



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:24 PM UTC

PDB ID : 7R46 / pdb_00007r46
EMDB ID : EMD-14277
Title : Bovine complex I in the presence of IM1761092, deactive class ii (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

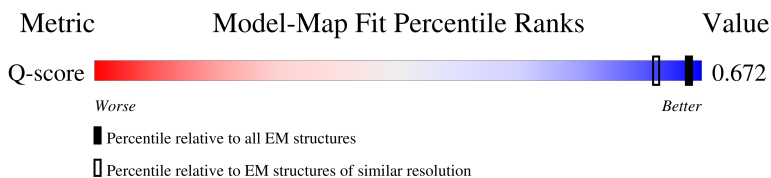
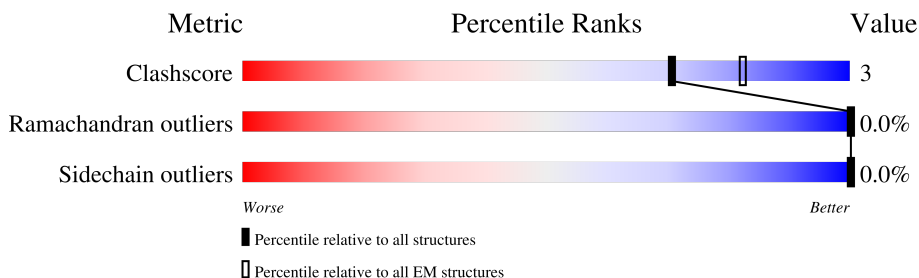
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	216	
3	C	266	
4	D	463	

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

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

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 67614 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	101	Total	C	N	O	S	0	0
			814	555	118	136	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	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	421	Total	C	N	O	S	0	0
			3395	2168	586	616	25		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3310	2085	591	614	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	312	Total	C	N	O	S	0	0
			2462	1651	378	410	23		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			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	289	Total	C	N	O	S	0	0
			2298	1469	415	409	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	82	Total	C	N	O	S	0	0
			663	416	124	121	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	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	97	Total	C	N	O	S	0	0
			813	523	133	153	4		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	N	O		0	0
			1050	672	186	192			

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

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

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

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

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

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

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

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

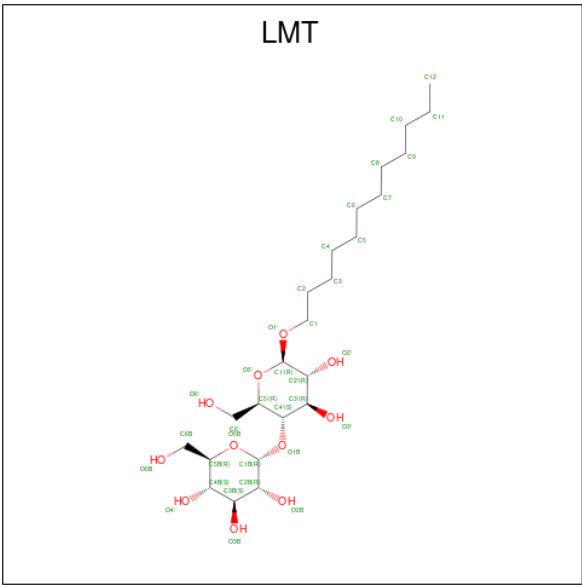
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



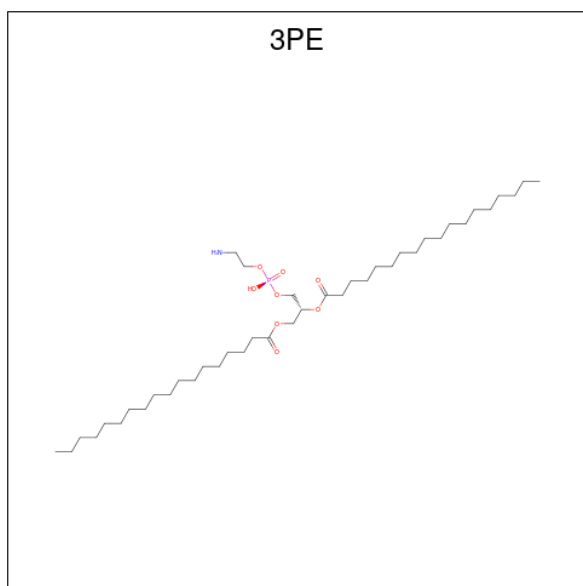
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	N	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
45	h	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: $C_{41}H_{82}NO_8P$).



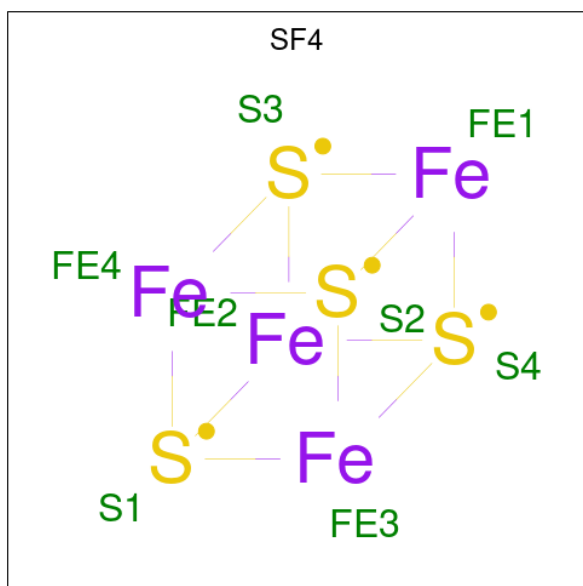
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	H	1	Total	C	N	O	P	0
			24	14	1	8	1	
46	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	I	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	N	1	Total	C	N	O	P	0
			43	33	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
			46	36	1	8	1	
46	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	Z	1	Total	C	N	O	P	0
			25	15	1	8	1	
46	d	1	Total	C	N	O	P	0
			38	28	1	8	1	

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



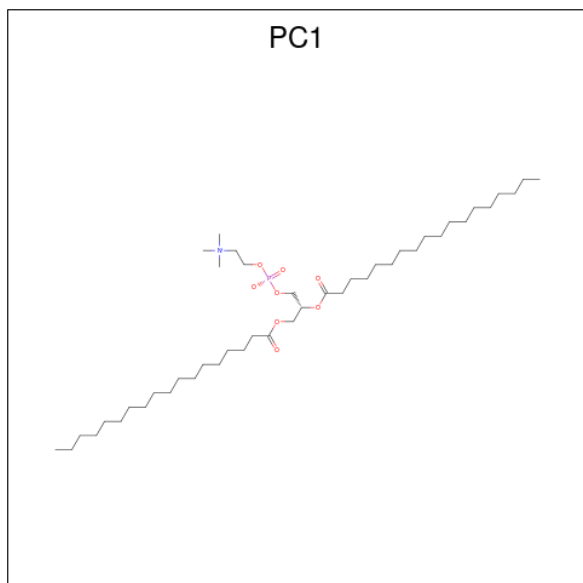
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	

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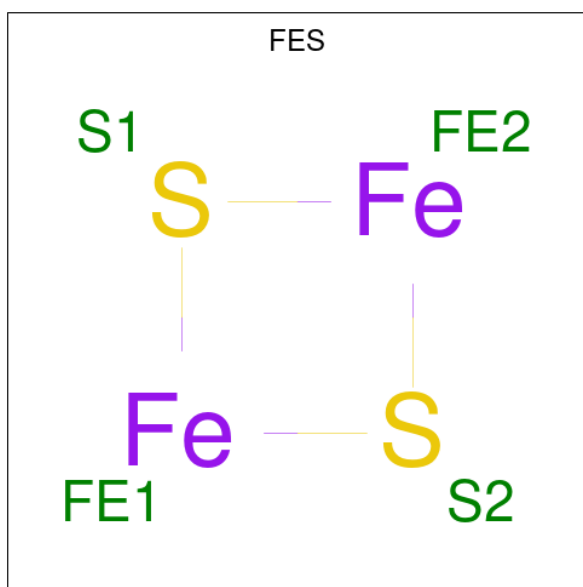
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



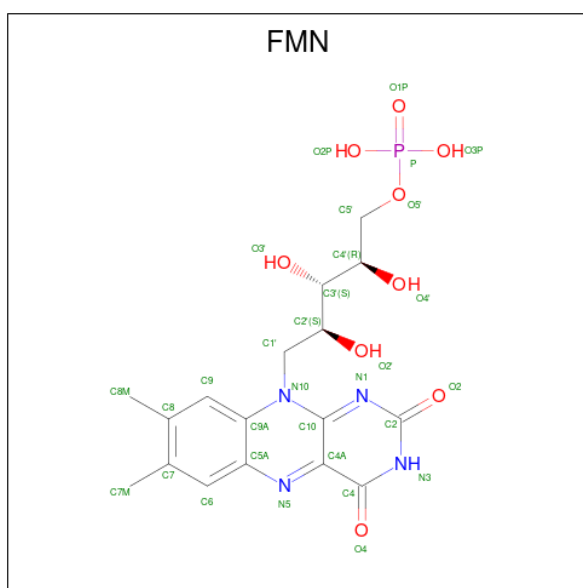
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	g	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



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

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

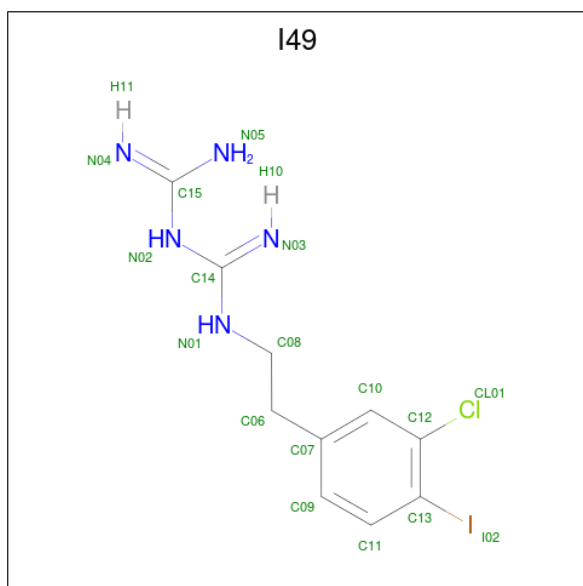


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

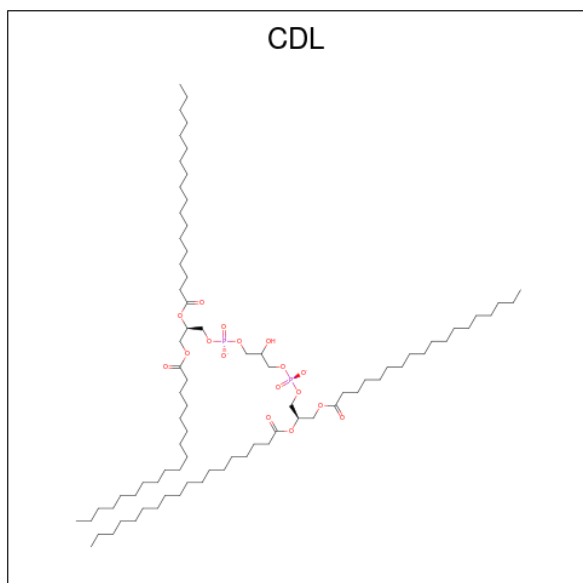
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

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



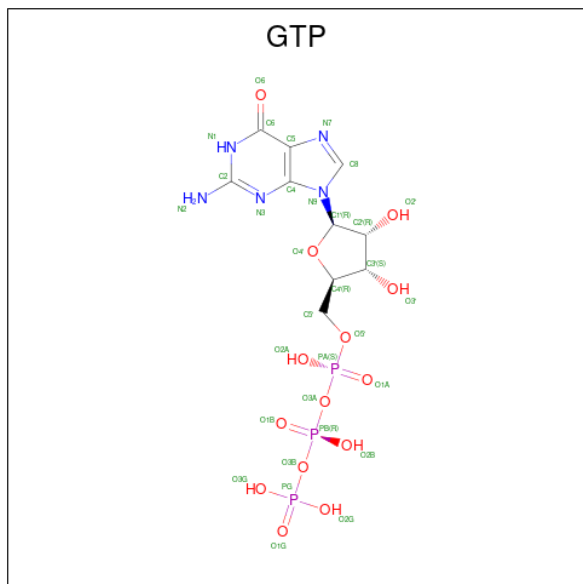
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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



Mol	Chain	Residues	Atoms				AltConf
53	K	1	Total	C	O	P	0
			50	35	13	2	
53	L	1	Total	C	O	P	0
			64	45	17	2	
53	X	1	Total	C	O	P	0
			72	53	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			67	48	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

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

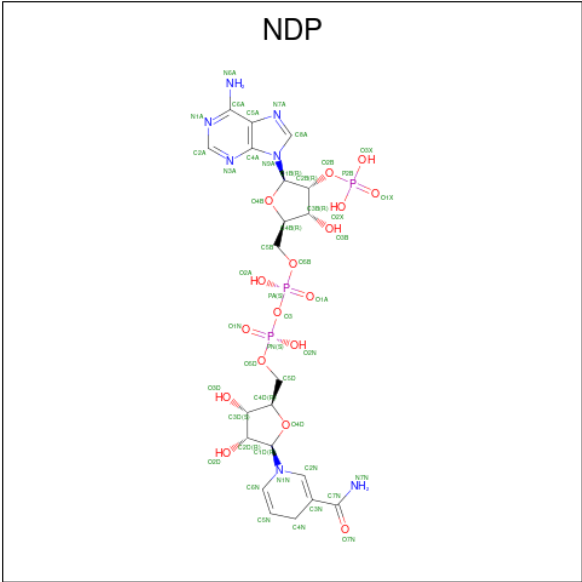


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

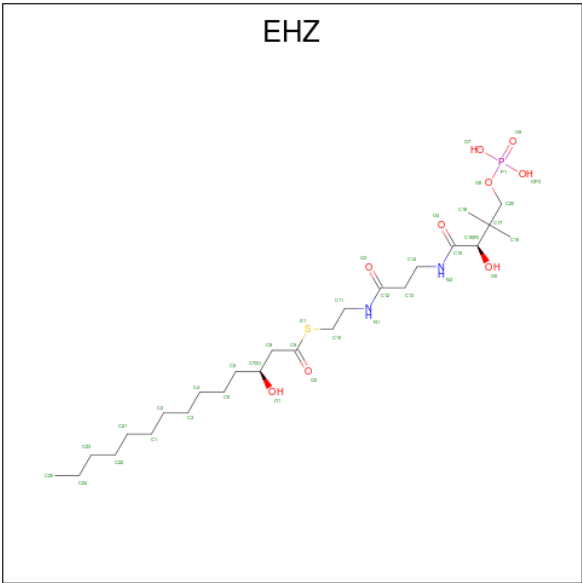


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

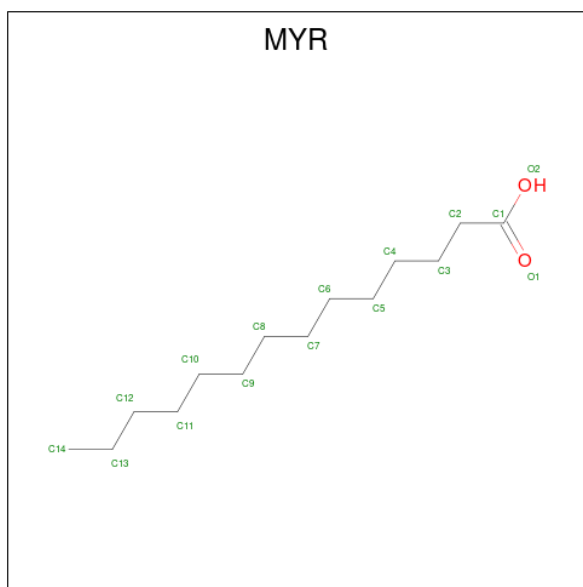
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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: C₂₅H₄₉N₂O₉PS).



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

- Molecule 59 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	4	Total	O	
			4	4	0
60	B	42	Total	O	
			42	42	0
60	C	61	Total	O	
			61	61	0
60	D	96	Total	O	
			96	96	0
60	E	11	Total	O	
			11	11	0
60	F	44	Total	O	
			44	44	0
60	G	139	Total	O	
			139	139	0

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Mol	Chain	Residues	Atoms		AltConf
60	H	30	Total 30	O 30	0
60	I	76	Total 76	O 76	0
60	J	3	Total 3	O 3	0
60	K	2	Total 2	O 2	0
60	L	25	Total 25	O 25	0
60	M	26	Total 26	O 26	0
60	N	17	Total 17	O 17	0
60	O	5	Total 5	O 5	0
60	P	25	Total 25	O 25	0
60	Q	51	Total 51	O 51	0
60	R	18	Total 18	O 18	0
60	U	2	Total 2	O 2	0
60	V	10	Total 10	O 10	0
60	W	3	Total 3	O 3	0
60	X	10	Total 10	O 10	0
60	Y	1	Total 1	O 1	0
60	Z	11	Total 11	O 11	0
60	a	9	Total 9	O 9	0
60	b	3	Total 3	O 3	0
60	d	7	Total 7	O 7	0
60	e	8	Total 8	O 8	0

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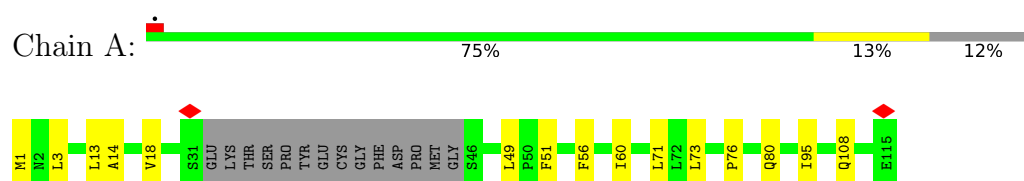
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	f	3	Total 3	O 3	0
60	g	7	Total 7	O 7	0
60	h	8	Total 8	O 8	0
60	i	4	Total 4	O 4	0
60	j	2	Total 2	O 2	0
60	k	3	Total 3	O 3	0
60	l	13	Total 13	O 13	0
60	m	7	Total 7	O 7	0
60	n	14	Total 14	O 14	0
60	o	7	Total 7	O 7	0
60	p	14	Total 14	O 14	0
60	q	21	Total 21	O 21	0
60	r	14	Total 14	O 14	0
60	s	3	Total 3	O 3	0

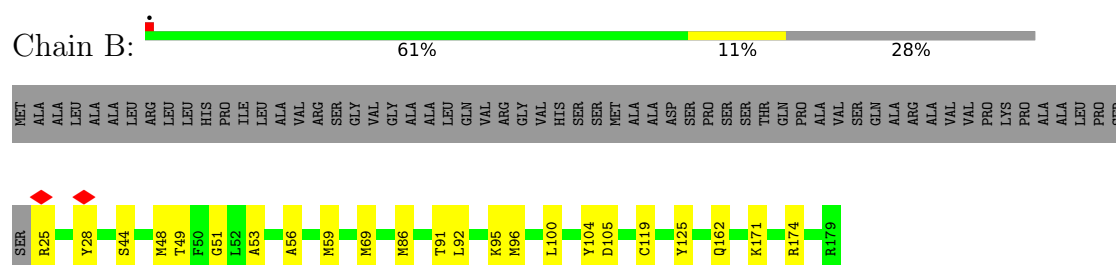
3 Residue-property plots [i](#)

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

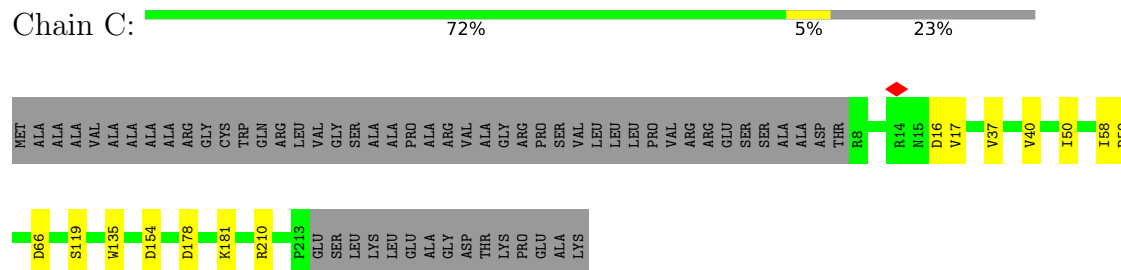
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



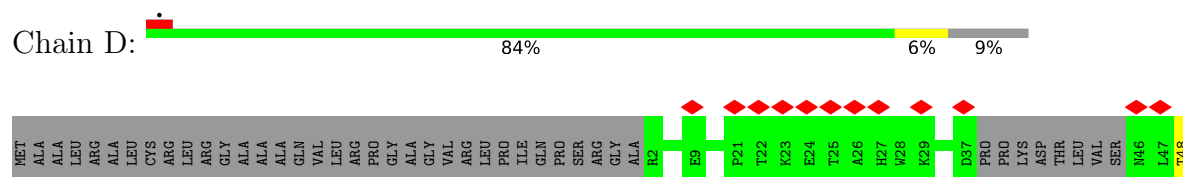
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

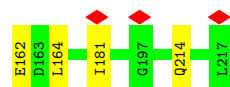
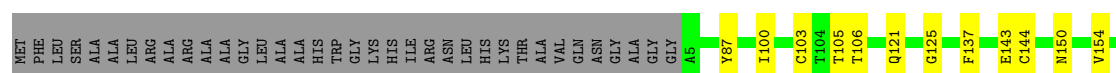
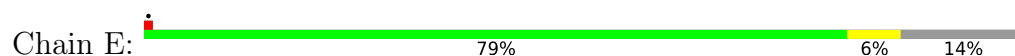


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

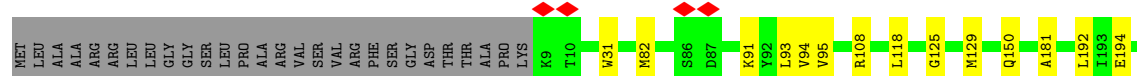
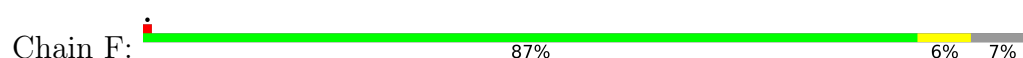




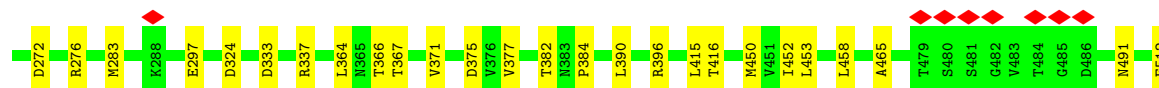
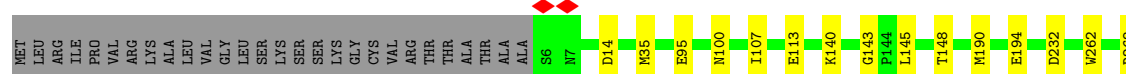
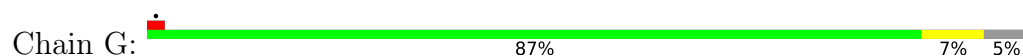
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



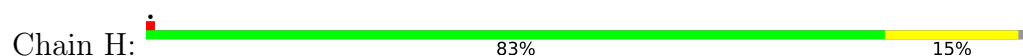
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

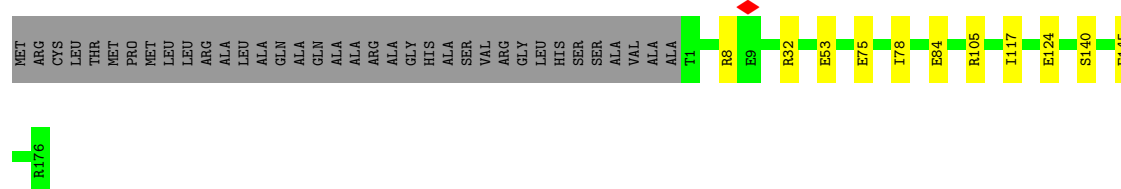


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



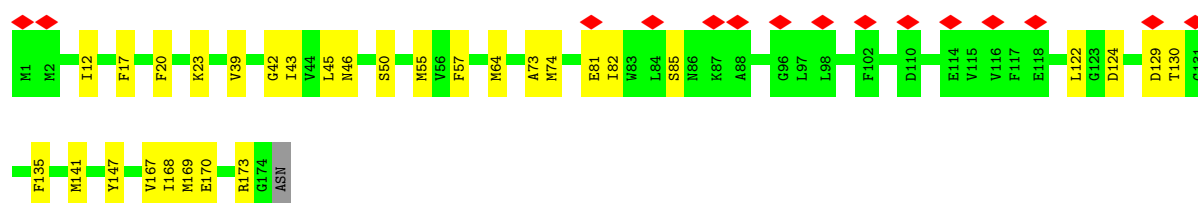
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  78% 5% 17%

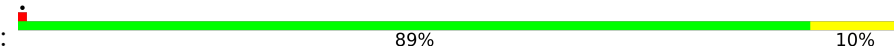


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  9% 82% 17%



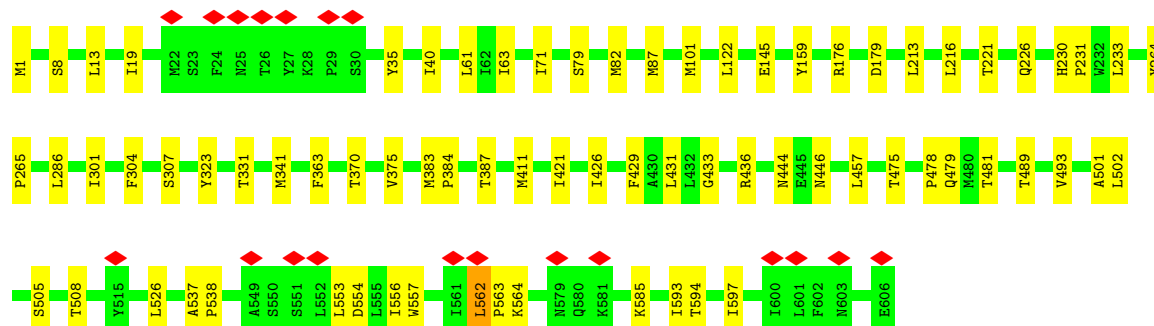
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  89% 10%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

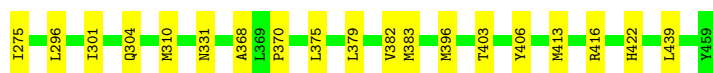
Chain L:  88% 12%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  89% 11%





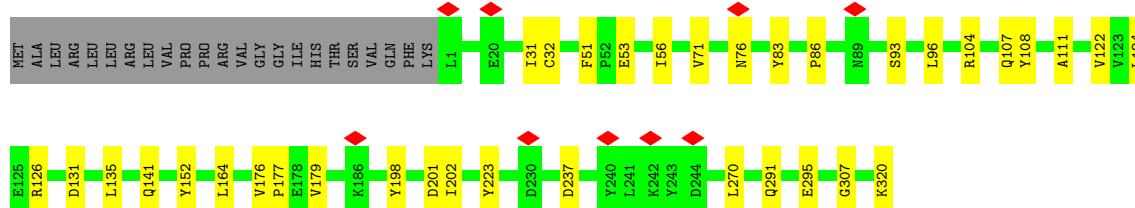
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 92% 8%



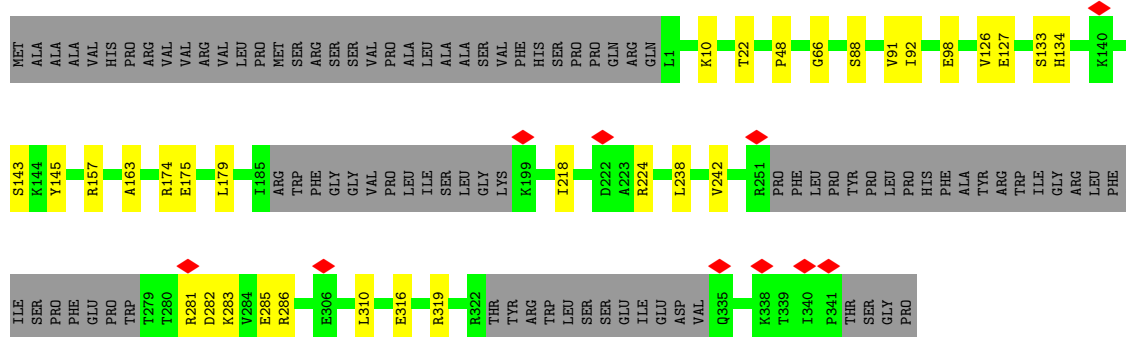
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 83% 10% 7%



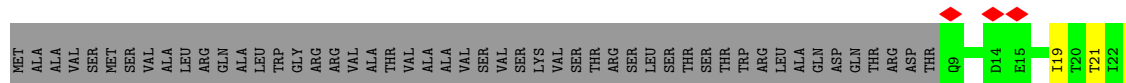
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 68% 8% 24%

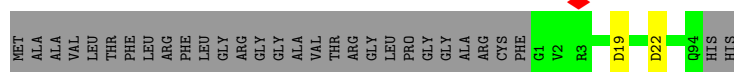
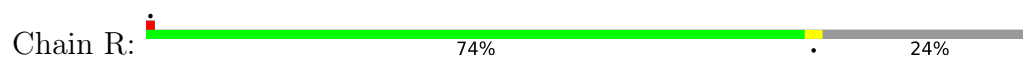


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

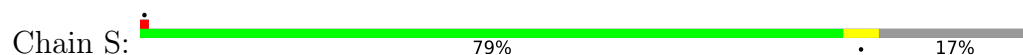
Chain Q: 67% 29%



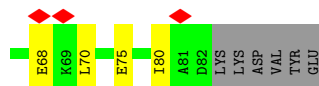
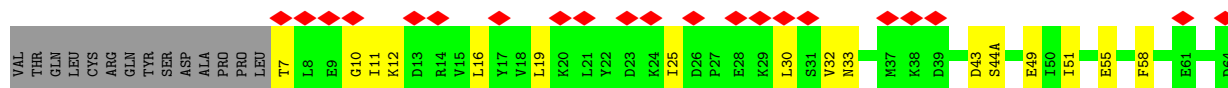
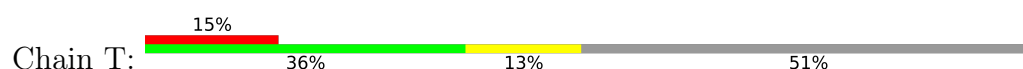
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



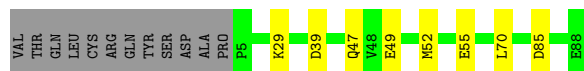
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



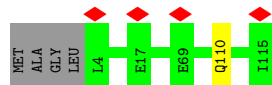
- Molecule 20: Acyl carrier protein, mitochondrial



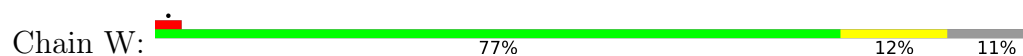
- Molecule 20: Acyl carrier protein, mitochondrial

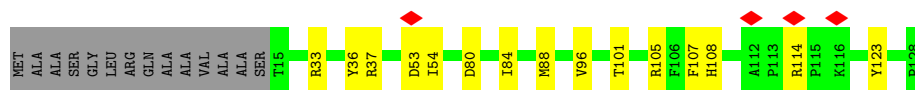


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



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

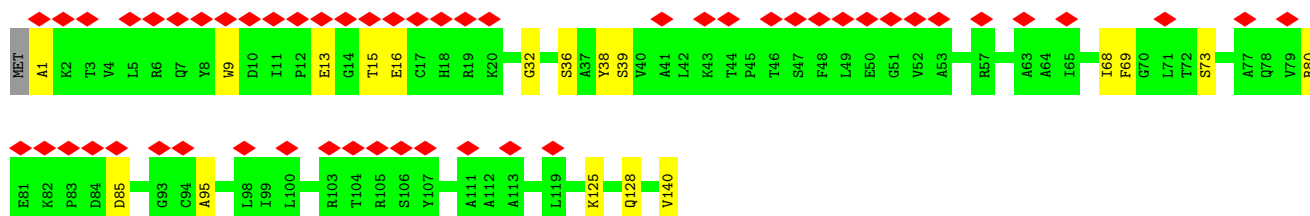
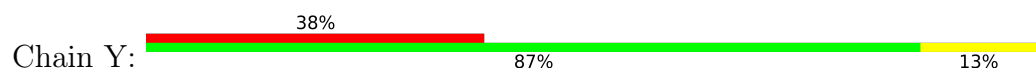




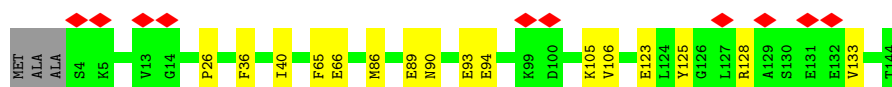
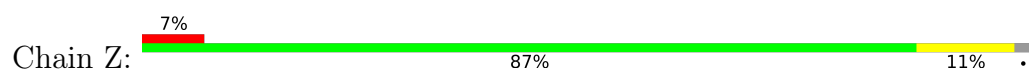
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



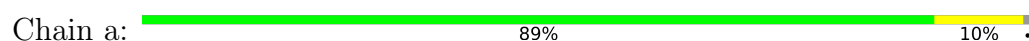
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



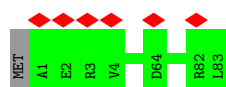
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

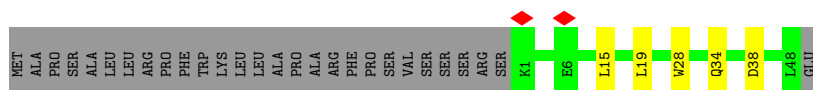


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

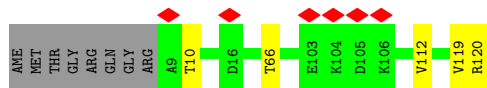
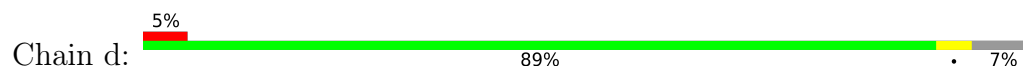


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

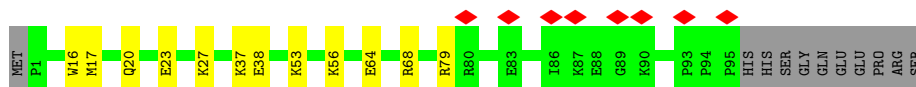
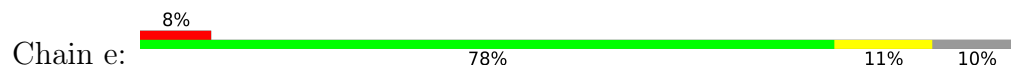




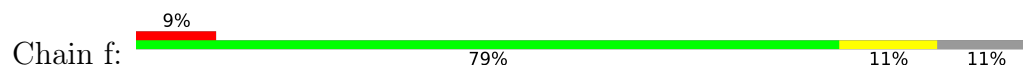
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



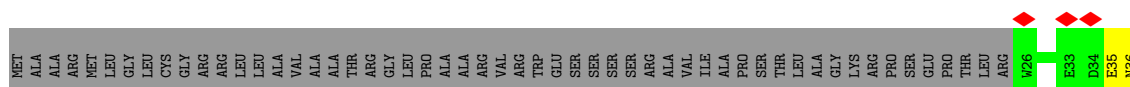
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



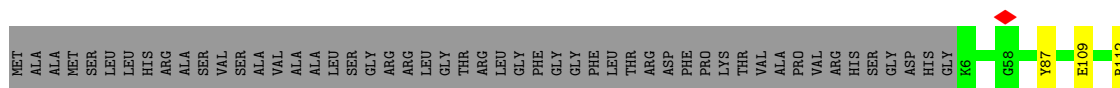
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



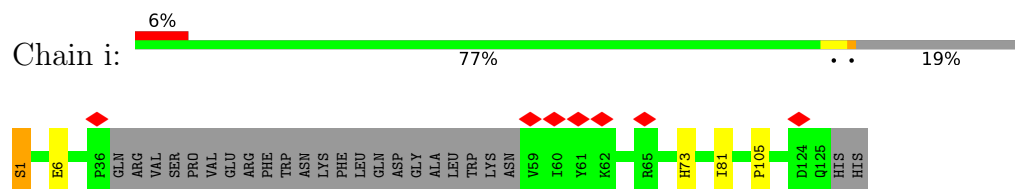
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



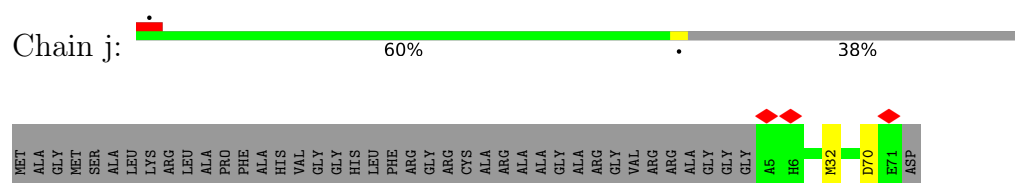
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



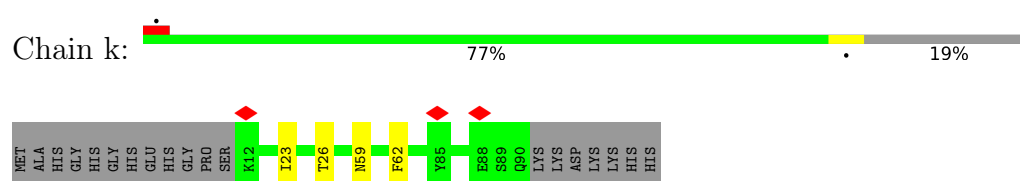
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



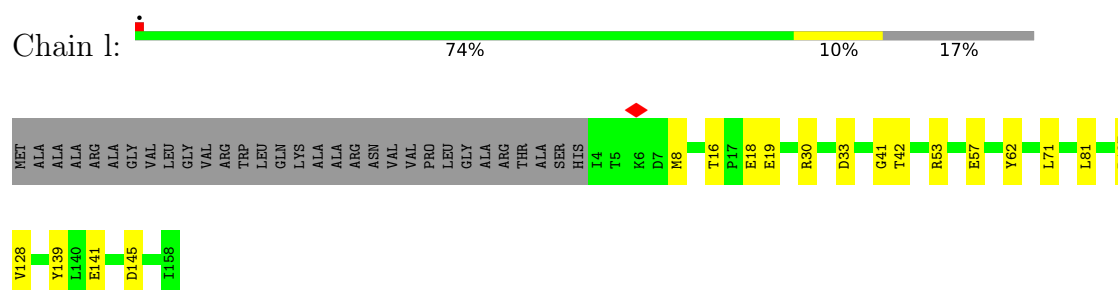
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



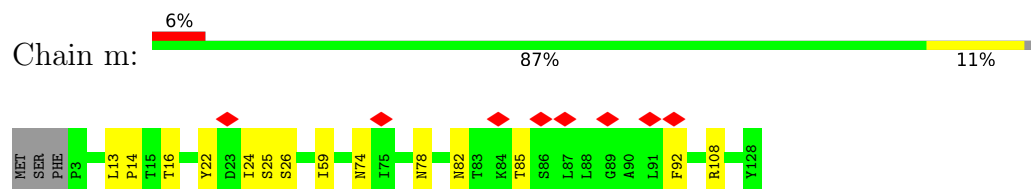
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



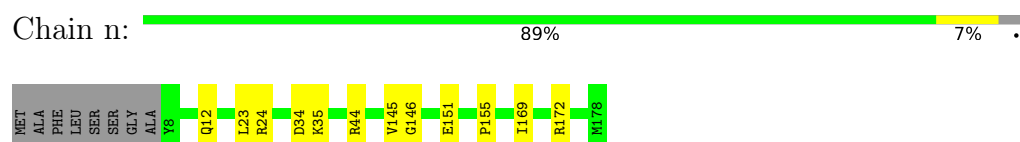
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

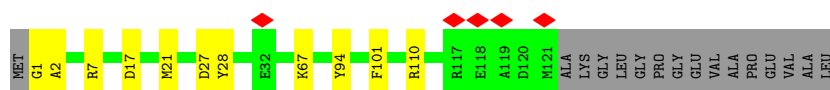


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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

Chain o:  80% 8% 12%

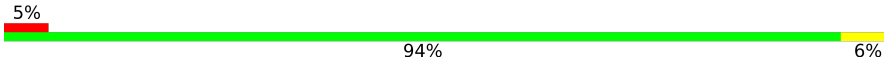


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  88% 9%



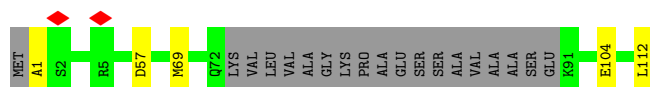
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  5% 94% 6%



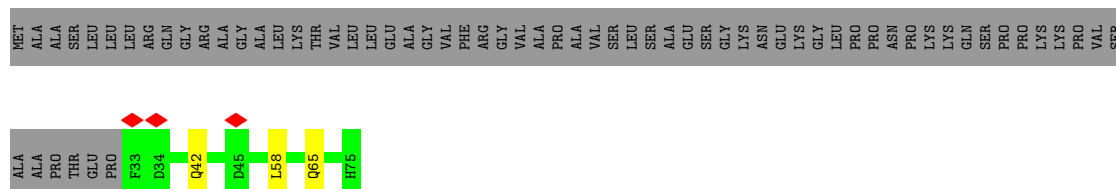
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  79% 17%



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

Chain s:  37% 61%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35448	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	32.083	Depositor
Minimum map value	-12.979	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EHZ, FES, MYR, AYA, LMT, SF4, NDP, GTP, ZN, I49, 2MR, PC1, K, FMN, 3PE, CDL, FME, SAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/824	0.29	0/1128
2	B	0.30	0/1272	0.40	0/1720
3	C	0.25	0/1765	0.31	0/2403
4	D	0.25	0/3470	0.30	0/4699
5	E	0.22	0/1695	0.29	0/2307
6	F	0.23	0/3384	0.30	0/4573
7	G	0.24	0/5367	0.32	0/7274
8	H	0.27	0/2522	0.35	0/3445
9	I	0.27	0/1445	0.36	0/1956
10	J	0.22	0/1362	0.32	0/1848
11	K	0.26	0/739	0.34	0/1000
12	L	0.26	0/4900	0.30	0/6667
13	M	0.27	0/3738	0.31	0/5097
14	N	0.25	0/2792	0.29	0/3800
15	O	0.23	0/2651	0.29	0/3587
16	P	0.22	0/2348	0.31	0/3172
17	Q	0.25	0/1039	0.30	0/1404
18	R	0.24	0/731	0.28	0/984
19	S	0.21	0/674	0.30	0/908
20	T	0.19	0/621	0.29	0/837
20	U	0.29	0/692	0.30	0/932
21	V	0.21	0/931	0.25	0/1261
22	W	0.22	0/995	0.30	0/1337
23	X	0.24	0/1439	0.31	0/1942
24	Y	0.16	0/1042	0.28	0/1414
25	Z	0.23	0/1181	0.27	0/1592
26	a	0.25	0/576	0.30	0/775
27	b	0.23	0/672	0.30	0/923
28	c	0.19	0/418	0.25	0/567
29	d	0.24	0/964	0.29	0/1305
30	e	0.23	0/818	0.34	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.22	0/457	0.32	0/616
32	g	0.24	0/839	0.29	0/1140
33	h	0.25	0/1188	0.29	0/1607
34	i	0.28	0/904	0.32	0/1230
35	j	0.27	0/607	0.32	0/833
36	k	0.24	0/657	0.28	0/887
37	l	0.27	0/1358	0.29	0/1858
38	m	0.25	0/1076	0.30	0/1455
39	n	0.28	0/1540	0.32	0/2085
40	o	0.31	0/1068	0.36	0/1430
41	p	0.27	0/1468	0.30	0/1979
42	q	0.21	0/1250	0.30	0/1698
43	r	0.23	0/780	0.31	0/1056
44	s	0.20	0/375	0.25	0/507
All	All	0.25	0/66634	0.31	0/90331

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
34	i	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	i	1	SAC	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	814	0	858	11	0
2	B	1241	0	1251	17	0
3	C	1714	0	1668	11	0
4	D	3395	0	3332	18	0
5	E	1655	0	1661	12	0
6	F	3310	0	3261	19	0
7	G	5279	0	5301	37	0
8	H	2462	0	2575	35	0
9	I	1414	0	1370	11	0
10	J	1337	0	1346	27	0
11	K	739	0	780	14	0
12	L	4784	0	4937	51	0
13	M	3654	0	3852	37	0
14	N	2733	0	2912	21	0
15	O	2589	0	2566	21	0
16	P	2298	0	2330	19	0
17	Q	1016	0	1014	5	0
18	R	720	0	700	1	0
19	S	663	0	672	2	0
20	T	612	0	604	14	0
20	U	681	0	677	7	0
21	V	911	0	950	1	0
22	W	971	0	989	13	0
23	X	1402	0	1383	8	0
24	Y	1030	0	1041	11	0
25	Z	1152	0	1151	12	0
26	a	561	0	564	5	0
27	b	651	0	662	0	0
28	c	405	0	409	3	0
29	d	934	0	919	6	0
30	e	799	0	807	10	0
31	f	444	0	444	4	0
32	g	813	0	759	10	0
33	h	1154	0	1168	2	0
34	i	884	0	905	5	0
35	j	580	0	519	2	0
36	k	638	0	621	3	0
37	l	1304	0	1203	14	0
38	m	1050	0	1051	10	0
39	n	1487	0	1433	9	0
40	o	1043	0	1011	7	0
41	p	1435	0	1411	11	0
42	q	1209	0	1182	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	767	0	776	5	0
44	s	364	0	336	3	0
45	A	35	0	46	1	0
45	L	35	0	46	2	0
45	M	70	0	92	3	0
45	N	70	0	92	0	0
45	Y	35	0	46	1	0
45	h	70	0	92	1	0
45	j	35	0	46	0	0
45	l	35	0	46	0	0
46	A	40	0	54	0	0
46	B	36	0	49	0	0
46	H	24	0	24	2	0
46	I	82	0	118	0	0
46	L	123	0	174	1	0
46	N	84	0	116	2	0
46	Y	81	0	113	2	0
46	Z	25	0	24	1	0
46	d	38	0	53	0	0
47	B	8	0	0	0	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	B	35	0	44	0	0
48	g	49	0	75	2	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	H	17	0	0	1	0
53	K	50	0	61	2	0
53	L	64	0	72	0	0
53	X	72	0	88	2	0
53	d	65	0	77	0	0
53	h	67	0	81	3	0
53	q	61	0	66	0	0
54	O	32	0	12	1	0
55	O	1	0	0	0	0
56	P	48	0	26	1	0
57	R	1	0	0	0	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	o	15	0	27	0	0
60	A	4	0	0	0	0
60	B	42	0	0	0	0
60	C	61	0	0	1	0
60	D	96	0	0	2	0
60	E	11	0	0	0	0
60	F	44	0	0	1	0
60	G	139	0	0	5	0
60	H	30	0	0	1	0
60	I	76	0	0	2	0
60	J	3	0	0	0	0
60	K	2	0	0	0	0
60	L	25	0	0	1	0
60	M	26	0	0	3	0
60	N	17	0	0	2	0
60	O	5	0	0	1	0
60	P	25	0	0	1	0
60	Q	51	0	0	2	0
60	R	18	0	0	0	0
60	U	2	0	0	1	0
60	V	10	0	0	1	0
60	W	3	0	0	1	0
60	X	10	0	0	2	0
60	Y	1	0	0	0	0
60	Z	11	0	0	0	0
60	a	9	0	0	0	0
60	b	3	0	0	0	0
60	d	7	0	0	0	0
60	e	8	0	0	0	0
60	f	3	0	0	0	0
60	g	7	0	0	2	0
60	h	8	0	0	0	0
60	i	4	0	0	0	0
60	j	2	0	0	0	0
60	k	3	0	0	0	0
60	l	13	0	0	1	0
60	m	7	0	0	0	0
60	n	14	0	0	0	0
60	o	7	0	0	0	0
60	p	14	0	0	0	0
60	q	21	0	0	0	0
60	r	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	s	3	0	0	1	0
All	All	67614	0	67240	467	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 (467) 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)
7:G:232:ASP:OD1	60:G:901:HOH:O	1.96	0.83
15:O:83:TYR:OH	54:O:401:GTP:O3'	1.97	0.81
45:h:1003:LMT:H6'	45:h:1003:LMT:H6B	0.82	0.81
7:G:366:THR:O	7:G:367:THR:OG1	1.97	0.81
16:P:48:PRO:O	60:P:601:HOH:O	1.98	0.81
38:m:16:THR:O	38:m:22:TYR:OH	1.99	0.80
42:q:78:ASP:OD1	42:q:80:SER:OG	2.00	0.78
24:Y:80:ARG:NH2	24:Y:85:ASP:OD1	2.16	0.78
23:X:87:CYS:SG	23:X:102:GLN:NE2	2.57	0.78
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.66	0.77
36:k:23:ILE:O	36:k:26:THR:OG1	2.04	0.76
17:Q:21:THR:OG1	60:Q:201:HOH:O	2.03	0.75
14:N:337:LEU:HD23	53:X:1701:CDL:H601	1.67	0.75
15:O:307:GLY:O	15:O:320:LYS:NZ	2.11	0.74
4:D:219:SER:OG	60:D:501:HOH:O	2.04	0.74
9:I:32:ARG:NH2	25:Z:26:PRO:O	2.20	0.74
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.69	0.73
13:M:87:GLU:OE2	13:M:91:ARG:NE	2.22	0.73
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.22	0.72
7:G:113:GLU:OE2	60:G:902:HOH:O	2.05	0.72
16:P:174:ARG:NH1	16:P:316:GLU:OE2	2.22	0.72
2:B:44:SER:OG	8:H:51:ASP:OD1	2.06	0.72
13:M:198:ALA:O	60:M:901:HOH:O	2.07	0.72
23:X:102:GLN:O	60:X:1801:HOH:O	2.07	0.71
10:J:141:MET:HA	10:J:141:MET:HE2	1.72	0.71
31:f:53:GLU:N	31:f:53:GLU:OE1	2.23	0.70
1:A:71:LEU:O	10:J:147:TYR:OH	2.09	0.70
13:M:208:PRO:O	60:M:902:HOH:O	2.10	0.70
9:I:124:GLU:OE2	60:I:301:HOH:O	2.09	0.70
4:D:303:GLU:OE1	60:D:502:HOH:O	2.09	0.70
17:Q:36:ARG:NE	17:Q:106:GLU:OE1	2.24	0.69
7:G:95:GLU:OE2	60:G:904:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:ARG:NH1	19:S:87:THR:OG1	2.26	0.69
11:K:59:MET:HE3	14:N:84:TRP:CH2	2.27	0.69
22:W:80:ASP:OD2	60:W:201:HOH:O	2.11	0.68
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.75	0.68
25:Z:89:GLU:OE1	25:Z:128:ARG:NH2	2.26	0.68
14:N:214:THR:HG22	14:N:218:MET:HE2	1.74	0.68
9:I:84:GLU:OE2	60:I:302:HOH:O	2.10	0.68
13:M:413:MET:O	60:M:903:HOH:O	2.10	0.67
39:n:34:ASP:OD1	39:n:35:LYS:N	2.26	0.67
12:L:479:GLN:NE2	12:L:481:THR:O	2.27	0.67
17:Q:44:ASN:ND2	17:Q:44:ASN:O	2.27	0.67
20:T:19:LEU:HB3	20:T:30:LEU:HD11	1.77	0.67
3:C:210:ARG:NH2	7:G:35:MET:SD	2.68	0.67
20:U:85:ASP:OD1	60:U:201:HOH:O	2.13	0.67
10:J:81:GLU:OE2	10:J:85:SER:OG	2.11	0.67
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.77	0.67
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.25	0.67
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.27	0.67
13:M:57:PHE:HB3	13:M:113:MET:HE2	1.75	0.66
44:s:65:GLN:OE1	60:s:101:HOH:O	2.14	0.66
4:D:161:ILE:HD11	4:D:235:TRP:CZ3	2.30	0.66
20:U:29:LYS:NZ	20:U:39:ASP:O	2.28	0.66
5:E:214:GLN:NE2	6:F:235:CYS:O	2.28	0.66
37:l:53:ARG:NH2	37:l:57:GLU:OE1	2.29	0.66
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.28	0.65
7:G:684:MET:HA	7:G:684:MET:HE2	1.78	0.65
3:C:66:ASP:OD2	60:C:301:HOH:O	2.15	0.65
8:H:240:ILE:O	60:H:701:HOH:O	2.15	0.64
12:L:478:PRO:O	60:L:801:HOH:O	2.15	0.64
16:P:10:LYS:O	22:W:114:ARG:NH2	2.30	0.64
13:M:382:VAL:HG22	13:M:396:MET:HE3	1.77	0.64
1:A:56:PHE:HB2	10:J:74:MET:HE1	1.79	0.64
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.30	0.64
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.23	0.64
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.64
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.80	0.64
45:M:802:LMT:O1'	45:M:802:LMT:O6'	2.13	0.64
8:H:111:LEU:HD11	10:J:57:PHE:HD1	1.62	0.63
16:P:143:SER:OG	16:P:282:ASP:OD1	2.07	0.63
8:H:318:THR:HG21	10:J:135:PHE:CE2	2.33	0.63
6:F:367:GLU:OE2	7:G:100:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:MET:HE2	8:H:118:TRP:CD1	2.33	0.63
7:G:194:GLU:N	7:G:194:GLU:OE1	2.31	0.63
22:W:96:VAL:HG12	22:W:96:VAL:O	1.97	0.63
13:M:105:PHE:O	13:M:109:THR:OG1	2.17	0.62
7:G:396:ARG:NH1	7:G:416:THR:O	2.32	0.62
8:H:111:LEU:HD11	10:J:57:PHE:CD1	2.34	0.62
11:K:53:PHE:CE2	11:K:56:ALA:HB2	2.33	0.62
7:G:276:ARG:NH2	7:G:680:ALA:O	2.33	0.62
6:F:373:ASN:ND2	60:F:602:HOH:O	2.32	0.61
11:K:59:MET:HE3	14:N:84:TRP:HH2	1.65	0.61
15:O:53:GLU:OE2	15:O:126:ARG:NH2	2.33	0.61
12:L:8:SER:HB2	12:L:82:MET:HE2	1.83	0.61
15:O:104:ARG:NE	15:O:131:ASP:OD2	2.32	0.61
15:O:51:PHE:HB2	15:O:124:LEU:HD23	1.83	0.61
20:T:7:THR:O	20:T:10:GLY:N	2.33	0.60
8:H:68:ALA:O	8:H:72:ILE:HD12	2.00	0.60
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.34	0.60
20:U:49:GLU:OE1	39:n:44:ARG:NH1	2.31	0.60
3:C:37:VAL:HG12	43:r:69:MET:HE1	1.82	0.60
4:D:48:THR:C	4:D:49:LEU:HD12	2.25	0.60
15:O:56:ILE:HD11	15:O:96:LEU:HD13	1.83	0.60
24:Y:69:PHE:O	24:Y:73:SER:OG	2.05	0.60
30:e:37:LYS:NZ	30:e:38:GLU:OE1	2.34	0.60
7:G:14:ASP:OD2	60:G:905:HOH:O	2.16	0.60
41:p:98:ASP:OD2	41:p:141:ARG:NH1	2.34	0.60
16:P:127:GLU:O	16:P:224:ARG:NH1	2.35	0.60
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.28	0.59
10:J:23:LYS:NZ	11:K:21:MET:O	2.31	0.59
15:O:31:ILE:O	15:O:179:VAL:HG13	2.02	0.59
58:U:101:EHZ:O7	39:n:12:GLN:NE2	2.35	0.59
38:m:74:ASN:O	38:m:78:ASN:ND2	2.36	0.59
41:p:88:GLU:OE2	41:p:92:ARG:NE	2.36	0.59
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.84	0.59
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.84	0.59
20:T:75:GLU:OE1	20:T:75:GLU:N	2.34	0.58
22:W:54:ILE:HD13	22:W:107:PHE:CZ	2.38	0.58
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.86	0.58
12:L:594:THR:OG1	24:Y:38:TYR:OH	2.17	0.58
8:H:318:THR:HG22	26:a:41:TYR:CE2	2.38	0.58
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.84	0.58
8:H:258:ASN:ND2	46:H:601:3PE:O32	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.85	0.57
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.39	0.57
24:Y:39:SER:OG	46:Y:602:3PE:O14	2.17	0.57
33:h:109:GLU:OE2	33:h:112:ARG:NH1	2.37	0.57
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.38	0.57
21:V:110:GLN:OE1	60:V:201:HOH:O	2.17	0.57
2:B:49:THR:HG21	2:B:59:MET:HG2	1.86	0.57
2:B:86:MET:HE1	2:B:104:TYR:HB2	1.85	0.57
10:J:42:GLY:O	10:J:46:ASN:ND2	2.37	0.57
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.86	0.57
37:l:139:TYR:OH	37:l:145:ASP:O	2.14	0.57
12:L:505:SER:O	12:L:508:THR:OG1	2.22	0.57
2:B:25:ARG:O	2:B:28:TYR:N	2.38	0.57
12:L:363:PHE:CD1	12:L:370:THR:HG21	2.40	0.57
23:X:162:HIS:O	60:X:1802:HOH:O	2.18	0.57
12:L:341:MET:CE	12:L:457:LEU:HD12	2.33	0.56
45:M:802:LMT:H6'	45:M:802:LMT:C1'	2.18	0.56
11:K:53:PHE:CD1	30:e:20:GLN:HB3	2.40	0.56
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.87	0.56
32:g:91:ARG:NH2	60:g:1602:HOH:O	2.38	0.56
16:P:319:ARG:NH2	22:W:53:ASP:OD1	2.37	0.56
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.35	0.56
43:r:57:ASP:OD1	60:r:201:HOH:O	2.18	0.56
37:l:16:THR:HG23	37:l:19:GLU:H	1.70	0.56
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.89	0.55
10:J:23:LYS:NZ	53:K:401:CDL:OA9	2.38	0.55
45:L:704:LMT:C11	46:Y:601:3PE:H2I1	2.36	0.55
20:T:51:ILE:HD12	20:T:70:LEU:HD12	1.88	0.55
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.88	0.55
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.36	0.55
12:L:383:MET:HE3	12:L:384:PRO:HD2	1.88	0.55
20:T:7:THR:O	20:T:11:ILE:N	2.34	0.55
32:g:35:GLU:OE2	32:g:36:ASN:N	2.40	0.55
42:q:25:ARG:HH21	42:q:66:THR:HG21	1.72	0.55
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.87	0.54
14:N:337:LEU:HD23	53:X:1701:CDL:C60	2.37	0.54
3:C:16:ASP:OD1	3:C:17:VAL:N	2.40	0.54
16:P:133:SER:OG	16:P:134:HIS:N	2.39	0.54
11:K:70:GLU:OE2	14:N:64:SER:OG	2.14	0.54
28:c:34:GLN:NE2	28:c:38:ASP:OD1	2.40	0.54
23:X:3:ILE:HD11	25:Z:105:LYS:NZ	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.88	0.54
3:C:37:VAL:HG12	43:r:69:MET:CE	2.38	0.53
12:L:323:TYR:CE1	12:L:475:THR:HG21	2.42	0.53
24:Y:9:TRP:CD1	45:Y:603:LMT:H3O2	2.25	0.53
37:l:8:MET:HE2	37:l:8:MET:HA	1.91	0.53
30:e:53:LYS:O	30:e:56:LYS:NZ	2.39	0.53
6:F:31:TRP:NE1	44:s:42:GLN:OE1	2.41	0.53
13:M:53:SER:O	13:M:113:MET:HE3	2.08	0.53
20:T:25:ILE:HG21	20:T:30:LEU:HD12	1.89	0.53
12:L:444:ASN:OD1	12:L:446:ASN:ND2	2.41	0.53
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.39	0.53
39:n:169:ILE:O	39:n:172:ARG:NH1	2.41	0.53
11:K:53:PHE:CE1	30:e:20:GLN:HA	2.43	0.53
12:L:331:THR:HB	12:L:387:THR:HG22	1.90	0.53
29:d:112:VAL:O	41:p:159:LYS:NZ	2.40	0.53
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.91	0.52
7:G:333:ASP:O	7:G:337:ARG:NH1	2.42	0.52
15:O:291:GLN:NE2	15:O:295:GLU:OE1	2.43	0.52
25:Z:36:PHE:O	25:Z:40:ILE:HD12	2.10	0.52
29:d:112:VAL:HG21	41:p:78:GLU:OE2	2.09	0.52
29:d:120:ARG:O	38:m:108:ARG:NH2	2.42	0.52
31:f:42:LEU:O	41:p:68:ARG:NH1	2.40	0.52
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.92	0.52
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.45	0.52
40:o:21:MET:HE1	40:o:101:PHE:CD2	2.46	0.52
3:C:58:ILE:HD11	3:C:119:SER:O	2.10	0.51
48:g:1501:PC1:H142	53:h:1001:CDL:OA3	2.11	0.51
30:e:23:GLU:OE2	30:e:27:LYS:NZ	2.44	0.51
37:l:62:TYR:OH	39:n:151:GLU:OE2	2.27	0.51
13:M:126:LEU:HD11	13:M:153:THR:HG21	1.93	0.51
6:F:438:GLN:N	6:F:438:GLN:OE1	2.43	0.51
15:O:56:ILE:HD11	15:O:96:LEU:CD1	2.41	0.51
14:N:314:LYS:NZ	15:O:270:LEU:O	2.44	0.50
8:H:62:ARG:N	8:H:63:PRO:CD	2.75	0.50
12:L:286:LEU:HD13	12:L:411:MET:SD	2.52	0.50
15:O:107:GLN:OE1	60:O:501:HOH:O	2.19	0.50
8:H:93:TYR:OH	26:a:35:GLU:OE1	2.22	0.50
25:Z:94:GLU:HG2	25:Z:106:VAL:HG13	1.92	0.50
2:B:162:GLN:OE1	9:I:140:SER:OG	2.24	0.50
37:l:16:THR:OG1	37:l:18:GLU:OE1	2.27	0.50
2:B:92:LEU:HD22	2:B:100:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:301:ILE:CG2	12:L:426:ILE:HD11	2.41	0.50
20:T:32:VAL:HG13	20:T:33:ASN:OD1	2.11	0.49
20:T:58:PHE:CE2	20:T:80:ILE:HD13	2.47	0.49
13:M:78:MET:HE1	13:M:439:LEU:HD12	1.92	0.49
40:o:27:ASP:OD2	40:o:27:ASP:N	2.45	0.49
7:G:415:LEU:O	7:G:416:THR:OG1	2.18	0.49
7:G:465:ALA:HB2	7:G:654:GLN:OE1	2.12	0.49
13:M:80:SER:OG	13:M:226:ALA:HB2	2.12	0.49
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.94	0.49
17:Q:42:ARG:O	60:Q:202:HOH:O	2.20	0.49
32:g:107:ILE:HD11	41:p:134:VAL:HB	1.94	0.49
43:r:104:GLU:HA	43:r:104:GLU:OE2	2.12	0.49
4:D:117:ALA:HB2	4:D:367:ILE:HG12	1.94	0.49
13:M:403:THR:HA	13:M:406:TYR:CE1	2.48	0.49
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.95	0.48
2:B:105:ASP:O	8:H:62:ARG:NH1	2.45	0.48
12:L:19:ILE:CD1	12:L:122:LEU:HD23	2.42	0.48
13:M:42:MET:HE1	32:g:77:VAL:HG22	1.94	0.48
12:L:562:LEU:CB	12:L:563:PRO:CD	2.91	0.48
32:g:57:ASN:ND2	32:g:57:ASN:O	2.46	0.48
7:G:640:ASN:CG	7:G:641:TYR:H	2.22	0.48
14:N:174:GLN:OE1	60:N:1001:HOH:O	2.20	0.48
4:D:64:LEU:HD22	4:D:76:CYS:SG	2.54	0.48
11:K:53:PHE:HE2	11:K:56:ALA:HB2	1.77	0.48
5:E:105:THR:HG22	5:E:106:THR:H	1.79	0.48
53:h:1001:CDL:H172	34:i:81:ILE:HD13	1.96	0.48
23:X:17:VAL:HG12	23:X:19:VAL:HG22	1.96	0.47
37:l:30:ARG:NH1	37:l:33:ASP:OD1	2.46	0.47
12:L:230:HIS:N	12:L:231:PRO:CD	2.77	0.47
20:T:12:LYS:O	20:T:16:LEU:HD23	2.14	0.47
5:E:121:GLN:O	5:E:125:GLY:N	2.45	0.47
8:H:228:TYR:OH	52:H:602:I49:N04	2.47	0.47
12:L:593:ILE:HG22	12:L:597:ILE:HD12	1.97	0.47
13:M:368:ALA:O	13:M:375:LEU:HD12	2.14	0.47
13:M:370:PRO:HB3	13:M:375:LEU:HD13	1.95	0.47
28:c:15:LEU:HD23	28:c:19:LEU:HD12	1.97	0.47
37:l:41:GLY:HA3	38:m:85:THR:HG21	1.96	0.47
12:L:71:ILE:HG23	13:M:310:MET:HE1	1.96	0.47
14:N:19:ILE:O	14:N:23:SER:OG	2.24	0.47
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.31	0.47
32:g:110:SER:O	41:p:161:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.96	0.47
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.96	0.47
12:L:264:TYR:N	12:L:265:PRO:CD	2.77	0.47
5:E:100:ILE:HD11	5:E:137:PHE:CD1	2.50	0.47
20:U:55:GLU:OE2	39:n:24:ARG:NH2	2.45	0.47
24:Y:32:GLY:O	24:Y:36:SER:OG	2.27	0.47
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.95	0.47
8:H:195:ARG:NH2	8:H:274:ARG:HD2	2.30	0.47
32:g:101:GLU:OE1	60:g:1601:HOH:O	2.20	0.47
12:L:489:THR:O	12:L:493:VAL:HG22	2.15	0.46
38:m:82:ASN:OD1	38:m:85:THR:OG1	2.12	0.46
29:d:10:THR:HG23	29:d:10:THR:O	2.15	0.46
8:H:102:VAL:HG11	8:H:154:LEU:HD11	1.96	0.46
6:F:82:MET:O	6:F:91:LYS:NZ	2.35	0.46
7:G:145:LEU:HD21	7:G:687:CYS:SG	2.55	0.46
7:G:382:THR:HG23	7:G:384:PRO:HD3	1.96	0.46
12:L:556:ILE:HG22	12:L:557:TRP:N	2.31	0.46
33:h:87:TYR:OH	41:p:86:GLU:HG2	2.15	0.46
2:B:51:GLY:HA2	2:B:56:ALA:HB2	1.98	0.46
10:J:17:PHE:HA	10:J:20:PHE:CE1	2.51	0.46
10:J:64:MET:HE2	11:K:68:ALA:HA	1.98	0.46
20:T:25:ILE:CG2	20:T:30:LEU:HD12	2.46	0.46
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.96	0.46
8:H:169:GLN:O	46:H:601:3PE:N	2.34	0.46
10:J:82:ILE:O	10:J:85:SER:OG	2.34	0.46
13:M:216:LEU:HB3	13:M:217:PRO:HD3	1.98	0.46
10:J:45:LEU:HD23	10:J:50:SER:HA	1.98	0.46
4:D:161:ILE:HD11	4:D:235:TRP:HZ3	1.80	0.45
12:L:221:THR:HG21	46:L:701:3PE:H2I2	1.98	0.45
7:G:140:LYS:O	7:G:148:THR:OG1	2.31	0.45
53:K:401:CDL:OA3	12:L:585:LYS:NZ	2.50	0.45
12:L:63:ILE:O	12:L:79:SER:HA	2.16	0.45
20:T:68:GLU:OE2	22:W:33:ARG:NE	2.49	0.45
22:W:107:PHE:O	22:W:108:HIS:C	2.59	0.45
38:m:22:TYR:O	38:m:24:ILE:N	2.49	0.45
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.46	0.45
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.44	0.45
7:G:143:GLY:HA2	7:G:190:MET:HE2	1.98	0.45
8:H:87:ILE:N	8:H:88:PRO:CD	2.79	0.45
13:M:153:THR:HG23	13:M:206:LYS:HE3	1.98	0.45
16:P:133:SER:O	56:P:501:NDP:H6N	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:1:MET:HG2	26:a:3:PHE:CE2	2.51	0.45
1:A:73:LEU:O	1:A:76:PRO:HD2	2.17	0.45
3:C:178:ASP:O	3:C:181:LYS:NZ	2.49	0.45
8:H:18:ALA:O	8:H:21:THR:OG1	2.26	0.45
11:K:53:PHE:HE1	30:e:20:GLN:HA	1.82	0.45
12:L:502:LEU:HD21	36:k:62:PHE:CG	2.51	0.45
13:M:75:LEU:HA	13:M:78:MET:HE2	1.97	0.45
13:M:207:MET:SD	13:M:240:GLY:N	2.90	0.45
15:O:198:TYR:CE2	15:O:202:ILE:HD11	2.51	0.45
34:i:105:PRO:O	40:o:67:LYS:NZ	2.47	0.45
12:L:554:ASP:OD2	13:M:275:ILE:HD13	2.16	0.45
41:p:143:HIS:O	41:p:157:LYS:NZ	2.42	0.45
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.50	0.45
12:L:19:ILE:HD11	12:L:122:LEU:HD23	1.99	0.45
9:I:145:GLU:OE2	16:P:66:GLY:N	2.46	0.45
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.98	0.45
22:W:101:THR:O	22:W:105:ARG:HG3	2.17	0.45
14:N:242:VAL:HG11	46:N:902:3PE:C33	2.47	0.45
6:F:403:THR:HB	47:F:502:SF4:S4	2.56	0.44
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.17	0.44
31:f:11:TRP:O	31:f:14:VAL:HG22	2.16	0.44
2:B:171:LYS:HD3	2:B:174:ARG:NH2	2.31	0.44
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.98	0.44
8:H:24:GLU:HG3	8:H:271:LEU:HG	1.99	0.44
5:E:181:ILE:O	5:E:181:ILE:HG13	2.16	0.44
6:F:94:VAL:HG11	6:F:192:LEU:CD2	2.48	0.44
12:L:301:ILE:HG21	12:L:426:ILE:HD11	1.98	0.44
13:M:370:PRO:CB	13:M:375:LEU:HD13	2.47	0.44
22:W:84:ILE:HG22	22:W:88:MET:HE3	2.00	0.44
35:j:70:ASP:O	35:j:70:ASP:OD2	2.36	0.44
8:H:72:ILE:HG22	8:H:76:ILE:HD12	2.00	0.44
12:L:82:MET:HE3	12:L:87:MET:HE3	1.97	0.44
12:L:429:PHE:O	12:L:436:ARG:NH2	2.48	0.44
23:X:79:GLU:HB2	23:X:80:PRO:HD3	1.99	0.44
3:C:135:TRP:CE2	22:W:88:MET:HE1	2.53	0.44
12:L:61:LEU:HD12	12:L:61:LEU:C	2.43	0.44
18:R:19:ASP:OD2	18:R:22:ASP:HB2	2.17	0.44
19:S:33:ARG:O	19:S:37:GLU:HG3	2.17	0.44
37:l:41:GLY:O	37:l:42:THR:C	2.60	0.44
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.48	0.44
45:A:301:LMT:O5B	45:A:301:LMT:O3'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:THR:HG22	5:E:106:THR:N	2.33	0.44
9:I:8:ARG:NH1	43:r:112:LEU:O	2.44	0.44
20:T:49:GLU:OE1	22:W:36:TYR:OH	2.34	0.44
13:M:375:LEU:HD23	13:M:375:LEU:C	2.43	0.44
32:g:110:SER:OG	41:p:140:ASP:OD2	2.16	0.44
5:E:143:GLU:O	5:E:144:CYS:C	2.60	0.44
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.18	0.44
14:N:270:MET:HE1	14:N:282:MET:SD	2.57	0.44
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.52	0.44
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.51	0.43
12:L:82:MET:HB3	12:L:87:MET:HE3	2.00	0.43
12:L:553:LEU:HD11	38:m:92:PHE:CD2	2.53	0.43
16:P:22:THR:OG1	16:P:88:SER:OG	2.14	0.43
20:T:55:GLU:OE1	22:W:37:ARG:NH2	2.51	0.43
37:l:16:THR:HG22	37:l:19:GLU:CD	2.43	0.43
30:e:16:TRP:CE3	30:e:17:MET:HG3	2.52	0.43
38:m:25:SER:OG	38:m:26:SER:N	2.51	0.43
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.99	0.43
25:Z:90:ASN:ND2	25:Z:123:GLU:O	2.51	0.43
7:G:366:THR:C	7:G:367:THR:HG1	2.03	0.43
24:Y:16:GLU:O	24:Y:16:GLU:HG2	2.19	0.43
7:G:616:LEU:HA	7:G:619:VAL:HG12	2.00	0.43
20:U:47:GLN:NE2	20:U:70:LEU:O	2.51	0.43
1:A:49:LEU:O	1:A:51:PHE:N	2.51	0.43
1:A:80:GLN:HG3	8:H:317:GLN:HG2	2.01	0.43
25:Z:40:ILE:HD12	25:Z:40:ILE:H	1.84	0.43
4:D:202:ASP:N	4:D:323:ILE:HD13	2.34	0.43
7:G:512:GLU:CD	7:G:512:GLU:H	2.26	0.43
10:J:135:PHE:CD2	10:J:135:PHE:O	2.72	0.43
37:l:141:GLU:OE2	37:l:141:GLU:N	2.49	0.43
39:n:145:VAL:HG23	39:n:146:GLY:N	2.33	0.43
12:L:176:ARG:O	12:L:179:ASP:OD1	2.36	0.43
16:P:175:GLU:N	16:P:175:GLU:OE2	2.51	0.43
13:M:304:GLN:O	29:d:119:VAL:HG11	2.19	0.43
34:i:6:GLU:HG3	39:n:155:PRO:HD3	2.00	0.43
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.54	0.43
15:O:108:TYR:OH	15:O:164:LEU:O	2.36	0.43
1:A:3:LEU:HD22	46:Z:401:3PE:C3	2.49	0.42
1:A:13:LEU:CD2	8:H:10:ILE:HG21	2.49	0.42
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.54	0.42
15:O:176:VAL:N	15:O:177:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:THR:HA	2:B:119:CYS:HB3	2.01	0.42
40:o:7:ARG:NH2	40:o:17:ASP:OD1	2.52	0.42
8:H:176:LEU:HB3	8:H:177:PRO:HD3	2.02	0.42
14:N:261:MET:HG3	14:N:340:THR:HG23	2.01	0.42
15:O:31:ILE:HG22	15:O:32:CYS:SG	2.59	0.42
25:Z:86:MET:HE1	25:Z:125:TYR:CE2	2.54	0.42
31:f:7:VAL:HG12	31:f:9:ASP:H	1.84	0.42
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.54	0.42
8:H:249:PRO:O	26:a:28:ARG:NH2	2.52	0.42
6:F:95:VAL:HG11	6:F:118:LEU:HD11	2.01	0.42
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.52	0.42
4:D:322:GLU:OE1	4:D:322:GLU:N	2.40	0.42
12:L:433:GLY:O	36:k:59:ASN:ND2	2.40	0.42
13:M:116:ILE:HG12	13:M:174:LEU:HD13	2.01	0.42
2:B:59:MET:HE1	2:B:69:MET:HE1	2.01	0.42
5:E:103:CYS:SG	5:E:144:CYS:HA	2.59	0.42
8:H:121:TRP:HE1	10:J:73:ALA:HB2	1.85	0.42
4:D:134:ALA:HB2	4:D:323:ILE:O	2.19	0.42
12:L:13:LEU:HD22	34:i:81:ILE:HD11	2.02	0.42
12:L:145:GLU:OE2	12:L:179:ASP:OD2	2.38	0.42
12:L:159:TYR:HB2	13:M:416:ARG:HG2	2.02	0.42
13:M:126:LEU:HD11	13:M:153:THR:CG2	2.48	0.42
16:P:92:ILE:HD11	16:P:218:ILE:HD11	2.02	0.42
16:P:281:ARG:O	16:P:285:GLU:HG2	2.20	0.42
2:B:95:LYS:HA	3:C:154:ASP:OD2	2.19	0.42
10:J:135:PHE:CE2	25:Z:65:PHE:CE1	3.07	0.42
14:N:237:THR:HG21	14:N:319:LEU:HD11	2.02	0.42
15:O:86:PRO:O	15:O:93:SER:OG	2.29	0.42
16:P:98:GLU:OE2	16:P:283:LYS:NZ	2.48	0.42
8:H:2:PHE:HE2	8:H:6:ILE:HD11	1.83	0.42
12:L:233:LEU:HD23	12:L:307:SER:OG	2.20	0.42
13:M:243:MET:HA	13:M:246:ILE:HG22	2.02	0.42
16:P:238:LEU:O	16:P:242:VAL:HG23	2.20	0.42
11:K:59:MET:HG3	11:K:60:PRO:HD3	2.01	0.41
13:M:193:VAL:HG21	45:M:801:LMT:H41	2.02	0.41
41:p:40:VAL:O	41:p:44:VAL:HG23	2.20	0.41
4:D:259:MET:HE1	4:D:405:MET:HE1	2.00	0.41
7:G:333:ASP:HB3	7:G:611:LEU:HD22	2.01	0.41
12:L:564:LYS:NZ	45:L:704:LMT:O5B	2.53	0.41
12:L:375:VAL:HG22	35:j:32:MET:SD	2.60	0.41
53:h:1001:CDL:OA7	53:h:1001:CDL:H131	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:ILE:HD13	4:D:330:VAL:HG11	2.01	0.41
6:F:93:LEU:HD13	6:F:129:MET:HE1	2.02	0.41
10:J:12:ILE:HG22	10:J:39:VAL:HG21	2.01	0.41
10:J:55:MET:HA	10:J:55:MET:HE2	2.03	0.41
16:P:157:ARG:NH2	16:P:163:ALA:O	2.47	0.41
24:Y:13:GLU:OE1	24:Y:125:LYS:NZ	2.52	0.41
24:Y:68:ILE:CG2	24:Y:95:ALA:HB1	2.51	0.41
30:e:64:GLU:O	30:e:68:ARG:N	2.49	0.41
4:D:104:ASP:OD1	4:D:115:GLU:OE2	2.38	0.41
14:N:242:VAL:HG11	46:N:902:3PE:H331	2.02	0.41
58:T:101:EHZ:O2	58:T:101:EHZ:O1	2.37	0.41
6:F:125:GLY:O	6:F:129:MET:HE3	2.20	0.41
23:X:25:LYS:NZ	23:X:94:GLN:O	2.49	0.41
30:e:16:TRP:CZ3	30:e:17:MET:HG3	2.56	0.41
1:A:108:GLN:HB2	10:J:169:MET:HE1	2.03	0.41
6:F:248:GLU:O	6:F:249:ARG:HB2	2.21	0.41
12:L:286:LEU:HD23	12:L:286:LEU:C	2.45	0.41
12:L:421:ILE:HA	12:L:501:ALA:HB2	2.02	0.41
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.03	0.41
4:D:69:SER:OG	4:D:74:ARG:CZ	2.69	0.41
7:G:375:ASP:OD1	7:G:375:ASP:N	2.54	0.41
10:J:122:LEU:HD22	30:e:79:ARG:HD2	2.01	0.41
14:N:289:ASN:OD1	60:N:1002:HOH:O	2.22	0.41
24:Y:15:THR:O	24:Y:16:GLU:C	2.63	0.41
25:Z:89:GLU:O	25:Z:93:GLU:OE1	2.39	0.41
1:A:14:ALA:O	1:A:18:VAL:HG23	2.21	0.41
2:B:96:MET:HE1	4:D:60:GLY:HA2	2.03	0.41
2:B:96:MET:O	2:B:96:MET:HG3	2.20	0.41
2:B:125:TYR:HB2	9:I:117:ILE:HG21	2.02	0.41
5:E:87:TYR:HB3	6:F:181:ALA:O	2.21	0.41
7:G:268:ARG:NH1	60:G:929:HOH:O	2.51	0.41
9:I:75:GLU:O	9:I:105:ARG:NH1	2.53	0.41
12:L:213:LEU:HD23	12:L:216:LEU:HD12	2.02	0.41
13:M:379:LEU:O	13:M:383:MET:HG2	2.21	0.41
23:X:122:GLY:N	25:Z:66:GLU:OE2	2.52	0.41
37:l:127:PRO:O	60:l:301:HOH:O	2.22	0.41
7:G:377:VAL:HG13	7:G:452:ILE:CD1	2.51	0.41
8:H:77:MET:HE3	8:H:81:LEU:CD1	2.50	0.41
10:J:43:ILE:HG22	11:K:46:LEU:HD11	2.03	0.41
20:U:52:MET:HE1	39:n:23:LEU:CB	2.51	0.41
13:M:42:MET:HE1	32:g:77:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:140:VAL:O	24:Y:140:VAL:HG23	2.21	0.40
32:g:100:ARG:NH1	32:g:107:ILE:O	2.50	0.40
48:g:1501:PC1:O13	48:g:1501:PC1:H132	2.20	0.40
2:B:48:MET:O	2:B:48:MET:SD	2.79	0.40
8:H:301:CYS:O	8:H:305:VAL:HG23	2.20	0.40
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.03	0.40
14:N:250:SER:O	14:N:259:GLY:HA3	2.21	0.40
16:P:179:LEU:HD11	16:P:310:LEU:HD11	2.03	0.40
38:m:13:LEU:HD12	38:m:14:PRO:HD2	2.02	0.40
7:G:272:ASP:OD1	7:G:681:SER:OG	2.37	0.40
7:G:371:VAL:HG22	7:G:450:MET:HE1	2.02	0.40
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.03	0.40
12:L:40:ILE:HG13	12:L:101:MET:SD	2.61	0.40
14:N:230:LEU:HD11	14:N:244:ILE:HD13	2.02	0.40
20:T:43:ASP:CG	20:T:44(A):SER:H	2.29	0.40
20:U:29:LYS:HG2	20:U:29:LYS:O	2.22	0.40
40:o:1:GLY:O	40:o:2:ALA:HB3	2.22	0.40
42:q:1:MET:O	42:q:5:GLN:OE1	2.39	0.40
3:C:40:VAL:HG13	3:C:50:ILE:HD13	2.03	0.40
6:F:150:GLN:HE21	44:s:58:LEU:HD12	1.87	0.40
7:G:627:SER:OG	7:G:629:ASN:OD1	2.38	0.40
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.04	0.40
4:D:155:THR:HB	4:D:167:PHE:HA	2.04	0.40
7:G:297:GLU:HG3	22:W:123:TYR:CZ	2.57	0.40
10:J:129:ASP:OD1	10:J:130:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/115 (84%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	153/216 (71%)	144 (94%)	8 (5%)	1 (1%)	18	28
3	C	204/266 (77%)	198 (97%)	6 (3%)	0	100	100
4	D	416/463 (90%)	398 (96%)	18 (4%)	0	100	100
5	E	211/249 (85%)	207 (98%)	4 (2%)	0	100	100
6	F	428/464 (92%)	419 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	661 (96%)	25 (4%)	0	100	100
8	H	308/318 (97%)	294 (96%)	14 (4%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	172/175 (98%)	157 (91%)	15 (9%)	0	100	100
11	K	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	580 (96%)	23 (4%)	1 (0%)	43	58
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	311 (98%)	7 (2%)	0	100	100
16	P	281/380 (74%)	275 (98%)	6 (2%)	0	100	100
17	Q	123/175 (70%)	122 (99%)	1 (1%)	0	100	100
18	R	92/124 (74%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99 (81%)	78 (98%)	2 (2%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	82/156 (53%)	82 (100%)	0	0	100	100
21	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	109 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	131 (94%)	8 (6%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
29	d	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	95/154 (62%)	89 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	77 (100%)	0	0	100	100
37	l	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
38	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	119/137 (87%)	113 (95%)	6 (5%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	41/109 (38%)	38 (93%)	3 (7%)	0	100	100
All	All	7993/9212 (87%)	7757 (97%)	234 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
2	B	53	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/100 (88%)	88 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	187/228 (82%)	187 (100%)	0	100	100
4	D	362/392 (92%)	362 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	344/368 (94%)	344 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	268/274 (98%)	268 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	84/85 (99%)	84 (100%)	0	100	100
12	L	529/533 (99%)	529 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	248/327 (76%)	248 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	77/97 (79%)	77 (100%)	0	100	100
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	78/135 (58%)	78 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	100 (99%)	1 (1%)	68	84
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	58/59 (98%)	58 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100
31	f	48/54 (89%)	48 (100%)	0	100	100
32	g	88/131 (67%)	88 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	98/120 (82%)	98 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	110 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	131/131 (100%)	131 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	42/92 (46%)	42 (100%)	0	100	100
All	All	7059/7892 (89%)	7058 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
24	Y	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	HIS
3	C	88	ASN
4	D	59	HIS
4	D	157	HIS
4	D	200	HIS
6	F	200	GLN
6	F	356	HIS
7	G	82	ASN
7	G	141	ASN
7	G	313	ASN
12	L	170	GLN
12	L	200	GLN
12	L	248	HIS
12	L	354	GLN
12	L	442	ASN
12	L	514	HIS
13	M	251	ASN
13	M	366	ASN
13	M	415	GLN

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Mol	Chain	Res	Type
14	N	120	GLN
14	N	174	GLN
15	O	190	HIS
16	P	8	HIS
16	P	103	ASN
17	Q	44	ASN
17	Q	50	ASN
19	S	72	GLN
19	S	85	GLN
22	W	70	ASN
22	W	126	HIS
23	X	29	HIS
23	X	142	HIS
24	Y	128	GLN
24	Y	133	GLN
28	c	9	HIS
33	h	124	HIS
33	h	143	ASN
34	i	66	HIS
38	m	32	GLN
38	m	74	ASN
39	n	12	GLN
39	n	50	HIS
40	o	42	GLN
40	o	109	GLN
42	q	112	ASN
43	r	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FME	K	1	11	8,9,10	0.95	0	8,9,11	0.87	0
12	FME	L	1	12	8,9,10	1.01	1 (12%)	8,9,11	1.03	1 (12%)
1	FME	A	1	1	8,9,10	1.00	1 (12%)	8,9,11	0.93	0
34	SAC	i	1	34	7,8,9	1.95	2 (28%)	7,9,11	1.98	1 (14%)
8	FME	H	1	8	8,9,10	1.02	1 (12%)	8,9,11	0.90	0
13	FME	M	1	13	8,9,10	1.00	1 (12%)	8,9,11	1.13	1 (12%)
14	FME	N	1	14	8,9,10	1.06	1 (12%)	8,9,11	0.83	0
4	2MR	D	85	4	10,12,13	2.74	4 (40%)	5,13,15	0.84	0
24	AYA	Y	1	24	6,7,8	1.87	1 (16%)	6,8,10	1.19	1 (16%)
43	AYA	r	1	43	6,7,8	1.83	2 (33%)	6,8,10	1.32	1 (16%)
10	FME	J	1	10	8,9,10	0.96	0	8,9,11	0.84	0

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.26	1.44	1.33
4	D	85	2MR	CZ-NE	4.79	1.44	1.34
34	i	1	SAC	O-C	4.38	1.36	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	O-C	4.12	1.35	1.20
24	Y	1	AYA	CT-N	3.48	1.45	1.34
43	r	1	AYA	CT-N	3.30	1.45	1.34
14	N	1	FME	CA-N	-2.20	1.43	1.46
8	H	1	FME	CA-N	-2.12	1.43	1.46
1	A	1	FME	CA-N	-2.11	1.43	1.46
13	M	1	FME	CA-N	-2.10	1.43	1.46
4	D	85	2MR	CQ1-NH1	-2.08	1.42	1.46
43	r	1	AYA	OT-CT	-2.06	1.18	1.23
12	L	1	FME	CA-N	-2.05	1.43	1.46
34	i	1	SAC	CA-N	-2.05	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	O-C-CA	-4.58	112.98	124.77
13	M	1	FME	C-CA-N	2.64	114.59	109.50
43	r	1	AYA	CM-CT-N	2.28	119.90	116.12
12	L	1	FME	C-CA-N	2.17	113.69	109.50
24	Y	1	AYA	CM-CT-N	2.10	119.61	116.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
10	J	1	FME	CB-CA-N-CN
24	Y	1	AYA	C-CA-N-CT

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
46	3PE	H	601	-	23,23,50	1.53	4 (17%)	24,27,55	1.17	2 (8%)
54	GTP	O	401	55	33,34,34	3.28	15 (45%)	50,54,54	1.91	14 (28%)
45	LMT	N	903	-	36,36,36	1.18	3 (8%)	47,47,47	0.91	1 (2%)
46	3PE	L	705	-	28,28,50	1.13	4 (14%)	31,33,55	1.18	2 (6%)
45	LMT	h	1002	-	36,36,36	1.18	3 (8%)	47,47,47	1.31	5 (10%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
46	3PE	d	1201	-	37,37,50	1.00	4 (10%)	40,42,55	1.11	2 (5%)
46	3PE	A	302	-	39,39,50	0.95	4 (10%)	42,44,55	1.24	2 (4%)
46	3PE	B	1001	-	35,35,50	1.04	4 (11%)	38,40,55	1.07	2 (5%)
45	LMT	h	1003	-	36,36,36	1.17	2 (5%)	47,47,47	0.98	2 (4%)
45	LMT	M	801	-	36,36,36	1.12	2 (5%)	47,47,47	1.22	4 (8%)
48	PC1	B	1003	-	34,34,53	1.17	4 (11%)	40,42,61	1.14	2 (5%)
47	SF4	B	1002	2	0,12,12	-	-	-	-	-
53	CDL	q	201	-	60,60,99	1.13	8 (13%)	66,72,111	1.12	4 (6%)
49	FES	E	301	5	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	G	802	7	0,12,12	-	-	-		
46	3PE	I	204	-	30,30,50	1.10	3 (10%)	33,35,55	1.21	3 (9%)
58	EHZ	T	101	20	31,36,37	1.55	4 (12%)	36,44,47	1.52	5 (13%)
49	FES	G	803	7	0,4,4	-	-	-		
52	I49	H	602	-	15,17,17	0.85	1 (6%)	17,22,22	2.06	5 (29%)
50	FMN	F	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.24	5 (10%)
53	CDL	K	401	-	49,49,99	1.03	5 (10%)	53,58,111	1.03	2 (3%)
53	CDL	h	1001	-	66,66,99	1.07	7 (10%)	72,78,111	1.20	4 (5%)
45	LMT	Y	603	-	36,36,36	1.21	2 (5%)	47,47,47	1.02	1 (2%)
48	PC1	g	1501	-	48,48,53	1.01	3 (6%)	54,56,61	0.99	2 (3%)
47	SF4	F	502	6	0,12,12	-	-	-		
45	LMT	l	201	-	36,36,36	1.22	3 (8%)	47,47,47	1.08	3 (6%)
46	3PE	N	902	-	42,42,50	0.95	3 (7%)	45,47,55	1.14	2 (4%)
53	CDL	d	1202	-	64,64,99	1.08	7 (10%)	70,76,111	1.13	4 (5%)
56	NDP	P	501	-	51,52,52	2.16	5 (9%)	71,80,80	1.49	15 (21%)
53	CDL	L	702	-	63,63,99	1.10	6 (9%)	69,75,111	1.12	4 (5%)
45	LMT	M	802	-	36,36,36	1.17	2 (5%)	47,47,47	1.38	3 (6%)
45	LMT	N	901	-	36,36,36	1.17	3 (8%)	47,47,47	0.80	0
45	LMT	j	101	-	36,36,36	1.18	2 (5%)	47,47,47	0.82	0
46	3PE	Y	601	-	45,45,50	0.91	3 (6%)	48,50,55	1.17	3 (6%)
45	LMT	A	301	-	36,36,36	1.21	2 (5%)	47,47,47	0.95	1 (2%)
46	3PE	L	701	-	48,48,50	0.89	2 (4%)	51,53,55	1.05	2 (3%)
47	SF4	I	203	9	0,12,12	-	-	-		
59	MYR	o	201	40	13,14,15	0.86	0	12,13,15	0.53	0
45	LMT	L	704	-	36,36,36	1.18	2 (5%)	47,47,47	0.93	1 (2%)
58	EHZ	U	101	20	31,36,37	1.52	4 (12%)	36,44,47	1.51	5 (13%)
46	3PE	L	703	-	44,44,50	0.92	3 (6%)	47,49,55	1.12	2 (4%)
46	3PE	Z	401	-	24,24,50	1.23	4 (16%)	27,29,55	1.17	2 (7%)
53	CDL	X	1701	-	71,71,99	1.04	7 (9%)	77,83,111	1.21	5 (6%)
46	3PE	I	201	-	50,50,50	0.88	3 (6%)	53,55,55	1.06	2 (3%)
47	SF4	G	801	7	0,12,12	-	-	-		
46	3PE	N	904	-	40,40,50	0.96	4 (10%)	43,45,55	1.14	2 (4%)
46	3PE	Y	602	-	34,34,50	1.06	4 (11%)	37,39,55	1.18	2 (5%)

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
46	3PE	H	601	-	-	9/26/26/54	-
54	GTP	O	401	55	-	6/22/38/38	0/3/3/3
45	LMT	N	903	-	-	10/21/61/61	0/2/2/2
46	3PE	L	705	-	-	13/32/32/54	-
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
47	SF4	I	202	9	-	-	0/6/5/5
46	3PE	d	1201	-	-	21/41/41/54	-
46	3PE	A	302	-	-	23/43/43/54	-
46	3PE	B	1001	-	-	17/39/39/54	-
45	LMT	h	1003	-	-	6/21/61/61	0/2/2/2
45	LMT	M	801	-	-	5/21/61/61	0/2/2/2
48	PC1	B	1003	-	-	14/38/38/57	-
47	SF4	B	1002	2	-	-	0/6/5/5
53	CDL	q	201	-	-	36/71/71/110	-
49	FES	E	301	5	-	-	0/1/1/1
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	I	204	-	-	17/34/34/54	-
58	EHZ	T	101	20	-	15/42/44/45	-
52	I49	H	602	-	-	7/10/10/10	0/1/1/1
49	FES	G	803	7	-	-	0/1/1/1
50	FMN	F	501	-	-	2/18/18/18	0/3/3/3
53	CDL	K	401	-	-	19/54/54/110	-
53	CDL	h	1001	-	-	34/77/77/110	-
45	LMT	Y	603	-	-	7/21/61/61	0/2/2/2
48	PC1	g	1501	-	-	19/52/52/57	-
53	CDL	d	1202	-	-	36/75/75/110	-
45	LMT	l	201	-	-	7/21/61/61	0/2/2/2
46	3PE	N	902	-	-	19/46/46/54	-
47	SF4	F	502	6	-	-	0/6/5/5
56	NDP	P	501	-	-	5/34/77/77	0/5/5/5
53	CDL	L	702	-	-	30/74/74/110	-
45	LMT	M	802	-	-	7/21/61/61	0/2/2/2
45	LMT	N	901	-	-	3/21/61/61	0/2/2/2
45	LMT	j	101	-	-	5/21/61/61	0/2/2/2
46	3PE	Y	601	-	-	24/49/49/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	A	301	-	-	8/21/61/61	0/2/2/2
46	3PE	L	701	-	-	21/52/52/54	-
47	SF4	I	203	9	-	-	0/6/5/5
59	MYR	o	201	40	-	7/12/12/13	-
45	LMT	L	704	-	-	8/21/61/61	0/2/2/2
58	EHZ	U	101	20	-	10/42/44/45	-
46	3PE	L	703	-	-	25/48/48/54	-
46	3PE	Z	401	-	-	14/28/28/54	-
53	CDL	X	1701	-	-	45/82/82/110	-
46	3PE	I	201	-	-	25/54/54/54	-
47	SF4	G	801	7	-	-	0/6/5/5
46	3PE	N	904	-	-	15/44/44/54	-
46	3PE	Y	602	-	-	16/38/38/54	-

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.14	1.80	1.59
54	O	401	GTP	O6-C6	8.76	1.40	1.23
54	O	401	GTP	C5-N7	6.69	1.52	1.39
58	T	101	EHZ	C15-N2	5.04	1.45	1.33
54	O	401	GTP	PA-O3A	4.99	1.64	1.59
54	O	401	GTP	PB-O3B	4.90	1.64	1.59
54	O	401	GTP	C2-N1	4.89	1.49	1.37
58	U	101	EHZ	C15-N2	4.87	1.45	1.33
58	T	101	EHZ	C12-N1	4.83	1.44	1.33
54	O	401	GTP	PB-O3A	4.80	1.64	1.59
58	U	101	EHZ	C12-N1	4.74	1.44	1.33
54	O	401	GTP	C2-N3	4.70	1.44	1.33
54	O	401	GTP	C2-N2	4.61	1.45	1.34
46	H	601	3PE	O21-C2	-4.48	1.40	1.46
54	O	401	GTP	C8-N9	-4.41	1.27	1.37
54	O	401	GTP	C4-N9	-3.84	1.28	1.38
56	P	501	NDP	PA-O3	3.73	1.63	1.59
56	P	501	NDP	PN-O5D	3.58	1.73	1.59
45	l	201	LMT	O5B-C1B	3.57	1.51	1.41
45	Y	603	LMT	O5B-C1B	3.49	1.50	1.41
45	j	101	LMT	O5B-C1B	3.40	1.50	1.41
50	F	501	FMN	C4A-N5	3.38	1.38	1.30
45	h	1003	LMT	O5B-C1B	3.38	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O2B-C2B	-3.34	1.32	1.44
45	N	903	LMT	O5B-C1B	3.33	1.50	1.41
45	L	704	LMT	O5B-C1B	3.33	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.33	1.50	1.41
45	A	301	LMT	O5B-C1B	3.29	1.50	1.41
45	N	901	LMT	O5B-C1B	3.25	1.50	1.41
45	A	301	LMT	O5'-C1'	3.24	1.50	1.41
45	M	801	LMT	O5B-C1B	3.18	1.50	1.41
45	Y	603	LMT	O5'-C1'	3.18	1.50	1.41
45	N	903	LMT	O5'-C1'	3.16	1.50	1.41
46	H	601	3PE	O21-C21	3.15	1.40	1.33
45	M	802	LMT	O5'-C1'	3.15	1.49	1.41
45	L	704	LMT	O5'-C1'	3.07	1.49	1.41
48	g	1501	PC1	O21-C2	-3.00	1.39	1.46
45	j	101	LMT	O5'-C1'	3.00	1.49	1.41
53	L	702	CDL	OB6-CB4	-2.98	1.39	1.46
53	X	1701	CDL	OB6-CB4	-2.98	1.39	1.46
45	M	802	LMT	O5B-C1B	2.97	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.92	1.49	1.41
45	l	201	LMT	O5'-C1'	2.92	1.49	1.41
46	Y	601	3PE	O21-C2	-2.91	1.39	1.46
53	d	1202	CDL	OA6-CA4	-2.89	1.39	1.46
53	h	1001	CDL	OB6-CB4	-2.88	1.39	1.46
45	N	901	LMT	O5'-C1'	2.88	1.49	1.41
53	K	401	CDL	OA6-CA4	-2.87	1.39	1.46
53	h	1001	CDL	OA6-CA4	-2.87	1.39	1.46
53	q	201	CDL	OA6-CA4	-2.87	1.39	1.46
46	I	201	3PE	O21-C2	-2.87	1.39	1.46
53	d	1202	CDL	OB6-CB4	-2.83	1.39	1.46
45	h	1003	LMT	O5'-C1'	2.82	1.49	1.41
46	L	701	3PE	O21-C2	-2.82	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.82	1.40	1.46
53	L	702	CDL	OA6-CA4	-2.81	1.40	1.46
46	B	1001	3PE	O21-C2	-2.80	1.40	1.46
46	L	703	3PE	O21-C2	-2.79	1.40	1.46
46	N	902	3PE	O21-C2	-2.78	1.40	1.46
53	K	401	CDL	PB2-OB5	2.76	1.65	1.54
54	O	401	GTP	O4'-C1'	2.76	1.48	1.42
46	d	1201	3PE	O21-C2	-2.76	1.40	1.46
45	M	801	LMT	O5'-C1'	2.75	1.48	1.41
46	I	204	3PE	O21-C2	-2.73	1.40	1.46
46	L	701	3PE	O31-C3	-2.73	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Z	401	3PE	O21-C2	-2.69	1.40	1.46
46	N	904	3PE	O21-C2	-2.67	1.40	1.46
53	X	1701	CDL	OA6-CA4	-2.67	1.40	1.46
46	Y	602	3PE	O21-C2	-2.65	1.40	1.46
58	T	101	EHZ	O4-C15	-2.59	1.18	1.23
46	Z	401	3PE	O31-C3	-2.57	1.39	1.45
58	U	101	EHZ	O4-C15	-2.57	1.18	1.23
46	L	705	3PE	O21-C2	-2.57	1.40	1.46
53	h	1001	CDL	OB8-CB6	-2.56	1.39	1.45
48	B	1003	PC1	O21-C2	-2.51	1.40	1.46
53	X	1701	CDL	OB8-CB7	2.50	1.40	1.33
46	L	703	3PE	O31-C3	-2.49	1.39	1.45
46	I	201	3PE	O31-C3	-2.44	1.39	1.45
53	q	201	CDL	OA8-CA6	-2.43	1.39	1.45
46	H	601	3PE	O31-C31	2.43	1.40	1.33
58	T	101	EHZ	O3-C12	-2.43	1.18	1.23
53	d	1202	CDL	OA8-CA6	-2.43	1.39	1.45
58	U	101	EHZ	O3-C12	-2.42	1.18	1.23
53	q	201	CDL	OB8-CB7	2.41	1.40	1.33
53	L	702	CDL	OB8-CB7	2.41	1.40	1.33
46	Y	602	3PE	O31-C31	2.40	1.40	1.33
46	B	1001	3PE	O31-C3	-2.39	1.39	1.45
53	d	1202	CDL	OB8-CB7	2.39	1.40	1.33
45	h	1002	LMT	O5B-C5B	2.39	1.50	1.44
52	H	602	I49	C15-N02	-2.38	1.31	1.36
46	N	902	3PE	O31-C31	2.38	1.40	1.33
53	K	401	CDL	OA8-CA6	-2.36	1.39	1.45
53	L	702	CDL	OA8-CA6	-2.35	1.39	1.45
48	B	1003	PC1	O21-C21	2.35	1.40	1.34
46	N	902	3PE	O31-C3	-2.35	1.39	1.45
53	X	1701	CDL	OA8-CA7	2.35	1.40	1.33
53	d	1202	CDL	OB8-CB6	-2.34	1.39	1.45
46	N	904	3PE	O31-C3	-2.34	1.39	1.45
53	L	702	CDL	OA8-CA7	2.34	1.40	1.33
54	O	401	GTP	PG-O3G	-2.34	1.46	1.54
46	I	204	3PE	O31-C31	2.34	1.40	1.33
46	d	1201	3PE	O31-C31	2.32	1.40	1.33
53	q	201	CDL	OB8-CB6	-2.32	1.40	1.45
54	O	401	GTP	PG-O2G	-2.32	1.46	1.54
46	L	705	3PE	O31-C31	2.31	1.40	1.33
46	Y	602	3PE	O31-C3	-2.31	1.40	1.45
45	l	201	LMT	O5B-C5B	2.30	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g	1501	PC1	O31-C31	2.30	1.40	1.33
46	B	1001	3PE	O31-C31	2.27	1.40	1.33
54	O	401	GTP	C2'-C3'	-2.27	1.47	1.53
53	h	1001	CDL	OA8-CA6	-2.26	1.40	1.45
53	X	1701	CDL	OA8-CA6	-2.26	1.40	1.45
46	Y	601	3PE	O31-C31	2.25	1.39	1.33
53	h	1001	CDL	OA8-CA7	2.23	1.39	1.33
48	g	1501	PC1	O31-C3	-2.23	1.40	1.45
46	N	904	3PE	O31-C31	2.23	1.39	1.33
46	A	302	3PE	O31-C3	-2.23	1.40	1.45
53	K	401	CDL	OA8-CA7	2.23	1.39	1.33
48	B	1003	PC1	O31-C3	-2.22	1.40	1.45
53	X	1701	CDL	OA6-CA5	2.22	1.40	1.34
46	d	1201	3PE	O31-C3	-2.22	1.40	1.45
56	P	501	NDP	O5D-C5D	-2.22	1.36	1.44
46	A	302	3PE	O31-C31	2.20	1.39	1.33
48	B	1003	PC1	O31-C31	2.20	1.39	1.33
53	X	1701	CDL	OB8-CB6	-2.18	1.40	1.45
46	I	204	3PE	O31-C3	-2.18	1.40	1.45
53	h	1001	CDL	OB8-CB7	2.18	1.39	1.33
46	A	302	3PE	O21-C2	-2.17	1.41	1.46
53	h	1001	CDL	OB6-CB5	2.17	1.40	1.34
46	H	601	3PE	O31-C3	-2.17	1.40	1.45
53	q	201	CDL	OA8-CA7	2.15	1.39	1.33
46	Z	401	3PE	O31-C31	2.15	1.39	1.33
46	A	302	3PE	O21-C21	2.14	1.40	1.34
46	B	1001	3PE	O21-C21	2.14	1.40	1.34
46	Y	601	3PE	O31-C3	-2.13	1.40	1.45
46	L	703	3PE	O31-C31	2.13	1.39	1.33
46	Z	401	3PE	O21-C21	2.12	1.40	1.34
46	I	201	3PE	O31-C31	2.12	1.39	1.33
53	d	1202	CDL	OA8-CA7	2.12	1.39	1.33
53	d	1202	CDL	OB6-CB5	2.11	1.40	1.34
45	N	901	LMT	O5B-C5B	2.11	1.49	1.44
46	L	705	3PE	O21-C21	2.10	1.40	1.34
53	q	201	CDL	OA6-CA5	2.10	1.40	1.34
53	L	702	CDL	OB8-CB6	-2.10	1.40	1.45
46	L	705	3PE	O31-C3	-2.08	1.40	1.45
53	K	401	CDL	OA6-CA5	2.08	1.40	1.34
46	Y	602	3PE	O21-C21	2.06	1.40	1.34
46	N	904	3PE	O21-C21	2.05	1.40	1.34
50	F	501	FMN	C10-N1	2.05	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	q	201	CDL	OB6-CB5	2.04	1.40	1.34
46	d	1201	3PE	O21-C21	2.03	1.40	1.34
45	N	903	LMT	O5B-C5B	2.01	1.49	1.44
54	O	401	GTP	PB-O2B	-2.01	1.46	1.55

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	GTP	C8-N9-C4	7.59	120.26	106.03
58	U	101	EHZ	C8-C9-S1	5.77	120.84	113.56
58	T	101	EHZ	C8-C9-S1	5.54	120.55	113.56
45	M	802	LMT	C3B-C4B-C5B	5.11	119.51	110.23
52	H	602	I49	N01-C14-N03	4.92	129.32	120.26
53	h	1001	CDL	OB6-CB5-C51	4.48	121.17	111.48
46	A	302	3PE	O21-C21-C22	4.43	121.06	111.48
46	N	904	3PE	O21-C21-C22	4.30	120.78	111.48
48	B	1003	PC1	O21-C21-C22	4.30	120.78	111.48
46	L	705	3PE	O21-C21-C22	4.26	120.70	111.48
46	I	201	3PE	O21-C21-C22	4.17	120.49	111.48
53	X	1701	CDL	OA6-CA5-C11	4.12	120.40	111.48
46	L	703	3PE	O21-C21-C22	4.12	120.39	111.48
46	Y	602	3PE	O21-C21-C22	4.10	120.35	111.48
56	P	501	NDP	P2B-O2B-C2B	-4.10	112.49	123.43
46	H	601	3PE	O21-C21-O22	-4.07	120.48	125.70
53	X	1701	CDL	OB6-CB5-C51	4.05	120.25	111.48
53	q	201	CDL	OA6-CA5-C11	4.05	120.24	111.48
53	d	1202	CDL	OA6-CA5-C11	4.05	120.24	111.48
46	d	1201	3PE	O21-C21-C22	4.02	120.18	111.48
46	I	204	3PE	O21-C21-C22	3.99	120.10	111.48
53	h	1001	CDL	OA6-CA5-C11	3.96	120.04	111.48
53	L	702	CDL	OB6-CB5-C51	3.91	119.95	111.48
46	N	902	3PE	O21-C21-C22	3.85	119.80	111.48
53	L	702	CDL	OA6-CA5-C11	3.80	119.70	111.48
46	Z	401	3PE	O21-C21-C22	3.78	119.66	111.48
46	L	701	3PE	O21-C21-C22	3.78	119.65	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.73	96.02	109.33
45	M	801	LMT	C1'-C2'-C3'	3.73	117.85	110.01
53	K	401	CDL	OA6-CA5-C11	3.62	119.31	111.48
45	h	1002	LMT	O5B-C5B-C4B	3.51	116.02	109.70
46	Y	601	3PE	O21-C21-C22	3.50	119.05	111.48
48	g	1501	PC1	O21-C21-C22	3.48	119.01	111.48
45	M	802	LMT	O5B-C5B-C4B	3.47	115.95	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	O3-PA-O1A	-3.47	100.28	110.70
53	q	201	CDL	OB6-CB5-C51	3.37	118.77	111.48
46	Y	601	3PE	O31-C31-C32	3.37	122.10	111.83
50	F	501	FMN	C4-N3-C2	-3.35	119.70	125.64
45	h	1002	LMT	C2'-C3'-C4'	3.27	117.09	109.68
53	X	1701	CDL	OB8-CB7-C71	3.26	121.77	111.83
45	h	1002	LMT	C1'-C2'-C3'	3.21	116.75	110.01
54	O	401	GTP	C2-N1-C6	-3.13	119.43	125.11
46	N	902	3PE	O31-C31-C32	3.12	121.34	111.83
46	A	302	3PE	O31-C31-C32	3.09	121.26	111.83
45	M	801	LMT	C2'-C3'-C4'	3.06	116.63	109.68
52	H	602	I49	N05-C15-N04	-3.04	111.42	120.07
45	h	1003	LMT	O5'-C5'-C4'	3.04	116.01	109.72
46	Y	602	3PE	O31-C31-C32	3.04	121.10	111.83
48	B	1003	PC1	O31-C31-C32	2.97	120.89	111.83
48	g	1501	PC1	O31-C31-C32	2.95	120.82	111.83
54	O	401	GTP	O2G-PG-O3B	2.93	114.47	104.64
50	F	501	FMN	C4A-C10-N10	2.92	120.66	116.48
54	O	401	GTP	O3G-PG-O3B	2.85	114.20	104.64
46	I	204	3PE	O31-C31-C32	2.84	120.50	111.83
53	h	1001	CDL	OA8-CA7-C31	2.83	120.48	111.83
53	q	201	CDL	OA8-CA7-C31	2.83	120.46	111.83
54	O	401	GTP	C3'-C2'-C1'	2.81	106.78	101.46
46	L	703	3PE	O31-C31-C32	2.81	120.40	111.83
53	X	1701	CDL	OA8-CA7-C31	2.80	120.37	111.83
45	Y	603	LMT	C1B-O1B-C4'	-2.80	111.35	117.98
46	B	1001	3PE	O31-C31-C32	2.79	120.33	111.83
45	l	201	LMT	O5B-C5B-C4B	2.77	114.70	109.70
56	P	501	NDP	PA-O5B-C5B	-2.76	105.52	121.35
46	H	601	3PE	O31-C31-C32	2.76	120.25	111.83
50	F	501	FMN	C4A-C4-N3	2.76	120.27	113.25
53	d	1202	CDL	OA8-CA7-C31	2.72	120.11	111.83
53	h	1001	CDL	OB8-CB7-C71	2.70	120.08	111.83
56	P	501	NDP	O2N-PN-O3	2.69	114.54	107.27
52	H	602	I49	C06-C07-C10	-2.69	116.03	120.54
45	M	802	LMT	C4B-C3B-C2B	2.68	115.53	110.83
45	M	801	LMT	C1'-O5'-C5'	-2.67	108.50	113.72
53	d	1202	CDL	OB8-CB7-C71	2.67	119.97	111.83
58	U	101	EHZ	O2-C9-C8	-2.66	119.55	123.74
52	H	602	I49	C08-C06-C07	2.64	118.79	112.83
46	L	705	3PE	O31-C31-C32	2.60	119.77	111.83
53	K	401	CDL	OA8-CA7-C31	2.60	119.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	O3X-P2B-O2X	2.59	117.53	107.80
45	h	1002	LMT	C1'-O5'-C5'	-2.57	108.70	113.72
56	P	501	NDP	PN-O5D-C5D	-2.57	106.62	121.35
54	O	401	GTP	C2'-C3'-C4'	2.56	107.56	102.61
54	O	401	GTP	C1'-N9-C8	-2.56	119.47	126.73
46	I	201	3PE	O31-C31-C32	2.53	119.54	111.83
58	T	101	EHZ	O2-C9-C8	-2.52	119.77	123.74
46	B	1001	3PE	O21-C21-C22	2.52	120.20	110.93
56	P	501	NDP	C2A-N1A-C6A	-2.52	114.60	118.73
46	Z	401	3PE	O31-C31-C32	2.52	119.51	111.83
53	L	702	CDL	OB8-CB7-C71	2.50	119.47	111.83
46	d	1201	3PE	O31-C31-C32	2.50	119.45	111.83
50	F	501	FMN	O4-C4-C4A	-2.50	119.94	126.53
45	h	1002	LMT	C3B-C4B-C5B	2.49	114.75	110.23
53	d	1202	CDL	OB6-CB5-C51	2.47	120.02	110.93
54	O	401	GTP	O2A-PA-O1A	-2.47	100.95	112.44
58	T	101	EHZ	C13-C12-N1	2.46	120.83	116.34
53	q	201	CDL	OB8-CB7-C71	2.45	119.32	111.83
45	M	801	LMT	C1B-O5B-C5B	-2.45	108.93	113.72
52	H	602	I49	N02-C14-N01	-2.44	111.80	118.08
46	N	904	3PE	O31-C31-C32	2.43	119.25	111.83
53	L	702	CDL	OA8-CA7-C31	2.42	119.22	111.83
45	l	201	LMT	C6B-C5B-C4B	-2.42	107.07	113.02
58	U	101	EHZ	O2-C9-S1	-2.41	119.61	122.68
56	P	501	NDP	N3A-C4A-N9A	2.40	131.26	127.17
54	O	401	GTP	C5-C6-N1	2.40	119.36	113.25
45	A	301	LMT	O1B-C4'-C3'	2.39	113.31	107.23
50	F	501	FMN	C10-C4A-N5	-2.39	119.94	124.81
54	O	401	GTP	O2B-PB-O1B	-2.38	101.36	112.44
56	P	501	NDP	O2N-PN-O1N	2.38	123.52	112.44
46	L	701	3PE	O31-C31-C32	2.37	119.06	111.83
58	T	101	EHZ	O2-C9-S1	-2.36	119.68	122.68
58	T	101	EHZ	C16-C15-N2	2.36	120.96	116.48
45	N	903	LMT	O1B-C4'-C3'	2.34	113.19	107.23
53	X	1701	CDL	CB4-OB6-CB5	-2.32	112.24	117.80
54	O	401	GTP	C5-C4-N9	-2.32	101.51	105.66
56	P	501	NDP	O4B-C4B-C3B	2.31	109.74	105.15
54	O	401	GTP	O6-C6-C5	-2.30	120.47	126.53
56	P	501	NDP	O5D-PN-O1N	-2.28	99.88	108.94
46	I	204	3PE	C2-O21-C21	-2.26	112.39	117.80
54	O	401	GTP	N9-C8-N7	-2.23	109.27	113.40
56	P	501	NDP	C5A-C4A-N3A	-2.23	123.65	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	L	704	LMT	C1B-O1B-C4'	-2.19	112.79	117.98
45	h	1003	LMT	C1B-O1B-C4'	-2.17	112.84	117.98
56	P	501	NDP	O7N-C7N-N7N	-2.15	118.08	122.89
58	U	101	EHZ	C7-C8-C9	-2.11	109.14	113.86
54	O	401	GTP	C1'-N9-C4	-2.11	120.26	126.49
56	P	501	NDP	O3X-P2B-O2B	-2.07	97.80	105.85
46	Y	601	3PE	O31-C31-O32	-2.05	118.50	123.63
45	l	201	LMT	C2'-C3'-C4'	2.04	114.31	109.68
58	U	101	EHZ	C16-C15-N2	2.01	120.29	116.48

There are no chirality outliers.

All (618) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
46	A	302	3PE	O21-C2-C3-O31
46	A	302	3PE	O22-C21-O21-C2
46	A	302	3PE	C22-C21-O21-C2
46	B	1001	3PE	C1-O11-P-O12
46	B	1001	3PE	C1-O11-P-O13
46	B	1001	3PE	C1-O11-P-O14
46	B	1001	3PE	C11-O13-P-O14
46	B	1001	3PE	O13-C11-C12-N
46	B	1001	3PE	C22-C21-O21-C2
46	H	601	3PE	C11-O13-P-O11
46	H	601	3PE	C11-O13-P-O12
46	H	601	3PE	O13-C11-C12-N
46	H	601	3PE	O22-C21-O21-C2
46	I	201	3PE	O13-C11-C12-N
46	I	201	3PE	O22-C21-O21-C2
46	I	201	3PE	C22-C21-O21-C2
46	I	204	3PE	C11-O13-P-O11
46	I	204	3PE	C11-O13-P-O12
46	I	204	3PE	C11-O13-P-O14
46	I	204	3PE	O13-C11-C12-N
46	L	701	3PE	O13-C11-C12-N
46	L	703	3PE	C1-O11-P-O12
46	L	703	3PE	C1-O11-P-O13
46	L	703	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
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	L	705	3PE	C1-O11-P-O12
46	L	705	3PE	C1-O11-P-O13
46	L	705	3PE	C1-O11-P-O14
46	L	705	3PE	O22-C21-O21-C2
46	N	902	3PE	O13-C11-C12-N
46	N	904	3PE	C1-O11-P-O14
46	N	904	3PE	O13-C11-C12-N
46	Y	601	3PE	C11-O13-P-O11
46	Y	601	3PE	C11-O13-P-O12
46	Y	601	3PE	C11-O13-P-O14
46	Y	602	3PE	O13-C11-C12-N
46	Y	602	3PE	C22-C21-O21-C2
46	Z	401	3PE	C1-O11-P-O12
46	Z	401	3PE	C1-O11-P-O13
46	Z	401	3PE	C1-O11-P-O14
46	Z	401	3PE	O13-C11-C12-N
46	d	1201	3PE	C22-C21-O21-C2
52	H	602	I49	C07-C06-C08-N01
52	H	602	I49	N04-C15-N02-C14
52	H	602	I49	N05-C15-N02-C14
53	K	401	CDL	CB2-OB2-PB2-OB4
53	K	401	CDL	CB2-OB2-PB2-OB5
53	L	702	CDL	CB2-C1-CA2-OA2
53	L	702	CDL	CA2-OA2-PA1-OA4
53	L	702	CDL	CA2-OA2-PA1-OA5
53	L	702	CDL	CA3-OA5-PA1-OA3
53	X	1701	CDL	OA7-CA5-OA6-CA4
53	X	1701	CDL	CB2-OB2-PB2-OB3
53	X	1701	CDL	CB2-OB2-PB2-OB5
53	d	1202	CDL	CA2-OA2-PA1-OA3
53	d	1202	CDL	CA2-OA2-PA1-OA4
53	d	1202	CDL	CA3-OA5-PA1-OA2
53	d	1202	CDL	CA3-OA5-PA1-OA3
53	d	1202	CDL	CB2-OB2-PB2-OB4
53	d	1202	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	CA2-OA2-PA1-OA3
53	h	1001	CDL	CA2-OA2-PA1-OA4
53	h	1001	CDL	CA2-OA2-PA1-OA5
53	h	1001	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
53	h	1001	CDL	CA3-OA5-PA1-OA4
53	h	1001	CDL	CB2-OB2-PB2-OB3
53	h	1001	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	CA2-OA2-PA1-OA4
53	q	201	CDL	CA2-OA2-PA1-OA5
53	q	201	CDL	CA3-OA5-PA1-OA2
53	q	201	CDL	CA3-OA5-PA1-OA4
53	q	201	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CB2-OB2-PB2-OB5
53	q	201	CDL	OB5-CB3-CB4-OB6
54	O	401	GTP	PB-O3B-PG-O2G
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-C17
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	O4-C15-C16-C17
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
59	o	201	MYR	O1-C1-C2-C3
45	A	301	LMT	C3'-C4'-O1B-C1B
53	X	1701	CDL	OB9-CB7-OB8-CB6
45	M	802	LMT	O5B-C1B-O1B-C4'
53	X	1701	CDL	C71-CB7-OB8-CB6
46	N	902	3PE	O32-C31-O31-C3
46	Y	602	3PE	O32-C31-O31-C3
46	Z	401	3PE	O32-C31-O31-C3
53	X	1701	CDL	OA9-CA7-OA8-CA6
53	d	1202	CDL	OB9-CB7-OB8-CB6
53	h	1001	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	O22-C21-O21-C2
46	L	703	3PE	O22-C21-O21-C2
46	Y	602	3PE	O22-C21-O21-C2
46	d	1201	3PE	O22-C21-O21-C2
53	d	1202	CDL	OB7-CB5-OB6-CB4
53	q	201	CDL	OA7-CA5-OA6-CA4
45	M	802	LMT	C2B-C1B-O1B-C4'
46	N	902	3PE	C32-C31-O31-C3
46	Z	401	3PE	C32-C31-O31-C3
46	d	1201	3PE	C32-C31-O31-C3
53	h	1001	CDL	C71-CB7-OB8-CB6
45	l	201	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
46	L	701	3PE	C22-C21-O21-C2
46	L	703	3PE	C22-C21-O21-C2
46	L	705	3PE	C22-C21-O21-C2
53	X	1701	CDL	C11-CA5-OA6-CA4
53	h	1001	CDL	C51-CB5-OB6-CB4
53	q	201	CDL	C11-CA5-OA6-CA4
45	N	903	LMT	C3'-C4'-O1B-C1B
46	Y	602	3PE	C32-C31-O31-C3
53	X	1701	CDL	C31-CA7-OA8-CA6
53	d	1202	CDL	C71-CB7-OB8-CB6
53	q	201	CDL	C31-CA7-OA8-CA6
45	j	101	LMT	O5'-C5'-C6'-O6'
46	d	1201	3PE	O32-C31-O31-C3
46	B	1001	3PE	O22-C21-O21-C2
53	d	1202	CDL	O1-C1-CA2-OA2
45	A	301	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	O5B-C5B-C6B-O6B
45	h	1003	LMT	C4'-C5'-C6'-O6'
46	Y	601	3PE	C22-C21-O21-C2
48	B	1003	PC1	C22-C21-O21-C2
53	d	1202	CDL	C11-CA5-OA6-CA4
45	h	1002	LMT	O5B-C1B-O1B-C4'
45	h	1003	LMT	O5'-C5'-C6'-O6'
45	j	101	LMT	C4'-C5'-C6'-O6'
56	P	501	NDP	O4D-C4D-C5D-O5D
45	Y	603	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	CB4-CB3-OB5-PB2
53	q	201	CDL	OA9-CA7-OA8-CA6
45	L	704	LMT	O5'-C1'-O1'-C1
45	N	903	LMT	O5'-C1'-O1'-C1
45	h	1002	LMT	C3'-C4'-O1B-C1B
45	l	201	LMT	O5'-C5'-C6'-O6'
45	M	801	LMT	C4B-C5B-C6B-O6B
46	N	904	3PE	O32-C31-O31-C3
46	Y	601	3PE	O22-C21-O21-C2
48	B	1003	PC1	O22-C21-O21-C2
53	d	1202	CDL	OA7-CA5-OA6-CA4
53	h	1001	CDL	CA2-C1-CB2-OB2
46	L	701	3PE	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
46	N	904	3PE	C32-C31-O31-C3
48	B	1003	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
48	g	1501	PC1	C32-C31-O31-C3
45	Y	603	LMT	C4B-C5B-C6B-O6B
45	A	301	LMT	C2'-C1'-O1'-C1
45	L	704	LMT	C2'-C1'-O1'-C1
48	g	1501	PC1	O32-C31-O31-C3
45	N	903	LMT	C4'-C5'-C6'-O6'
45	N	901	LMT	C4B-C5B-C6B-O6B
46	B	1001	3PE	O11-C1-C2-O21
45	N	901	LMT	O5B-C5B-C6B-O6B
53	L	702	CDL	C71-CB7-OB8-CB6
45	M	802	LMT	C3'-C4'-O1B-C1B
45	M	801	LMT	O5B-C5B-C6B-O6B
46	d	1201	3PE	C31-C32-C33-C34
46	I	204	3PE	C21-C22-C23-C24
46	N	902	3PE	C31-C32-C33-C34
48	B	1003	PC1	C21-C22-C23-C24
53	h	1001	CDL	CB5-C51-C52-C53
48	B	1003	PC1	O32-C31-O31-C3
45	A	301	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	C31-C32-C33-C34
46	L	701	3PE	C21-C22-C23-C24
53	X	1701	CDL	CB7-C71-C72-C73
46	L	701	3PE	O32-C31-O31-C3
45	h	1002	LMT	C5'-C4'-O1B-C1B
53	L	702	CDL	O1-C1-CA2-OA2
53	h	1001	CDL	O1-C1-CB2-OB2
46	L	703	3PE	O32-C31-O31-C3
46	Z	401	3PE	C31-C32-C33-C34
53	L	702	CDL	CB5-C51-C52-C53
53	L	702	CDL	OB9-CB7-OB8-CB6
45	M	802	LMT	C5'-C4'-O1B-C1B
46	Y	602	3PE	C31-C32-C33-C34
53	d	1202	CDL	CB2-C1-CA2-OA2
46	L	703	3PE	C21-C22-C23-C24
46	I	204	3PE	C22-C21-O21-C2
46	I	204	3PE	O22-C21-O21-C2
46	I	204	3PE	C32-C31-O31-C3
45	N	903	LMT	O5'-C5'-C6'-O6'
58	U	101	EHZ	C5-C6-C7-O1
53	h	1001	CDL	C31-CA7-OA8-CA6
48	g	1501	PC1	C31-C32-C33-C34
59	o	201	MYR	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
46	N	902	3PE	C35-C36-C37-C38
46	N	904	3PE	C22-C23-C24-C25
46	N	904	3PE	C23-C24-C25-C26
46	d	1201	3PE	C33-C34-C35-C36
53	L	702	CDL	C54-C55-C56-C57
53	d	1202	CDL	C33-C34-C35-C36
53	q	201	CDL	C59-C60-C61-C62
58	U	101	EHZ	C3-C4-C5-C6
46	d	1201	3PE	C21-C22-C23-C24
48	g	1501	PC1	C24-C25-C26-C27
48	g	1501	PC1	C2A-C2B-C2C-C2D
53	X	1701	CDL	C57-C58-C59-C60
53	h	1001	CDL	C71-C72-C73-C74
45	h	1003	LMT	C2-C1-O1'-C1'
48	g	1501	PC1	C21-C22-C23-C24
46	A	302	3PE	C2A-C2B-C2C-C2D
53	X	1701	CDL	C56-C57-C58-C59
59	o	201	MYR	C11-C10-C9-C8
58	T	101	EHZ	C5-C6-C7-C8
46	I	201	3PE	C21-C22-C23-C24
53	K	401	CDL	CA5-C11-C12-C13
53	d	1202	CDL	CB7-C71-C72-C73
45	N	903	LMT	C1-C2-C3-C4
45	Y	603	LMT	C2-C3-C4-C5
48	g	1501	PC1	C28-C29-C2A-C2B
46	N	904	3PE	C32-C33-C34-C35
46	A	302	3PE	C26-C27-C28-C29
46	Y	602	3PE	C1-C2-C3-O31
46	A	302	3PE	C28-C29-C2A-C2B
53	X	1701	CDL	C72-C73-C74-C75
53	h	1001	CDL	C17-C18-C19-C20
46	L	703	3PE	C3C-C3D-C3E-C3F
46	Y	601	3PE	C2A-C2B-C2C-C2D
53	h	1001	CDL	C20-C21-C22-C23
59	o	201	MYR	C4-C5-C6-C7
45	N	903	LMT	C11-C10-C9-C8
53	X	1701	CDL	CA5-C11-C12-C13
53	d	1202	CDL	CA7-C31-C32-C33
46	I	204	3PE	O32-C31-O31-C3
46	I	204	3PE	C23-C24-C25-C26
53	h	1001	CDL	C12-C13-C14-C15
53	h	1001	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	K	401	CDL	C31-C32-C33-C34
53	L	702	CDL	C34-C35-C36-C37
53	d	1202	CDL	C32-C33-C34-C35
53	L	702	CDL	C51-C52-C53-C54
45	A	301	LMT	C1-C2-C3-C4
45	A	301	LMT	O5B-C5B-C6B-O6B
53	X	1701	CDL	C11-C12-C13-C14
53	X	1701	CDL	O1-C1-CB2-OB2
53	X	1701	CDL	C51-CB5-OB6-CB4
53	h	1001	CDL	C11-CA5-OA6-CA4
53	X	1701	CDL	C20-C21-C22-C23
53	X	1701	CDL	OB7-CB5-OB6-CB4
45	Y	603	LMT	C3-C4-C5-C6
46	I	201	3PE	C33-C34-C35-C36
45	h	1002	LMT	C4B-C5B-C6B-O6B
53	q	201	CDL	C51-C52-C53-C54
45	L	704	LMT	C5-C6-C7-C8
46	d	1201	3PE	C37-C38-C39-C3A
58	T	101	EHZ	C5-C6-C7-O1
53	X	1701	CDL	C19-C20-C21-C22
45	Y	603	LMT	O5'-C5'-C6'-O6'
46	H	601	3PE	C2-C1-O11-P
46	d	1201	3PE	C2-C1-O11-P
46	N	902	3PE	C37-C38-C39-C3A
48	B	1003	PC1	C32-C33-C34-C35
58	U	101	EHZ	C1-C2-C3-C4
53	L	702	CDL	C35-C36-C37-C38
46	A	302	3PE	C27-C28-C29-C2A
46	A	302	3PE	C2C-C2D-C2E-C2F
46	H	601	3PE	C32-C33-C34-C35
53	q	201	CDL	C52-C53-C54-C55
48	g	1501	PC1	C2C-C2D-C2E-C2F
58	T	101	EHZ	O4-C15-C16-O5
46	B	1001	3PE	O11-C1-C2-C3
53	X	1701	CDL	OB5-CB3-CB4-CB6
45	N	903	LMT	O5B-C5B-C6B-O6B
46	B	1001	3PE	C35-C36-C37-C38
48	B	1003	PC1	C24-C25-C26-C27
46	L	703	3PE	C31-C32-C33-C34
53	L	702	CDL	C11-CA5-OA6-CA4
46	L	705	3PE	C33-C34-C35-C36
46	L	701	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	d	1201	3PE	C1-C2-C3-O31
48	B	1003	PC1	C1-C2-C3-O31
53	L	702	CDL	CA3-CA4-CA6-OA8
46	N	902	3PE	C33-C34-C35-C36
46	N	904	3PE	C26-C27-C28-C29
53	L	702	CDL	C31-C32-C33-C34
53	K	401	CDL	C36-C37-C38-C39
53	K	401	CDL	CB2-OB2-PB2-OB3
46	N	904	3PE	C33-C34-C35-C36
46	A	302	3PE	C1-C2-O21-C21
46	A	302	3PE	C35-C36-C37-C38
45	l	201	LMT	C3'-C4'-O1B-C1B
53	X	1701	CDL	CB2-C1-CA2-OA2
53	X	1701	CDL	CA2-C1-CB2-OB2
46	A	302	3PE	C32-C31-O31-C3
46	Y	602	3PE	C3B-C3C-C3D-C3E
53	q	201	CDL	C57-C58-C59-C60
46	I	204	3PE	C35-C36-C37-C38
53	h	1001	CDL	C16-C17-C18-C19
45	l	201	LMT	C5'-C4'-O1B-C1B
46	L	703	3PE	C22-C23-C24-C25
46	L	703	3PE	C34-C35-C36-C37
46	Z	401	3PE	C32-C33-C34-C35
46	L	701	3PE	O21-C2-C3-O31
53	L	702	CDL	OB6-CB4-CB6-OB8
53	X	1701	CDL	OA6-CA4-CA6-OA8
53	X	1701	CDL	O1-C1-CA2-OA2
46	I	201	3PE	C3A-C3B-C3C-C3D
53	X	1701	CDL	C21-C22-C23-C24
53	d	1202	CDL	C31-C32-C33-C34
46	Y	602	3PE	C23-C24-C25-C26
46	d	1201	3PE	C3F-C3G-C3H-C3I
53	h	1001	CDL	C15-C16-C17-C18
46	I	204	3PE	C25-C26-C27-C28
46	L	701	3PE	C22-C23-C24-C25
46	N	902	3PE	C2E-C2F-C2G-C2H
53	q	201	CDL	CA5-C11-C12-C13
46	I	201	3PE	C2B-C2C-C2D-C2E
53	L	702	CDL	C38-C39-C40-C41
45	M	801	LMT	C2-C1-O1'-C1'
53	q	201	CDL	C1-CA2-OA2-PA1
46	B	1001	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
46	Y	601	3PE	C33-C34-C35-C36
53	h	1001	CDL	C51-C52-C53-C54
59	o	201	MYR	C7-C8-C9-C10
46	A	302	3PE	O11-C1-C2-C3
46	L	703	3PE	O11-C1-C2-C3
53	X	1701	CDL	OA5-CA3-CA4-CA6
53	q	201	CDL	OB5-CB3-CB4-CB6
48	g	1501	PC1	C22-C21-O21-C2
48	g	1501	PC1	C2E-C2F-C2G-C2H
53	X	1701	CDL	C74-C75-C76-C77
52	H	602	I49	C08-C06-C07-C09
53	h	1001	CDL	OA7-CA5-OA6-CA4
46	I	204	3PE	C24-C25-C26-C27
46	L	701	3PE	C28-C29-C2A-C2B
45	l	201	LMT	O1'-C1-C2-C3
53	K	401	CDL	C18-C19-C20-C21
53	K	401	CDL	C16-C17-C18-C19
53	L	702	CDL	OA7-CA5-OA6-CA4
52	H	602	I49	C08-C06-C07-C10
46	A	302	3PE	O11-C1-C2-O21
46	Z	401	3PE	O11-C1-C2-O21
46	A	302	3PE	C2-C1-O11-P
48	g	1501	PC1	C2-C1-O11-P
45	l	201	LMT	C4-C5-C6-C7
58	T	101	EHZ	O1-C7-C8-C9
46	Y	601	3PE	C32-C33-C34-C35
53	h	1001	CDL	C24-C25-C26-C27
46	I	204	3PE	O21-C2-C3-O31
48	B	1003	PC1	O21-C2-C3-O31
53	X	1701	CDL	OB6-CB4-CB6-OB8
53	q	201	CDL	OB6-CB4-CB6-OB8
56	P	501	NDP	C3D-C4D-C5D-O5D
46	L	705	3PE	C31-C32-C33-C34
46	L	701	3PE	C3B-C3C-C3D-C3E
48	B	1003	PC1	C34-C35-C36-C37
46	B	1001	3PE	C32-C33-C34-C35
46	L	703	3PE	C29-C2A-C2B-C2C
46	I	201	3PE	C29-C2A-C2B-C2C
53	L	702	CDL	C60-C61-C62-C63
58	T	101	EHZ	C6-C7-C8-C9
48	g	1501	PC1	C3A-C3B-C3C-C3D
53	K	401	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
46	I	201	3PE	C37-C38-C39-C3A
48	g	1501	PC1	C29-C2A-C2B-C2C
53	q	201	CDL	OA5-CA3-CA4-CA6
46	N	902	3PE	C38-C39-C3A-C3B
46	Y	601	3PE	C28-C29-C2A-C2B
46	A	302	3PE	O32-C31-O31-C3
53	L	702	CDL	C51-CB5-OB6-CB4
58	T	101	EHZ	C21-C22-C23-C24
46	Y	601	3PE	C29-C2A-C2B-C2C
53	h	1001	CDL	C72-C73-C74-C75
48	g	1501	PC1	C23-C24-C25-C26
45	N	903	LMT	C5'-C4'-O1B-C1B
46	H	601	3PE	C33-C34-C35-C36
53	K	401	CDL	OA7-CA5-OA6-CA4
46	L	705	3PE	O11-C1-C2-O21
53	X	1701	CDL	OA5-CA3-CA4-OA6
53	q	201	CDL	OA5-CA3-CA4-OA6
46	A	302	3PE	C1-C2-C3-O31
53	L	702	CDL	CB3-CB4-CB6-OB8
53	X	1701	CDL	CA3-CA4-CA6-OA8
53	X	1701	CDL	CB3-CB4-CB6-OB8
46	I	201	3PE	C12-C11-O13-P
46	N	902	3PE	C12-C11-O13-P
46	Y	601	3PE	C12-C11-O13-P
46	L	701	3PE	C2C-C2D-C2E-C2F
45	M	802	LMT	C7-C8-C9-C10
46	d	1201	3PE	O21-C2-C3-O31
48	g	1501	PC1	O22-C21-O21-C2
53	d	1202	CDL	C38-C39-C40-C41
53	d	1202	CDL	C41-C42-C43-C44
46	I	201	3PE	C32-C33-C34-C35
53	h	1001	CDL	C23-C24-C25-C26
48	B	1003	PC1	C31-C32-C33-C34
53	L	702	CDL	C32-C33-C34-C35
45	L	704	LMT	O1'-C1-C2-C3
45	L	704	LMT	C9-C10-C11-C12
46	N	904	3PE	C22-C21-O21-C2
46	L	701	3PE	C33-C34-C35-C36
45	Y	603	LMT	C2-C1-O1'-C1'
45	A	301	LMT	C3-C4-C5-C6
53	h	1001	CDL	C31-C32-C33-C34
56	P	501	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
46	Z	401	3PE	O11-C1-C2-C3
53	L	702	CDL	OB7-CB5-OB6-CB4
58	T	101	EHZ	C18-C17-C20-O6
53	L	702	CDL	CB7-C71-C72-C73
46	d	1201	3PE	C3A-C3B-C3C-C3D
53	q	201	CDL	CA4-CA3-OA5-PA1
46	L	701	3PE	C27-C28-C29-C2A
46	L	703	3PE	O11-C1-C2-O21
53	X	1701	CDL	OB5-CB3-CB4-OB6
53	d	1202	CDL	OB5-CB3-CB4-OB6
53	q	201	CDL	C56-C57-C58-C59
46	N	902	3PE	C36-C37-C38-C39
52	H	602	I49	N01-C14-N02-C15
46	Y	602	3PE	O21-C2-C3-O31
53	L	702	CDL	OA6-CA4-CA6-OA8
46	Y	601	3PE	C26-C27-C28-C29
46	L	705	3PE	C21-C22-C23-C24
58	U	101	EHZ	C2-C3-C4-C5
53	q	201	CDL	CB3-CB4-CB6-OB8
58	T	101	EHZ	C16-C17-C20-O6
53	q	201	CDL	C15-C16-C17-C18
46	L	703	3PE	C27-C28-C29-C2A
46	L	701	3PE	C2F-C2G-C2H-C2I
46	Y	601	3PE	C36-C37-C38-C39
46	Y	601	3PE	C34-C35-C36-C37
46	A	302	3PE	C11-O13-P-O11
46	A	302	3PE	C11-O13-P-O14
46	B	1001	3PE	C11-O13-P-O11
46	B	1001	3PE	C11-O13-P-O12
46	I	201	3PE	C1-O11-P-O14
46	L	701	3PE	C1-O11-P-O12
46	L	701	3PE	C1-O11-P-O13
46	L	705	3PE	C11-O13-P-O14
46	N	904	3PE	C1-O11-P-O13
46	Y	601	3PE	O13-C11-C12-N
46	d	1201	3PE	O13-C11-C12-N
53	K	401	CDL	CA3-OA5-PA1-OA2
53	K	401	CDL	CA3-OA5-PA1-OA3
53	K	401	CDL	CA3-OA5-PA1-OA4
53	L	702	CDL	CA2-OA2-PA1-OA3
53	X	1701	CDL	CA2-OA2-PA1-OA5
53	d	1202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	d	1202	CDL	CB2-OB2-PB2-OB3
53	d	1202	CDL	CB2-OB2-PB2-OB5
53	h	1001	CDL	CA3-OA5-PA1-OA3
53	h	1001	CDL	CB2-OB2-PB2-OB4
53	q	201	CDL	CA2-OA2-PA1-OA3
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CB3-OB5-PB2-OB3
53	q	201	CDL	CB3-OB5-PB2-OB4
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A
48	g	1501	PC1	C39-C3A-C3B-C3C
46	N	902	3PE	C22-C23-C24-C25
58	U	101	EHZ	C1-C21-C22-C23
50	F	501	FMN	C5'-O5'-P-O1P
53	h	1001	CDL	CA6-CA4-OA6-CA5
46	I	201	3PE	C23-C24-C25-C26
46	I	201	3PE	C24-C25-C26-C27
53	d	1202	CDL	OB5-CB3-CB4-CB6
46	L	701	3PE	C2D-C2E-C2F-C2G
53	d	1202	CDL	C71-C72-C73-C74
45	N	903	LMT	C3-C4-C5-C6
46	I	201	3PE	C25-C26-C27-C28
46	B	1001	3PE	O31-C31-C32-C33
46	L	703	3PE	C25-C26-C27-C28
46	N	904	3PE	O22-C21-O21-C2
45	M	801	LMT	C1-C2-C3-C4
53	X	1701	CDL	C52-C51-CB5-OB6
46	Y	601	3PE	C23-C24-C25-C26
46	N	902	3PE	C26-C27-C28-C29
53	X	1701	CDL	C54-C55-C56-C57
45	N	903	LMT	C5-C6-C7-C8
46	d	1201	3PE	C3E-C3F-C3G-C3H
46	I	201	3PE	C2D-C2E-C2F-C2G
54	O	401	GTP	PG-O3B-PB-O2B
46	Y	601	3PE	O21-C21-C22-C23
45	M	802	LMT	C4'-C5'-C6'-O6'
46	L	701	3PE	C2E-C2F-C2G-C2H
46	Y	601	3PE	C35-C36-C37-C38
53	d	1202	CDL	C44-C45-C46-C47
53	L	702	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
59	o	201	MYR	C11-C12-C13-C14
46	I	204	3PE	C33-C34-C35-C36
46	Y	601	3PE	C37-C38-C39-C3A
46	L	703	3PE	C3B-C3C-C3D-C3E
46	A	302	3PE	C2B-C2C-C2D-C2E
46	d	1201	3PE	C3B-C3C-C3D-C3E
46	L	703	3PE	C39-C3A-C3B-C3C
46	N	902	3PE	C2A-C2B-C2C-C2D
46	N	902	3PE	O21-C2-C3-O31
48	g	1501	PC1	C33-C34-C35-C36
53	d	1202	CDL	C76-C77-C78-C79
46	B	1001	3PE	C36-C37-C38-C39
46	I	204	3PE	C1-C2-C3-O31
45	h	1002	LMT	C5-C6-C7-C8
46	N	902	3PE	O11-C1-C2-O21
45	l	201	LMT	C11-C10-C9-C8
46	Y	602	3PE	C33-C34-C35-C36
45	L	704	LMT	C4B-C5B-C6B-O6B
58	U	101	EHZ	C22-C23-C24-C25
53	K	401	CDL	O1-C1-CB2-OB2
56	P	501	NDP	PN-O3-PA-O1A
46	N	904	3PE	C2-C1-O11-P
46	Y	601	3PE	C2-C1-O11-P
53	X	1701	CDL	C1-CB2-OB2-PB2
46	N	904	3PE	C27-C28-C29-C2A
46	Y	601	3PE	C27-C28-C29-C2A
52	H	602	I49	N03-C14-N02-C15
46	N	904	3PE	C3A-C3B-C3C-C3D
46	I	201	3PE	C3B-C3C-C3D-C3E
58	T	101	EHZ	C12-C13-C14-N2
46	Y	602	3PE	C39-C3A-C3B-C3C
53	q	201	CDL	CA2-C1-CB2-OB2
46	L	701	3PE	C3C-C3D-C3E-C3F
46	Y	602	3PE	C34-C35-C36-C37
46	L	705	3PE	O11-C1-C2-C3
46	L	703	3PE	C2-C1-O11-P
46	I	201	3PE	C2E-C2F-C2G-C2H
46	H	601	3PE	C1-C2-O21-C21
46	H	601	3PE	C3-C2-O21-C21
48	g	1501	PC1	C38-C39-C3A-C3B
59	o	201	MYR	C10-C11-C12-C13
46	L	705	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
46	L	703	3PE	C33-C34-C35-C36
46	A	302	3PE	C23-C24-C25-C26
46	N	902	3PE	C23-C24-C25-C26
53	X	1701	CDL	C16-C17-C18-C19
46	I	204	3PE	C32-C33-C34-C35
53	d	1202	CDL	OA5-CA3-CA4-OA6
46	d	1201	3PE	C35-C36-C37-C38
46	N	902	3PE	C1-C2-C3-O31
53	d	1202	CDL	CA3-CA4-CA6-OA8
46	A	302	3PE	C22-C23-C24-C25
53	X	1701	CDL	C53-C54-C55-C56
53	h	1001	CDL	C32-C33-C34-C35
53	d	1202	CDL	C11-C12-C13-C14
46	I	201	3PE	C27-C28-C29-C2A
46	Y	601	3PE	C38-C39-C3A-C3B
58	T	101	EHZ	C22-C23-C24-C25
46	Z	401	3PE	C12-C11-O13-P
53	d	1202	CDL	OA6-CA4-CA6-OA8
53	q	201	CDL	OA6-CA4-CA6-OA8
46	Y	602	3PE	O11-C1-C2-C3
53	K	401	CDL	C33-C34-C35-C36
46	B	1001	3PE	C37-C38-C39-C3A
53	L	702	CDL	C55-C56-C57-C58
53	X	1701	CDL	C59-C60-C61-C62
53	L	702	CDL	C52-C51-CB5-OB6
53	d	1202	CDL	C40-C41-C42-C43
48	B	1003	PC1	O21-C21-C22-C23
46	Z	401	3PE	O22-C21-O21-C2
45	M	801	LMT	C4'-C5'-C6'-O6'
46	L	703	3PE	C38-C39-C3A-C3B
53	K	401	CDL	C12-C11-CA5-OA6
53	K	401	CDL	C32-C31-CA7-OA8
46	N	902	3PE	C27-C28-C29-C2A
53	X	1701	CDL	C77-C78-C79-C80
45	L	704	LMT	O5B-C5B-C6B-O6B
46	Y	602	3PE	C2-C1-O11-P
46	I	201	3PE	O32-C31-O31-C3
48	B	1003	PC1	C35-C36-C37-C38
53	h	1001	CDL	C22-C23-C24-C25
46	d	1201	3PE	O21-C21-C22-C23
53	X	1701	CDL	C12-C11-CA5-OA6
46	I	201	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	I	201	3PE	C26-C27-C28-C29
46	I	201	3PE	C32-C31-O31-C3
53	q	201	CDL	C32-C31-CA7-OA8
53	d	1202	CDL	CA5-C11-C12-C13
54	O	401	GTP	PB-O3B-PG-O1G
53	d	1202	CDL	C72-C71-CB7-OB8
53	q	201	CDL	C52-C51-CB5-OB6
45	M	802	LMT	C5-C6-C7-C8
50	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C19-C17-C20-O6
45	j	101	LMT	O5B-C5B-C6B-O6B
46	A	302	3PE	C33-C34-C35-C36
45	h	1003	LMT	C7-C8-C9-C10
45	N	901	LMT	C4'-C5'-C6'-O6'
46	L	705	3PE	C32-C33-C34-C35
56	P	501	NDP	C2B-O2B-P2B-O1X
46	Y	602	3PE	O11-C1-C2-O21
45	Y	603	LMT	O5'-C1'-O1'-C1
46	I	201	3PE	C28-C29-C2A-C2B
45	h	1003	LMT	C6-C7-C8-C9
53	K	401	CDL	C12-C11-CA5-OA7
53	K	401	CDL	C32-C31-CA7-OA9
53	X	1701	CDL	C12-C11-CA5-OA7
46	d	1201	3PE	C36-C37-C38-C39
53	q	201	CDL	C52-C51-CB5-OB7
46	A	302	3PE	C25-C26-C27-C28
45	j	101	LMT	C1-C2-C3-C4
58	U	101	EHZ	C10-C11-N1-C12
53	L	702	CDL	C52-C51-CB5-OB7
46	Y	601	3PE	C3A-C3B-C3C-C3D
45	L	704	LMT	C6-C7-C8-C9
45	h	1003	LMT	C11-C10-C9-C8
46	Z	401	3PE	O31-C31-C32-C33
46	I	201	3PE	C2C-C2D-C2E-C2F
48	B	1003	PC1	O22-C21-C22-C23
48	g	1501	PC1	C2F-C2G-C2H-C2I
46	Y	601	3PE	C25-C26-C27-C28
53	d	1202	CDL	C72-C71-CB7-OB9
46	d	1201	3PE	C34-C35-C36-C37
53	q	201	CDL	C32-C31-CA7-OA9
53	X	1701	CDL	C55-C56-C57-C58
46	Z	401	3PE	C22-C21-O21-C2

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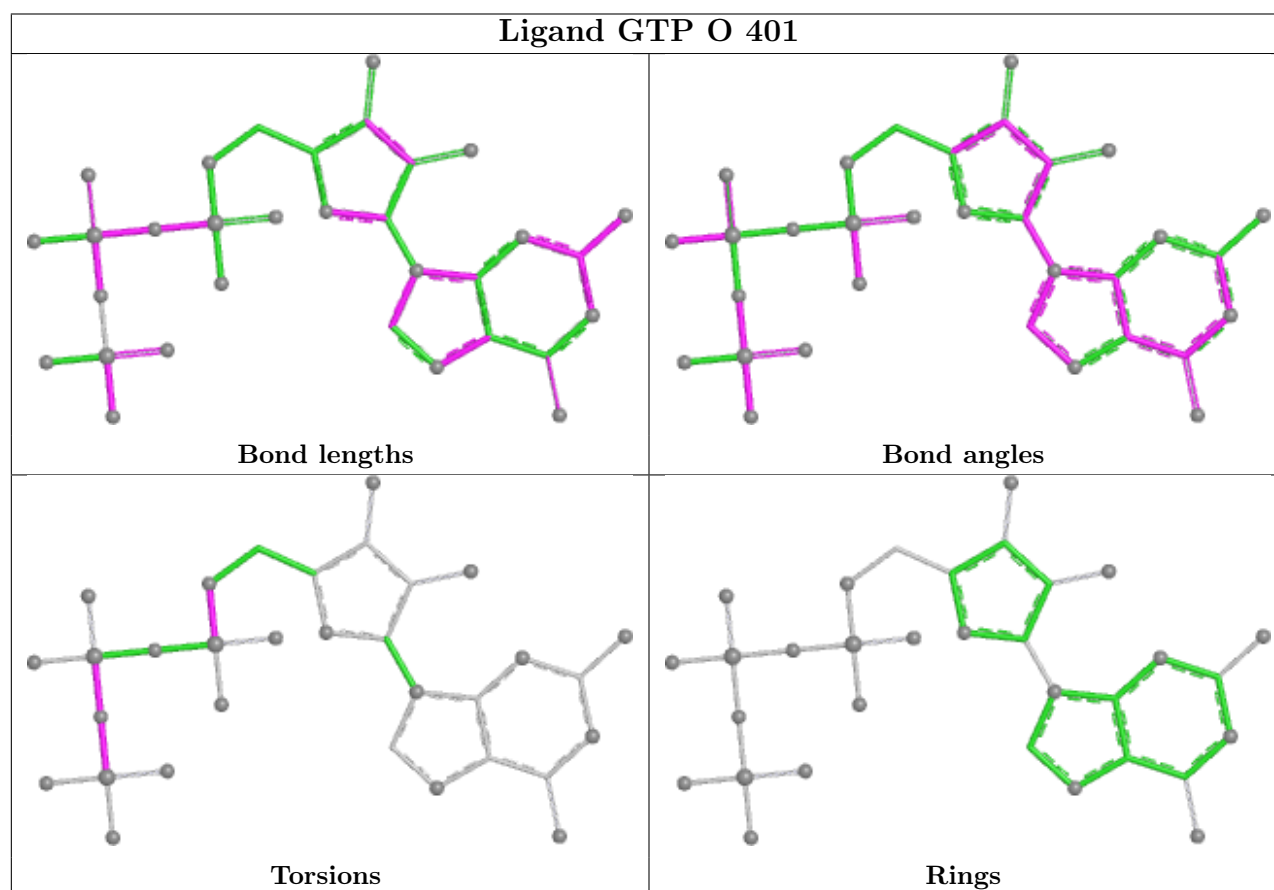
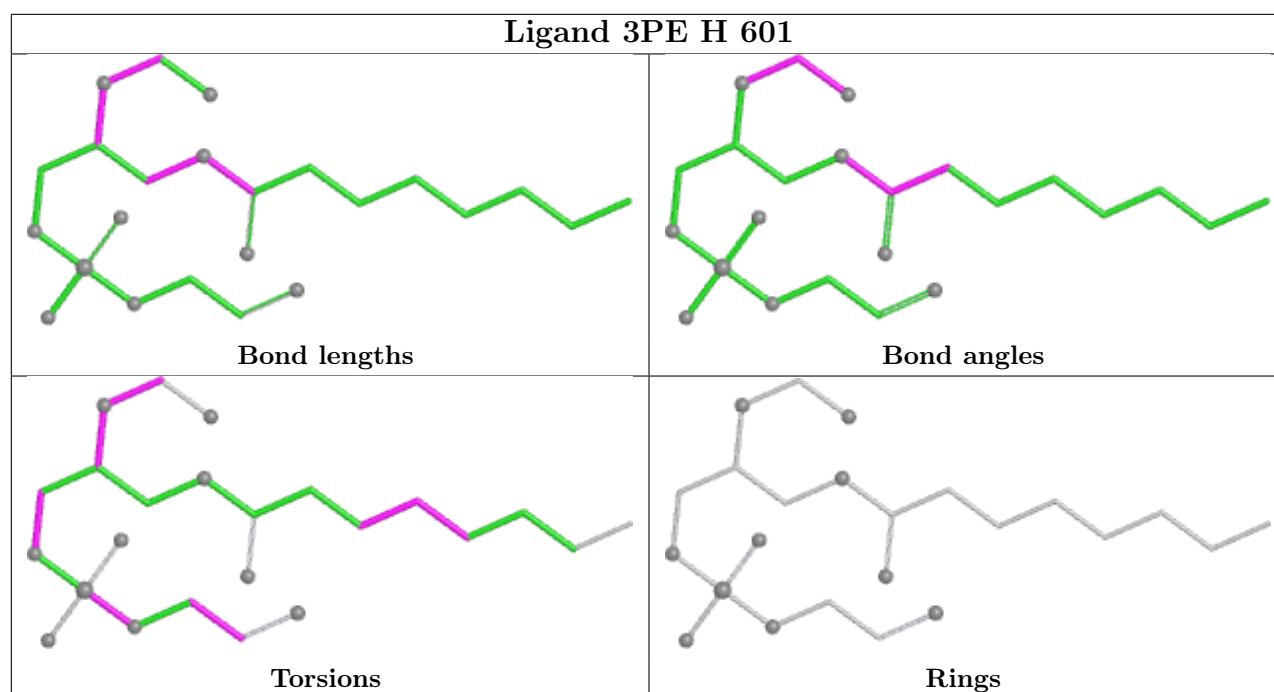
Mol	Chain	Res	Type	Atoms
46	d	1201	3PE	O22-C21-C22-C23
53	X	1701	CDL	C32-C31-CA7-OA8

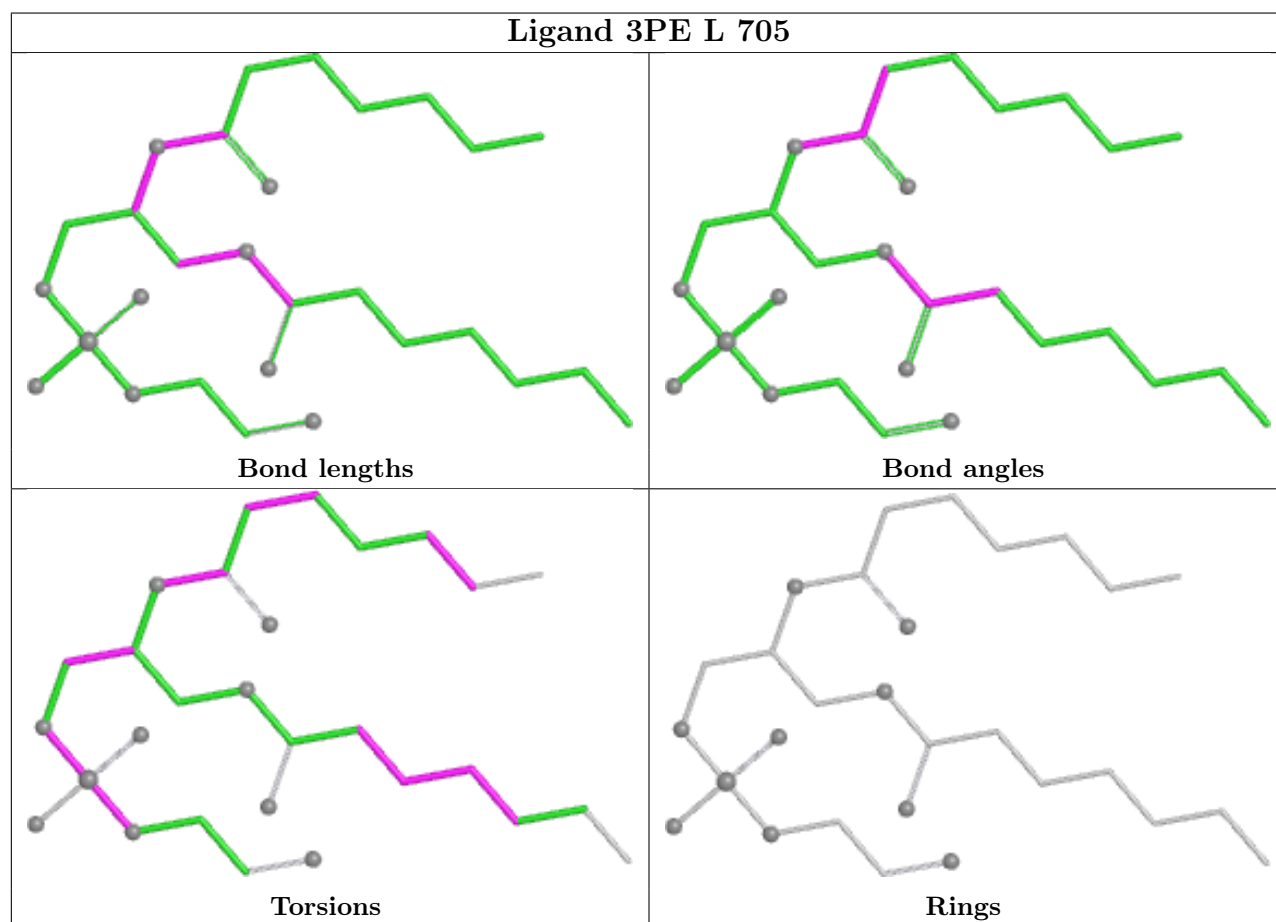
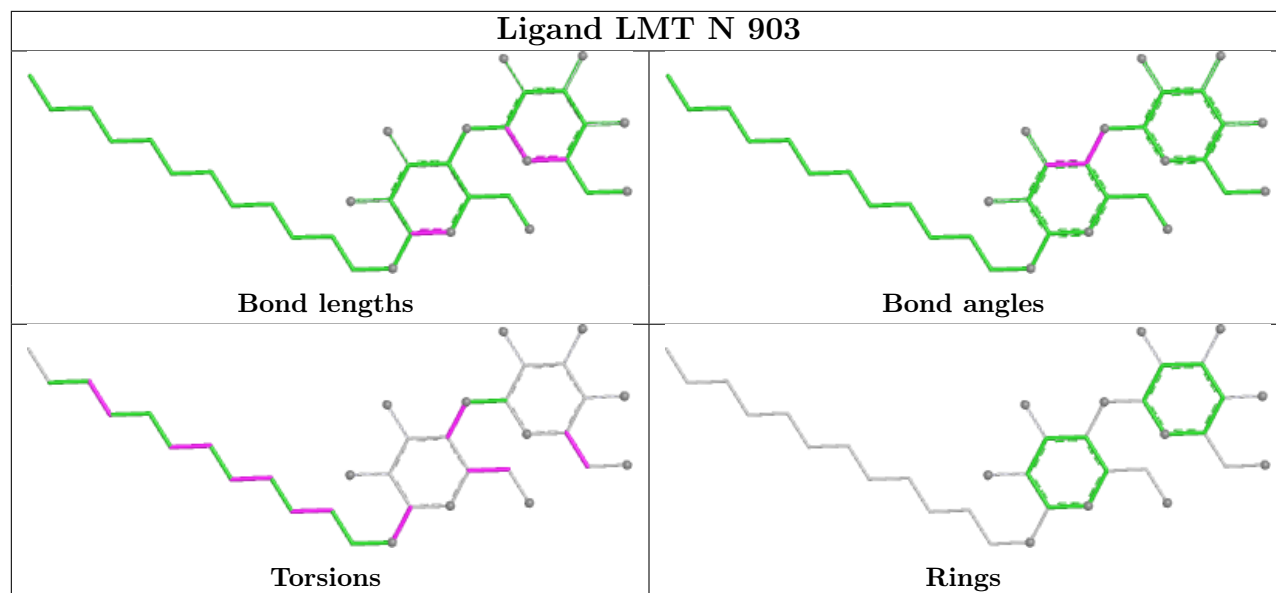
There are no ring outliers.

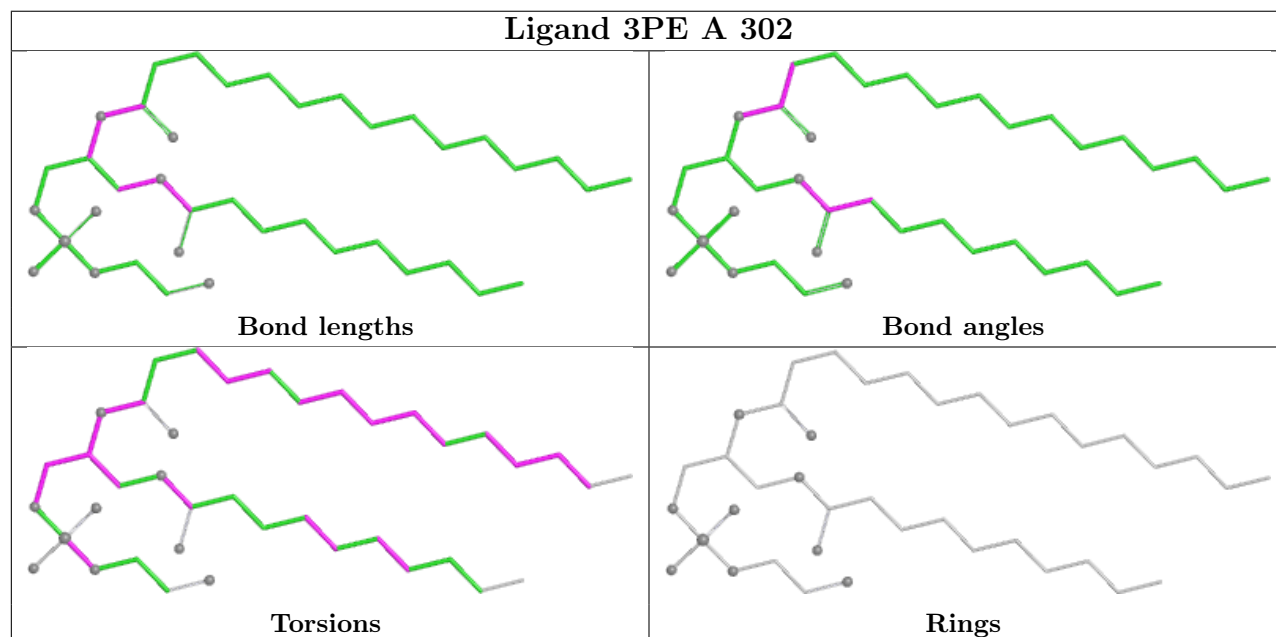
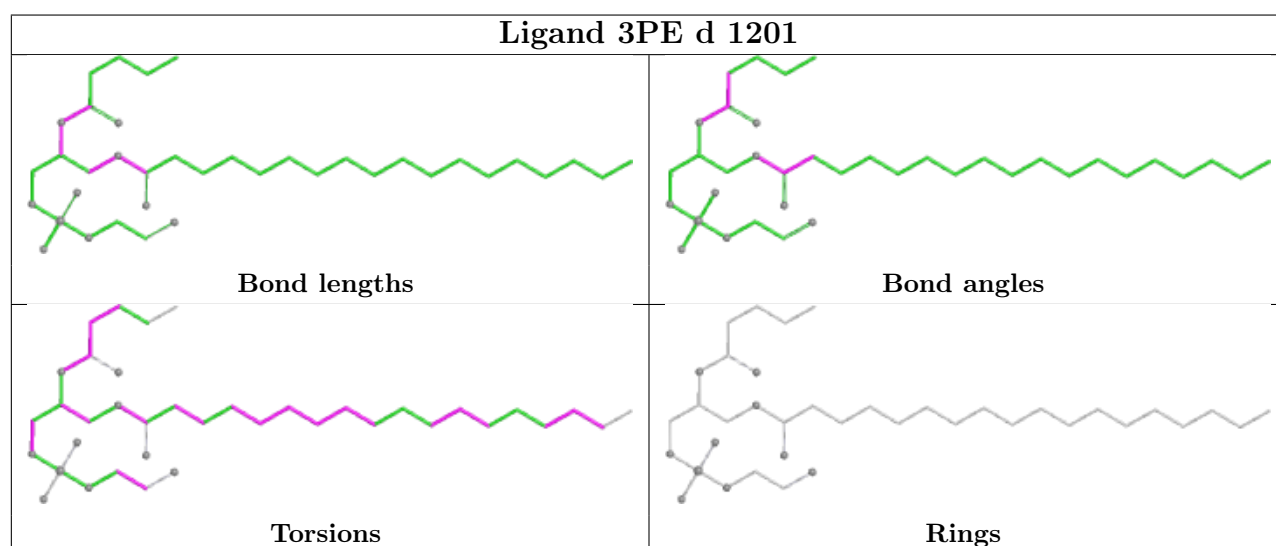
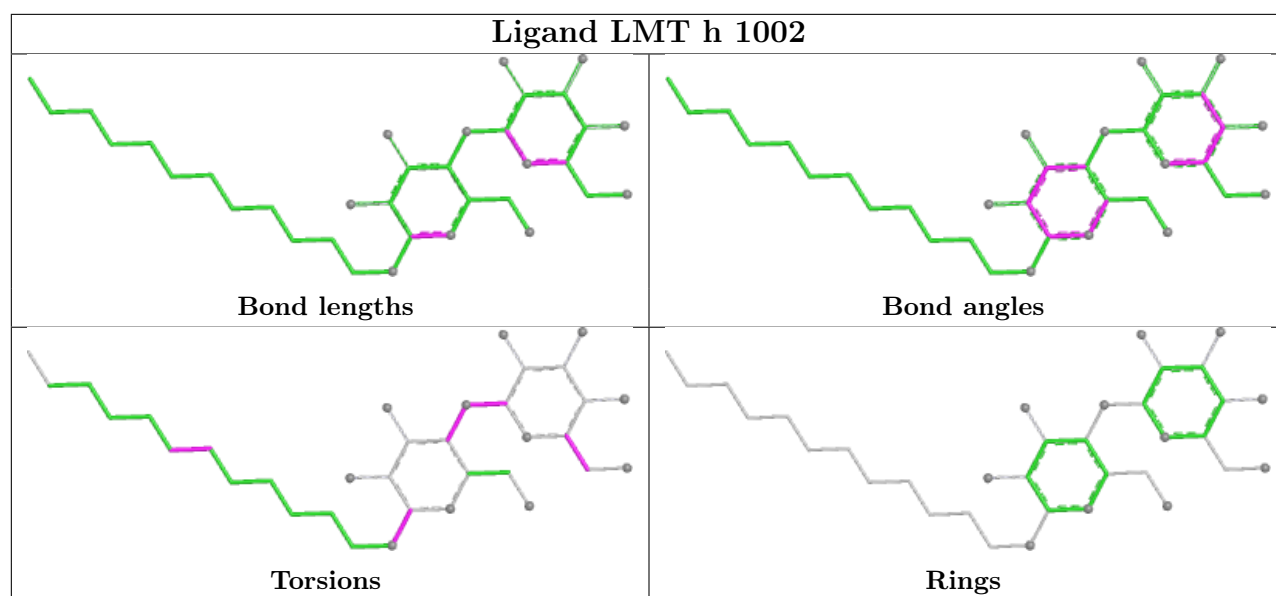
22 monomers are involved in 29 short contacts:

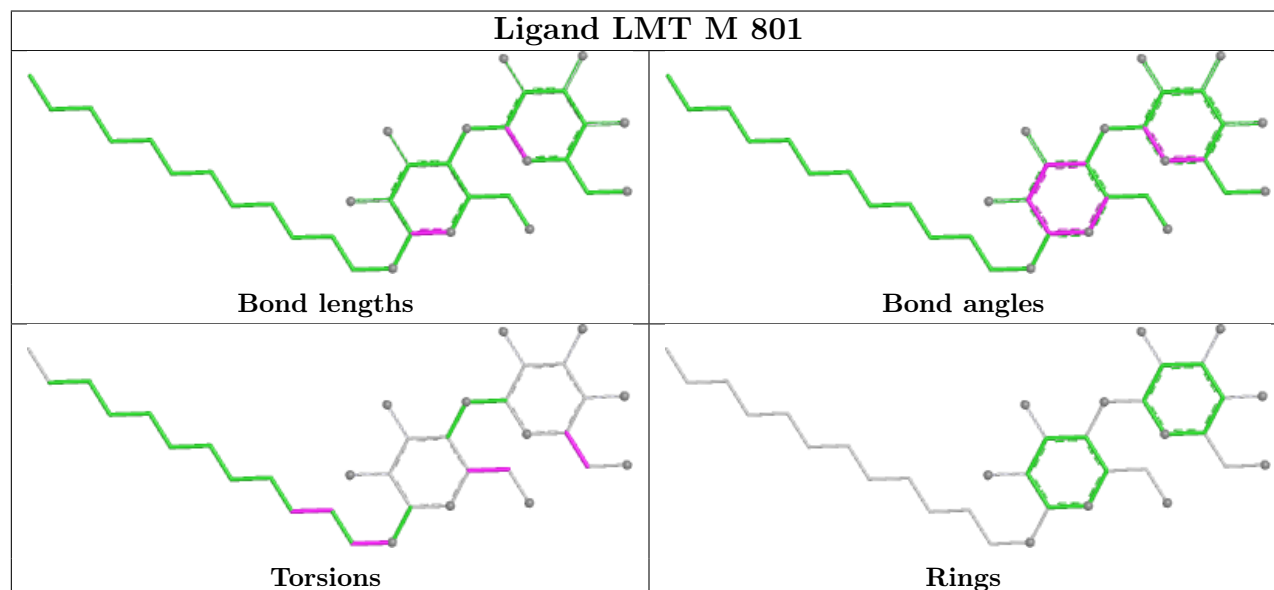
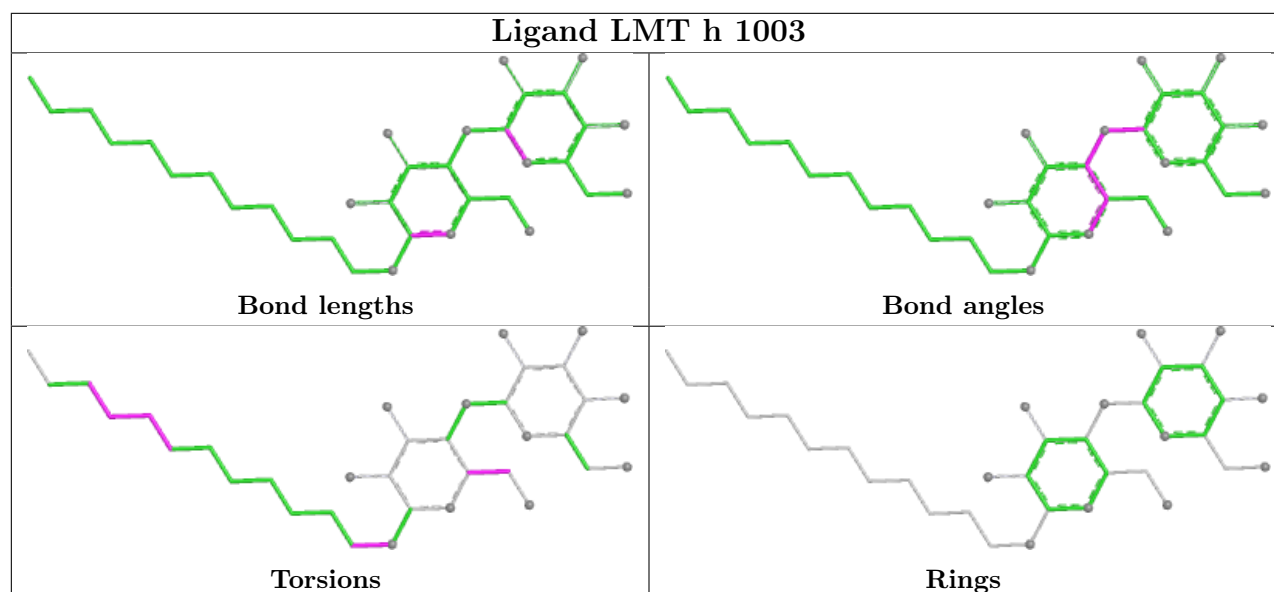
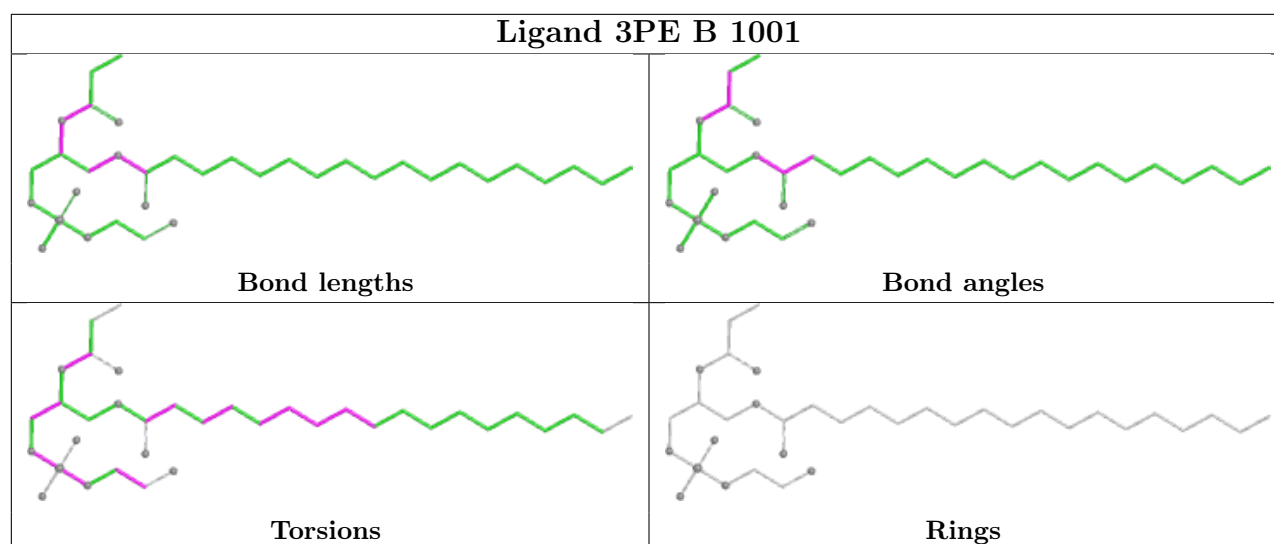
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	H	601	3PE	2	0
54	O	401	GTP	1	0
45	h	1003	LMT	1	0
45	M	801	LMT	1	0
58	T	101	EHZ	1	0
52	H	602	I49	1	0
53	K	401	CDL	2	0
53	h	1001	CDL	3	0
45	Y	603	LMT	1	0
48	g	1501	PC1	2	0
47	F	502	SF4	1	0
46	N	902	3PE	2	0
56	P	501	NDP	1	0
45	M	802	LMT	2	0
46	Y	601	3PE	1	0
45	A	301	LMT	1	0
46	L	701	3PE	1	0
45	L	704	LMT	2	0
58	U	101	EHZ	1	0
46	Z	401	3PE	1	0
53	X	1701	CDL	2	0
46	Y	602	3PE	1	0

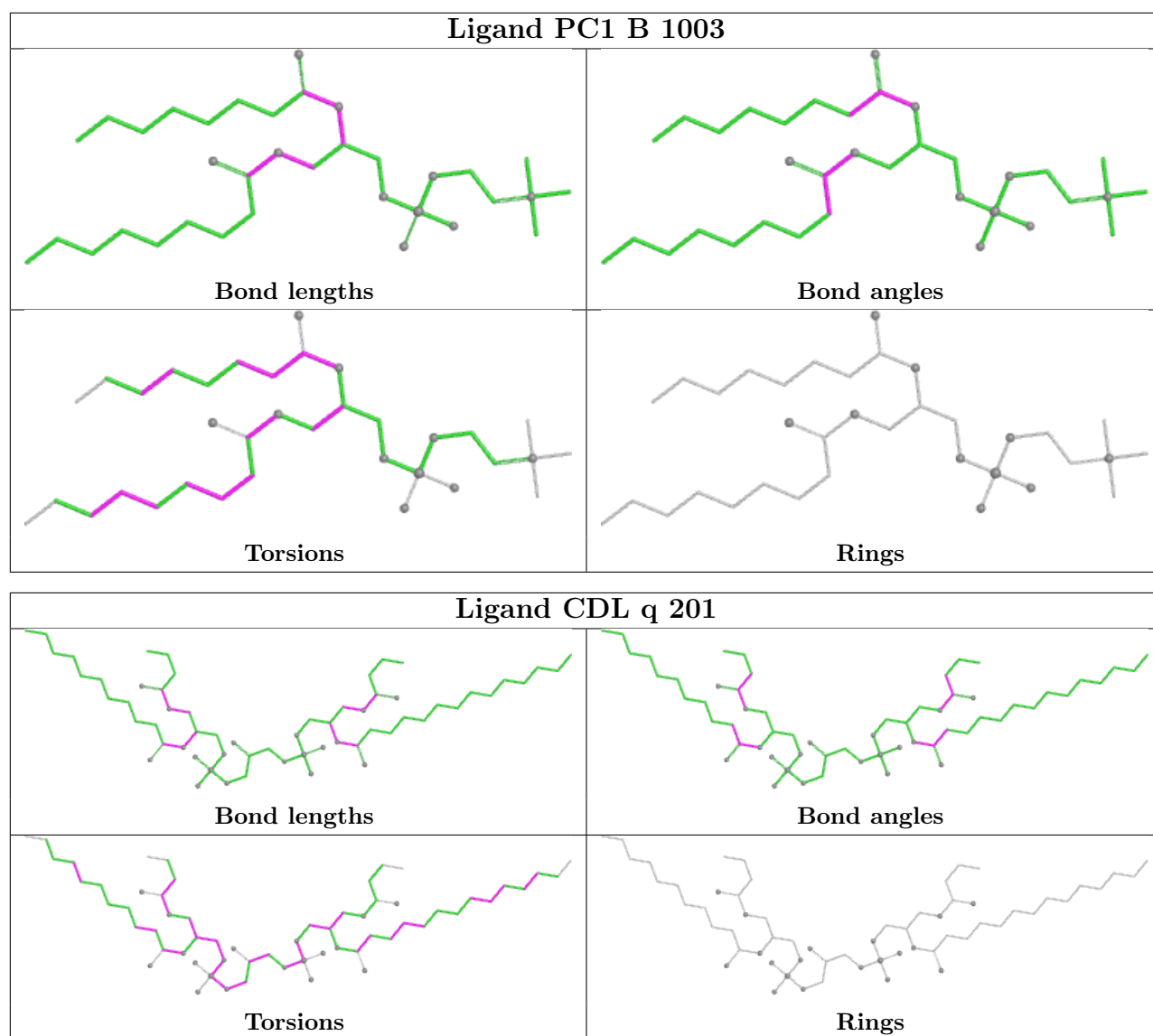
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

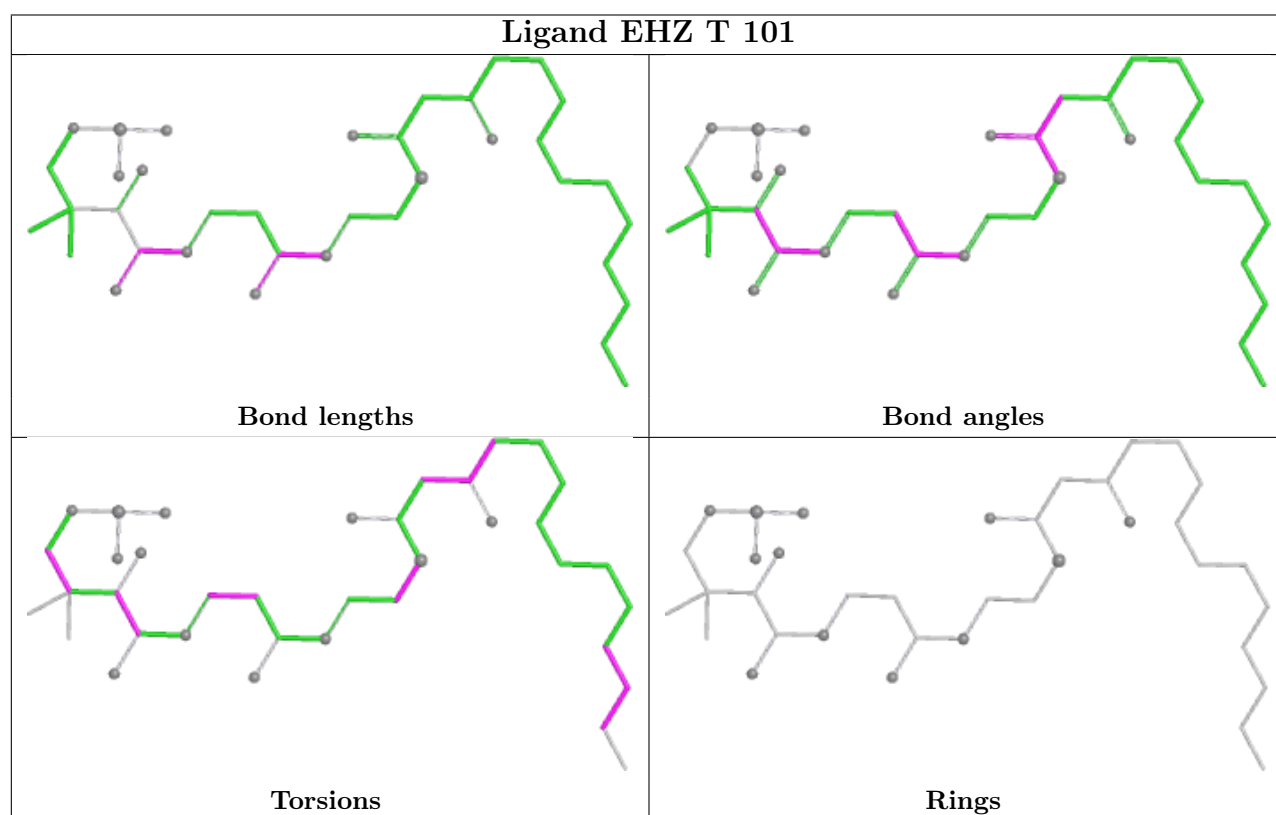
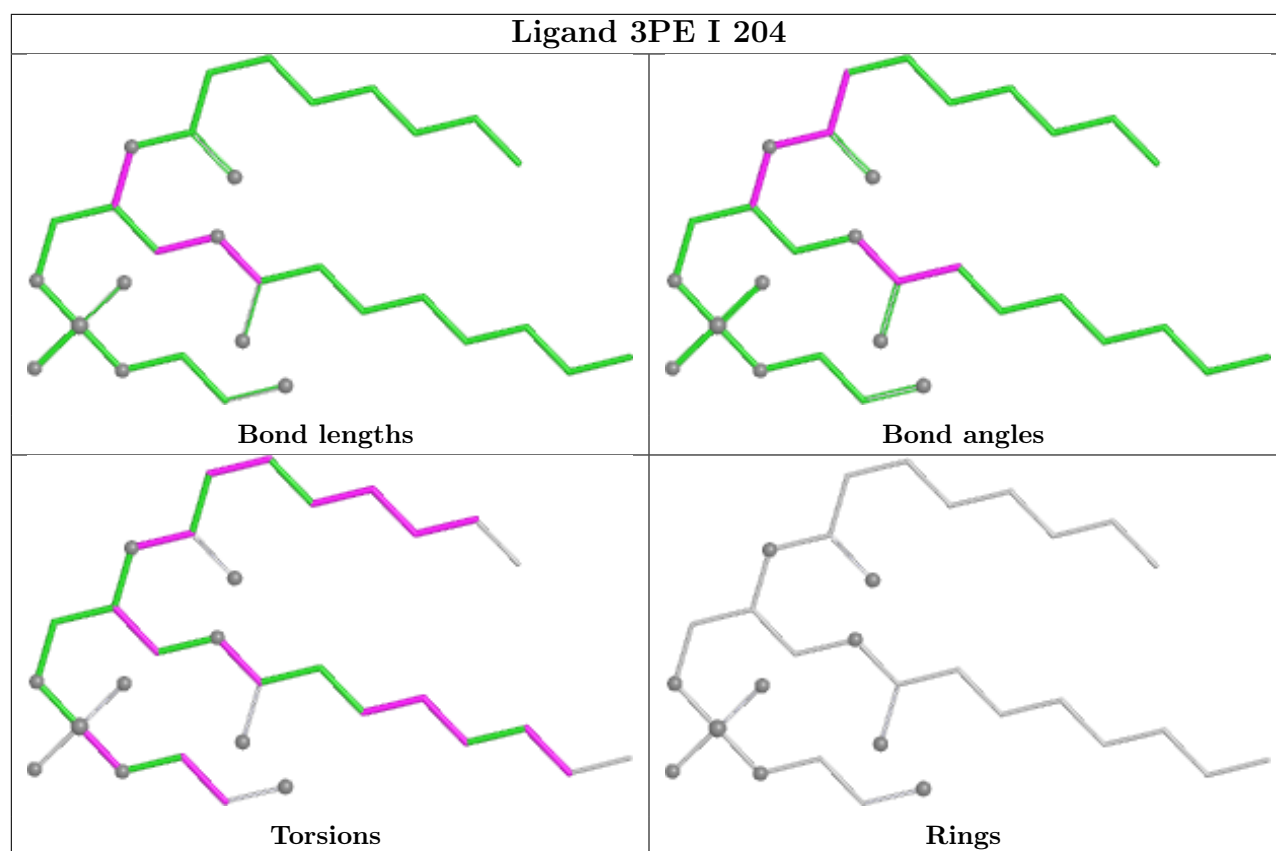


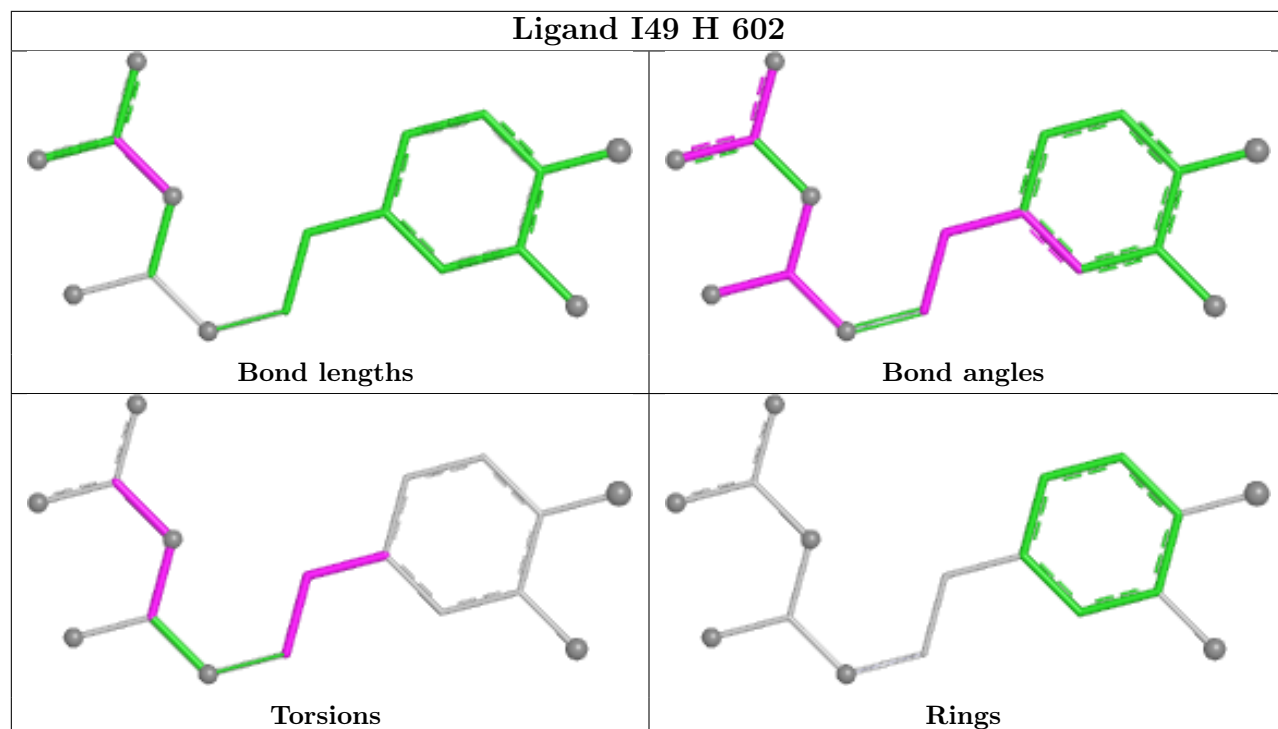


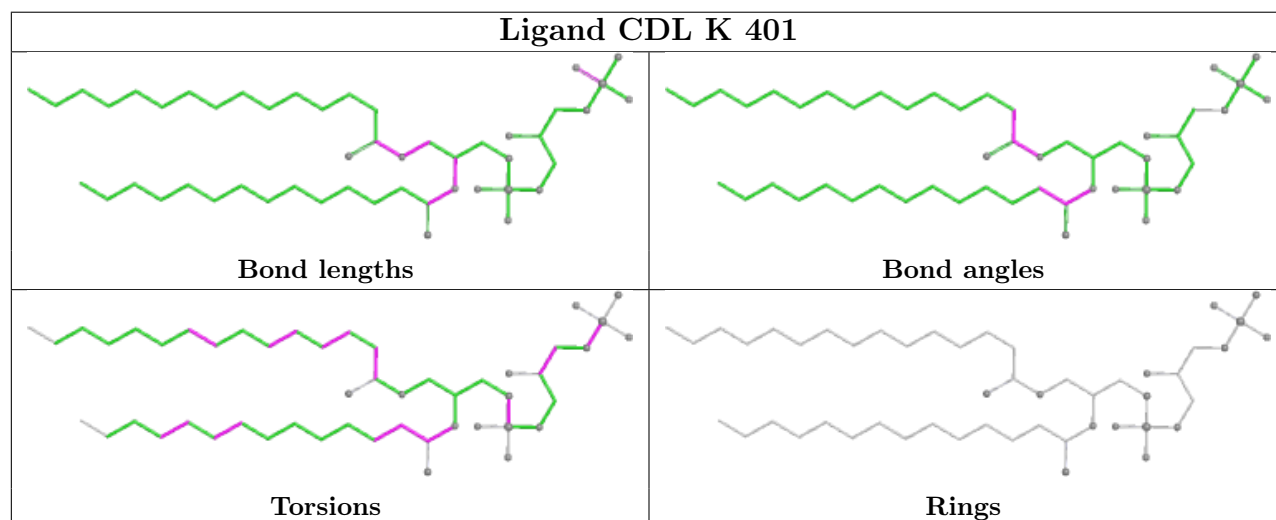
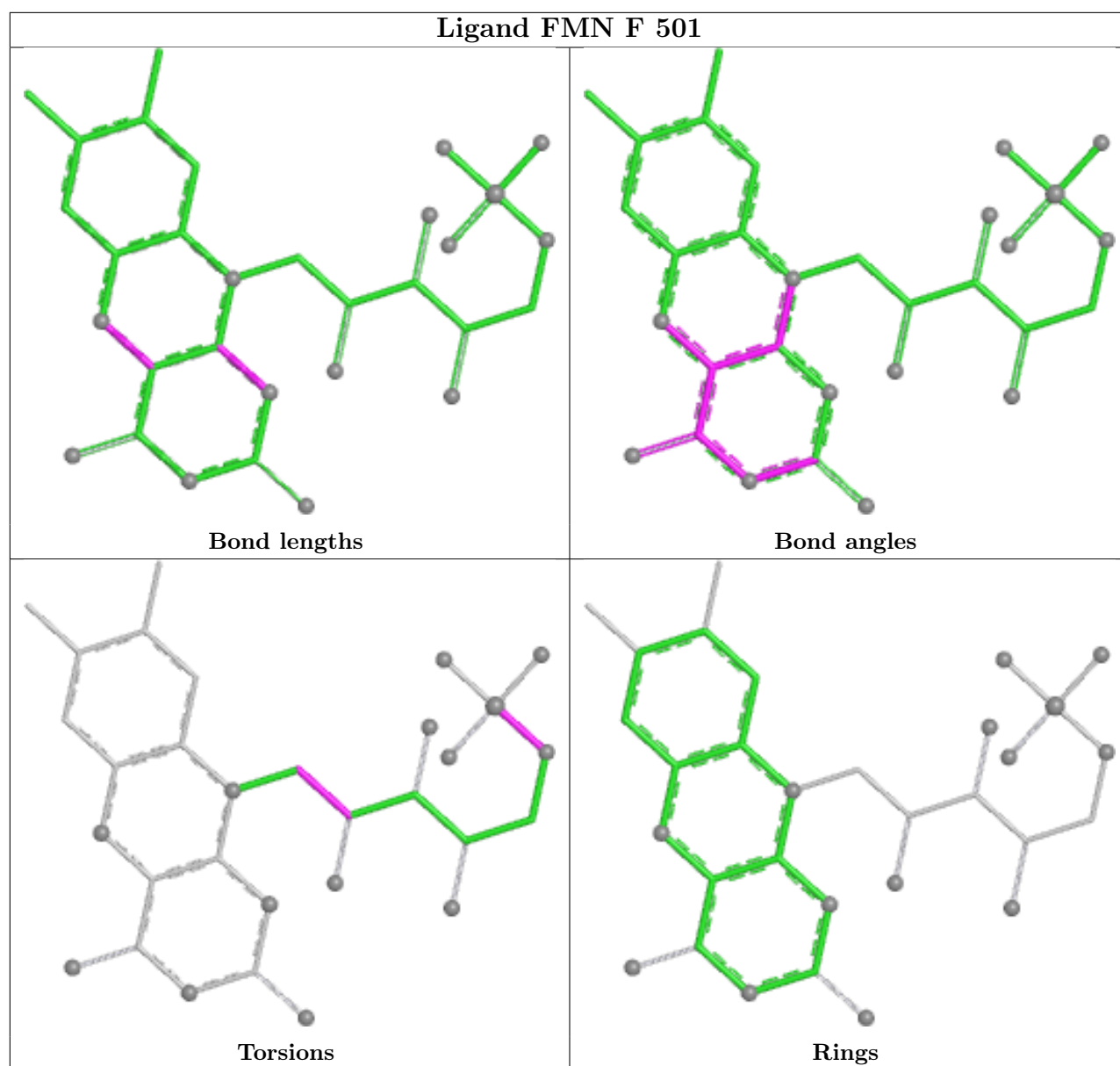


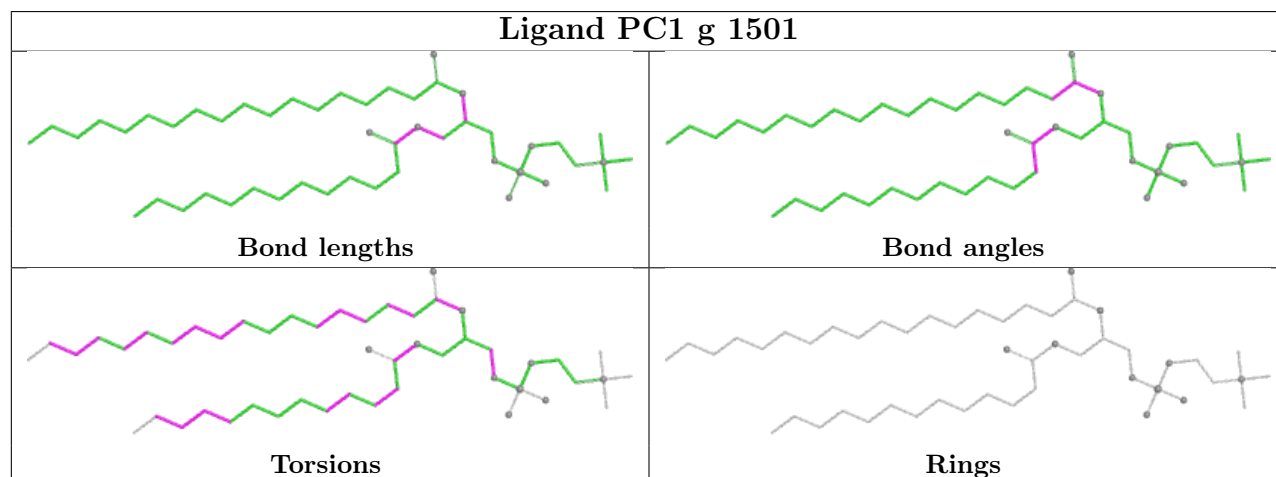
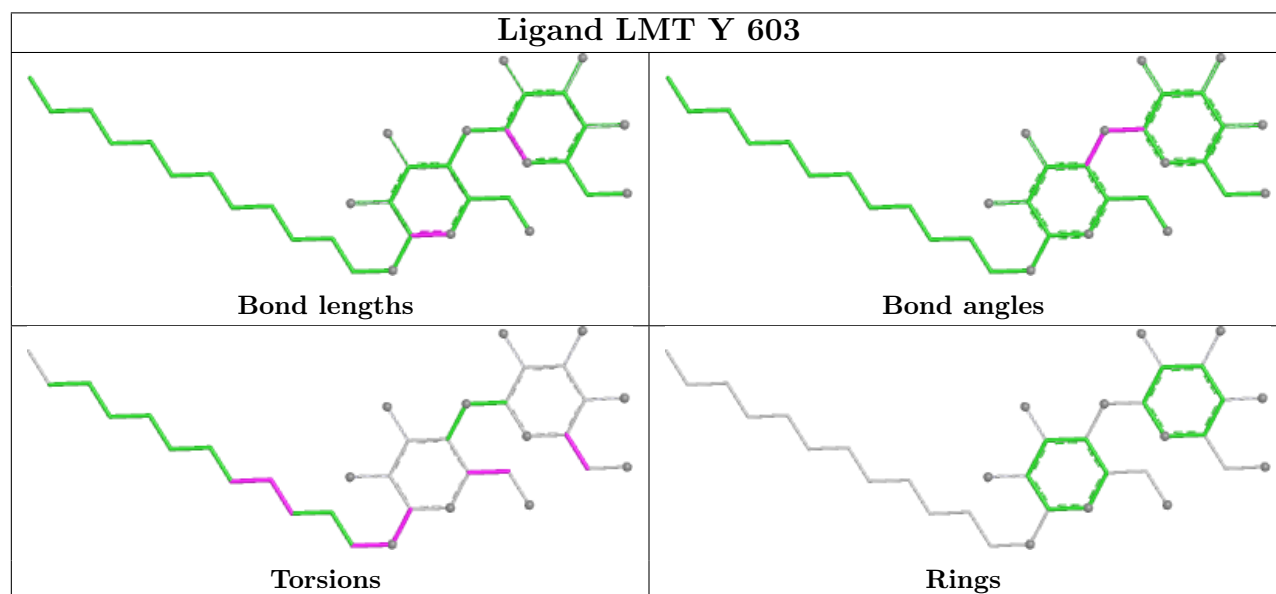
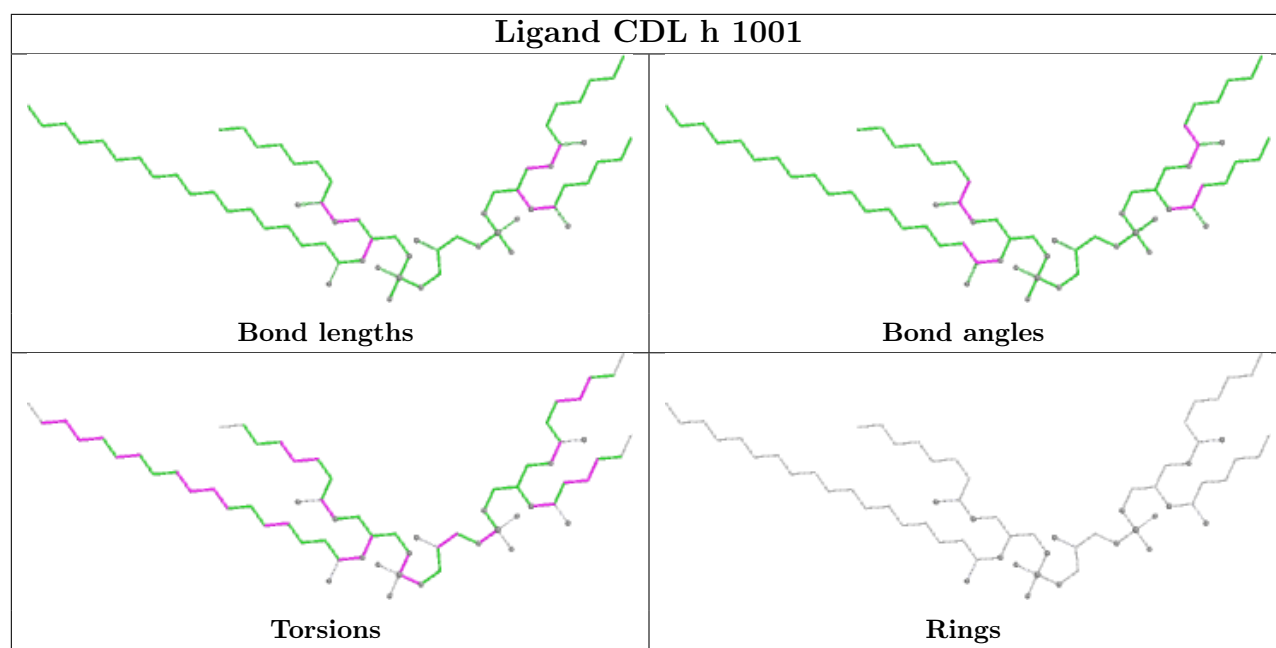


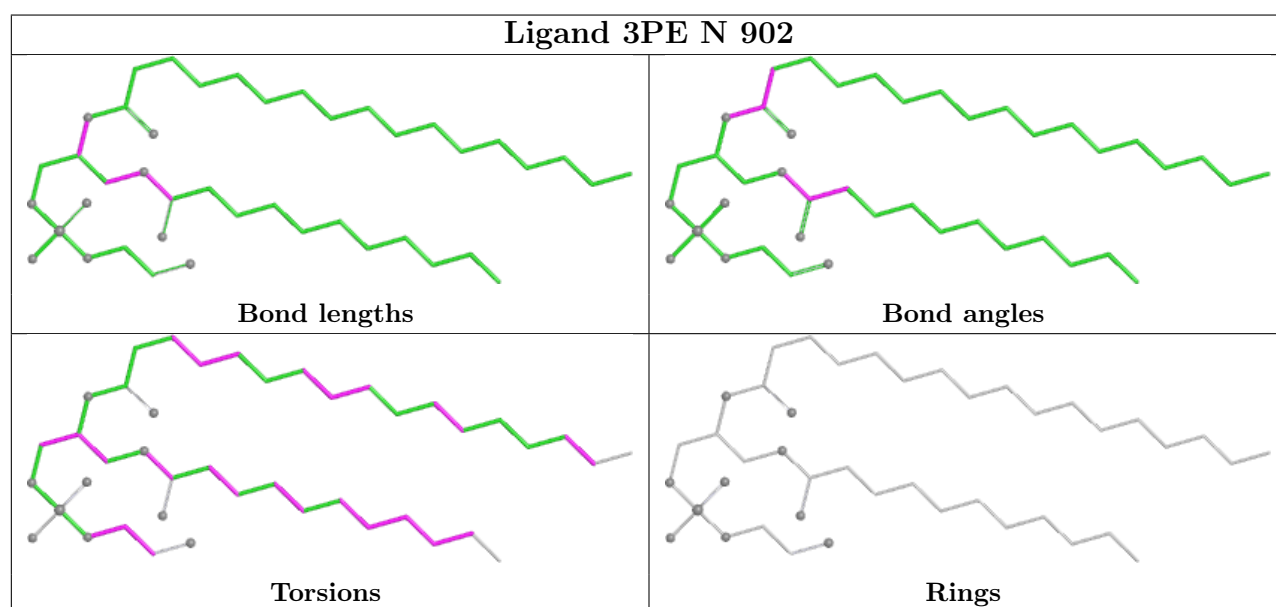
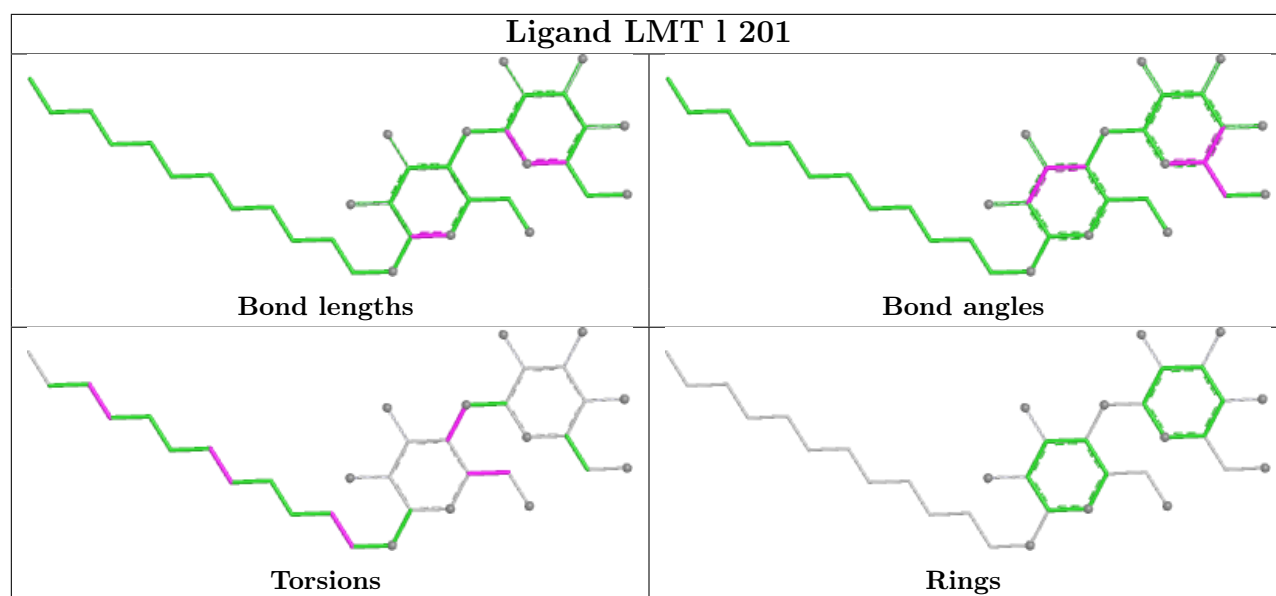


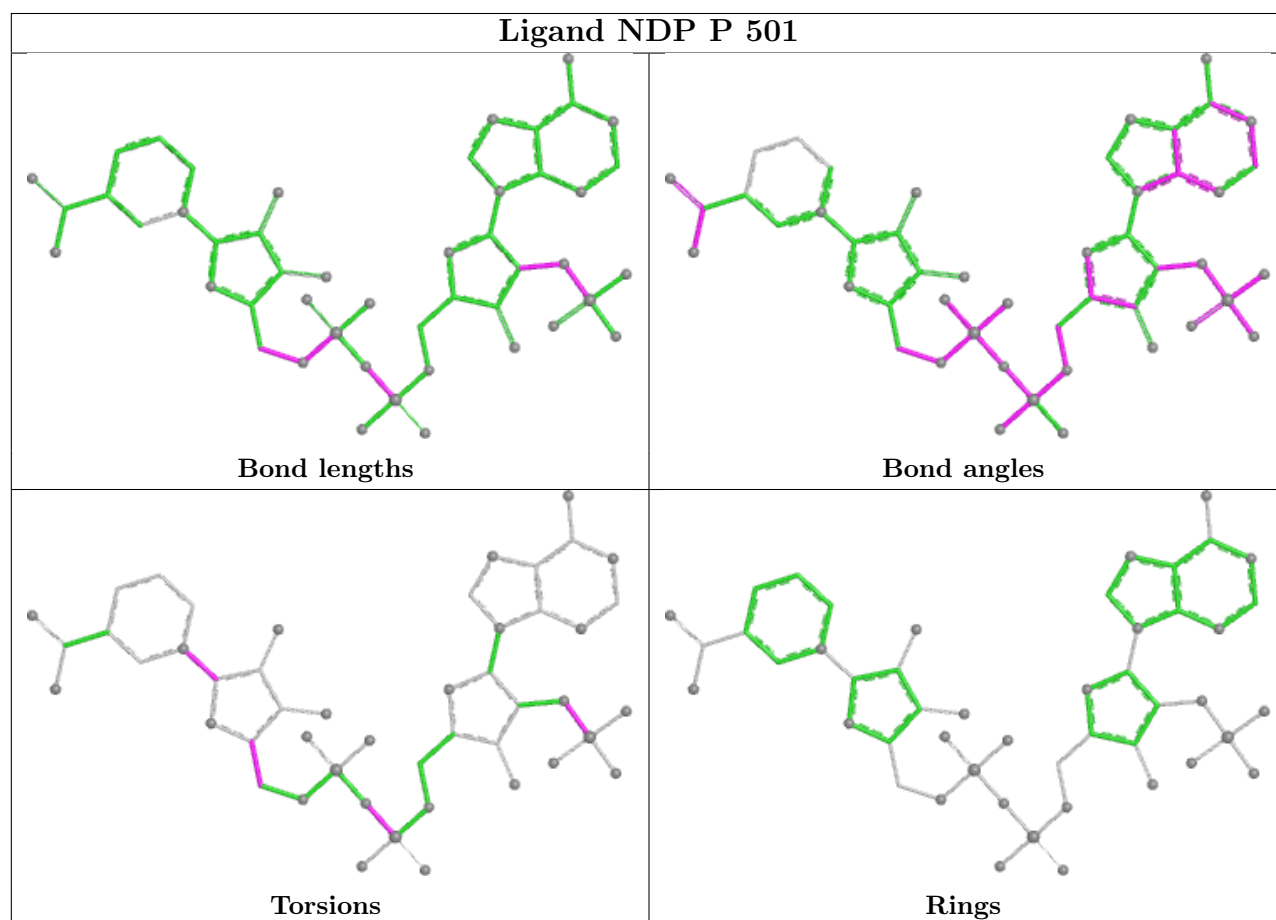
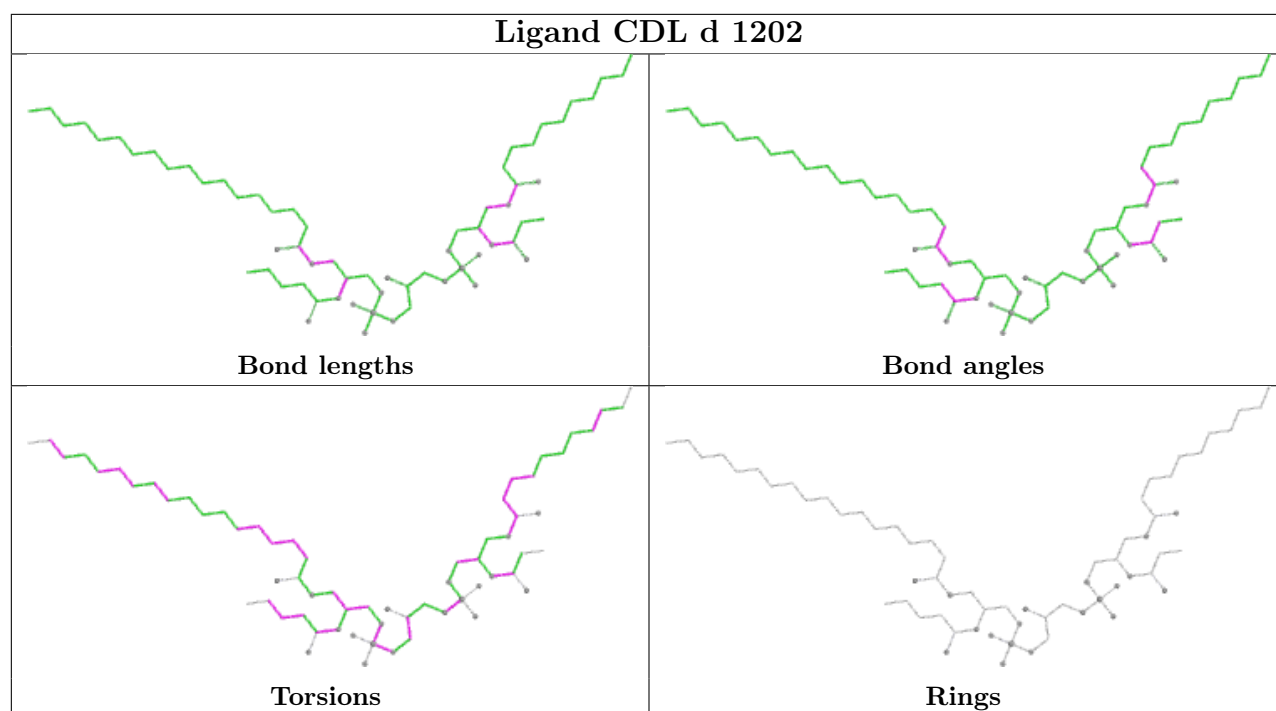


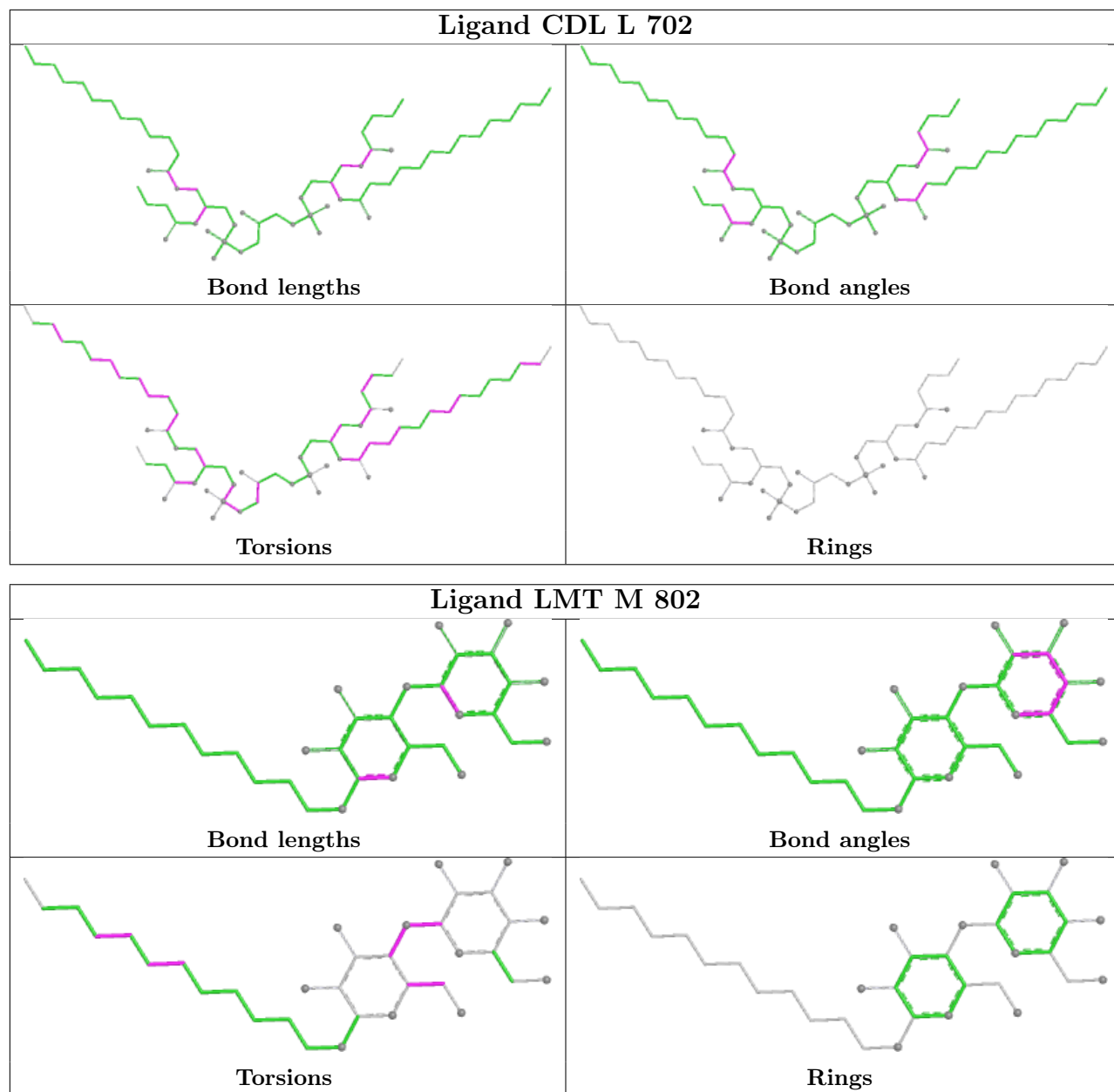


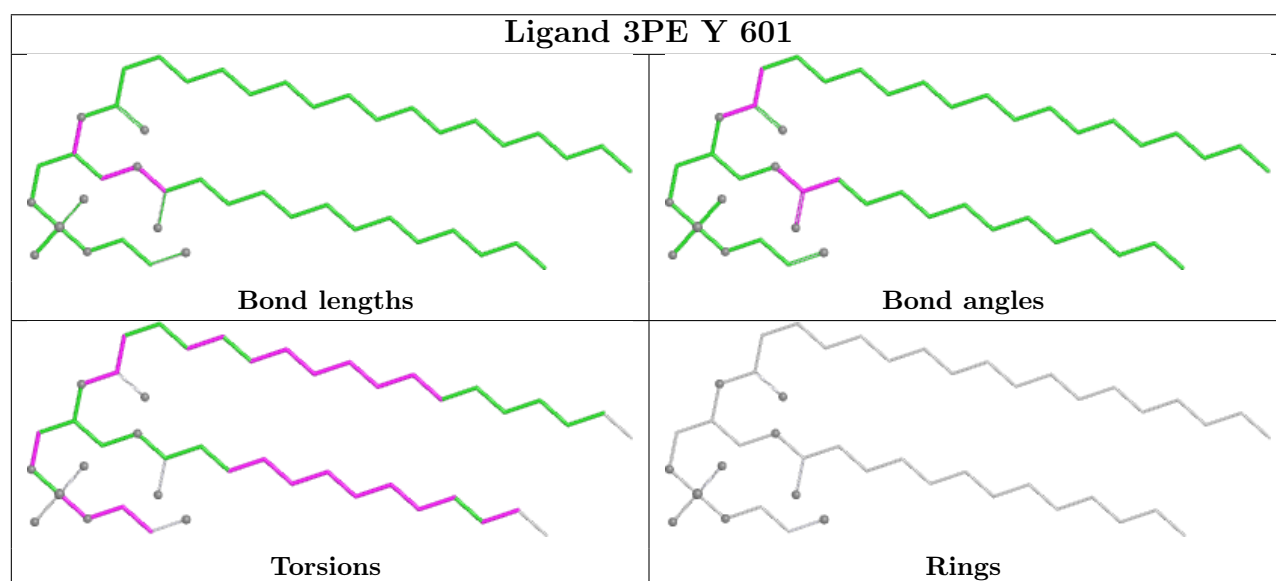
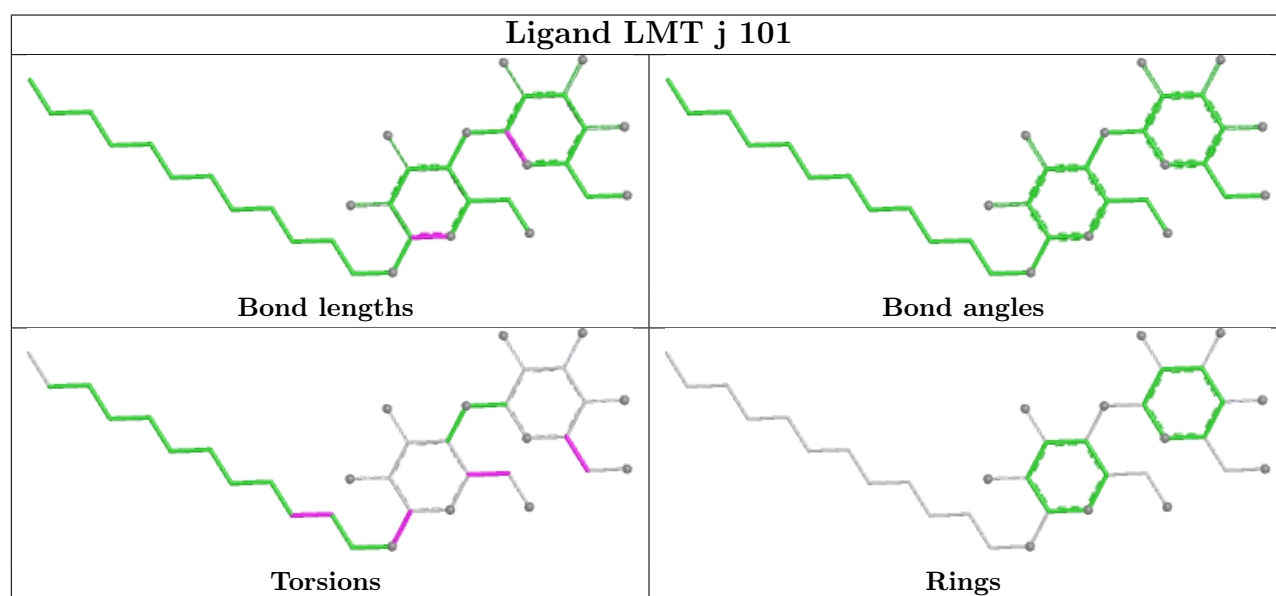
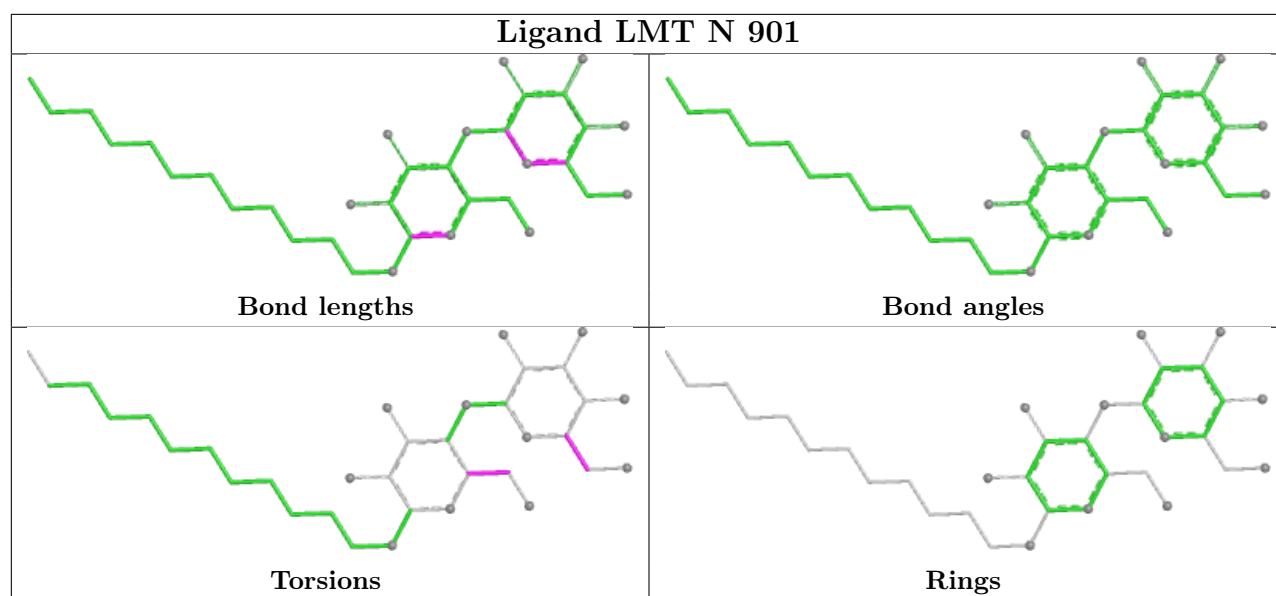


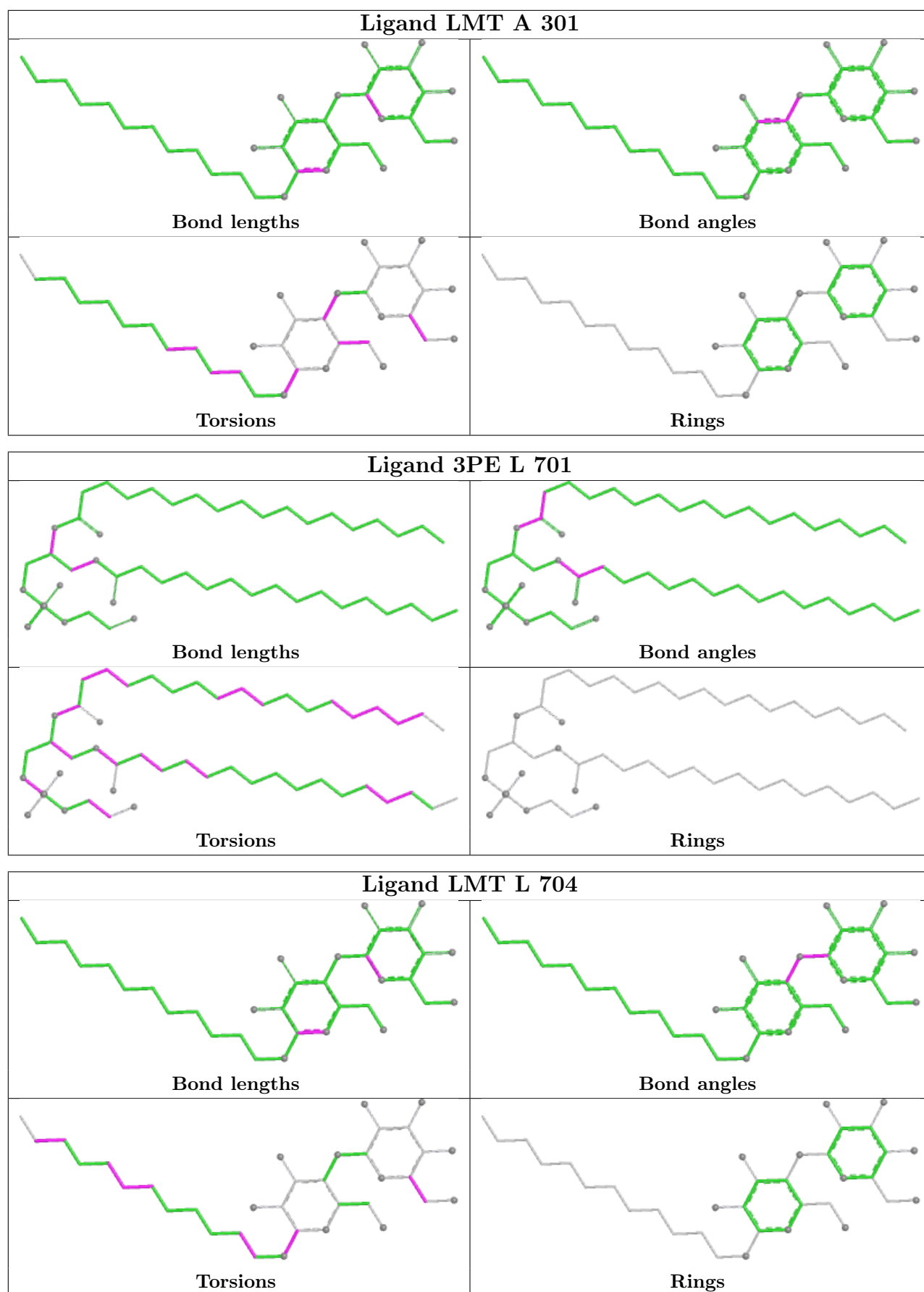


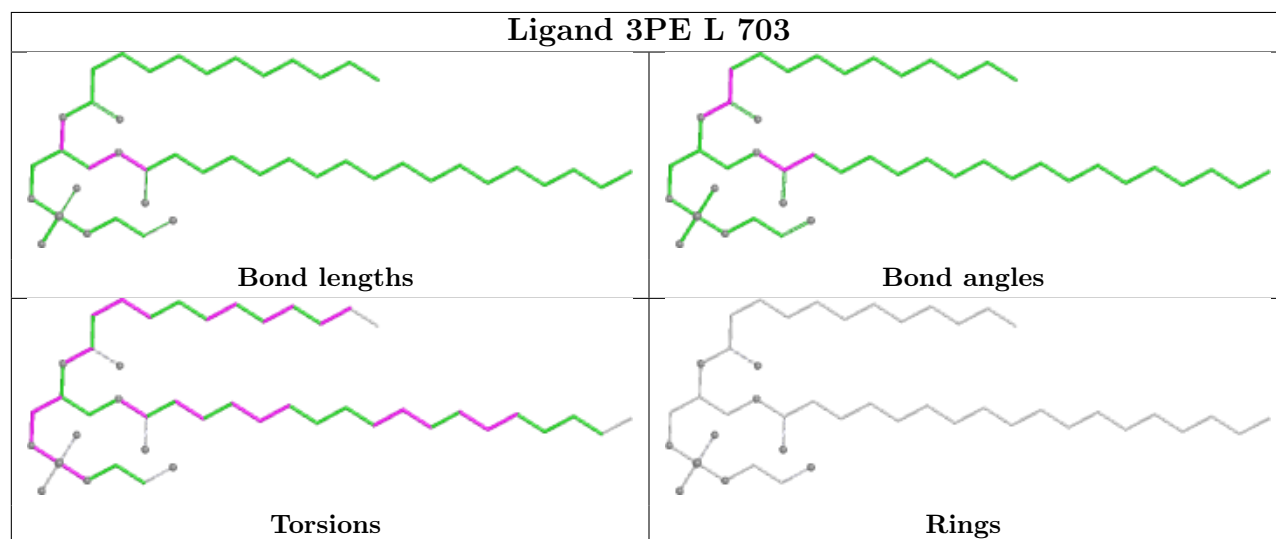
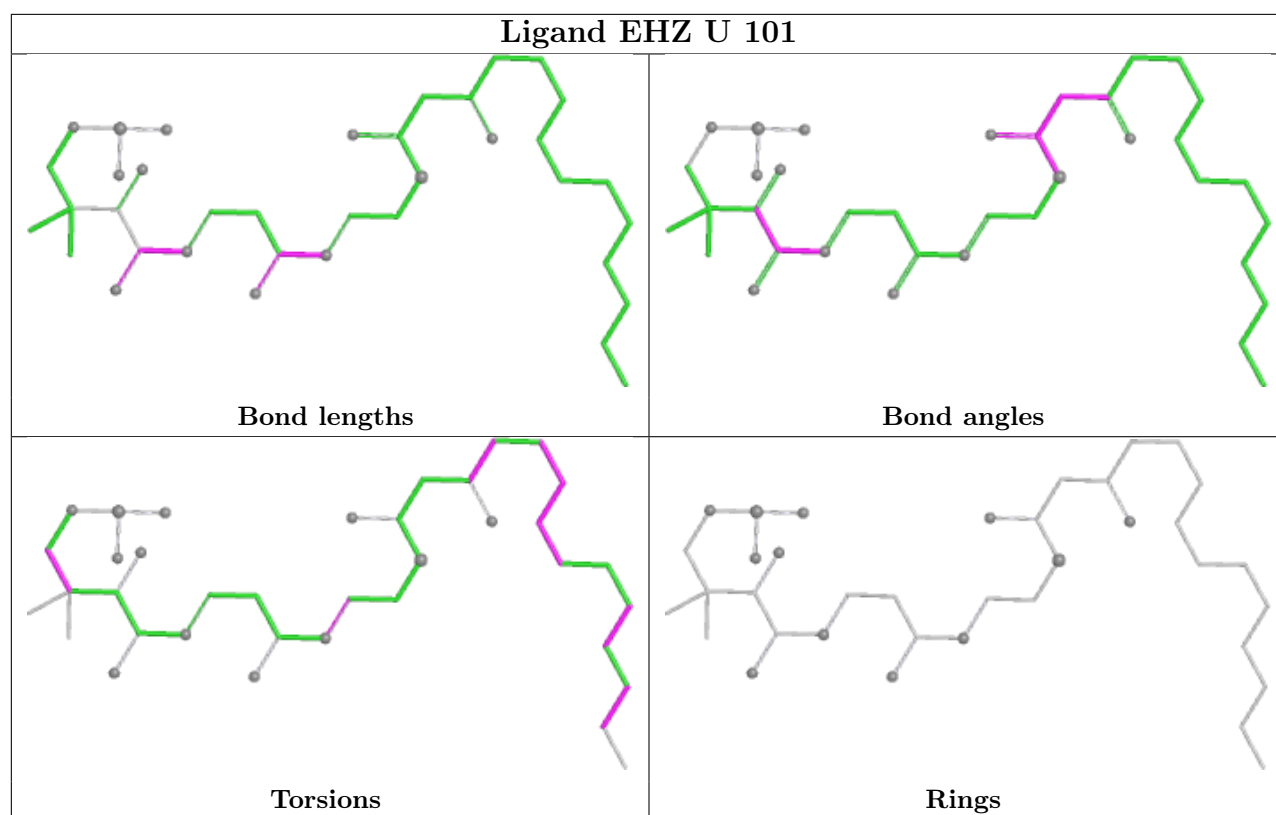




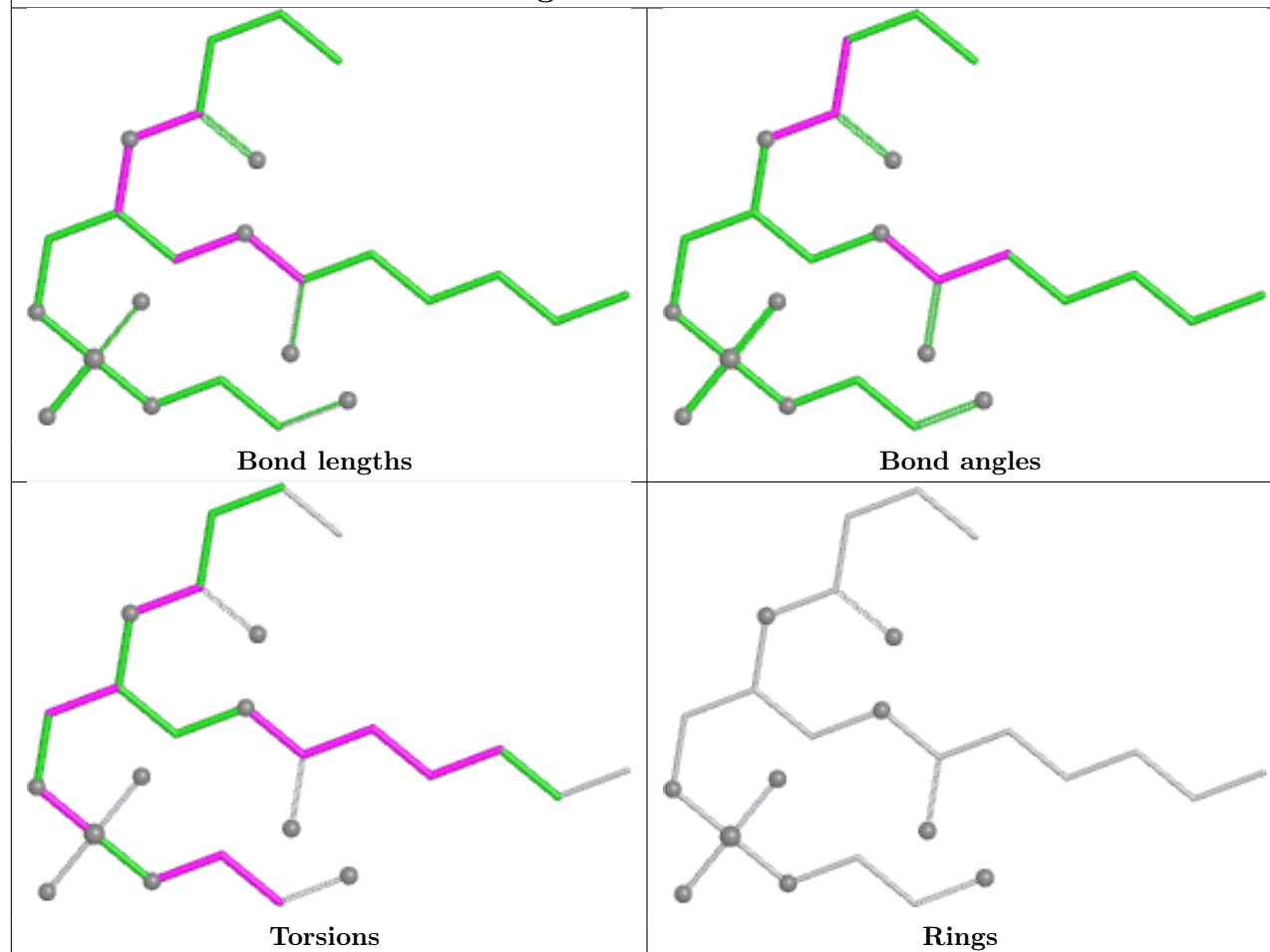




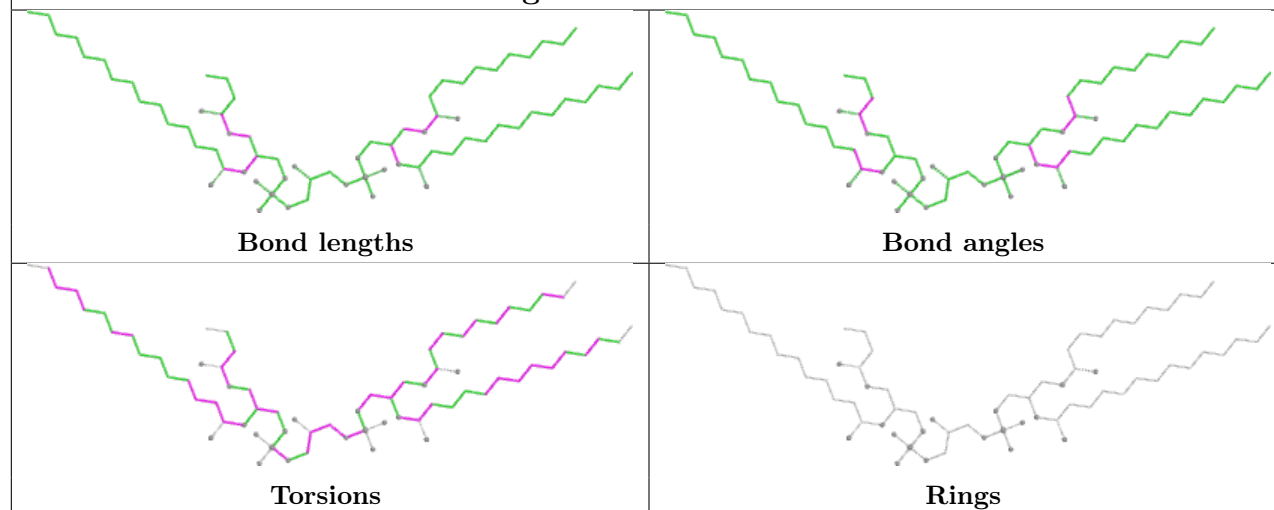


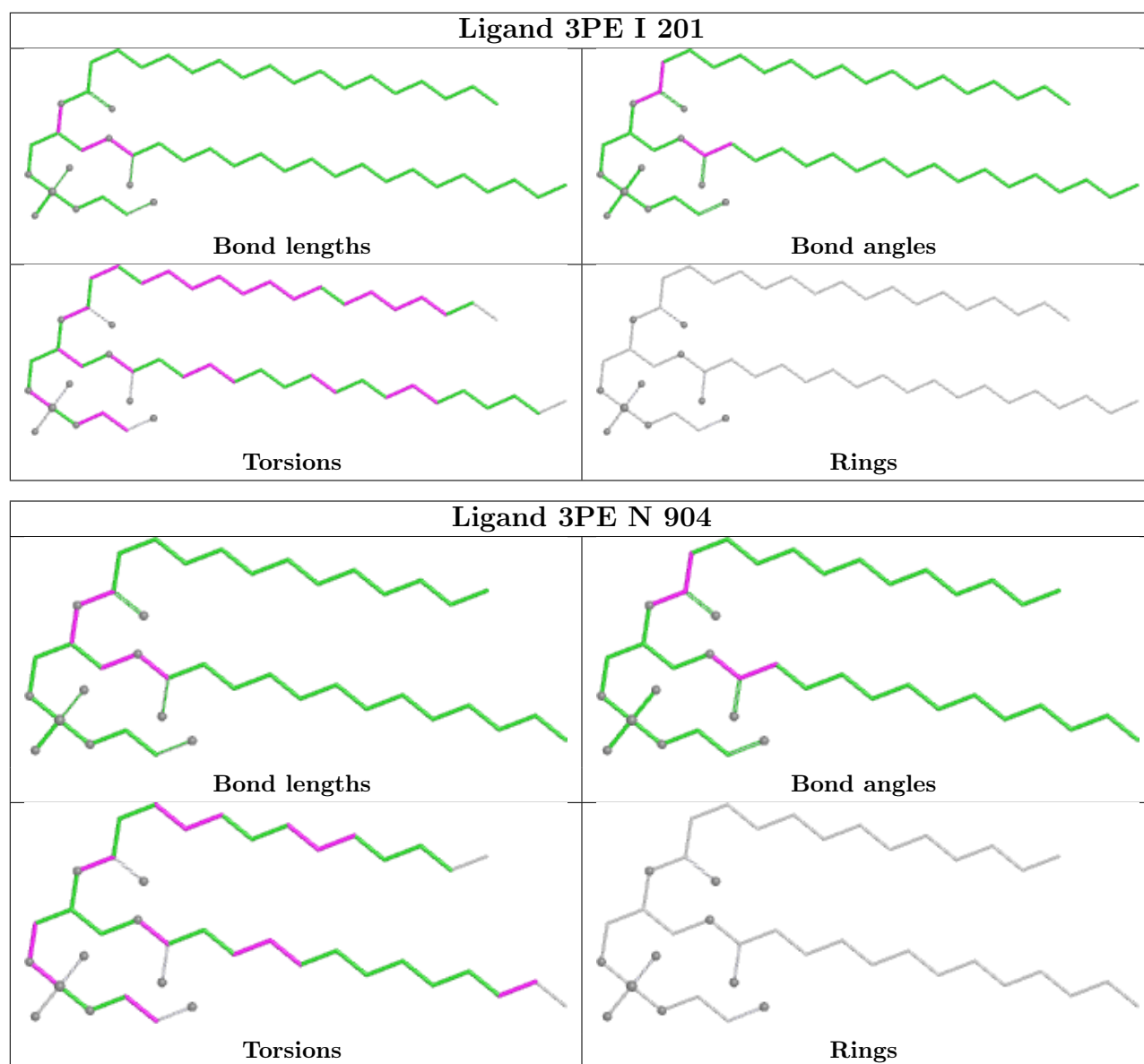


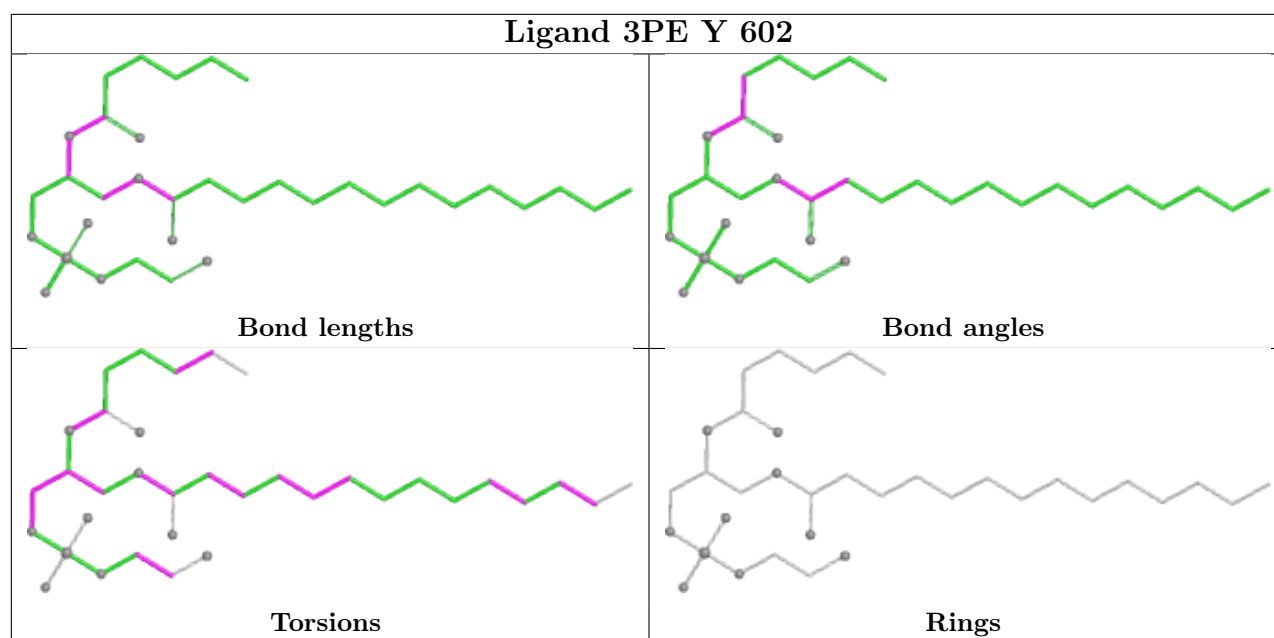
Ligand 3PE Z 401



Ligand CDL X 1701







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.

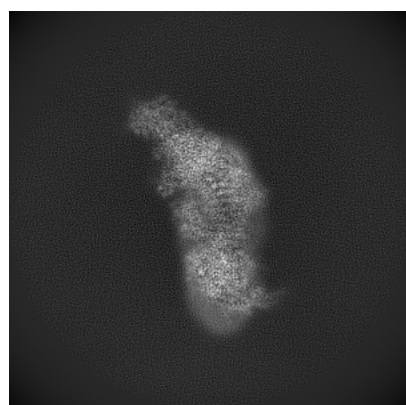
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14277. These allow visual inspection of the internal detail of the map and identification of artifacts.

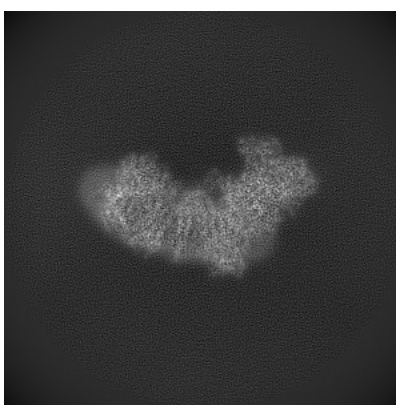
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

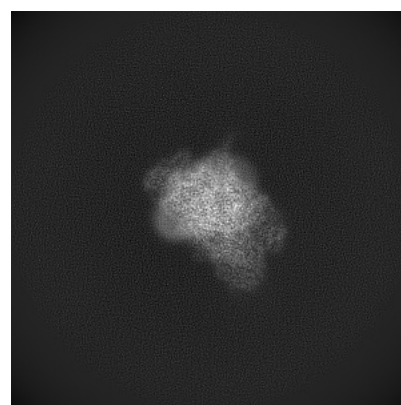
6.1.1 Primary map



X



Y

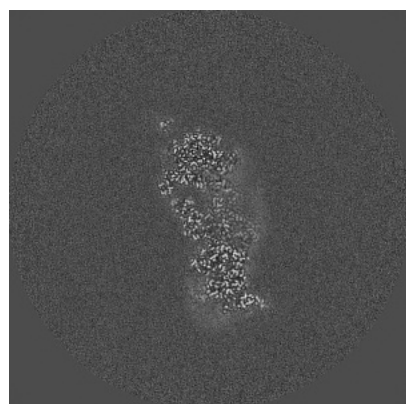


Z

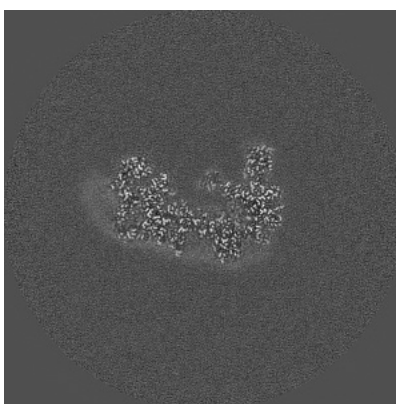
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

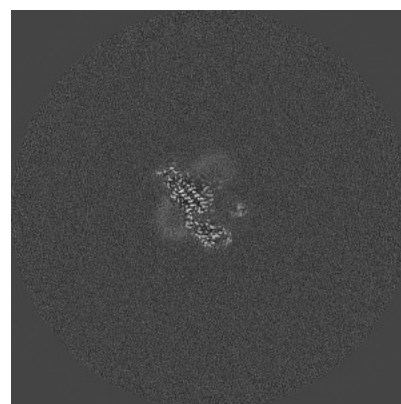
6.2.1 Primary map



X Index: 330



Y Index: 330

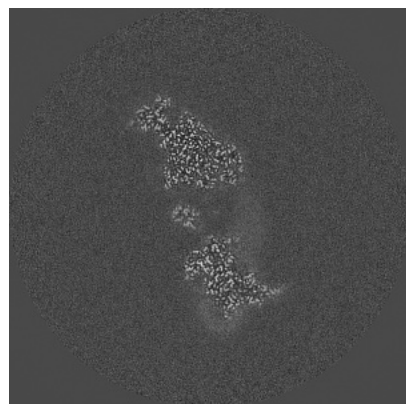


Z Index: 330

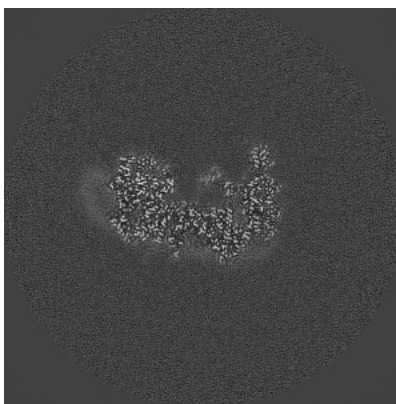
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

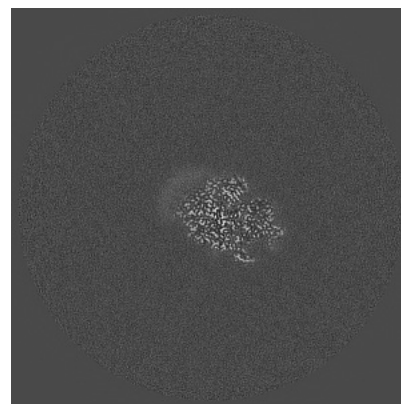
6.3.1 Primary map



X Index: 358



Y Index: 337

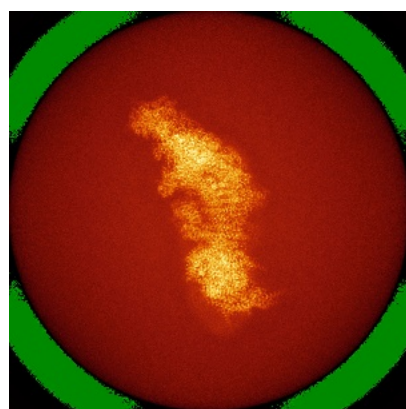


Z Index: 421

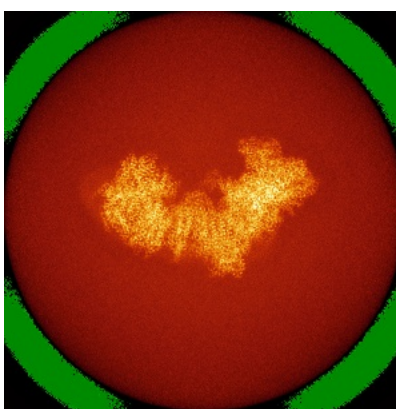
The images above show the largest variance slices of the map in three orthogonal directions.

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

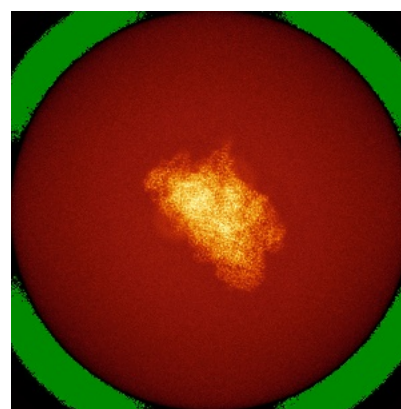
6.4.1 Primary map



X



Y

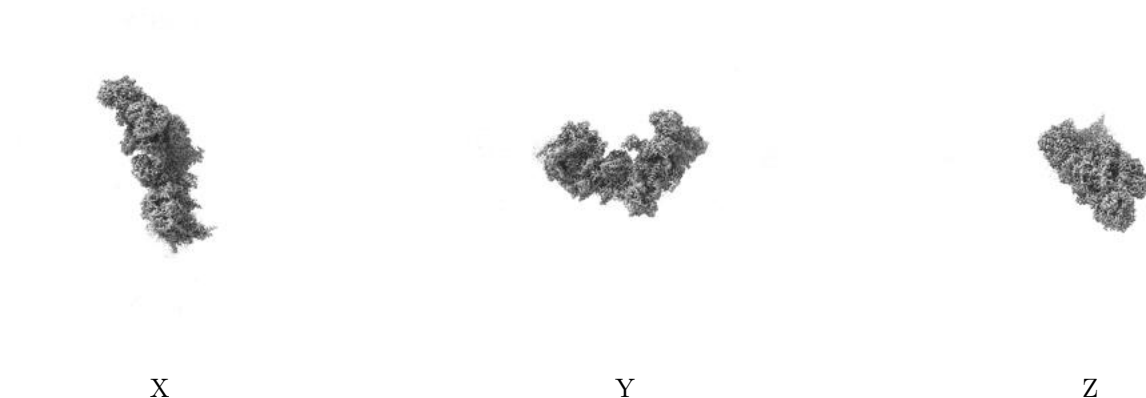


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

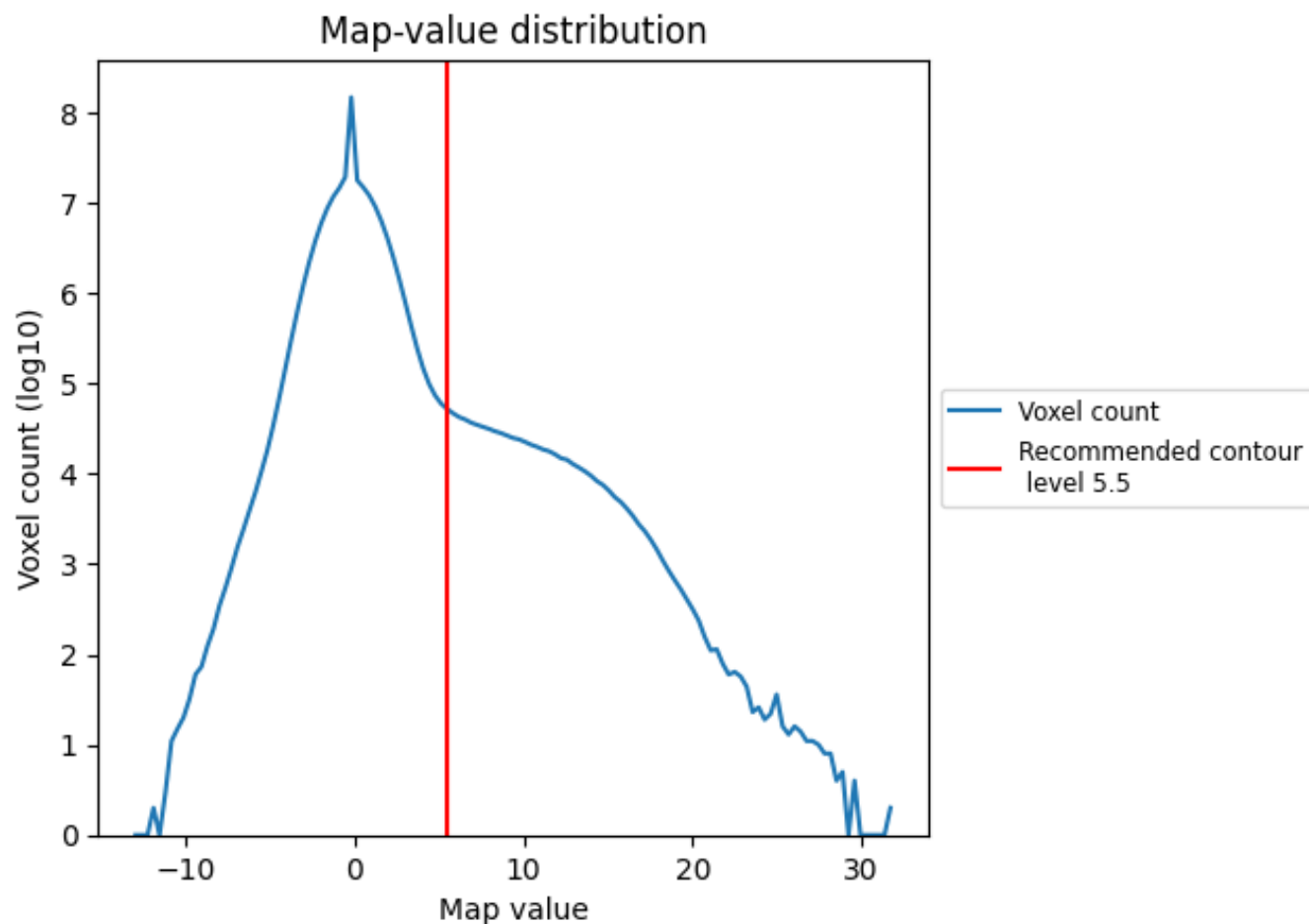
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

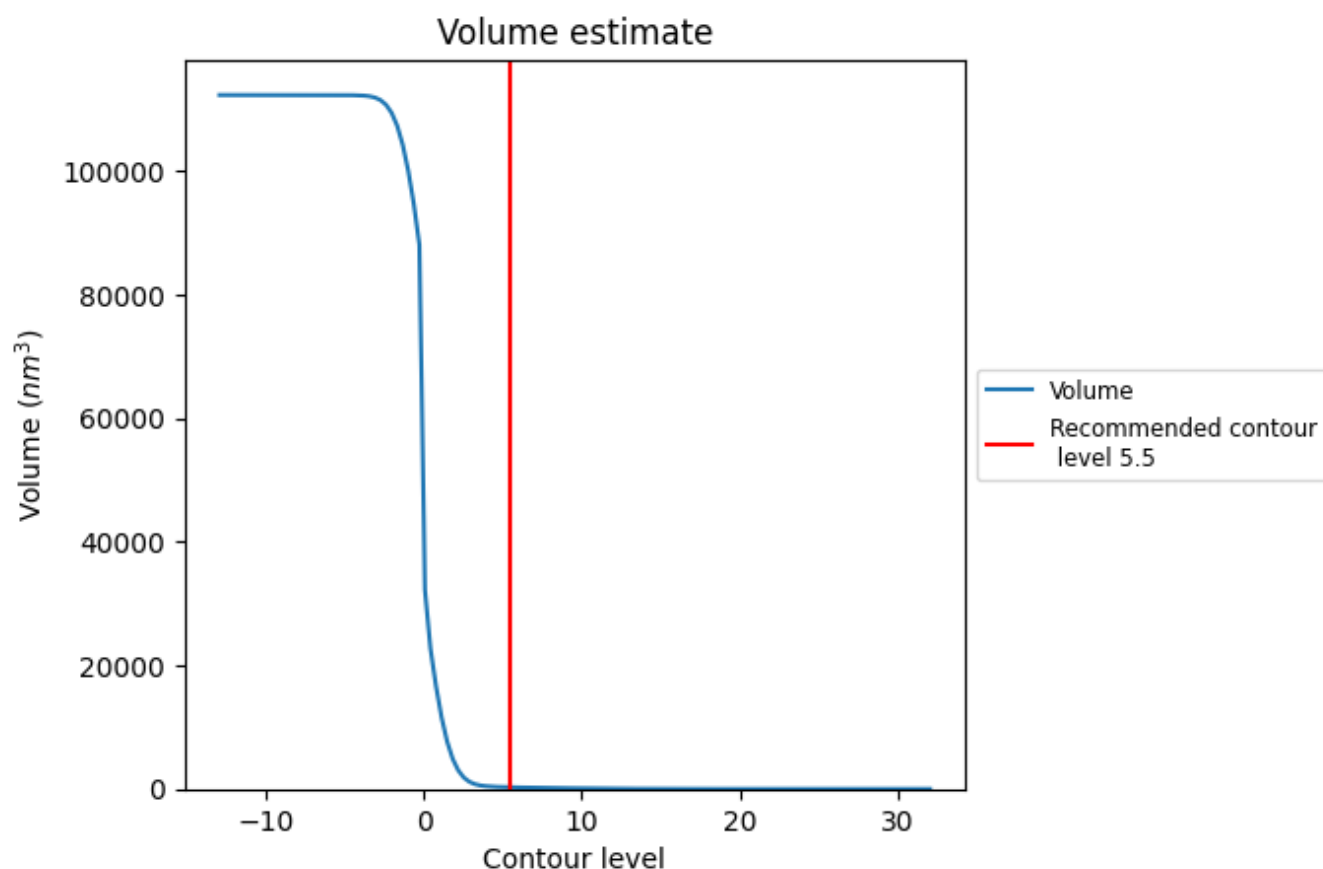
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

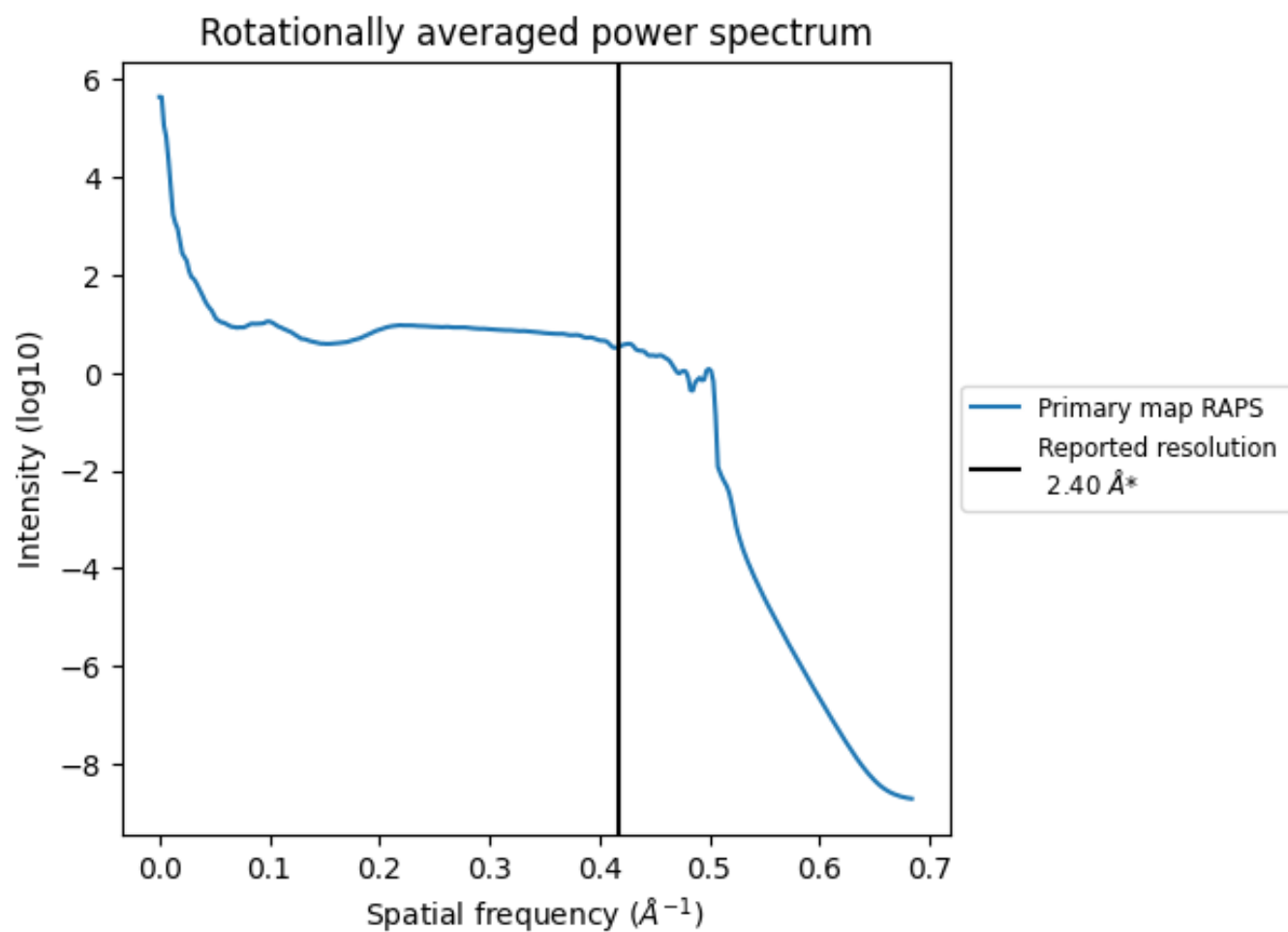
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm^3 ; this corresponds to an approximate mass of 244 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

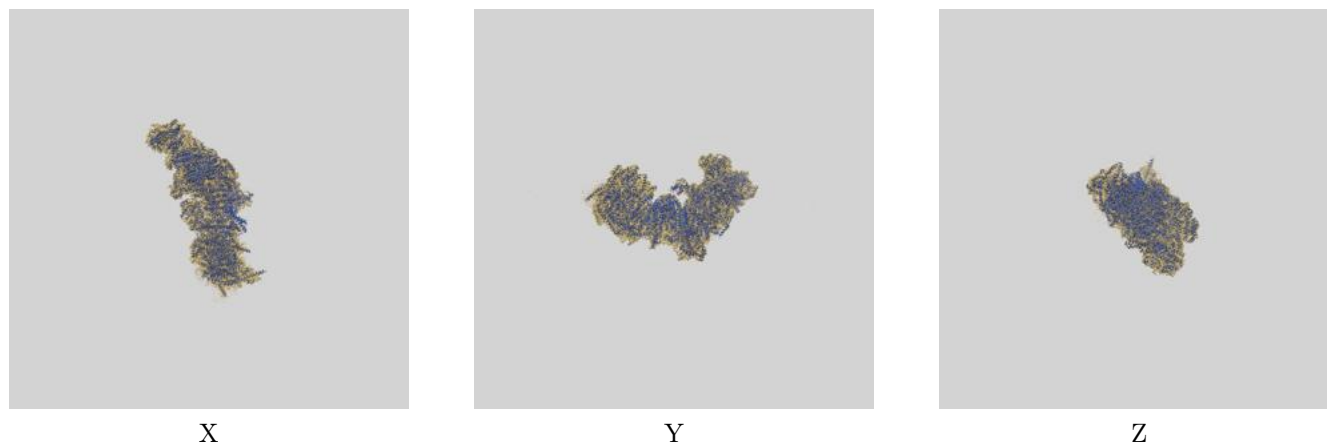
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

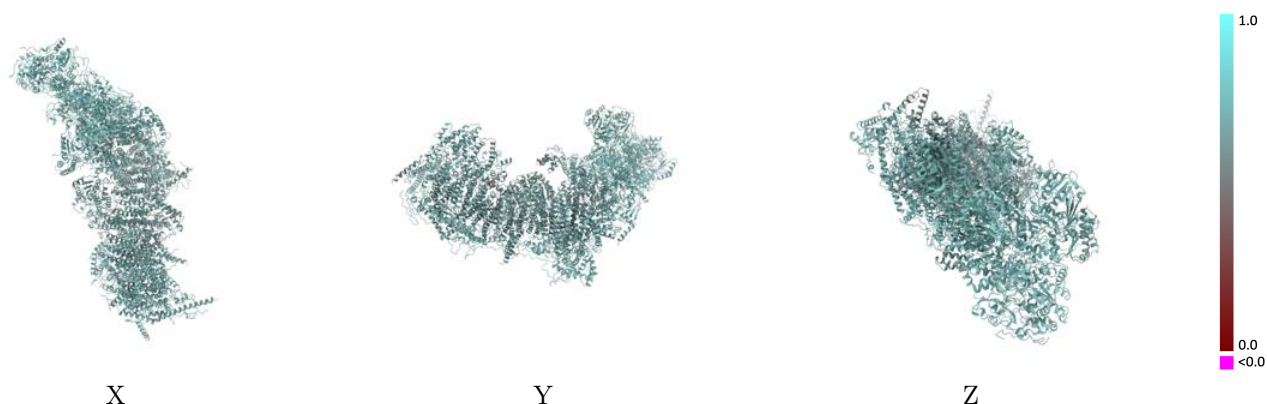
This section contains information regarding the fit between EMDB map EMD-14277 and PDB model 7R46. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



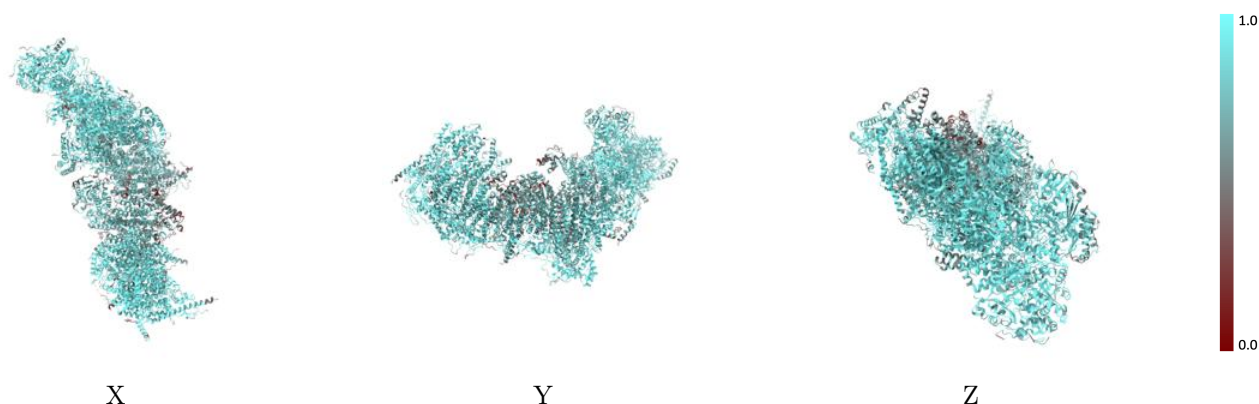
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



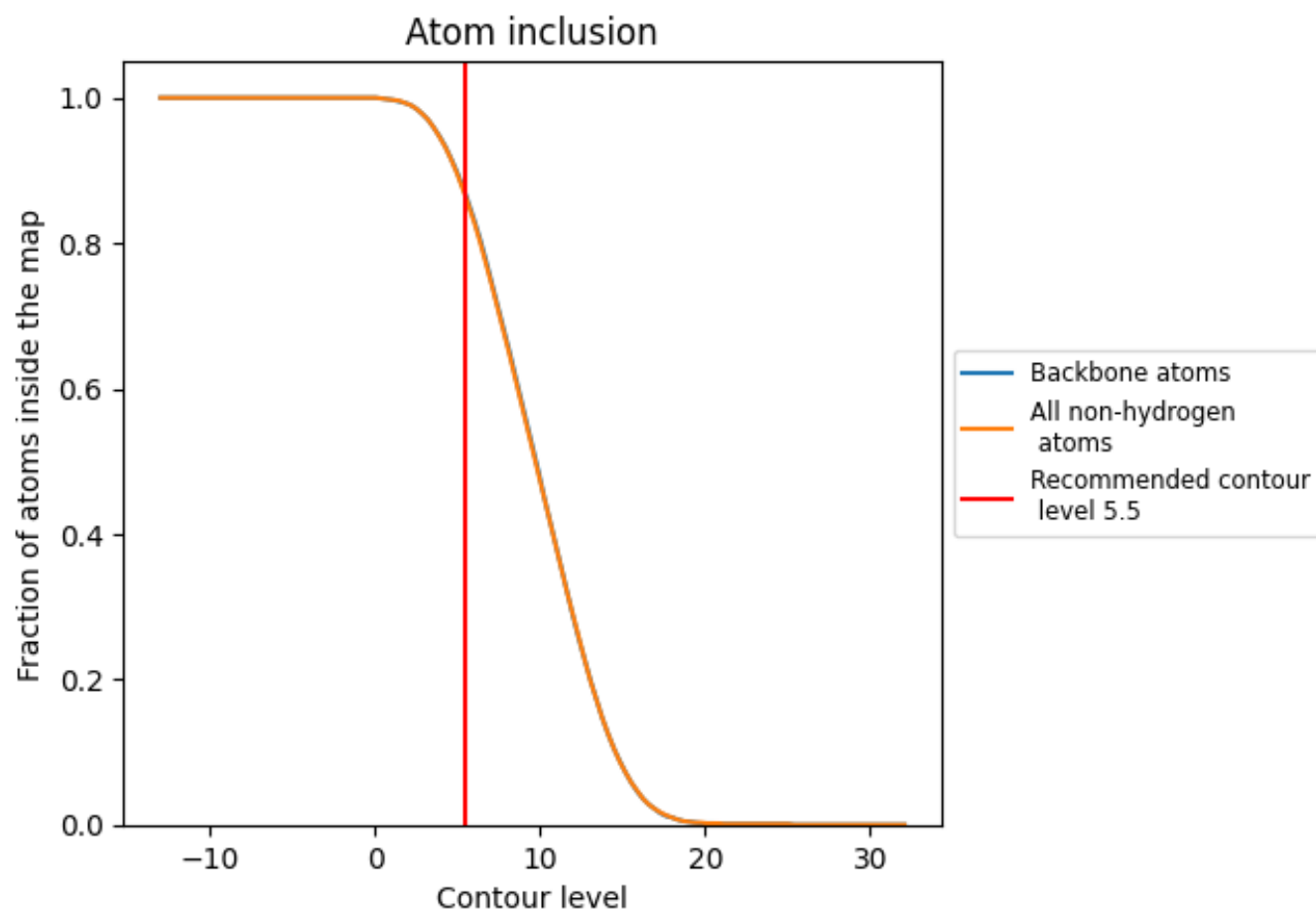
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.6720
A	 0.8220	 0.6570
B	 0.8890	 0.6930
C	 0.9500	 0.7160
D	 0.9080	 0.7050
E	 0.8560	 0.6700
F	 0.9000	 0.6840
G	 0.8950	 0.6920
H	 0.9230	 0.6810
I	 0.9410	 0.7170
J	 0.7930	 0.6500
K	 0.8510	 0.6780
L	 0.8860	 0.6640
M	 0.9460	 0.6890
N	 0.9220	 0.6890
O	 0.8200	 0.6420
P	 0.8440	 0.6720
Q	 0.8940	 0.6970
R	 0.8960	 0.6970
S	 0.8120	 0.6520
T	 0.5700	 0.5870
U	 0.9000	 0.6620
V	 0.8330	 0.6780
W	 0.8390	 0.6730
X	 0.8370	 0.6570
Y	 0.4880	 0.6040
Z	 0.8250	 0.6570
a	 0.9110	 0.6800
b	 0.8320	 0.6530
c	 0.7050	 0.6200
d	 0.8200	 0.6650
e	 0.8050	 0.6480
f	 0.8000	 0.6360
g	 0.8550	 0.6590
h	 0.8610	 0.6670



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Chain	Atom inclusion	Q-score
i	 0.8450	 0.6350
j	 0.8420	 0.6310
k	 0.8470	 0.6310
l	 0.8800	 0.6570
m	 0.8170	 0.6370
n	 0.9040	 0.6580
o	 0.8580	 0.6380
p	 0.8850	 0.6590
q	 0.8310	 0.6810
r	 0.8500	 0.6860
s	 0.8340	 0.6650