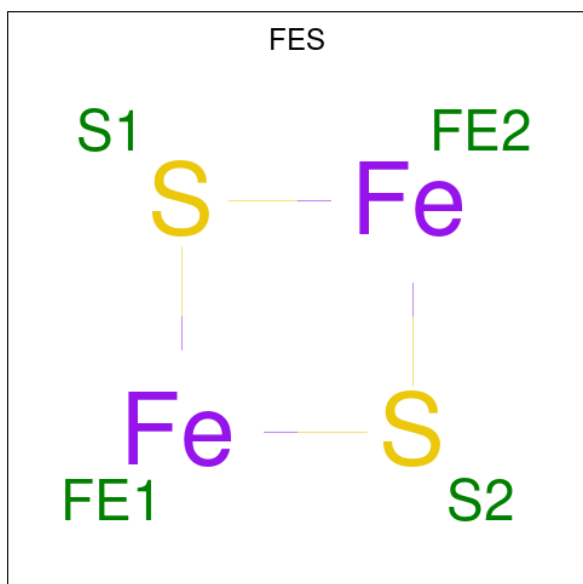
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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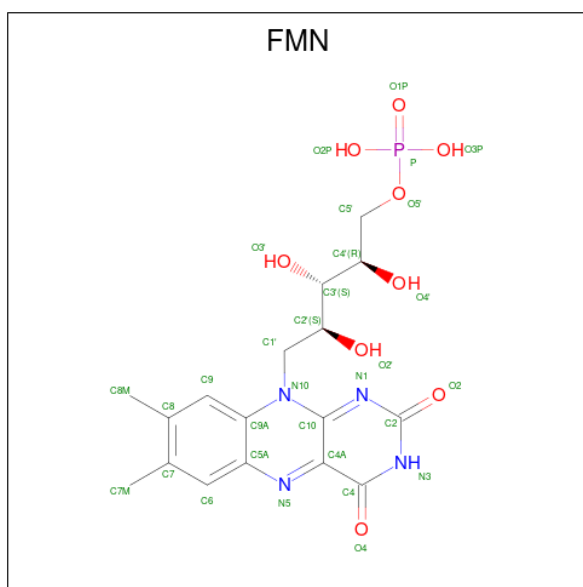
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

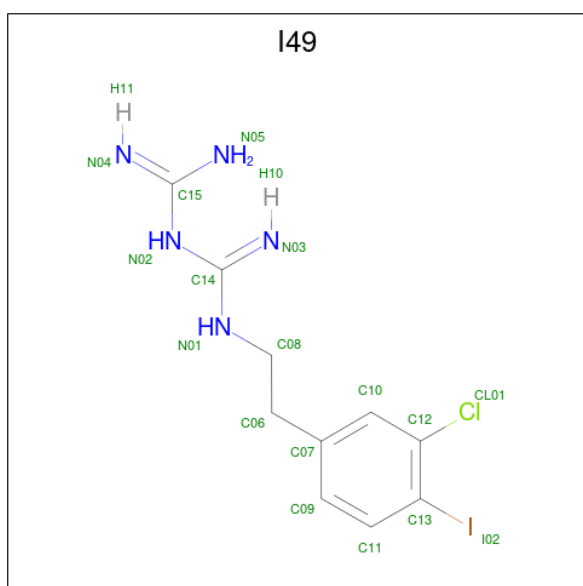


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

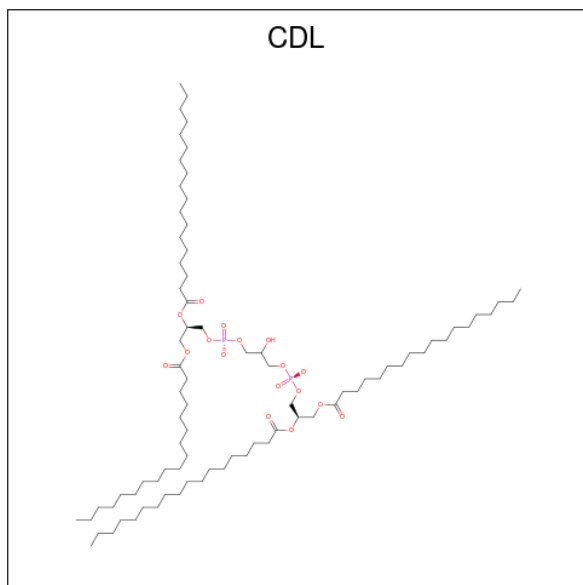
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (CCD ID: I49) (formula: C₁₀H₁₃ClIN₅) (labeled as "Ligand of Interest" by depositor).



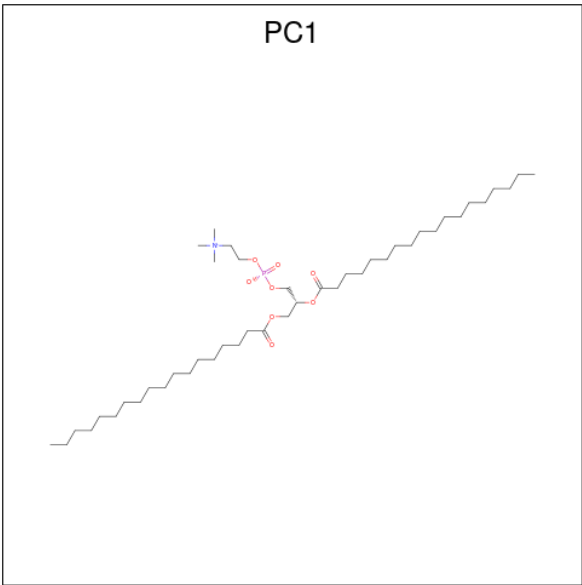
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	
51	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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



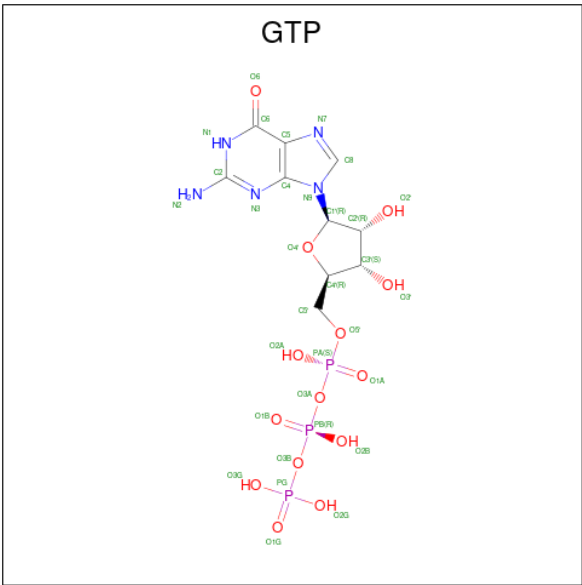
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	X	1	Total	C	O	P	0
			72	53	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	q	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
53	q	1	Total	C	N	O	P	0
			35	25	1	8	1	

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

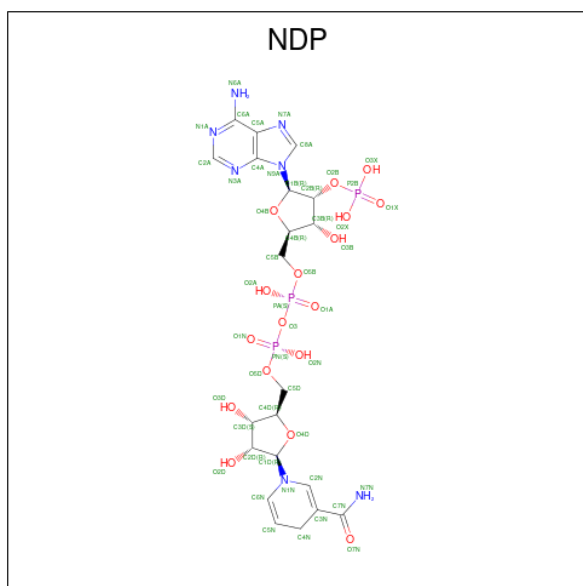


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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: $C_{21}H_{30}N_7O_{17}P_3$).

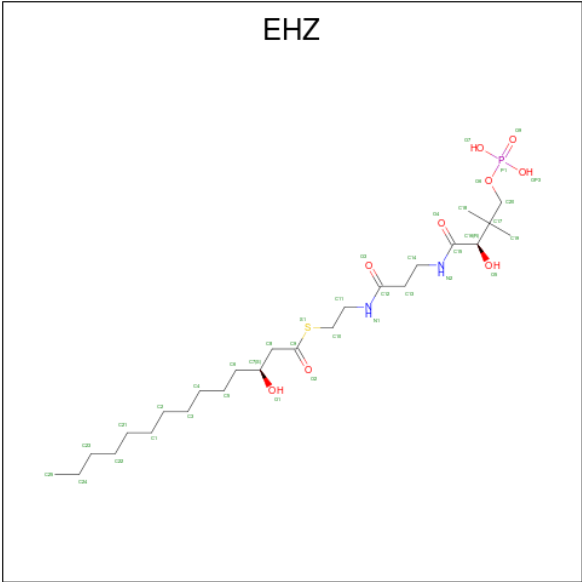


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

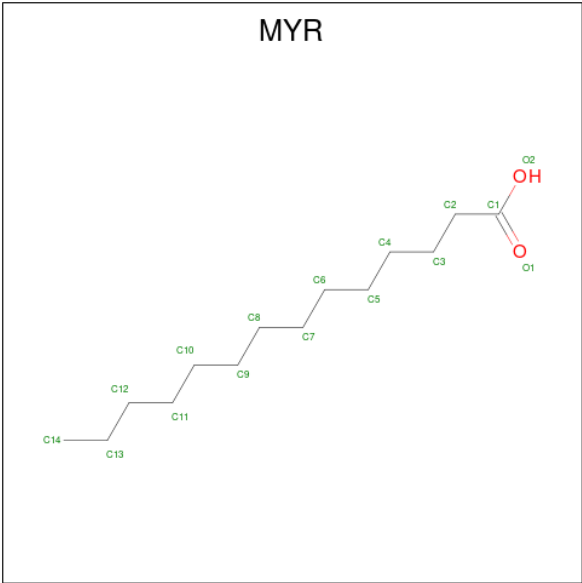
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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: $C_{25}H_{49}N_2O_9PS$).



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	11	Total 11	O 11	0
60	B	60	Total 60	O 60	0
60	C	109	Total 109	O 109	0
60	D	177	Total 177	O 177	0
60	E	27	Total 27	O 27	0
60	F	78	Total 78	O 78	0
60	G	228	Total 228	O 228	0
60	H	56	Total 56	O 56	0
60	I	107	Total 107	O 107	0
60	J	15	Total 15	O 15	0
60	K	12	Total 12	O 12	0
60	L	71	Total 71	O 71	0
60	M	83	Total 83	O 83	0
60	N	56	Total 56	O 56	0
60	O	30	Total 30	O 30	0
60	P	47	Total 47	O 47	0
60	Q	80	Total 80	O 80	0
60	R	46	Total 46	O 46	0
60	S	3	Total 3	O 3	0
60	U	23	Total 23	O 23	0
60	V	16	Total 16	O 16	0
60	W	21	Total 21	O 21	0

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Mol	Chain	Residues	Atoms		AltConf
60	X	34	Total 34	O 34	0
60	Y	2	Total 2	O 2	0
60	Z	32	Total 32	O 32	0
60	a	23	Total 23	O 23	0
60	b	10	Total 10	O 10	0
60	c	1	Total 1	O 1	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	16	Total 16	O 16	0
60	h	33	Total 33	O 33	0
60	i	12	Total 12	O 12	0
60	j	4	Total 4	O 4	0
60	k	10	Total 10	O 10	0
60	l	38	Total 38	O 38	0
60	m	20	Total 20	O 20	0
60	n	40	Total 40	O 40	0
60	o	24	Total 24	O 24	0
60	p	39	Total 39	O 39	0
60	q	42	Total 42	O 42	0
60	r	33	Total 33	O 33	0

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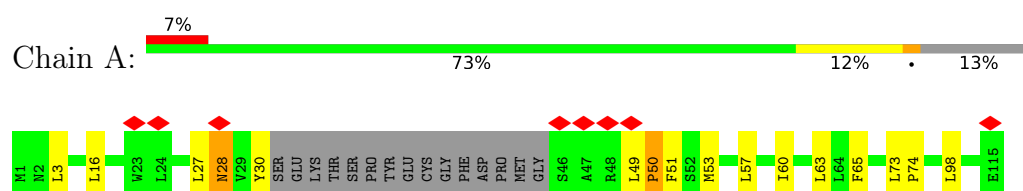
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	s	11	Total	O	0
			11	11	

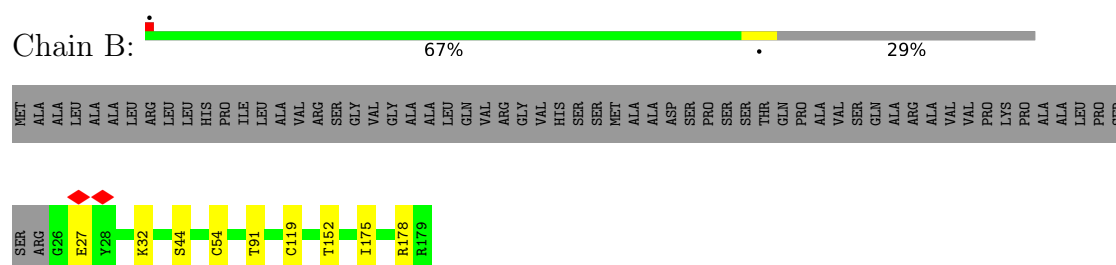
3 Residue-property plots [i](#)

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.

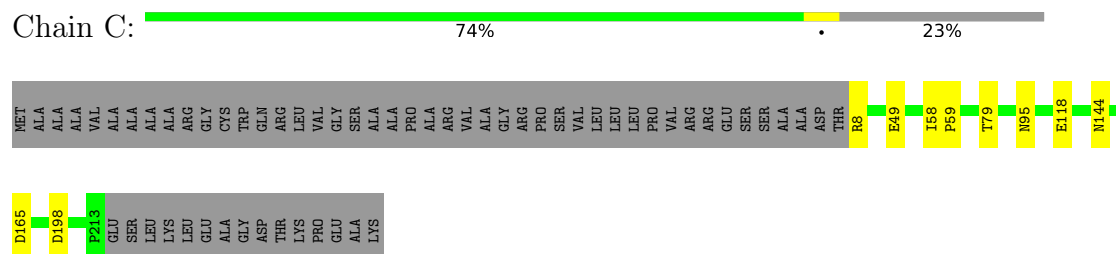
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



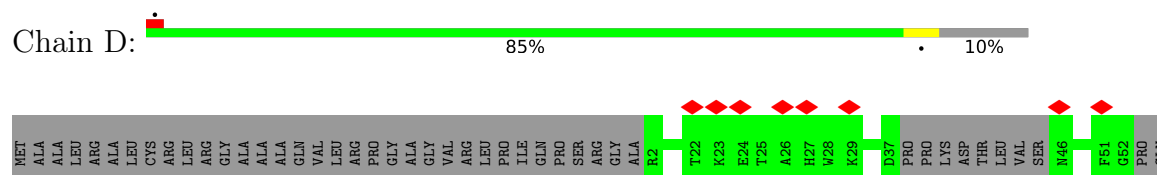
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



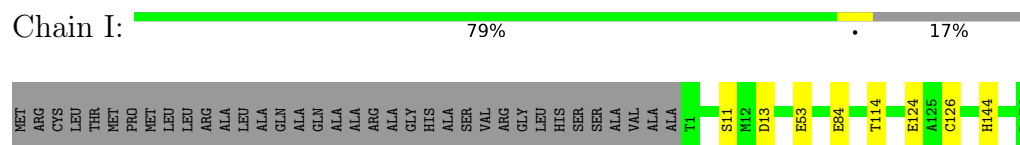
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



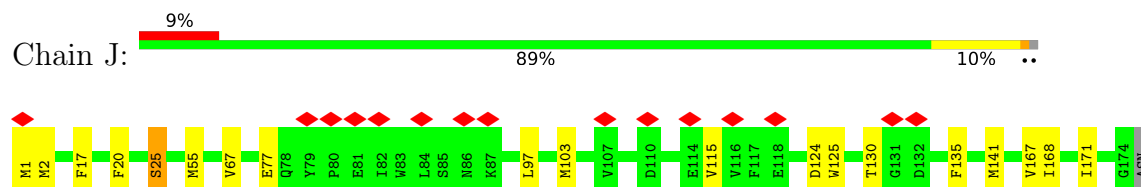
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



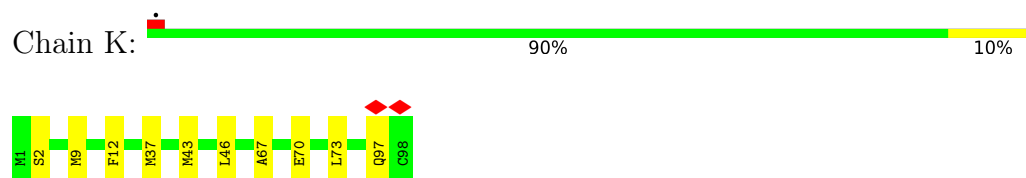
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



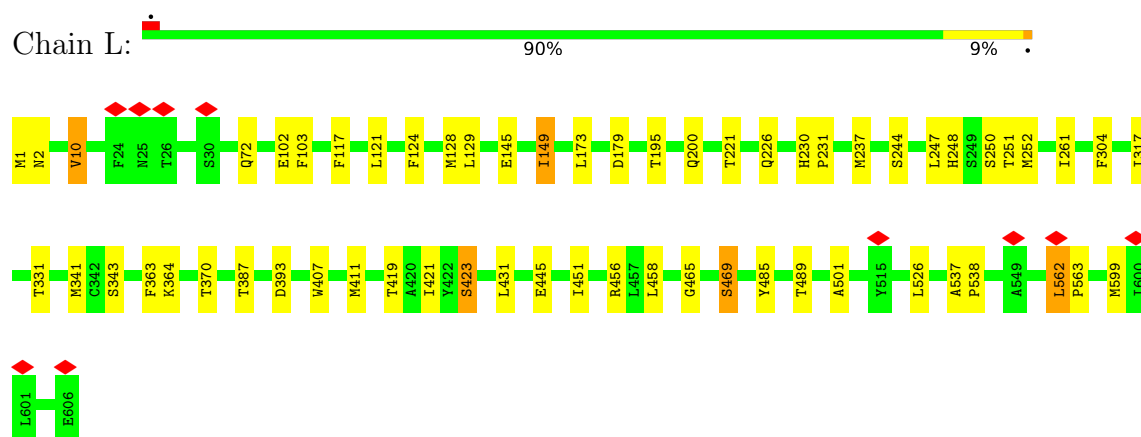
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



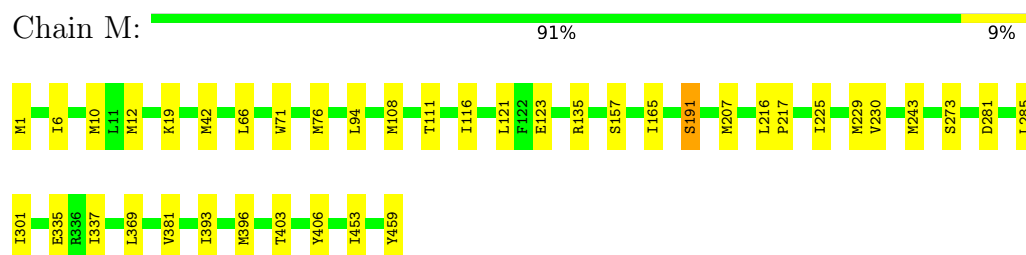
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

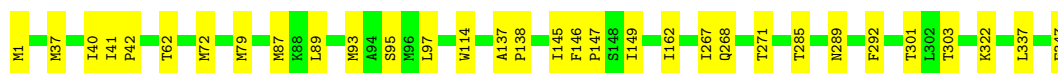


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



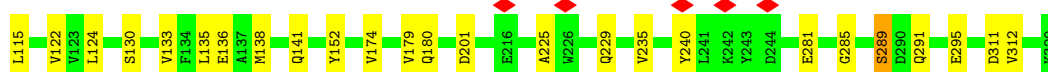
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2





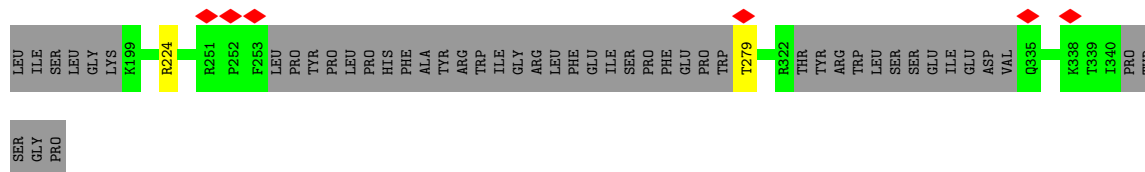
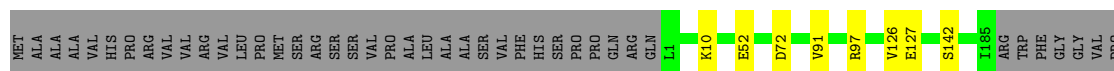
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 80% 12% 7%



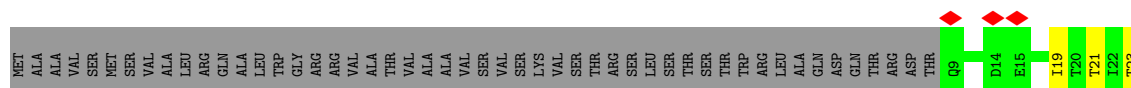
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 74% 24%



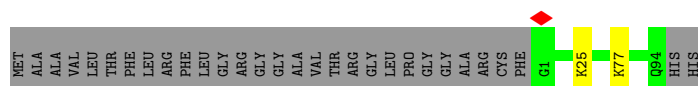
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 67% 29%



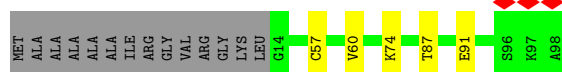
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 74% 24%



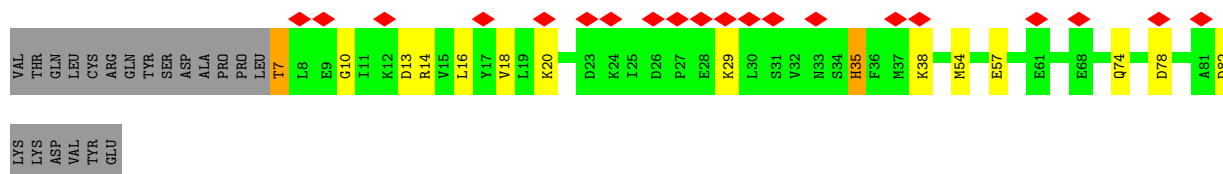
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 



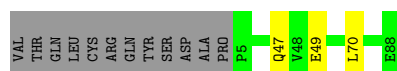
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T: 

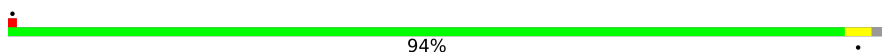


- Molecule 20: Acyl carrier protein, mitochondrial

Chain U: 



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

Chain V: 

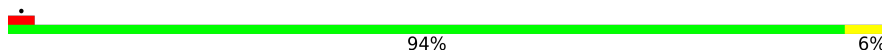


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W: 

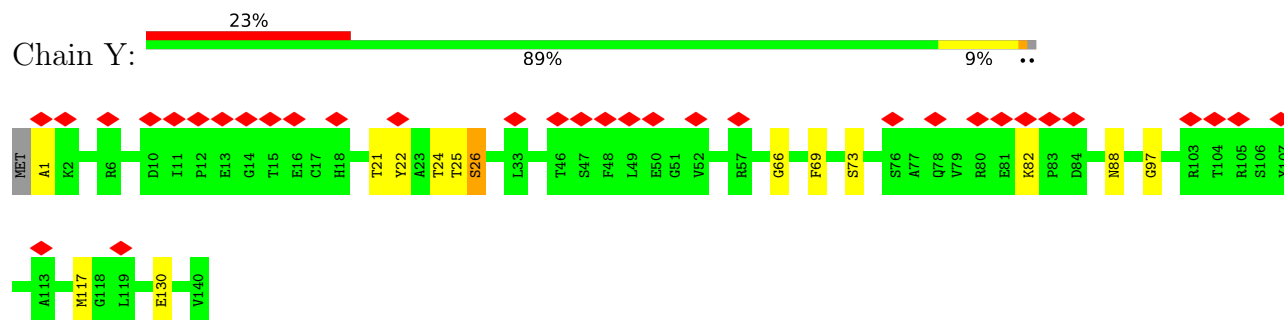


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

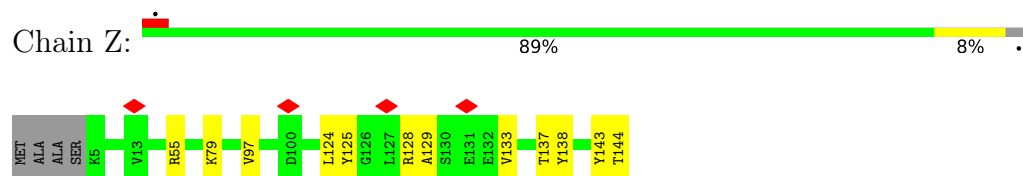
Chain X: 



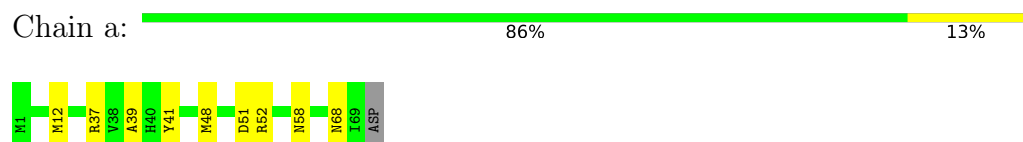
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



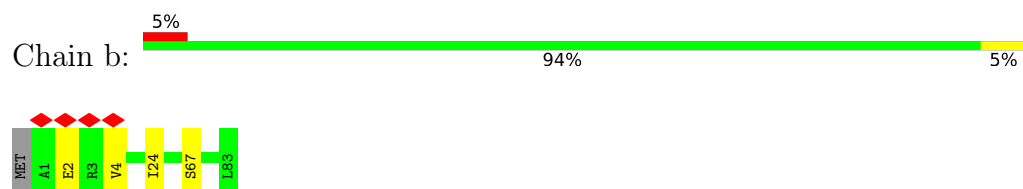
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



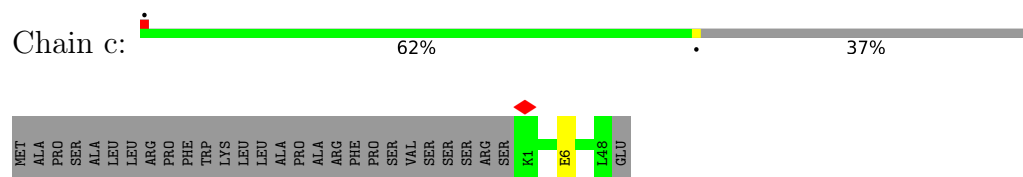
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



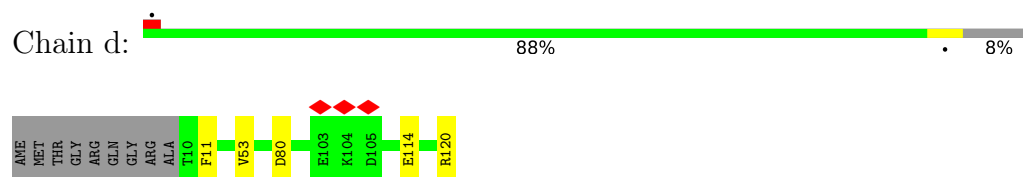
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



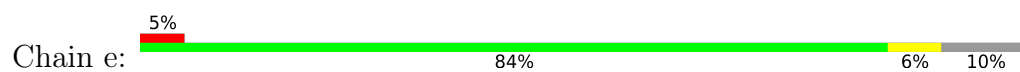
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



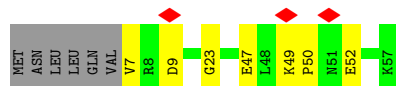
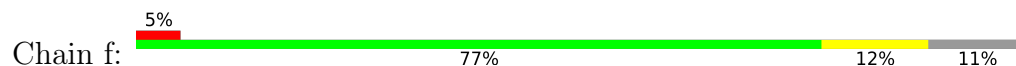
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



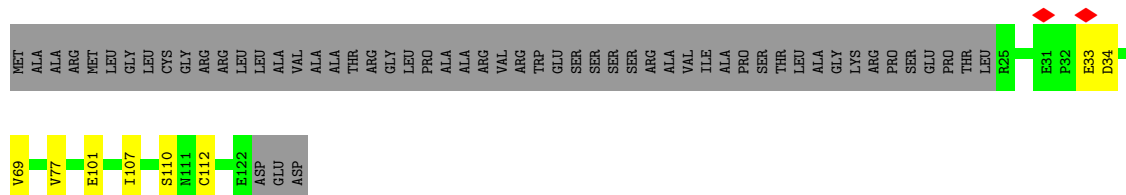
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



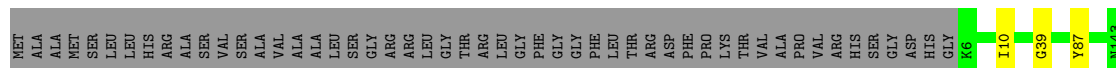
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



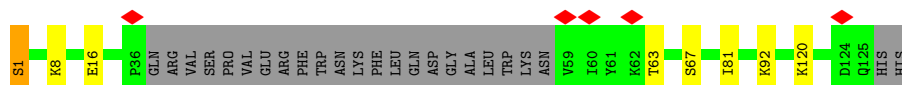
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



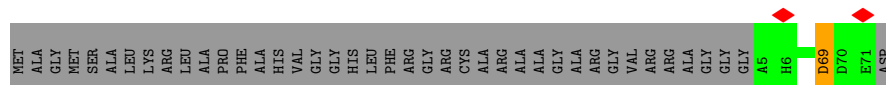
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



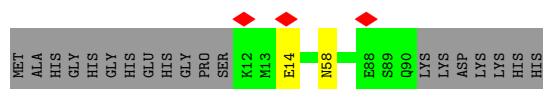
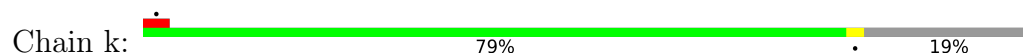
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



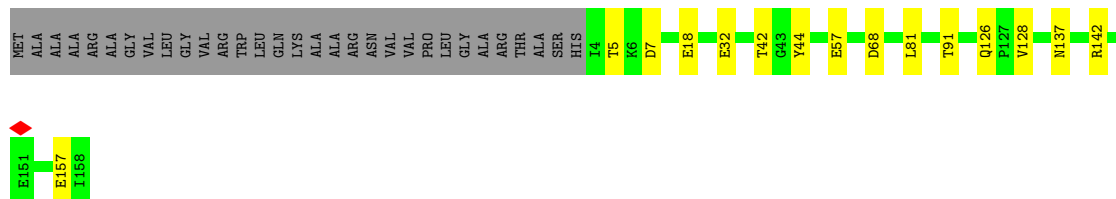
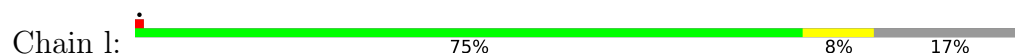
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



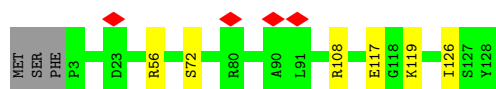
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



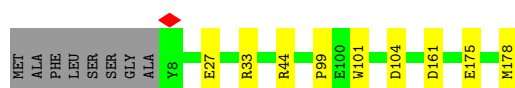
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



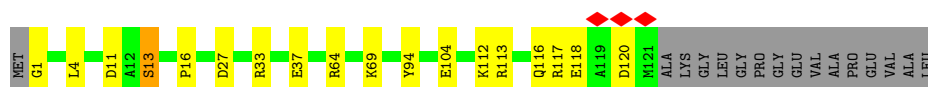
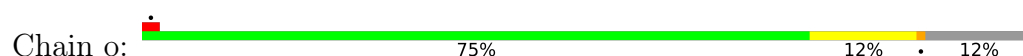
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



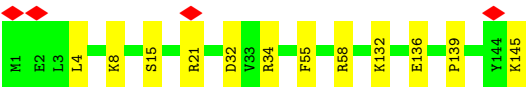
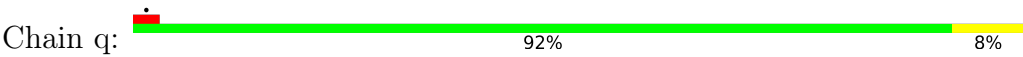
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



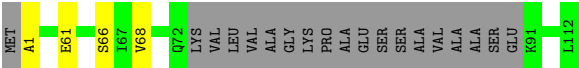
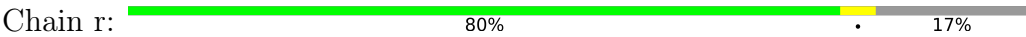
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



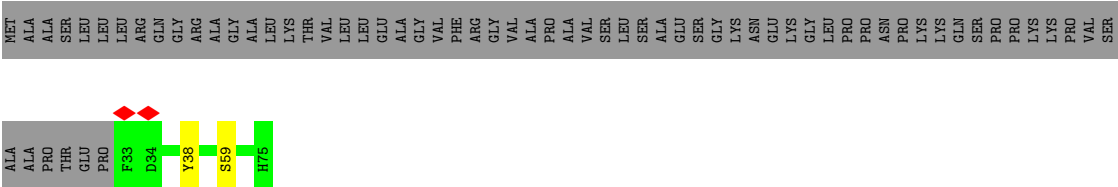
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	124012	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	44.627	Depositor
Minimum map value	-18.628	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.075	Depositor
Recommended contour level	6	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: I49, MG, ZN, LMT, NDP, SAC, AYA, EHZ, 2MR, PC1, FME, MYR, FES, 3PE, SF4, FMN, CDL, GTP, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/818	0.30	0/1120
2	B	0.26	0/1261	0.36	0/1706
3	C	0.24	0/1765	0.34	0/2403
4	D	0.23	0/3417	0.31	0/4623
5	E	0.21	0/1690	0.30	0/2300
6	F	0.22	0/3375	0.30	0/4561
7	G	0.22	0/5367	0.32	0/7274
8	H	0.25	0/2479	0.34	0/3384
9	I	0.25	0/1445	0.34	0/1956
10	J	0.19	0/1362	0.28	0/1848
11	K	0.21	0/745	0.25	0/1008
12	L	0.24	0/4900	0.30	0/6667
13	M	0.25	0/3738	0.31	0/5097
14	N	0.23	0/2792	0.31	0/3800
15	O	0.22	0/2651	0.29	0/3587
16	P	0.22	0/2360	0.31	0/3188
17	Q	0.22	0/1039	0.32	0/1404
18	R	0.23	0/731	0.30	0/984
19	S	0.20	0/694	0.30	0/934
20	T	0.17	0/621	0.32	0/837
20	U	0.26	0/692	0.28	0/932
21	V	0.19	0/931	0.27	0/1261
22	W	0.22	0/995	0.30	0/1337
23	X	0.22	0/1439	0.31	0/1942
24	Y	0.14	0/1042	0.25	0/1414
25	Z	0.22	0/1175	0.28	0/1584
26	a	0.23	0/576	0.31	0/775
27	b	0.21	0/672	0.29	0/923
28	c	0.21	0/418	0.31	0/567
29	d	0.23	0/959	0.30	0/1298
30	e	0.21	0/818	0.31	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.21	0/457	0.31	0/616
32	g	0.24	0/850	0.30	0/1154
33	h	0.24	0/1188	0.31	0/1607
34	i	0.27	0/904	0.34	0/1230
35	j	0.25	0/607	0.28	0/833
36	k	0.22	0/657	0.27	0/887
37	l	0.26	0/1358	0.29	0/1858
38	m	0.24	0/1076	0.30	0/1455
39	n	0.26	0/1540	0.31	0/2085
40	o	0.30	0/1068	0.35	0/1430
41	p	0.25	0/1468	0.29	0/1979
42	q	0.20	0/1250	0.33	0/1698
43	r	0.21	0/780	0.32	0/1056
44	s	0.19	0/375	0.28	0/507
All	All	0.23	0/66545	0.31	0/90202

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
34	i	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	808	0	853	14	0
2	B	1230	0	1238	6	0
3	C	1714	0	1668	7	0
4	D	3347	0	3287	12	0
5	E	1650	0	1656	10	0
6	F	3301	0	3253	16	0
7	G	5279	0	5301	27	0
8	H	2422	0	2538	30	0
9	I	1414	0	1370	6	0
10	J	1337	0	1346	13	0
11	K	745	0	785	8	0
12	L	4784	0	4937	35	0
13	M	3654	0	3852	29	0
14	N	2733	0	2912	26	0
15	O	2589	0	2566	26	0
16	P	2309	0	2339	8	0
17	Q	1016	0	1014	4	0
18	R	720	0	700	2	0
19	S	683	0	695	2	0
20	T	612	0	604	8	0
20	U	681	0	677	2	0
21	V	911	0	950	2	0
22	W	971	0	989	6	0
23	X	1402	0	1381	2	0
24	Y	1030	0	1041	7	0
25	Z	1146	0	1146	10	0
26	a	561	0	564	6	0
27	b	651	0	662	1	0
28	c	405	0	409	1	0
29	d	929	0	914	5	0
30	e	799	0	807	3	0
31	f	444	0	444	4	0
32	g	824	0	772	6	0
33	h	1154	0	1168	3	0
34	i	884	0	905	5	0
35	j	580	0	519	1	0
36	k	638	0	621	2	0
37	l	1304	0	1203	11	0
38	m	1050	0	1051	5	0
39	n	1487	0	1433	7	0
40	o	1043	0	1011	11	0
41	p	1435	0	1411	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	q	1209	0	1182	8	0
43	r	767	0	776	1	0
44	s	364	0	336	1	0
45	A	35	0	46	0	0
45	B	35	0	46	2	0
45	L	35	0	46	0	0
45	N	70	0	92	3	0
45	Y	35	0	46	0	0
45	d	35	0	46	0	0
45	e	35	0	46	2	0
45	f	70	0	92	0	0
45	h	35	0	46	2	0
45	j	35	0	46	2	0
45	l	35	0	46	0	0
46	A	38	0	50	1	0
46	H	34	0	47	0	0
46	I	51	0	82	1	0
46	L	94	0	142	1	0
46	M	95	0	144	1	0
46	N	41	0	56	0	0
46	Y	35	0	44	0	0
46	b	48	0	73	0	0
46	d	47	0	71	2	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	1	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	0	0
50	G	1	0	0	0	0
51	H	17	0	0	3	0
51	N	17	0	0	1	0
52	J	71	0	86	0	0
52	L	69	0	82	0	0
52	X	72	0	88	1	0
52	d	65	0	77	0	0
52	h	67	0	81	0	0
52	q	76	0	96	0	0
53	M	40	0	57	1	0
53	q	35	0	44	0	0
54	O	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	O	1	0	0	0	0
56	P	48	0	26	2	0
57	R	1	0	0	0	0
58	T	37	0	0	1	0
58	U	37	0	0	0	0
59	o	15	0	27	0	0
60	A	11	0	0	0	0
60	B	60	0	0	0	0
60	C	109	0	0	4	0
60	D	177	0	0	2	0
60	E	27	0	0	0	0
60	F	78	0	0	1	0
60	G	228	0	0	5	0
60	H	56	0	0	0	0
60	I	107	0	0	2	0
60	J	15	0	0	0	0
60	K	12	0	0	0	0
60	L	71	0	0	2	0
60	M	83	0	0	2	0
60	N	56	0	0	2	0
60	O	30	0	0	2	0
60	P	47	0	0	1	0
60	Q	80	0	0	0	0
60	R	46	0	0	1	0
60	S	3	0	0	0	0
60	U	23	0	0	0	0
60	V	16	0	0	0	0
60	W	21	0	0	2	0
60	X	34	0	0	0	0
60	Y	2	0	0	0	0
60	Z	32	0	0	2	0
60	a	23	0	0	2	0
60	b	10	0	0	0	0
60	c	1	0	0	0	0
60	d	16	0	0	2	0
60	e	30	0	0	1	0
60	f	10	0	0	0	0
60	g	16	0	0	1	0
60	h	33	0	0	0	0
60	i	12	0	0	2	0
60	j	4	0	0	0	0
60	k	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	l	38	0	0	1	0
60	m	20	0	0	3	0
60	n	40	0	0	3	0
60	o	24	0	0	1	0
60	p	39	0	0	1	0
60	q	42	0	0	1	0
60	r	33	0	0	0	0
60	s	11	0	0	0	0
All	All	68578	0	67288	358	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 (358) 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)
8:H:225:MET:HE3	51:H:602:I49:I02	2.35	0.96
9:I:11:SER:OG	9:I:13:ASP:OD1	1.92	0.86
38:m:72:SER:O	60:m:201:HOH:O	1.93	0.85
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.12	0.83
32:g:101:GLU:OE2	60:g:201:HOH:O	1.97	0.82
4:D:279:ASP:OD2	60:D:501:HOH:O	1.98	0.82
37:l:157:GLU:O	40:o:33:ARG:NH1	2.14	0.81
45:j:101:LMT:O3'	45:j:101:LMT:O2B	1.98	0.81
12:L:364:LYS:NZ	36:k:58:ASN:O	2.12	0.81
22:W:111:GLU:OE1	60:W:201:HOH:O	1.97	0.81
39:n:175:GLU:OE1	60:n:201:HOH:O	1.98	0.81
7:G:232:ASP:OD2	60:G:901:HOH:O	1.98	0.80
7:G:346:GLU:OE2	60:G:902:HOH:O	2.00	0.80
8:H:225:MET:CE	51:H:602:I49:I02	3.00	0.80
12:L:465:GLY:O	12:L:469:SER:OG	2.00	0.79
14:N:347:GLU:OE2	60:N:1001:HOH:O	1.99	0.79
29:d:80:ASP:OD2	60:d:1301:HOH:O	1.99	0.79
17:Q:36:ARG:NE	17:Q:106:GLU:OE1	2.16	0.77
40:o:64:ARG:O	60:o:301:HOH:O	2.03	0.77
25:Z:138:TYR:OH	60:Z:201:HOH:O	2.02	0.77
39:n:161:ASP:O	60:n:202:HOH:O	2.04	0.76
7:G:260:GLU:OE1	60:G:903:HOH:O	2.02	0.76
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.03	0.76
7:G:139:ASP:O	18:R:77:LYS:NZ	2.18	0.76
13:M:335:GLU:OE2	60:M:701:HOH:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:8:LYS:NZ	60:i:202:HOH:O	2.18	0.76
29:d:114:GLU:OE1	60:d:1302:HOH:O	2.03	0.75
10:J:141:MET:HA	10:J:141:MET:HE2	1.69	0.74
37:l:137:ASN:O	37:l:142:ARG:NH2	2.19	0.74
9:I:124:GLU:OE2	60:I:301:HOH:O	2.06	0.74
45:h:1002:LMT:O6B	41:p:58:ASN:OD1	2.02	0.74
6:F:108:ARG:NH1	60:F:601:HOH:O	2.21	0.73
13:M:42:MET:HE1	13:M:453:ILE:HD12	1.70	0.73
12:L:599:MET:HE3	14:N:93:MET:HE1	1.71	0.72
38:m:126:ILE:O	60:m:202:HOH:O	2.07	0.71
23:X:68:GLU:OE1	23:X:71:ARG:NH1	2.23	0.71
45:e:201:LMT:O2B	45:e:201:LMT:O3'	2.04	0.71
24:Y:69:PHE:O	24:Y:73:SER:OG	2.06	0.71
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.72	0.70
3:C:95:ASN:OD1	60:C:301:HOH:O	2.09	0.70
45:e:201:LMT:O6B	45:e:201:LMT:O3B	2.09	0.70
15:O:103:SER:OG	60:O:501:HOH:O	2.09	0.70
12:L:2:ASN:OD1	60:L:801:HOH:O	2.08	0.70
2:B:27:GLU:OE2	2:B:178:ARG:NH2	2.24	0.70
14:N:303:THR:O	60:N:1002:HOH:O	2.10	0.70
10:J:25:SER:OG	10:J:77:GLU:OE1	2.08	0.69
3:C:165:ASP:OD2	60:C:302:HOH:O	2.10	0.69
8:H:20:LEU:HD13	26:a:12:MET:HE1	1.74	0.68
22:W:123:TYR:O	60:W:202:HOH:O	2.12	0.68
7:G:140:LYS:O	7:G:148:THR:OG1	2.08	0.68
41:p:88:GLU:OE1	60:p:201:HOH:O	2.12	0.68
42:q:32:ASP:OD1	60:q:301:HOH:O	2.12	0.67
31:f:7:VAL:HG12	31:f:9:ASP:H	1.60	0.67
37:l:18:GLU:N	37:l:18:GLU:OE2	2.27	0.67
34:i:92:LYS:O	60:i:201:HOH:O	2.11	0.67
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.09	0.66
30:e:42:CYS:O	60:e:301:HOH:O	2.12	0.66
20:T:74:GLN:NE2	20:T:78:ASP:OD2	2.29	0.66
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.28	0.66
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.25	0.66
3:C:49:GLU:OE1	60:C:303:HOH:O	2.13	0.66
37:l:5:THR:OG1	37:l:7:ASP:OD2	2.05	0.65
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.65
39:n:104:ASP:OD2	60:n:203:HOH:O	2.13	0.65
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.78	0.65
12:L:599:MET:CE	14:N:93:MET:HE1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:598:LYS:NZ	60:G:905:HOH:O	2.22	0.64
10:J:124:ASP:OD1	11:K:2:SER:OG	2.15	0.64
15:O:60:ASP:OD1	15:O:60:ASP:N	2.32	0.63
13:M:10:MET:HE2	13:M:10:MET:HA	1.79	0.63
15:O:291:GLN:NE2	15:O:295:GLU:OE1	2.28	0.63
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.82	0.62
1:A:49:LEU:O	1:A:50:PRO:C	2.42	0.62
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.82	0.62
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.81	0.62
5:E:71:GLU:O	5:E:74:GLN:NE2	2.33	0.62
15:O:104:ARG:NH1	54:O:401:GTP:O6	2.32	0.62
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.80	0.62
36:k:14:GLU:N	36:k:14:GLU:OE2	2.33	0.61
24:Y:21:THR:O	24:Y:25:THR:OG1	2.11	0.61
26:a:37:ARG:NE	60:a:102:HOH:O	2.25	0.60
12:L:10:VAL:HG23	34:i:81:ILE:HD12	1.84	0.59
25:Z:97:VAL:HG21	30:e:82:ARG:HG3	1.84	0.59
16:P:72:ASP:O	60:P:601:HOH:O	2.16	0.59
18:R:25:LYS:O	60:R:301:HOH:O	2.17	0.59
3:C:118:GLU:OE2	3:C:144:ASN:ND2	2.36	0.58
5:E:181:ILE:HG23	5:E:181:ILE:O	2.03	0.57
34:i:63:THR:O	34:i:67:SER:N	2.36	0.57
1:A:49:LEU:O	1:A:51:PHE:N	2.38	0.57
15:O:26:THR:HG21	60:O:511:HOH:O	2.05	0.57
1:A:28:ASN:OD1	1:A:28:ASN:N	2.38	0.56
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.88	0.56
28:c:6:GLU:OE2	28:c:6:GLU:HA	2.05	0.56
8:H:203:GLY:O	8:H:207:LEU:HD22	2.05	0.56
7:G:441:GLN:HA	7:G:441:GLN:OE1	2.06	0.56
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.39	0.56
15:O:83:TYR:OH	54:O:401:GTP:O3'	2.04	0.56
9:I:84:GLU:OE2	60:I:302:HOH:O	2.18	0.56
11:K:12:PHE:CG	14:N:72:MET:HE2	2.41	0.55
12:L:128:MET:HB2	12:L:251:THR:HG23	1.87	0.55
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.87	0.55
37:l:57:GLU:OE1	37:l:91:THR:OG1	2.21	0.55
12:L:173:LEU:HD13	46:L:701:3PE:H222	1.89	0.55
8:H:200:LEU:HD22	8:H:285:LEU:HD21	1.88	0.55
19:S:57:CYS:O	19:S:60:VAL:HG22	2.07	0.55
45:j:101:LMT:H3O2	45:j:101:LMT:H2O1	1.52	0.54
12:L:72:GLN:OE1	60:L:803:HOH:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.37	0.54
13:M:296:LEU:HD22	13:M:381:VAL:HG11	1.90	0.54
15:O:311:ASP:OD1	15:O:312:VAL:HG13	2.08	0.54
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.90	0.54
16:P:10:LYS:NZ	17:Q:28:GLU:OE2	2.41	0.54
12:L:237:MET:HE1	12:L:248:HIS:NE2	2.24	0.53
5:E:105:THR:HG22	5:E:106:THR:H	1.73	0.53
13:M:135:ARG:NH1	14:N:301:THR:O	2.41	0.53
4:D:415:VAL:HG21	8:H:207:LEU:HG	1.90	0.53
1:A:30:TYR:OH	56:P:501:NDP:O3X	2.22	0.53
12:L:195:THR:HG21	12:L:200:GLN:HB3	1.91	0.52
15:O:138:MET:HE3	54:O:401:GTP:HN21	1.73	0.52
40:o:117:ARG:NH2	40:o:118:GLU:OE2	2.42	0.52
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.44	0.52
10:J:1:FME:SD	10:J:2:MET:N	2.83	0.52
45:N:902:LMT:O1B	45:N:902:LMT:O6'	2.26	0.52
7:G:170:ASP:OD2	60:G:904:HOH:O	2.18	0.52
7:G:315:VAL:O	7:G:340:SER:OG	2.23	0.52
7:G:366:THR:O	7:G:367:THR:OG1	2.18	0.52
8:H:70:MET:HE1	8:H:121:TRP:CE3	2.45	0.52
14:N:267:ILE:O	14:N:271:THR:HG23	2.10	0.52
38:m:56:ARG:NH2	60:m:203:HOH:O	2.37	0.51
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.92	0.51
11:K:9:MET:CE	14:N:79:MET:HE1	2.40	0.51
14:N:87:MET:O	14:N:145:ILE:HG22	2.10	0.51
3:C:8:ARG:NH2	43:r:61:GLU:OE1	2.33	0.51
15:O:281:GLU:N	15:O:281:GLU:OE1	2.43	0.51
5:E:123:LYS:NZ	5:E:174:ASP:OD1	2.23	0.51
14:N:97:LEU:HD21	45:N:902:LMT:H122	1.93	0.51
12:L:124:PHE:CD1	12:L:251:THR:HG21	2.45	0.51
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.46	0.51
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.46	0.51
31:f:47:GLU:OE2	31:f:47:GLU:HA	2.11	0.50
12:L:485:TYR:O	12:L:489:THR:OG1	2.29	0.50
26:a:51:ASP:OD2	60:a:101:HOH:O	2.20	0.50
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.42	0.50
5:E:194:GLU:OE1	5:E:194:GLU:N	2.43	0.50
7:G:377:VAL:HG23	7:G:404:LEU:HD11	1.94	0.50
15:O:285:GLY:O	15:O:289:SER:OG	2.29	0.50
45:B:202:LMT:O6'	45:B:202:LMT:O2B	2.26	0.50
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD11	45:B:202:LMT:H22	1.94	0.50
8:H:225:MET:HE2	51:H:602:I49:I02	2.81	0.49
19:S:87:THR:O	19:S:91:GLU:HG3	2.12	0.49
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.95	0.49
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.94	0.49
13:M:296:LEU:HD21	13:M:396:MET:SD	2.52	0.49
15:O:174:VAL:HG22	15:O:225:ALA:HB2	1.95	0.49
20:T:29:LYS:HD2	20:T:29:LYS:O	2.13	0.49
40:o:1:GLY:O	40:o:4:LEU:N	2.39	0.49
22:W:25:MET:HE1	22:W:79:VAL:HG21	1.94	0.49
29:d:11:PHE:O	30:e:8:ARG:NH2	2.44	0.49
35:j:69:ASP:OD1	40:o:113:ARG:NH1	2.46	0.49
6:F:99:GLU:OE1	6:F:107:ASP:N	2.46	0.48
16:P:97:ARG:NH2	56:P:501:NDP:O2X	2.44	0.48
37:l:42:THR:HG21	37:l:44:TYR:CE2	2.47	0.48
8:H:11:ILE:HB	8:H:12:PRO:HD3	1.94	0.48
6:F:367:GLU:OE2	7:G:100:ASN:ND2	2.45	0.48
29:d:120:ARG:O	38:m:108:ARG:NH2	2.45	0.48
17:Q:21:THR:HG21	22:W:73:ILE:HD11	1.95	0.48
15:O:136:GLU:HA	15:O:136:GLU:OE2	2.14	0.48
14:N:337:LEU:HD23	52:X:1701:CDL:C60	2.44	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.96	0.48
12:L:251:THR:HG22	12:L:252:MET:N	2.29	0.48
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.49	0.48
13:M:207:MET:HE3	13:M:298:ILE:HG13	1.95	0.48
16:P:224:ARG:HG2	16:P:224:ARG:HH11	1.78	0.48
16:P:279:THR:O	16:P:279:THR:HG23	2.14	0.47
25:Z:129:ALA:O	25:Z:133:VAL:HG23	2.14	0.47
13:M:207:MET:HE1	13:M:297:VAL:CG1	2.44	0.47
8:H:201:THR:O	8:H:205:SER:OG	2.25	0.47
10:J:103:MET:HG2	10:J:115:VAL:HG21	1.95	0.47
13:M:285:LEU:HD23	13:M:285:LEU:C	2.40	0.47
37:l:68:ASP:OD1	37:l:68:ASP:N	2.43	0.47
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.47	0.47
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.96	0.47
2:B:175:ILE:HD12	16:P:52:GLU:HG2	1.96	0.47
15:O:225:ALA:O	15:O:229:GLN:NE2	2.44	0.47
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.14	0.47
37:l:126:GLN:O	60:l:301:HOH:O	2.21	0.47
6:F:276:LEU:HD13	6:F:317:MET:SD	2.54	0.47
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:43:MET:HE1	14:N:72:MET:HE1	1.97	0.47
12:L:124:PHE:CE1	12:L:251:THR:HG21	2.50	0.47
13:M:225:ILE:O	13:M:229:MET:HG3	2.15	0.47
20:U:47:GLN:NE2	20:U:70:LEU:O	2.47	0.47
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.45	0.46
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.98	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.97	0.46
5:E:87:TYR:HB3	6:F:181:ALA:O	2.16	0.46
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.50	0.46
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.50	0.46
20:T:7:THR:O	20:T:10:GLY:N	2.49	0.46
13:M:108:MET:HB3	13:M:121:LEU:HD13	1.98	0.46
45:N:902:LMT:O1B	45:N:902:LMT:O4'	2.28	0.46
20:T:82:ASP:OD2	20:T:82:ASP:N	2.48	0.46
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.97	0.46
38:m:117:GLU:HB3	38:m:119:LYS:HE3	1.98	0.46
42:q:21:ARG:HH21	42:q:21:ARG:HG3	1.81	0.46
12:L:445:GLU:O	12:L:451:ILE:HD11	2.16	0.46
11:K:43:MET:HE1	14:N:72:MET:SD	2.55	0.46
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.97	0.46
15:O:82:PHE:CE1	15:O:138:MET:HE2	2.51	0.46
34:i:120:LYS:NZ	40:o:37:GLU:OE2	2.48	0.46
14:N:347:GLU:HG3	51:N:904:I49:I02	2.86	0.46
29:d:53:VAL:HG21	46:d:1201:3PE:H2	1.98	0.46
12:L:331:THR:HB	12:L:387:THR:HG22	1.98	0.45
13:M:459:TYR:OH	60:M:702:HOH:O	2.19	0.45
22:W:117:ASP:OD1	22:W:120:SER:OG	2.32	0.45
2:B:44:SER:OG	8:H:51:ASP:OD1	2.19	0.45
6:F:165:ASN:OD1	6:F:170:GLY:N	2.46	0.45
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.99	0.45
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.48	0.45
11:K:70:GLU:OE2	14:N:37:MET:HE1	2.16	0.45
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.99	0.45
42:q:4:LEU:HD11	42:q:8:LYS:HE3	1.98	0.45
42:q:132:LYS:NZ	42:q:136:GLU:OE1	2.50	0.45
6:F:98:ASP:O	6:F:99:GLU:C	2.60	0.45
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.98	0.45
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.98	0.45
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.99	0.45
13:M:191:SER:OG	24:Y:130:GLU:OE1	2.35	0.45
24:Y:82:LYS:O	24:Y:88:ASN:ND2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:I:201:3PE:H3C1	27:b:24:ILE:HD11	1.98	0.45
13:M:19:LYS:CE	13:M:19:LYS:H	2.30	0.45
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.42	0.44
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.99	0.44
58:T:101:EHZ:O2	58:T:101:EHZ:O1	2.34	0.44
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.52	0.44
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.44
1:A:51:PHE:HE1	1:A:53:MET:HE2	1.82	0.44
6:F:113:HIS:NE2	44:s:38:TYR:OH	2.32	0.44
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.98	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
24:Y:22:TYR:O	24:Y:26:SER:OG	2.32	0.44
6:F:93:LEU:O	6:F:134:ALA:HA	2.17	0.44
7:G:281:GLU:HG2	7:G:592:LEU:HD12	2.00	0.44
7:G:289:GLY:HA2	42:q:145:LYS:HE2	2.00	0.44
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.53	0.44
8:H:179:TRP:N	8:H:180:PRO:CD	2.81	0.44
13:M:123:GLU:OE2	13:M:157:SER:HB2	2.16	0.44
8:H:285:LEU:HD12	8:H:285:LEU:C	2.43	0.44
20:T:35:HIS:CE1	20:T:38:LYS:HE2	2.53	0.44
25:Z:124:LEU:O	25:Z:128:ARG:NH1	2.51	0.44
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.47	0.44
40:o:11:ASP:OD1	40:o:13:SER:OG	2.36	0.44
7:G:437:HIS:O	7:G:440:SER:OG	2.27	0.43
8:H:73:LEU:HD23	8:H:118:TRP:CZ3	2.53	0.43
14:N:146:PHE:HA	14:N:149:ILE:HD12	1.99	0.43
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.98	0.43
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.00	0.43
12:L:247:LEU:HD22	12:L:248:HIS:CD2	2.54	0.43
14:N:41:ILE:N	14:N:42:PRO:HD2	2.34	0.43
6:F:306:LEU:C	6:F:306:LEU:HD12	2.44	0.43
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.99	0.43
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.99	0.43
53:M:603:PC1:O13	53:M:603:PC1:H132	2.18	0.43
15:O:58:TYR:O	15:O:61:SER:OG	2.34	0.43
4:D:157:HIS:ND1	60:D:502:HOH:O	2.27	0.43
4:D:417:ILE:O	4:D:420:THR:HG22	2.18	0.43
4:D:259:MET:HE1	4:D:405:MET:HE1	2.01	0.43
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.99	0.43
12:L:562:LEU:CB	12:L:563:PRO:CD	2.96	0.43
16:P:127:GLU:O	16:P:224:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:39:GLY:HA3	45:h:1002:LMT:H123	2.00	0.43
12:L:363:PHE:CD1	12:L:370:THR:HG21	2.54	0.43
13:M:281:ASP:OD1	13:M:281:ASP:C	2.61	0.43
23:X:154:GLU:OE1	23:X:154:GLU:N	2.51	0.43
1:A:63:LEU:HB2	10:J:67:VAL:HG21	2.01	0.43
11:K:37:MET:HG3	11:K:67:ALA:CB	2.48	0.43
4:D:328:ALA:HB3	7:G:126:ASP:HB2	2.01	0.42
5:E:108:CYS:HA	5:E:151:ALA:HB1	2.01	0.42
37:l:81:LEU:HD13	37:l:81:LEU:C	2.44	0.42
10:J:130:THR:HG21	25:Z:124:LEU:HD12	2.01	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.01	0.42
8:H:221:ALA:O	8:H:225:MET:HG3	2.18	0.42
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.55	0.42
15:O:31:ILE:O	15:O:179:VAL:HG13	2.19	0.42
15:O:88:SER:OG	15:O:90:ASP:OD1	2.17	0.42
26:a:39:ALA:HB2	26:a:48:MET:HE2	2.02	0.42
37:l:32:GLU:OE1	37:l:32:GLU:N	2.50	0.42
21:V:17:GLU:OE1	21:V:17:GLU:HA	2.19	0.42
8:H:113:VAL:HG22	8:H:136:VAL:HG22	2.01	0.42
9:I:126:CYS:HA	47:I:203:SF4:S2	2.59	0.42
13:M:42:MET:HE3	32:g:77:VAL:HG22	2.00	0.42
25:Z:143:TYR:O	25:Z:144:THR:C	2.63	0.42
33:h:87:TYR:OH	41:p:86:GLU:OE2	2.29	0.42
41:p:72:ASP:OD2	41:p:74:THR:OG1	2.37	0.42
7:G:568:GLU:HA	7:G:587:VAL:O	2.20	0.42
8:H:102:VAL:HG13	8:H:150:LEU:HD21	2.00	0.42
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.55	0.42
12:L:145:GLU:OE1	12:L:179:ASP:OD2	2.37	0.42
15:O:130:SER:O	15:O:133:VAL:HG22	2.19	0.42
4:D:117:ALA:HB2	4:D:367:ILE:HG12	2.01	0.42
20:U:49:GLU:OE1	39:n:44:ARG:NH1	2.51	0.42
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.55	0.42
40:o:16:PRO:HB3	40:o:104:GLU:HG2	2.02	0.42
1:A:3:LEU:HD22	46:A:302:3PE:H31	2.01	0.41
13:M:12:MET:HE1	46:d:1201:3PE:H3C2	2.02	0.41
20:T:16:LEU:O	20:T:20:LYS:HG3	2.20	0.41
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.41
16:P:91:VAL:HG23	16:P:126:VAL:HG11	2.02	0.41
20:T:18:VAL:HG11	20:T:54:MET:HE2	2.00	0.41
25:Z:79:LYS:NZ	60:Z:205:HOH:O	2.53	0.41
32:g:33:GLU:OE1	32:g:34:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.49	0.41
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.53	0.41
7:G:535:GLN:OE1	7:G:535:GLN:HA	2.20	0.41
32:g:110:SER:OG	41:p:140:ASP:OD2	2.35	0.41
40:o:27:ASP:OD1	40:o:27:ASP:C	2.63	0.41
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.01	0.41
4:D:322:GLU:OE1	4:D:322:GLU:N	2.43	0.41
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.56	0.41
40:o:112:LYS:O	40:o:116:GLN:HG2	2.20	0.41
24:Y:97:GLY:CA	24:Y:117:MET:HE2	2.51	0.41
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.55	0.41
14:N:89:LEU:HD12	14:N:95:SER:HA	2.03	0.41
6:F:403:THR:HB	47:F:502:SF4:S4	2.60	0.41
8:H:312:SER:HG	25:Z:55:ARG:HH21	1.67	0.41
15:O:46:LEU:HD21	15:O:235:VAL:HG13	2.03	0.41
21:V:71:LEU:HD13	21:V:79:VAL:HG11	2.02	0.41
31:f:49:LYS:HB3	31:f:50:PRO:HD2	2.02	0.41
1:A:73:LEU:N	1:A:74:PRO:CD	2.84	0.41
3:C:198:ASP:O	60:C:304:HOH:O	2.22	0.41
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.56	0.41
7:G:450:MET:HE2	7:G:452:ILE:HD11	2.03	0.41
15:O:22:SER:HB3	15:O:115:LEU:HD11	2.02	0.41
1:A:49:LEU:HD21	8:H:130:ILE:HG13	2.03	0.41
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.03	0.41
10:J:125:TRP:HB2	25:Z:137:THR:HG21	2.03	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.55	0.41
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.56	0.40
14:N:162:ILE:HG22	14:N:285:THR:HG21	2.02	0.40
20:T:14:ARG:HD2	20:T:57:GLU:OE2	2.22	0.40
24:Y:24:THR:OG1	24:Y:66:GLY:O	2.32	0.40
39:n:99:PRO:HB2	39:n:101:TRP:CD1	2.56	0.40
12:L:261:ILE:HG13	12:L:317:ILE:HD11	2.03	0.40
2:B:32:LYS:HA	2:B:32:LYS:HD3	1.92	0.40
6:F:192:LEU:HD23	6:F:192:LEU:C	2.46	0.40
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.55	0.40
13:M:94:LEU:HD21	46:M:602:3PE:O32	2.21	0.40
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.03	0.40
7:G:254:MET:HA	7:G:260:GLU:O	2.22	0.40
8:H:233:MET:HE1	8:H:234:MET:HE3	2.02	0.40
8:H:318:THR:HG23	26:a:41:TYR:HE2	1.87	0.40
12:L:419:THR:O	12:L:423:SER:OG	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:MET:SD	13:M:230:VAL:HB	2.62	0.40
15:O:240:TYR:N	15:O:240:TYR:CD2	2.89	0.40
8:H:172:MET:HE2	8:H:172:MET:HB3	1.96	0.40
13:M:406:TYR:CD1	13:M:406:TYR:C	2.99	0.40
33:h:10:ILE:HG23	39:n:178:MET:HG2	2.03	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	96/115 (84%)	93 (97%)	2 (2%)	1 (1%)	12	15
2	B	152/216 (70%)	147 (97%)	5 (3%)	0	100	100
3	C	204/266 (77%)	199 (98%)	5 (2%)	0	100	100
4	D	408/463 (88%)	397 (97%)	11 (3%)	0	100	100
5	E	210/249 (84%)	207 (99%)	3 (1%)	0	100	100
6	F	427/464 (92%)	422 (99%)	5 (1%)	0	100	100
7	G	686/727 (94%)	670 (98%)	16 (2%)	0	100	100
8	H	301/318 (95%)	293 (97%)	8 (3%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	164 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	586 (97%)	17 (3%)	1 (0%)	43	55
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	282/380 (74%)	276 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	92/124 (74%)	91 (99%)	1 (1%)	0	100	100
19	S	83/99 (84%)	81 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	110 (100%)	0	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	96/154 (62%)	92 (96%)	4 (4%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	95 (96%)	4 (4%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
38	m	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	119/137 (87%)	114 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	s	41/109 (38%)	40 (98%)	1 (2%)	0	100	100
All	All	7978/9212 (87%)	7809 (98%)	167 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
12	L	562	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/100 (87%)	84 (97%)	3 (3%)	32	49
2	B	130/175 (74%)	129 (99%)	1 (1%)	73	86
3	C	187/228 (82%)	186 (100%)	1 (0%)	81	90
4	D	357/392 (91%)	353 (99%)	4 (1%)	65	81
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	343/368 (93%)	342 (100%)	1 (0%)	86	93
7	G	578/608 (95%)	574 (99%)	4 (1%)	76	87
8	H	265/274 (97%)	261 (98%)	4 (2%)	57	75
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	136 (97%)	4 (3%)	37	55
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	62
12	L	529/533 (99%)	519 (98%)	10 (2%)	50	69
13	M	412/412 (100%)	407 (99%)	5 (1%)	63	79
14	N	315/315 (100%)	313 (99%)	2 (1%)	78	89
15	O	283/303 (93%)	278 (98%)	5 (2%)	51	70
16	P	249/327 (76%)	248 (100%)	1 (0%)	84	92
17	Q	112/153 (73%)	111 (99%)	1 (1%)	70	84
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	75/82 (92%)	74 (99%)	1 (1%)	61	77
20	T	70/135 (52%)	67 (96%)	3 (4%)	26	39
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W	107/114 (94%)	104 (97%)	3 (3%)	38	56
23	X	154/155 (99%)	147 (96%)	7 (4%)	24	37
24	Y	101/102 (99%)	100 (99%)	1 (1%)	68	82
25	Z	119/121 (98%)	119 (100%)	0	100	100
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%)	83 (96%)	3 (4%)	32	48
31	f	48/54 (89%)	47 (98%)	1 (2%)	47	66
32	g	89/131 (68%)	88 (99%)	1 (1%)	65	81
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	97 (99%)	1 (1%)	68	82
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	73
36	k	61/76 (80%)	61 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	112/115 (97%)	112 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	107 (97%)	3 (3%)	39	58
41	p	154/157 (98%)	152 (99%)	2 (1%)	61	77
42	q	131/131 (100%)	130 (99%)	1 (1%)	73	86
43	r	84/97 (87%)	82 (98%)	2 (2%)	43	62
44	s	42/92 (46%)	41 (98%)	1 (2%)	43	62
All	All	7052/7892 (89%)	6969 (99%)	83 (1%)	61	79

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	28	ASN
1	A	57	LEU
2	B	54	CYS
3	C	79	THR
4	D	69	SER

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Mol	Chain	Res	Type
4	D	109	VAL
4	D	341	SER
4	D	420	THR
6	F	288	THR
7	G	17	SER
7	G	364	LEU
7	G	444	GLN
7	G	577	GLU
8	H	66	SER
8	H	121	TRP
8	H	163	SER
8	H	194	ASN
10	J	25	SER
10	J	97	LEU
10	J	135	PHE
10	J	171	ILE
11	K	46	LEU
11	K	97	GLN
12	L	10	VAL
12	L	129	LEU
12	L	149	ILE
12	L	244	SER
12	L	250	SER
12	L	343	SER
12	L	393	ASP
12	L	423	SER
12	L	458	LEU
12	L	469	SER
13	M	116	ILE
13	M	191	SER
13	M	273	SER
13	M	337	ILE
13	M	393	ILE
14	N	40	ILE
14	N	322	LYS
15	O	19	THR
15	O	44	GLU
15	O	60	ASP
15	O	180	GLN
15	O	289	SER
16	P	142	SER
17	Q	115	SER

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Mol	Chain	Res	Type
19	S	74	LYS
20	T	7	THR
20	T	13	ASP
20	T	35	HIS
22	W	96	VAL
22	W	99	GLN
22	W	116	LYS
23	X	17	VAL
23	X	22	SER
23	X	63	ASN
23	X	77	CYS
23	X	98	ARG
23	X	101	LYS
23	X	130	VAL
24	Y	26	SER
26	a	68	ASN
27	b	2	GLU
27	b	4	VAL
27	b	67	SER
30	e	17	MET
30	e	86	ILE
30	e	92	THR
31	f	52	GLU
32	g	112	CYS
34	i	16	GLU
35	j	69	ASP
40	o	13	SER
40	o	69	LYS
40	o	120	ASP
41	p	3	SER
41	p	68	ARG
42	q	15	SER
43	r	66	SER
43	r	68	VAL
44	s	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
3	C	39	GLN
3	C	71	GLN

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Mol	Chain	Res	Type
3	C	160	HIS
4	D	127	ASN
5	E	42	HIS
5	E	99	HIS
6	F	29	HIS
6	F	148	ASN
6	F	200	GLN
6	F	257	ASN
7	G	155	GLN
7	G	472	ASN
7	G	581	GLN
7	G	644	GLN
8	H	47	GLN
8	H	235	ASN
11	K	52	HIS
12	L	296	ASN
12	L	354	GLN
12	L	471	ASN
13	M	180	GLN
13	M	415	GLN
14	N	63	GLN
14	N	268	GLN
14	N	274	ASN
15	O	114	HIS
15	O	154	GLN
15	O	200	GLN
15	O	251	GLN
15	O	271	ASN
16	P	3	HIS
16	P	8	HIS
16	P	243	GLN
16	P	250	HIS
16	P	288	HIS
22	W	51	GLN
25	Z	85	GLN
28	c	46	ASN
33	h	63	HIS
33	h	124	HIS
34	i	125	GLN
35	j	6	HIS
35	j	24	GLN
35	j	42	HIS

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Mol	Chain	Res	Type
37	l	132	GLN
37	l	155	HIS
38	m	78	ASN
40	o	116	GLN
41	p	120	HIS
41	p	122	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
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.22	1 (16%)
1	FME	A	1	1	8,9,10	0.99	0	8,9,11	0.98	0
43	AYA	r	1	43	6,7,8	1.86	2 (33%)	6,8,10	1.44	1 (16%)
10	FME	J	1	10	8,9,10	1.03	0	8,9,11	0.80	0
4	2MR	D	85	4	10,12,13	2.72	4 (40%)	5,13,15	1.15	1 (20%)
13	FME	M	1	13	8,9,10	1.03	1 (12%)	8,9,11	0.99	1 (12%)
14	FME	N	1	14	8,9,10	1.01	0	8,9,11	0.99	1 (12%)
12	FME	L	1	12	8,9,10	1.01	1 (12%)	8,9,11	0.96	1 (12%)
11	FME	K	1	11	8,9,10	0.93	0	8,9,11	0.92	0
34	SAC	i	1	34	7,8,9	1.92	1 (14%)	7,9,11	1.90	1 (14%)
8	FME	H	1	8	8,9,10	0.98	0	8,9,11	0.93	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
24	AYA	Y	1	24	-	0/5/6/8	-
1	FME	A	1	1	-	3/7/9/11	-
43	AYA	r	1	43	-	1/5/6/8	-
10	FME	J	1	10	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
13	FME	M	1	13	-	0/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
34	SAC	i	1	34	-	3/7/8/10	-
8	FME	H	1	8	-	2/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.23	1.44	1.33
4	D	85	2MR	CZ-NE	4.61	1.44	1.34
34	i	1	SAC	O-C	4.35	1.36	1.20
4	D	85	2MR	O-C	4.05	1.35	1.20
24	Y	1	AYA	CT-N	3.48	1.45	1.34
43	r	1	AYA	CT-N	3.46	1.45	1.34
13	M	1	FME	CA-N	-2.17	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.07	1.42	1.46
12	L	1	FME	CA-N	-2.06	1.43	1.46
43	r	1	AYA	OT-CT	-2.03	1.18	1.23
24	Y	1	AYA	OT-CT	-2.03	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.53	113.12	124.77
43	r	1	AYA	CM-CT-N	2.55	120.35	116.12
14	N	1	FME	C-CA-N	2.17	113.69	109.50
24	Y	1	AYA	CM-CT-N	2.16	119.71	116.12
13	M	1	FME	C-CA-N	2.12	113.59	109.50
4	D	85	2MR	NE-CZ-NH2	-2.10	117.56	119.48
12	L	1	FME	C-CA-N	2.00	113.36	109.50

There are no chirality outliers.

All (17) 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
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	N-CA-CB-CG
34	i	1	SAC	O-C-CA-CB
34	i	1	SAC	C-CA-CB-OG
43	r	1	AYA	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
10	J	1	FME	C-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
34	i	1	SAC	N-CA-CB-OG

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 51 ligands modelled in this entry, 3 are monoatomic - leaving 48 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	N	901	-	36,36,36	1.20	3 (8%)	47,47,47	0.82	2 (4%)
46	3PE	L	703	-	44,44,50	0.93	3 (6%)	47,49,55	1.08	2 (4%)
51	I49	H	602	-	15,17,17	0.88	1 (6%)	17,22,22	1.82	3 (17%)
46	3PE	M	601	-	45,45,50	0.90	4 (8%)	48,50,55	1.10	2 (4%)
52	CDL	X	1701	-	71,71,99	1.04	8 (11%)	77,83,111	1.18	4 (5%)
45	LMT	d	1203	-	36,36,36	1.23	4 (11%)	47,47,47	1.02	3 (6%)
45	LMT	Y	402	-	36,36,36	1.20	3 (8%)	47,47,47	1.01	2 (4%)
45	LMT	B	202	-	36,36,36	1.20	2 (5%)	47,47,47	0.95	2 (4%)
49	FMN	F	501	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	6 (12%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
46	3PE	b	901	-	47,47,50	0.88	4 (8%)	50,52,55	1.06	2 (4%)
45	LMT	N	902	-	36,36,36	1.17	3 (8%)	47,47,47	0.90	1 (2%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
48	FES	G	803	7	0,4,4	-	-	-	-	-
58	EHZ	T	101	20	31,36,37	1.55	5 (16%)	36,44,47	1.43	5 (13%)
52	CDL	q	202	-	75,75,99	1.01	8 (10%)	81,87,111	1.06	4 (4%)
46	3PE	L	701	-	48,48,50	0.88	2 (4%)	51,53,55	1.01	2 (3%)
45	LMT	f	1802	-	36,36,36	1.21	3 (8%)	47,47,47	0.93	0
45	LMT	h	1002	-	36,36,36	1.16	2 (5%)	47,47,47	1.09	3 (6%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
45	LMT	e	201	-	36,36,36	1.21	3 (8%)	47,47,47	1.19	5 (10%)
46	3PE	H	601	-	33,33,50	1.34	3 (9%)	34,37,55	1.07	2 (5%)
53	PC1	q	201	-	34,34,53	1.17	4 (11%)	40,42,61	1.16	2 (5%)
54	GTP	O	401	55	33,34,34	3.29	15 (45%)	50,54,54	1.86	12 (24%)
52	CDL	L	702	-	68,68,99	1.05	8 (11%)	74,80,111	1.10	4 (5%)
46	3PE	A	302	-	37,37,50	0.99	4 (10%)	40,42,55	1.09	2 (5%)
51	I49	N	904	-	15,17,17	0.87	1 (6%)	17,22,22	1.93	5 (29%)
46	3PE	M	602	-	48,48,50	0.88	3 (6%)	51,53,55	1.15	2 (3%)
45	LMT	l	201	-	36,36,36	1.21	3 (8%)	47,47,47	0.98	3 (6%)
45	LMT	A	301	-	36,36,36	1.21	3 (8%)	47,47,47	0.91	1 (2%)
52	CDL	d	1202	-	64,64,99	1.09	8 (12%)	70,76,111	1.11	4 (5%)
52	CDL	h	1001	-	66,66,99	1.07	7 (10%)	72,78,111	1.21	5 (6%)
53	PC1	M	603	-	39,39,53	1.12	3 (7%)	45,47,61	1.01	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
46	3PE	I	201	-	50,50,50	0.88	4 (8%)	53,55,55	0.97	2 (3%)
46	3PE	N	903	-	40,40,50	0.97	4 (10%)	43,45,55	1.07	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	LMT	f	1801	-	36,36,36	1.19	3 (8%)	47,47,47	1.19	4 (8%)
56	NDP	P	501	-	51,52,52	2.28	7 (13%)	71,80,80	1.49	16 (22%)
58	EHZ	U	101	20	31,36,37	1.54	5 (16%)	36,44,47	1.48	4 (11%)
45	LMT	L	704	-	36,36,36	1.19	3 (8%)	47,47,47	0.80	1 (2%)
59	MYR	o	201	40	13,14,15	0.97	0	12,13,15	0.57	0
52	CDL	J	401	-	70,70,99	1.04	7 (10%)	76,82,111	1.10	4 (5%)
46	3PE	d	1201	-	46,46,50	0.92	4 (8%)	49,51,55	1.12	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
46	3PE	Y	401	-	34,34,50	1.05	4 (11%)	37,39,55	1.19	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
45	LMT	j	101	-	36,36,36	1.16	2 (5%)	47,47,47	0.89	1 (2%)
48	FES	E	301	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	N	901	-	-	2/21/61/61	0/2/2/2
46	3PE	L	703	-	-	23/48/48/54	-
51	I49	H	602	-	-	6/10/10/10	0/1/1/1
46	3PE	M	601	-	-	21/49/49/54	-
52	CDL	X	1701	-	-	36/82/82/110	-
45	LMT	d	1203	-	-	7/21/61/61	0/2/2/2
45	LMT	Y	402	-	-	9/21/61/61	0/2/2/2
45	LMT	B	202	-	-	7/21/61/61	0/2/2/2
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
47	SF4	B	201	2	-	-	0/6/5/5
46	3PE	b	901	-	-	27/51/51/54	-
45	LMT	N	902	-	-	7/21/61/61	0/2/2/2
47	SF4	I	203	9	-	-	0/6/5/5
48	FES	G	803	7	-	-	0/1/1/1
58	EHZ	T	101	20	-	9/42/44/45	-
52	CDL	q	202	-	-	40/86/86/110	-
46	3PE	L	701	-	-	20/52/52/54	-
45	LMT	f	1802	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	h	1002	-	-	6/21/61/61	0/2/2/2
47	SF4	G	802	7	-	-	0/6/5/5
45	LMT	e	201	-	-	8/21/61/61	0/2/2/2
46	3PE	H	601	-	-	13/36/36/54	-
53	PC1	q	201	-	-	9/38/38/57	-
54	GTP	O	401	55	-	4/22/38/38	0/3/3/3
52	CDL	L	702	-	-	28/79/79/110	-
46	3PE	A	302	-	-	11/41/41/54	-
51	I49	N	904	-	-	5/10/10/10	0/1/1/1
46	3PE	M	602	-	-	20/52/52/54	-
45	LMT	l	201	-	-	5/21/61/61	0/2/2/2
45	LMT	A	301	-	-	9/21/61/61	0/2/2/2
52	CDL	d	1202	-	-	28/75/75/110	-
52	CDL	h	1001	-	-	30/77/77/110	-
53	PC1	M	603	-	-	12/43/43/57	-
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	I	201	-	-	20/54/54/54	-
46	3PE	N	903	-	-	21/44/44/54	-
45	LMT	f	1801	-	-	9/21/61/61	0/2/2/2
56	NDP	P	501	-	-	8/34/77/77	0/5/5/5
58	EHZ	U	101	20	-	10/42/44/45	-
45	LMT	L	704	-	-	9/21/61/61	0/2/2/2
59	MYR	o	201	40	-	4/12/12/13	-
52	CDL	J	401	-	-	29/81/81/110	-
46	3PE	d	1201	-	-	22/50/50/54	-
47	SF4	F	502	6	-	-	0/6/5/5
46	3PE	Y	401	-	-	20/38/38/54	-
47	SF4	I	202	9	-	-	0/6/5/5
45	LMT	j	101	-	-	7/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.40	1.81	1.59
54	O	401	GTP	O6-C6	8.60	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	O	401	GTP	C5-N7	6.74	1.52	1.39
56	P	501	NDP	PA-O3	5.61	1.65	1.59
54	O	401	GTP	PA-O3A	5.27	1.65	1.59
58	T	101	EHZ	C12-N1	5.03	1.45	1.33
58	U	101	EHZ	C15-N2	5.01	1.45	1.33
54	O	401	GTP	PB-O3B	4.95	1.64	1.59
54	O	401	GTP	PB-O3A	4.90	1.64	1.59
46	H	601	3PE	O21-C2	-4.86	1.40	1.46
54	O	401	GTP	C2-N1	4.80	1.49	1.37
58	T	101	EHZ	C15-N2	4.74	1.44	1.33
58	U	101	EHZ	C12-N1	4.73	1.44	1.33
54	O	401	GTP	C2-N2	4.60	1.44	1.34
54	O	401	GTP	C2-N3	4.51	1.44	1.33
54	O	401	GTP	C8-N9	-4.49	1.27	1.37
56	P	501	NDP	PN-O5D	3.77	1.74	1.59
54	O	401	GTP	C4-N9	-3.76	1.28	1.38
45	N	901	LMT	O5B-C1B	3.57	1.51	1.41
45	l	201	LMT	O5B-C1B	3.57	1.51	1.41
45	f	1802	LMT	O5B-C1B	3.52	1.50	1.41
45	e	201	LMT	O5B-C1B	3.50	1.50	1.41
45	B	202	LMT	O5B-C1B	3.45	1.50	1.41
45	f	1801	LMT	O5B-C1B	3.45	1.50	1.41
45	A	301	LMT	O5B-C1B	3.35	1.50	1.41
45	N	902	LMT	O5B-C1B	3.35	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.34	1.32	1.44
45	L	704	LMT	O5B-C1B	3.33	1.50	1.41
45	d	1203	LMT	O5B-C1B	3.32	1.50	1.41
45	d	1203	LMT	O5'-C1'	3.31	1.50	1.41
45	Y	402	LMT	O5B-C1B	3.30	1.50	1.41
46	H	601	3PE	O21-C21	3.29	1.40	1.33
45	j	101	LMT	O5B-C1B	3.26	1.50	1.41
45	Y	402	LMT	O5'-C1'	3.22	1.50	1.41
45	L	704	LMT	O5'-C1'	3.21	1.50	1.41
49	F	501	FMN	C4A-N5	3.20	1.37	1.30
45	f	1802	LMT	O5'-C1'	3.18	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.16	1.50	1.41
45	j	101	LMT	O5'-C1'	3.15	1.49	1.41
45	A	301	LMT	O5'-C1'	3.15	1.49	1.41
52	h	1001	CDL	OA6-CA4	-3.06	1.39	1.46
45	N	902	LMT	O5'-C1'	3.04	1.49	1.41
45	l	201	LMT	O5'-C1'	3.00	1.49	1.41
46	L	703	3PE	O21-C2	-2.95	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B	202	LMT	O5'-C1'	2.95	1.49	1.41
45	f	1801	LMT	O5'-C1'	2.94	1.49	1.41
52	h	1001	CDL	OB6-CB4	-2.94	1.39	1.46
53	M	603	PC1	O21-C2	-2.93	1.39	1.46
45	e	201	LMT	O5'-C1'	2.90	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.90	1.49	1.41
46	M	602	3PE	O21-C2	-2.90	1.39	1.46
45	N	901	LMT	O5'-C1'	2.89	1.49	1.41
52	d	1202	CDL	OA6-CA4	-2.87	1.39	1.46
54	O	401	GTP	O4'-C1'	2.86	1.48	1.42
52	L	702	CDL	OB6-CB4	-2.84	1.39	1.46
52	q	202	CDL	OB6-CB4	-2.82	1.40	1.46
52	X	1701	CDL	OA6-CA4	-2.80	1.40	1.46
46	L	701	3PE	O21-C2	-2.78	1.40	1.46
52	L	702	CDL	OA6-CA4	-2.78	1.40	1.46
46	N	903	3PE	O21-C2	-2.77	1.40	1.46
52	q	202	CDL	OA6-CA4	-2.76	1.40	1.46
52	d	1202	CDL	OB6-CB4	-2.75	1.40	1.46
52	J	401	CDL	OA6-CA4	-2.72	1.40	1.46
46	d	1201	3PE	O21-C2	-2.72	1.40	1.46
46	I	201	3PE	O21-C2	-2.71	1.40	1.46
52	X	1701	CDL	OB6-CB4	-2.70	1.40	1.46
58	U	101	EHZ	O4-C15	-2.64	1.18	1.23
58	T	101	EHZ	O4-C15	-2.61	1.18	1.23
52	J	401	CDL	OB6-CB4	-2.59	1.40	1.46
46	A	302	3PE	O21-C2	-2.59	1.40	1.46
46	L	701	3PE	O31-C3	-2.56	1.39	1.45
46	I	201	3PE	O31-C3	-2.56	1.39	1.45
46	N	903	3PE	O31-C3	-2.55	1.39	1.45
46	H	601	3PE	O31-C31	2.55	1.40	1.33
53	q	201	PC1	O21-C2	-2.55	1.40	1.46
46	Y	401	3PE	O21-C2	-2.52	1.40	1.46
51	N	904	I49	C15-N02	-2.52	1.31	1.36
52	q	202	CDL	OB8-CB7	2.49	1.40	1.33
52	J	401	CDL	OB8-CB7	2.48	1.40	1.33
52	h	1001	CDL	OB8-CB6	-2.48	1.39	1.45
46	M	601	3PE	O21-C2	-2.46	1.40	1.46
52	d	1202	CDL	OB8-CB7	2.46	1.40	1.33
54	O	401	GTP	C2'-C3'	-2.45	1.46	1.53
52	d	1202	CDL	OA8-CA6	-2.43	1.39	1.45
46	b	901	3PE	O31-C31	2.42	1.40	1.33
58	T	101	EHZ	O3-C12	-2.42	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	401	CDL	OA8-CA6	-2.42	1.39	1.45
52	X	1701	CDL	OB8-CB7	2.41	1.40	1.33
46	M	602	3PE	O31-C3	-2.40	1.39	1.45
58	U	101	EHZ	O3-C12	-2.40	1.18	1.23
52	X	1701	CDL	OA8-CA7	2.40	1.40	1.33
52	X	1701	CDL	OB8-CB6	-2.39	1.39	1.45
52	L	702	CDL	OB8-CB6	-2.39	1.39	1.45
54	O	401	GTP	PG-O2G	-2.38	1.45	1.54
52	q	202	CDL	OA8-CA6	-2.38	1.39	1.45
52	L	702	CDL	OA8-CA7	2.37	1.40	1.33
53	M	603	PC1	O31-C3	-2.37	1.39	1.45
54	O	401	GTP	PG-O3G	-2.36	1.46	1.54
52	L	702	CDL	OB8-CB7	2.36	1.40	1.33
46	d	1201	3PE	O31-C31	2.35	1.40	1.33
52	d	1202	CDL	OB8-CB6	-2.35	1.39	1.45
46	L	703	3PE	O31-C3	-2.35	1.39	1.45
51	H	602	I49	C15-N02	-2.35	1.31	1.36
46	Y	401	3PE	O31-C31	2.34	1.40	1.33
46	b	901	3PE	O21-C2	-2.32	1.41	1.46
46	L	703	3PE	O31-C31	2.32	1.40	1.33
52	J	401	CDL	OA8-CA7	2.31	1.40	1.33
46	A	302	3PE	O31-C3	-2.31	1.40	1.45
53	q	201	PC1	O21-C21	2.30	1.40	1.34
45	f	1801	LMT	O5B-C5B	2.29	1.50	1.44
53	M	603	PC1	O31-C31	2.28	1.40	1.33
46	I	201	3PE	O31-C31	2.28	1.40	1.33
46	A	302	3PE	O31-C31	2.26	1.40	1.33
46	Y	401	3PE	O31-C3	-2.26	1.40	1.45
46	M	601	3PE	O31-C31	2.26	1.39	1.33
52	X	1701	CDL	OA8-CA6	-2.24	1.40	1.45
46	d	1201	3PE	O31-C3	-2.23	1.40	1.45
46	M	602	3PE	O31-C31	2.22	1.39	1.33
53	q	201	PC1	O31-C31	2.22	1.39	1.33
46	d	1201	3PE	O21-C21	2.21	1.40	1.34
52	h	1001	CDL	OA8-CA6	-2.19	1.40	1.45
53	q	201	PC1	O31-C3	-2.19	1.40	1.45
45	e	201	LMT	O5B-C5B	2.19	1.49	1.44
52	J	401	CDL	OB6-CB5	2.18	1.40	1.34
52	h	1001	CDL	OA8-CA7	2.18	1.39	1.33
52	q	202	CDL	OA8-CA7	2.18	1.39	1.33
52	L	702	CDL	OA8-CA6	-2.18	1.40	1.45
46	b	901	3PE	O21-C21	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	401	3PE	O21-C21	2.17	1.40	1.34
46	M	601	3PE	O21-C21	2.15	1.40	1.34
45	f	1802	LMT	O5B-C5B	2.15	1.49	1.44
46	A	302	3PE	O21-C21	2.15	1.40	1.34
52	h	1001	CDL	OB8-CB7	2.14	1.39	1.33
46	M	601	3PE	O31-C3	-2.14	1.40	1.45
52	q	202	CDL	OB8-CB6	-2.14	1.40	1.45
52	q	202	CDL	OB6-CB5	2.13	1.40	1.34
52	d	1202	CDL	OA8-CA7	2.13	1.39	1.33
46	N	903	3PE	O31-C31	2.11	1.39	1.33
52	d	1202	CDL	OB6-CB5	2.10	1.40	1.34
45	l	201	LMT	O5B-C5B	2.10	1.49	1.44
56	P	501	NDP	C5A-C4A	2.10	1.42	1.39
49	F	501	FMN	C10-N1	2.10	1.37	1.33
45	Y	402	LMT	O5B-C5B	2.09	1.49	1.44
56	P	501	NDP	C2A-N1A	2.09	1.37	1.33
52	L	702	CDL	OB6-CB5	2.08	1.40	1.34
45	N	901	LMT	O5B-C5B	2.08	1.49	1.44
56	P	501	NDP	O5D-C5D	-2.08	1.36	1.44
46	I	201	3PE	O21-C21	2.07	1.40	1.34
46	b	901	3PE	O31-C3	-2.07	1.40	1.45
52	X	1701	CDL	OA6-CA5	2.06	1.40	1.34
58	T	101	EHZ	C9-S1	2.06	1.81	1.76
45	N	902	LMT	O5B-C5B	2.06	1.49	1.44
46	N	903	3PE	O21-C21	2.05	1.40	1.34
45	A	301	LMT	O1B-C4'	2.05	1.49	1.43
52	J	401	CDL	OB8-CB6	-2.05	1.40	1.45
52	q	202	CDL	OA6-CA5	2.04	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.04	1.40	1.34
52	d	1202	CDL	OA6-CA5	2.04	1.40	1.34
52	X	1701	CDL	OB6-CB5	2.04	1.40	1.34
45	d	1203	LMT	O5B-C5B	2.03	1.49	1.44
58	U	101	EHZ	C9-S1	2.02	1.81	1.76
45	L	704	LMT	O5B-C5B	2.02	1.49	1.44
52	L	702	CDL	OA6-CA5	2.00	1.39	1.34
54	O	401	GTP	PA-O2A	-2.00	1.46	1.55
45	d	1203	LMT	O5'-C5'	2.00	1.49	1.44

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	GTP	C8-N9-C4	7.54	120.17	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	U	101	EHZ	C8-C9-S1	5.90	121.00	113.56
58	T	101	EHZ	C8-C9-S1	5.62	120.65	113.56
51	N	904	I49	N01-C14-N03	5.20	129.85	120.26
52	h	1001	CDL	OB6-CB5-C51	4.40	121.00	111.48
53	q	201	PC1	O21-C21-C22	4.37	120.93	111.48
52	X	1701	CDL	OB6-CB5-C51	4.28	120.73	111.48
46	d	1201	3PE	O21-C21-C22	4.27	120.71	111.48
46	Y	401	3PE	O21-C21-C22	4.21	120.58	111.48
46	M	602	3PE	O21-C21-C22	4.09	120.33	111.48
51	H	602	I49	N01-C14-N03	4.07	127.76	120.26
52	q	202	CDL	OA6-CA5-C11	4.07	120.28	111.48
46	H	601	3PE	O21-C21-O22	-4.04	120.52	125.70
52	d	1202	CDL	OA6-CA5-C11	4.03	120.19	111.48
46	N	903	3PE	O21-C21-C22	3.93	119.99	111.48
46	b	901	3PE	O21-C21-C22	3.91	119.94	111.48
46	M	601	3PE	O21-C21-C22	3.90	119.92	111.48
52	h	1001	CDL	OA6-CA5-C11	3.89	119.90	111.48
52	X	1701	CDL	OA6-CA5-C11	3.88	119.88	111.48
46	L	701	3PE	O21-C21-C22	3.86	119.84	111.48
52	L	702	CDL	OA6-CA5-C11	3.81	119.73	111.48
46	A	302	3PE	O21-C21-C22	3.78	119.67	111.48
52	J	401	CDL	OA6-CA5-C11	3.77	119.63	111.48
56	P	501	NDP	P2B-O2B-C2B	-3.76	113.38	123.43
56	P	501	NDP	O2B-P2B-O1X	-3.74	96.01	109.33
52	J	401	CDL	OB6-CB5-C51	3.68	119.44	111.48
46	I	201	3PE	O21-C21-C22	3.58	119.22	111.48
52	L	702	CDL	OB6-CB5-C51	3.51	119.08	111.48
46	L	703	3PE	O21-C21-C22	3.51	119.08	111.48
53	M	603	PC1	O21-C21-C22	3.50	119.06	111.48
52	q	202	CDL	OB6-CB5-C51	3.50	119.05	111.48
56	P	501	NDP	O3-PA-O1A	-3.35	100.62	110.70
45	h	1002	LMT	O5'-C5'-C4'	3.28	116.51	109.72
49	F	501	FMN	C4-N3-C2	-3.26	119.86	125.64
54	O	401	GTP	C2-N1-C6	-3.20	119.31	125.11
52	X	1701	CDL	OB8-CB7-C71	3.17	121.51	111.83
45	e	201	LMT	O5'-C5'-C4'	3.15	116.23	109.72
49	F	501	FMN	C4A-C10-N10	3.14	120.97	116.48
46	M	601	3PE	O31-C31-C32	3.10	121.28	111.83
58	U	101	EHZ	O2-C9-C8	-3.04	118.96	123.74
45	f	1801	LMT	C1'-C2'-C3'	2.99	116.30	110.01
46	Y	401	3PE	O31-C31-C32	2.98	120.93	111.83
52	h	1001	CDL	OA8-CA7-C31	2.94	120.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	q	201	PC1	O31-C31-C32	2.94	120.79	111.83
46	A	302	3PE	O31-C31-C32	2.86	120.56	111.83
45	h	1002	LMT	C1B-O1B-C4'	-2.86	111.20	117.98
58	T	101	EHZ	O2-C9-S1	-2.86	119.05	122.68
46	d	1201	3PE	O31-C31-C32	2.85	120.53	111.83
51	H	602	I49	C08-N01-C14	-2.85	118.23	123.46
54	O	401	GTP	O2G-PG-O3B	2.84	114.17	104.64
56	P	501	NDP	PA-O5B-C5B	-2.83	105.11	121.35
54	O	401	GTP	O3G-PG-O3B	2.83	114.14	104.64
52	J	401	CDL	OB8-CB7-C71	2.82	120.44	111.83
46	L	703	3PE	O31-C31-C32	2.80	120.36	111.83
53	M	603	PC1	O31-C31-C32	2.77	120.30	111.83
52	q	202	CDL	OB8-CB7-C71	2.77	120.28	111.83
52	d	1202	CDL	OB8-CB7-C71	2.77	120.28	111.83
46	M	602	3PE	O31-C31-C32	2.77	120.27	111.83
52	h	1001	CDL	OB8-CB7-C71	2.74	120.18	111.83
51	N	904	I49	N05-C15-N04	-2.73	112.30	120.07
51	N	904	I49	N05-C15-N02	2.71	127.50	117.97
51	H	602	I49	N05-C15-N04	-2.71	112.36	120.07
45	f	1801	LMT	C1'-O5'-C5'	-2.70	108.45	113.72
52	X	1701	CDL	OA8-CA7-C31	2.68	120.00	111.83
54	O	401	GTP	C1'-N9-C8	-2.64	119.22	126.73
49	F	501	FMN	C4A-C4-N3	2.62	119.93	113.25
46	b	901	3PE	O31-C31-C32	2.61	119.81	111.83
56	P	501	NDP	PN-O5D-C5D	-2.61	106.38	121.35
52	J	401	CDL	OA8-CA7-C31	2.60	119.77	111.83
56	P	501	NDP	O2N-PN-O3	2.60	114.29	107.27
52	L	702	CDL	OB8-CB7-C71	2.59	119.73	111.83
46	H	601	3PE	O31-C31-C32	2.59	119.72	111.83
52	d	1202	CDL	OB6-CB5-C51	2.57	120.38	110.93
45	f	1801	LMT	C2'-C3'-C4'	2.56	115.50	109.68
56	P	501	NDP	O3X-P2B-O2X	2.55	117.34	107.80
54	O	401	GTP	O2B-PB-O1B	-2.54	100.64	112.44
52	d	1202	CDL	OA8-CA7-C31	2.52	119.52	111.83
45	j	101	LMT	C1B-O1B-C4'	-2.52	112.01	117.98
52	L	702	CDL	OA8-CA7-C31	2.50	119.45	111.83
45	e	201	LMT	O5B-C5B-C4B	2.49	114.18	109.70
45	l	201	LMT	C1B-O1B-C4'	-2.47	112.13	117.98
45	N	901	LMT	C1B-O1B-C4'	-2.46	112.14	117.98
49	F	501	FMN	C10-C4A-N5	-2.46	119.78	124.81
54	O	401	GTP	O2A-PA-O1A	-2.45	101.04	112.44
54	O	401	GTP	C5-C6-N1	2.45	119.49	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	f	1801	LMT	O5B-C5B-C4B	2.45	114.11	109.70
56	P	501	NDP	O4B-C4B-C3B	2.44	109.99	105.15
45	e	201	LMT	C3B-C4B-C5B	2.43	114.64	110.23
56	P	501	NDP	N3A-C4A-N9A	2.43	131.30	127.17
49	F	501	FMN	O4-C4-C4A	-2.43	120.12	126.53
46	I	201	3PE	O31-C31-C32	2.41	119.19	111.83
56	P	501	NDP	O5D-PN-O1N	-2.41	99.39	108.94
56	P	501	NDP	C2A-N1A-C6A	-2.40	114.78	118.73
45	d	1203	LMT	C3B-C4B-C5B	2.39	114.56	110.23
56	P	501	NDP	O2N-PN-O1N	2.34	123.34	112.44
58	T	101	EHZ	C13-C12-N1	2.32	120.57	116.34
45	d	1203	LMT	O5B-C5B-C4B	2.31	113.86	109.70
54	O	401	GTP	N9-C8-N7	-2.29	109.16	113.40
46	L	701	3PE	O31-C31-C32	2.25	118.71	111.83
45	Y	402	LMT	C3B-C4B-C5B	2.25	114.32	110.23
52	h	1001	CDL	CA4-OA6-CA5	-2.25	112.41	117.80
45	e	201	LMT	C4B-C3B-C2B	2.25	114.78	110.83
46	N	903	3PE	O31-C31-C32	2.24	118.66	111.83
54	O	401	GTP	O6-C6-C5	-2.20	120.71	126.53
45	L	704	LMT	C1B-O5B-C5B	-2.20	109.42	113.72
45	Y	402	LMT	C1B-O1B-C4'	-2.20	112.76	117.98
45	e	201	LMT	C3'-C4'-C5'	2.19	115.79	110.93
45	A	301	LMT	O1B-C4'-C3'	2.19	112.80	107.23
58	T	101	EHZ	O2-C9-C8	-2.19	120.30	123.74
54	O	401	GTP	C5-C4-N9	-2.16	101.78	105.66
45	N	902	LMT	O1B-C4'-C3'	2.16	112.72	107.23
51	N	904	I49	N02-C14-N01	-2.15	112.54	118.08
51	N	904	I49	C09-C07-C10	2.15	121.51	118.55
56	P	501	NDP	O7N-C7N-N7N	-2.15	118.08	122.89
54	O	401	GTP	C6-C5-N7	2.13	134.17	130.29
45	l	201	LMT	O5B-C5B-C4B	2.13	113.53	109.70
45	d	1203	LMT	O5'-C5'-C4'	2.12	114.11	109.72
45	l	201	LMT	C6B-C5B-C4B	-2.11	107.83	113.02
58	T	101	EHZ	C13-C14-N2	-2.11	107.51	112.00
56	P	501	NDP	C2B-C1B-N9A	-2.10	110.30	113.75
58	U	101	EHZ	O2-C9-S1	-2.08	120.04	122.68
45	N	901	LMT	O1'-C1'-C2'	2.08	111.43	108.27
56	P	501	NDP	O3X-P2B-O2B	-2.07	97.77	105.85
45	B	202	LMT	O1'-C1'-C2'	2.05	111.39	108.27
45	B	202	LMT	C6'-C5'-C4'	-2.03	107.66	113.38
49	F	501	FMN	C4A-C10-N1	-2.02	119.63	124.59
52	q	202	CDL	OA8-CA7-C31	2.02	118.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	U	101	EHZ	C13-C12-N1	2.02	120.02	116.34
56	P	501	NDP	C5A-C4A-N3A	-2.02	123.94	126.72
45	h	1002	LMT	C1B-O5B-C5B	-2.00	109.81	113.72

There are no chirality outliers.

All (569) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	202	LMT	O5'-C1'-O1'-C1
45	e	201	LMT	C2-C1-O1'-C1'
45	f	1801	LMT	O5'-C1'-O1'-C1
45	f	1802	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	O22-C21-O21-C2
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	C1-O11-P-O14
46	L	703	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	M	601	3PE	O13-C11-C12-N
46	M	602	3PE	O13-C11-C12-N
46	N	903	3PE	C11-O13-P-O11
46	N	903	3PE	C11-O13-P-O12
46	N	903	3PE	C11-O13-P-O14
46	N	903	3PE	O13-C11-C12-N
46	Y	401	3PE	C1-O11-P-O12
46	Y	401	3PE	C1-O11-P-O13
46	Y	401	3PE	C11-O13-P-O11
46	Y	401	3PE	C11-O13-P-O14
46	Y	401	3PE	O13-C11-C12-N
46	Y	401	3PE	C22-C21-O21-C2
46	b	901	3PE	C1-O11-P-O12
46	b	901	3PE	C1-O11-P-O13
46	b	901	3PE	C1-O11-P-O14
46	b	901	3PE	O13-C11-C12-N
46	b	901	3PE	O21-C2-C3-O31
46	b	901	3PE	O22-C21-O21-C2
46	d	1201	3PE	C1-O11-P-O12
46	d	1201	3PE	C1-O11-P-O13
46	d	1201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	d	1201	3PE	O13-C11-C12-N
46	d	1201	3PE	C22-C21-O21-C2
51	H	602	I49	C07-C06-C08-N01
51	N	904	I49	C07-C06-C08-N01
51	N	904	I49	N05-C15-N02-C14
52	J	401	CDL	CA3-OA5-PA1-OA2
52	J	401	CDL	CB2-OB2-PB2-OB3
52	J	401	CDL	CB2-OB2-PB2-OB4
52	J	401	CDL	CB3-OB5-PB2-OB2
52	J	401	CDL	CB3-OB5-PB2-OB3
52	J	401	CDL	CB3-OB5-PB2-OB4
52	X	1701	CDL	CA2-C1-CB2-OB2
52	X	1701	CDL	CA2-OA2-PA1-OA4
52	X	1701	CDL	C11-CA5-OA6-CA4
52	d	1202	CDL	CA3-OA5-PA1-OA2
52	d	1202	CDL	CA3-OA5-PA1-OA4
52	d	1202	CDL	C11-CA5-OA6-CA4
52	d	1202	CDL	CB2-OB2-PB2-OB3
52	d	1202	CDL	CB2-OB2-PB2-OB5
52	d	1202	CDL	C51-CB5-OB6-CB4
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	q	202	CDL	O1-C1-CB2-OB2
52	q	202	CDL	CA2-OA2-PA1-OA3
52	q	202	CDL	CA2-OA2-PA1-OA4
52	q	202	CDL	CA2-OA2-PA1-OA5
52	q	202	CDL	C11-CA5-OA6-CA4
52	q	202	CDL	CB3-OB5-PB2-OB2
52	q	202	CDL	CB3-OB5-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O3A
58	T	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
45	d	1203	LMT	O5B-C1B-O1B-C4'
45	d	1203	LMT	C2B-C1B-O1B-C4'
46	M	602	3PE	O32-C31-O31-C3
45	A	301	LMT	C3'-C4'-O1B-C1B
46	M	602	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	A	302	3PE	O32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	d	1201	3PE	O32-C31-O31-C3
52	X	1701	CDL	OA9-CA7-OA8-CA6
52	X	1701	CDL	OB9-CB7-OB8-CB6
52	d	1202	CDL	OB9-CB7-OB8-CB6
52	J	401	CDL	OA7-CA5-OA6-CA4
52	X	1701	CDL	OA7-CA5-OA6-CA4
52	d	1202	CDL	OA7-CA5-OA6-CA4
52	d	1202	CDL	OB7-CB5-OB6-CB4
52	q	202	CDL	OA7-CA5-OA6-CA4
46	A	302	3PE	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
52	X	1701	CDL	C31-CA7-OA8-CA6
52	X	1701	CDL	C71-CB7-OB8-CB6
46	b	901	3PE	C22-C21-O21-C2
52	J	401	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C51-CB5-OB6-CB4
45	N	902	LMT	C3'-C4'-O1B-C1B
46	d	1201	3PE	C32-C31-O31-C3
52	d	1202	CDL	C71-CB7-OB8-CB6
46	Y	401	3PE	O22-C21-O21-C2
46	d	1201	3PE	O22-C21-O21-C2
45	N	901	LMT	C4B-C5B-C6B-O6B
45	N	902	LMT	C4'-C5'-C6'-O6'
45	Y	402	LMT	C4'-C5'-C6'-O6'
46	Y	401	3PE	C32-C31-O31-C3
46	Y	401	3PE	O32-C31-O31-C3
45	A	301	LMT	C4B-C5B-C6B-O6B
45	e	201	LMT	C4B-C5B-C6B-O6B
45	L	704	LMT	O5'-C5'-C6'-O6'
52	J	401	CDL	CB4-CB3-OB5-PB2
45	f	1801	LMT	O5'-C5'-C6'-O6'
45	e	201	LMT	O5'-C1'-O1'-C1
45	N	901	LMT	O5B-C5B-C6B-O6B
45	N	902	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	O5B-C5B-C6B-O6B
45	Y	402	LMT	O5'-C5'-C6'-O6'
52	q	202	CDL	CA2-C1-CB2-OB2
46	N	903	3PE	C32-C31-O31-C3
52	L	702	CDL	C31-CA7-OA8-CA6
52	h	1001	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
53	M	603	PC1	C32-C31-O31-C3
53	q	201	PC1	C32-C31-O31-C3
46	N	903	3PE	O32-C31-O31-C3
52	X	1701	CDL	O1-C1-CB2-OB2
45	f	1801	LMT	C4'-C5'-C6'-O6'
45	e	201	LMT	O5B-C5B-C6B-O6B
45	B	202	LMT	C3'-C4'-O1B-C1B
52	h	1001	CDL	OB9-CB7-OB8-CB6
53	M	603	PC1	O32-C31-O31-C3
45	f	1801	LMT	C5'-C4'-O1B-C1B
46	N	903	3PE	O21-C2-C3-O31
52	h	1001	CDL	CB5-C51-C52-C53
52	L	702	CDL	OA9-CA7-OA8-CA6
53	q	201	PC1	O32-C31-O31-C3
45	A	301	LMT	C2-C3-C4-C5
52	J	401	CDL	CA5-C11-C12-C13
52	X	1701	CDL	CB7-C71-C72-C73
45	j	101	LMT	O5'-C5'-C6'-O6'
45	L	704	LMT	C4'-C5'-C6'-O6'
45	d	1203	LMT	C3'-C4'-O1B-C1B
46	A	302	3PE	C31-C32-C33-C34
46	I	201	3PE	C21-C22-C23-C24
46	L	701	3PE	C31-C32-C33-C34
46	M	602	3PE	C31-C32-C33-C34
45	f	1802	LMT	C4B-C5B-C6B-O6B
52	J	401	CDL	C31-CA7-OA8-CA6
46	M	601	3PE	C21-C22-C23-C24
45	j	101	LMT	O5B-C1B-O1B-C4'
52	L	702	CDL	C71-CB7-OB8-CB6
45	j	101	LMT	C2B-C1B-O1B-C4'
53	q	201	PC1	C31-C32-C33-C34
52	J	401	CDL	CB7-C71-C72-C73
52	q	202	CDL	C71-CB7-OB8-CB6
45	f	1802	LMT	C5'-C4'-O1B-C1B
45	A	301	LMT	O5'-C5'-C6'-O6'
45	d	1203	LMT	C5'-C4'-O1B-C1B
45	e	201	LMT	O5'-C5'-C6'-O6'
45	f	1801	LMT	C3'-C4'-O1B-C1B
52	L	702	CDL	C11-CA5-OA6-CA4
52	L	702	CDL	C51-CB5-OB6-CB4
45	h	1002	LMT	C4'-C5'-C6'-O6'
52	L	702	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
52	L	702	CDL	OB7-CB5-OB6-CB4
45	A	301	LMT	C2'-C1'-O1'-C1
45	L	704	LMT	C2'-C1'-O1'-C1
46	b	901	3PE	C1-C2-O21-C21
52	L	702	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	C22-C21-O21-C2
45	f	1802	LMT	C3'-C4'-O1B-C1B
46	b	901	3PE	C2A-C2B-C2C-C2D
52	X	1701	CDL	C54-C55-C56-C57
45	Y	402	LMT	C3-C4-C5-C6
46	L	701	3PE	C29-C2A-C2B-C2C
46	Y	401	3PE	C37-C38-C39-C3A
52	h	1001	CDL	C72-C73-C74-C75
46	L	701	3PE	C37-C38-C39-C3A
46	b	901	3PE	C28-C29-C2A-C2B
52	X	1701	CDL	C15-C16-C17-C18
45	L	704	LMT	O1'-C1-C2-C3
52	J	401	CDL	OA9-CA7-OA8-CA6
45	N	902	LMT	C1-C2-C3-C4
52	h	1001	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	O1-C1-CB2-OB2
46	M	602	3PE	C2B-C2C-C2D-C2E
46	N	903	3PE	C29-C2A-C2B-C2C
52	q	202	CDL	C57-C58-C59-C60
46	d	1201	3PE	C21-C22-C23-C24
59	o	201	MYR	C2-C3-C4-C5
52	q	202	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	O22-C21-O21-C2
46	M	602	3PE	C26-C27-C28-C29
52	h	1001	CDL	C31-CA7-OA8-CA6
52	L	702	CDL	C55-C56-C57-C58
46	I	201	3PE	C33-C34-C35-C36
52	X	1701	CDL	C11-C12-C13-C14
45	e	201	LMT	C11-C10-C9-C8
46	I	201	3PE	C23-C24-C25-C26
46	L	703	3PE	C38-C39-C3A-C3B
46	b	901	3PE	C26-C27-C28-C29
51	N	904	I49	N04-C15-N02-C14
52	X	1701	CDL	CB5-C51-C52-C53
52	X	1701	CDL	C20-C21-C22-C23
52	h	1001	CDL	OA7-CA5-OA6-CA4
46	I	201	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C22-C23-C24-C25
46	L	701	3PE	C2E-C2F-C2G-C2H
46	b	901	3PE	C3E-C3F-C3G-C3H
52	q	202	CDL	C39-C40-C41-C42
46	N	903	3PE	C32-C33-C34-C35
52	h	1001	CDL	C12-C13-C14-C15
52	h	1001	CDL	C22-C23-C24-C25
46	d	1201	3PE	C33-C34-C35-C36
46	L	703	3PE	C32-C33-C34-C35
45	l	201	LMT	O1'-C1-C2-C3
46	d	1201	3PE	C37-C38-C39-C3A
52	d	1202	CDL	C33-C34-C35-C36
52	q	202	CDL	C31-C32-C33-C34
46	M	602	3PE	C22-C21-O21-C2
46	N	903	3PE	C21-C22-C23-C24
46	H	601	3PE	C3C-C3D-C3E-C3F
52	L	702	CDL	C34-C35-C36-C37
46	M	602	3PE	C3C-C3D-C3E-C3F
52	q	202	CDL	C72-C73-C74-C75
53	M	603	PC1	C29-C2A-C2B-C2C
46	L	701	3PE	C34-C35-C36-C37
46	M	602	3PE	C23-C24-C25-C26
52	h	1001	CDL	OA9-CA7-OA8-CA6
52	J	401	CDL	C16-C17-C18-C19
46	M	602	3PE	O22-C21-O21-C2
46	N	903	3PE	C22-C21-O21-C2
51	H	602	I49	N05-C15-N02-C14
45	L	704	LMT	C5-C6-C7-C8
46	M	601	3PE	C31-C32-C33-C34
52	d	1202	CDL	CB7-C71-C72-C73
45	f	1801	LMT	O5B-C5B-C6B-O6B
52	h	1001	CDL	C31-C32-C33-C34
46	b	901	3PE	C37-C38-C39-C3A
45	l	201	LMT	C4-C5-C6-C7
46	M	602	3PE	C3D-C3E-C3F-C3G
52	h	1001	CDL	C71-C72-C73-C74
52	q	202	CDL	C51-C52-C53-C54
52	q	202	CDL	C1-CA2-OA2-PA1
46	b	901	3PE	C2C-C2D-C2E-C2F
52	h	1001	CDL	CA2-C1-CB2-OB2
52	J	401	CDL	C36-C37-C38-C39
46	N	903	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
52	q	202	CDL	C11-C12-C13-C14
45	B	202	LMT	C5'-C4'-O1B-C1B
46	N	903	3PE	C33-C34-C35-C36
46	L	703	3PE	O11-C1-C2-C3
52	X	1701	CDL	OA5-CA3-CA4-CA6
52	d	1202	CDL	OA5-CA3-CA4-CA6
52	q	202	CDL	OA5-CA3-CA4-CA6
46	I	201	3PE	C3B-C3C-C3D-C3E
53	M	603	PC1	C2C-C2D-C2E-C2F
59	o	201	MYR	C9-C10-C11-C12
46	M	601	3PE	C22-C21-O21-C2
46	A	302	3PE	C1-C2-C3-O31
46	L	701	3PE	C1-C2-C3-O31
46	Y	401	3PE	C1-C2-C3-O31
46	d	1201	3PE	C1-C2-C3-O31
52	J	401	CDL	CA3-CA4-CA6-OA8
52	L	702	CDL	CA3-CA4-CA6-OA8
53	q	201	PC1	C1-C2-C3-O31
45	Y	402	LMT	C2-C3-C4-C5
45	B	202	LMT	O5'-C5'-C6'-O6'
46	M	601	3PE	C36-C37-C38-C39
53	M	603	PC1	C2B-C2C-C2D-C2E
45	N	902	LMT	O5B-C5B-C6B-O6B
58	T	101	EHZ	C1-C2-C3-C4
46	I	201	3PE	C32-C31-O31-C3
52	q	202	CDL	C59-C60-C61-C62
45	e	201	LMT	C2B-C1B-O1B-C4'
46	A	302	3PE	C32-C33-C34-C35
52	J	401	CDL	C12-C13-C14-C15
52	X	1701	CDL	C74-C75-C76-C77
46	M	601	3PE	C37-C38-C39-C3A
58	T	101	EHZ	C3-C4-C5-C6
58	U	101	EHZ	C1-C21-C22-C23
52	X	1701	CDL	CB2-C1-CA2-OA2
46	L	703	3PE	O11-C1-C2-O21
46	M	602	3PE	O11-C1-C2-O21
46	M	602	3PE	C3A-C3B-C3C-C3D
46	L	703	3PE	C25-C26-C27-C28
45	f	1802	LMT	O5B-C5B-C6B-O6B
52	L	702	CDL	OB6-CB4-CB6-OB8
53	M	603	PC1	O21-C2-C3-O31
52	X	1701	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C28-C29-C2A-C2B
45	L	704	LMT	C6-C7-C8-C9
46	b	901	3PE	C35-C36-C37-C38
45	h	1002	LMT	C4B-C5B-C6B-O6B
52	q	202	CDL	C35-C36-C37-C38
54	O	401	GTP	PG-O3B-PB-O1B
58	U	101	EHZ	C1-C2-C3-C4
46	Y	401	3PE	C31-C32-C33-C34
46	b	901	3PE	C39-C3A-C3B-C3C
45	f	1802	LMT	C1-C2-C3-C4
46	H	601	3PE	C35-C36-C37-C38
46	L	701	3PE	C2A-C2B-C2C-C2D
52	X	1701	CDL	C75-C76-C77-C78
46	H	601	3PE	C37-C38-C39-C3A
45	L	704	LMT	C2-C1-O1'-C1'
45	Y	402	LMT	C2-C1-O1'-C1'
45	d	1203	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2-C1-O1'-C1'
46	d	1201	3PE	C35-C36-C37-C38
53	M	603	PC1	C2-C1-O11-P
46	I	201	3PE	C37-C38-C39-C3A
52	X	1701	CDL	C57-C58-C59-C60
53	M	603	PC1	C2E-C2F-C2G-C2H
46	M	601	3PE	C2A-C2B-C2C-C2D
46	H	601	3PE	C3E-C3F-C3G-C3H
58	T	101	EHZ	C1-C21-C22-C23
46	M	601	3PE	O11-C1-C2-C3
46	Y	401	3PE	O11-C1-C2-C3
45	j	101	LMT	O5B-C5B-C6B-O6B
52	J	401	CDL	C39-C40-C41-C42
58	T	101	EHZ	C5-C6-C7-C8
52	q	202	CDL	O1-C1-CA2-OA2
56	P	501	NDP	O4D-C4D-C5D-O5D
46	I	201	3PE	C27-C28-C29-C2A
45	e	201	LMT	O5B-C1B-O1B-C4'
52	J	401	CDL	C19-C20-C21-C22
45	f	1801	LMT	O5B-C1B-O1B-C4'
46	A	302	3PE	C24-C25-C26-C27
45	L	704	LMT	O5'-C1'-O1'-C1
45	A	301	LMT	O1'-C1-C2-C3
46	L	701	3PE	C38-C39-C3A-C3B
46	I	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	N	903	3PE	C1-C2-C3-O31
46	b	901	3PE	C1-C2-C3-O31
52	h	1001	CDL	CB3-CB4-CB6-OB8
52	q	202	CDL	CA3-CA4-CA6-OA8
46	L	701	3PE	C36-C37-C38-C39
46	b	901	3PE	C27-C28-C29-C2A
52	q	202	CDL	C37-C38-C39-C40
46	N	903	3PE	O22-C21-O21-C2
52	X	1701	CDL	OB5-CB3-CB4-OB6
52	d	1202	CDL	OA5-CA3-CA4-OA6
52	q	202	CDL	OA5-CA3-CA4-OA6
52	q	202	CDL	C15-C16-C17-C18
53	M	603	PC1	C23-C24-C25-C26
46	H	601	3PE	C2-C1-O11-P
58	T	101	EHZ	O1-C7-C8-C9
46	A	302	3PE	C39-C3A-C3B-C3C
46	A	302	3PE	O21-C2-C3-O31
46	L	703	3PE	O21-C2-C3-O31
46	M	601	3PE	O21-C2-C3-O31
46	Y	401	3PE	O21-C2-C3-O31
46	d	1201	3PE	O21-C2-C3-O31
52	q	202	CDL	OB6-CB4-CB6-OB8
53	q	201	PC1	O21-C2-C3-O31
52	h	1001	CDL	C15-C16-C17-C18
58	T	101	EHZ	C6-C7-C8-C9
46	I	201	3PE	C2B-C2C-C2D-C2E
52	J	401	CDL	C54-C55-C56-C57
52	X	1701	CDL	C60-C61-C62-C63
46	M	602	3PE	O11-C1-C2-C3
52	X	1701	CDL	OB5-CB3-CB4-CB6
59	o	201	MYR	C11-C12-C13-C14
46	d	1201	3PE	C38-C39-C3A-C3B
52	L	702	CDL	CB5-C51-C52-C53
45	N	902	LMT	C5'-C4'-O1B-C1B
46	M	601	3PE	O22-C21-O21-C2
46	M	601	3PE	C3-C2-O21-C21
53	M	603	PC1	C31-C32-C33-C34
46	L	701	3PE	C24-C25-C26-C27
52	X	1701	CDL	C53-C54-C55-C56
52	h	1001	CDL	C73-C74-C75-C76
46	M	601	3PE	O11-C1-C2-O21
52	L	702	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
52	d	1202	CDL	CA5-C11-C12-C13
46	d	1201	3PE	C3A-C3B-C3C-C3D
46	A	302	3PE	C12-C11-O13-P
46	M	602	3PE	C12-C11-O13-P
52	q	202	CDL	C56-C57-C58-C59
46	L	701	3PE	O21-C2-C3-O31
52	J	401	CDL	OA6-CA4-CA6-OA8
52	h	1001	CDL	OB6-CB4-CB6-OB8
46	I	201	3PE	C32-C33-C34-C35
52	q	202	CDL	C38-C39-C40-C41
52	d	1202	CDL	C31-C32-C33-C34
53	q	201	PC1	C22-C23-C24-C25
46	L	701	3PE	C21-C22-C23-C24
52	X	1701	CDL	C52-C53-C54-C55
52	d	1202	CDL	C52-C51-CB5-OB6
46	L	703	3PE	C3C-C3D-C3E-C3F
52	J	401	CDL	C71-CB7-OB8-CB6
46	I	201	3PE	C26-C27-C28-C29
54	O	401	GTP	PB-O3A-PA-O1A
56	P	501	NDP	PN-O3-PA-O1A
52	h	1001	CDL	C17-C18-C19-C20
46	A	302	3PE	C35-C36-C37-C38
52	d	1202	CDL	O1-C1-CB2-OB2
45	B	202	LMT	C7-C8-C9-C10
59	o	201	MYR	C7-C8-C9-C10
46	Y	401	3PE	O11-C1-C2-O21
45	B	202	LMT	C3-C4-C5-C6
52	L	702	CDL	C38-C39-C40-C41
51	N	904	I49	N01-C14-N02-C15
52	L	702	CDL	OA6-CA4-CA6-OA8
52	q	202	CDL	OA6-CA4-CA6-OA8
52	d	1202	CDL	CA2-C1-CB2-OB2
46	M	601	3PE	C1-C2-C3-O31
52	q	202	CDL	CB3-CB4-CB6-OB8
53	M	603	PC1	C1-C2-C3-O31
52	X	1701	CDL	C52-C51-CB5-OB6
52	J	401	CDL	OB9-CB7-OB8-CB6
46	b	901	3PE	C34-C35-C36-C37
46	H	601	3PE	C11-O13-P-O14
46	I	201	3PE	C11-O13-P-O11
46	I	201	3PE	C11-O13-P-O12
46	I	201	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	M	601	3PE	C1-O11-P-O12
46	M	601	3PE	C1-O11-P-O13
46	M	602	3PE	C1-O11-P-O14
46	Y	401	3PE	C11-O13-P-O12
52	J	401	CDL	CA3-OA5-PA1-OA3
52	J	401	CDL	CB2-OB2-PB2-OB5
52	L	702	CDL	CA2-OA2-PA1-OA3
52	L	702	CDL	CB3-OB5-PB2-OB2
52	X	1701	CDL	CA2-OA2-PA1-OA5
52	X	1701	CDL	CA3-OA5-PA1-OA2
52	X	1701	CDL	CA3-OA5-PA1-OA3
52	d	1202	CDL	CA3-OA5-PA1-OA3
52	d	1202	CDL	CB2-OB2-PB2-OB4
52	q	202	CDL	CA3-OA5-PA1-OA3
52	q	202	CDL	CB2-OB2-PB2-OB3
54	O	401	GTP	C5'-O5'-PA-O1A
52	L	702	CDL	C33-C34-C35-C36
52	q	202	CDL	C54-C55-C56-C57
52	L	702	CDL	C54-C55-C56-C57
52	L	702	CDL	CA4-CA3-OA5-PA1
52	X	1701	CDL	CB4-CB3-OB5-PB2
45	B	202	LMT	C5-C6-C7-C8
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	f	1801	LMT	C2B-C1B-O1B-C4'
58	T	101	EHZ	C5-C6-C7-O1
45	d	1203	LMT	C9-C10-C11-C12
52	L	702	CDL	OB5-CB3-CB4-CB6
52	q	202	CDL	C17-C18-C19-C20
52	X	1701	CDL	OA5-CA3-CA4-OA6
46	I	201	3PE	C25-C26-C27-C28
52	L	702	CDL	C14-C15-C16-C17
46	L	701	3PE	C2C-C2D-C2E-C2F
46	L	703	3PE	O21-C21-C22-C23
46	Y	401	3PE	C32-C33-C34-C35
46	N	903	3PE	O31-C31-C32-C33
46	b	901	3PE	C21-C22-C23-C24
56	P	501	NDP	PN-O3-PA-O2A
45	d	1203	LMT	C5-C6-C7-C8
45	j	101	LMT	C4'-C5'-C6'-O6'
52	d	1202	CDL	C52-C51-CB5-OB7
58	U	101	EHZ	C2-C3-C4-C5
56	P	501	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
52	q	202	CDL	CA4-CA3-OA5-PA1
45	Y	402	LMT	C3'-C4'-O1B-C1B
52	q	202	CDL	OB5-CB3-CB4-OB6
45	L	704	LMT	C9-C10-C11-C12
46	M	601	3PE	C3A-C3B-C3C-C3D
52	d	1202	CDL	C38-C39-C40-C41
46	M	601	3PE	C23-C24-C25-C26
56	P	501	NDP	O4D-C1D-N1N-C6N
46	M	602	3PE	C35-C36-C37-C38
52	L	702	CDL	C56-C57-C58-C59
46	L	703	3PE	C2-C1-O11-P
49	F	501	FMN	C4'-C5'-O5'-P
46	L	703	3PE	C1-C2-C3-O31
52	L	702	CDL	C31-C32-C33-C34
46	H	601	3PE	C3D-C3E-C3F-C3G
46	b	901	3PE	C22-C23-C24-C25
46	Y	401	3PE	C39-C3A-C3B-C3C
45	Y	402	LMT	C5'-C4'-O1B-C1B
51	H	602	I49	C08-C06-C07-C09
46	M	602	3PE	C33-C34-C35-C36
52	h	1001	CDL	C16-C17-C18-C19
46	d	1201	3PE	C2-C1-O11-P
53	q	201	PC1	C2-C1-O11-P
52	d	1202	CDL	C77-C78-C79-C80
46	I	201	3PE	O22-C21-O21-C2
58	U	101	EHZ	C21-C1-C2-C3
46	L	703	3PE	C36-C37-C38-C39
46	H	601	3PE	C3A-C3B-C3C-C3D
51	H	602	I49	C08-C06-C07-C10
52	h	1001	CDL	C24-C25-C26-C27
45	Y	402	LMT	C11-C10-C9-C8
46	L	703	3PE	C22-C23-C24-C25
56	P	501	NDP	C2B-O2B-P2B-O1X
53	q	201	PC1	C24-C25-C26-C27
52	J	401	CDL	O1-C1-CB2-OB2
52	h	1001	CDL	C52-C53-C54-C55
46	L	701	3PE	C32-C31-O31-C3
46	M	601	3PE	C25-C26-C27-C28
46	Y	401	3PE	C3B-C3C-C3D-C3E
46	L	703	3PE	C3E-C3F-C3G-C3H
58	U	101	EHZ	C5-C6-C7-O1
46	N	903	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
45	h	1002	LMT	C11-C10-C9-C8
46	I	201	3PE	C22-C21-O21-C2
46	b	901	3PE	C23-C24-C25-C26
51	H	602	I49	N03-C14-N02-C15
51	N	904	I49	N03-C14-N02-C15
46	L	701	3PE	O32-C31-O31-C3
52	h	1001	CDL	C32-C33-C34-C35
46	L	703	3PE	C35-C36-C37-C38
46	M	601	3PE	C26-C27-C28-C29
52	J	401	CDL	C52-C53-C54-C55
46	N	903	3PE	C22-C23-C24-C25
46	b	901	3PE	C32-C33-C34-C35
52	L	702	CDL	C35-C36-C37-C38
56	P	501	NDP	C2D-C1D-N1N-C6N
45	A	301	LMT	C4'-C5'-C6'-O6'
46	d	1201	3PE	C31-C32-C33-C34
45	Y	402	LMT	C1-C2-C3-C4
45	h	1002	LMT	O5B-C5B-C6B-O6B
52	J	401	CDL	C53-C54-C55-C56
46	b	901	3PE	C2B-C2C-C2D-C2E
46	d	1201	3PE	C39-C3A-C3B-C3C
52	L	702	CDL	C53-C54-C55-C56
52	J	401	CDL	C33-C34-C35-C36
46	H	601	3PE	C36-C37-C38-C39
46	M	601	3PE	C12-C11-O13-P
46	d	1201	3PE	C32-C33-C34-C35
52	q	202	CDL	C52-C53-C54-C55
45	l	201	LMT	C5-C6-C7-C8
46	Y	401	3PE	C23-C24-C25-C26
46	L	703	3PE	C28-C29-C2A-C2B
46	N	903	3PE	O11-C1-C2-C3
46	H	601	3PE	C33-C34-C35-C36
52	L	702	CDL	C71-C72-C73-C74
46	I	201	3PE	C3A-C3B-C3C-C3D
46	L	701	3PE	O21-C21-C22-C23
52	q	202	CDL	C52-C51-CB5-OB6
46	N	903	3PE	O21-C21-C22-C23
52	d	1202	CDL	C72-C71-CB7-OB8
45	f	1801	LMT	C5-C6-C7-C8
46	M	602	3PE	C27-C28-C29-C2A
56	P	501	NDP	O4B-C4B-C5B-O5B
46	M	602	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	C51-C52-C53-C54
45	l	201	LMT	C1-C2-C3-C4
45	N	902	LMT	O5'-C1'-O1'-C1
46	d	1201	3PE	O21-C21-C22-C23
46	b	901	3PE	O21-C21-C22-C23
53	M	603	PC1	O31-C31-C32-C33
52	d	1202	CDL	C32-C33-C34-C35
52	X	1701	CDL	C32-C31-CA7-OA8
49	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C22-C23-C24-C25
58	U	101	EHZ	C3-C4-C5-C6
52	X	1701	CDL	CA5-C11-C12-C13
46	H	601	3PE	O11-C1-C2-O21
52	d	1202	CDL	C72-C71-CB7-OB9
51	H	602	I49	N01-C14-N02-C15
52	X	1701	CDL	C32-C31-CA7-OA9
52	h	1001	CDL	OA6-CA4-CA6-OA8
45	j	101	LMT	C2'-C1'-O1'-C1
46	L	701	3PE	O22-C21-C22-C23
46	N	903	3PE	O22-C21-C22-C23
46	b	901	3PE	O22-C21-C22-C23
52	q	202	CDL	C52-C51-CB5-OB7
45	l	201	LMT	O5B-C1B-O1B-C4'
45	A	301	LMT	O5'-C1'-O1'-C1
53	q	201	PC1	O21-C21-C22-C23
46	I	201	3PE	C39-C3A-C3B-C3C
46	A	302	3PE	O31-C31-C32-C33
46	b	901	3PE	O31-C31-C32-C33
52	X	1701	CDL	C58-C59-C60-C61
46	d	1201	3PE	O22-C21-C22-C23
52	d	1202	CDL	C71-C72-C73-C74

There are no ring outliers.

19 monomers are involved in 31 short contacts:

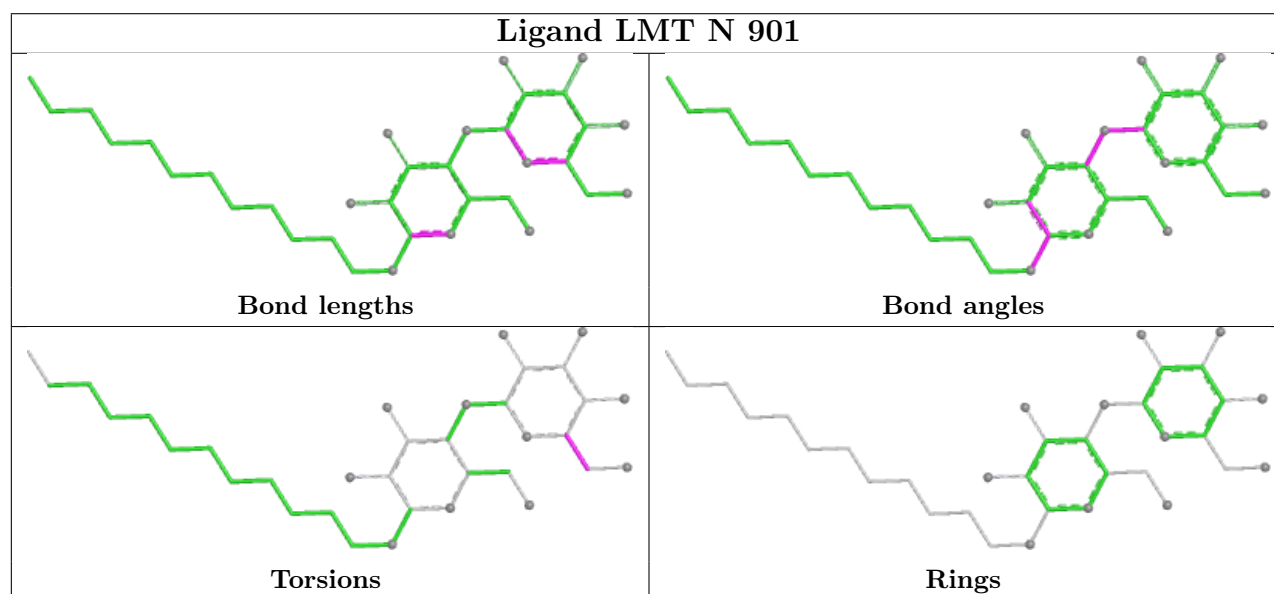
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51	H	602	I49	3	0
52	X	1701	CDL	1	0
45	B	202	LMT	2	0
45	N	902	LMT	3	0
47	I	203	SF4	1	0
58	T	101	EHZ	1	0

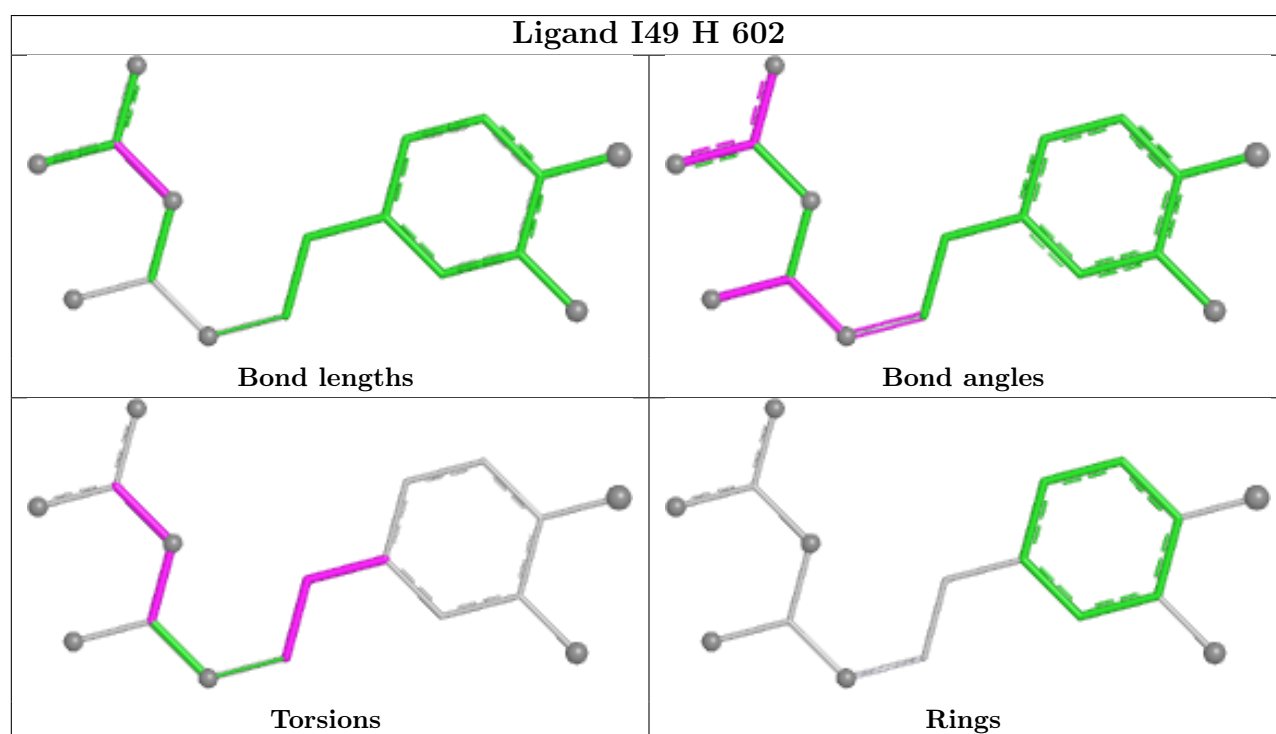
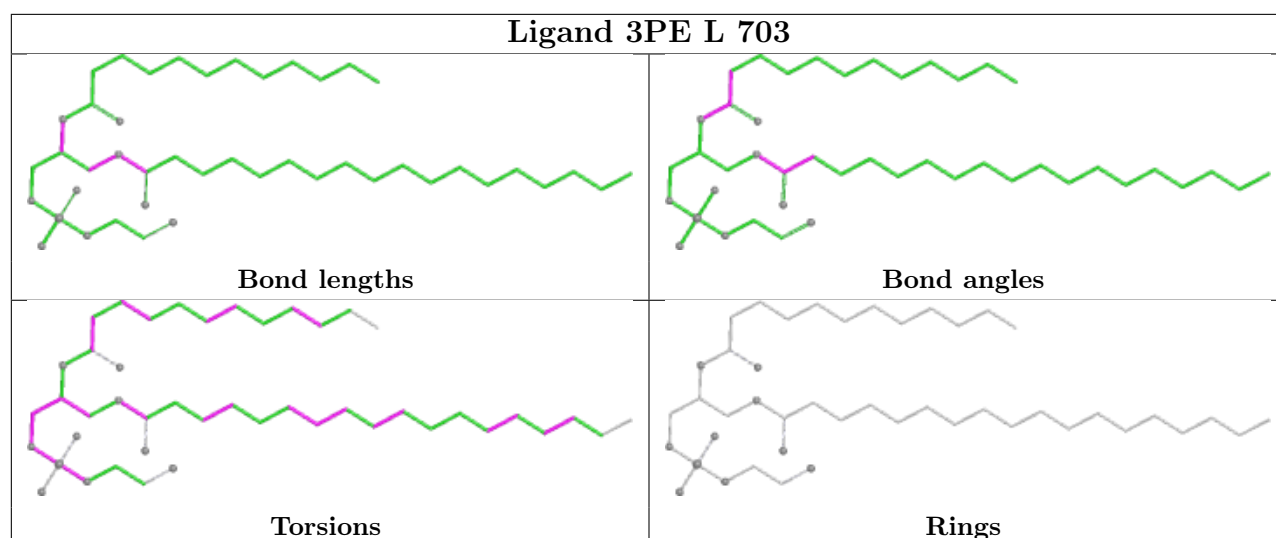
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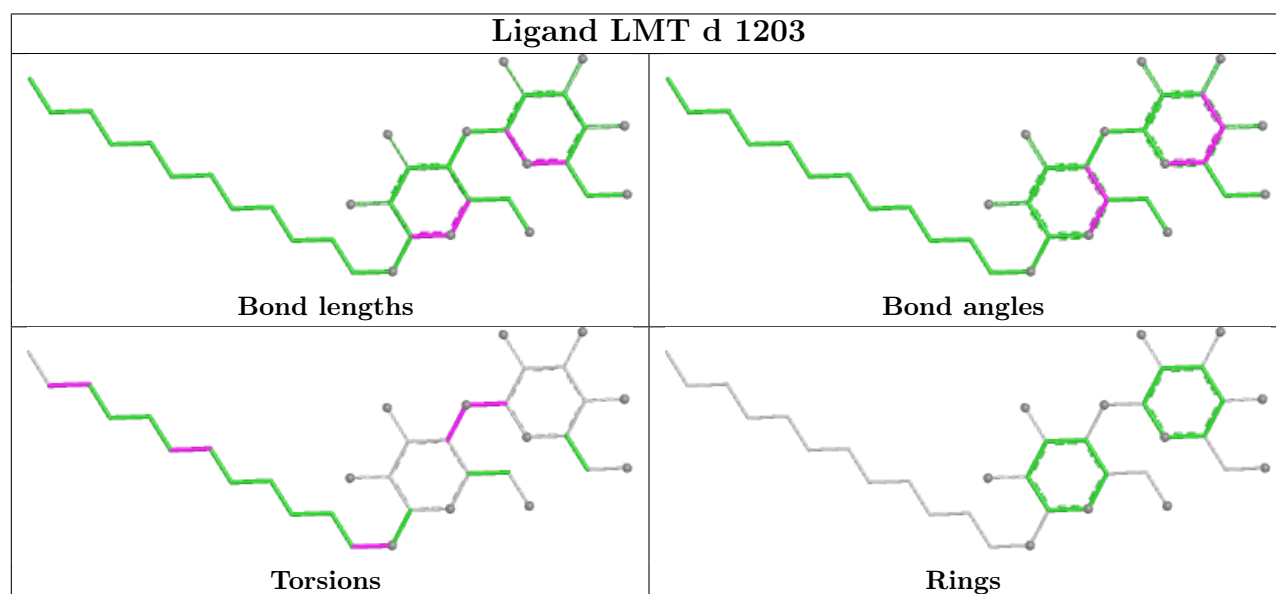
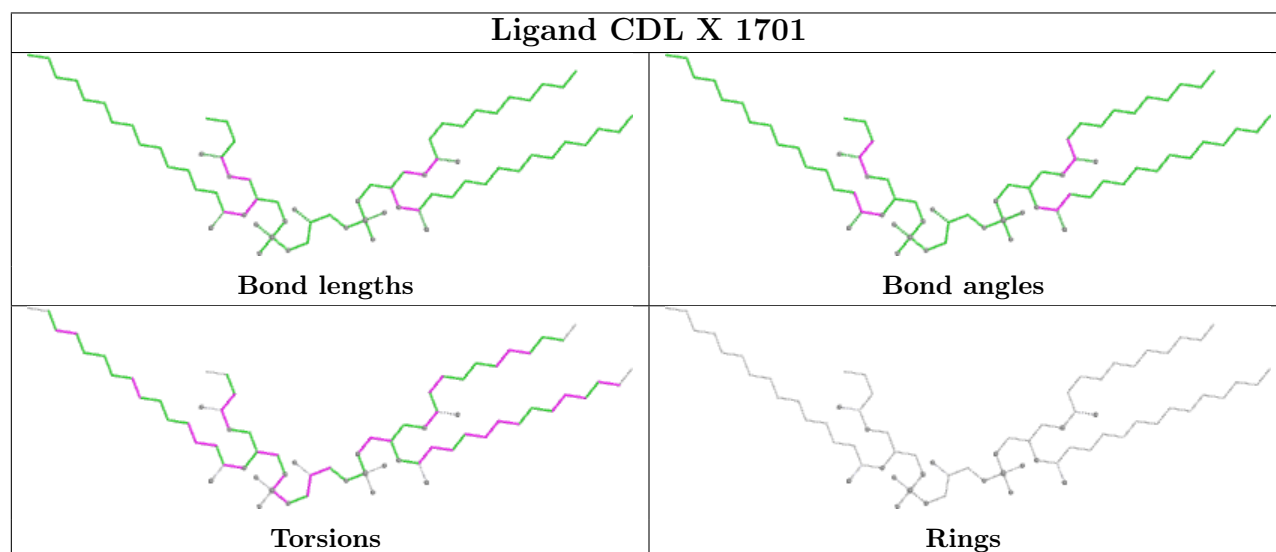
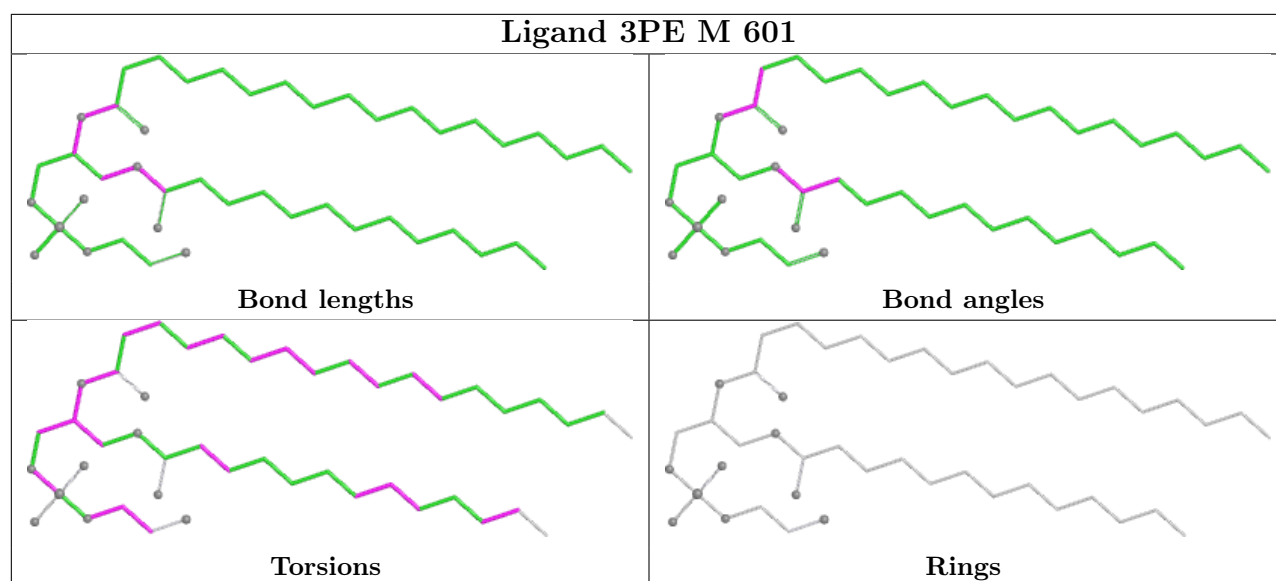
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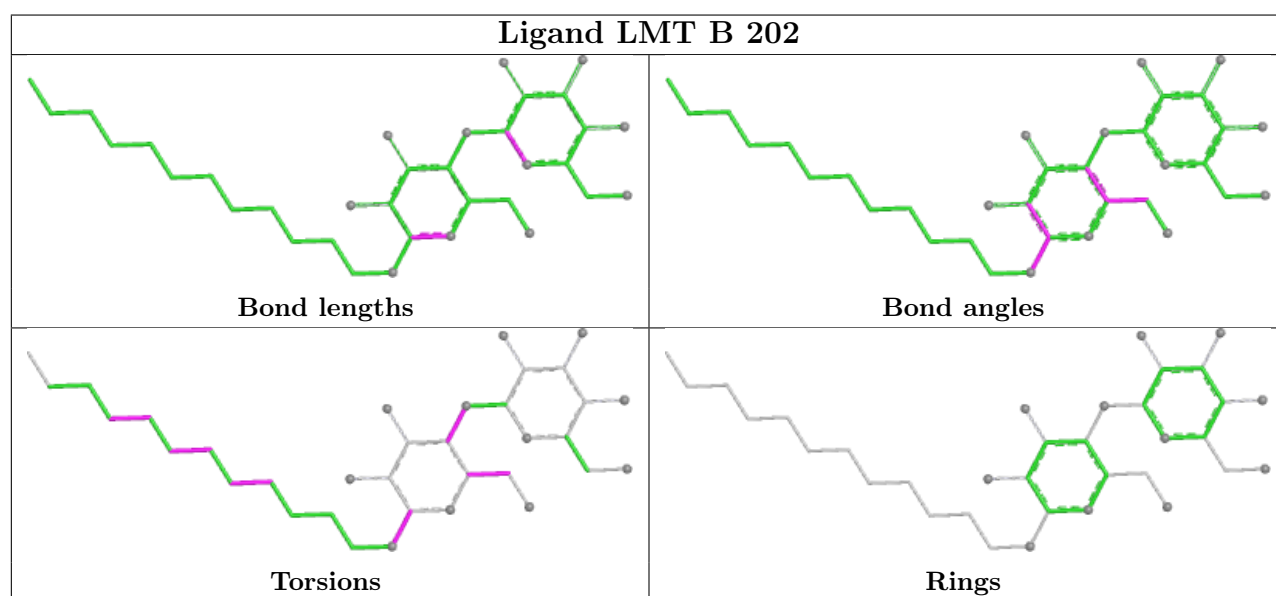
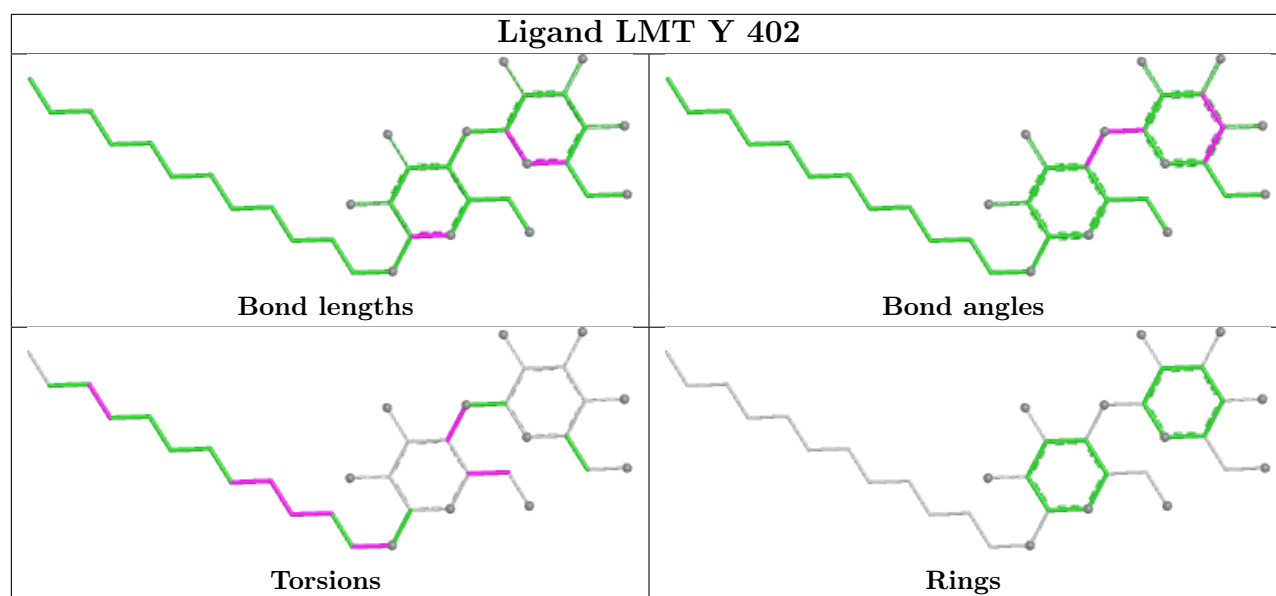
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	L	701	3PE	1	0
45	h	1002	LMT	2	0
45	e	201	LMT	2	0
54	O	401	GTP	3	0
46	A	302	3PE	1	0
51	N	904	I49	1	0
46	M	602	3PE	1	0
53	M	603	PC1	1	0
46	I	201	3PE	1	0
56	P	501	NDP	2	0
46	d	1201	3PE	2	0
47	F	502	SF4	1	0
45	j	101	LMT	2	0

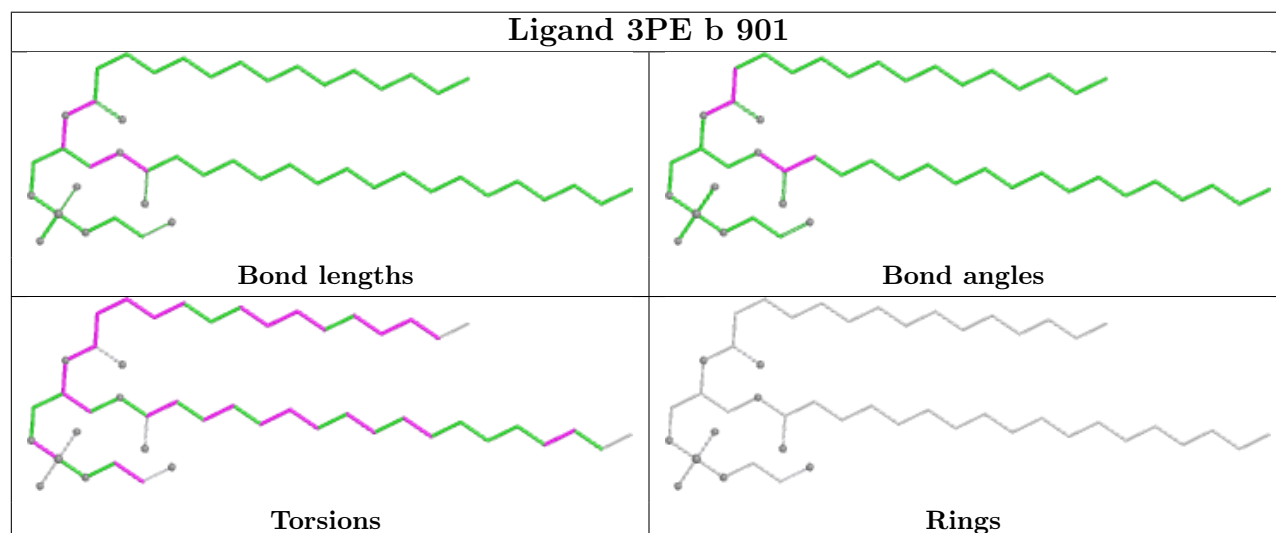
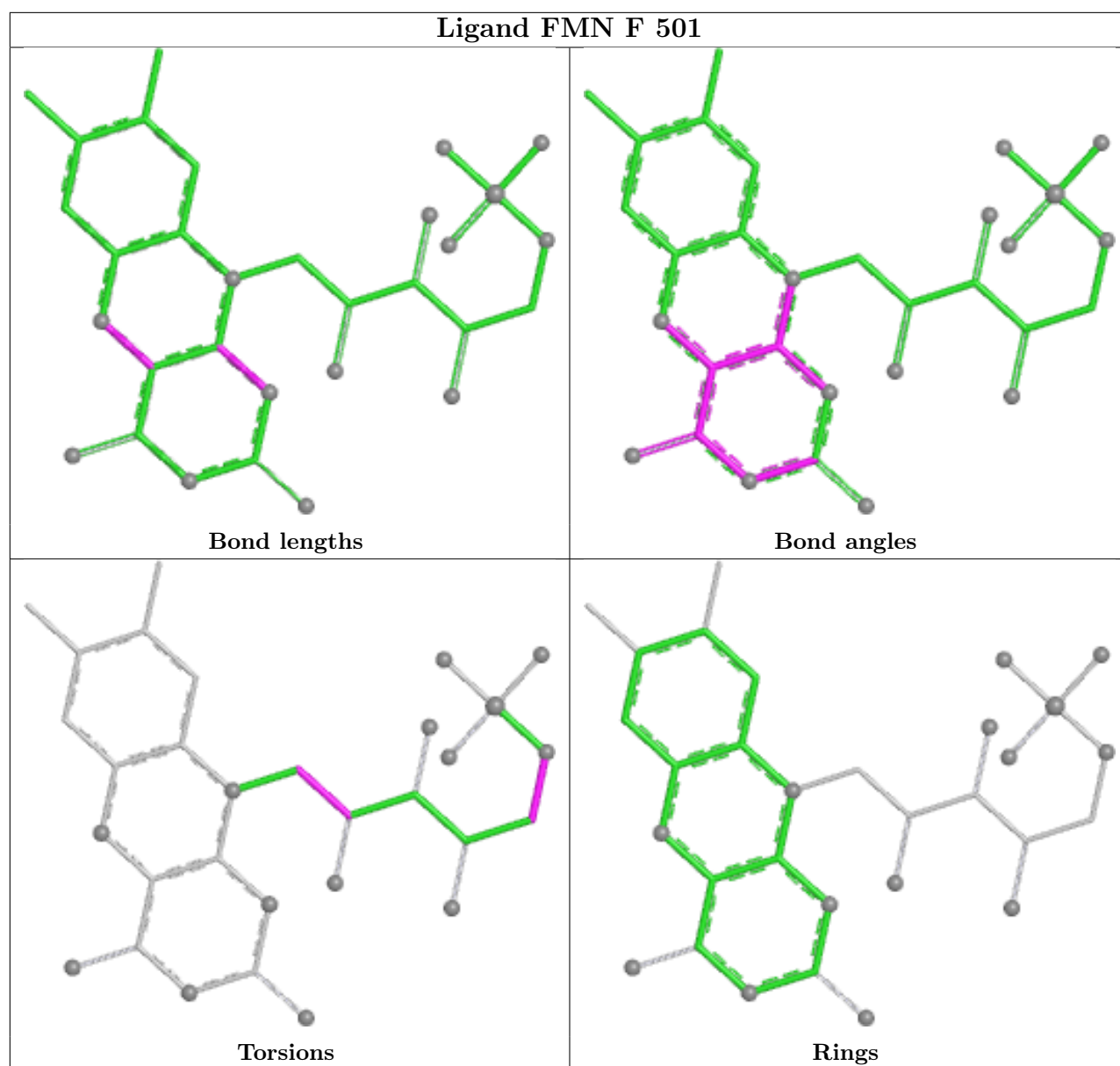
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

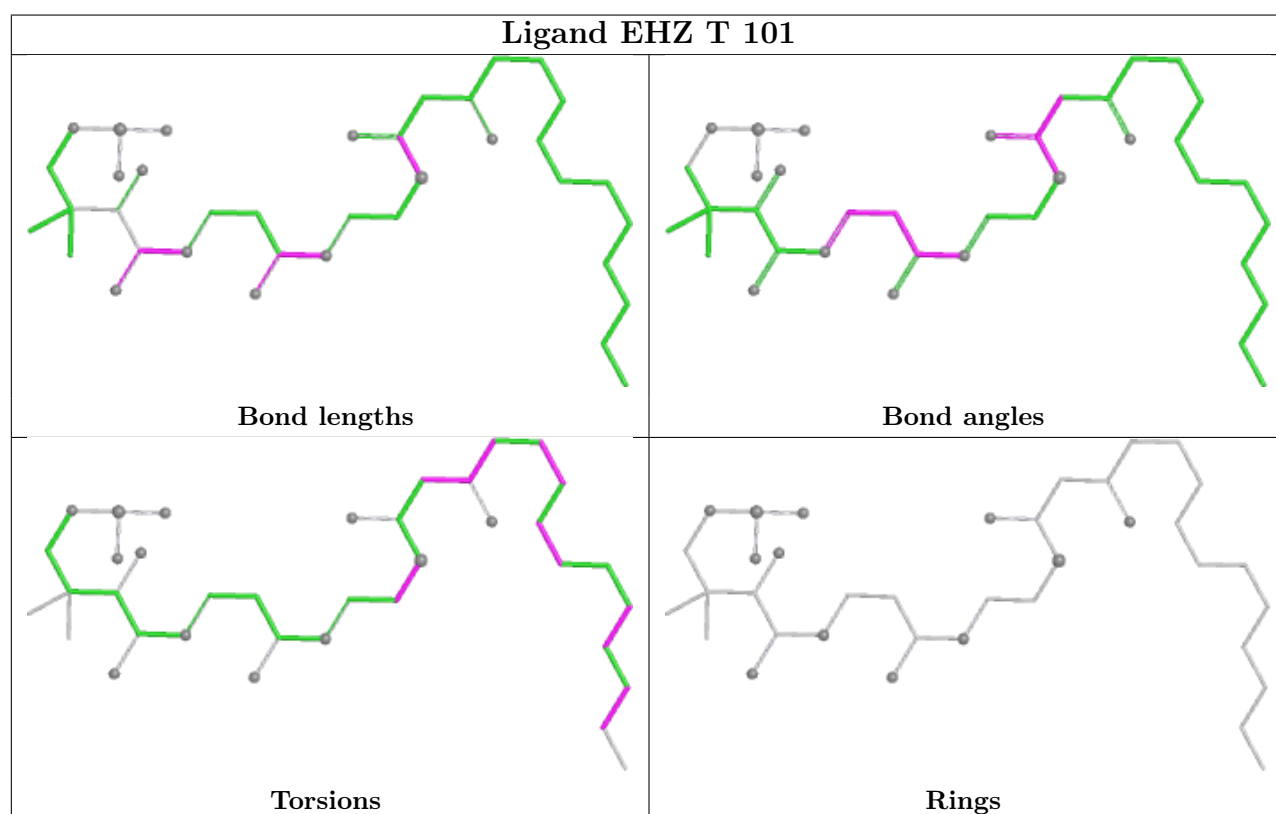
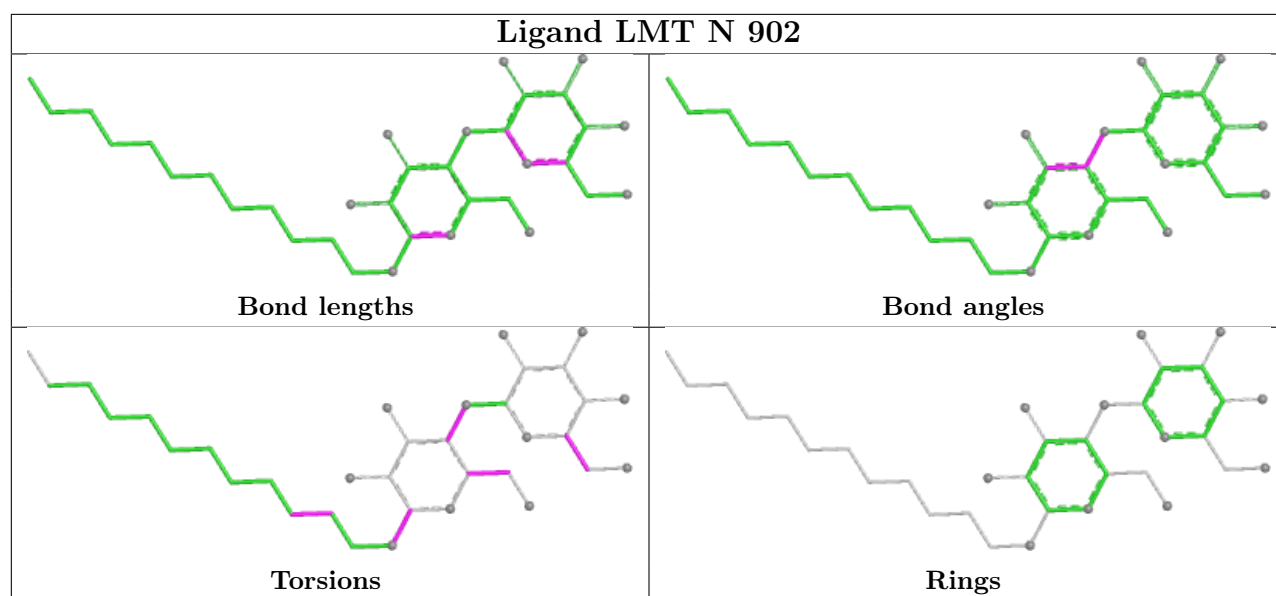


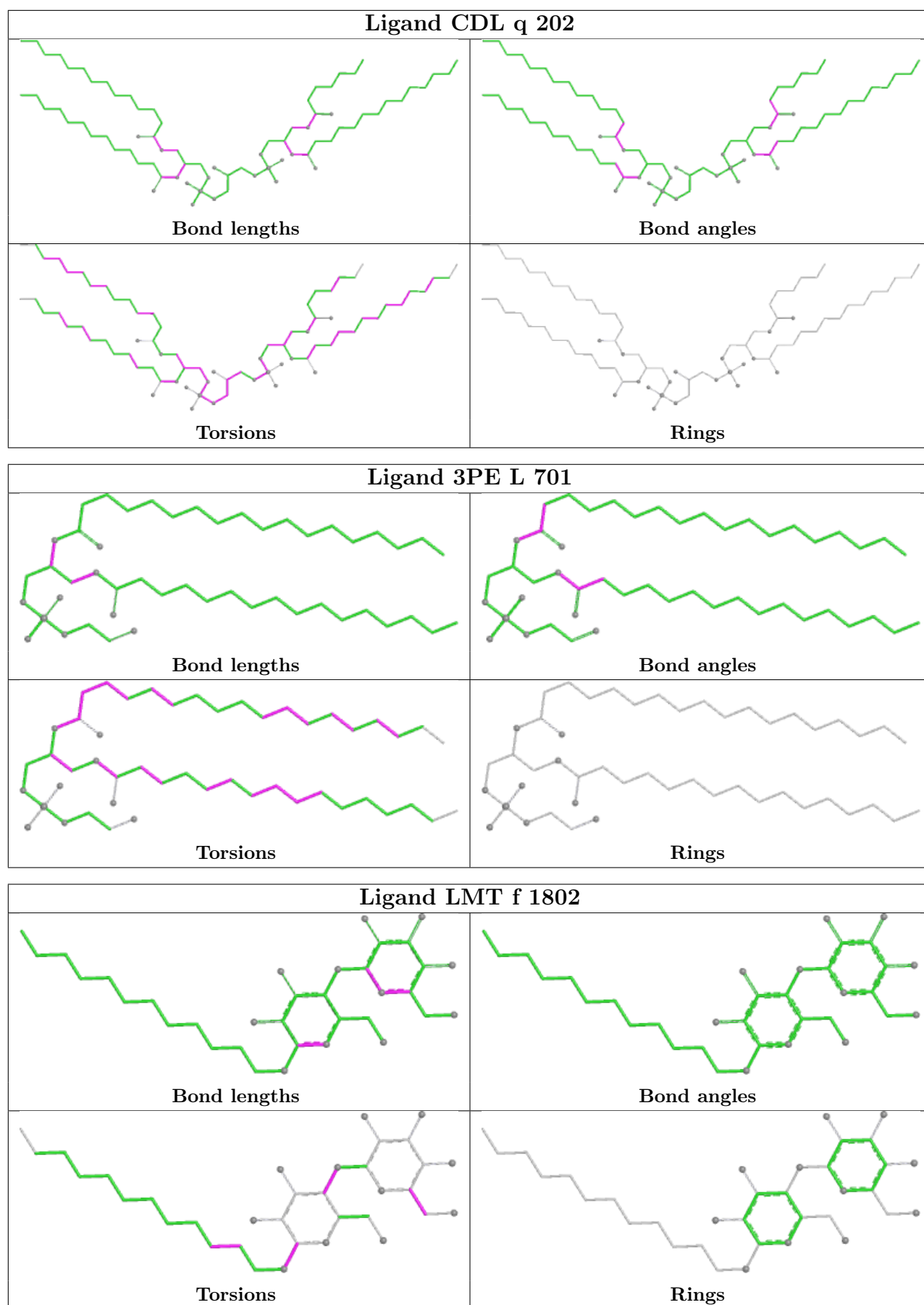


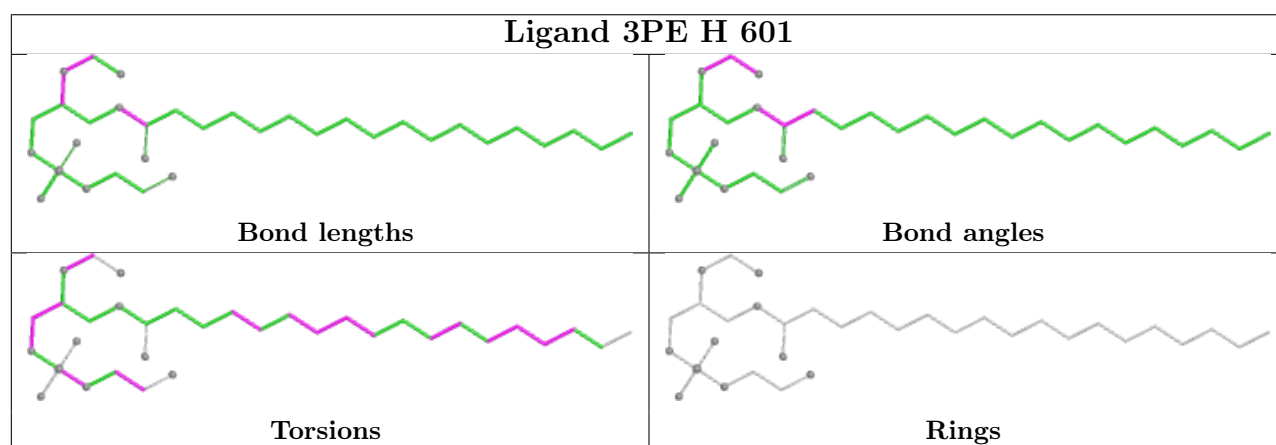
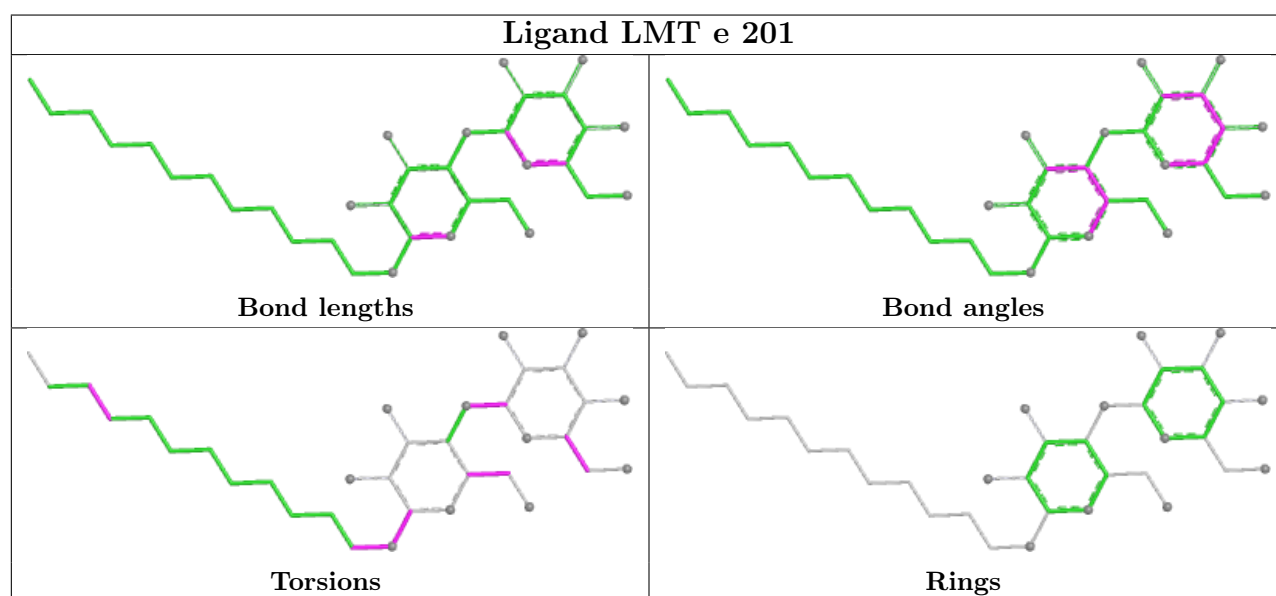
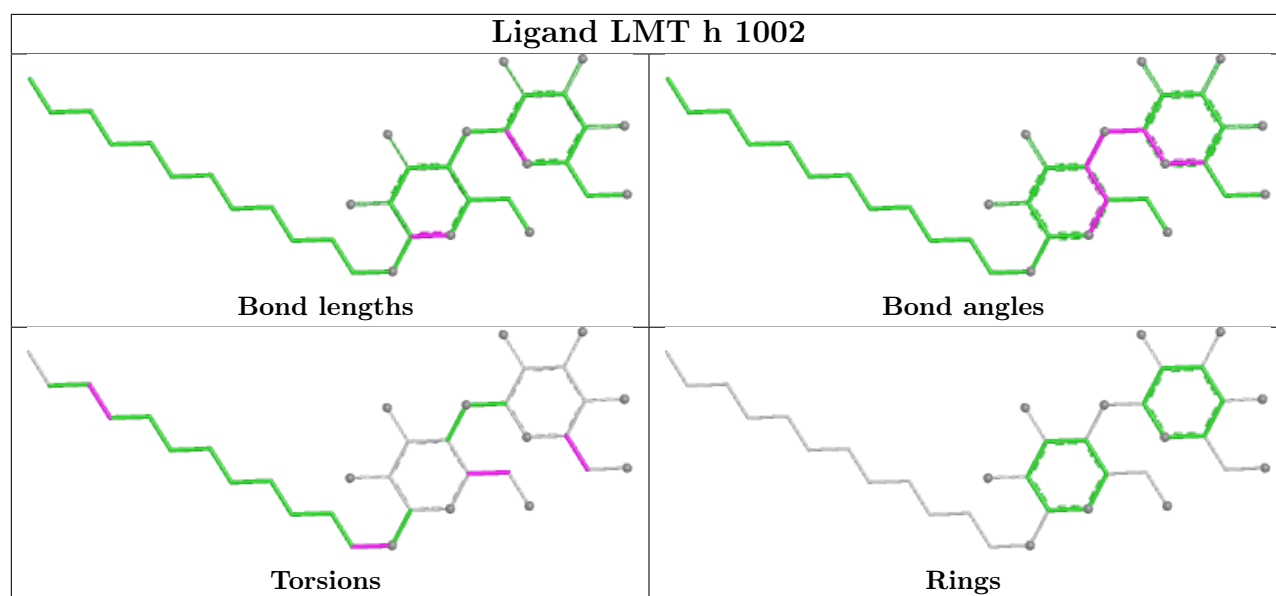


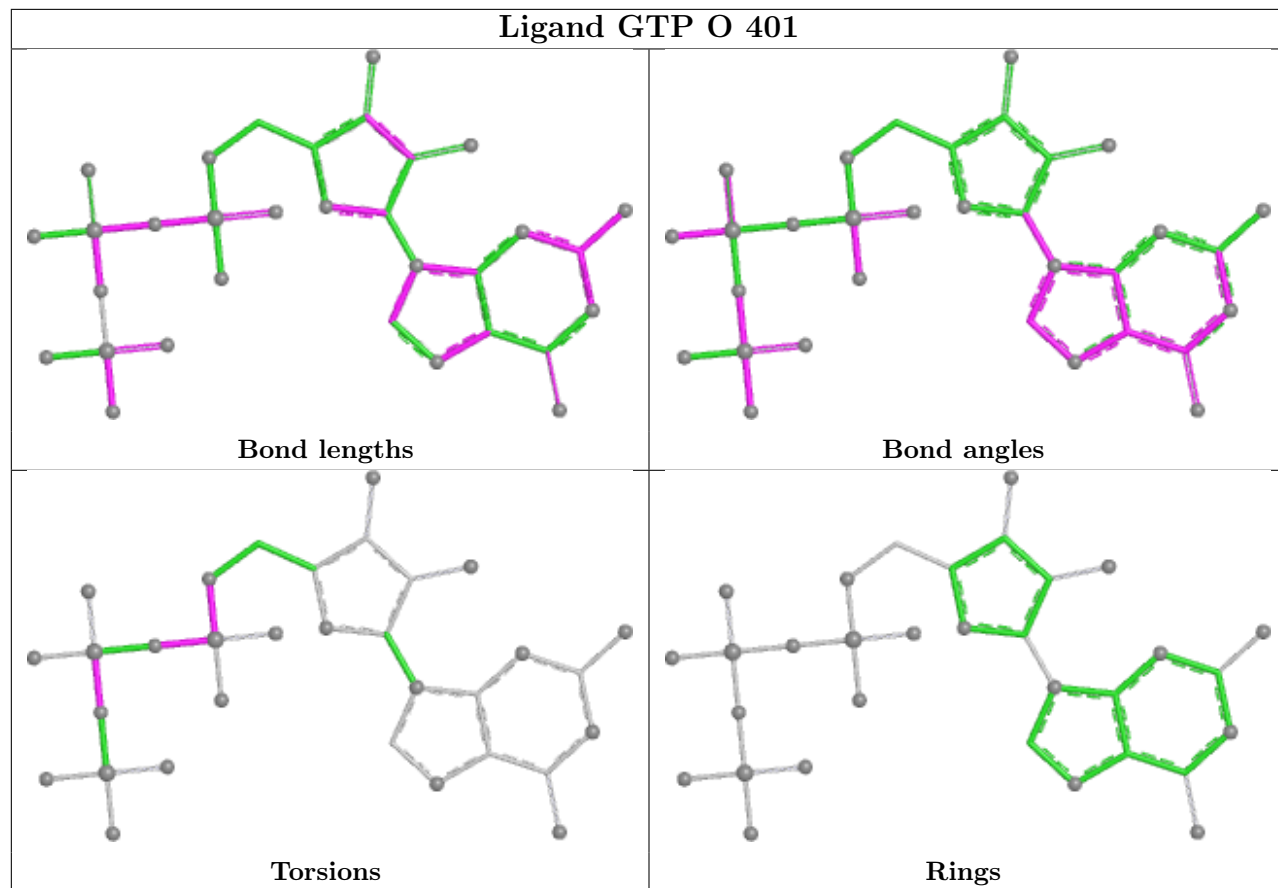
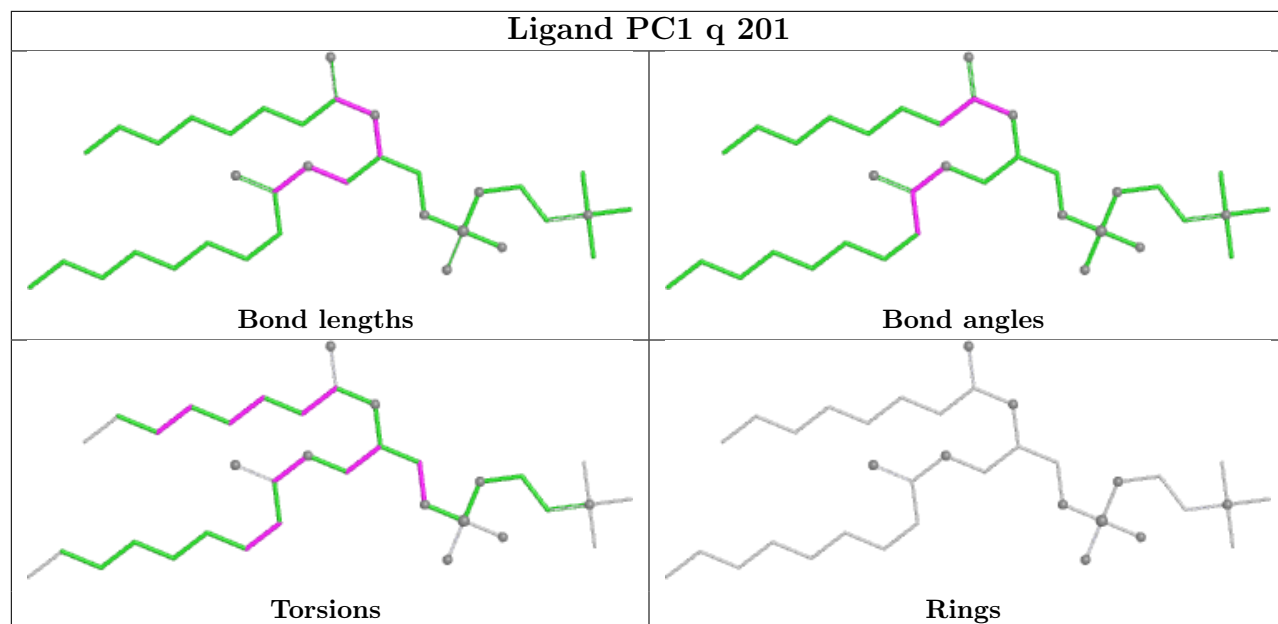


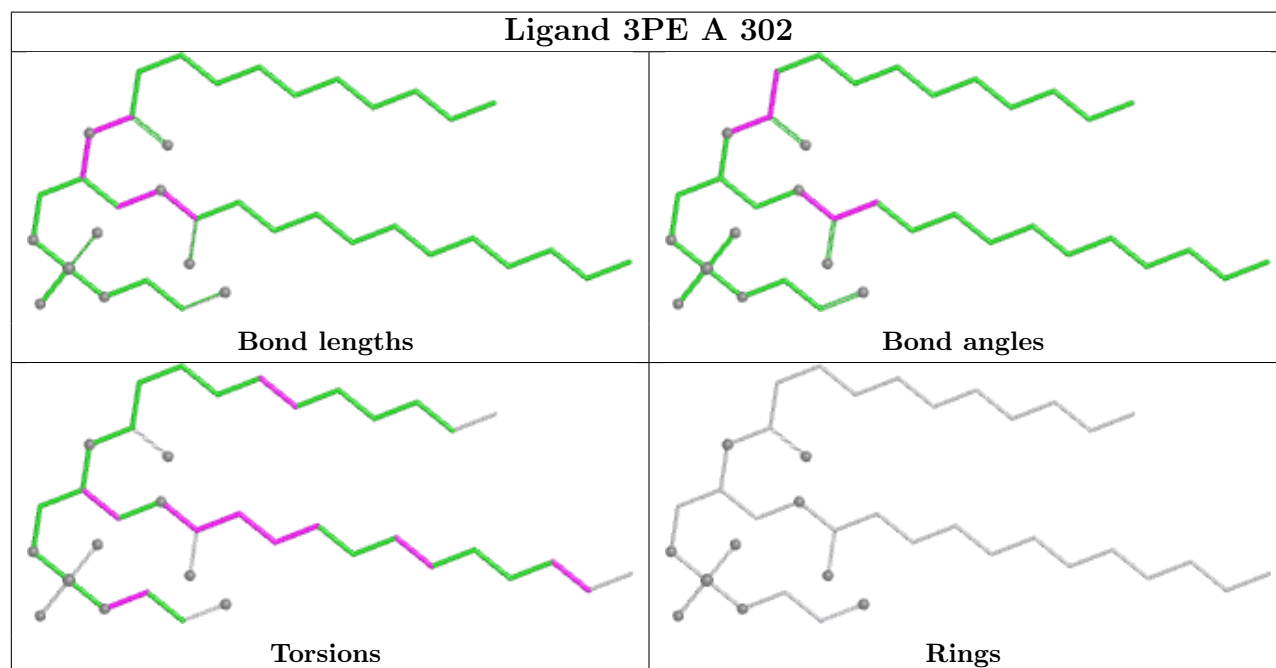
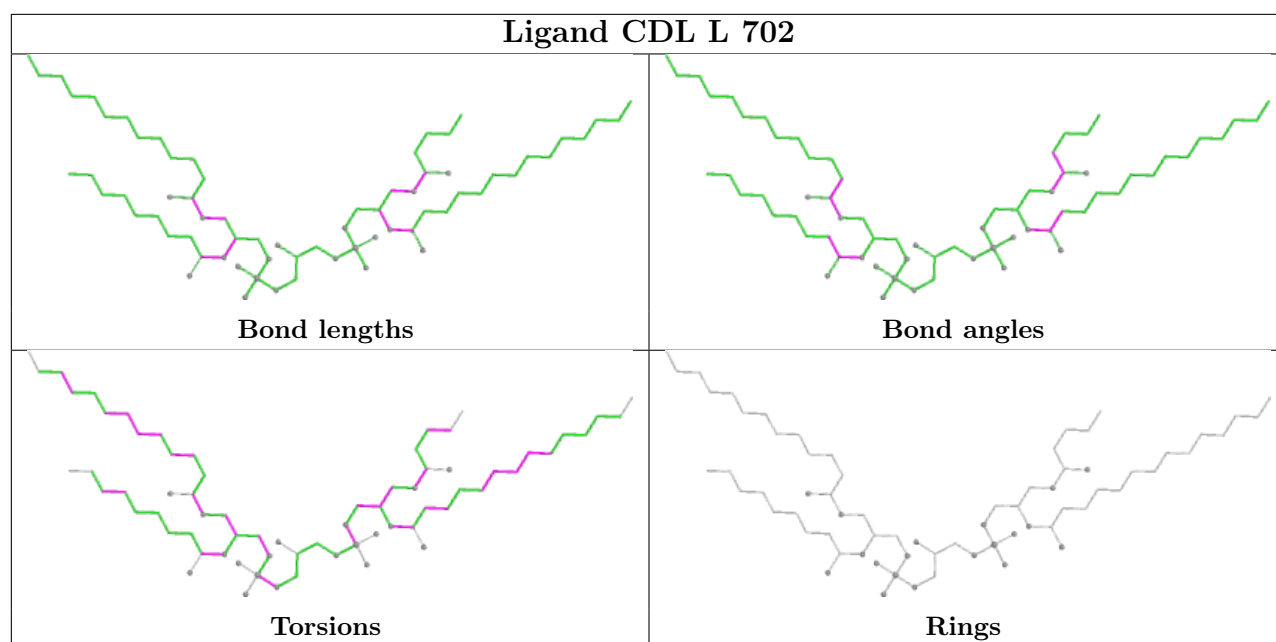


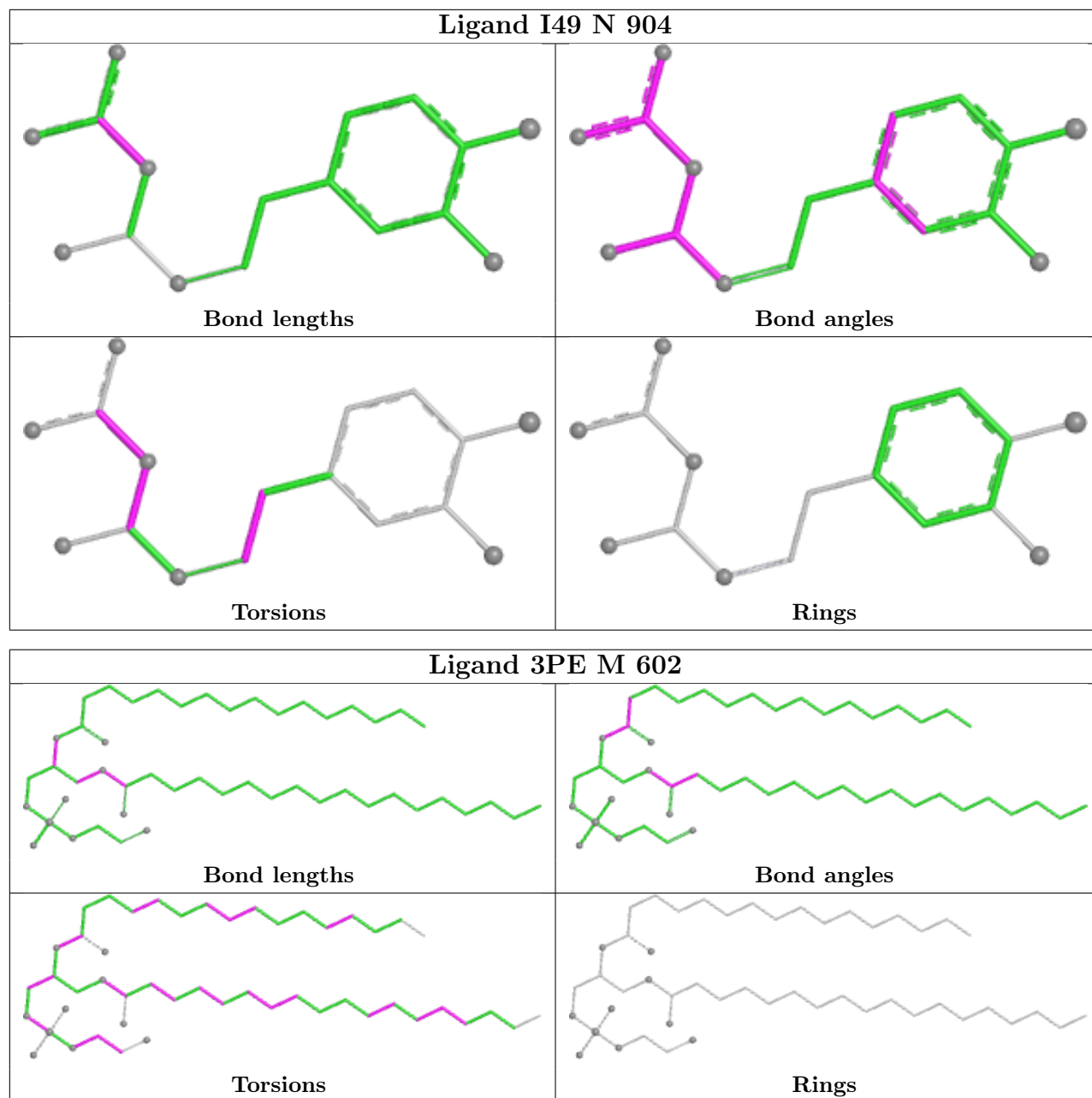


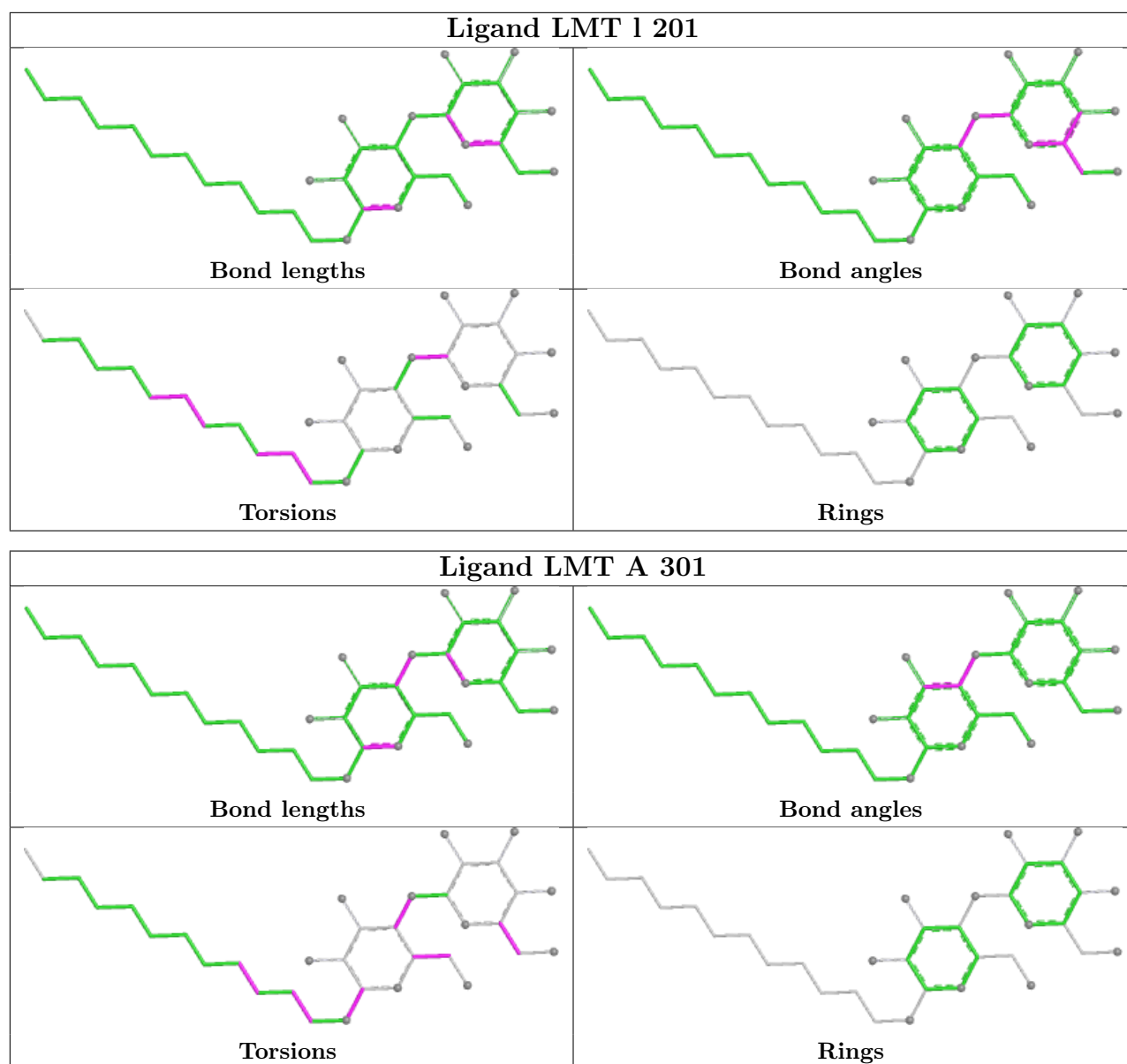


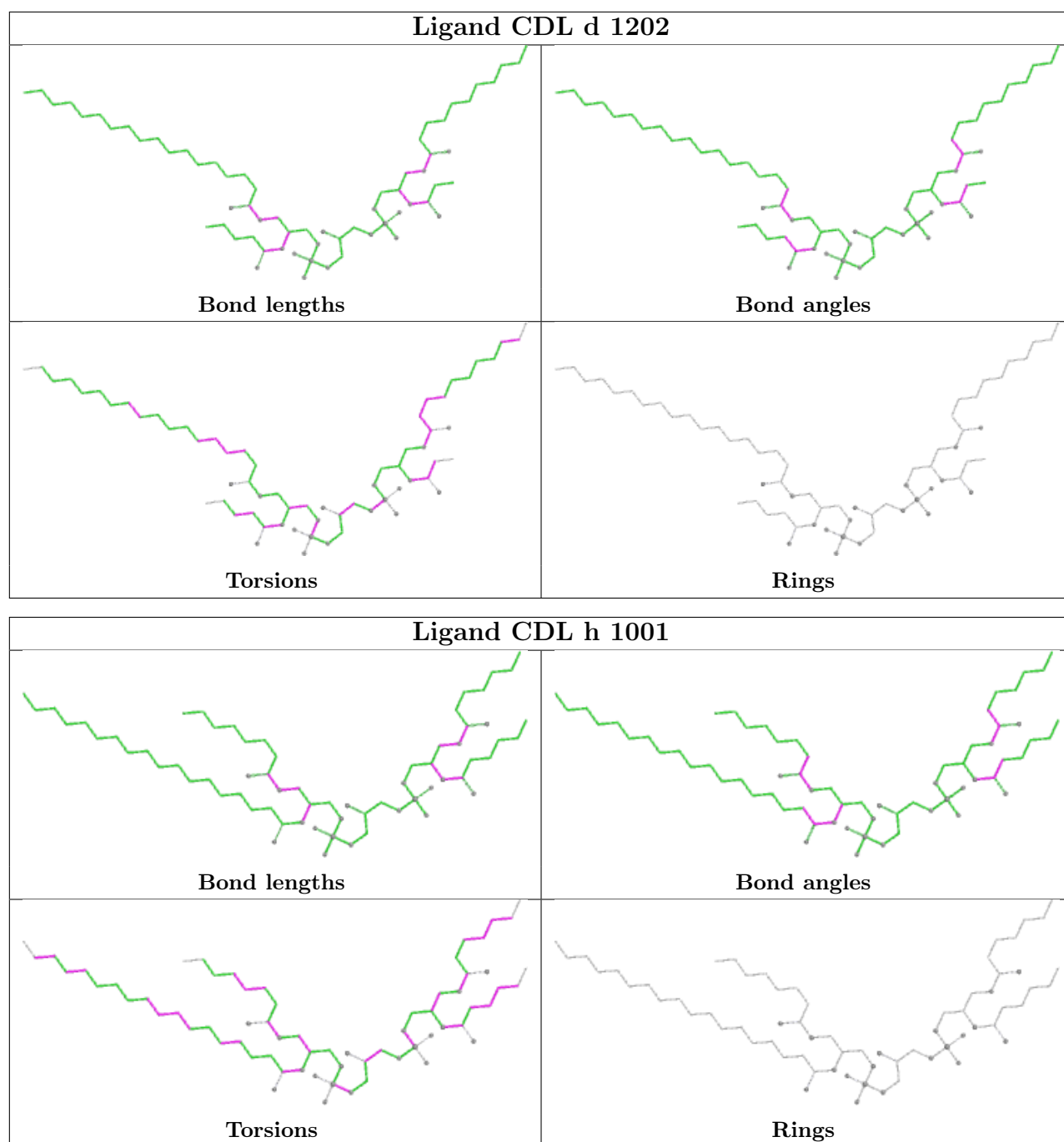


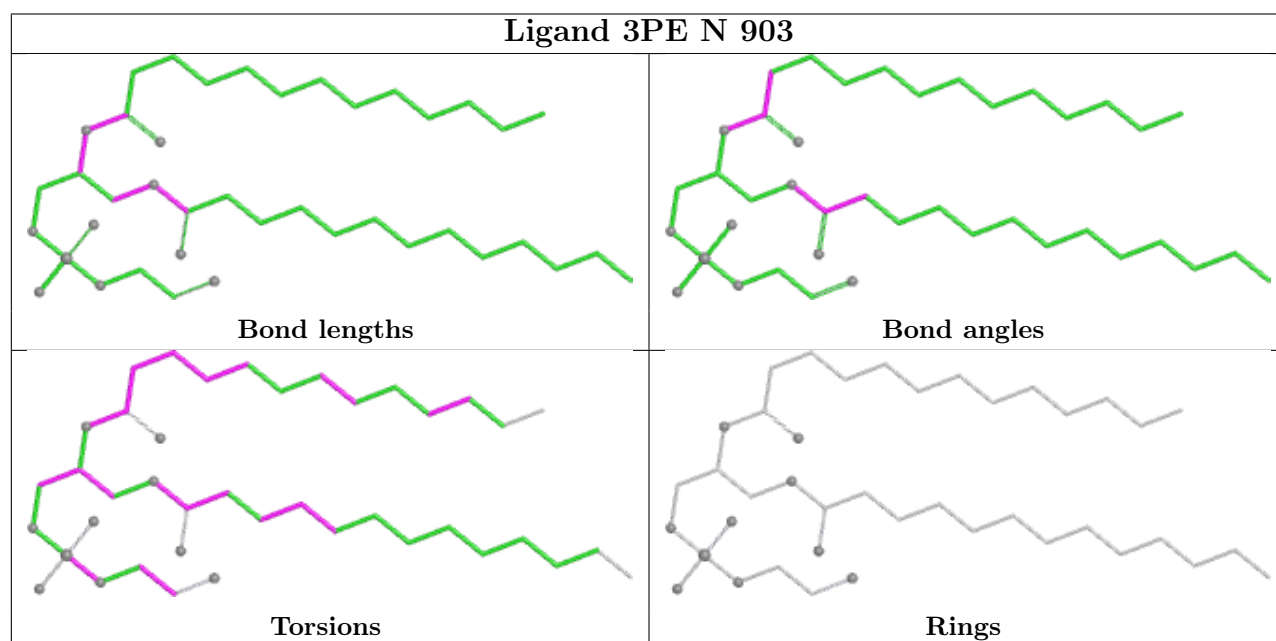
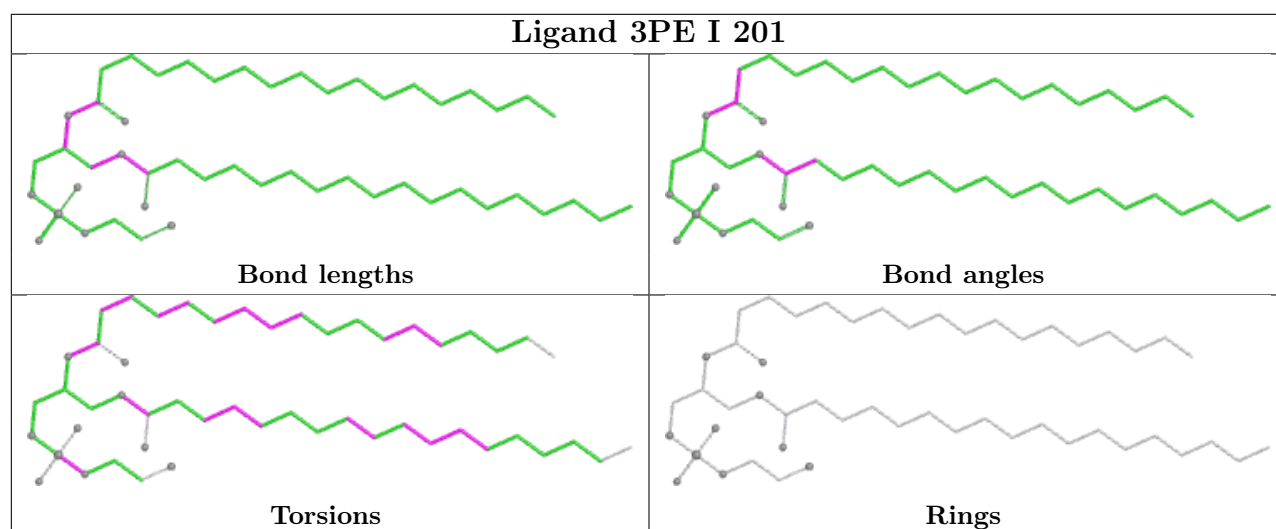
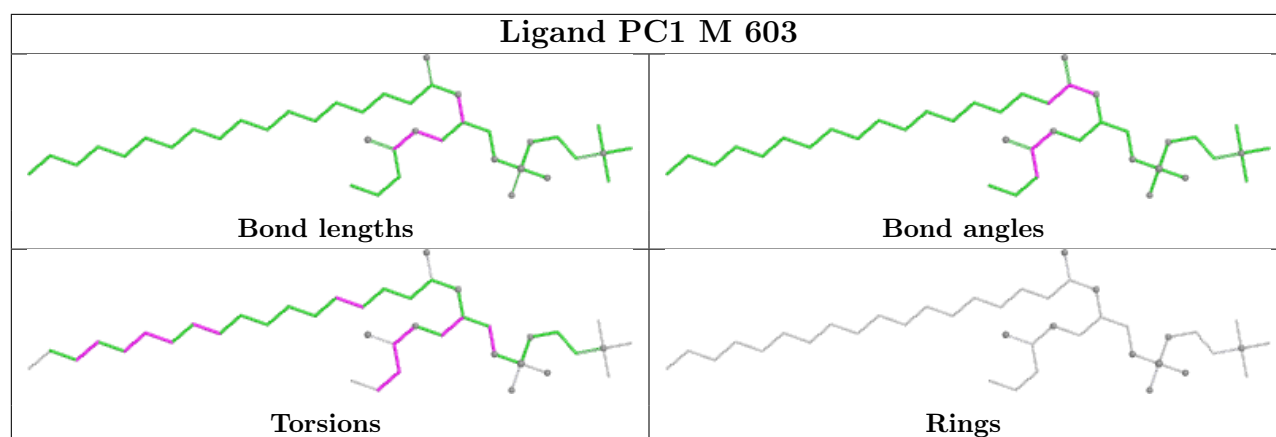


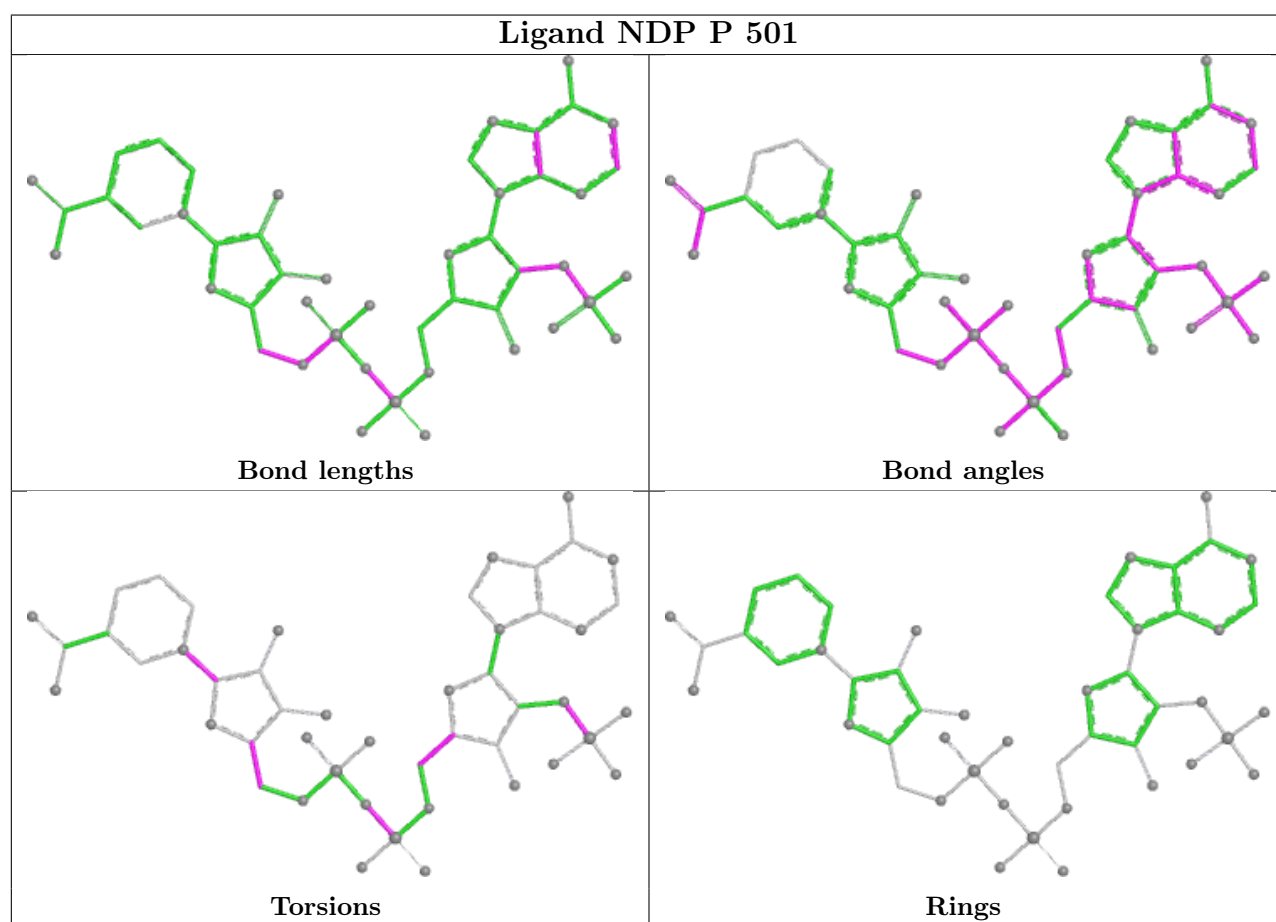
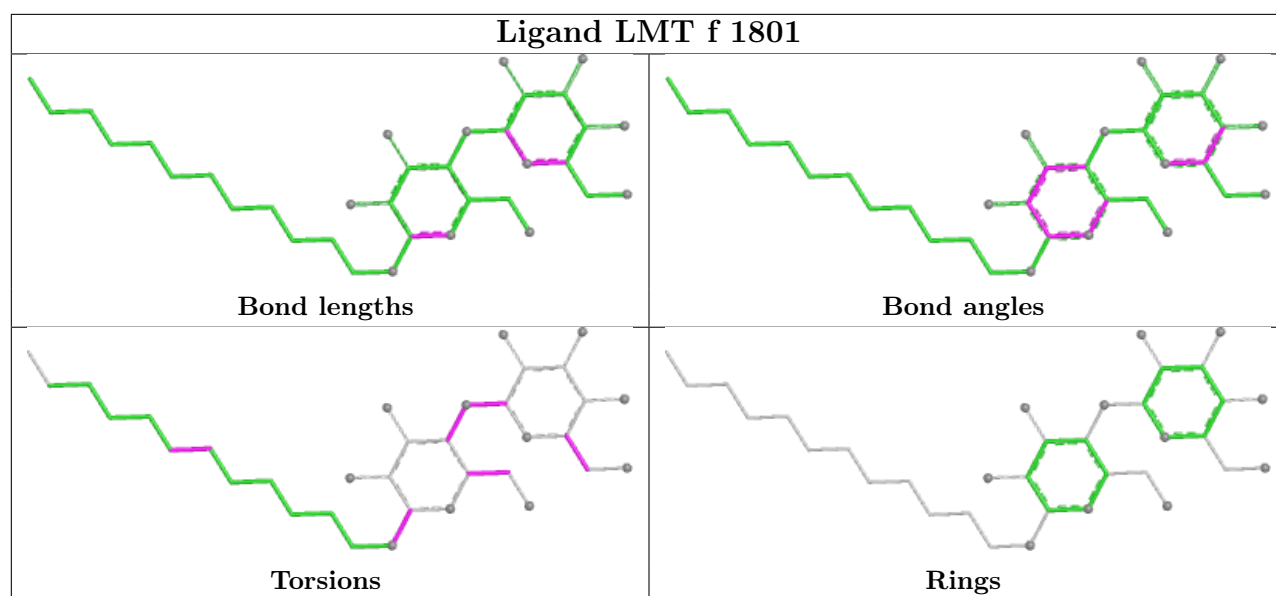


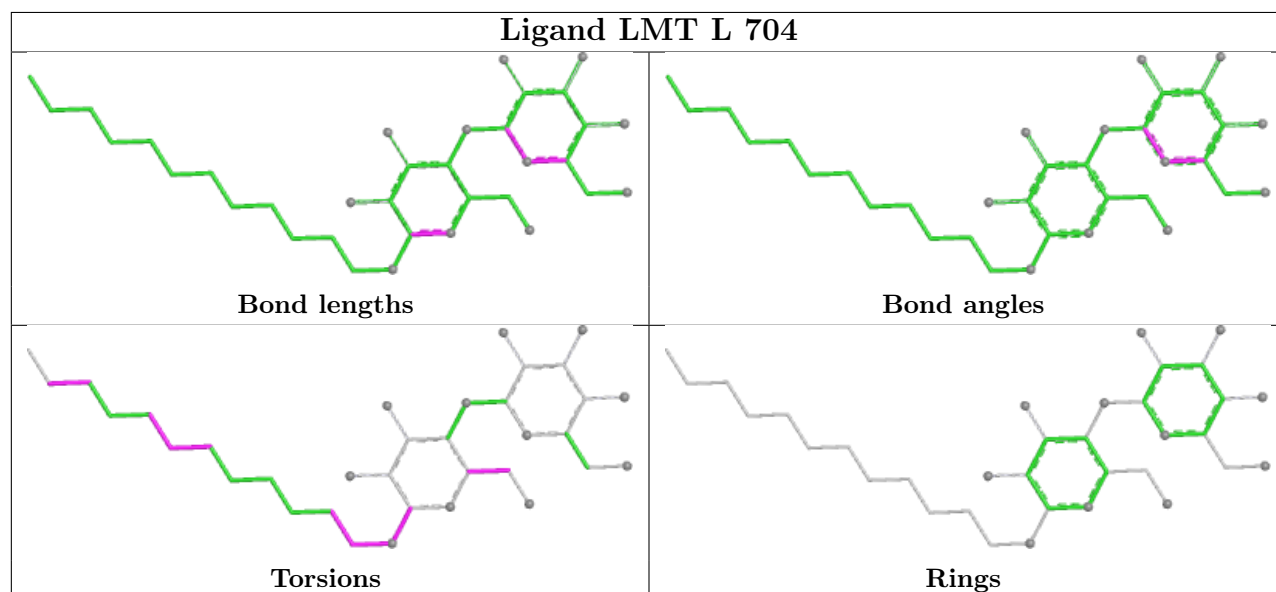
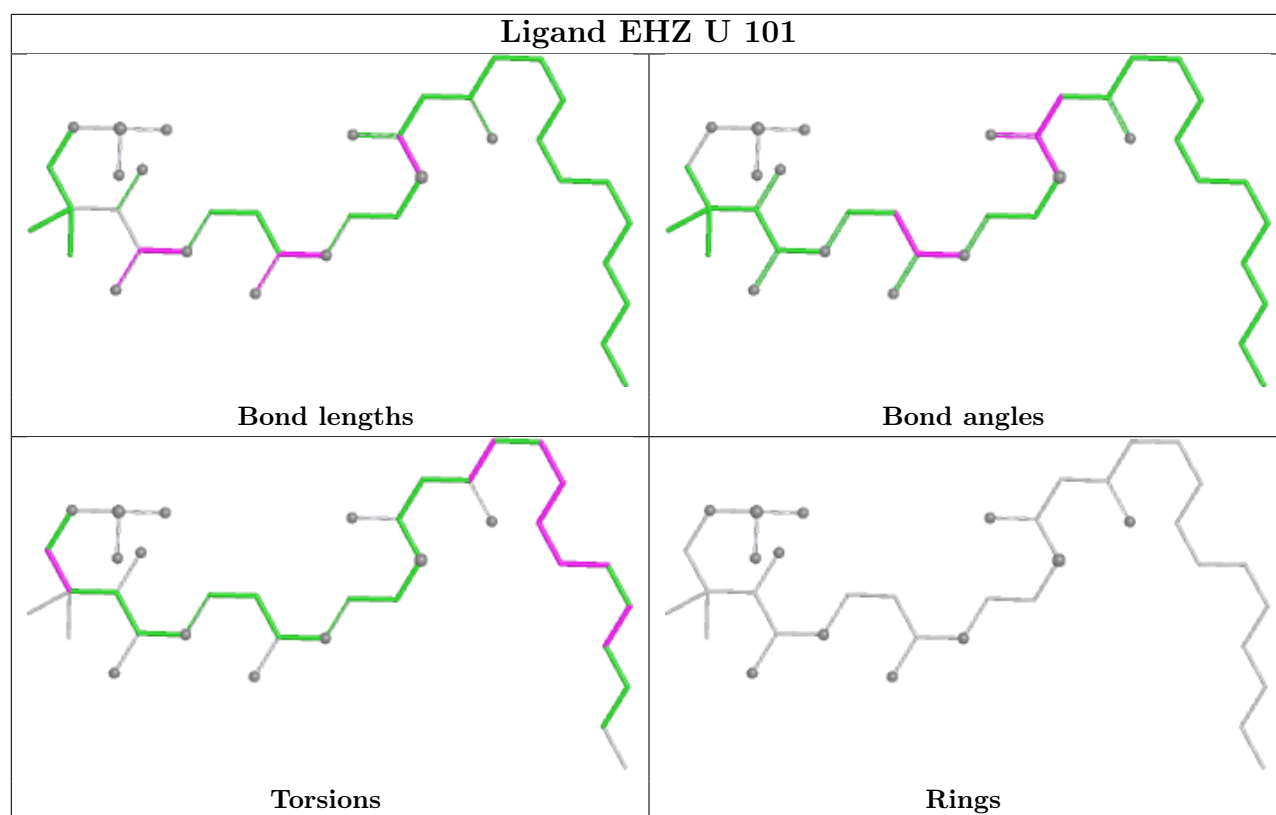


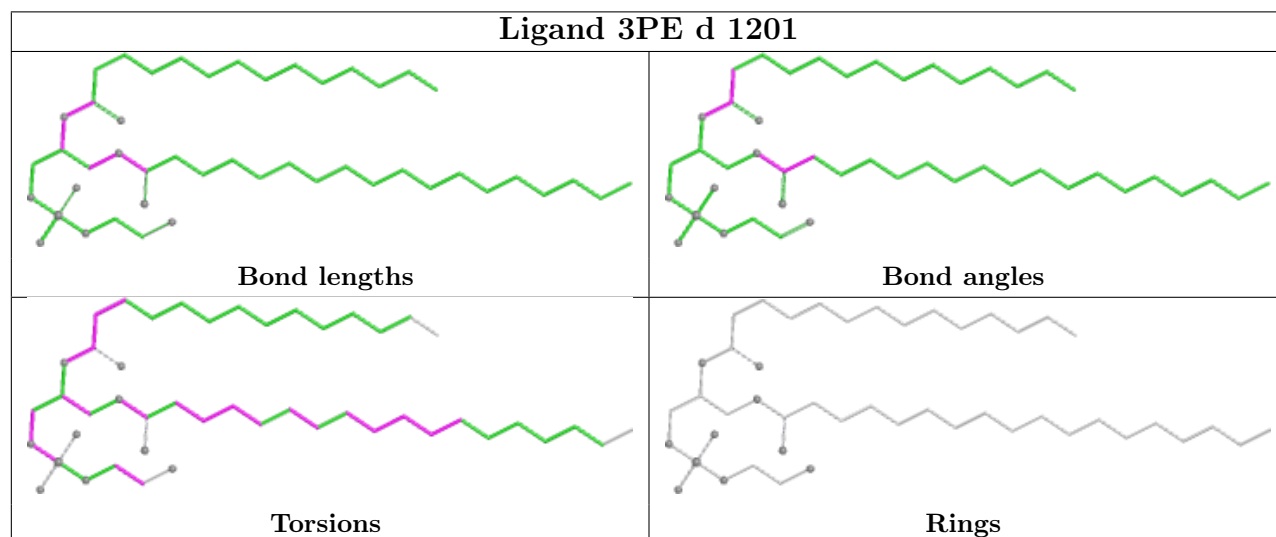
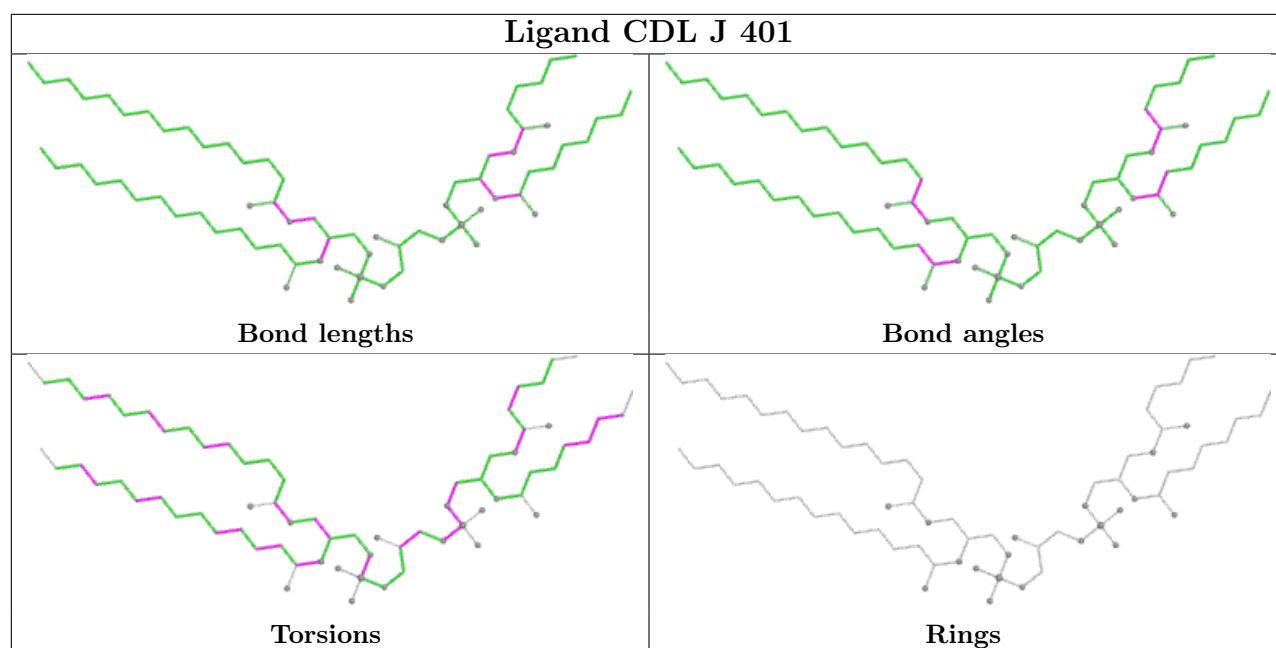


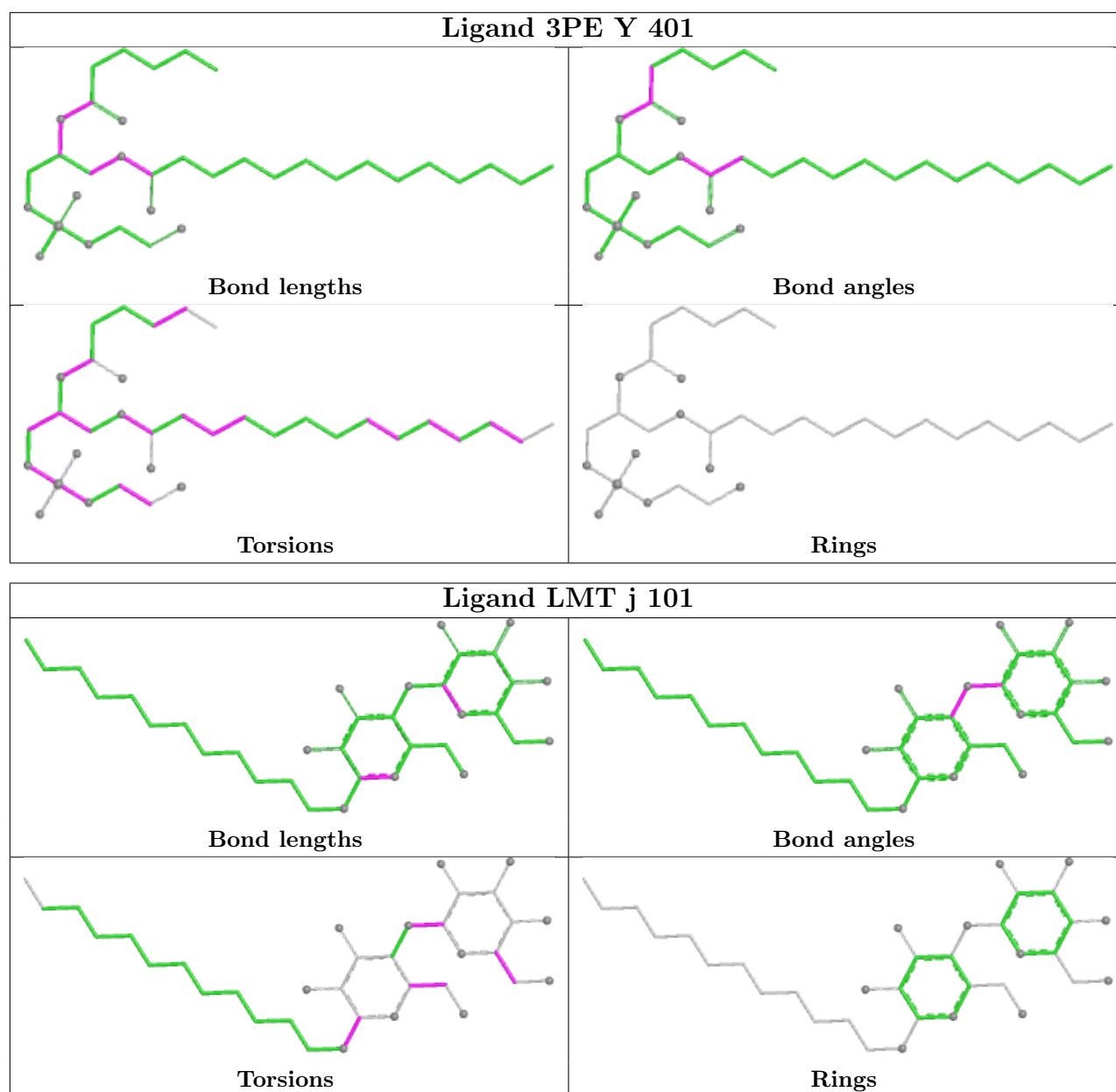












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

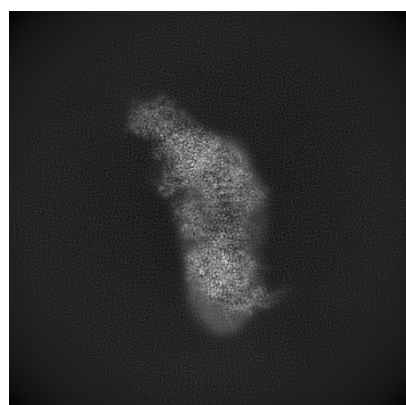
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14282. These allow visual inspection of the internal detail of the map and identification of artifacts.

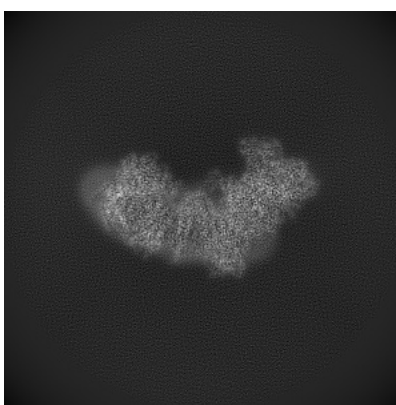
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

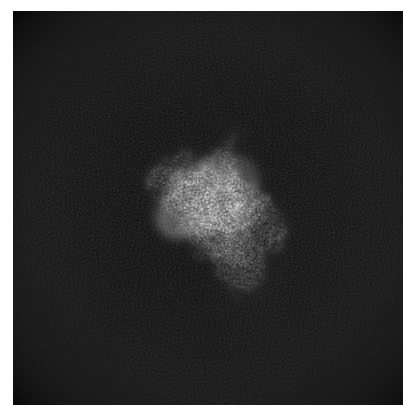
6.1.1 Primary map



X



Y

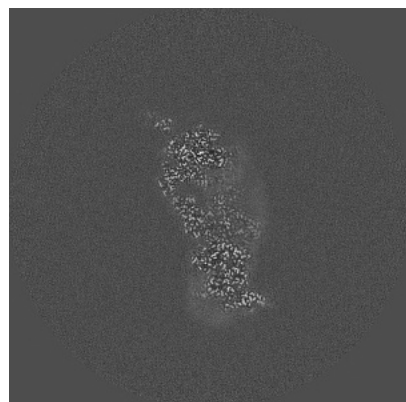


Z

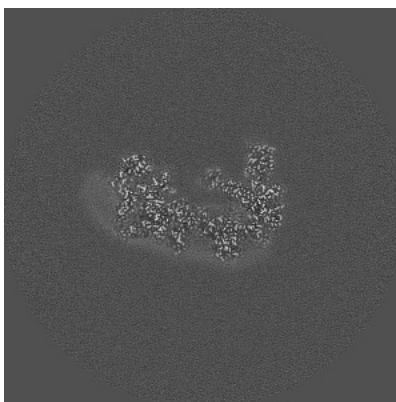
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

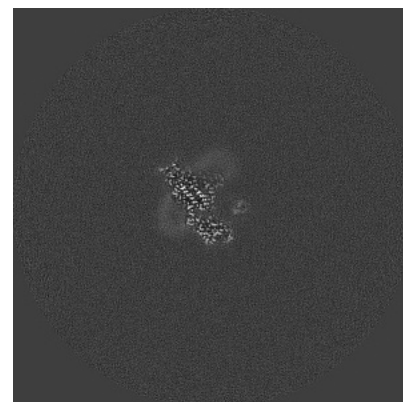
6.2.1 Primary map



X Index: 330



Y Index: 330

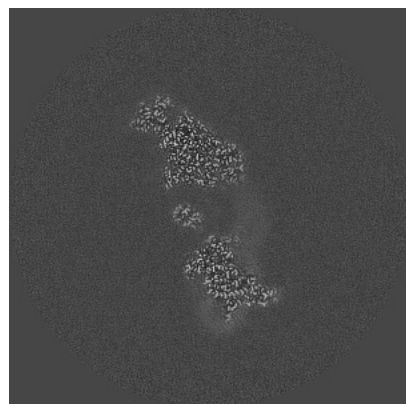


Z Index: 330

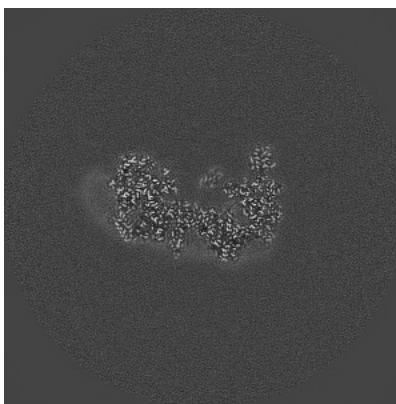
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

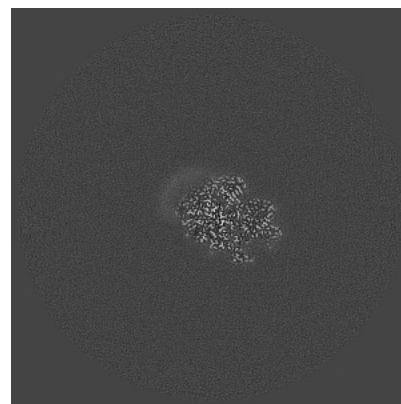
6.3.1 Primary map



X Index: 356



Y Index: 336

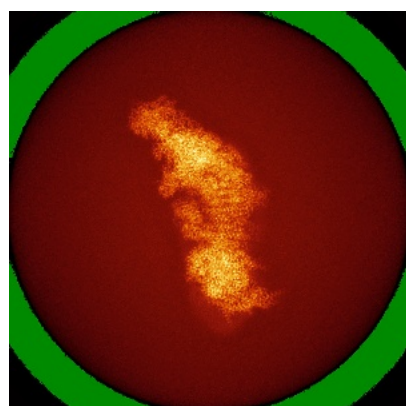


Z Index: 422

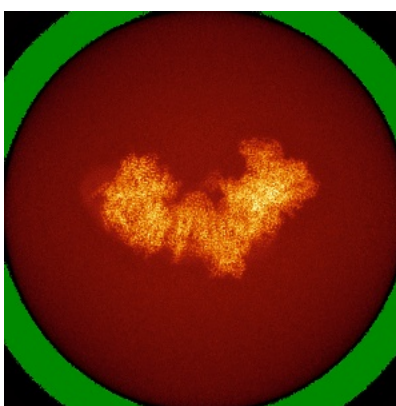
The images above show the largest variance slices of the map in three orthogonal directions.

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

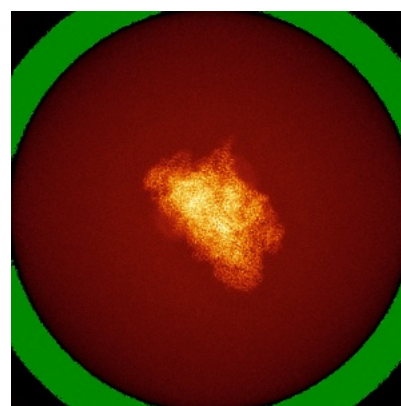
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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

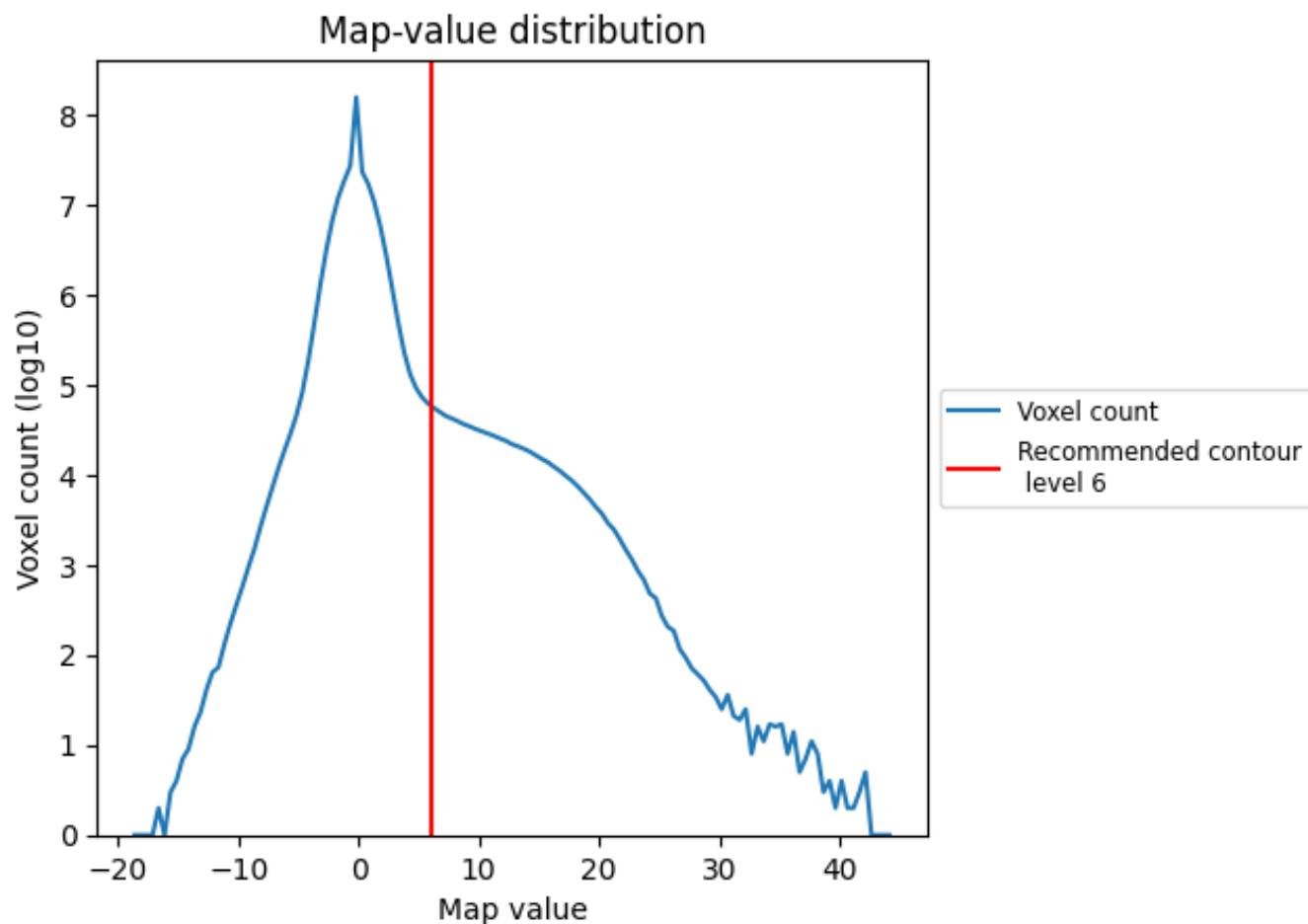
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

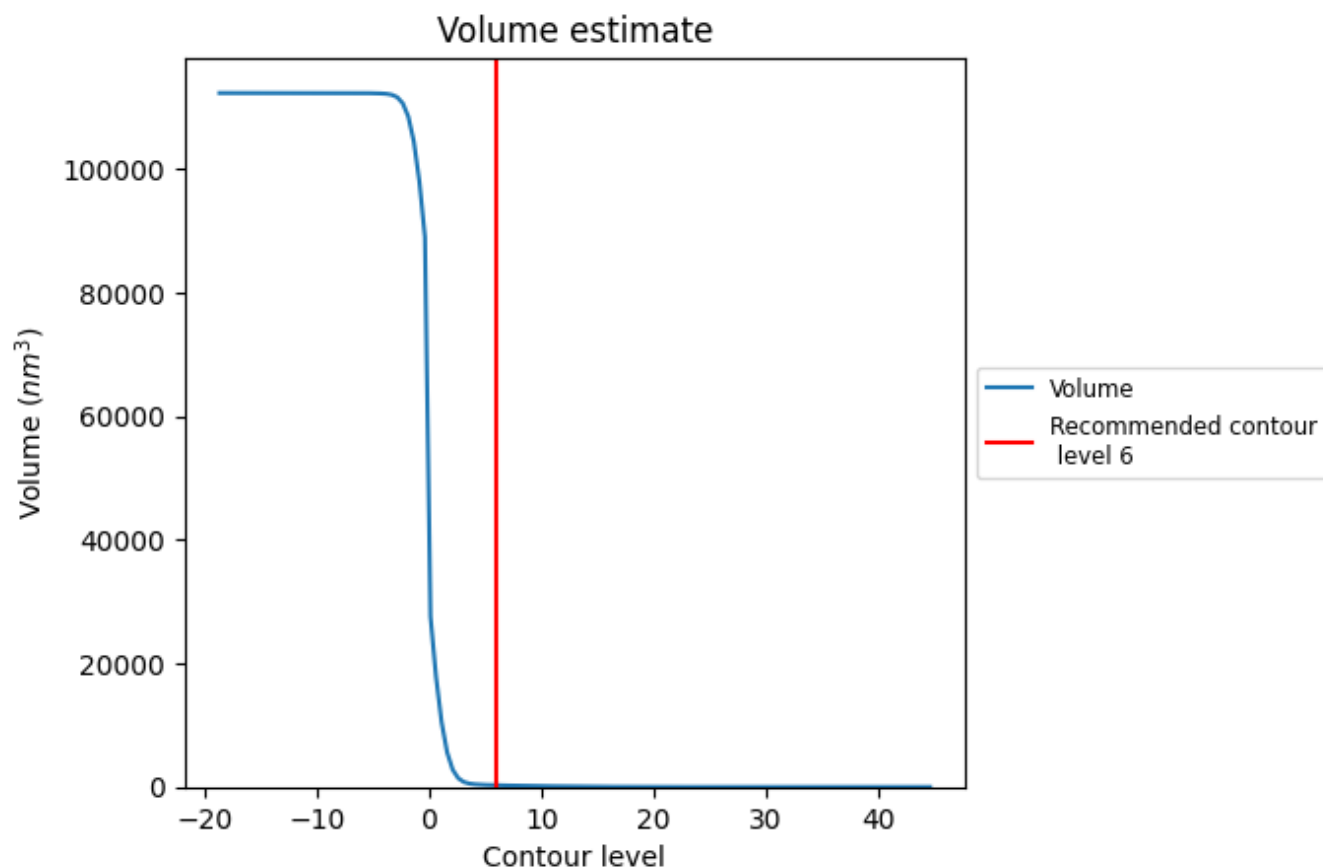
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

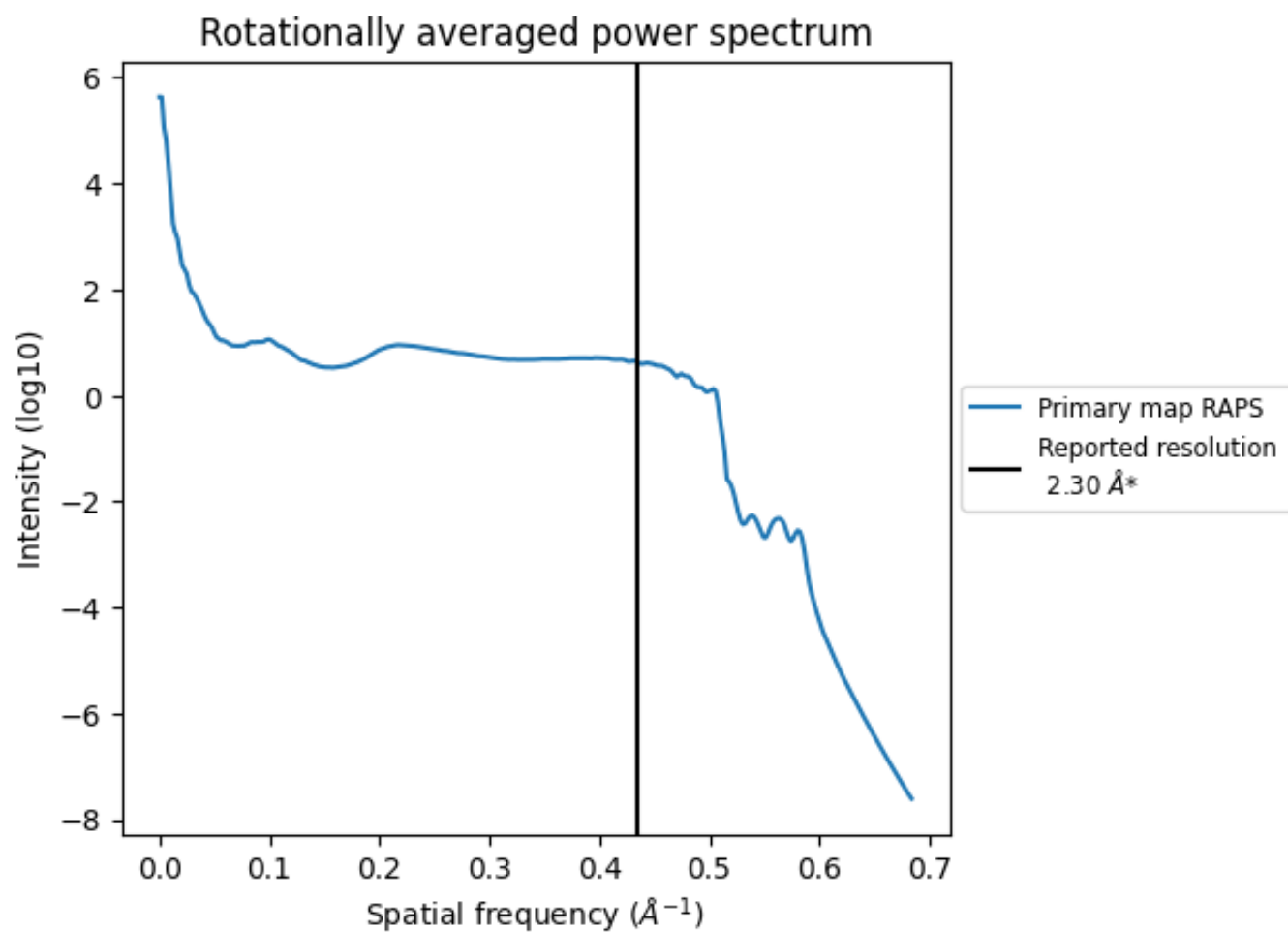
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm^3 ; this corresponds to an approximate mass of 251 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

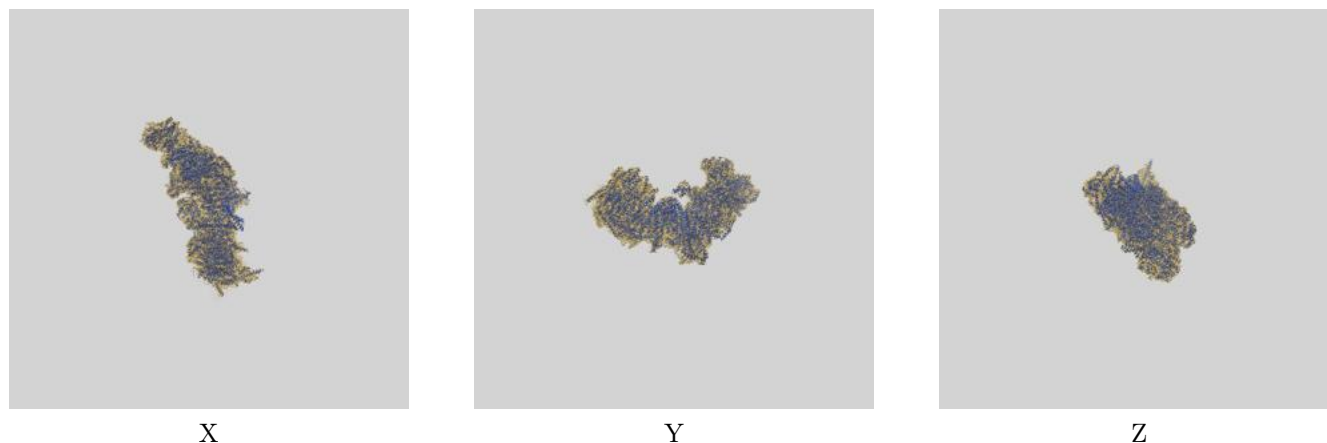
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

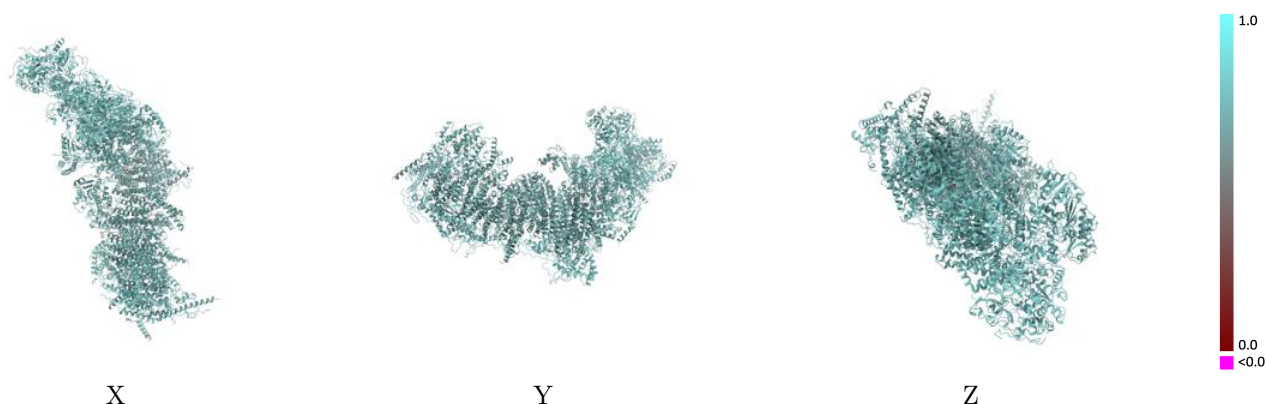
This section contains information regarding the fit between EMDB map EMD-14282 and PDB model 7R47. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



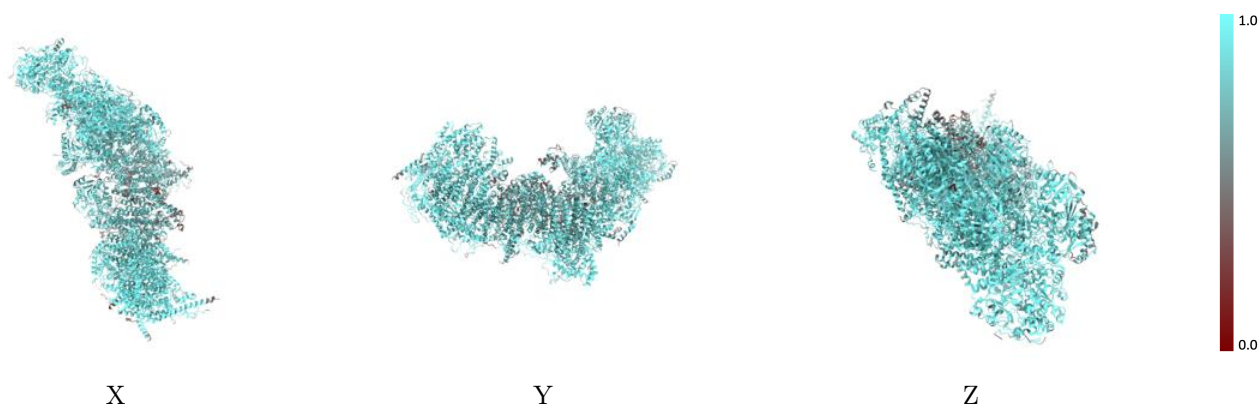
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



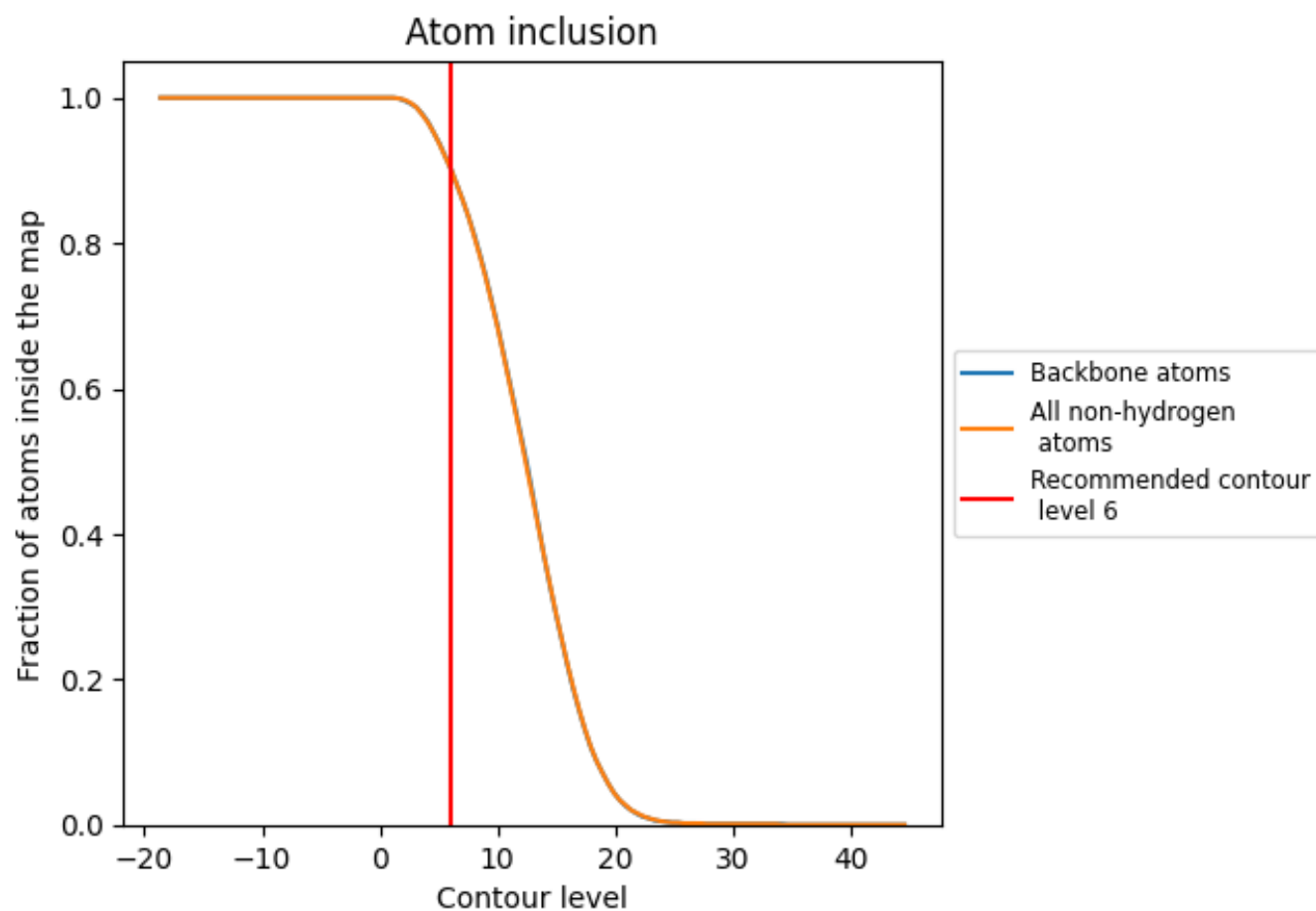
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9040	 0.7150
A	 0.8270	 0.6910
B	 0.9330	 0.7420
C	 0.9720	 0.7530
D	 0.9470	 0.7490
E	 0.9050	 0.7110
F	 0.9460	 0.7250
G	 0.9280	 0.7310
H	 0.9430	 0.7240
I	 0.9740	 0.7570
J	 0.8040	 0.7000
K	 0.9500	 0.7330
L	 0.9360	 0.7100
M	 0.9740	 0.7320
N	 0.9550	 0.7300
O	 0.8800	 0.6950
P	 0.8880	 0.7150
Q	 0.9210	 0.7410
R	 0.9170	 0.7370
S	 0.8460	 0.6980
T	 0.6290	 0.6360
U	 0.9480	 0.7010
V	 0.8770	 0.7210
W	 0.8810	 0.7190
X	 0.8750	 0.7000
Y	 0.5920	 0.6590
Z	 0.8820	 0.7070
a	 0.9580	 0.7170
b	 0.8510	 0.6830
c	 0.8380	 0.6710
d	 0.8360	 0.6990
e	 0.8270	 0.6890
f	 0.7820	 0.6640
g	 0.9000	 0.7040
h	 0.9130	 0.7070



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Chain	Atom inclusion	Q-score
i	 0.8800	 0.6800
j	 0.8630	 0.6720
k	 0.8920	 0.6710
l	 0.9250	 0.6990
m	 0.8660	 0.6960
n	 0.9320	 0.7060
o	 0.9000	 0.6790
p	 0.9270	 0.7040
q	 0.8590	 0.7210
r	 0.9190	 0.7340
s	 0.8870	 0.7110