



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:08 AM UTC

PDB ID : 7R42 / pdb_00007r42
EMDB ID : EMD-14256
Title : Bovine complex I in the presence of IM1761092, active class ii (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

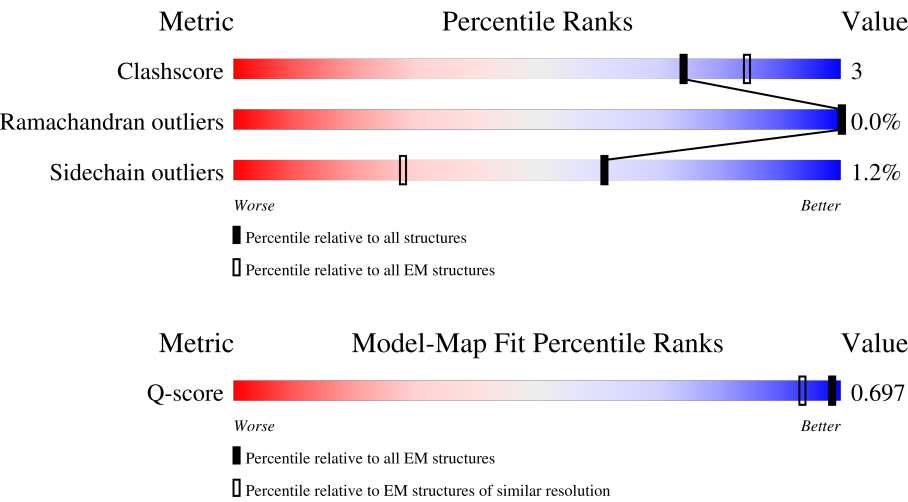
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 Å.

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



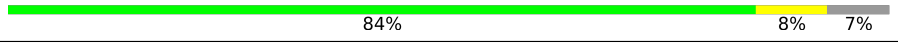
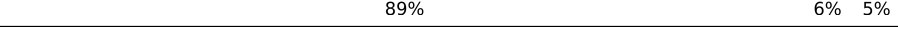
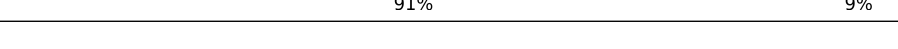
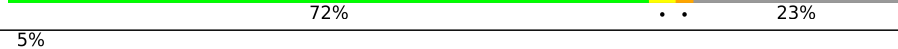
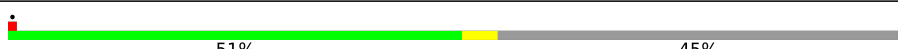
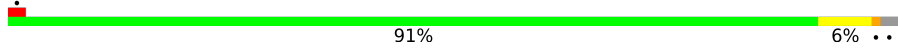
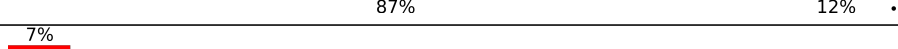
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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

Mol	Chain	Length	Quality of chain
1	A	115	95%5%
2	B	216	67%28%
3	C	266	74%22%
4	D	463	83%10%7%

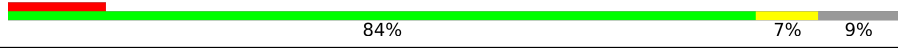
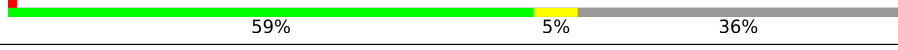
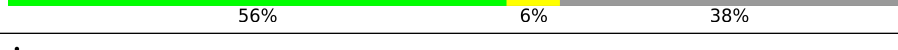
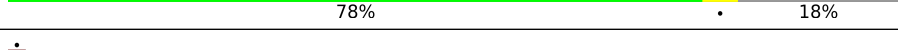
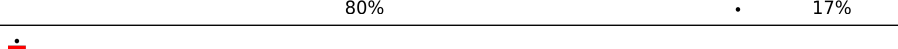
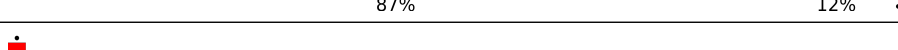
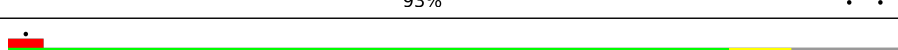
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

There are 60 unique types of molecules in this entry. The entry contains 69480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4780	3178	735	824	43		

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	113	Total	C	N	O	S	0	0
			945	619	161	162	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	104	Total	C	N	O	S	0	0
			898	590	155	152	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	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	127	Total	C	N	O	S	0	0
			1061	681	187	193			

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

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

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

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

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

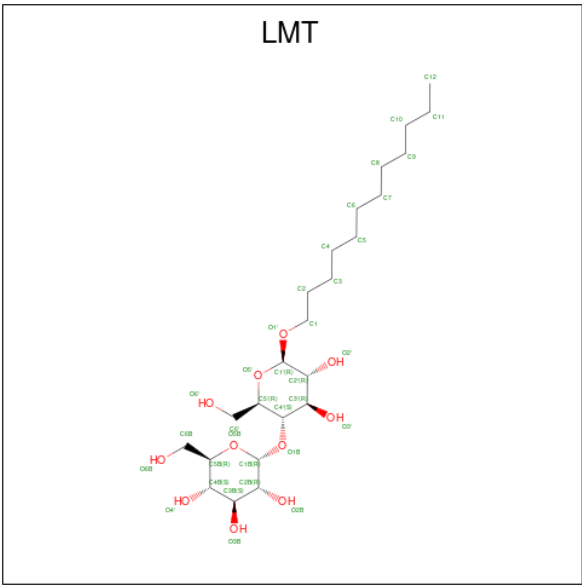
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

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



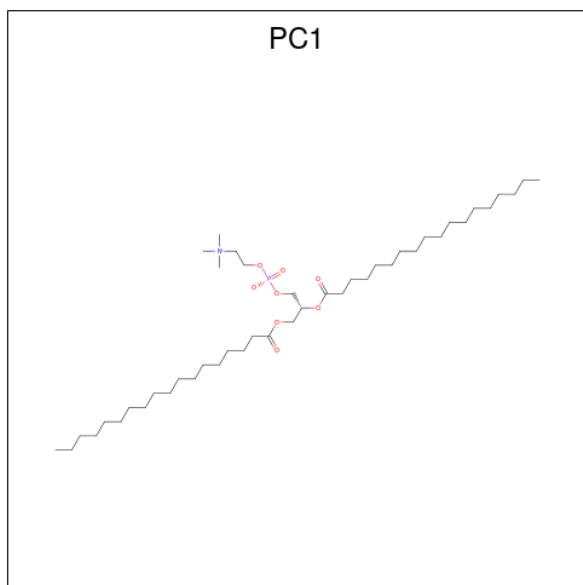
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	K	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	

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

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



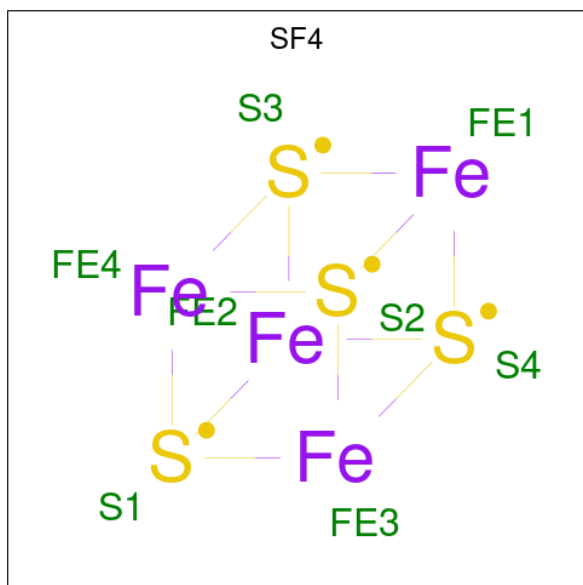
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			21	11	1	8	1	

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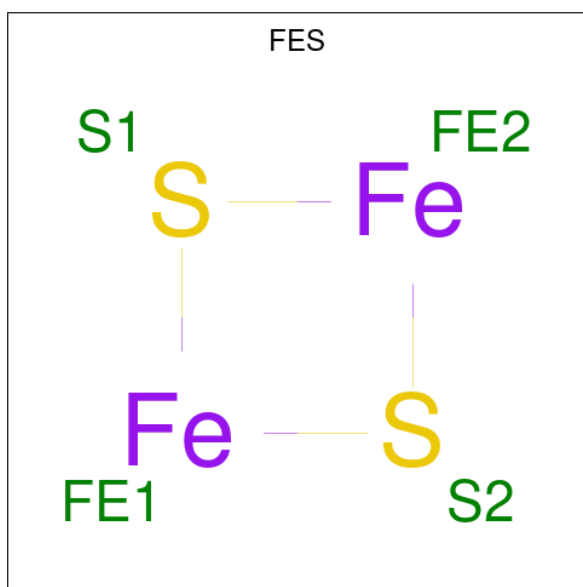
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	L	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



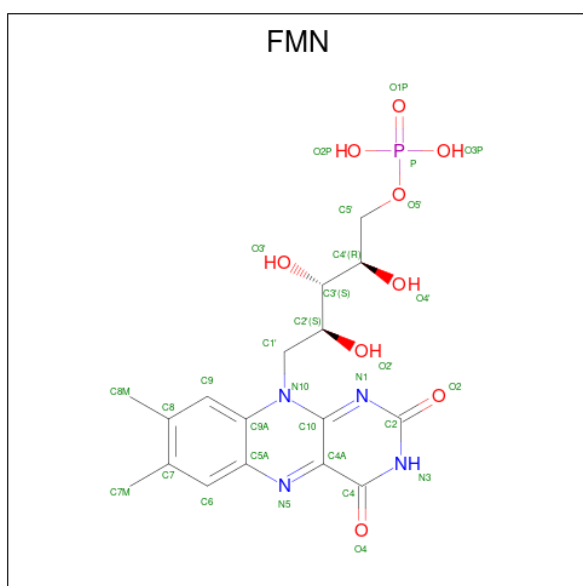
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



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

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

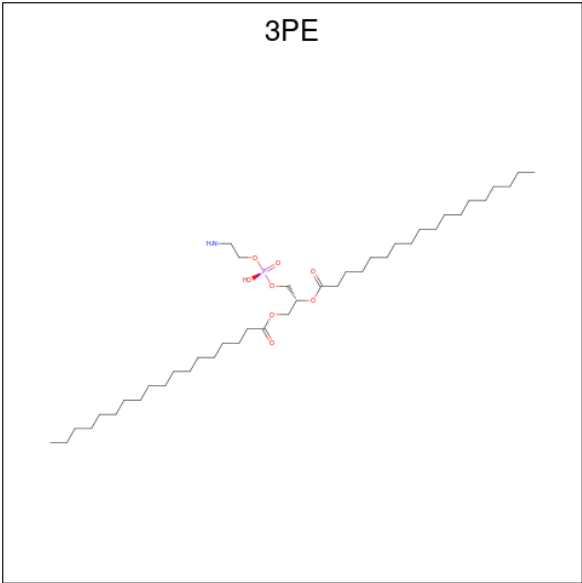


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



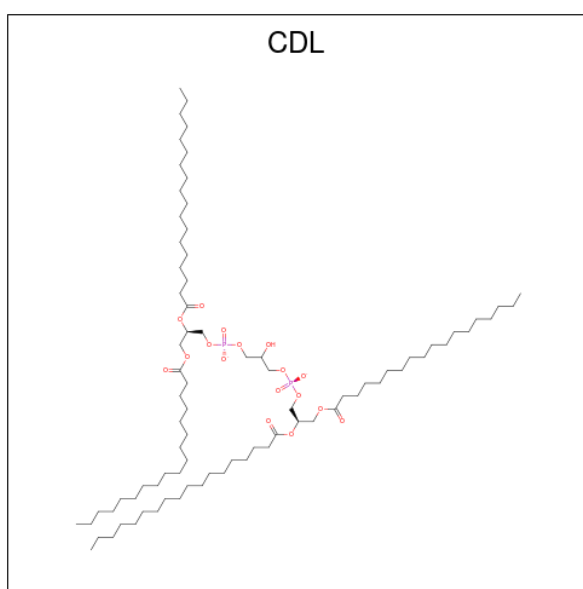
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
51	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
51	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
51	N	1	Total	C	N	O	P	0
			29	19	1	8	1	
51	P	1	Total	C	N	O	P	0
			37	27	1	8	1	

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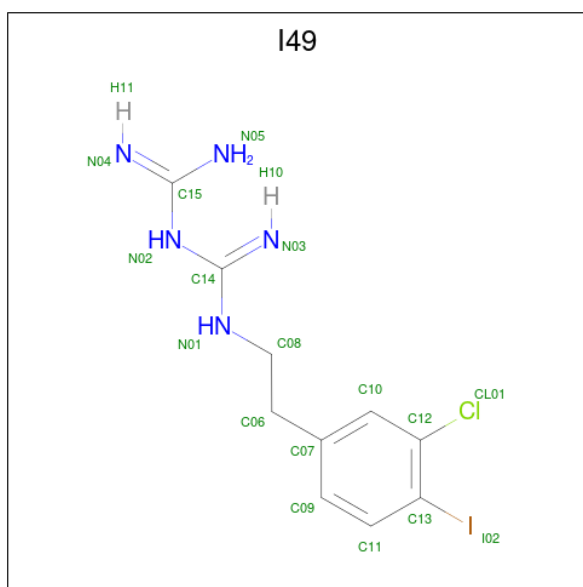
Mol	Chain	Residues	Atoms					AltConf
51	X	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



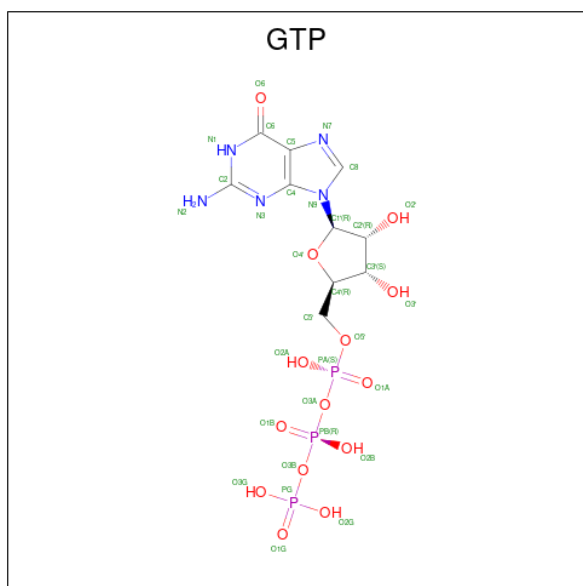
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			62	43	17	2	
52	K	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	r	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 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
53	N	1	Total	C	Cl	I	N	0
			17	10	1	1	5	

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

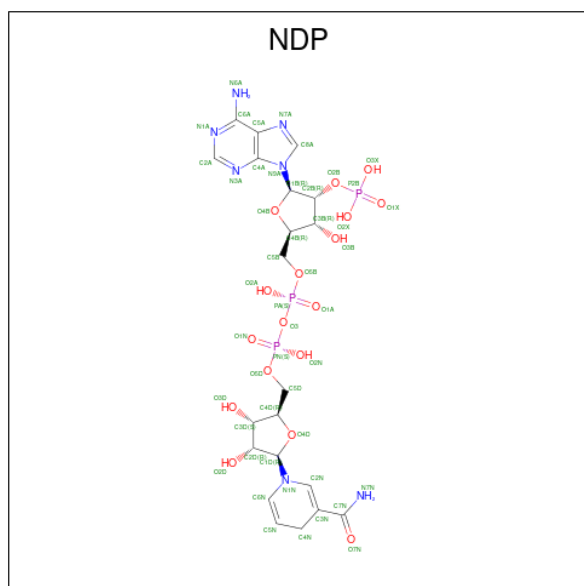


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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

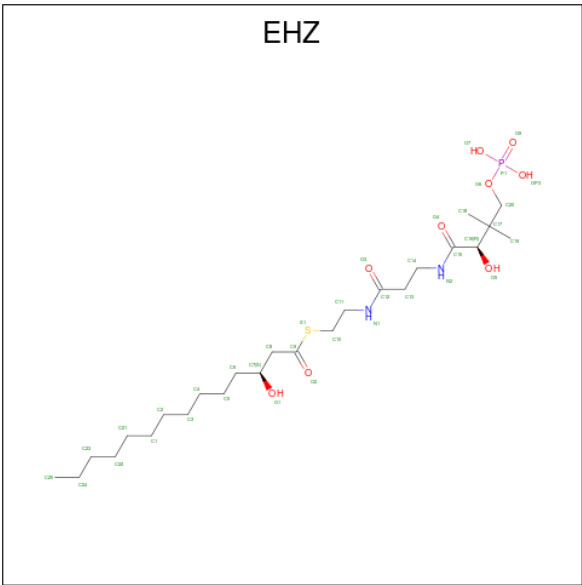


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

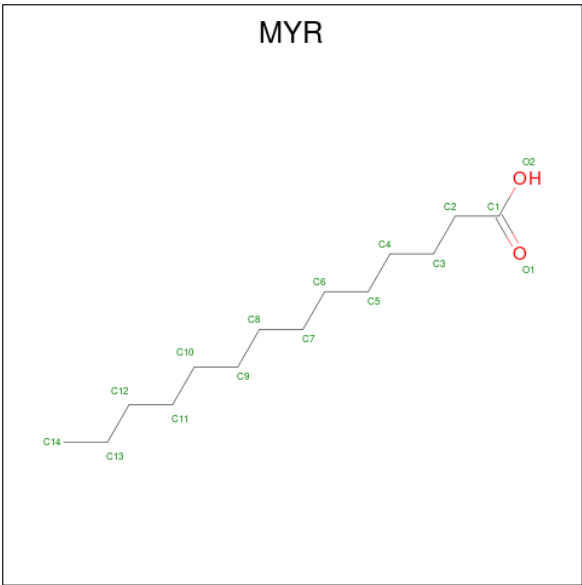
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	S
			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	0
			15	14	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	30	Total 30	O 30	0
60	B	65	Total 65	O 65	0
60	C	92	Total 92	O 92	0
60	D	168	Total 168	O 168	0
60	E	15	Total 15	O 15	0
60	F	63	Total 63	O 63	0
60	G	203	Total 203	O 203	0
60	H	70	Total 70	O 70	0
60	I	92	Total 92	O 92	0
60	J	27	Total 27	O 27	0
60	K	18	Total 18	O 18	0
60	L	52	Total 52	O 52	0
60	M	65	Total 65	O 65	0
60	N	52	Total 52	O 52	0
60	O	27	Total 27	O 27	0
60	P	80	Total 80	O 80	0
60	Q	64	Total 64	O 64	0
60	R	44	Total 44	O 44	0
60	S	4	Total 4	O 4	0
60	U	1	Total 1	O 1	0
60	V	17	Total 17	O 17	0
60	W	13	Total 13	O 13	0

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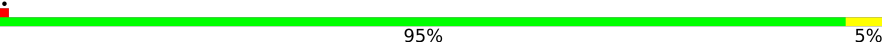
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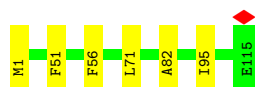
Mol	Chain	Residues	Atoms		AltConf
60	X	28	Total 28	O 28	0
60	Y	2	Total 2	O 2	0
60	Z	22	Total 22	O 22	0
60	a	16	Total 16	O 16	0
60	b	8	Total 8	O 8	0
60	d	17	Total 17	O 17	0
60	e	18	Total 18	O 18	0
60	f	3	Total 3	O 3	0
60	g	5	Total 5	O 5	0
60	h	23	Total 23	O 23	0
60	i	3	Total 3	O 3	0
60	j	2	Total 2	O 2	0
60	k	1	Total 1	O 1	0
60	l	13	Total 13	O 13	0
60	m	11	Total 11	O 11	0
60	n	7	Total 7	O 7	0
60	o	2	Total 2	O 2	0
60	p	16	Total 16	O 16	0
60	q	47	Total 47	O 47	0
60	r	33	Total 33	O 33	0
60	s	6	Total 6	O 6	0

3 Residue-property plots [i](#)

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

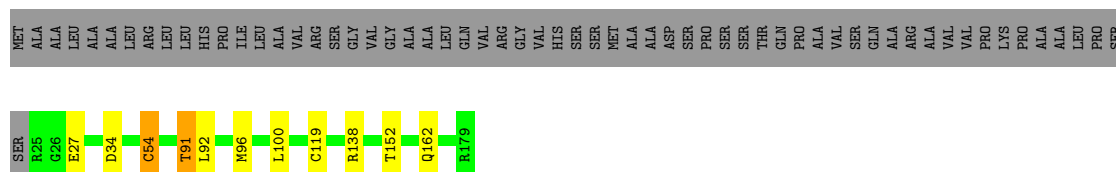
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



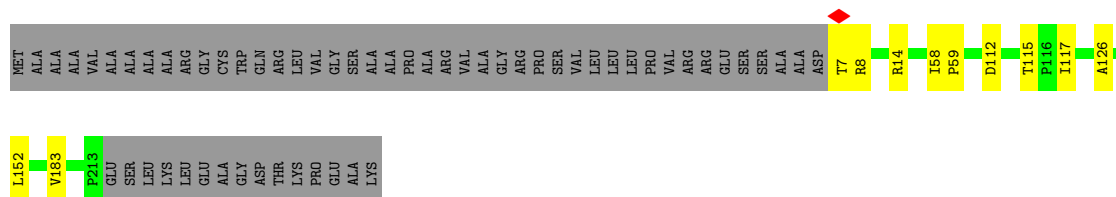
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



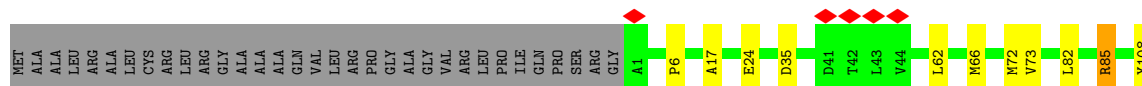
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



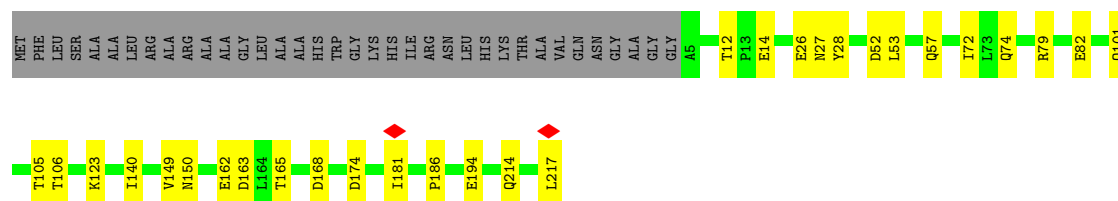
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

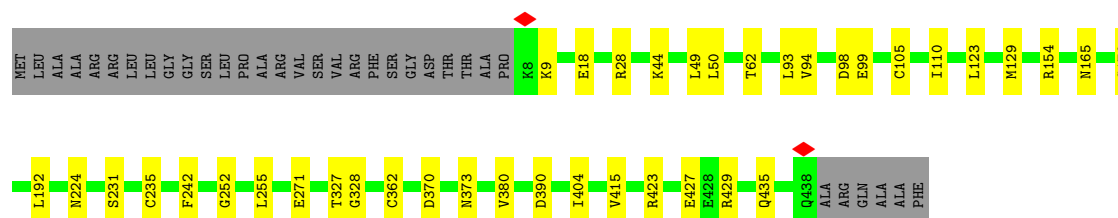
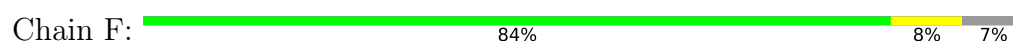




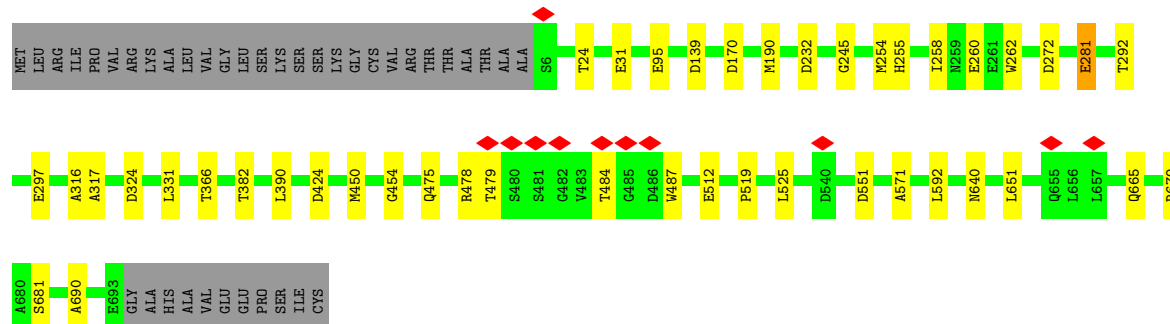
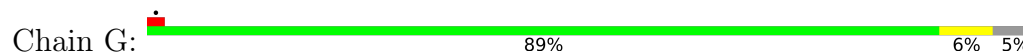
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



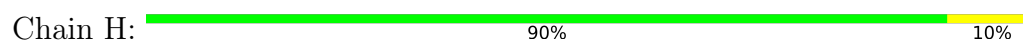
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

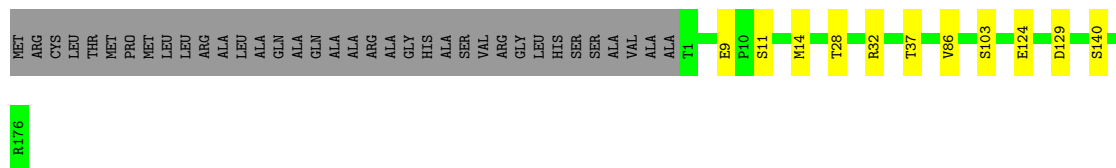


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



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

Chain I:  78% 5% 17%

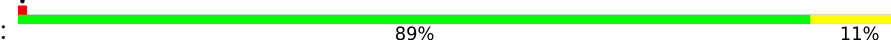


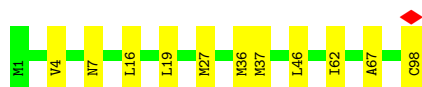
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  89% 10% .



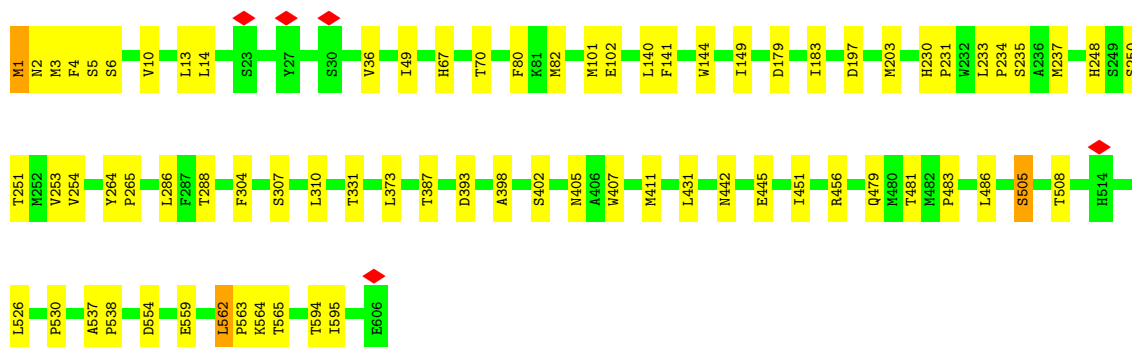
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  89% 11%

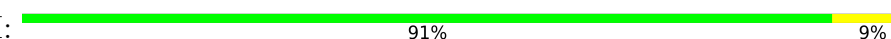


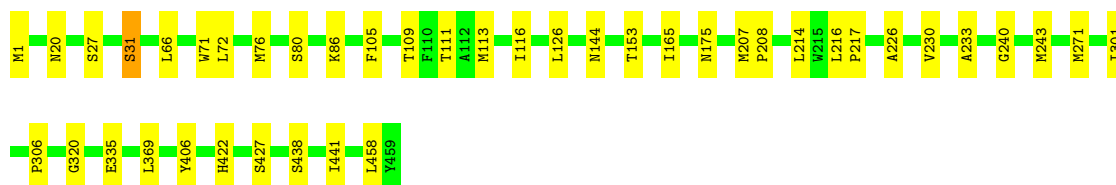
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

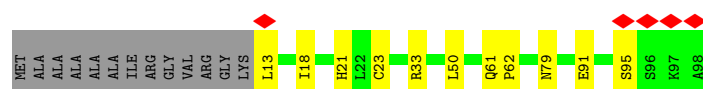
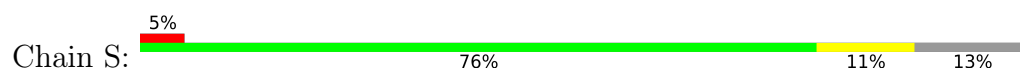
Chain L:  88% 12%



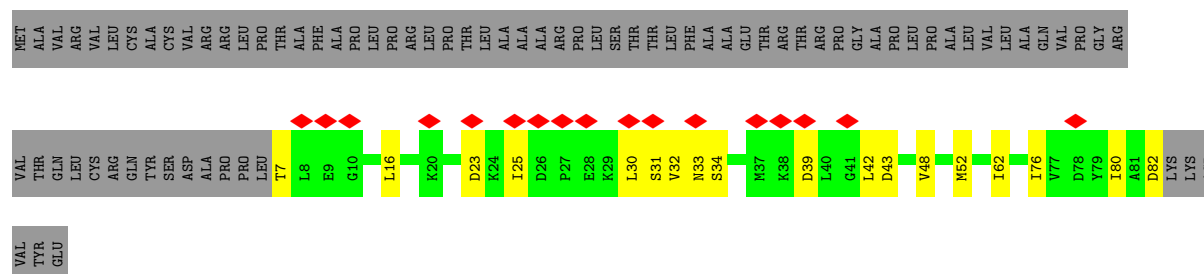
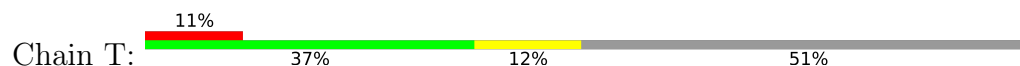
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  91% 9%

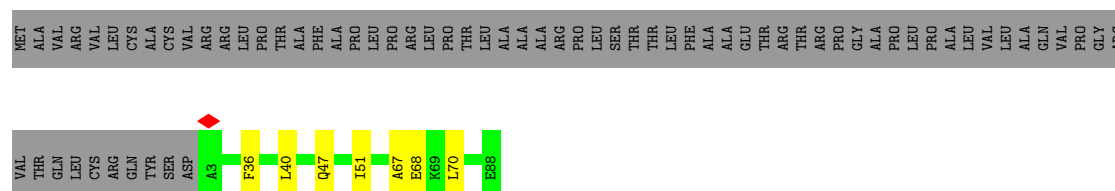




- Molecule 20: Acyl carrier protein, mitochondrial



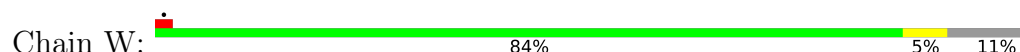
- Molecule 20: Acyl carrier protein, mitochondrial



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



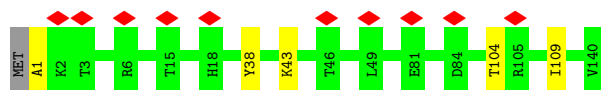
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



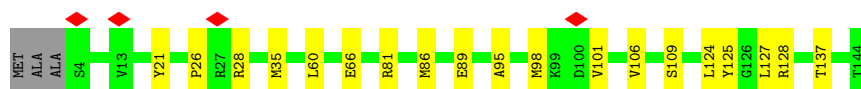
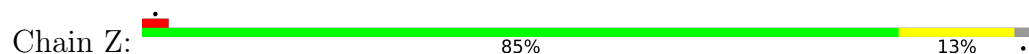
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



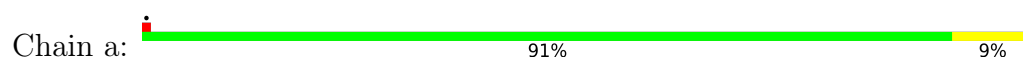
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



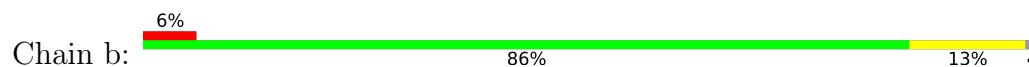
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



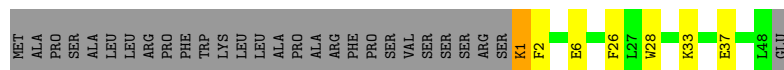
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



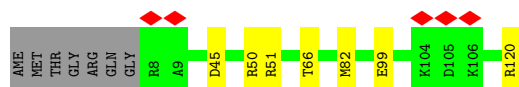
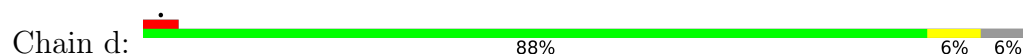
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



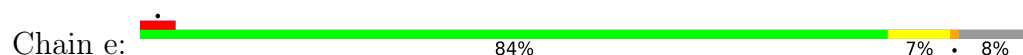
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

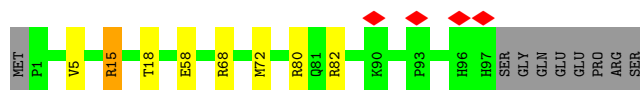


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

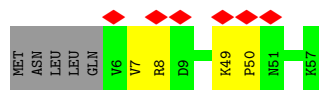
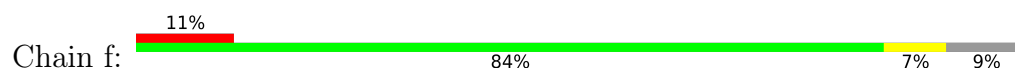


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

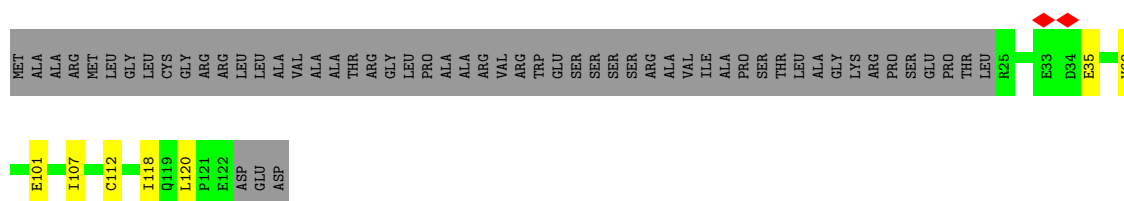




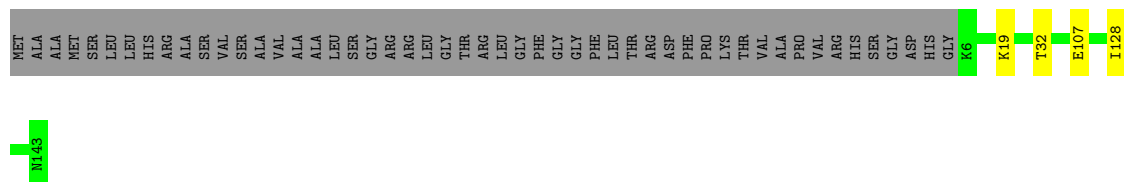
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



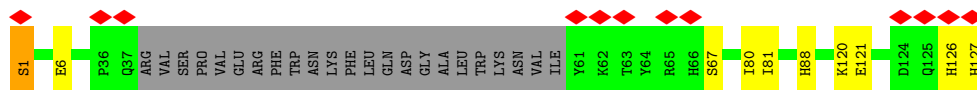
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



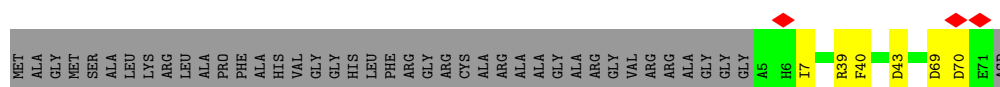
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

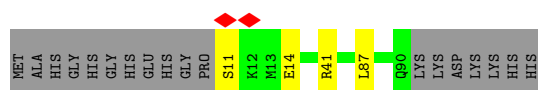


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



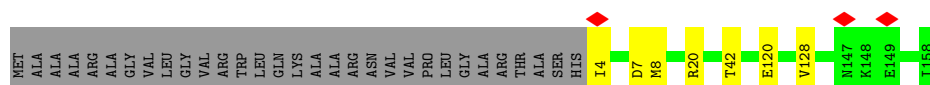
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:  78% 18%



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

Chain l:  80% 17%



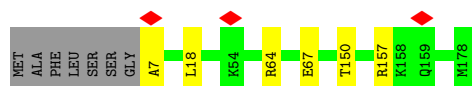
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  87% 12%



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

Chain n:  93% 7%

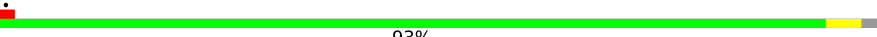


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  81% 7% 12%



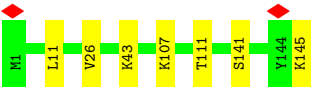
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  93% 7%

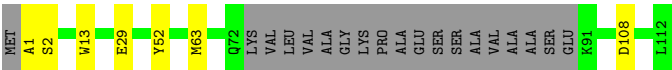


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

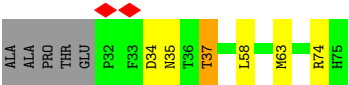
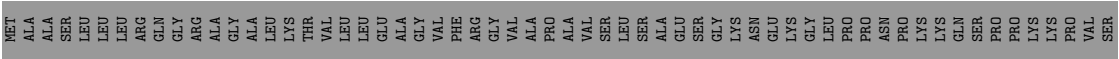
Chain q:  95% 5%



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53763	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	32.833	Depositor
Minimum map value	-14.121	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.032	Depositor
Recommended contour level	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: LMT, MG, K, FME, I49, NDP, 3PE, FES, CDL, FMN, PC1, ZN, MYR, 2MR, EHZ, SF4, AYA, GTP, 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	0.23	0/936	0.28	0/1281
2	B	0.27	0/1272	0.37	0/1720
3	C	0.25	0/1772	0.32	0/2413
4	D	0.26	0/3537	0.33	0/4794
5	E	0.22	0/1695	0.31	0/2307
6	F	0.23	0/3393	0.30	0/4584
7	G	0.24	0/5367	0.32	0/7274
8	H	0.27	0/2571	0.35	0/3513
9	I	0.27	0/1445	0.35	0/1956
10	J	0.24	0/1362	0.31	0/1848
11	K	0.24	0/745	0.28	0/1008
12	L	0.26	0/4896	0.30	0/6663
13	M	0.27	0/3738	0.31	0/5097
14	N	0.26	0/2792	0.30	0/3800
15	O	0.24	0/2651	0.29	0/3587
16	P	0.23	0/2824	0.32	0/3831
17	Q	0.24	0/1039	0.32	0/1404
18	R	0.26	0/742	0.33	0/999
19	S	0.22	0/702	0.31	0/945
20	T	0.18	0/621	0.31	0/837
20	U	0.28	0/705	0.30	0/952
21	V	0.21	0/943	0.27	0/1277
22	W	0.24	0/995	0.31	0/1337
23	X	0.24	0/1439	0.33	0/1942
24	Y	0.19	0/1042	0.29	0/1414
25	Z	0.23	0/1181	0.29	0/1592
26	a	0.25	0/584	0.32	0/786
27	b	0.22	0/672	0.31	0/923
28	c	0.22	0/418	0.28	0/567
29	d	0.24	0/975	0.31	0/1319
30	e	0.23	0/840	0.36	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.22	0/464	0.33	0/626
32	g	0.23	0/850	0.29	0/1154
33	h	0.25	0/1188	0.31	0/1607
34	i	0.25	0/920	0.34	0/1251
35	j	0.25	0/607	0.29	0/833
36	k	0.24	0/663	0.30	0/895
37	l	0.25	0/1358	0.30	0/1858
38	m	0.26	0/1088	0.31	0/1472
39	n	0.25	0/1545	0.29	0/2092
40	o	0.26	0/1060	0.34	0/1420
41	p	0.27	0/1476	0.28	0/1990
42	q	0.23	0/1250	0.32	0/1698
43	r	0.22	0/780	0.31	0/1056
44	s	0.20	0/383	0.28	0/518
All	All	0.25	0/67526	0.31	0/91563

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	275	TYR	Peptide
4	D	85	2MR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	5	0
2	B	1241	0	1251	8	0
3	C	1721	0	1675	8	0
4	D	3459	0	3404	32	0
5	E	1655	0	1661	18	0
6	F	3319	0	3274	24	0
7	G	5279	0	5301	28	0
8	H	2509	0	2621	18	0
9	I	1414	0	1370	8	0
10	J	1337	0	1346	17	0
11	K	745	0	785	10	0
12	L	4780	0	4926	46	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	20	0
15	O	2589	0	2565	22	0
16	P	2747	0	2766	18	0
17	Q	1016	0	1014	3	0
18	R	730	0	707	4	0
19	S	691	0	706	4	0
20	T	612	0	604	9	0
20	U	693	0	688	4	0
21	V	923	0	964	5	0
22	W	971	0	989	4	0
23	X	1402	0	1385	14	0
24	Y	1030	0	1039	5	0
25	Z	1152	0	1151	18	0
26	a	569	0	568	5	0
27	b	651	0	662	8	0
28	c	405	0	409	6	0
29	d	945	0	932	9	0
30	e	819	0	821	6	0
31	f	451	0	453	2	0
32	g	824	0	772	6	0
33	h	1154	0	1168	3	0
34	i	898	0	907	7	0
35	j	580	0	519	3	0
36	k	644	0	626	1	0
37	l	1304	0	1203	9	0
38	m	1061	0	1059	14	0
39	n	1492	0	1438	6	0
40	o	1035	0	1004	7	0
41	p	1443	0	1415	6	0
42	q	1209	0	1182	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	767	0	776	6	0
44	s	371	0	344	5	0
45	A	70	0	92	2	0
45	J	35	0	46	2	0
45	K	35	0	46	0	0
45	L	105	0	138	0	0
45	M	105	0	138	6	0
45	Y	105	0	138	1	0
45	b	35	0	46	0	0
45	h	35	0	46	1	0
45	j	35	0	46	0	0
45	l	35	0	46	0	0
46	A	21	0	18	1	0
46	B	89	0	132	4	0
46	L	49	0	75	3	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	1	0
50	G	1	0	0	0	0
51	H	129	0	194	0	0
51	L	94	0	142	2	0
51	M	97	0	151	4	0
51	N	70	0	88	0	0
51	P	37	0	48	0	0
51	X	51	0	82	2	0
51	Y	35	0	44	1	0
51	d	102	0	164	0	0
52	J	62	0	68	1	0
52	K	71	0	86	0	0
52	L	69	0	82	0	0
52	h	67	0	81	2	0
52	r	76	0	96	1	0
53	N	17	0	0	4	0
54	O	32	0	12	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	U	37	0	0	0	0
59	o	15	0	27	0	0
60	A	30	0	0	0	0
60	B	65	0	0	3	0
60	C	92	0	0	2	0
60	D	168	0	0	7	0
60	E	15	0	0	1	0
60	F	63	0	0	4	0
60	G	203	0	0	8	0
60	H	70	0	0	0	0
60	I	92	0	0	1	0
60	J	27	0	0	1	0
60	K	18	0	0	0	0
60	L	52	0	0	1	0
60	M	65	0	0	3	0
60	N	52	0	0	2	0
60	O	27	0	0	5	0
60	P	80	0	0	4	0
60	Q	64	0	0	1	0
60	R	44	0	0	1	0
60	S	4	0	0	0	0
60	U	1	0	0	0	0
60	V	17	0	0	2	0
60	W	13	0	0	0	0
60	X	28	0	0	2	0
60	Y	2	0	0	0	0
60	Z	22	0	0	1	0
60	a	16	0	0	1	0
60	b	8	0	0	0	0
60	d	17	0	0	0	0
60	e	18	0	0	0	0
60	f	3	0	0	0	0
60	g	5	0	0	0	0
60	h	23	0	0	2	0
60	i	3	0	0	0	0
60	j	2	0	0	0	0
60	k	1	0	0	0	0
60	l	13	0	0	1	0
60	m	11	0	0	2	0
60	n	7	0	0	0	0
60	o	2	0	0	0	0
60	p	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	q	47	0	0	0	0
60	r	33	0	0	2	0
60	s	6	0	0	0	0
All	All	69480	0	68583	434	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 (434) 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)
53:N:703:I49:I02	29:d:82:MET:HB3	2.31	1.01
53:N:703:I49:I02	29:d:82:MET:O	2.57	0.92
16:P:51:CYS:O	60:P:601:HOH:O	1.93	0.85
16:P:98:GLU:OE1	60:P:602:HOH:O	1.97	0.81
52:J:701:CDL:OB4	60:J:801:HOH:O	1.97	0.81
35:j:69:ASP:OD2	40:o:113:ARG:NH1	2.15	0.80
7:G:31:GLU:OE1	60:G:901:HOH:O	2.01	0.78
25:Z:98:MET:HE3	25:Z:101:VAL:HG21	1.64	0.78
33:h:107:GLU:OE1	60:h:1101:HOH:O	2.01	0.78
6:F:373:ASN:OD1	60:F:1201:HOH:O	2.01	0.77
37:l:20:ARG:NH1	60:l:301:HOH:O	2.18	0.77
13:M:20:ASN:OD1	60:M:701:HOH:O	2.03	0.76
15:O:83:TYR:OH	54:O:401:GTP:O3'	1.95	0.75
45:h:1002:LMT:H6'	45:h:1002:LMT:H6B	1.35	0.75
12:L:479:GLN:NE2	12:L:481:THR:O	2.20	0.75
4:D:6:PRO:O	60:D:501:HOH:O	2.05	0.74
28:c:33:LYS:NZ	28:c:37:GLU:OE1	2.21	0.73
15:O:146:LYS:NZ	15:O:150:ASP:OD1	2.22	0.72
12:L:594:THR:HG1	24:Y:38:TYR:HH	1.21	0.72
13:M:335:GLU:OE2	60:M:702:HOH:O	2.07	0.72
27:b:10:ASN:OD1	27:b:14:LYS:NZ	2.16	0.72
1:A:71:LEU:O	10:J:147:TYR:OH	2.05	0.72
6:F:99:GLU:OE1	60:F:1202:HOH:O	2.07	0.72
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.08	0.71
6:F:28:ARG:NH1	44:s:35:ASN:O	2.23	0.71
21:V:110:GLN:OE1	60:V:202:HOH:O	2.10	0.70
12:L:562:LEU:HD13	45:M:602:LMT:C12	2.21	0.70
21:V:105:GLU:O	60:V:201:HOH:O	2.09	0.70
38:m:24:ILE:O	38:m:24:ILE:HD12	1.92	0.70
7:G:139:ASP:OD1	60:G:902:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:38:VAL:O	60:a:101:HOH:O	2.10	0.69
20:T:31:SER:N	20:T:34:SER:OG	2.26	0.69
38:m:74:ASN:OD1	60:m:201:HOH:O	2.10	0.68
51:M:601:3PE:H2I1	45:M:602:LMT:H111	1.76	0.68
53:N:703:I49:I02	29:d:82:MET:C	3.06	0.68
2:B:34:ASP:OD1	60:B:301:HOH:O	2.12	0.67
21:V:57:MET:CE	21:V:71:LEU:HD23	2.25	0.67
12:L:197:ASP:OD1	60:L:801:HOH:O	2.13	0.67
7:G:665:GLN:OE1	60:G:904:HOH:O	2.13	0.67
20:U:47:GLN:NE2	20:U:70:LEU:O	2.27	0.67
46:B:202:PC1:O12	60:B:302:HOH:O	2.13	0.66
12:L:102:GLU:OE2	12:L:456:ARG:NH2	2.28	0.66
37:l:4:ILE:HD12	37:l:8:MET:HB2	1.77	0.66
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.28	0.66
25:Z:66:GLU:OE1	60:Z:201:HOH:O	2.14	0.66
37:l:4:ILE:HB	37:l:8:MET:HE3	1.78	0.66
6:F:98:ASP:OD2	60:F:1203:HOH:O	2.14	0.66
39:n:18:LEU:HD13	39:n:67:GLU:OE1	1.96	0.66
13:M:86:LYS:NZ	32:g:35:GLU:OE1	2.26	0.66
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.06	0.65
5:E:12:THR:OG1	5:E:14:GLU:OE2	2.11	0.65
7:G:232:ASP:O	60:G:903:HOH:O	2.12	0.65
15:O:21:LYS:O	60:O:501:HOH:O	2.13	0.65
7:G:95:GLU:OE2	60:G:905:HOH:O	2.13	0.65
42:q:43:LYS:NZ	42:q:111:THR:O	2.25	0.65
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.79	0.64
14:N:347:GLU:OE1	60:N:802:HOH:O	2.15	0.64
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.31	0.64
12:L:562:LEU:HD13	45:M:602:LMT:H123	1.80	0.64
15:O:129:TYR:O	60:O:502:HOH:O	2.15	0.64
45:J:702:LMT:O3'	45:J:702:LMT:O2B	2.08	0.63
38:m:70:ALA:O	60:m:202:HOH:O	2.15	0.63
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.28	0.63
16:P:72:ASP:O	60:P:603:HOH:O	2.15	0.63
12:L:1:FME:O	12:L:5:SER:OG	2.14	0.62
12:L:564:LYS:NZ	45:M:602:LMT:O6B	2.25	0.62
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.29	0.62
10:J:77:GLU:OE2	10:J:77:GLU:N	2.33	0.62
25:Z:86:MET:HE1	25:Z:125:TYR:CZ	2.34	0.62
5:E:214:GLN:NE2	6:F:235:CYS:O	2.33	0.62
5:E:52:ASP:OD2	60:E:401:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:LEU:HD13	26:a:12:MET:HE1	1.82	0.61
11:K:19:LEU:HD22	11:K:36:MET:HE1	1.82	0.61
15:O:250:ASP:OD1	15:O:250:ASP:N	2.32	0.61
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.82	0.60
13:M:208:PRO:O	60:M:703:HOH:O	2.16	0.60
46:A:303:PC1:O13	46:A:303:PC1:H132	2.00	0.60
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.84	0.60
4:D:249:ASP:OD2	60:D:502:HOH:O	2.16	0.60
23:X:152:GLU:OE2	23:X:153:VAL:N	2.34	0.60
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.83	0.60
13:M:27:SER:O	13:M:31:SER:OG	2.17	0.60
23:X:29:HIS:ND1	60:X:502:HOH:O	2.31	0.60
29:d:120:ARG:NH1	38:m:112:GLU:OE1	2.33	0.60
16:P:143:SER:OG	16:P:282:ASP:OD1	2.17	0.60
3:C:8:ARG:O	4:D:129:ARG:NH2	2.35	0.60
18:R:2:VAL:HG11	18:R:37:GLU:OE1	2.02	0.59
5:E:194:GLU:OE1	5:E:194:GLU:N	2.34	0.59
7:G:366:THR:HB	7:G:450:MET:HE3	1.84	0.59
10:J:103:MET:HG2	10:J:115:VAL:HG11	1.85	0.59
20:T:7:THR:HG22	20:T:7:THR:O	2.03	0.59
51:M:601:3PE:H2I1	45:M:602:LMT:C11	2.33	0.59
37:l:7:ASP:OD2	37:l:7:ASP:N	2.34	0.59
38:m:32:GLN:OE1	39:n:7:ALA:N	2.36	0.59
15:O:88:SER:OG	15:O:90:ASP:OD1	2.17	0.59
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.86	0.58
12:L:483:PRO:HD2	12:L:486:LEU:HD12	1.85	0.58
43:r:29:GLU:O	60:r:301:HOH:O	2.17	0.58
25:Z:98:MET:CE	25:Z:101:VAL:HG21	2.32	0.58
34:i:6:GLU:OE1	39:n:157:ARG:NH1	2.35	0.58
7:G:475:GLN:O	7:G:479:THR:HG23	2.04	0.58
44:s:63:MET:HE3	44:s:63:MET:HA	1.86	0.58
20:T:32:VAL:HG13	20:T:33:ASN:OD1	2.04	0.57
15:O:83:TYR:HH	54:O:401:GTP:HO3'	1.25	0.57
23:X:149:PRO:O	60:X:501:HOH:O	2.17	0.57
6:F:9:LYS:NZ	6:F:271:GLU:OE2	2.36	0.57
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.40	0.57
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.39	0.57
11:K:19:LEU:CD2	11:K:36:MET:HE1	2.35	0.57
10:J:115:VAL:HG23	10:J:115:VAL:O	2.04	0.57
12:L:6:SER:O	12:L:10:VAL:HG13	2.05	0.57
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:4:ILE:HD12	37:l:8:MET:CB	2.35	0.56
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.40	0.56
34:i:121:GLU:OE2	34:i:121:GLU:HA	2.04	0.56
6:F:423:ARG:NH1	6:F:427:GLU:OE2	2.37	0.56
20:T:23:ASP:OD2	20:T:23:ASP:N	2.35	0.56
7:G:331:LEU:HD22	7:G:525:LEU:HD22	1.88	0.56
7:G:260:GLU:OE2	60:G:906:HOH:O	2.17	0.55
22:W:30:ARG:HG3	22:W:30:ARG:HH11	1.71	0.55
3:C:14:ARG:NH1	60:C:308:HOH:O	2.38	0.55
14:N:70:LEU:HD22	14:N:98:MET:HE2	1.88	0.55
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.88	0.55
25:Z:89:GLU:OE2	25:Z:128:ARG:NH2	2.39	0.55
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.89	0.55
12:L:80:PHE:HB3	12:L:82:MET:HE2	1.88	0.54
32:g:101:GLU:CG	32:g:107:ILE:HD11	2.37	0.54
23:X:97:ARG:HD2	25:Z:60:LEU:HD13	1.89	0.54
10:J:70:TYR:HB3	11:K:27:MET:HE1	1.90	0.54
14:N:214:THR:HG22	14:N:218:MET:HE2	1.90	0.54
10:J:153:LEU:O	10:J:157:THR:HG23	2.07	0.54
12:L:445:GLU:O	12:L:451:ILE:HD11	2.07	0.54
32:g:118:ILE:HG21	41:p:162:MET:HE1	1.90	0.54
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.90	0.54
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.41	0.54
13:M:306:PRO:HA	13:M:458:LEU:HD22	1.90	0.54
12:L:288:THR:HG21	12:L:307:SER:HB3	1.89	0.54
15:O:260:ARG:NH1	60:O:504:HOH:O	2.35	0.54
32:g:120:LEU:HD21	41:p:162:MET:HE3	1.90	0.53
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.91	0.53
29:d:99:GLU:CD	29:d:99:GLU:H	2.17	0.53
5:E:105:THR:HG22	5:E:106:THR:H	1.74	0.53
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.43	0.53
12:L:13:LEU:HD22	34:i:81:ILE:HD11	1.89	0.53
4:D:24:GLU:N	4:D:24:GLU:OE2	2.41	0.53
25:Z:127:LEU:HD22	30:e:82:ARG:NH1	2.24	0.53
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.36	0.52
18:R:78:GLU:OE2	18:R:78:GLU:HA	2.09	0.52
53:N:703:I49:I02	29:d:82:MET:CB	3.18	0.52
15:O:28:ASP:OD1	15:O:206:TYR:OH	2.23	0.52
13:M:66:LEU:HD11	13:M:111:THR:HG23	1.91	0.52
46:L:707:PC1:H142	52:h:1001:CDL:OA3	2.09	0.52
16:P:97:ARG:NH2	56:P:501:NDP:O2X	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:174:ARG:NH1	60:P:605:HOH:O	2.38	0.52
19:S:23:CYS:O	19:S:33:ARG:NH1	2.43	0.52
3:C:152:LEU:O	60:C:301:HOH:O	2.19	0.52
12:L:149:ILE:HG13	13:M:369:LEU:HD13	1.92	0.52
5:E:74:GLN:O	44:s:74:ARG:NH2	2.43	0.51
25:Z:86:MET:HE2	25:Z:124:LEU:HG	1.92	0.51
37:l:128:VAL:HG22	40:o:97:ARG:HB3	1.92	0.51
4:D:66:MET:HE1	4:D:411:LEU:HD11	1.92	0.51
4:D:385:ARG:NH1	60:D:518:HOH:O	2.39	0.51
38:m:72:SER:OG	38:m:73:ALA:N	2.44	0.51
40:o:11:ASP:OD2	40:o:14:VAL:HG22	2.10	0.51
4:D:279:ASP:OD2	60:D:503:HOH:O	2.19	0.51
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.93	0.51
23:X:87:CYS:SG	23:X:102:GLN:NE2	2.83	0.51
8:H:70:MET:HB3	8:H:122:ALA:HB2	1.92	0.51
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.92	0.51
38:m:121:ASP:OD1	38:m:123:THR:OG1	2.28	0.51
14:N:70:LEU:CD2	14:N:98:MET:HE2	2.40	0.51
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.46	0.51
25:Z:127:LEU:HD22	30:e:82:ARG:HH11	1.75	0.51
1:A:82:ALA:O	27:b:42:LEU:HD12	2.11	0.50
16:P:268:ARG:HD2	16:P:268:ARG:O	2.10	0.50
3:C:7:THR:O	3:C:7:THR:OG1	2.28	0.50
13:M:422:HIS:HB2	38:m:59:ILE:HD12	1.93	0.50
20:U:36:PHE:HD1	20:U:40:LEU:HD12	1.76	0.50
20:U:51:ILE:HG21	20:U:67:ALA:HB1	1.94	0.50
8:H:18:ALA:O	8:H:21:THR:OG1	2.23	0.50
12:L:505:SER:O	12:L:508:THR:OG1	2.28	0.50
5:E:79:ARG:NH1	5:E:82:GLU:OE1	2.44	0.50
16:P:138:ASP:OD1	16:P:140:LYS:N	2.37	0.50
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.94	0.50
10:J:11:VAL:HG11	45:J:702:LMT:H71	1.94	0.50
14:N:236:LYS:HD3	14:N:237:THR:HG23	1.94	0.50
27:b:58:ASP:HA	27:b:62:MET:HE2	1.93	0.49
7:G:170:ASP:OD1	60:G:907:HOH:O	2.18	0.49
16:P:260:HIS:NE2	16:P:285:GLU:OE1	2.42	0.49
14:N:72:MET:HE3	14:N:76:ILE:HD11	1.95	0.49
15:O:26:THR:HG21	60:O:513:HOH:O	2.12	0.49
40:o:30:PHE:HB3	40:o:33:ARG:HG3	1.93	0.49
4:D:123:GLU:OE1	4:D:138:ARG:NH2	2.45	0.49
4:D:296:ARG:HH21	4:D:420:THR:HG21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10:SER:OG	11:K:7:ASN:ND2	2.42	0.49
21:V:43:TYR:CD1	21:V:93:MET:HE2	2.48	0.49
28:c:6:GLU:OE2	28:c:6:GLU:HA	2.12	0.49
12:L:373:LEU:HD23	12:L:431:LEU:HD11	1.95	0.49
12:L:331:THR:HB	12:L:387:THR:HG22	1.95	0.49
12:L:594:THR:OG1	24:Y:38:TYR:OH	2.05	0.49
20:T:62:ILE:N	20:T:62:ILE:HD12	2.28	0.49
30:e:80:ARG:NH1	30:e:80:ARG:HB3	2.28	0.49
12:L:398:ALA:O	12:L:402:SER:OG	2.28	0.49
2:B:162:GLN:OE1	9:I:140:SER:OG	2.24	0.48
16:P:46:ILE:N	16:P:46:ILE:HD12	2.27	0.48
2:B:92:LEU:HD13	2:B:100:LEU:HD13	1.96	0.48
16:P:293:ILE:HG22	16:P:295:PRO:HD3	1.95	0.48
15:O:303:LYS:O	29:d:50:ARG:NH1	2.46	0.48
19:S:61:GLN:OE1	19:S:79:ASN:ND2	2.46	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.95	0.48
51:L:705:3PE:N	46:L:707:PC1:O12	2.47	0.48
12:L:562:LEU:CB	12:L:563:PRO:CD	2.92	0.48
4:D:228:MET:HE1	9:I:37:THR:HG23	1.96	0.48
40:o:20:ARG:HB3	40:o:20:ARG:NH1	2.28	0.47
10:J:55:MET:HE2	10:J:55:MET:HA	1.96	0.47
18:R:31:ARG:NH2	60:R:306:HOH:O	2.44	0.47
5:E:217:LEU:HD22	6:F:44:LYS:CE	2.44	0.47
9:I:32:ARG:NH2	25:Z:26:PRO:O	2.43	0.47
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.97	0.47
38:m:22:TYR:O	38:m:23:ASP:C	2.57	0.47
39:n:67:GLU:OE1	39:n:67:GLU:HA	2.15	0.47
3:C:112:ASP:OD1	3:C:115:THR:OG1	2.24	0.47
13:M:207:MET:SD	13:M:240:GLY:N	2.87	0.47
46:B:203:PC1:O13	46:B:203:PC1:H133	2.14	0.47
12:L:49:ILE:HG12	41:p:32:LEU:HD13	1.95	0.47
12:L:264:TYR:N	12:L:265:PRO:CD	2.78	0.47
46:B:202:PC1:H2A2	46:B:202:PC1:H2H2	1.97	0.47
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.45	0.47
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.97	0.47
28:c:1:LYS:CG	28:c:2:PHE:H	2.27	0.47
45:A:301:LMT:H6'1	27:b:42:LEU:HB2	1.96	0.47
4:D:72:MET:SD	4:D:410:MET:HG2	2.55	0.47
4:D:276:ASP:OD1	60:D:504:HOH:O	2.20	0.47
7:G:424:ASP:OD1	7:G:424:ASP:N	2.46	0.47
15:O:211:LEU:O	15:O:215:SER:OG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.51	0.46
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.50	0.46
4:D:151:ILE:HG23	4:D:170:MET:HB3	1.96	0.46
13:M:80:SER:OG	13:M:226:ALA:HB2	2.14	0.46
7:G:478:ARG:NH1	7:G:487:TRP:O	2.48	0.46
12:L:253:VAL:HB	12:L:310:LEU:HD11	1.96	0.46
43:r:52:TYR:OH	60:r:302:HOH:O	2.20	0.46
13:M:216:LEU:HD23	13:M:216:LEU:C	2.40	0.46
6:F:327:THR:OG1	6:F:328:GLY:N	2.49	0.46
20:T:48:VAL:HG12	20:T:52:MET:HE2	1.96	0.46
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.46	0.46
12:L:203:MET:HG2	41:p:109:LEU:HD11	1.96	0.46
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.96	0.46
13:M:406:TYR:CD1	13:M:406:TYR:C	2.94	0.46
14:N:316:GLN:OE1	60:N:803:HOH:O	2.21	0.46
6:F:110:ILE:HD11	6:F:255:LEU:CD1	2.45	0.46
5:E:149:VAL:HG13	6:F:105:CYS:SG	2.57	0.45
6:F:370:ASP:OD2	60:F:1204:HOH:O	2.20	0.45
4:D:261:ARG:NH2	4:D:303:GLU:OE2	2.49	0.45
9:I:14:MET:HE1	27:b:12:TRP:CD1	2.51	0.45
23:X:48:GLU:OE2	23:X:134:ARG:NH1	2.42	0.45
9:I:28:THR:HG21	25:Z:35:MET:HE1	1.98	0.45
13:M:105:PHE:O	13:M:109:THR:OG1	2.17	0.45
15:O:224:SER:OG	15:O:225:ALA:N	2.50	0.45
8:H:156:MET:HE3	8:H:174:LEU:HD22	1.98	0.45
12:L:1:FME:HCN	12:L:4:PHE:H	1.82	0.45
23:X:63:ASN:OD1	25:Z:81:ARG:NH2	2.48	0.45
24:Y:43:LYS:HB3	24:Y:43:LYS:NZ	2.32	0.45
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.50	0.45
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.57	0.45
5:E:217:LEU:HD22	6:F:44:LYS:HE3	1.98	0.45
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.15	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.45
16:P:311:GLU:OE1	16:P:311:GLU:N	2.50	0.45
51:X:401:3PE:H3I1	51:X:401:3PE:H261	1.98	0.45
25:Z:21:TYR:OH	43:r:108:ASP:OD1	2.26	0.45
38:m:74:ASN:O	38:m:78:ASN:ND2	2.50	0.45
22:W:35:LEU:HD21	22:W:86:GLY:HA3	1.99	0.44
40:o:30:PHE:HB3	40:o:33:ARG:CG	2.47	0.44
12:L:2:ASN:OD1	12:L:3:MET:N	2.48	0.44
12:L:407:TRP:CZ2	12:L:411:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:132:THR:O	60:Q:201:HOH:O	2.21	0.44
28:c:26:PHE:CD1	28:c:26:PHE:C	2.94	0.44
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.98	0.44
13:M:76:MET:SD	13:M:230:VAL:HB	2.57	0.44
20:T:76:ILE:O	20:T:80:ILE:HG12	2.17	0.44
38:m:29:ARG:NH2	39:n:7:ALA:O	2.50	0.44
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.99	0.44
7:G:272:ASP:OD1	7:G:681:SER:OG	2.20	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.80	0.44
11:K:37:MET:HE3	11:K:67:ALA:HB2	1.99	0.44
7:G:317:ALA:HB1	7:G:331:LEU:HD21	2.00	0.44
14:N:337:LEU:HD23	51:X:401:3PE:H391	2.00	0.44
25:Z:86:MET:HE1	25:Z:125:TYR:CE2	2.53	0.44
13:M:438:SER:HA	13:M:441:ILE:HG22	1.99	0.44
17:Q:89:LYS:NZ	17:Q:107:GLU:OE1	2.24	0.44
58:T:101:EHZ:O5	22:W:32:VAL:HG11	2.17	0.44
4:D:62:LEU:HB2	4:D:425:PHE:CZ	2.52	0.44
7:G:551:ASP:OD2	7:G:679:ARG:NH2	2.46	0.44
8:H:179:TRP:N	8:H:180:PRO:CD	2.81	0.44
51:L:705:3PE:H291	34:i:80:ILE:HG23	2.00	0.44
44:s:34:ASP:OD2	44:s:37:THR:OG1	2.35	0.44
4:D:35:ASP:OD1	60:D:505:HOH:O	2.21	0.44
45:Y:804:LMT:O6'	45:Y:804:LMT:O4'	2.26	0.44
1:A:51:PHE:CD1	8:H:133:LEU:HD13	2.53	0.44
33:h:19:LYS:HD2	33:h:19:LYS:HA	1.87	0.44
12:L:80:PHE:CB	12:L:82:MET:HE2	2.47	0.43
25:Z:28:ARG:NH2	43:r:13:TRP:O	2.48	0.43
20:T:25:ILE:HD11	20:T:42:LEU:HD11	2.00	0.43
26:a:69:ILE:HD12	26:a:69:ILE:C	2.43	0.43
4:D:264:GLY:O	60:D:506:HOH:O	2.21	0.43
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.01	0.43
6:F:192:LEU:HD23	6:F:192:LEU:O	2.19	0.43
7:G:297:GLU:OE2	7:G:297:GLU:N	2.46	0.43
12:L:36:VAL:HG12	12:L:101:MET:SD	2.59	0.43
13:M:271:MET:HE2	13:M:271:MET:HA	2.01	0.43
15:O:42:ILE:HD11	15:O:234:VAL:HG11	1.99	0.43
3:C:126:ALA:HB2	4:D:253:TYR:C	2.43	0.43
7:G:254:MET:HA	7:G:260:GLU:O	2.18	0.43
6:F:380:VAL:O	6:F:429:ARG:HD3	2.18	0.43
27:b:42:LEU:HD21	27:b:46:ARG:HE	1.83	0.43
12:L:144:TRP:NE1	12:L:179:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:603:LMT:H112	38:m:97:LEU:HD13	2.00	0.43
41:p:16:THR:HG23	41:p:16:THR:O	2.19	0.43
43:r:2:SER:O	52:r:201:CDL:O1	2.28	0.43
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.00	0.43
14:N:204:ASN:C	14:N:204:ASN:HD22	2.24	0.43
18:R:94:GLN:O	18:R:95:HIS:C	2.61	0.43
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.01	0.43
37:l:42:THR:O	37:l:42:THR:CG2	2.67	0.43
4:D:409:HIS:HB3	4:D:413:ASP:HB2	2.01	0.43
30:e:58:GLU:OE1	30:e:58:GLU:N	2.52	0.43
11:K:16:LEU:HA	11:K:36:MET:HE2	2.01	0.42
7:G:281:GLU:HG2	7:G:592:LEU:HD12	2.00	0.42
10:J:101:PHE:CD1	10:J:101:PHE:C	2.97	0.42
51:M:605:3PE:C33	14:N:242:VAL:HG11	2.49	0.42
7:G:651:LEU:N	7:G:651:LEU:HD23	2.34	0.42
8:H:142:TYR:CD1	8:H:142:TYR:C	2.96	0.42
15:O:178:GLU:OE2	15:O:182:ARG:NH1	2.51	0.42
29:d:45:ASP:OD2	29:d:51:ARG:NH1	2.51	0.42
35:j:70:ASP:OD2	35:j:70:ASP:N	2.52	0.42
4:D:407:LYS:HA	4:D:407:LYS:HD3	1.90	0.42
6:F:94:VAL:HG11	6:F:192:LEU:HD22	2.01	0.42
12:L:10:VAL:O	12:L:14:LEU:HB2	2.19	0.42
12:L:250:SER:O	12:L:251:THR:C	2.63	0.42
23:X:8:SER:HG	23:X:11:ASP:CG	2.27	0.42
30:e:15:ARG:HA	30:e:18:THR:HG23	2.00	0.42
4:D:66:MET:HE1	4:D:411:LEU:CD1	2.49	0.42
12:L:286:LEU:C	12:L:286:LEU:HD13	2.44	0.42
12:L:526:LEU:HD12	12:L:530:PRO:HG2	2.00	0.42
15:O:138:MET:CE	54:O:401:GTP:HN21	2.33	0.42
28:c:33:LYS:HZ2	28:c:37:GLU:CD	2.23	0.42
8:H:255:TYR:CD1	8:H:255:TYR:C	2.98	0.42
12:L:405:ASN:ND2	37:l:120:GLU:OE1	2.46	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.01	0.42
38:m:24:ILE:HD12	38:m:24:ILE:C	2.44	0.42
12:L:141:PHE:CZ	12:L:183:ILE:HD11	2.55	0.42
23:X:122:GLY:HA2	25:Z:66:GLU:OE2	2.20	0.42
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.55	0.42
6:F:49:LEU:HD11	6:F:123:LEU:HD21	2.02	0.42
19:S:18:ILE:HD12	19:S:50:LEU:HD21	2.02	0.42
24:Y:43:LYS:HD3	51:Y:802:3PE:O14	2.19	0.42
37:l:128:VAL:HG22	40:o:97:ARG:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:390:ASP:OD1	6:F:423:ARG:NH2	2.53	0.42
12:L:559:GLU:HG2	13:M:214:LEU:HD13	2.02	0.42
8:H:251:MET:SD	8:H:254:LEU:HD11	2.60	0.42
9:I:124:GLU:OE2	60:I:301:HOH:O	2.22	0.42
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.55	0.42
12:L:237:MET:HE1	12:L:248:HIS:NE2	2.34	0.42
5:E:101:GLN:HG2	5:E:140:ILE:HD11	2.02	0.41
5:E:163:ASP:OD2	5:E:186:PRO:HB3	2.20	0.41
8:H:236:ILE:HG23	8:H:259:PHE:CE1	2.54	0.41
11:K:37:MET:HE1	14:N:30:TRP:CH2	2.55	0.41
51:M:605:3PE:H332	14:N:242:VAL:HG11	2.02	0.41
16:P:176:ASP:OD1	16:P:176:ASP:C	2.62	0.41
3:C:183:VAL:O	22:W:101:THR:OG1	2.31	0.41
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.55	0.41
10:J:136:PHE:CD1	10:J:136:PHE:C	2.97	0.41
16:P:181:TYR:CE2	16:P:287:ILE:HD13	2.55	0.41
21:V:4:LEU:HD21	21:V:17:GLU:OE1	2.20	0.41
23:X:133:ASP:O	23:X:134:ARG:C	2.63	0.41
33:h:128:ILE:O	60:h:1102:HOH:O	2.22	0.41
43:r:63:MET:HE3	43:r:63:MET:HB3	1.96	0.41
15:O:30:ASN:O	15:O:33:SER:OG	2.26	0.41
13:M:113:MET:HE3	13:M:175:ASN:HD21	1.86	0.41
16:P:182:PHE:HA	16:P:185:ILE:HD12	2.03	0.41
34:i:126:HIS:O	34:i:127:HIS:HB2	2.21	0.41
46:B:203:PC1:O13	46:B:203:PC1:C13	2.68	0.41
14:N:329:MET:O	14:N:333:SER:OG	2.29	0.41
16:P:185:ILE:HG21	16:P:191:VAL:HG13	2.03	0.41
4:D:73:VAL:HG21	4:D:414:VAL:CG2	2.50	0.41
5:E:27:ASN:OD1	5:E:53:LEU:HD11	2.21	0.41
10:J:125:TRP:HB2	25:Z:137:THR:HG21	2.01	0.41
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.50	0.41
15:O:221:LEU:HD21	15:O:241:LEU:HD21	2.03	0.41
16:P:184:ASN:O	16:P:187:TRP:HD1	2.03	0.41
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.21	0.41
19:S:21:HIS:O	19:S:62:PRO:HA	2.20	0.41
20:U:68:GLU:O	34:i:1:SAC:OG	2.39	0.41
2:B:96:MET:SD	4:D:82:LEU:HD23	2.60	0.41
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.86	0.41
8:H:264:LEU:HD11	26:a:13:GLY:HA2	2.03	0.41
10:J:55:MET:HE2	10:J:55:MET:CA	2.50	0.41
46:L:707:PC1:O13	46:L:707:PC1:H132	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.55	0.41
25:Z:95:ALA:HA	25:Z:106:VAL:HG21	2.03	0.41
38:m:22:TYR:CG	39:n:64:ARG:HD3	2.54	0.41
7:G:512:GLU:H	7:G:512:GLU:CD	2.29	0.41
26:a:37:ARG:NH2	26:a:51:ASP:OD2	2.46	0.41
31:f:49:LYS:O	31:f:50:PRO:C	2.64	0.41
2:B:54:CYS:HB3	4:D:108:TYR:HB2	2.02	0.41
7:G:245:GLY:O	60:G:908:HOH:O	2.22	0.41
12:L:595:ILE:HA	14:N:100:MET:HE1	2.02	0.41
23:X:129:LYS:HE2	27:b:65:VAL:O	2.21	0.41
24:Y:104:THR:HG21	24:Y:109:ILE:HD12	2.03	0.41
31:f:7:VAL:HG12	31:f:8:ARG:N	2.36	0.41
35:j:39:ARG:NE	35:j:43:ASP:OD2	2.45	0.41
1:A:56:PHE:O	10:J:70:TYR:OH	2.38	0.41
45:A:301:LMT:O5B	27:b:38:THR:HG22	2.21	0.41
7:G:382:THR:HB	7:G:454:GLY:HA3	2.02	0.41
13:M:233:ALA:HA	13:M:320:GLY:HA2	2.02	0.41
23:X:10:GLU:N	23:X:10:GLU:CD	2.79	0.41
4:D:151:ILE:HG21	4:D:174:ARG:HG3	2.03	0.40
5:E:28:TYR:CE1	5:E:72:ILE:HD11	2.55	0.40
5:E:123:LYS:HE2	5:E:174:ASP:OD1	2.21	0.40
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.03	0.40
7:G:316:ALA:HB3	7:G:519:PRO:HG3	2.02	0.40
30:e:68:ARG:O	30:e:72:MET:HG3	2.22	0.40
41:p:158:GLN:HG2	41:p:162:MET:HE2	2.01	0.40
2:B:138:ARG:NH1	60:B:305:HOH:O	2.32	0.40
13:M:126:LEU:HD21	13:M:153:THR:HG21	2.03	0.40
52:h:1001:CDL:OB4	34:i:88:HIS:NE2	2.55	0.40
36:k:14:GLU:OE2	36:k:14:GLU:HA	2.22	0.40
6:F:165:ASN:OD1	6:F:170:GLY:N	2.51	0.40
15:O:151:HIS:HB2	15:O:279:LEU:HD11	2.04	0.40
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.04	0.40
11:K:62:ILE:HG21	14:N:31:ILE:HD11	2.03	0.40
15:O:301:GLY:O	60:O:503:HOH:O	2.22	0.40
20:T:16:LEU:HD13	20:T:30:LEU:HD21	2.03	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	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	153/216 (71%)	147 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	409 (96%)	18 (4%)	0	100	100
5	E	211/249 (85%)	204 (97%)	7 (3%)	0	100	100
6	F	429/464 (92%)	419 (98%)	10 (2%)	0	100	100
7	G	686/727 (94%)	673 (98%)	13 (2%)	0	100	100
8	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	582 (96%)	21 (4%)	1 (0%)	43	55
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	339/380 (89%)	330 (97%)	9 (3%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	74/156 (47%)	72 (97%)	2 (3%)	0	100	100
20	U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	V	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	111/120 (92%)	111 (100%)	0	0	100	100
30	e	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	96/154 (62%)	91 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	63 (97%)	2 (3%)	0	100	100
36	k	78/98 (80%)	77 (99%)	1 (1%)	0	100	100
37	l	153/186 (82%)	150 (98%)	3 (2%)	0	100	100
38	m	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
39	n	170/179 (95%)	167 (98%)	3 (2%)	0	100	100
40	o	118/137 (86%)	113 (96%)	5 (4%)	0	100	100
41	p	169/176 (96%)	168 (99%)	1 (1%)	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	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
All	All	8109/9212 (88%)	7899 (97%)	209 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	128 (98%)	3 (2%)	44	63
3	C	188/228 (82%)	187 (100%)	1 (0%)	81	90
4	D	370/392 (94%)	368 (100%)	2 (0%)	81	90
5	E	183/205 (89%)	181 (99%)	2 (1%)	65	81
6	F	345/368 (94%)	339 (98%)	6 (2%)	53	72
7	G	578/608 (95%)	573 (99%)	5 (1%)	70	84
8	H	274/274 (100%)	273 (100%)	1 (0%)	84	92
9	I	151/175 (86%)	148 (98%)	3 (2%)	48	67
10	J	140/141 (99%)	139 (99%)	1 (1%)	76	87
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	79
12	L	528/533 (99%)	520 (98%)	8 (2%)	57	75
13	M	412/412 (100%)	407 (99%)	5 (1%)	63	79
14	N	315/315 (100%)	314 (100%)	1 (0%)	86	93
15	O	283/303 (93%)	275 (97%)	8 (3%)	38	56
16	P	295/327 (90%)	293 (99%)	2 (1%)	76	87
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	76 (97%)	2 (3%)	40	59
19	S	76/82 (93%)	73 (96%)	3 (4%)	28	43
20	T	70/135 (52%)	67 (96%)	3 (4%)	26	39
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	82
22	W	107/114 (94%)	106 (99%)	1 (1%)	70	84
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	89
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	86
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	56
28	c	44/68 (65%)	43 (98%)	1 (2%)	44	63
29	d	101/105 (96%)	101 (100%)	0	100	100
30	e	88/96 (92%)	86 (98%)	2 (2%)	44	63
31	f	49/54 (91%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	89/131 (68%)	88 (99%)	1 (1%)	65	81
33	h	121/158 (77%)	120 (99%)	1 (1%)	73	86
34	i	99/120 (82%)	97 (98%)	2 (2%)	48	67
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	50
36	k	62/76 (82%)	59 (95%)	3 (5%)	23	35
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	155 (99%)	1 (1%)	78	89
40	o	109/120 (91%)	107 (98%)	2 (2%)	51	70
41	p	155/157 (99%)	153 (99%)	2 (1%)	61	77
42	q	131/131 (100%)	126 (96%)	5 (4%)	29	44
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	43/92 (47%)	42 (98%)	1 (2%)	44	63
All	All	7150/7892 (91%)	7064 (99%)	86 (1%)	61	79

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	27	GLU
2	B	54	CYS
2	B	91	THR
3	C	117	ILE
4	D	109	VAL
4	D	376	VAL
5	E	26	GLU
5	E	181	ILE
6	F	18	GLU
6	F	50	LEU
6	F	62	THR
6	F	231	SER
6	F	415	VAL
6	F	435	GLN
7	G	24	THR
7	G	281	GLU
7	G	292	THR
7	G	484	THR
7	G	640	ASN

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Mol	Chain	Res	Type
8	H	176	LEU
9	I	9	GLU
9	I	11	SER
9	I	103	SER
10	J	135	PHE
11	K	46	LEU
12	L	140	LEU
12	L	235	SER
12	L	254	VAL
12	L	393	ASP
12	L	442	ASN
12	L	505	SER
12	L	554	ASP
12	L	565	THR
13	M	31	SER
13	M	72	LEU
13	M	116	ILE
13	M	144	ASN
13	M	427	SER
14	N	125	SER
15	O	1	LEU
15	O	17	LYS
15	O	60	ASP
15	O	203	GLU
15	O	206	TYR
15	O	250	ASP
15	O	289	SER
15	O	317	ILE
16	P	142	SER
16	P	170	GLU
18	R	2	VAL
18	R	95	HIS
19	S	13	LEU
19	S	91	GLU
19	S	95	SER
20	T	39	ASP
20	T	43	ASP
20	T	82	ASP
21	V	57	MET
22	W	68	LYS
23	X	154	GLU
25	Z	109	SER

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Mol	Chain	Res	Type
27	b	4	VAL
27	b	33	THR
28	c	1	LYS
30	e	5	VAL
30	e	15	ARG
32	g	112	CYS
33	h	32	THR
34	i	67	SER
34	i	120	LYS
35	j	7	ILE
35	j	40	PHE
36	k	11	SER
36	k	41	ARG
36	k	87	LEU
39	n	150	THR
40	o	58	CYS
40	o	115	GLU
41	p	30	THR
41	p	74	THR
42	q	11	LEU
42	q	26	VAL
42	q	107	LYS
42	q	141	SER
42	q	145	LYS
44	s	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	39	GLN
3	C	88	ASN
3	C	192	GLN
4	D	13	GLN
4	D	157	HIS
6	F	29	HIS
6	F	257	ASN
6	F	264	ASN
6	F	421	HIS
6	F	431	GLN
7	G	155	GLN
7	G	182	GLN
7	G	293	HIS

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Mol	Chain	Res	Type
7	G	308	GLN
7	G	402	ASN
7	G	430	GLN
7	G	517	ASN
7	G	581	GLN
7	G	640	ASN
11	K	7	ASN
11	K	50	ASN
11	K	52	HIS
12	L	296	ASN
13	M	399	ASN
14	N	36	ASN
14	N	47	ASN
14	N	134	GLN
14	N	204	ASN
14	N	268	GLN
14	N	289	ASN
15	O	89	ASN
15	O	120	GLN
15	O	180	GLN
15	O	190	HIS
15	O	200	GLN
16	P	8	HIS
18	R	51	GLN
19	S	30	GLN
19	S	79	ASN
20	T	74	GLN
21	V	75	GLN
22	W	48	HIS
22	W	58	GLN
23	X	29	HIS
24	Y	128	GLN
29	d	88	HIS
31	f	10	HIS
33	h	63	HIS
33	h	143	ASN
35	j	24	GLN
35	j	50	HIS
38	m	32	GLN
38	m	74	ASN
38	m	78	ASN
39	n	77	GLN

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Mol	Chain	Res	Type
40	o	42	GLN
40	o	84	HIS
41	p	58	ASN
41	p	122	GLN
44	s	43	HIS

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
10	FME	J	1	10	8,9,10	0.95	0	8,9,11	1.01	0
12	FME	L	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.92	0
1	FME	A	1	1	8,9,10	0.95	0	8,9,11	1.04	1 (12%)
43	AYA	r	1	43	6,7,8	1.89	2 (33%)	6,8,10	1.28	1 (16%)
24	AYA	Y	1	24	6,7,8	1.83	2 (33%)	6,8,10	1.43	1 (16%)
34	SAC	i	1	34	7,8,9	0.99	0	7,9,11	1.82	2 (28%)
4	2MR	D	85	4	10,12,13	2.71	4 (40%)	5,13,15	1.19	1 (20%)
14	FME	N	1	14	8,9,10	1.01	0	8,9,11	0.95	0
8	FME	H	1	8	8,9,10	1.07	1 (12%)	8,9,11	0.92	0
13	FME	M	1	13	8,9,10	1.02	1 (12%)	8,9,11	0.94	0
11	FME	K	1	11	8,9,10	0.95	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
10	FME	J	1	10	-	3/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
24	AYA	Y	1	24	-	1/5/6/8	-
34	SAC	i	1	34	-	6/7/8/10	-
4	2MR	D	85	4	-	0/10/13/15	-
14	FME	N	1	14	-	5/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.21	1.44	1.33
4	D	85	2MR	CZ-NE	4.58	1.44	1.34
4	D	85	2MR	O-C	4.12	1.35	1.20
43	r	1	AYA	CT-N	3.48	1.45	1.34
24	Y	1	AYA	CT-N	3.33	1.45	1.34
8	H	1	FME	CA-N	-2.34	1.43	1.46
12	L	1	FME	CA-N	-2.19	1.43	1.46
13	M	1	FME	CA-N	-2.15	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
24	Y	1	AYA	OT-CT	-2.02	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C-CA-N	3.17	115.61	109.50
4	D	85	2MR	NE-CZ-NH2	-2.41	117.27	119.48
24	Y	1	AYA	CM-CT-N	2.40	120.10	116.12
43	r	1	AYA	CM-CT-N	2.34	120.00	116.12
1	A	1	FME	C-CA-N	2.20	113.75	109.50
34	i	1	SAC	C2A-C1A-N	2.06	119.54	116.12

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
24	Y	1	AYA	O-C-CA-CB
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
8	H	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
1	A	1	FME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
34	i	1	SAC	CB-CA-N-C1A
34	i	1	SAC	C-CA-N-C1A
10	J	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	1	FME	2	0
34	i	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 3 are monoatomic - leaving 55 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
51	3PE	Y	802	-	34,34,50	1.07	4 (11%)	37,39,55	1.21	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-		
53	I49	N	703	-	15,17,17	0.81	1 (6%)	17,22,22	1.89	5 (29%)
51	3PE	H	403	-	33,33,50	1.30	4 (12%)	34,37,55	1.25	2 (5%)
51	3PE	L	701	-	48,48,50	0.91	4 (8%)	51,53,55	1.15	2 (3%)
47	SF4	B	201	2	0,12,12	-	-	-		
51	3PE	H	401	-	43,43,50	0.95	3 (6%)	46,48,55	1.11	2 (4%)
51	3PE	X	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.15	2 (3%)
58	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.54	5 (13%)
45	LMT	h	1002	-	36,36,36	1.16	2 (5%)	47,47,47	0.94	3 (6%)
52	CDL	r	201	-	75,75,99	1.01	6 (8%)	81,87,111	1.12	4 (4%)
56	NDP	P	501	-	51,52,52	2.23	5 (9%)	71,80,80	1.50	18 (25%)
45	LMT	l	201	-	36,36,36	1.23	3 (8%)	47,47,47	1.15	3 (6%)
46	PC1	L	707	-	48,48,53	0.99	4 (8%)	54,56,61	1.08	2 (3%)
51	3PE	H	402	-	50,50,50	0.89	4 (8%)	53,55,55	1.07	3 (5%)
46	PC1	B	202	-	53,53,53	0.94	3 (5%)	59,61,61	1.06	2 (3%)
52	CDL	K	502	-	70,70,99	1.05	6 (8%)	76,82,111	1.09	4 (5%)
52	CDL	L	703	-	68,68,99	1.05	6 (8%)	74,80,111	1.11	4 (5%)
45	LMT	K	501	-	36,36,36	1.19	3 (8%)	47,47,47	1.02	0
45	LMT	A	302	-	36,36,36	1.23	2 (5%)	47,47,47	1.10	3 (6%)
45	LMT	j	101	-	36,36,36	1.21	3 (8%)	47,47,47	0.98	2 (4%)
52	CDL	J	701	-	61,61,99	1.08	7 (11%)	67,73,111	1.27	5 (7%)
51	3PE	P	502	-	36,36,50	1.04	4 (11%)	39,41,55	1.17	2 (5%)
45	LMT	A	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.14	3 (6%)
51	3PE	N	701	-	40,40,50	0.98	4 (10%)	43,45,55	1.10	2 (4%)
58	EHZ	T	101	20	31,36,37	1.55	5 (16%)	36,44,47	1.72	6 (16%)
45	LMT	b	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.18	3 (6%)
51	3PE	d	1201	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
45	LMT	M	604	-	36,36,36	1.23	4 (11%)	47,47,47	0.97	0
51	3PE	L	705	-	44,44,50	0.92	3 (6%)	47,49,55	1.08	2 (4%)
46	PC1	B	203	-	34,34,53	1.19	4 (11%)	40,42,61	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	A	303	-	20,20,53	1.78	3 (15%)	24,27,61	1.19	1 (4%)
54	GTP	O	401	55	33,34,34	3.25	15 (45%)	50,54,54	1.83	13 (26%)
45	LMT	L	704	-	36,36,36	1.23	3 (8%)	47,47,47	0.93	0
48	FES	E	301	5	0,4,4	-	-	-	-	-
45	LMT	Y	803	-	36,36,36	1.17	3 (8%)	47,47,47	1.02	2 (4%)
52	CDL	h	1001	-	66,66,99	1.07	8 (12%)	72,78,111	1.24	4 (5%)
45	LMT	M	603	-	36,36,36	1.15	2 (5%)	47,47,47	0.99	1 (2%)
45	LMT	M	602	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
45	LMT	L	702	-	36,36,36	1.18	2 (5%)	47,47,47	0.92	0
45	LMT	J	702	-	36,36,36	1.21	3 (8%)	47,47,47	1.12	2 (4%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
47	SF4	I	201	9	0,12,12	-	-	-	-	-
51	3PE	N	702	-	28,28,50	1.15	3 (10%)	31,33,55	1.17	2 (6%)
51	3PE	M	601	-	45,45,50	0.92	4 (8%)	48,50,55	0.99	2 (4%)
45	LMT	Y	801	-	36,36,36	1.15	3 (8%)	47,47,47	1.16	4 (8%)
45	LMT	Y	804	-	36,36,36	1.19	3 (8%)	47,47,47	1.08	2 (4%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
49	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	6 (12%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
59	MYR	o	201	40	13,14,15	0.95	0	12,13,15	0.57	0
45	LMT	L	706	-	36,36,36	1.19	2 (5%)	47,47,47	1.14	4 (8%)
51	3PE	M	605	-	50,50,50	0.88	3 (6%)	53,55,55	1.13	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
51	3PE	d	1202	-	50,50,50	0.83	3 (6%)	53,55,55	1.20	4 (7%)

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
51	3PE	Y	802	-	-	17/38/38/54	-
47	SF4	G	801	7	-	-	0/6/5/5
53	I49	N	703	-	-	5/10/10/10	0/1/1/1
51	3PE	H	403	-	-	18/36/36/54	-
51	3PE	L	701	-	-	24/52/52/54	-
51	3PE	X	401	-	-	24/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	H	401	-	-	23/47/47/54	-
58	EHZ	U	101	20	-	8/42/44/45	-
47	SF4	B	201	2	-	-	0/6/5/5
45	LMT	h	1002	-	-	6/21/61/61	0/2/2/2
52	CDL	r	201	-	-	31/86/86/110	-
56	NDP	P	501	-	-	4/34/77/77	0/5/5/5
45	LMT	l	201	-	-	6/21/61/61	0/2/2/2
46	PC1	L	707	-	-	25/52/52/57	-
51	3PE	H	402	-	-	17/54/54/54	-
46	PC1	B	202	-	-	22/57/57/57	-
52	CDL	K	502	-	-	31/81/81/110	-
52	CDL	L	703	-	-	31/79/79/110	-
45	LMT	K	501	-	-	10/21/61/61	0/2/2/2
45	LMT	A	302	-	-	14/21/61/61	0/2/2/2
45	LMT	j	101	-	-	9/21/61/61	0/2/2/2
52	CDL	J	701	-	-	29/71/71/110	-
51	3PE	P	502	-	-	22/40/40/54	-
45	LMT	A	301	-	-	1/21/61/61	0/2/2/2
51	3PE	N	701	-	-	19/44/44/54	-
58	EHZ	T	101	20	-	10/42/44/45	-
45	LMT	b	101	-	-	3/21/61/61	0/2/2/2
51	3PE	d	1201	-	-	27/54/54/54	-
45	LMT	M	604	-	-	11/21/61/61	0/2/2/2
51	3PE	L	705	-	-	14/48/48/54	-
46	PC1	B	203	-	-	13/38/38/57	-
46	PC1	A	303	-	-	8/22/22/57	-
54	GTP	O	401	55	-	3/22/38/38	0/3/3/3
45	LMT	L	704	-	-	8/21/61/61	0/2/2/2
48	FES	E	301	5	-	-	0/1/1/1
45	LMT	Y	803	-	-	11/21/61/61	0/2/2/2
52	CDL	h	1001	-	-	34/77/77/110	-
45	LMT	M	603	-	-	10/21/61/61	0/2/2/2
45	LMT	M	602	-	-	7/21/61/61	0/2/2/2
45	LMT	L	702	-	-	9/21/61/61	0/2/2/2
45	LMT	J	702	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	N	702	-	-	18/32/32/54	-
47	SF4	F	502	6	-	-	0/6/5/5
47	SF4	I	201	9	-	-	0/6/5/5
51	3PE	M	601	-	-	17/49/49/54	-
45	LMT	Y	801	-	-	8/21/61/61	0/2/2/2
45	LMT	Y	804	-	-	8/21/61/61	0/2/2/2
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
59	MYR	o	201	40	-	9/12/12/13	-
45	LMT	L	706	-	-	8/21/61/61	0/2/2/2
51	3PE	M	605	-	-	22/54/54/54	-
48	FES	G	803	7	-	-	0/1/1/1
51	3PE	d	1202	-	-	16/54/54/54	-

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.81	1.82	1.59
54	O	401	GTP	O6-C6	8.65	1.40	1.23
54	O	401	GTP	C5-N7	6.70	1.52	1.39
46	A	303	PC1	O21-C2	-5.11	1.40	1.46
54	O	401	GTP	PA-O3A	4.93	1.64	1.59
58	T	101	EHZ	C12-N1	4.90	1.45	1.33
58	U	101	EHZ	C12-N1	4.88	1.44	1.33
58	T	101	EHZ	C15-N2	4.83	1.45	1.33
58	U	101	EHZ	C15-N2	4.81	1.44	1.33
54	O	401	GTP	PB-O3A	4.79	1.64	1.59
54	O	401	GTP	C2-N1	4.70	1.49	1.37
51	H	403	3PE	O21-C2	-4.64	1.40	1.46
54	O	401	GTP	C2-N3	4.64	1.44	1.33
54	O	401	GTP	C8-N9	-4.50	1.27	1.37
54	O	401	GTP	C2-N2	4.45	1.44	1.34
54	O	401	GTP	PB-O3B	4.43	1.64	1.59
56	P	501	NDP	PA-O3	3.98	1.63	1.59
54	O	401	GTP	C4-N9	-3.84	1.28	1.38
45	K	501	LMT	O5B-C1B	3.68	1.51	1.41
56	P	501	NDP	PN-O5D	3.63	1.73	1.59
45	b	101	LMT	O5B-C1B	3.59	1.51	1.41
45	L	704	LMT	O5B-C1B	3.53	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	604	LMT	O5B-C1B	3.49	1.50	1.41
45	J	702	LMT	O5B-C1B	3.48	1.50	1.41
45	Y	804	LMT	O5B-C1B	3.45	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.44	1.32	1.44
45	l	201	LMT	O5B-C1B	3.44	1.50	1.41
45	A	302	LMT	O5'-C1'	3.42	1.50	1.41
45	Y	803	LMT	O5B-C1B	3.41	1.50	1.41
45	A	302	LMT	O5B-C1B	3.40	1.50	1.41
45	j	101	LMT	O5B-C1B	3.40	1.50	1.41
45	L	706	LMT	O5B-C1B	3.35	1.50	1.41
45	j	101	LMT	O5'-C1'	3.34	1.50	1.41
45	L	704	LMT	O5'-C1'	3.33	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.33	1.50	1.41
45	l	201	LMT	O5'-C1'	3.32	1.50	1.41
45	M	603	LMT	O5B-C1B	3.31	1.50	1.41
49	F	501	FMN	C4A-N5	3.26	1.37	1.30
45	L	702	LMT	O5B-C1B	3.25	1.50	1.41
45	M	602	LMT	O5B-C1B	3.25	1.50	1.41
45	M	604	LMT	O5'-C1'	3.24	1.50	1.41
45	A	301	LMT	O5B-C1B	3.15	1.50	1.41
45	Y	801	LMT	O5B-C1B	3.13	1.49	1.41
45	J	702	LMT	O5'-C1'	3.12	1.49	1.41
46	A	303	PC1	O21-C21	3.10	1.40	1.33
51	L	705	3PE	O21-C2	-3.03	1.39	1.46
51	H	403	3PE	O21-C21	3.01	1.39	1.33
45	K	501	LMT	O5'-C1'	3.00	1.49	1.41
51	H	401	3PE	O21-C2	-3.00	1.39	1.46
52	r	201	CDL	OB6-CB4	-2.97	1.39	1.46
52	r	201	CDL	OA6-CA4	-2.97	1.39	1.46
52	L	703	CDL	OA6-CA4	-2.96	1.39	1.46
45	L	702	LMT	O5'-C1'	2.93	1.49	1.41
51	M	605	3PE	O21-C2	-2.93	1.39	1.46
45	M	603	LMT	O5'-C1'	2.92	1.49	1.41
54	O	401	GTP	O4'-C1'	2.90	1.48	1.42
45	b	101	LMT	O5'-C1'	2.90	1.49	1.41
45	Y	804	LMT	O5'-C1'	2.89	1.49	1.41
45	L	706	LMT	O5'-C1'	2.88	1.49	1.41
45	Y	801	LMT	O5'-C1'	2.87	1.49	1.41
45	A	301	LMT	O5'-C1'	2.87	1.49	1.41
52	K	502	CDL	OA6-CA4	-2.86	1.39	1.46
45	Y	803	LMT	O5'-C1'	2.86	1.49	1.41
52	h	1001	CDL	OA6-CA4	-2.86	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	703	CDL	OB6-CB4	-2.85	1.39	1.46
51	L	701	3PE	O21-C2	-2.84	1.39	1.46
51	M	601	3PE	O21-C2	-2.83	1.39	1.46
52	h	1001	CDL	OB6-CB4	-2.83	1.39	1.46
58	U	101	EHZ	O4-C15	-2.82	1.18	1.23
52	J	701	CDL	OB6-CB4	-2.80	1.40	1.46
51	Y	802	3PE	O21-C2	-2.80	1.40	1.46
46	B	202	PC1	O21-C2	-2.80	1.40	1.46
52	K	502	CDL	OB6-CB4	-2.77	1.40	1.46
51	N	702	3PE	O21-C2	-2.77	1.40	1.46
45	h	1002	LMT	O5'-C1'	2.77	1.49	1.41
45	M	602	LMT	O5'-C1'	2.76	1.48	1.41
51	L	701	3PE	O31-C3	-2.73	1.39	1.45
46	B	203	PC1	O21-C2	-2.72	1.40	1.46
51	X	401	3PE	O21-C2	-2.69	1.40	1.46
51	H	402	3PE	O21-C2	-2.62	1.40	1.46
51	H	402	3PE	O31-C3	-2.62	1.39	1.45
51	N	701	3PE	O21-C2	-2.60	1.40	1.46
51	H	403	3PE	O31-C31	2.57	1.40	1.33
51	M	605	3PE	O31-C3	-2.55	1.39	1.45
54	O	401	GTP	C2'-C3'	-2.55	1.46	1.53
58	T	101	EHZ	O4-C15	-2.55	1.18	1.23
52	K	502	CDL	OA8-CA6	-2.54	1.39	1.45
51	d	1201	3PE	O31-C31	2.53	1.40	1.33
51	H	401	3PE	O31-C3	-2.52	1.39	1.45
52	K	502	CDL	OB8-CB7	2.52	1.40	1.33
51	P	502	3PE	O31-C31	2.51	1.40	1.33
52	r	201	CDL	OA8-CA6	-2.51	1.39	1.45
51	N	701	3PE	O31-C31	2.47	1.40	1.33
46	L	707	PC1	O31-C31	2.46	1.40	1.33
52	J	701	CDL	OA6-CA5	2.46	1.40	1.35
52	h	1001	CDL	OB8-CB6	-2.46	1.39	1.45
52	J	701	CDL	OA6-CA4	-2.45	1.40	1.46
58	U	101	EHZ	O3-C12	-2.43	1.18	1.23
51	L	705	3PE	O31-C3	-2.43	1.39	1.45
58	T	101	EHZ	O3-C12	-2.42	1.18	1.23
54	O	401	GTP	PG-O2G	-2.41	1.45	1.54
52	r	201	CDL	OB8-CB7	2.39	1.40	1.33
52	L	703	CDL	OA8-CA6	-2.39	1.39	1.45
46	B	202	PC1	O31-C3	-2.39	1.39	1.45
46	L	707	PC1	O21-C2	-2.37	1.41	1.46
51	Y	802	3PE	O31-C3	-2.36	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	L	703	CDL	OB8-CB7	2.35	1.40	1.33
52	J	701	CDL	OB8-CB6	-2.35	1.39	1.45
51	N	702	3PE	O31-C31	2.34	1.40	1.33
51	M	601	3PE	O31-C31	2.34	1.40	1.33
52	h	1001	CDL	OA8-CA7	2.33	1.40	1.33
51	d	1201	3PE	O21-C2	-2.31	1.41	1.46
56	P	501	NDP	O5D-C5D	-2.30	1.35	1.44
51	X	401	3PE	O31-C3	-2.30	1.40	1.45
51	P	502	3PE	O21-C21	2.30	1.40	1.34
54	O	401	GTP	PG-O3G	-2.29	1.46	1.54
51	Y	802	3PE	O31-C31	2.28	1.40	1.33
51	M	601	3PE	O31-C3	-2.28	1.40	1.45
52	K	502	CDL	OA8-CA7	2.28	1.40	1.33
46	B	203	PC1	O31-C31	2.27	1.40	1.33
51	H	401	3PE	O31-C31	2.27	1.40	1.33
52	J	701	CDL	OA8-CA6	-2.27	1.40	1.45
51	N	702	3PE	O31-C3	-2.25	1.40	1.45
51	L	705	3PE	O31-C31	2.25	1.39	1.33
45	l	201	LMT	O5B-C5B	2.25	1.49	1.44
51	H	402	3PE	O21-C21	2.25	1.40	1.34
52	L	703	CDL	OA8-CA7	2.24	1.39	1.33
46	B	203	PC1	O31-C3	-2.23	1.40	1.45
46	B	203	PC1	O21-C21	2.23	1.40	1.34
51	N	701	3PE	O21-C21	2.23	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.23	1.40	1.34
52	J	701	CDL	OA8-CA7	2.22	1.39	1.33
45	M	604	LMT	O5B-C5B	2.21	1.49	1.44
52	h	1001	CDL	OA8-CA6	-2.21	1.40	1.45
53	N	703	I49	C15-N02	-2.19	1.31	1.36
51	d	1202	3PE	O31-C3	-2.19	1.40	1.45
45	Y	804	LMT	O5B-C5B	2.19	1.49	1.44
51	P	502	3PE	O31-C3	-2.19	1.40	1.45
51	d	1201	3PE	O21-C21	2.18	1.40	1.34
51	d	1202	3PE	O31-C31	2.16	1.39	1.33
51	P	502	3PE	O21-C2	-2.16	1.41	1.46
46	B	202	PC1	O31-C31	2.16	1.39	1.33
46	L	707	PC1	O21-C21	2.14	1.40	1.34
51	L	701	3PE	O31-C31	2.14	1.39	1.33
45	j	101	LMT	O5B-C5B	2.13	1.49	1.44
51	d	1202	3PE	O21-C2	-2.13	1.41	1.46
52	K	502	CDL	OB6-CB5	2.12	1.40	1.34
46	A	303	PC1	O31-C3	-2.12	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	K	501	LMT	O5B-C5B	2.11	1.49	1.44
52	h	1001	CDL	OB8-CB7	2.11	1.39	1.33
51	H	402	3PE	O31-C31	2.10	1.39	1.33
58	U	101	EHZ	C9-S1	2.10	1.81	1.76
52	L	703	CDL	OB8-CB6	-2.10	1.40	1.45
51	X	401	3PE	O31-C31	2.07	1.39	1.33
51	M	601	3PE	O21-C21	2.07	1.40	1.34
51	X	401	3PE	O21-C21	2.07	1.40	1.34
46	L	707	PC1	O31-C3	-2.06	1.40	1.45
52	h	1001	CDL	OA6-CA5	2.05	1.40	1.34
52	r	201	CDL	OA6-CA5	2.05	1.40	1.34
51	Y	802	3PE	O21-C21	2.05	1.40	1.34
51	M	605	3PE	O21-C21	2.05	1.40	1.34
49	F	501	FMN	C10-N1	2.03	1.37	1.33
52	J	701	CDL	OB8-CB7	2.03	1.39	1.33
58	T	101	EHZ	C9-S1	2.03	1.81	1.76
45	Y	801	LMT	O5B-C5B	2.03	1.49	1.44
45	Y	803	LMT	O5B-C5B	2.03	1.49	1.44
51	N	701	3PE	O31-C3	-2.03	1.40	1.45
51	H	403	3PE	O31-C3	-2.02	1.40	1.45
45	L	704	LMT	O5'-C5'	2.02	1.49	1.44
51	L	701	3PE	O21-C21	2.02	1.40	1.34
54	O	401	GTP	PA-O2A	-2.02	1.46	1.55
51	d	1201	3PE	O31-C3	-2.02	1.40	1.45
52	r	201	CDL	OA8-CA7	2.02	1.39	1.33
45	M	604	LMT	O1B-C4'	2.01	1.49	1.43
45	J	702	LMT	O5'-C5'	2.01	1.49	1.44

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	GTP	C8-N9-C4	7.52	120.12	106.03
58	T	101	EHZ	C8-C9-S1	6.43	121.68	113.56
58	U	101	EHZ	C8-C9-S1	5.96	121.08	113.56
51	H	403	3PE	O21-C21-O22	-5.27	118.94	125.70
52	h	1001	CDL	OB6-CB5-C51	4.78	121.83	111.48
46	L	707	PC1	O21-C21-C22	4.68	121.61	111.48
52	J	701	CDL	OA6-CA5-C11	4.65	119.39	111.09
46	A	303	PC1	O21-C21-O22	-4.50	119.92	125.70
53	N	703	I49	N01-C14-N03	4.50	128.55	120.26
46	B	203	PC1	O21-C21-C22	4.45	121.10	111.48
46	B	202	PC1	O21-C21-C22	4.40	121.00	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	701	CDL	OB6-CB5-C51	4.28	120.74	111.48
51	d	1202	3PE	O21-C21-C22	4.26	120.71	111.48
51	Y	802	3PE	O21-C21-C22	4.18	120.53	111.48
51	X	401	3PE	O21-C21-C22	4.18	120.53	111.48
51	L	701	3PE	O21-C21-C22	4.16	120.48	111.48
51	N	702	3PE	O21-C21-C22	4.09	120.33	111.48
51	P	502	3PE	O21-C21-C22	4.06	120.27	111.48
52	h	1001	CDL	OA6-CA5-C11	4.04	120.22	111.48
51	d	1201	3PE	O21-C21-C22	4.02	120.19	111.48
51	H	402	3PE	O21-C21-C22	4.02	120.18	111.48
51	N	701	3PE	O21-C21-C22	4.01	120.16	111.48
52	r	201	CDL	OA6-CA5-C11	3.79	119.67	111.48
52	r	201	CDL	OB6-CB5-C51	3.76	119.61	111.48
51	M	605	3PE	O21-C21-C22	3.75	119.59	111.48
45	A	301	LMT	O1'-C1'-C2'	3.72	113.92	108.27
52	L	703	CDL	OB6-CB5-C51	3.70	119.49	111.48
56	P	501	NDP	P2B-O2B-C2B	-3.69	113.59	123.43
51	H	401	3PE	O21-C21-C22	3.68	119.44	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.64	96.34	109.33
51	L	705	3PE	O21-C21-C22	3.62	119.31	111.48
52	K	502	CDL	OB6-CB5-C51	3.62	119.30	111.48
52	L	703	CDL	OA6-CA5-C11	3.58	119.24	111.48
49	F	501	FMN	C4-N3-C2	-3.57	119.30	125.64
52	K	502	CDL	OA6-CA5-C11	3.48	119.00	111.48
56	P	501	NDP	O3-PA-O1A	-3.37	100.57	110.70
51	d	1201	3PE	O31-C31-C32	3.35	122.05	111.83
45	b	101	LMT	C2'-C3'-C4'	3.30	117.18	109.68
51	M	601	3PE	O21-C21-C22	3.27	118.55	111.48
45	b	101	LMT	C1'-C2'-C3'	3.22	116.78	110.01
53	N	703	I49	N05-C15-N04	-3.20	110.97	120.07
45	Y	801	LMT	C3B-C4B-C5B	3.18	116.00	110.23
51	P	502	3PE	O31-C31-C32	3.17	121.51	111.83
52	h	1001	CDL	OA8-CA7-C31	3.17	121.49	111.83
51	N	701	3PE	O31-C31-C32	3.15	121.44	111.83
54	O	401	GTP	C2-N1-C6	-3.09	119.50	125.11
58	T	101	EHZ	C10-S1-C9	3.08	110.95	101.84
52	J	701	CDL	OB8-CB7-C71	3.07	121.20	111.83
58	T	101	EHZ	O2-C9-C8	-3.04	118.95	123.74
49	F	501	FMN	C4A-C10-N10	3.03	120.83	116.48
51	Y	802	3PE	O31-C31-C32	3.00	120.99	111.83
51	H	401	3PE	O31-C31-C32	2.98	120.91	111.83
51	H	403	3PE	O31-C31-C32	2.97	120.89	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	L	707	PC1	O31-C31-C32	2.95	120.84	111.83
45	A	302	LMT	C1-O1'-C1'	2.95	118.72	113.68
51	d	1202	3PE	O31-C31-C32	2.95	120.83	111.83
46	B	203	PC1	O31-C31-C32	2.88	120.63	111.83
51	M	605	3PE	O31-C31-C32	2.84	120.50	111.83
56	P	501	NDP	PA-O5B-C5B	-2.81	105.25	121.35
52	r	201	CDL	OB8-CB7-C71	2.81	120.39	111.83
52	K	502	CDL	OB8-CB7-C71	2.80	120.36	111.83
45	b	101	LMT	C1'-O5'-C5'	-2.79	108.26	113.72
54	O	401	GTP	O2G-PG-O3B	2.78	113.97	104.64
52	r	201	CDL	OA8-CA7-C31	2.78	120.31	111.83
51	L	701	3PE	O31-C31-C32	2.76	120.25	111.83
49	F	501	FMN	C4A-C4-N3	2.75	120.25	113.25
56	P	501	NDP	O2N-PN-O3	2.73	114.64	107.27
51	X	401	3PE	O31-C31-C32	2.70	120.06	111.83
51	N	702	3PE	O31-C31-C32	2.70	120.06	111.83
45	J	702	LMT	C1B-O1B-C4'	-2.69	111.59	117.98
52	L	703	CDL	OB8-CB7-C71	2.69	120.04	111.83
52	K	502	CDL	OA8-CA7-C31	2.69	120.03	111.83
54	O	401	GTP	O3G-PG-O3B	2.68	113.61	104.64
58	U	101	EHZ	O2-C9-C8	-2.68	119.53	123.74
58	T	101	EHZ	C13-C14-N2	-2.66	106.33	112.00
45	l	201	LMT	C3B-C4B-C5B	2.66	115.05	110.23
45	j	101	LMT	C1B-O1B-C4'	-2.61	111.78	117.98
58	T	101	EHZ	O2-C9-S1	-2.60	119.37	122.68
52	J	701	CDL	OA8-CA7-C31	2.59	119.74	111.83
58	U	101	EHZ	O2-C9-S1	-2.59	119.39	122.68
56	P	501	NDP	PN-O5D-C5D	-2.58	106.55	121.35
54	O	401	GTP	C1'-N9-C8	-2.58	119.40	126.73
53	N	703	I49	N05-C15-N02	2.58	127.02	117.97
45	l	201	LMT	O5B-C5B-C4B	2.57	114.33	109.70
49	F	501	FMN	O4-C4-C4A	-2.53	119.84	126.53
56	P	501	NDP	C2B-C1B-N9A	-2.51	109.62	113.75
56	P	501	NDP	O3X-P2B-O2X	2.51	117.22	107.80
51	M	601	3PE	O31-C31-C32	2.50	119.47	111.83
45	Y	801	LMT	O5B-C5B-C4B	2.48	114.17	109.70
45	Y	801	LMT	C1B-O5B-C5B	-2.48	108.88	113.72
46	B	202	PC1	O31-C31-C32	2.48	119.39	111.83
45	L	706	LMT	O5'-C5'-C4'	2.48	114.85	109.72
58	T	101	EHZ	C13-C12-N1	2.47	120.85	116.34
52	h	1001	CDL	OB8-CB7-C71	2.45	119.31	111.83
54	O	401	GTP	C5-C6-N1	2.45	119.48	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	L	703	CDL	OA8-CA7-C31	2.45	119.30	111.83
56	P	501	NDP	C2A-N1A-C6A	-2.44	114.73	118.73
54	O	401	GTP	O2A-PA-O1A	-2.44	101.12	112.44
49	F	501	FMN	C10-C4A-N5	-2.43	119.84	124.81
51	L	705	3PE	O31-C31-C32	2.40	119.15	111.83
54	O	401	GTP	O2B-PB-O1B	-2.39	101.31	112.44
58	U	101	EHZ	C10-S1-C9	2.38	108.89	101.84
51	H	402	3PE	O31-C31-C32	2.35	119.01	111.83
56	P	501	NDP	O2N-PN-O1N	2.35	123.36	112.44
45	Y	804	LMT	C1B-O1B-C4'	-2.34	112.44	117.98
53	N	703	I49	C08-N01-C14	-2.34	119.17	123.46
56	P	501	NDP	O3X-P2B-O2B	-2.33	96.76	105.85
56	P	501	NDP	N3A-C4A-N9A	2.33	131.13	127.17
56	P	501	NDP	O4B-C4B-C3B	2.33	109.78	105.15
45	I	201	LMT	C4B-C3B-C2B	2.28	114.84	110.83
56	P	501	NDP	O5D-PN-O1N	-2.28	99.90	108.94
53	N	703	I49	C08-C06-C07	2.27	117.95	112.83
45	Y	801	LMT	C2'-C3'-C4'	2.27	114.84	109.68
54	O	401	GTP	C5-C4-N9	-2.27	101.60	105.66
45	J	702	LMT	O5'-C5'-C4'	2.26	114.40	109.72
45	A	302	LMT	O1B-C4'-C5'	2.25	115.38	109.48
45	A	301	LMT	C1B-O1B-C4'	-2.25	112.66	117.98
51	H	402	3PE	C3-C2-C1	-2.21	106.63	111.78
51	d	1202	3PE	O21-C2-C3	2.21	116.26	108.34
56	P	501	NDP	O7N-C7N-C3N	2.20	125.04	120.90
45	L	706	LMT	C3'-C4'-C5'	2.20	115.80	110.93
45	Y	803	LMT	C1'-O5'-C5'	-2.19	109.44	113.72
54	O	401	GTP	O6-C6-C5	-2.18	120.79	126.53
56	P	501	NDP	C5A-C4A-N3A	-2.17	123.72	126.72
52	J	701	CDL	OB8-CB7-OB9	-2.16	118.23	123.63
45	h	1002	LMT	C1B-O1B-C4'	-2.16	112.87	117.98
49	F	501	FMN	C4A-C10-N1	-2.16	119.31	124.59
51	d	1202	3PE	O21-C21-O22	-2.13	118.72	123.70
45	L	706	LMT	C1'-O5'-C5'	-2.10	109.61	113.72
56	P	501	NDP	O7N-C7N-N7N	-2.09	118.21	122.89
45	h	1002	LMT	O5'-C5'-C4'	2.09	114.03	109.72
54	O	401	GTP	N9-C8-N7	-2.07	109.56	113.40
45	M	603	LMT	C1B-C2B-C3B	2.07	114.36	110.01
45	A	301	LMT	C1-O1'-C1'	-2.07	110.15	113.68
45	Y	803	LMT	C1B-O1B-C4'	-2.06	113.09	117.98
45	M	602	LMT	C1B-O5B-C5B	-2.06	109.70	113.72
45	Y	804	LMT	C1'-O5'-C5'	-2.06	109.70	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	M	602	LMT	O5'-C5'-C4'	2.06	113.97	109.72
58	U	101	EHZ	C13-C12-N1	2.05	120.07	116.34
45	h	1002	LMT	C3'-C4'-C5'	2.04	115.46	110.93
54	O	401	GTP	C1'-N9-C4	-2.04	120.46	126.49
45	L	706	LMT	C6'-C5'-C4'	-2.03	107.67	113.38
56	P	501	NDP	C5B-C4B-C3B	-2.03	107.91	115.21
54	O	401	GTP	C6-C5-N7	2.03	133.98	130.29
45	j	101	LMT	O5B-C5B-C4B	2.02	113.34	109.70
45	A	302	LMT	O5B-C5B-C4B	2.01	113.32	109.70

There are no chirality outliers.

All (681) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	302	LMT	O5'-C1'-O1'-C1
45	L	702	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	O5'-C1'-O1'-C1
45	L	706	LMT	O5'-C1'-O1'-C1
45	M	603	LMT	C2'-C1'-O1'-C1
45	M	603	LMT	O5'-C1'-O1'-C1
45	M	604	LMT	O5'-C1'-O1'-C1
45	Y	803	LMT	O5'-C1'-O1'-C1
46	A	303	PC1	C1-O11-P-O14
46	A	303	PC1	C1-O11-P-O13
46	A	303	PC1	O22-C21-O21-C2
51	H	401	3PE	C1-O11-P-O13
51	H	401	3PE	C1-O11-P-O14
51	H	401	3PE	C11-O13-P-O12
51	H	401	3PE	O13-C11-C12-N
51	H	402	3PE	C11-O13-P-O11
51	H	402	3PE	C11-O13-P-O12
51	H	402	3PE	C11-O13-P-O14
51	H	402	3PE	O13-C11-C12-N
51	H	403	3PE	C11-O13-P-O11
51	H	403	3PE	C11-O13-P-O12
51	H	403	3PE	O13-C11-C12-N
51	H	403	3PE	O22-C21-O21-C2
51	L	701	3PE	C11-O13-P-O11
51	L	701	3PE	C11-O13-P-O12
51	L	701	3PE	C11-O13-P-O14
51	L	701	3PE	C22-C21-O21-C2
51	L	705	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
51	M	601	3PE	C1-O11-P-O13
51	M	601	3PE	O13-C11-C12-N
51	M	605	3PE	C1-O11-P-O13
51	M	605	3PE	C1-O11-P-O14
51	M	605	3PE	O13-C11-C12-N
51	N	701	3PE	C11-O13-P-O12
51	N	701	3PE	O13-C11-C12-N
51	N	702	3PE	C1-O11-P-O12
51	N	702	3PE	C1-O11-P-O13
51	N	702	3PE	C1-O11-P-O14
51	N	702	3PE	C11-O13-P-O11
51	N	702	3PE	C11-O13-P-O12
51	N	702	3PE	O22-C21-O21-C2
51	N	702	3PE	C22-C21-O21-C2
51	P	502	3PE	C1-O11-P-O13
51	P	502	3PE	C1-O11-P-O14
51	P	502	3PE	C22-C21-O21-C2
51	X	401	3PE	C11-O13-P-O11
51	X	401	3PE	C11-O13-P-O12
51	X	401	3PE	C11-O13-P-O14
51	X	401	3PE	C22-C21-O21-C2
51	Y	802	3PE	C1-O11-P-O12
51	Y	802	3PE	C1-O11-P-O13
51	Y	802	3PE	C11-O13-P-O11
51	Y	802	3PE	C11-O13-P-O12
51	Y	802	3PE	C11-O13-P-O14
51	Y	802	3PE	C22-C21-O21-C2
51	d	1201	3PE	C1-O11-P-O12
51	d	1201	3PE	C1-O11-P-O13
51	d	1201	3PE	C1-O11-P-O14
51	d	1201	3PE	O13-C11-C12-N
51	d	1201	3PE	O32-C31-O31-C3
51	d	1201	3PE	C32-C31-O31-C3
51	d	1201	3PE	O22-C21-O21-C2
51	d	1202	3PE	O22-C21-O21-C2
52	J	701	CDL	CB2-C1-CA2-OA2
52	J	701	CDL	CA3-OA5-PA1-OA2
52	J	701	CDL	CA3-OA5-PA1-OA4
52	J	701	CDL	OB7-CB5-OB6-CB4
52	J	701	CDL	C51-CB5-OB6-CB4
52	K	502	CDL	CA2-OA2-PA1-OA4
52	K	502	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
52	K	502	CDL	CB4-CB3-OB5-PB2
52	L	703	CDL	CB2-C1-CA2-OA2
52	L	703	CDL	CA2-OA2-PA1-OA4
52	L	703	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CA2-OA2-PA1-OA4
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CA3-OA5-PA1-OA4
52	h	1001	CDL	CB2-OB2-PB2-OB4
52	h	1001	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	OB7-CB5-OB6-CB4
52	h	1001	CDL	C51-CB5-OB6-CB4
52	r	201	CDL	O1-C1-CA2-OA2
52	r	201	CDL	CB2-C1-CA2-OA2
52	r	201	CDL	CB2-OB2-PB2-OB3
52	r	201	CDL	CB2-OB2-PB2-OB4
52	r	201	CDL	CB2-OB2-PB2-OB5
53	N	703	I49	C07-C06-C08-N01
53	N	703	I49	N01-C14-N02-C15
53	N	703	I49	N03-C14-N02-C15
54	O	401	GTP	PB-O3B-PG-O2G
54	O	401	GTP	C5'-O5'-PA-O1A
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-C17-C20-O6
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	C5-C6-C7-O1
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
59	o	201	MYR	O1-C1-C2-C3
59	o	201	MYR	C1-C2-C3-C4
52	J	701	CDL	C11-CA5-OA6-CA4
51	H	403	3PE	O32-C31-O31-C3
51	Y	802	3PE	O32-C31-O31-C3
45	J	702	LMT	O5B-C1B-O1B-C4'
51	H	403	3PE	C32-C31-O31-C3
51	H	401	3PE	O32-C31-O31-C3
45	A	302	LMT	C5'-C4'-O1B-C1B
45	J	702	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
45	j	101	LMT	O5B-C5B-C6B-O6B
51	L	701	3PE	O22-C21-O21-C2
51	P	502	3PE	O22-C21-O21-C2
51	X	401	3PE	O22-C21-O21-C2
51	Y	802	3PE	O22-C21-O21-C2
51	H	401	3PE	C32-C31-O31-C3
51	Y	802	3PE	C32-C31-O31-C3
52	J	701	CDL	C31-CA7-OA8-CA6
52	J	701	CDL	OA7-CA5-OA6-CA4
45	L	706	LMT	O5B-C5B-C6B-O6B
51	d	1201	3PE	C22-C21-O21-C2
51	d	1202	3PE	C22-C21-O21-C2
45	M	602	LMT	O5B-C5B-C6B-O6B
45	M	604	LMT	O5'-C5'-C6'-O6'
51	L	701	3PE	C32-C31-O31-C3
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	M	604	LMT	O5B-C5B-C6B-O6B
52	J	701	CDL	OA9-CA7-OA8-CA6
46	B	203	PC1	O22-C21-O21-C2
52	J	701	CDL	O1-C1-CA2-OA2
51	H	402	3PE	C32-C31-O31-C3
51	M	605	3PE	C32-C31-O31-C3
51	P	502	3PE	C32-C31-O31-C3
45	L	702	LMT	O5B-C5B-C6B-O6B
45	M	602	LMT	O5'-C5'-C6'-O6'
45	Y	803	LMT	O5B-C5B-C6B-O6B
45	Y	804	LMT	O5'-C5'-C6'-O6'
45	j	101	LMT	C4B-C5B-C6B-O6B
45	K	501	LMT	C4'-C5'-C6'-O6'
46	B	203	PC1	C22-C21-O21-C2
51	L	705	3PE	C22-C21-O21-C2
51	M	605	3PE	O32-C31-O31-C3
45	K	501	LMT	O5'-C5'-C6'-O6'
45	Y	804	LMT	O5B-C5B-C6B-O6B
45	L	706	LMT	C4B-C5B-C6B-O6B
56	P	501	NDP	O4D-C4D-C5D-O5D
51	L	701	3PE	O32-C31-O31-C3
45	L	702	LMT	C4B-C5B-C6B-O6B
45	Y	801	LMT	C4B-C5B-C6B-O6B
45	L	704	LMT	C4B-C5B-C6B-O6B
45	M	602	LMT	C4B-C5B-C6B-O6B
45	Y	803	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
45	j	101	LMT	O5B-C1B-O1B-C4'
51	H	402	3PE	O32-C31-O31-C3
51	P	502	3PE	O32-C31-O31-C3
45	l	201	LMT	O5'-C1'-O1'-C1
45	Y	801	LMT	O5B-C5B-C6B-O6B
45	A	302	LMT	C4'-C5'-C6'-O6'
45	M	604	LMT	C4B-C5B-C6B-O6B
45	M	604	LMT	C4'-C5'-C6'-O6'
45	h	1002	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	O5B-C5B-C6B-O6B
45	j	101	LMT	C2B-C1B-O1B-C4'
45	L	702	LMT	O5'-C5'-C6'-O6'
45	Y	801	LMT	O5'-C5'-C6'-O6'
45	A	302	LMT	C4B-C5B-C6B-O6B
45	h	1002	LMT	C2-C3-C4-C5
46	B	203	PC1	C32-C31-O31-C3
46	L	707	PC1	C32-C31-O31-C3
51	N	702	3PE	C32-C31-O31-C3
52	L	703	CDL	C71-CB7-OB8-CB6
52	h	1001	CDL	C31-CA7-OA8-CA6
52	h	1001	CDL	C71-CB7-OB8-CB6
52	r	201	CDL	C31-CA7-OA8-CA6
45	L	702	LMT	C4'-C5'-C6'-O6'
45	Y	804	LMT	C4B-C5B-C6B-O6B
45	L	706	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	C2'-C1'-O1'-C1
52	h	1001	CDL	O1-C1-CB2-OB2
45	M	602	LMT	C4'-C5'-C6'-O6'
45	Y	804	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	O5'-C5'-C6'-O6'
45	L	704	LMT	O5B-C5B-C6B-O6B
45	M	603	LMT	O5B-C1B-O1B-C4'
46	B	203	PC1	O32-C31-O31-C3
52	h	1001	CDL	OA9-CA7-OA8-CA6
52	h	1001	CDL	OB9-CB7-OB8-CB6
52	r	201	CDL	OA9-CA7-OA8-CA6
45	Y	801	LMT	C4'-C5'-C6'-O6'
51	L	705	3PE	O22-C21-O21-C2
52	K	502	CDL	C11-CA5-OA6-CA4
52	L	703	CDL	C11-CA5-OA6-CA4
52	K	502	CDL	C31-CA7-OA8-CA6
52	L	703	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
52	K	502	CDL	CA5-C11-C12-C13
51	N	702	3PE	O32-C31-O31-C3
52	L	703	CDL	OB9-CB7-OB8-CB6
45	J	702	LMT	O5B-C5B-C6B-O6B
45	M	603	LMT	O5B-C5B-C6B-O6B
51	N	702	3PE	C21-C22-C23-C24
51	X	401	3PE	C21-C22-C23-C24
52	L	703	CDL	CA5-C11-C12-C13
46	L	707	PC1	O32-C31-O31-C3
52	L	703	CDL	O1-C1-CA2-OA2
52	K	502	CDL	OA7-CA5-OA6-CA4
52	L	703	CDL	OA7-CA5-OA6-CA4
45	M	604	LMT	C3'-C4'-O1B-C1B
52	K	502	CDL	OA9-CA7-OA8-CA6
52	L	703	CDL	OA9-CA7-OA8-CA6
45	K	501	LMT	O5B-C5B-C6B-O6B
52	h	1001	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	OA7-CA5-OA6-CA4
45	L	704	LMT	C2'-C1'-O1'-C1
45	Y	803	LMT	C2'-C1'-O1'-C1
51	H	401	3PE	C31-C32-C33-C34
59	o	201	MYR	C3-C4-C5-C6
46	L	707	PC1	C21-C22-C23-C24
51	d	1202	3PE	C3-C2-O21-C21
51	d	1202	3PE	C2A-C2B-C2C-C2D
45	j	101	LMT	C4-C5-C6-C7
46	B	202	PC1	C2A-C2B-C2C-C2D
52	h	1001	CDL	C16-C17-C18-C19
51	M	605	3PE	C35-C36-C37-C38
51	X	401	3PE	C23-C24-C25-C26
52	h	1001	CDL	C22-C23-C24-C25
46	L	707	PC1	C24-C25-C26-C27
51	M	605	3PE	C23-C24-C25-C26
51	L	701	3PE	C23-C24-C25-C26
51	d	1202	3PE	C26-C27-C28-C29
52	r	201	CDL	C39-C40-C41-C42
45	L	702	LMT	C2-C1-O1'-C1'
45	b	101	LMT	C2-C1-O1'-C1'
46	B	202	PC1	C28-C29-C2A-C2B
52	r	201	CDL	C51-C52-C53-C54
51	H	403	3PE	C34-C35-C36-C37
51	M	601	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	L	707	PC1	C29-C2A-C2B-C2C
51	N	701	3PE	C22-C21-O21-C2
52	r	201	CDL	C11-CA5-OA6-CA4
58	U	101	EHZ	C5-C6-C7-C8
46	B	202	PC1	C33-C34-C35-C36
46	B	202	PC1	C35-C36-C37-C38
51	M	601	3PE	C34-C35-C36-C37
52	K	502	CDL	C40-C41-C42-C43
45	L	706	LMT	C1-C2-C3-C4
45	A	302	LMT	C7-C8-C9-C10
51	L	705	3PE	C25-C26-C27-C28
51	M	601	3PE	C37-C38-C39-C3A
51	N	702	3PE	C32-C33-C34-C35
51	d	1201	3PE	C3E-C3F-C3G-C3H
59	o	201	MYR	C10-C11-C12-C13
45	M	604	LMT	C5'-C4'-O1B-C1B
45	J	702	LMT	O5'-C5'-C6'-O6'
51	d	1201	3PE	C2D-C2E-C2F-C2G
46	L	707	PC1	C36-C37-C38-C39
51	H	403	3PE	C3C-C3D-C3E-C3F
51	H	403	3PE	C3D-C3E-C3F-C3G
51	L	705	3PE	C33-C34-C35-C36
52	J	701	CDL	C73-C74-C75-C76
46	L	707	PC1	C23-C24-C25-C26
46	L	707	PC1	C2D-C2E-C2F-C2G
51	M	601	3PE	C36-C37-C38-C39
58	U	101	EHZ	C21-C1-C2-C3
52	J	701	CDL	CA7-C31-C32-C33
52	L	703	CDL	CA7-C31-C32-C33
46	L	707	PC1	C34-C35-C36-C37
51	X	401	3PE	C32-C33-C34-C35
51	d	1202	3PE	C3E-C3F-C3G-C3H
52	r	201	CDL	C57-C58-C59-C60
51	L	701	3PE	C28-C29-C2A-C2B
51	L	701	3PE	C29-C2A-C2B-C2C
51	M	601	3PE	C38-C39-C3A-C3B
51	M	605	3PE	C2D-C2E-C2F-C2G
45	Y	803	LMT	C1-C2-C3-C4
46	B	202	PC1	C2C-C2D-C2E-C2F
46	L	707	PC1	C22-C21-O21-C2
45	L	702	LMT	C6-C7-C8-C9
51	d	1202	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
51	d	1201	3PE	C26-C27-C28-C29
51	d	1202	3PE	C39-C3A-C3B-C3C
51	N	701	3PE	O22-C21-O21-C2
52	r	201	CDL	OA7-CA5-OA6-CA4
45	M	603	LMT	C2-C3-C4-C5
59	o	201	MYR	C9-C10-C11-C12
46	B	202	PC1	C31-C32-C33-C34
51	L	701	3PE	C2D-C2E-C2F-C2G
51	X	401	3PE	C2A-C2B-C2C-C2D
45	L	704	LMT	O1'-C1-C2-C3
51	H	402	3PE	C38-C39-C3A-C3B
51	L	701	3PE	C2E-C2F-C2G-C2H
51	P	502	3PE	C33-C34-C35-C36
45	L	704	LMT	O5'-C1'-O1'-C1
51	d	1201	3PE	C29-C2A-C2B-C2C
45	M	604	LMT	C2'-C1'-O1'-C1
45	j	101	LMT	C2'-C1'-O1'-C1
59	o	201	MYR	C5-C6-C7-C8
52	L	703	CDL	C54-C55-C56-C57
45	M	602	LMT	C9-C10-C11-C12
52	L	703	CDL	C51-CB5-OB6-CB4
51	H	402	3PE	C21-C22-C23-C24
45	Y	804	LMT	C4-C5-C6-C7
46	L	707	PC1	C38-C39-C3A-C3B
52	r	201	CDL	C58-C59-C60-C61
45	h	1002	LMT	C6-C7-C8-C9
45	J	702	LMT	C1-C2-C3-C4
46	L	707	PC1	C2B-C2C-C2D-C2E
45	A	302	LMT	C11-C10-C9-C8
51	M	605	3PE	C3D-C3E-C3F-C3G
52	r	201	CDL	C31-C32-C33-C34
45	j	101	LMT	C1-C2-C3-C4
52	J	701	CDL	C78-C79-C80-C81
52	K	502	CDL	C19-C20-C21-C22
51	X	401	3PE	C3C-C3D-C3E-C3F
51	d	1202	3PE	C24-C25-C26-C27
51	d	1201	3PE	C2B-C2C-C2D-C2E
51	N	701	3PE	O21-C2-C3-O31
51	X	401	3PE	C38-C39-C3A-C3B
52	K	502	CDL	C16-C17-C18-C19
46	L	707	PC1	C2-C1-O11-P
51	X	401	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
52	L	703	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C25-C26-C27-C28
52	J	701	CDL	C77-C78-C79-C80
52	L	703	CDL	CB4-CB6-OB8-CB7
52	h	1001	CDL	C13-C14-C15-C16
51	H	401	3PE	C27-C28-C29-C2A
52	K	502	CDL	C36-C37-C38-C39
51	X	401	3PE	C28-C29-C2A-C2B
51	H	401	3PE	O11-C1-C2-C3
51	N	702	3PE	O11-C1-C2-C3
46	L	707	PC1	O22-C21-O21-C2
52	K	502	CDL	C51-CB5-OB6-CB4
51	H	403	3PE	C37-C38-C39-C3A
52	J	701	CDL	C79-C80-C81-C82
45	K	501	LMT	O5B-C1B-O1B-C4'
46	B	203	PC1	C1-C2-C3-O31
51	H	403	3PE	C1-C2-C3-O31
51	N	702	3PE	C1-C2-C3-O31
51	Y	802	3PE	C1-C2-C3-O31
51	d	1201	3PE	C1-C2-C3-O31
52	J	701	CDL	CB3-CB4-CB6-OB8
45	J	702	LMT	C4-C5-C6-C7
51	L	701	3PE	C34-C35-C36-C37
51	X	401	3PE	C26-C27-C28-C29
52	J	701	CDL	CA4-CA6-OA8-CA7
46	L	707	PC1	C37-C38-C39-C3A
51	Y	802	3PE	C34-C35-C36-C37
46	L	707	PC1	C26-C27-C28-C29
51	d	1201	3PE	C23-C24-C25-C26
45	b	101	LMT	O1'-C1-C2-C3
51	H	401	3PE	C22-C23-C24-C25
52	J	701	CDL	CA3-CA4-OA6-CA5
51	L	701	3PE	C38-C39-C3A-C3B
52	r	201	CDL	CA5-C11-C12-C13
51	Y	802	3PE	C37-C38-C39-C3A
46	A	303	PC1	O11-C1-C2-O21
51	d	1202	3PE	C27-C28-C29-C2A
52	L	703	CDL	C58-C59-C60-C61
52	J	701	CDL	C54-C55-C56-C57
45	L	706	LMT	C4-C5-C6-C7
51	P	502	3PE	O21-C2-C3-O31
52	K	502	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	C52-C53-C54-C55
52	J	701	CDL	C72-C73-C74-C75
52	h	1001	CDL	C14-C15-C16-C17
53	N	703	I49	C08-C06-C07-C09
51	H	403	3PE	C3A-C3B-C3C-C3D
51	L	701	3PE	C33-C34-C35-C36
45	K	501	LMT	C3'-C4'-O1B-C1B
45	A	302	LMT	C2-C1-O1'-C1'
45	L	704	LMT	C2-C1-O1'-C1'
45	L	706	LMT	C2-C1-O1'-C1'
45	M	603	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2-C1-O1'-C1'
45	j	101	LMT	C2-C1-O1'-C1'
51	M	601	3PE	C35-C36-C37-C38
51	P	502	3PE	C2-C1-O11-P
51	d	1201	3PE	C2-C1-O11-P
58	T	101	EHZ	S1-C10-C11-N1
52	h	1001	CDL	C11-C12-C13-C14
45	A	302	LMT	C2'-C1'-O1'-C1
45	J	702	LMT	C2'-C1'-O1'-C1
45	M	602	LMT	C2'-C1'-O1'-C1
45	b	101	LMT	C2'-C1'-O1'-C1
51	M	605	3PE	O11-C1-C2-C3
52	K	502	CDL	OB5-CB3-CB4-CB6
59	o	201	MYR	C11-C12-C13-C14
45	K	501	LMT	C5'-C4'-O1B-C1B
56	P	501	NDP	C3D-C4D-C5D-O5D
45	h	1002	LMT	C4-C5-C6-C7
51	N	701	3PE	C2A-C2B-C2C-C2D
45	L	704	LMT	C1-C2-C3-C4
46	B	202	PC1	O21-C21-C22-C23
52	r	201	CDL	C71-C72-C73-C74
51	L	701	3PE	C3D-C3E-C3F-C3G
45	M	603	LMT	C7-C8-C9-C10
51	L	705	3PE	C1-C2-C3-O31
51	N	701	3PE	C1-C2-C3-O31
51	P	502	3PE	C1-C2-C3-O31
52	J	701	CDL	CA3-CA4-CA6-OA8
52	K	502	CDL	CA3-CA4-CA6-OA8
52	L	703	CDL	CB3-CB4-CB6-OB8
51	H	402	3PE	C2B-C2C-C2D-C2E
45	M	602	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
45	M	604	LMT	C2-C3-C4-C5
51	X	401	3PE	C25-C26-C27-C28
59	o	201	MYR	C2-C3-C4-C5
46	L	707	PC1	C39-C3A-C3B-C3C
53	N	703	I49	C08-C06-C07-C10
52	L	703	CDL	C34-C35-C36-C37
51	N	702	3PE	O11-C1-C2-O21
52	J	701	CDL	OB5-CB3-CB4-OB6
52	K	502	CDL	OB5-CB3-CB4-OB6
51	H	403	3PE	C2-C1-O11-P
51	H	401	3PE	C3D-C3E-C3F-C3G
45	M	604	LMT	O1'-C1-C2-C3
51	M	605	3PE	C33-C34-C35-C36
51	N	701	3PE	C34-C35-C36-C37
46	B	203	PC1	O21-C2-C3-O31
51	L	705	3PE	O21-C2-C3-O31
51	Y	802	3PE	O21-C2-C3-O31
45	L	702	LMT	C5-C6-C7-C8
46	B	203	PC1	C21-C22-C23-C24
51	L	705	3PE	C38-C39-C3A-C3B
52	h	1001	CDL	C24-C25-C26-C27
51	H	402	3PE	C29-C2A-C2B-C2C
51	P	502	3PE	C35-C36-C37-C38
51	H	403	3PE	C32-C33-C34-C35
45	K	501	LMT	C6-C7-C8-C9
45	M	603	LMT	C3'-C4'-O1B-C1B
51	L	701	3PE	C37-C38-C39-C3A
52	r	201	CDL	C15-C16-C17-C18
46	A	303	PC1	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
51	Y	802	3PE	O11-C1-C2-C3
52	h	1001	CDL	OB5-CB3-CB4-CB6
51	H	401	3PE	C26-C27-C28-C29
45	M	603	LMT	C4B-C5B-C6B-O6B
52	K	502	CDL	OB7-CB5-OB6-CB4
59	o	201	MYR	C6-C7-C8-C9
51	d	1201	3PE	C34-C35-C36-C37
52	r	201	CDL	C54-C55-C56-C57
46	L	707	PC1	C3-C2-O21-C21
51	d	1201	3PE	C1-C2-O21-C21
51	d	1201	3PE	C32-C33-C34-C35
45	M	603	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	O11-C1-C2-O21
46	L	707	PC1	O11-C1-C2-O21
52	L	703	CDL	C13-C14-C15-C16
51	H	401	3PE	C12-C11-O13-P
51	M	601	3PE	C12-C11-O13-P
51	M	605	3PE	C12-C11-O13-P
51	P	502	3PE	C12-C11-O13-P
51	H	401	3PE	O21-C2-C3-O31
51	d	1201	3PE	O21-C2-C3-O31
52	J	701	CDL	OA6-CA4-CA6-OA8
52	K	502	CDL	OA6-CA4-CA6-OA8
52	L	703	CDL	OB6-CB4-CB6-OB8
52	r	201	CDL	OB6-CB4-CB6-OB8
51	N	701	3PE	C23-C24-C25-C26
58	T	101	EHZ	C2-C1-C21-C22
51	d	1202	3PE	C31-C32-C33-C34
51	d	1201	3PE	C37-C38-C39-C3A
54	O	401	GTP	PB-O3A-PA-O1A
45	l	201	LMT	O1'-C1-C2-C3
46	L	707	PC1	C3A-C3B-C3C-C3D
45	Y	801	LMT	C1-C2-C3-C4
51	N	701	3PE	C22-C23-C24-C25
51	N	701	3PE	C29-C2A-C2B-C2C
51	d	1202	3PE	C2E-C2F-C2G-C2H
51	X	401	3PE	C2-C3-O31-C31
45	A	302	LMT	O5B-C1B-O1B-C4'
52	r	201	CDL	C17-C18-C19-C20
51	H	402	3PE	C3A-C3B-C3C-C3D
51	d	1201	3PE	C2A-C2B-C2C-C2D
51	H	403	3PE	C3E-C3F-C3G-C3H
46	L	707	PC1	O11-C1-C2-C3
51	L	701	3PE	O11-C1-C2-C3
52	h	1001	CDL	OA5-CA3-CA4-CA6
58	T	101	EHZ	C21-C22-C23-C24
46	B	202	PC1	C2F-C2G-C2H-C2I
52	r	201	CDL	C1-CB2-OB2-PB2
51	X	401	3PE	C39-C3A-C3B-C3C
45	K	501	LMT	C2B-C1B-O1B-C4'
58	U	101	EHZ	C11-C10-S1-C9
51	P	502	3PE	C24-C25-C26-C27
51	H	401	3PE	O11-C1-C2-O21
51	L	701	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
51	M	605	3PE	O11-C1-C2-O21
51	P	502	3PE	O11-C1-C2-O21
51	Y	802	3PE	O11-C1-C2-O21
52	h	1001	CDL	OA5-CA3-CA4-OA6
52	h	1001	CDL	OB5-CB3-CB4-OB6
45	L	704	LMT	C5-C6-C7-C8
56	P	501	NDP	O4D-C1D-N1N-C6N
51	H	403	3PE	O21-C2-C3-O31
46	B	203	PC1	C32-C33-C34-C35
46	A	303	PC1	C1-C2-C3-O31
51	M	601	3PE	C25-C26-C27-C28
51	L	701	3PE	C3A-C3B-C3C-C3D
45	J	702	LMT	O5'-C1'-O1'-C1
45	j	101	LMT	O5'-C1'-O1'-C1
46	A	303	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	203	PC1	C11-O13-P-O14
51	H	401	3PE	C1-O11-P-O12
51	H	401	3PE	C11-O13-P-O11
51	H	401	3PE	C11-O13-P-O14
51	L	705	3PE	C11-O13-P-O14
51	M	601	3PE	C11-O13-P-O14
51	M	605	3PE	C1-O11-P-O12
51	N	701	3PE	C1-O11-P-O12
51	N	701	3PE	C11-O13-P-O11
51	N	701	3PE	C11-O13-P-O14
51	N	702	3PE	O13-C11-C12-N
51	P	502	3PE	C11-O13-P-O11
51	P	502	3PE	C11-O13-P-O12
51	P	502	3PE	C11-O13-P-O14
51	X	401	3PE	C1-O11-P-O13
51	X	401	3PE	C1-O11-P-O14
51	d	1202	3PE	C1-O11-P-O14
52	J	701	CDL	CB2-OB2-PB2-OB3
52	K	502	CDL	CA2-OA2-PA1-OA3
52	K	502	CDL	CA2-OA2-PA1-OA5
52	K	502	CDL	CB3-OB5-PB2-OB2
52	K	502	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
52	K	502	CDL	CB3-OB5-PB2-OB4
52	L	703	CDL	CA2-OA2-PA1-OA3
52	L	703	CDL	CB3-OB5-PB2-OB2
52	r	201	CDL	CA3-OA5-PA1-OA3
51	P	502	3PE	C39-C3A-C3B-C3C
51	d	1202	3PE	C2D-C2E-C2F-C2G
46	B	203	PC1	C24-C25-C26-C27
51	H	401	3PE	C37-C38-C39-C3A
51	M	605	3PE	C3A-C3B-C3C-C3D
46	L	707	PC1	C27-C28-C29-C2A
52	L	703	CDL	C38-C39-C40-C41
52	h	1001	CDL	C72-C73-C74-C75
52	L	703	CDL	C52-C53-C54-C55
51	d	1202	3PE	C32-C33-C34-C35
51	P	502	3PE	C1-C2-O21-C21
52	h	1001	CDL	CA3-CA4-OA6-CA5
51	P	502	3PE	C37-C38-C39-C3A
51	M	605	3PE	C3F-C3G-C3H-C3I
52	h	1001	CDL	CA2-C1-CB2-OB2
51	M	605	3PE	C21-C22-C23-C24
46	L	707	PC1	C35-C36-C37-C38
51	Y	802	3PE	C3B-C3C-C3D-C3E
52	r	201	CDL	CA4-CA3-OA5-PA1
51	X	401	3PE	C29-C2A-C2B-C2C
51	N	702	3PE	O21-C2-C3-O31
52	J	701	CDL	OB6-CB4-CB6-OB8
51	M	605	3PE	C34-C35-C36-C37
46	B	203	PC1	C35-C36-C37-C38
51	N	702	3PE	C34-C35-C36-C37
45	Y	803	LMT	C3-C4-C5-C6
51	H	401	3PE	C1-C2-C3-O31
52	K	502	CDL	C15-C16-C17-C18
45	Y	801	LMT	C2-C1-O1'-C1'
45	Y	804	LMT	C2-C1-O1'-C1'
45	l	201	LMT	C2-C1-O1'-C1'
45	Y	801	LMT	C3'-C4'-O1B-C1B
45	l	201	LMT	C4'-C5'-C6'-O6'
51	L	701	3PE	C2F-C2G-C2H-C2I
51	M	601	3PE	C28-C29-C2A-C2B
52	r	201	CDL	C32-C33-C34-C35
51	M	605	3PE	C3B-C3C-C3D-C3E
45	J	702	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
45	Y	803	LMT	C3'-C4'-O1B-C1B
51	H	402	3PE	C33-C34-C35-C36
46	B	202	PC1	C3B-C3C-C3D-C3E
45	Y	801	LMT	C5'-C4'-O1B-C1B
52	r	201	CDL	CB3-CB4-CB6-OB8
51	M	601	3PE	C2C-C2D-C2E-C2F
45	A	301	LMT	C2-C3-C4-C5
45	A	302	LMT	C2B-C1B-O1B-C4'
52	h	1001	CDL	CA6-CA4-OA6-CA5
45	Y	803	LMT	C5'-C4'-O1B-C1B
51	X	401	3PE	C31-C32-C33-C34
52	J	701	CDL	C1-CB2-OB2-PB2
51	M	601	3PE	C33-C34-C35-C36
52	r	201	CDL	C34-C35-C36-C37
52	J	701	CDL	C35-C36-C37-C38
51	X	401	3PE	C3F-C3G-C3H-C3I
46	L	707	PC1	C33-C34-C35-C36
51	M	601	3PE	C2A-C2B-C2C-C2D
46	A	303	PC1	O21-C2-C3-O31
45	l	201	LMT	O5'-C5'-C6'-O6'
56	P	501	NDP	C2B-O2B-P2B-O1X
52	J	701	CDL	C72-C71-CB7-OB8
51	H	401	3PE	C33-C34-C35-C36
45	Y	804	LMT	O5'-C1'-O1'-C1
46	L	707	PC1	C31-C32-C33-C34
51	M	601	3PE	C26-C27-C28-C29
46	B	202	PC1	O22-C21-C22-C23
51	M	605	3PE	C26-C27-C28-C29
52	K	502	CDL	C52-C53-C54-C55
51	H	402	3PE	O11-C1-C2-O21
51	d	1201	3PE	C33-C34-C35-C36
58	T	101	EHZ	C12-C13-C14-N2
51	M	605	3PE	C38-C39-C3A-C3B
51	H	402	3PE	C24-C25-C26-C27
52	r	201	CDL	C56-C57-C58-C59
51	H	402	3PE	C25-C26-C27-C28
51	P	502	3PE	O11-C1-C2-C3
52	J	701	CDL	OB5-CB3-CB4-CB6
51	N	701	3PE	C32-C33-C34-C35
49	F	501	FMN	C4'-C5'-O5'-P
51	N	701	3PE	C37-C38-C39-C3A
52	K	502	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C2B-C2C-C2D-C2E
51	H	403	3PE	C1-C2-O21-C21
51	H	403	3PE	C3-C2-O21-C21
52	h	1001	CDL	C18-C19-C20-C21
51	H	402	3PE	C3F-C3G-C3H-C3I
45	K	501	LMT	C4B-C5B-C6B-O6B
51	d	1201	3PE	C21-C22-C23-C24
51	L	705	3PE	C37-C38-C39-C3A
45	A	302	LMT	O1'-C1-C2-C3
51	d	1201	3PE	C31-C32-C33-C34
45	A	302	LMT	C3'-C4'-O1B-C1B
45	Y	803	LMT	C2-C3-C4-C5
52	L	703	CDL	C39-C40-C41-C42
52	h	1001	CDL	C19-C20-C21-C22
51	L	701	3PE	C22-C23-C24-C25
52	r	201	CDL	OA6-CA4-CA6-OA8
45	Y	803	LMT	C5-C6-C7-C8
52	L	703	CDL	C36-C37-C38-C39
52	L	703	CDL	CA4-CA3-OA5-PA1
51	X	401	3PE	O31-C31-C32-C33
51	M	605	3PE	C3E-C3F-C3G-C3H
52	L	703	CDL	C12-C13-C14-C15
46	B	202	PC1	O31-C31-C32-C33
45	K	501	LMT	O1'-C1-C2-C3
51	H	402	3PE	C26-C27-C28-C29
46	B	202	PC1	C39-C3A-C3B-C3C
52	L	703	CDL	C53-C54-C55-C56
51	L	705	3PE	O21-C21-C22-C23
52	h	1001	CDL	C31-C32-C33-C34
51	L	701	3PE	O21-C21-C22-C23
52	r	201	CDL	C32-C31-CA7-OA8
45	Y	804	LMT	O1'-C1-C2-C3
46	B	203	PC1	O21-C21-C22-C23
58	U	101	EHZ	C2-C3-C4-C5
49	F	501	FMN	N10-C1'-C2'-O2'
52	L	703	CDL	C55-C56-C57-C58
51	H	401	3PE	O21-C21-C22-C23
51	X	401	3PE	O32-C31-C32-C33
51	N	701	3PE	C2-C1-O11-P
45	M	604	LMT	C3-C4-C5-C6
52	K	502	CDL	C11-C12-C13-C14
51	d	1202	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
51	Y	802	3PE	C36-C37-C38-C39
51	N	702	3PE	C33-C34-C35-C36
45	Y	803	LMT	C4'-C5'-C6'-O6'
51	L	705	3PE	C39-C3A-C3B-C3C
52	K	502	CDL	C53-C54-C55-C56
46	B	203	PC1	O22-C21-C22-C23
51	L	705	3PE	O31-C31-C32-C33
51	N	701	3PE	O21-C21-C22-C23
52	r	201	CDL	C52-C51-CB5-OB6
51	d	1201	3PE	O21-C21-C22-C23
51	d	1201	3PE	C2F-C2G-C2H-C2I
58	U	101	EHZ	C4-C5-C6-C7
52	K	502	CDL	C35-C36-C37-C38
46	B	202	PC1	O32-C31-C32-C33
51	P	502	3PE	C36-C37-C38-C39
52	r	201	CDL	C32-C31-CA7-OA9
52	K	502	CDL	OB9-CB7-OB8-CB6
45	L	706	LMT	C6-C7-C8-C9
51	L	701	3PE	O22-C21-C22-C23
51	M	601	3PE	C21-C22-C23-C24
51	L	705	3PE	O22-C21-C22-C23
51	H	401	3PE	O22-C21-C22-C23
51	N	701	3PE	O22-C21-C22-C23

There are no ring outliers.

23 monomers are involved in 39 short contacts:

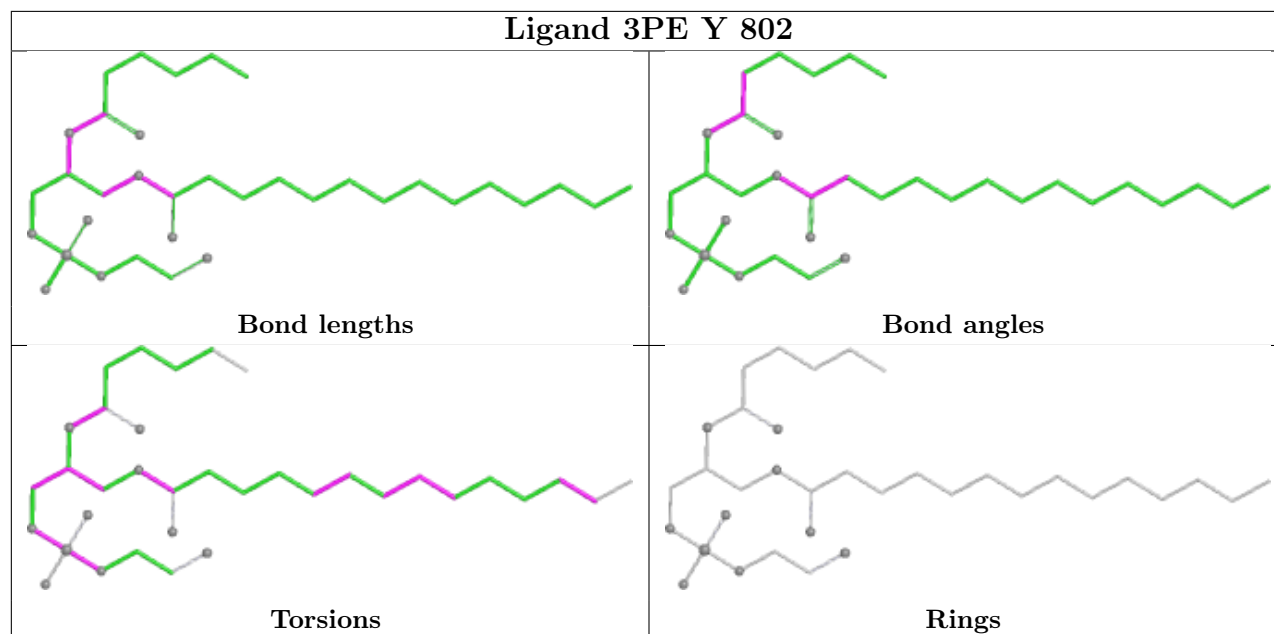
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	Y	802	3PE	1	0
53	N	703	I49	4	0
51	X	401	3PE	2	0
45	h	1002	LMT	1	0
52	r	201	CDL	1	0
56	P	501	NDP	1	0
46	L	707	PC1	3	0
46	B	202	PC1	2	0
52	J	701	CDL	1	0
45	A	301	LMT	2	0
58	T	101	EHZ	1	0
51	L	705	3PE	2	0
46	B	203	PC1	2	0
46	A	303	PC1	1	0

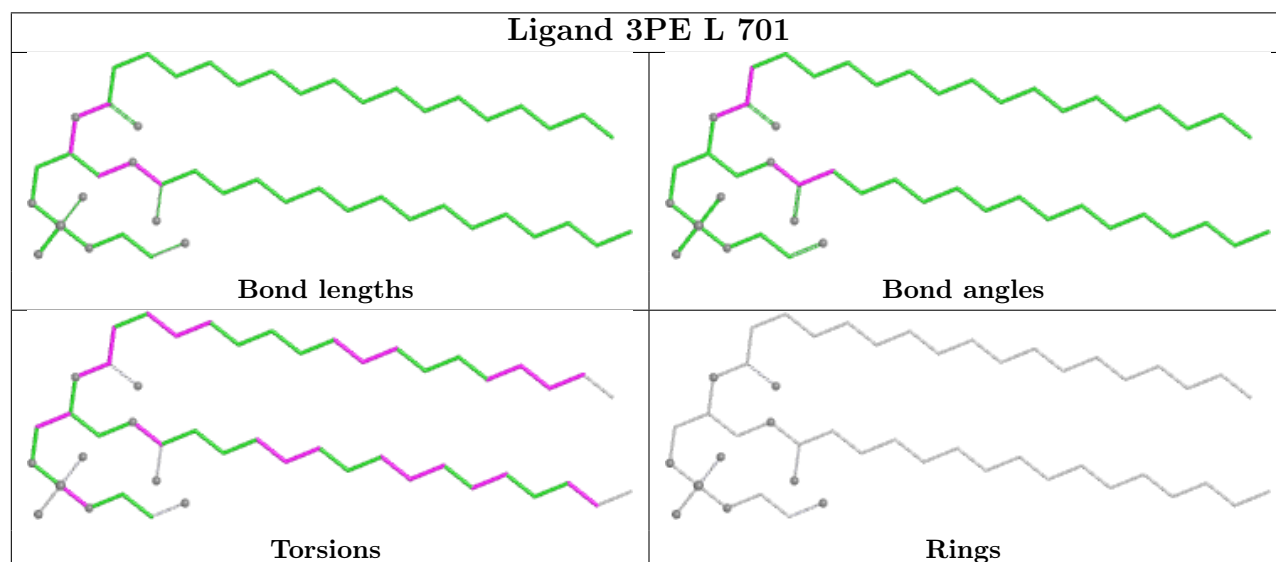
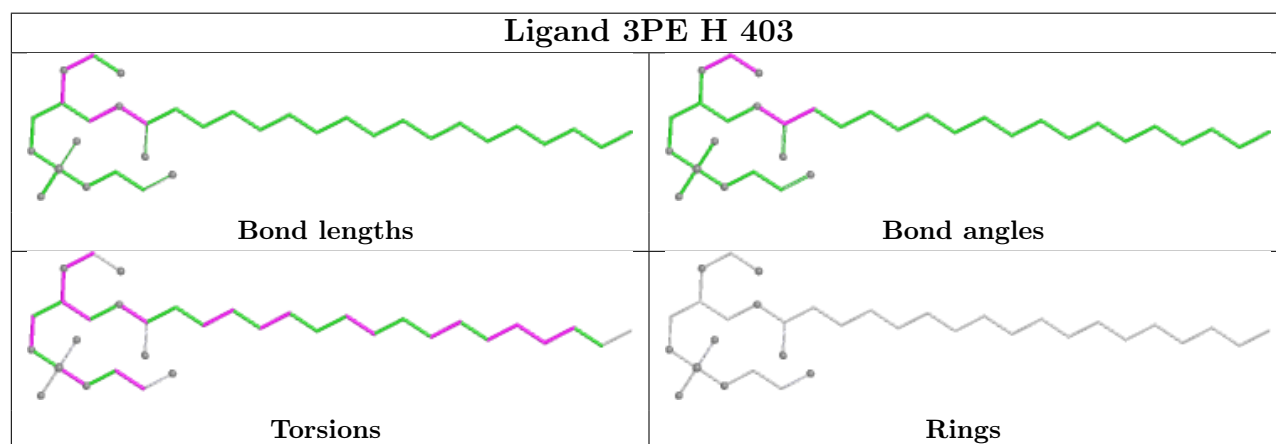
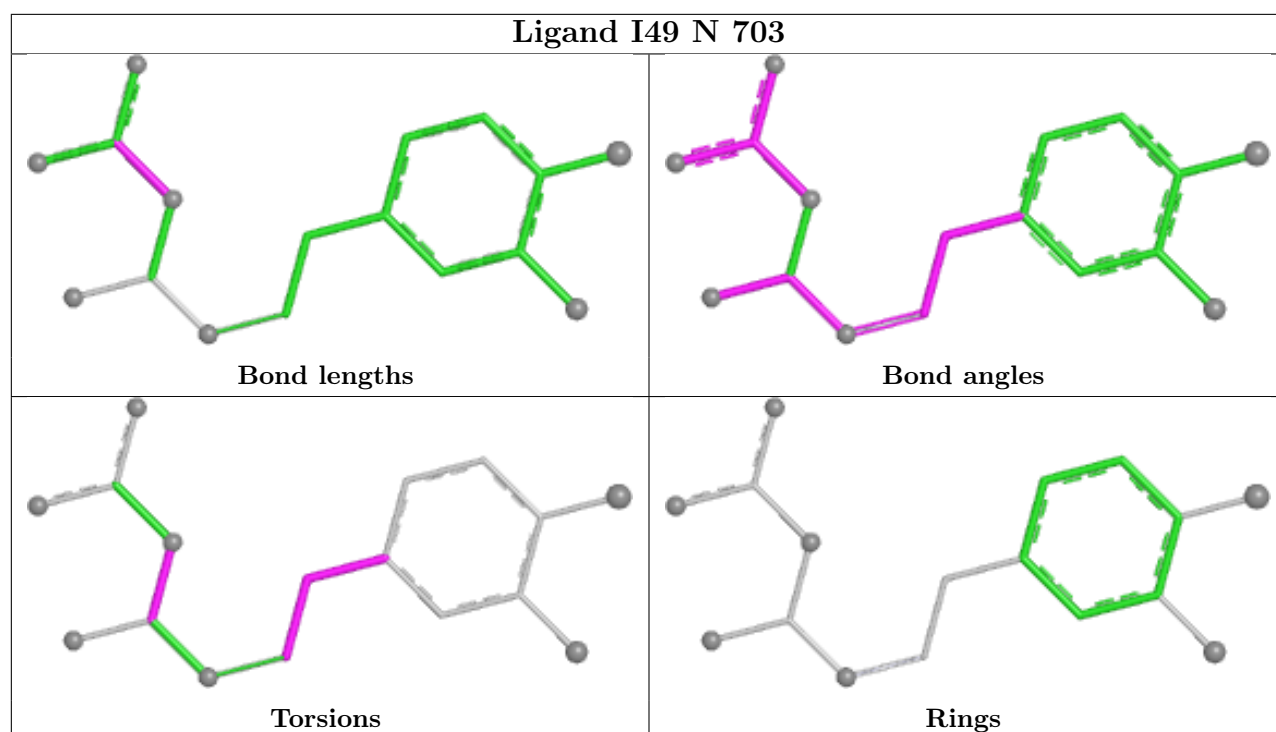
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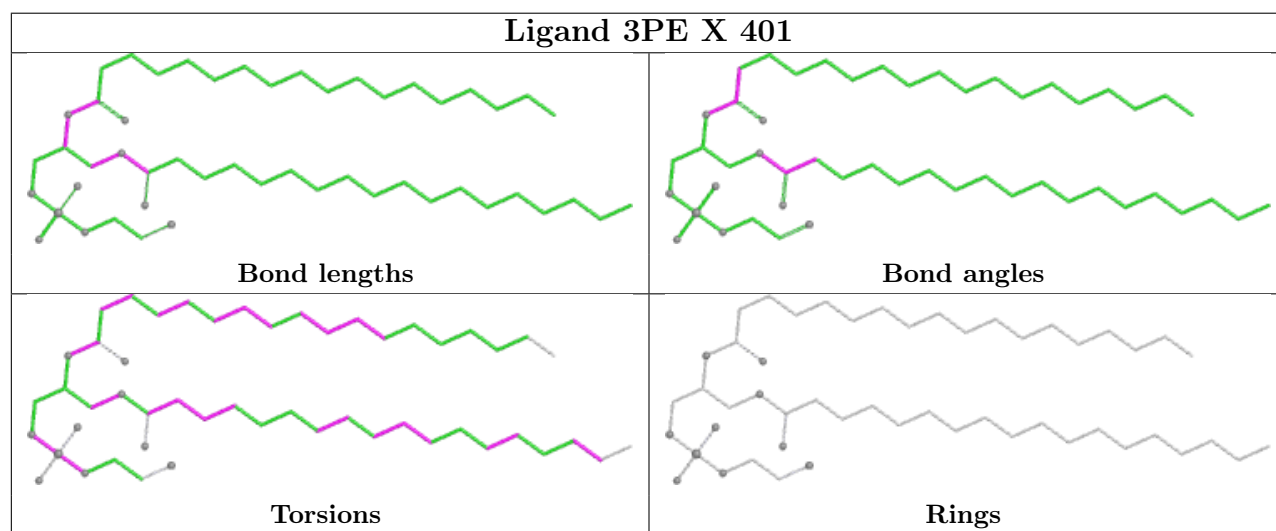
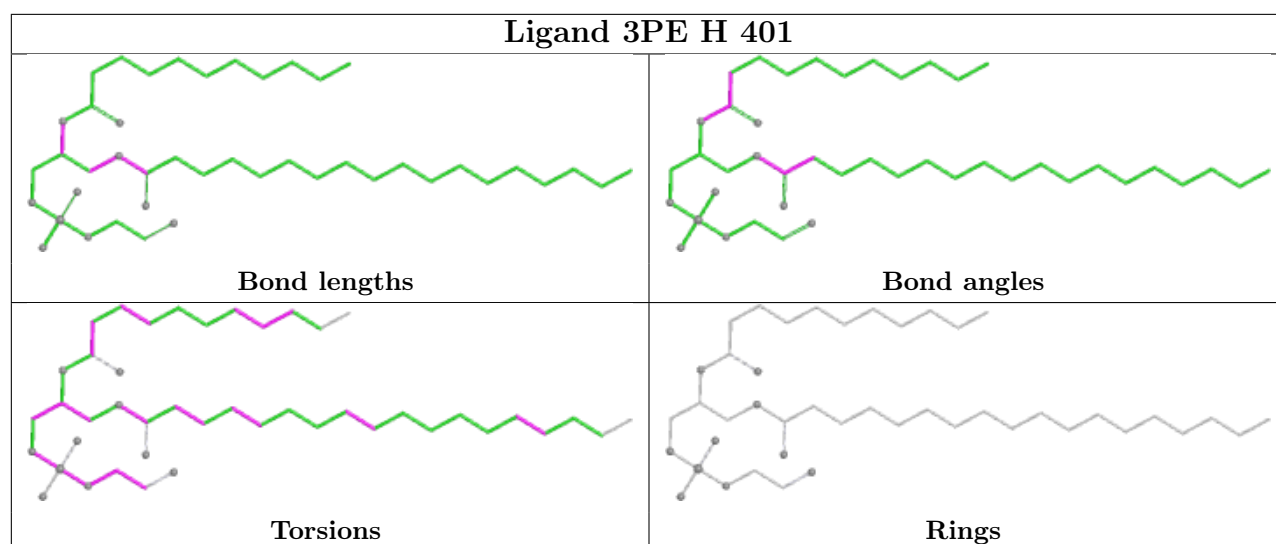
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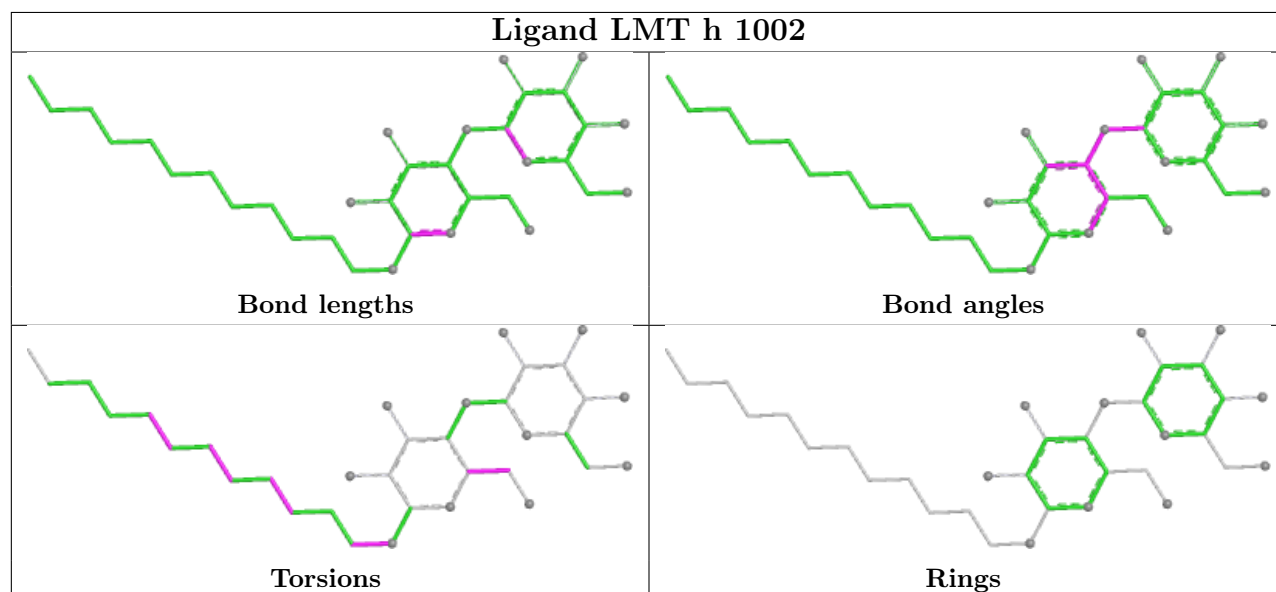
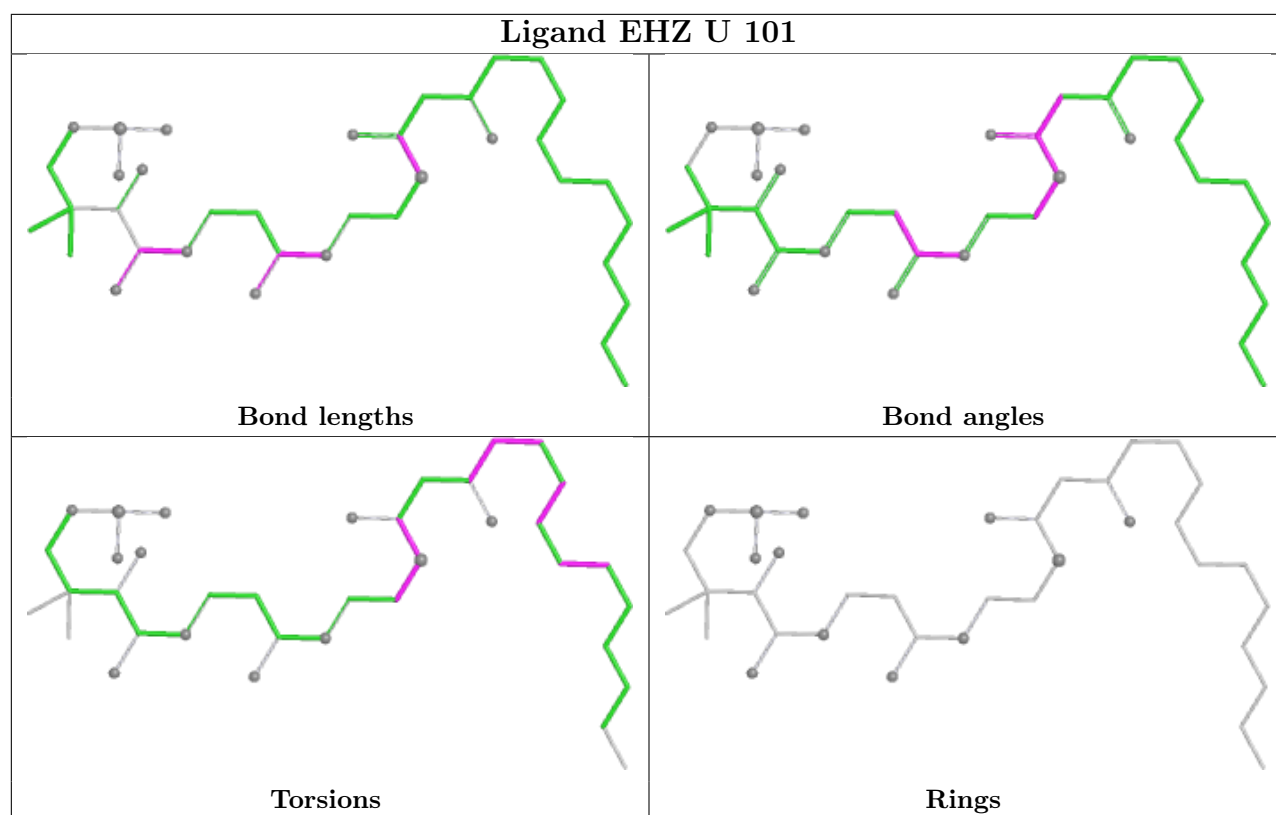
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	O	401	GTP	3	0
52	h	1001	CDL	2	0
45	M	603	LMT	1	0
45	M	602	LMT	5	0
45	J	702	LMT	2	0
51	M	601	3PE	2	0
45	Y	804	LMT	1	0
49	F	501	FMN	1	0
51	M	605	3PE	2	0

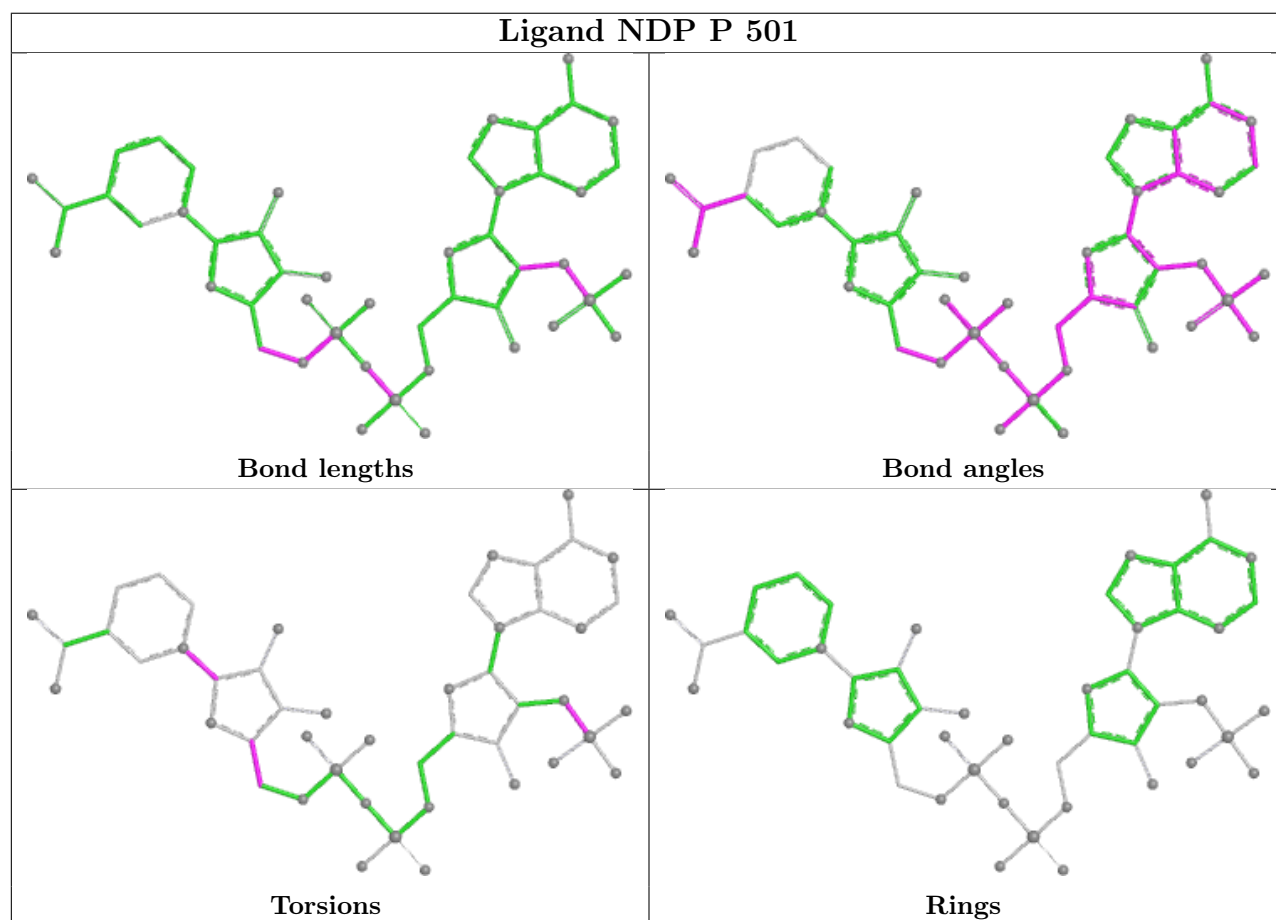
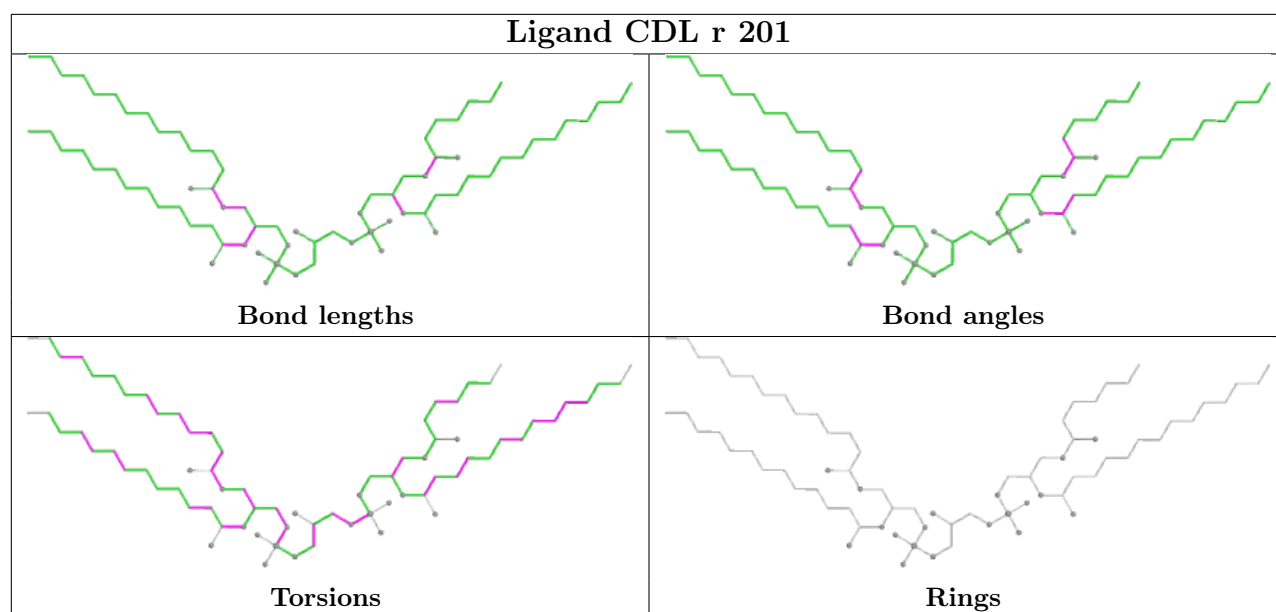
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

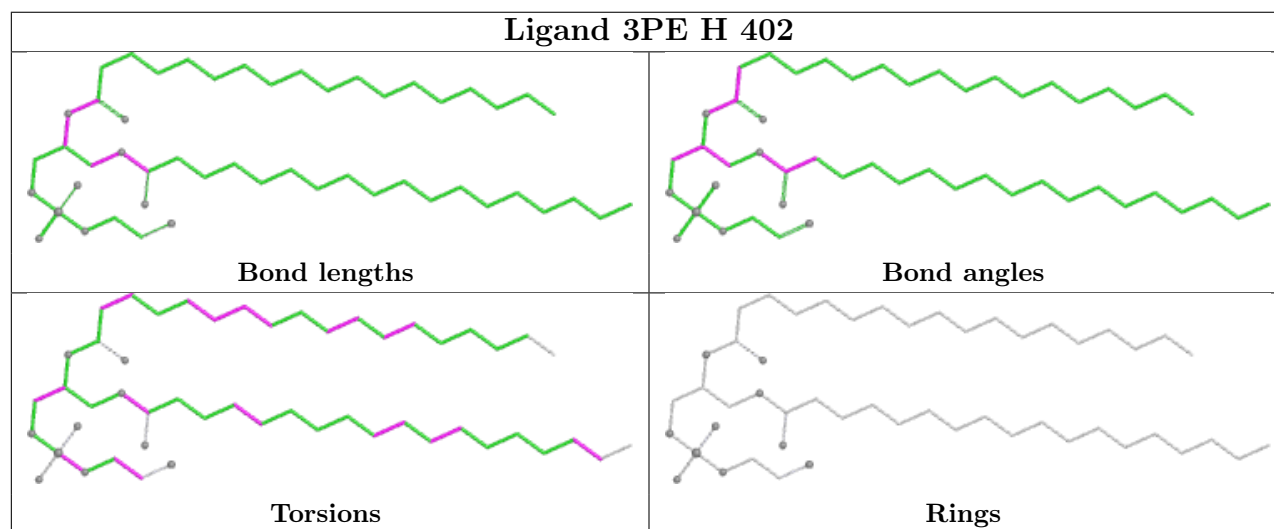
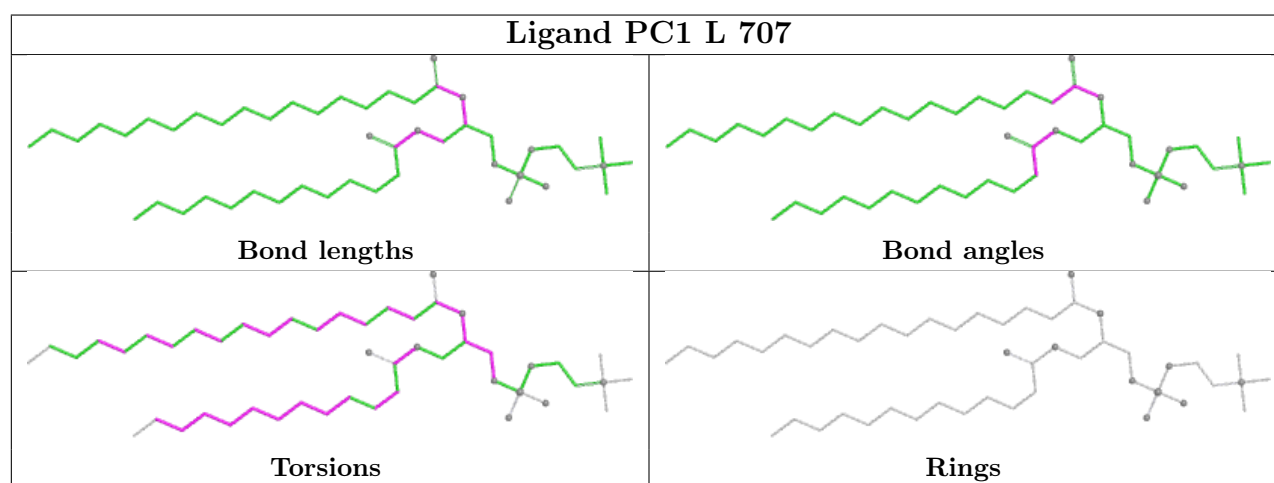
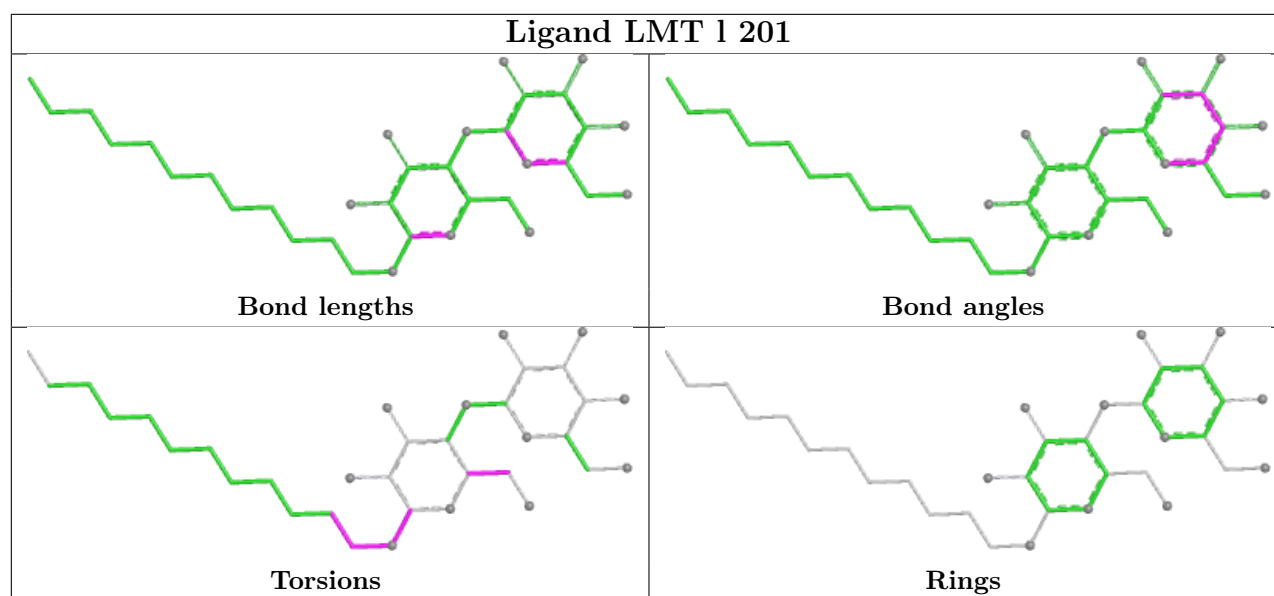


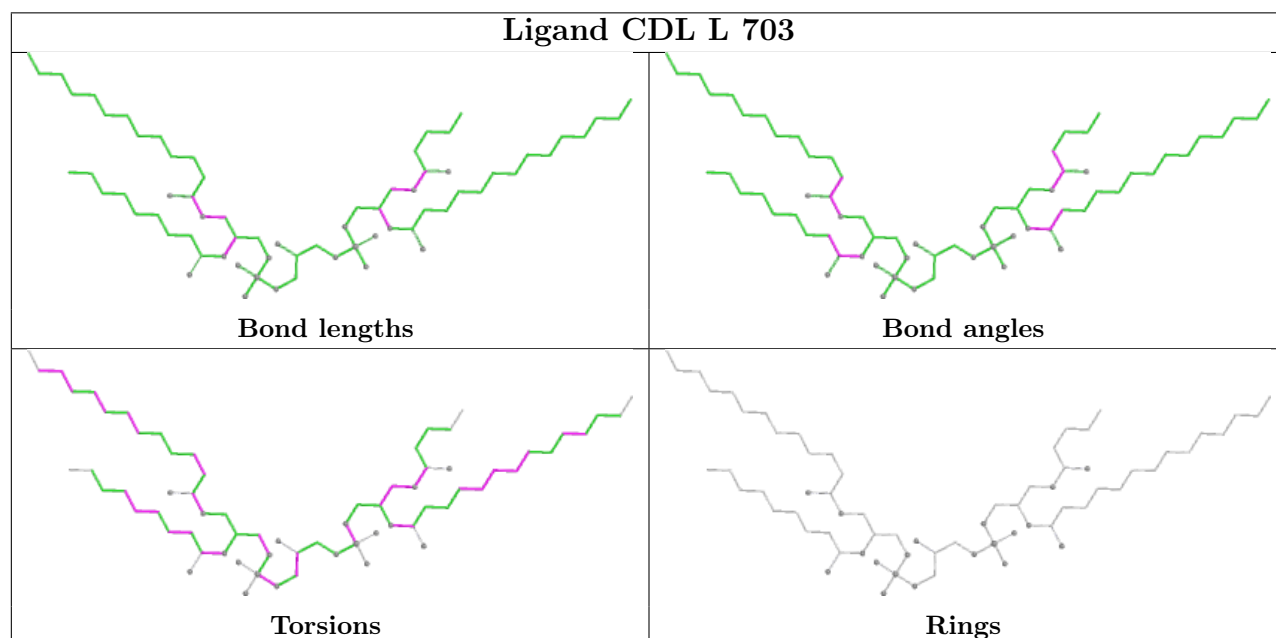
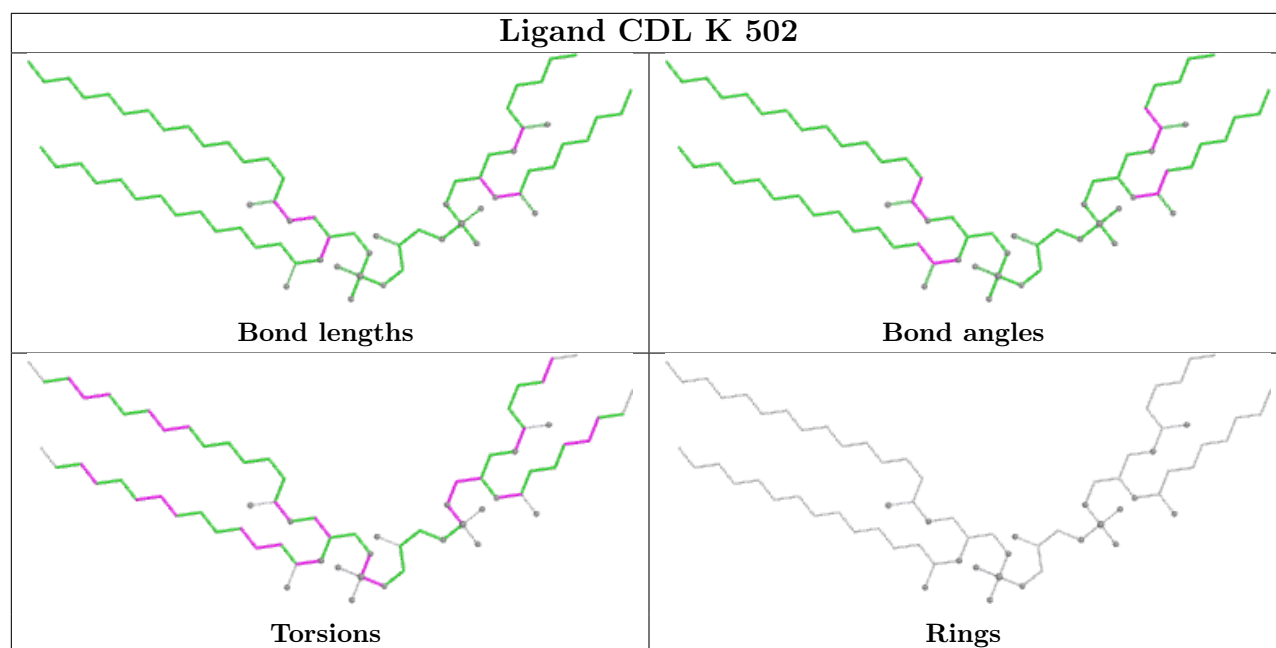
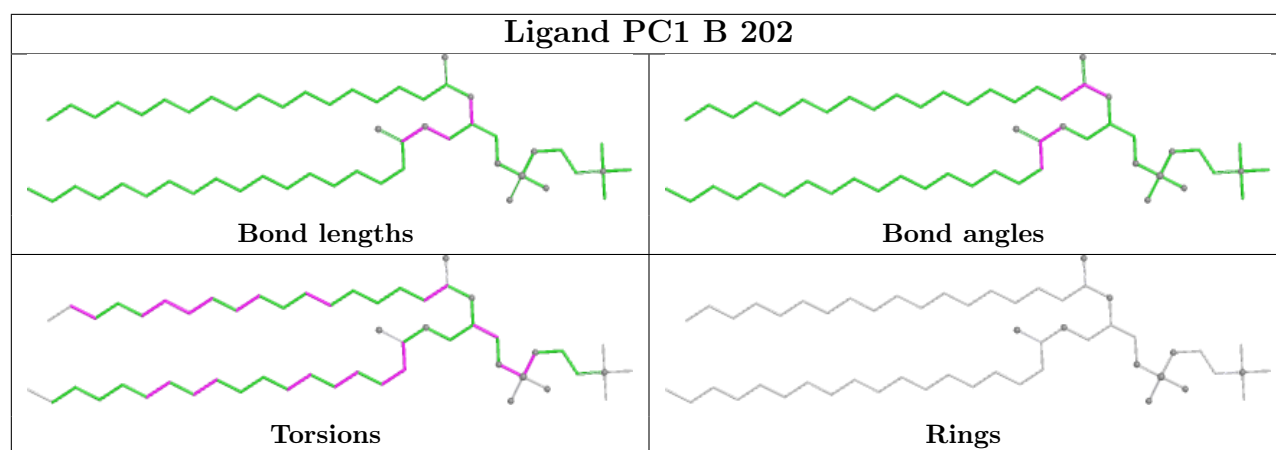


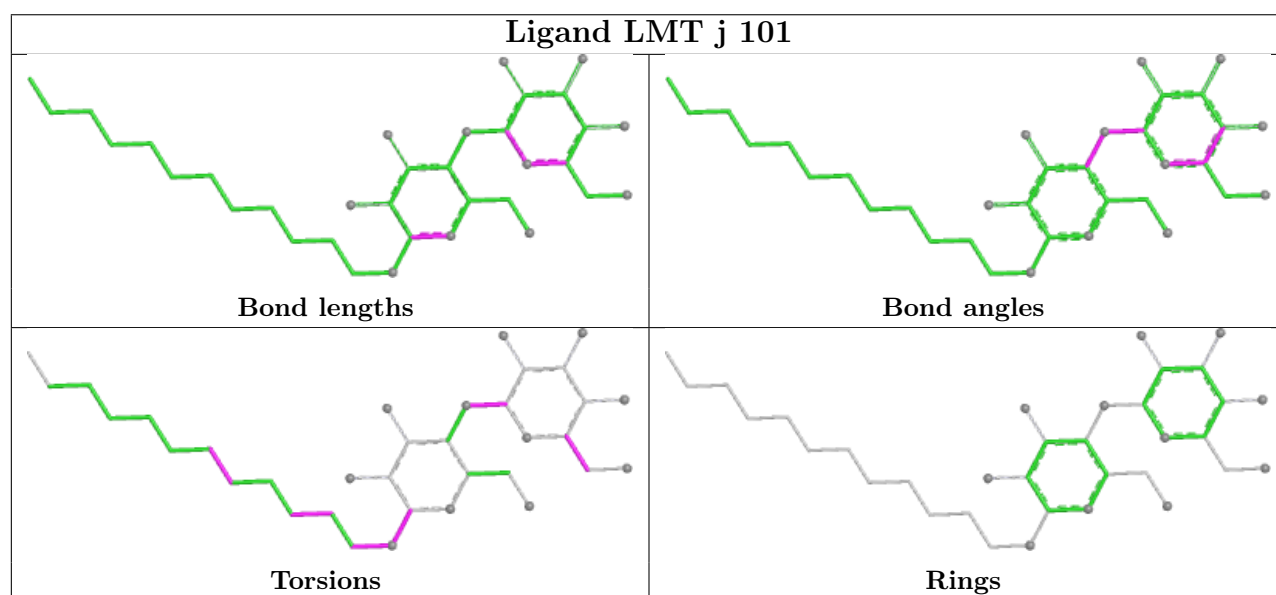
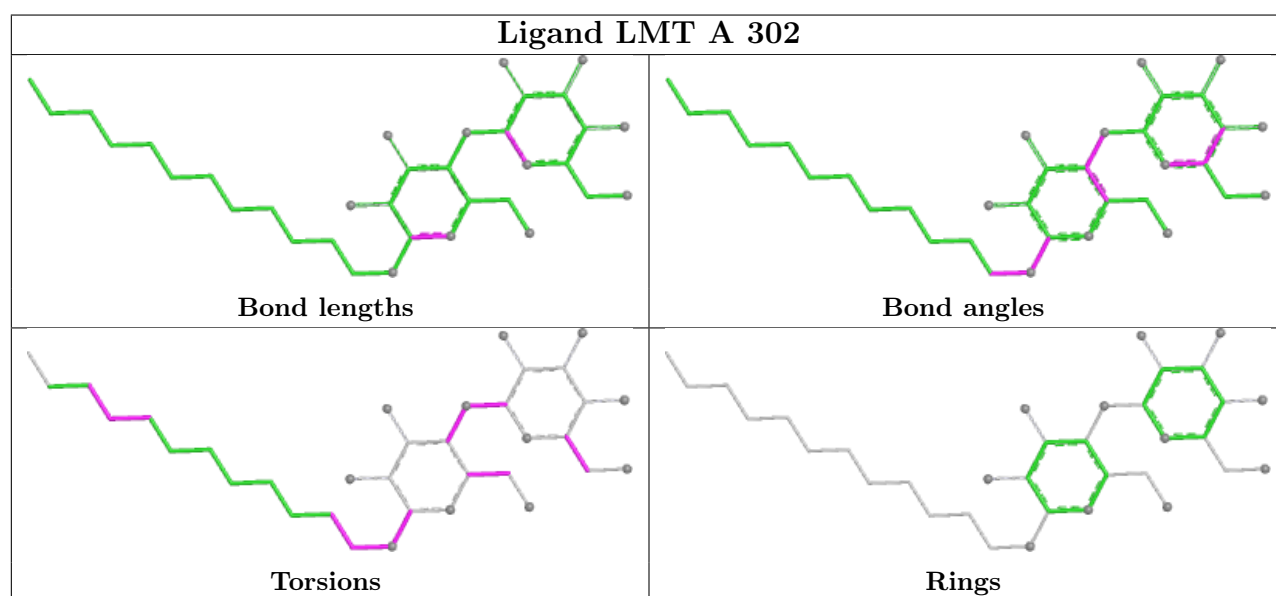
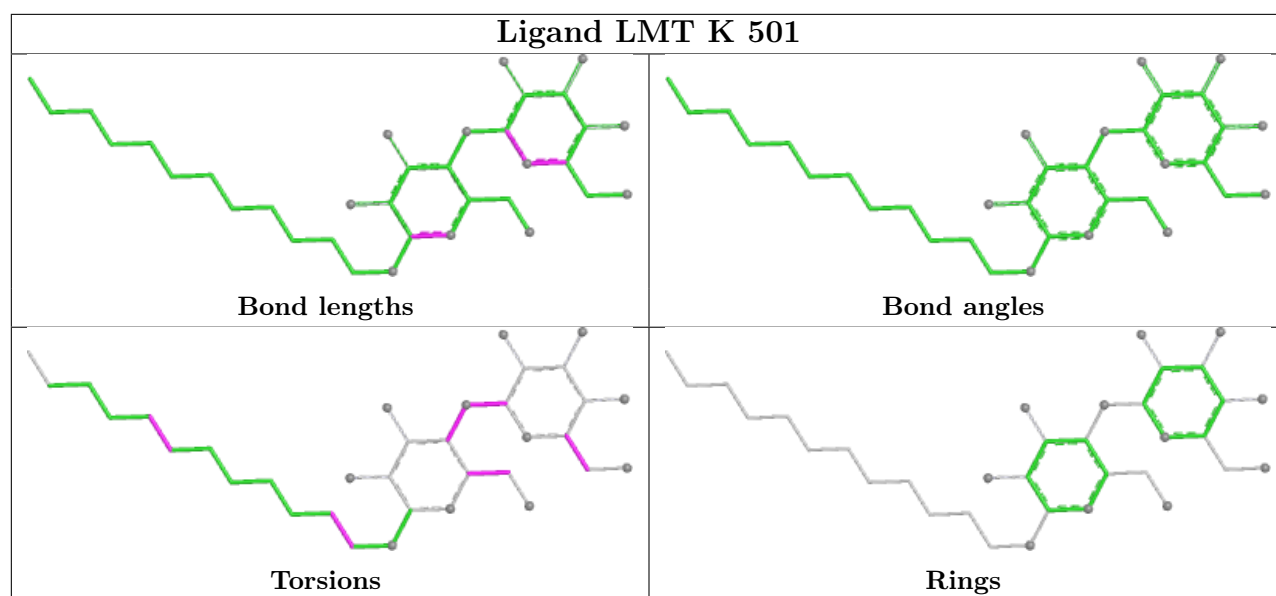


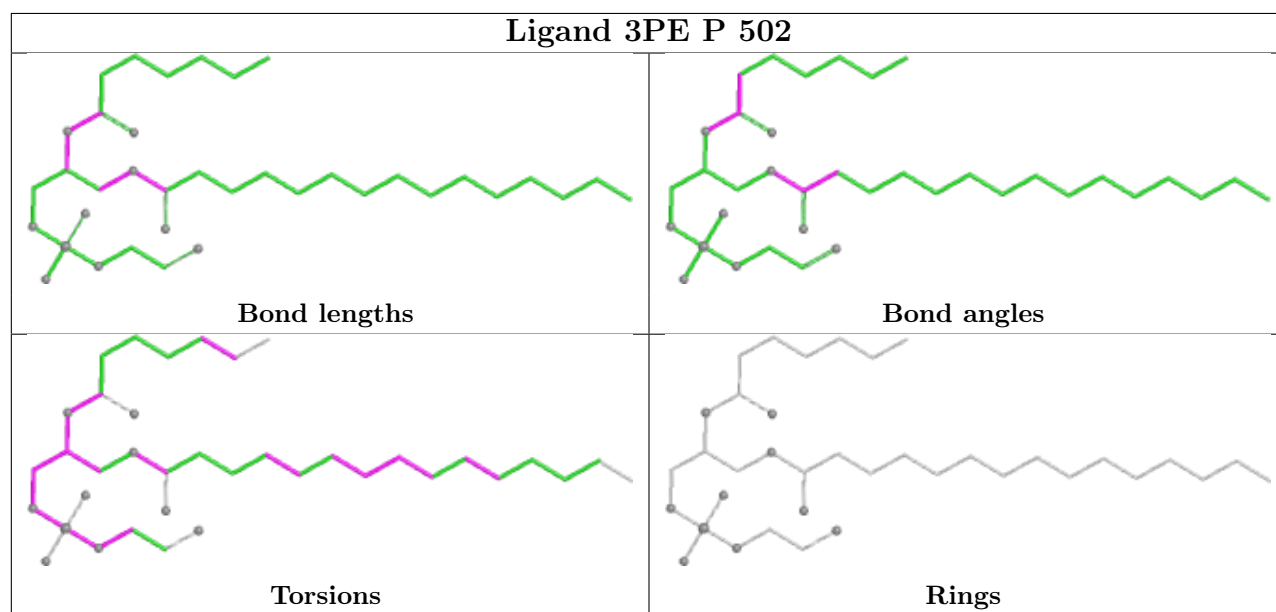
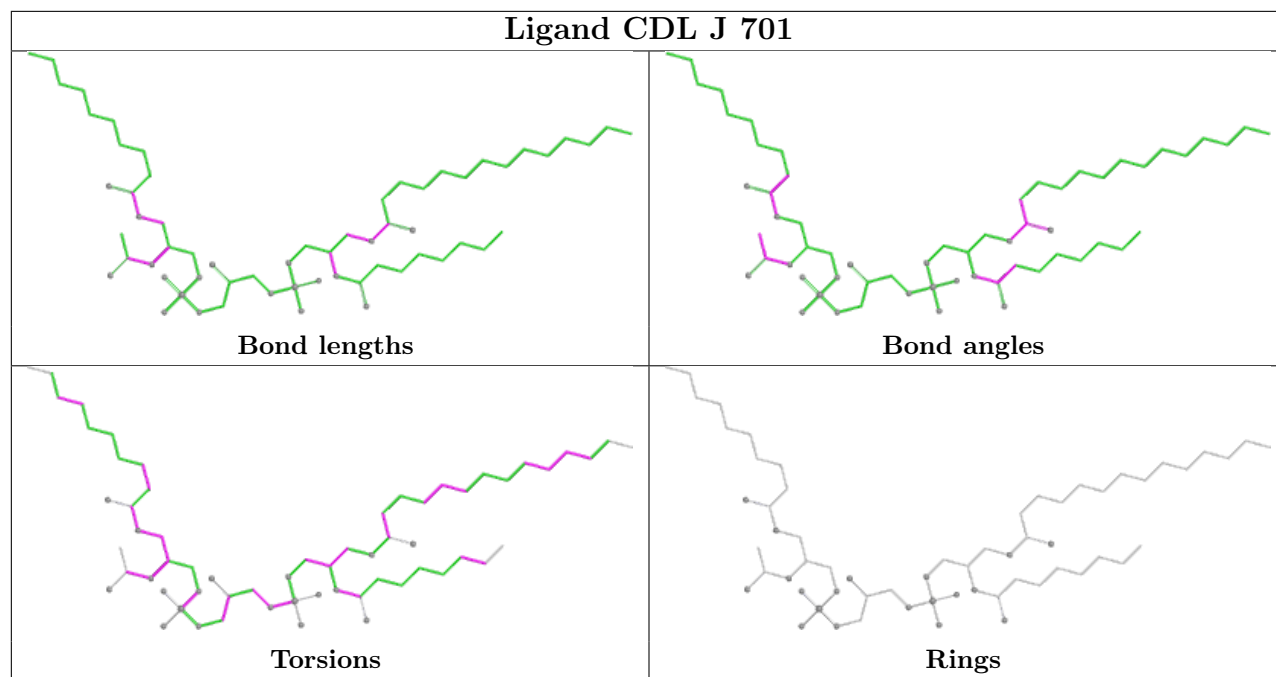


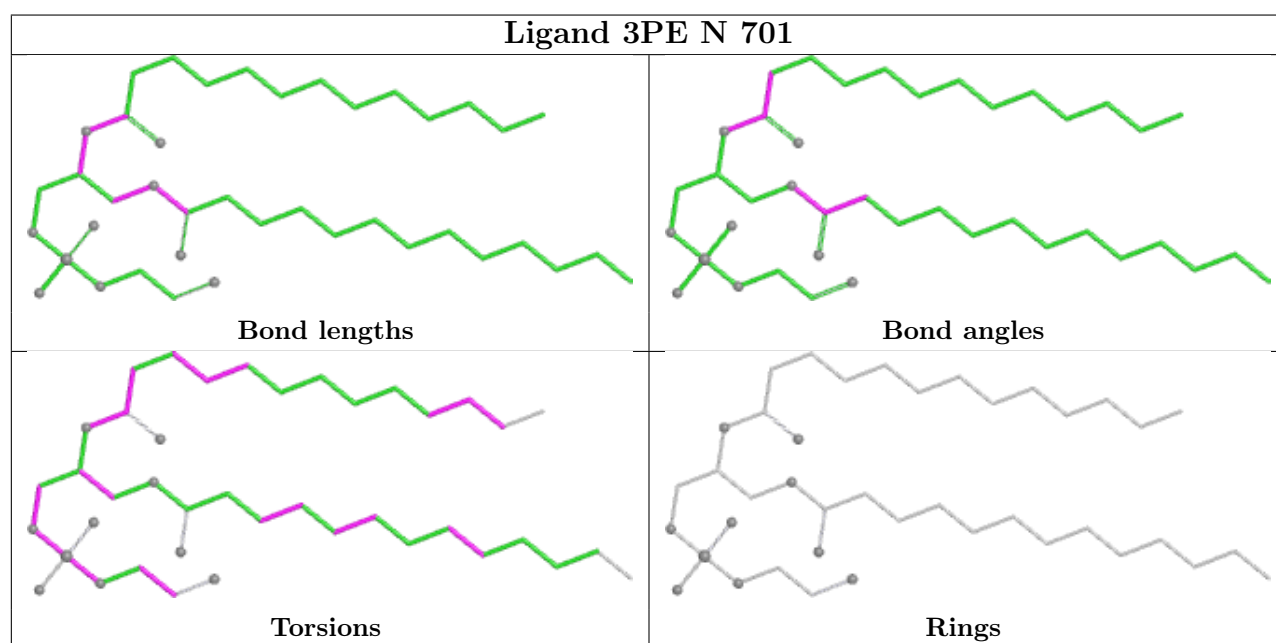
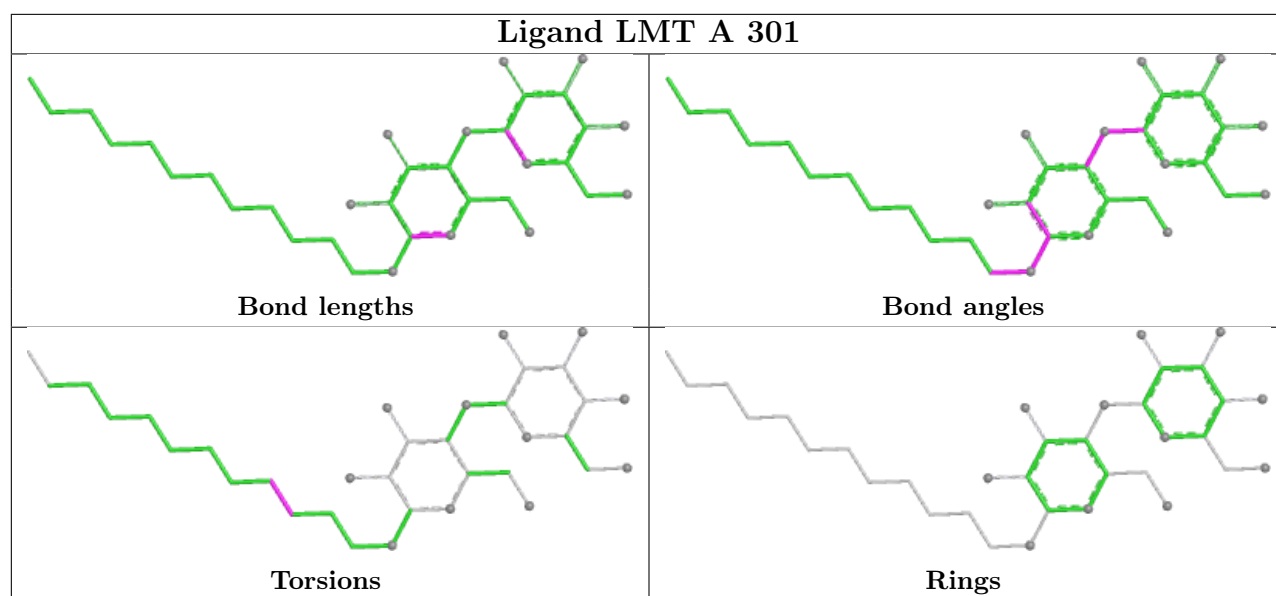


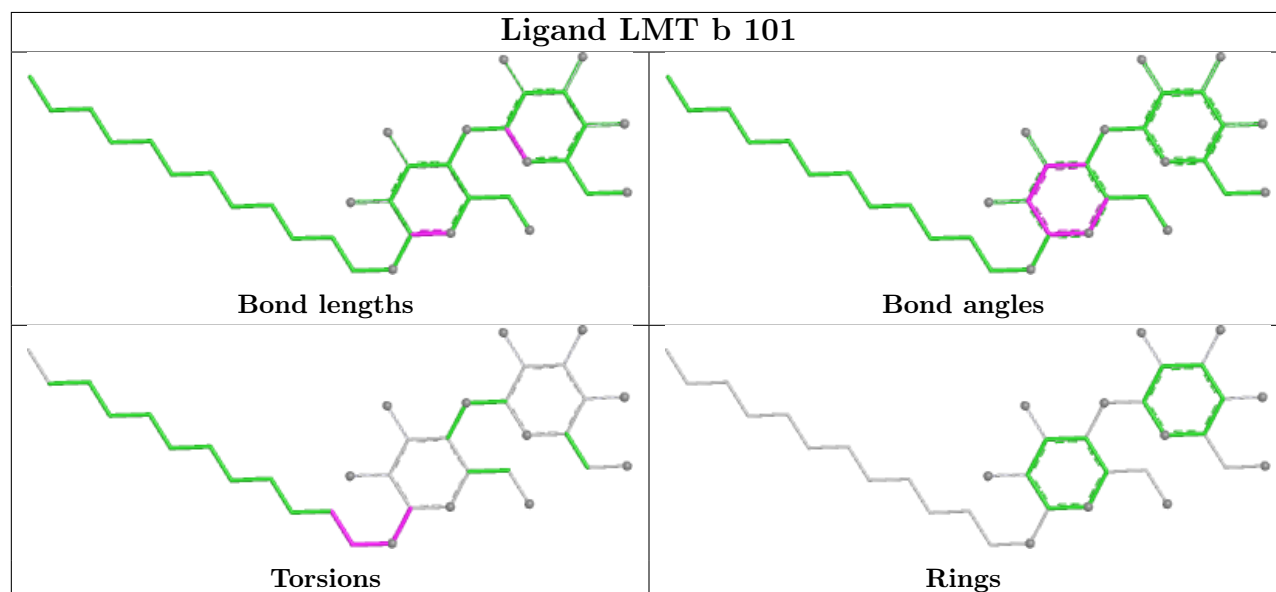
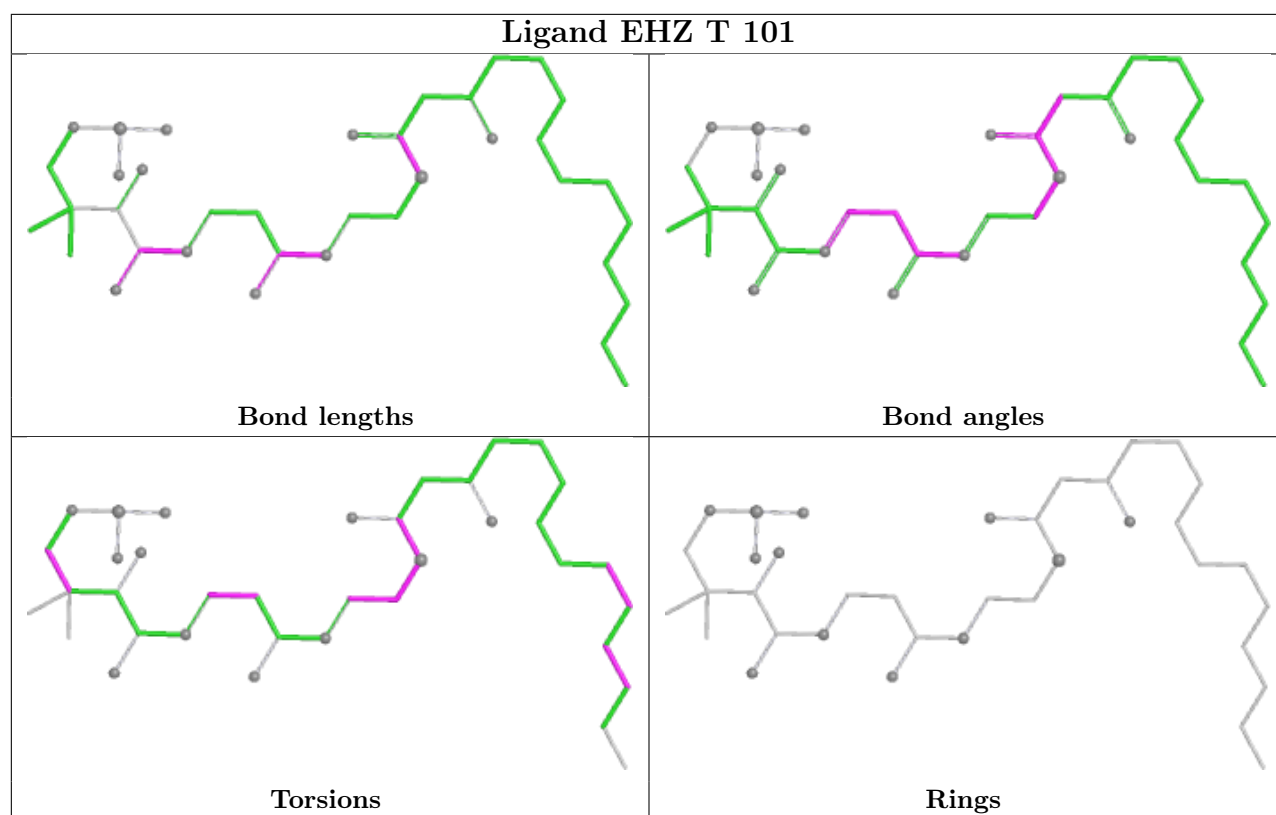


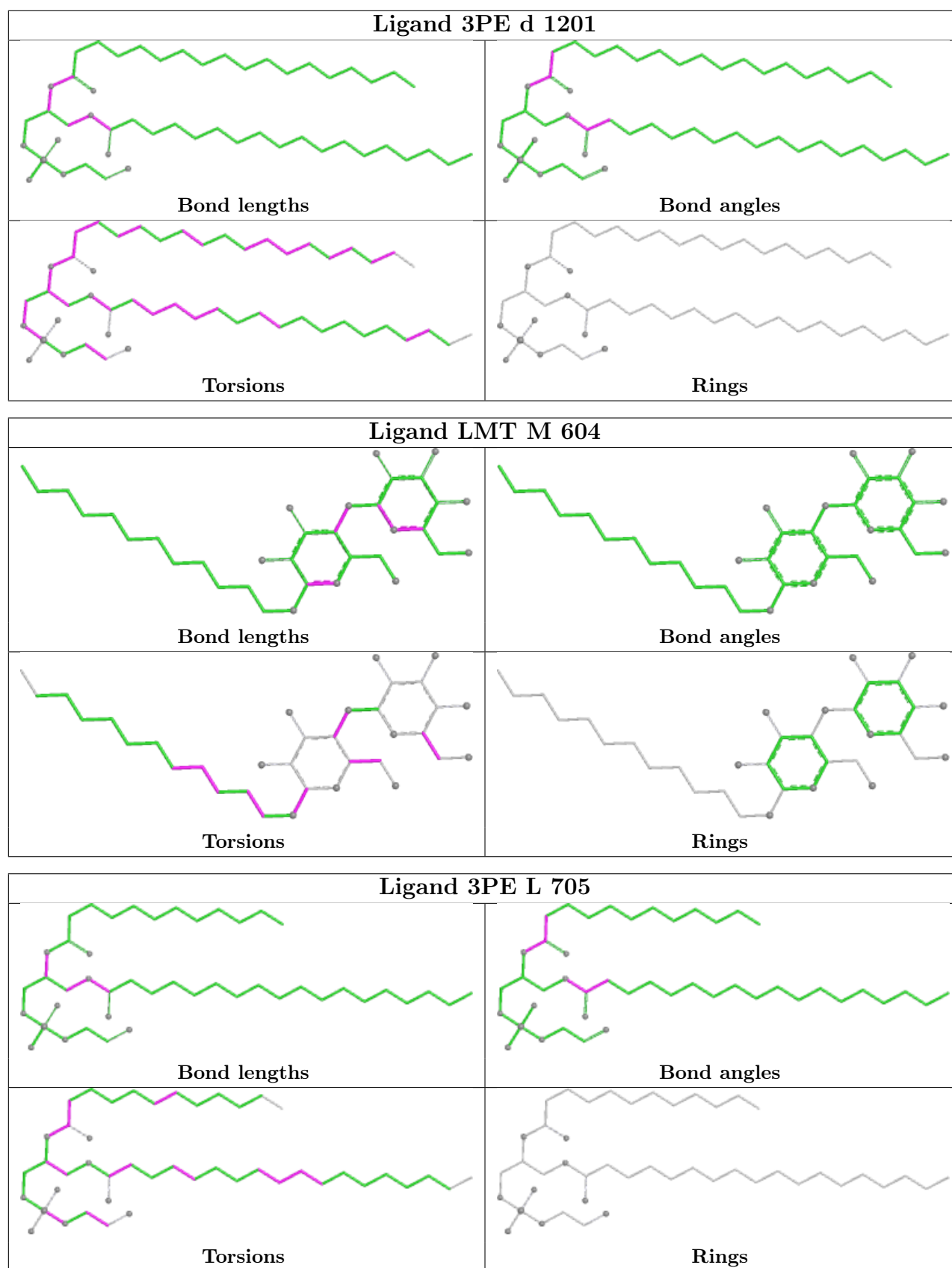


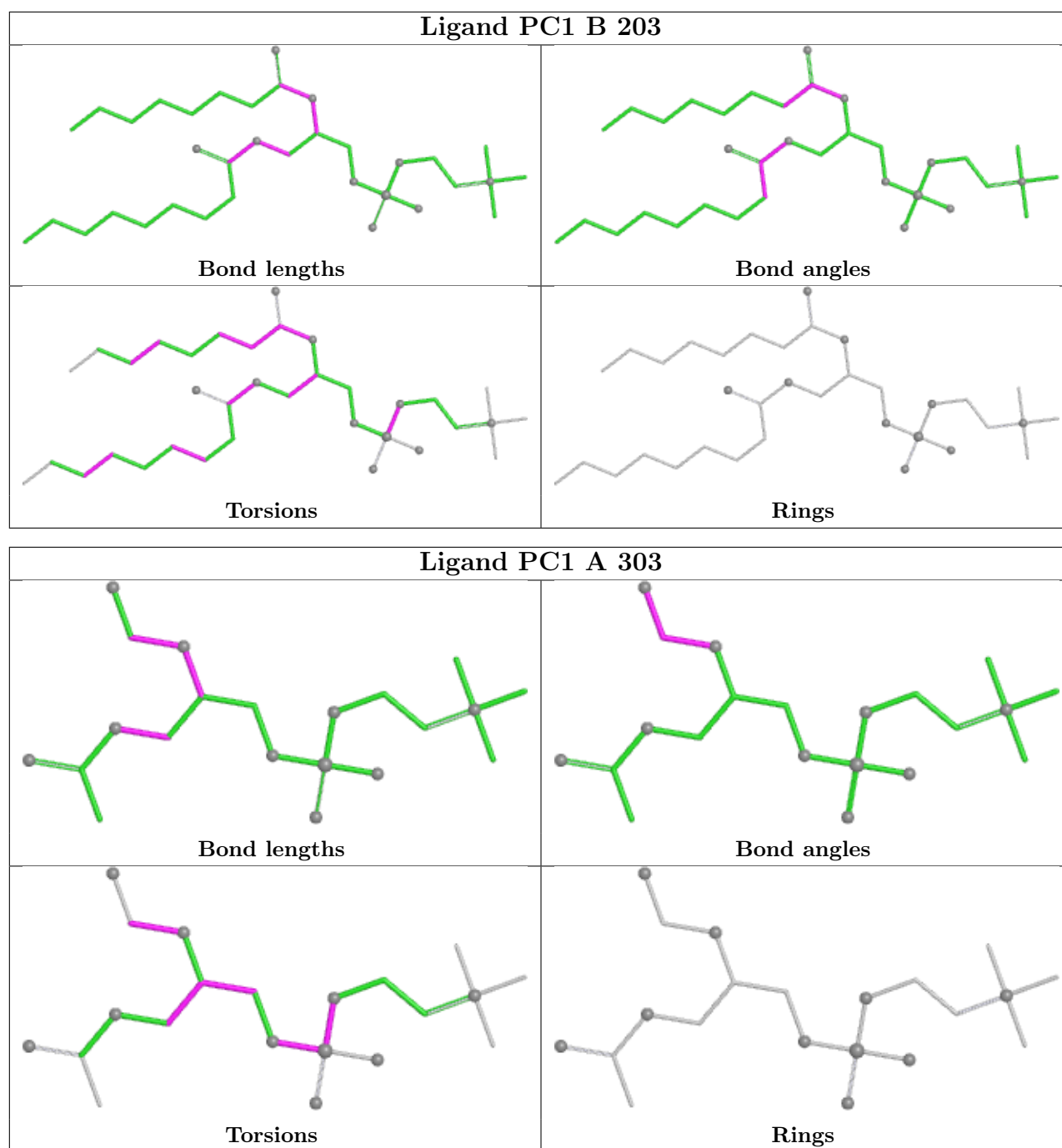


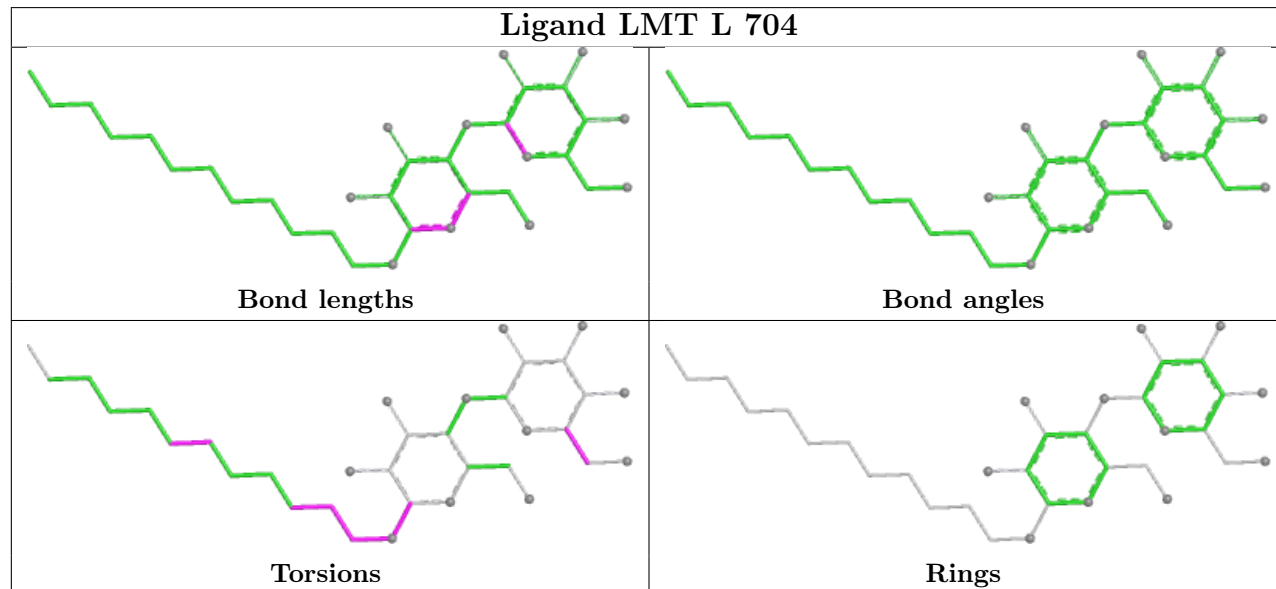
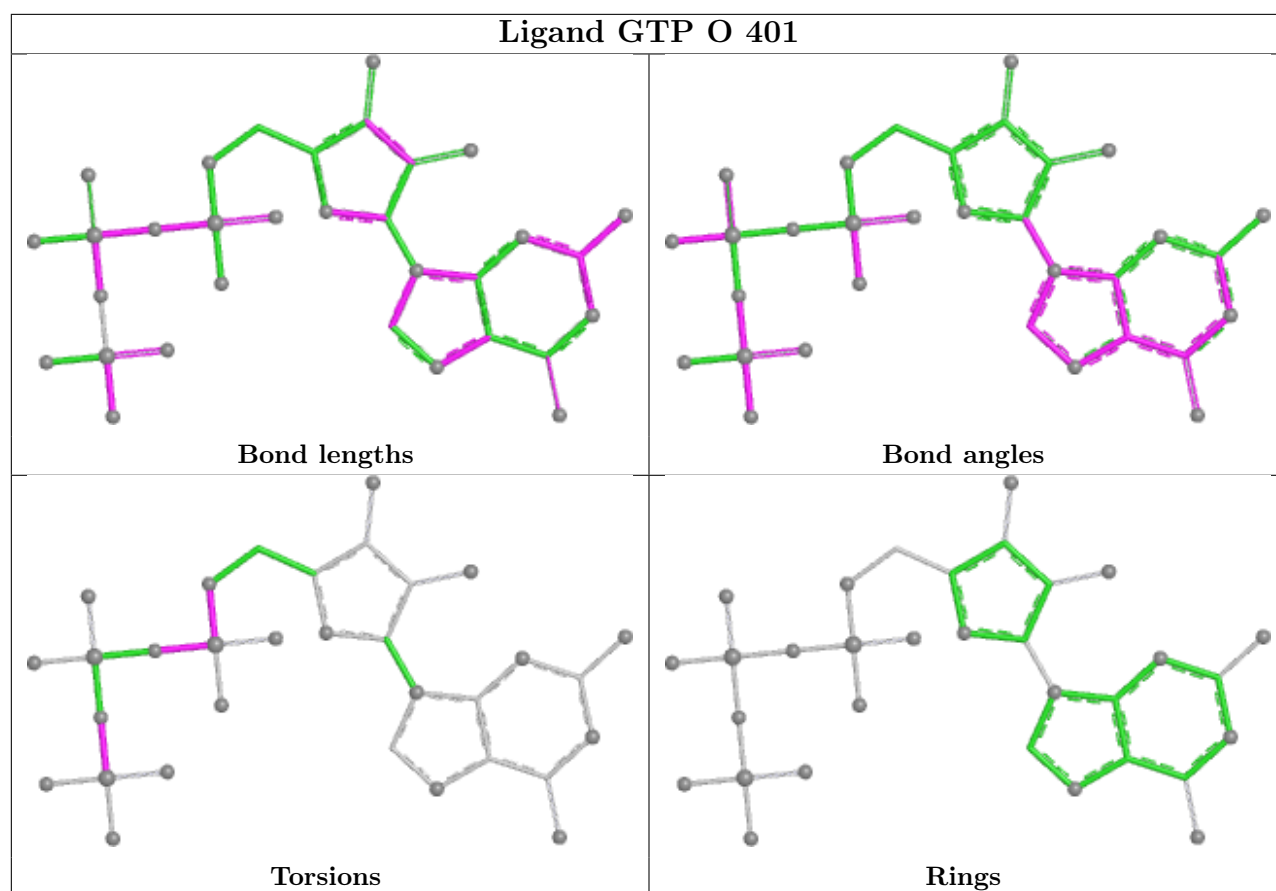


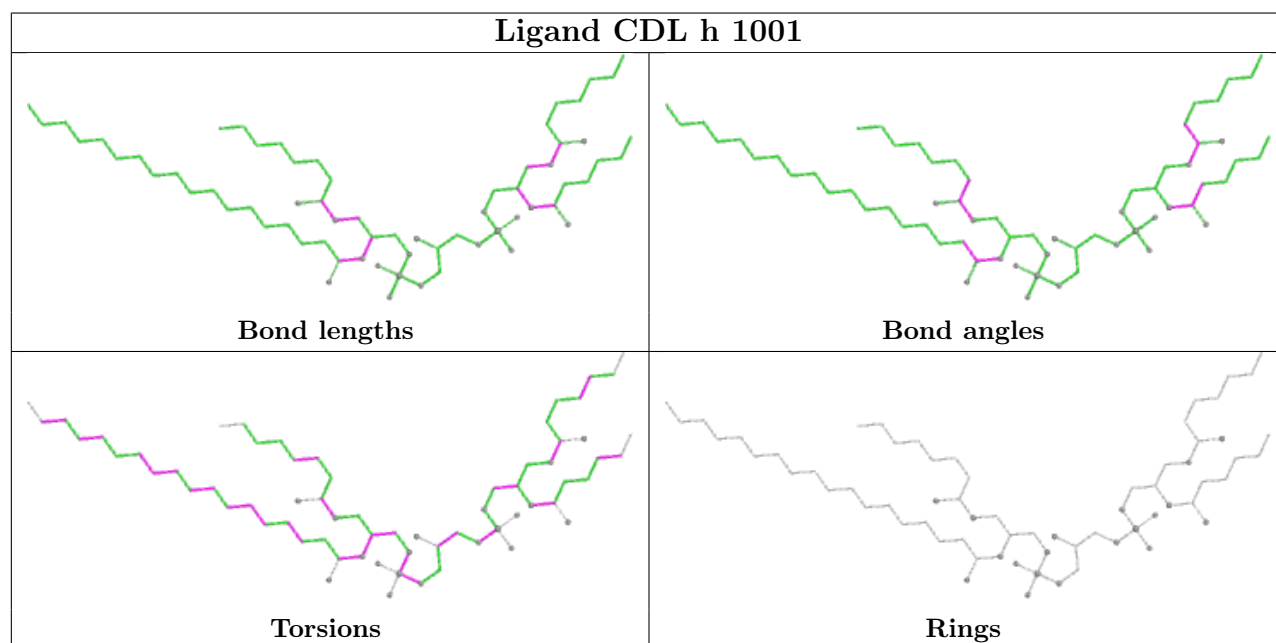
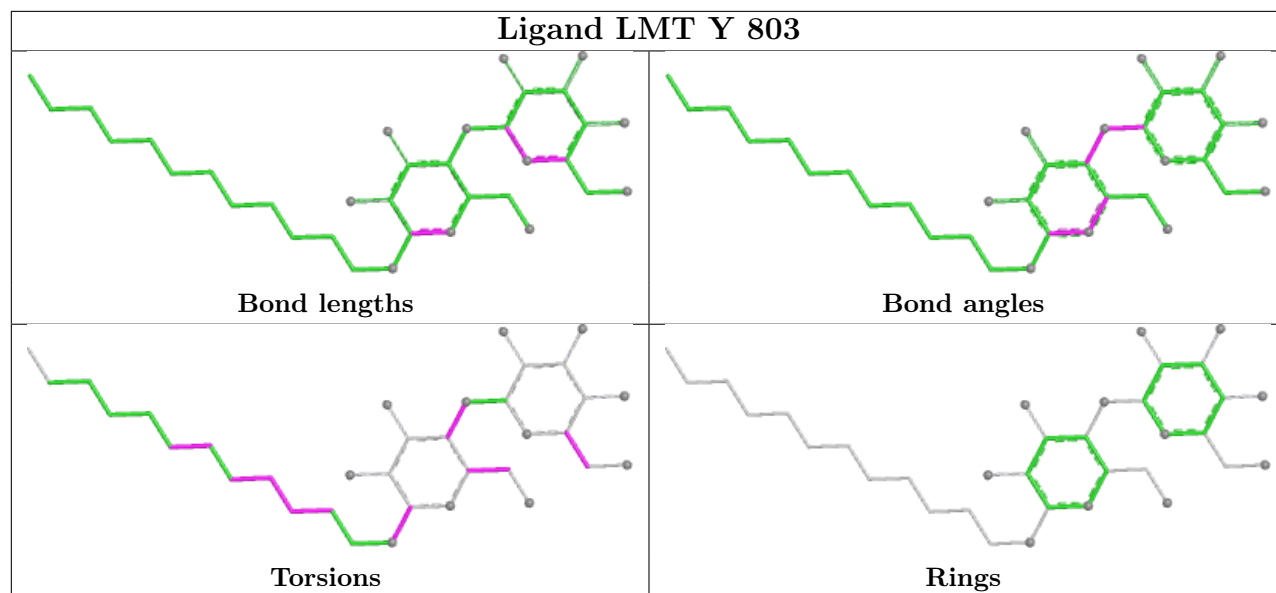


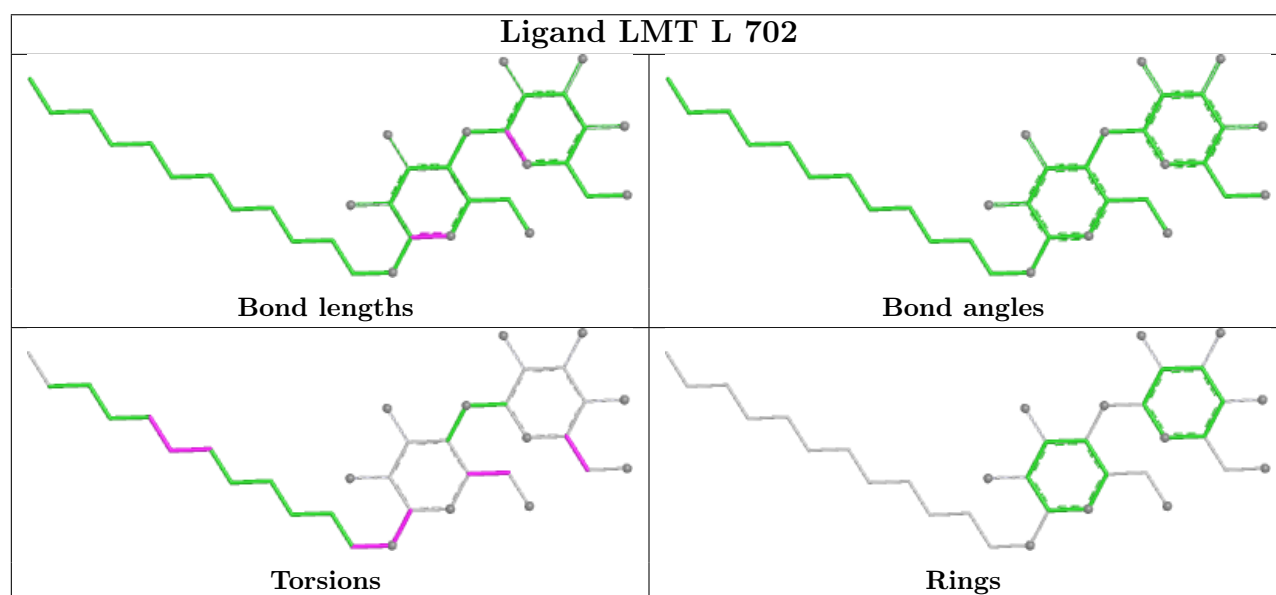
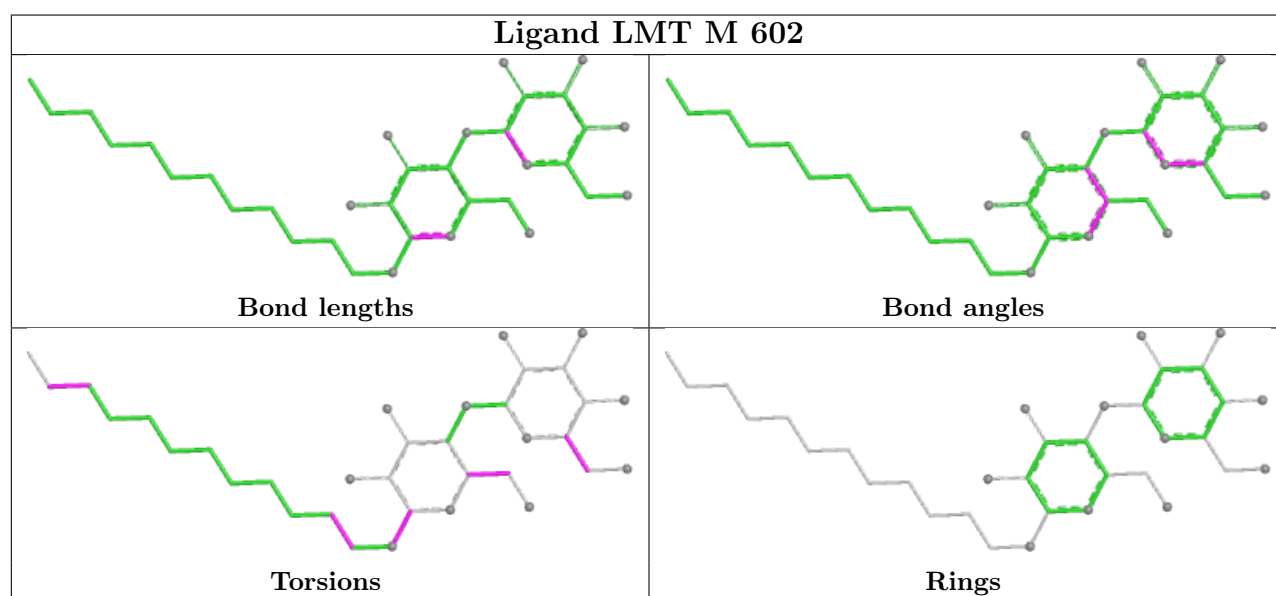
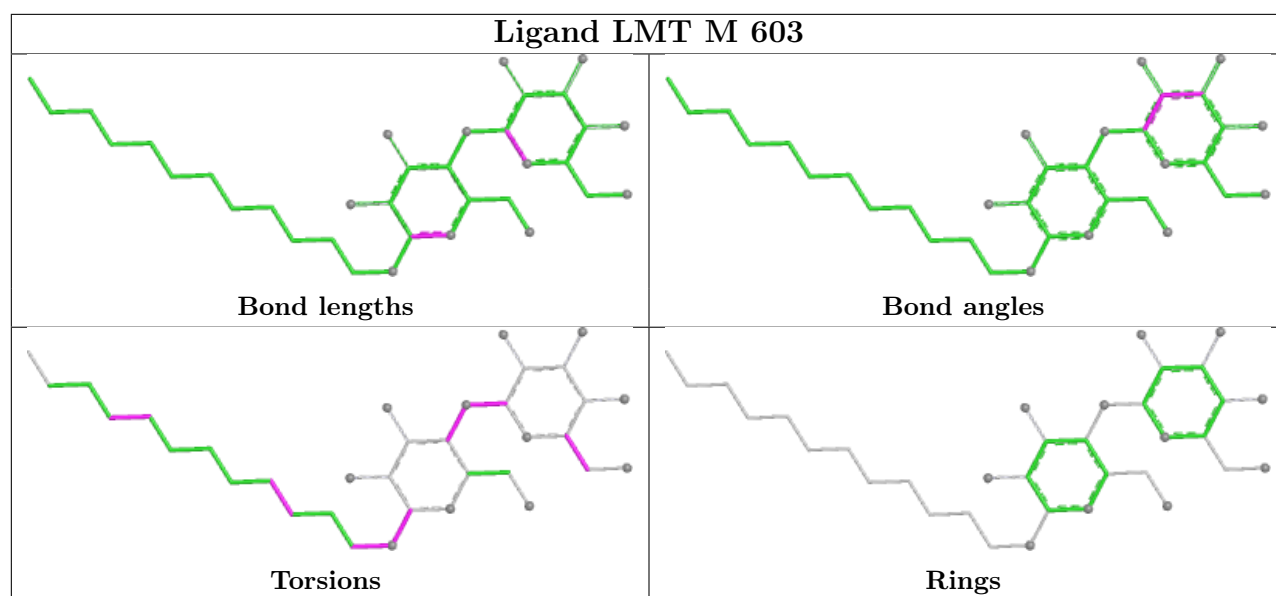


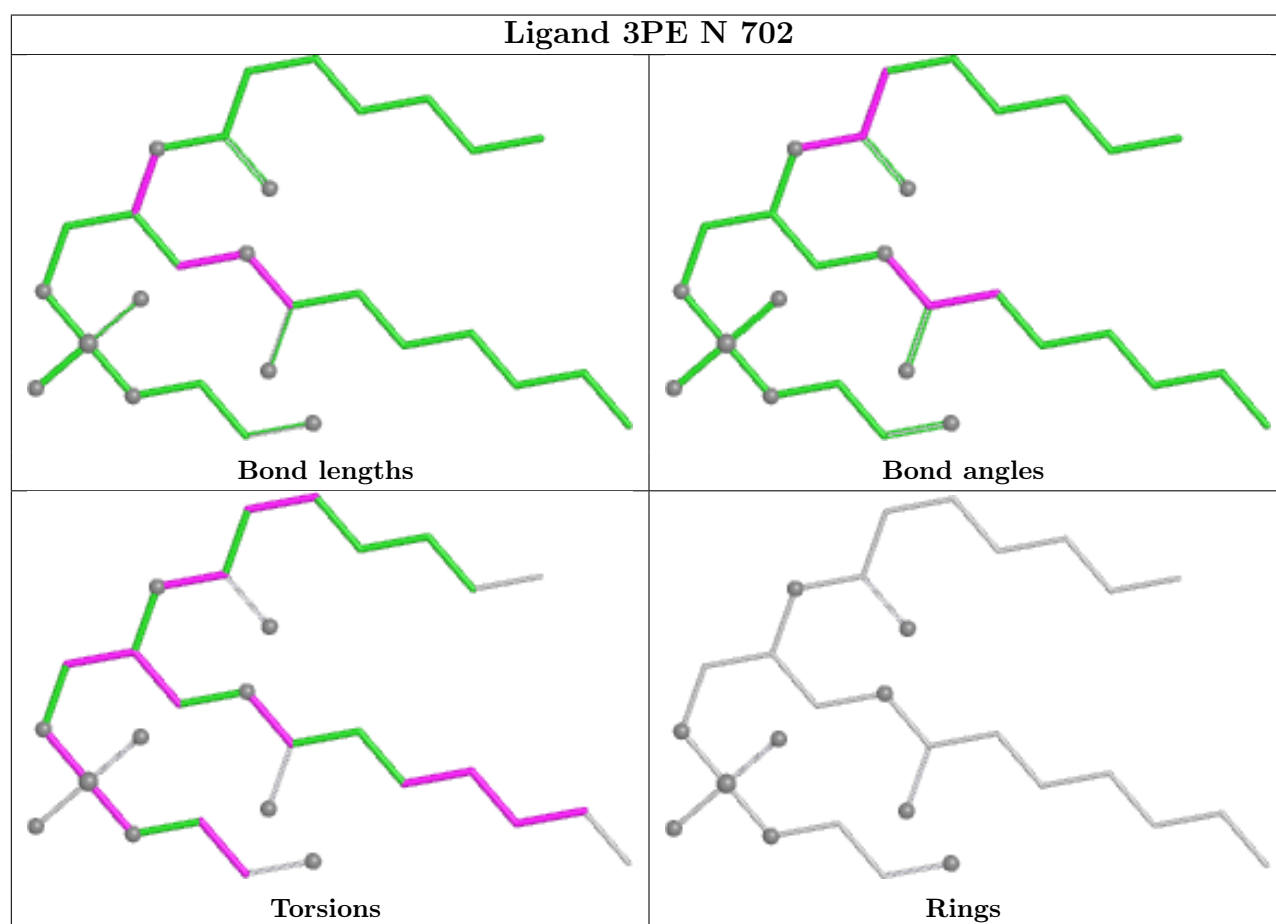
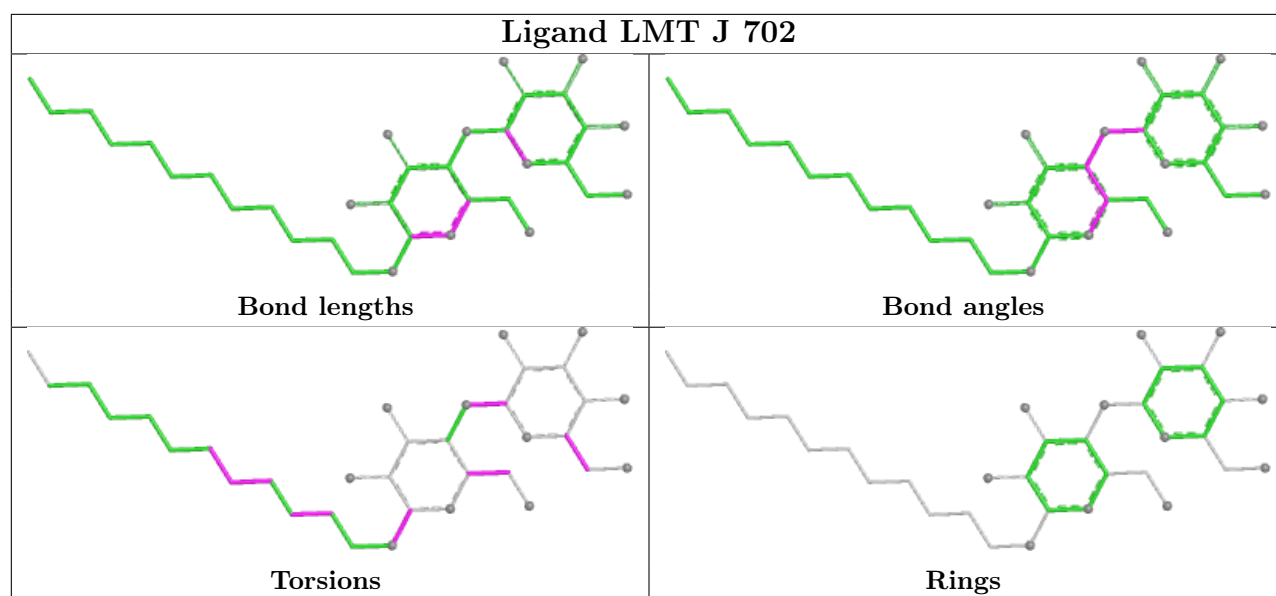


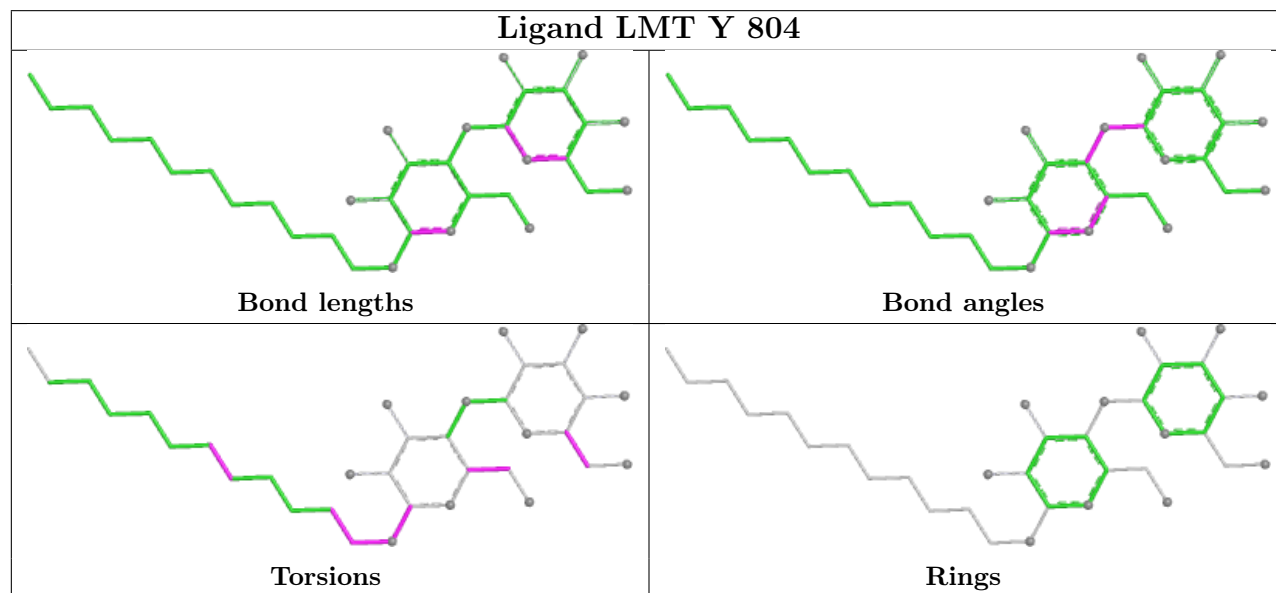
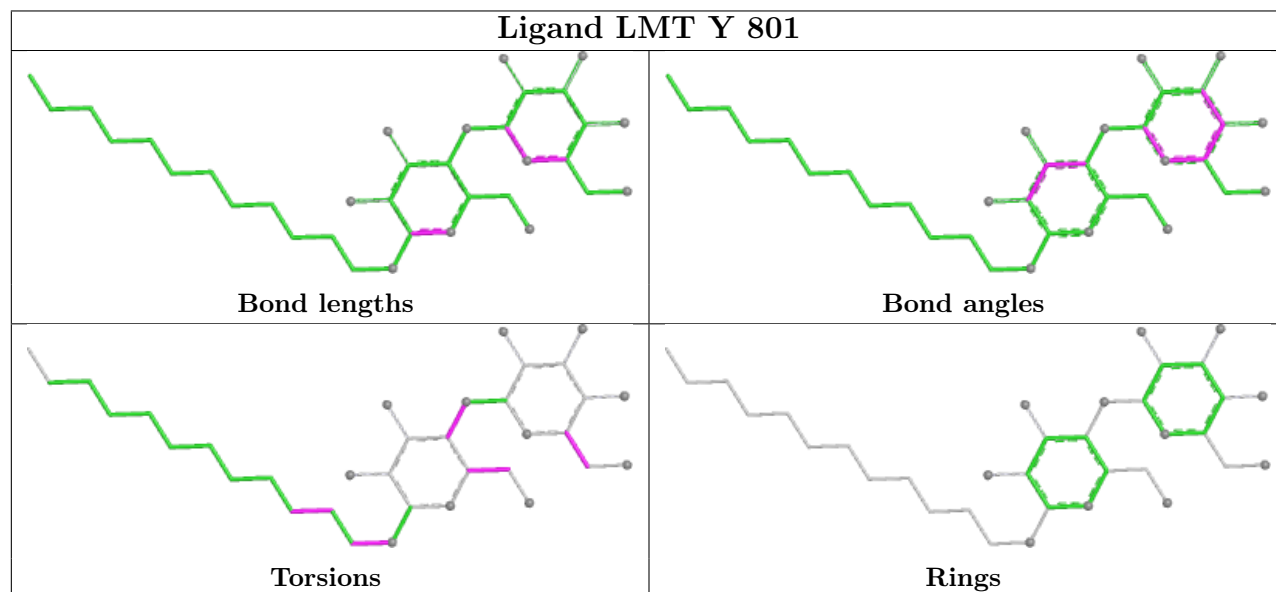
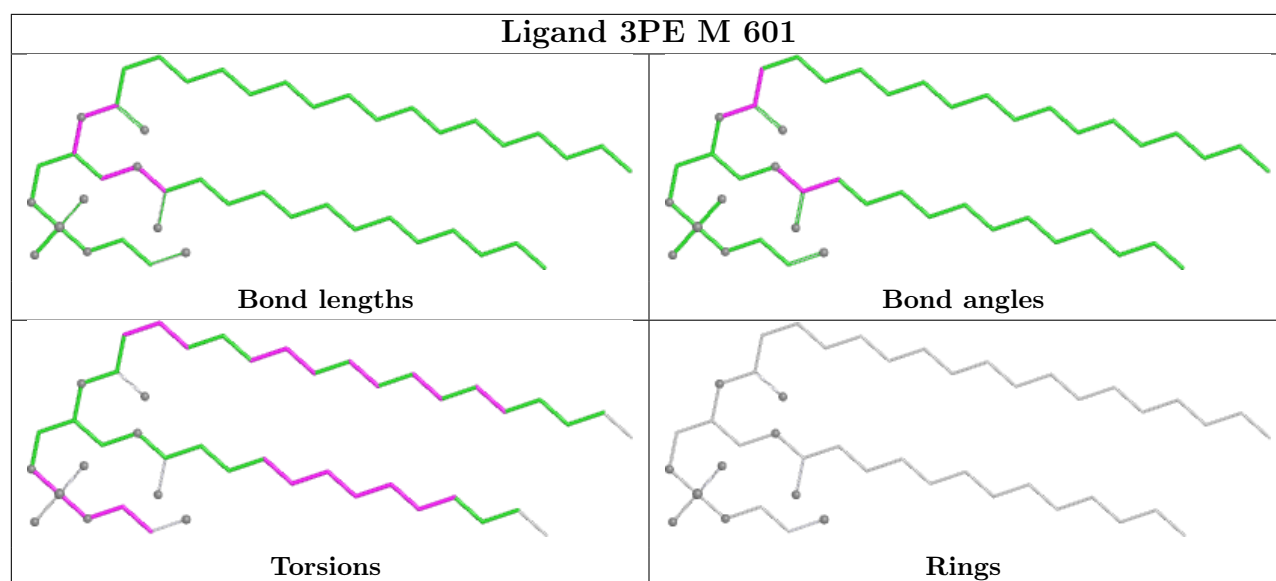


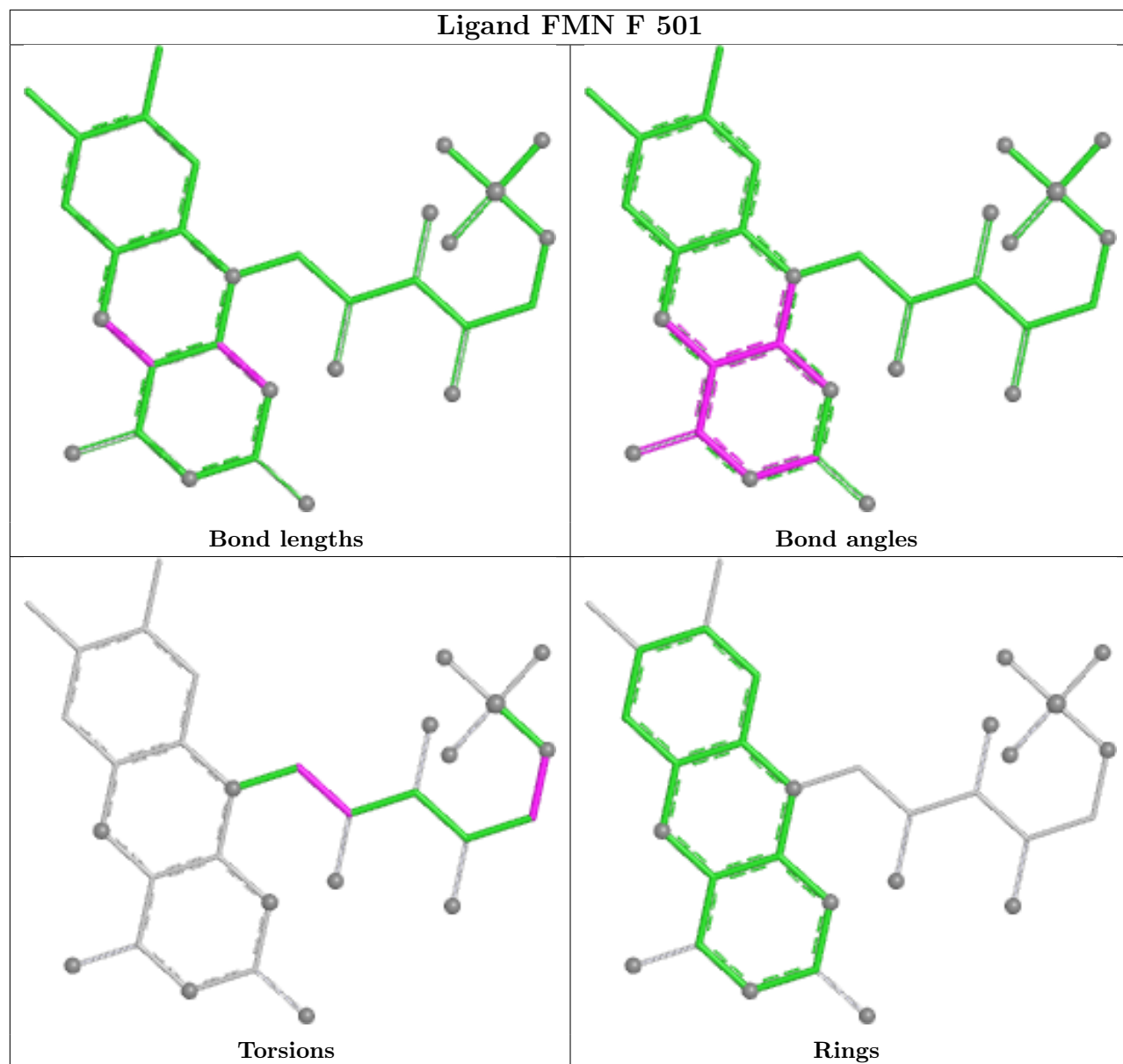


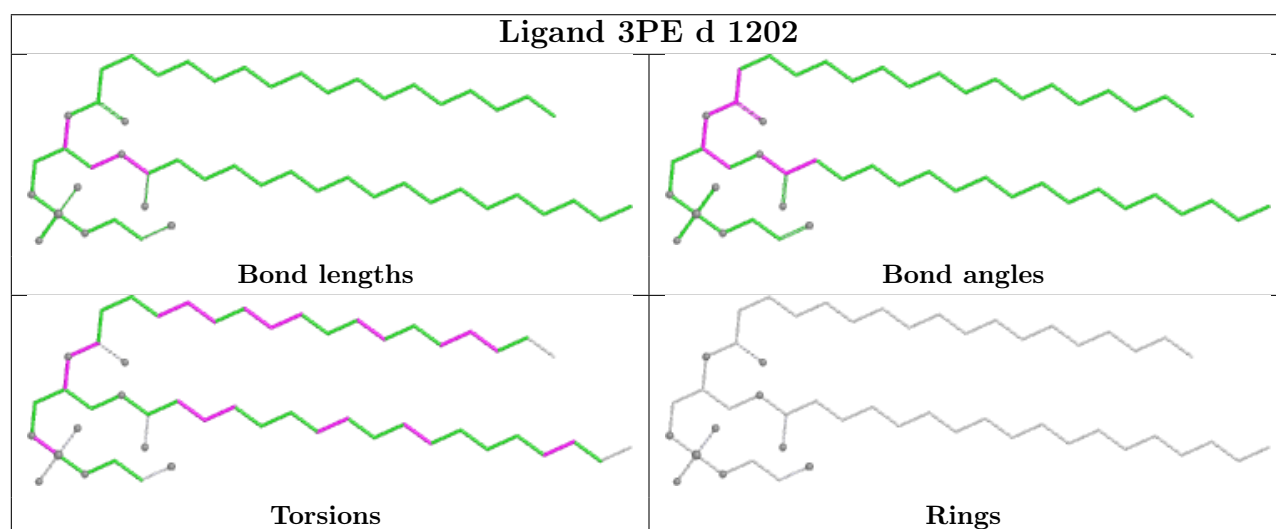
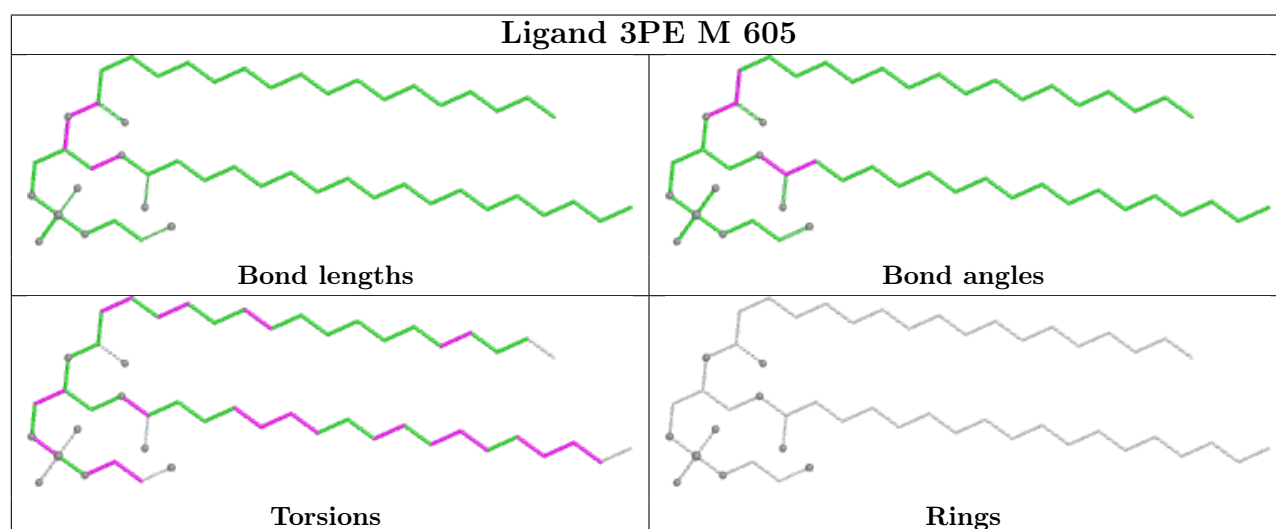
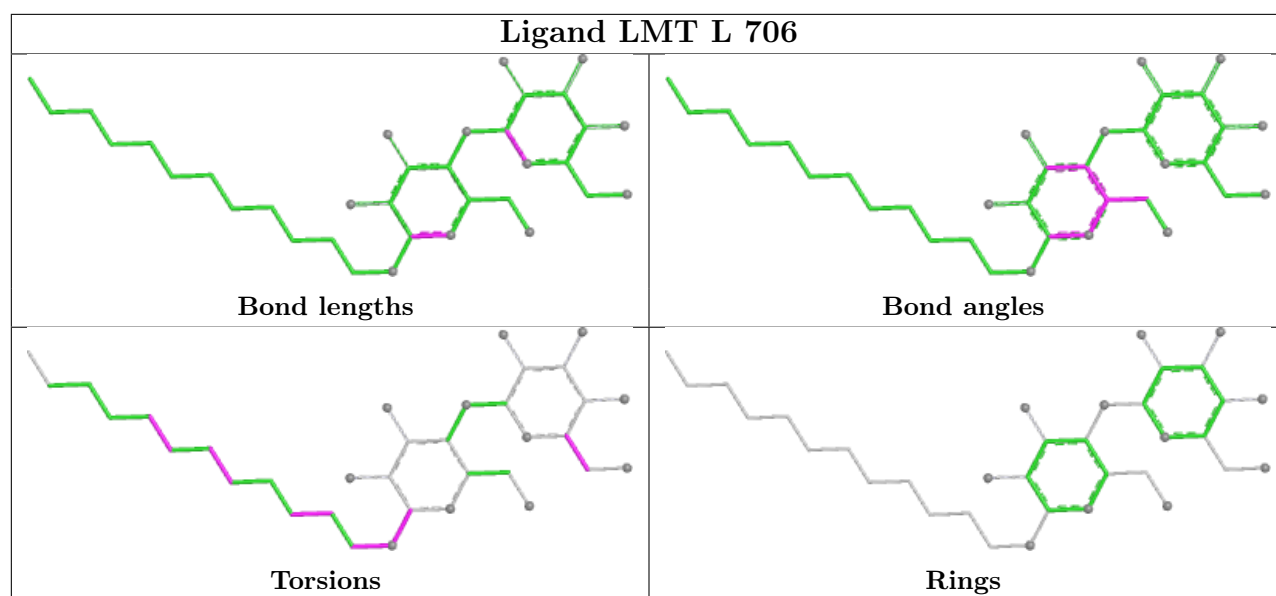












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

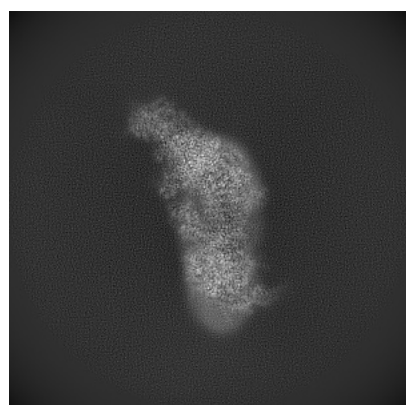
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14256. These allow visual inspection of the internal detail of the map and identification of artifacts.

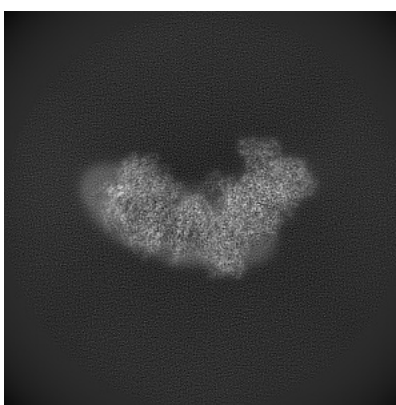
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

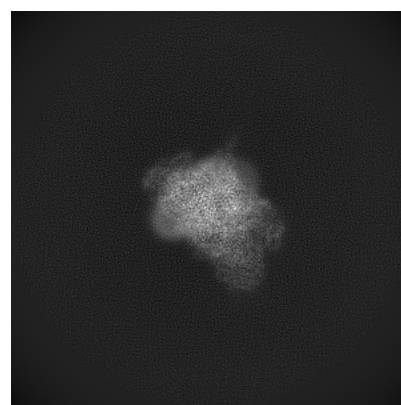
6.1.1 Primary map



X



Y

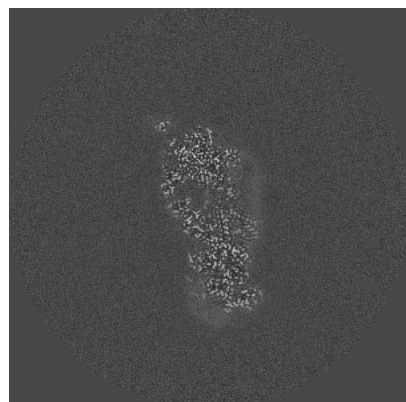


Z

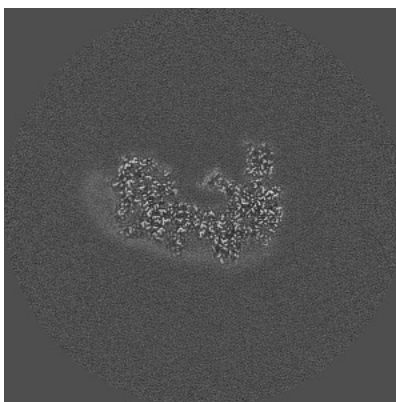
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

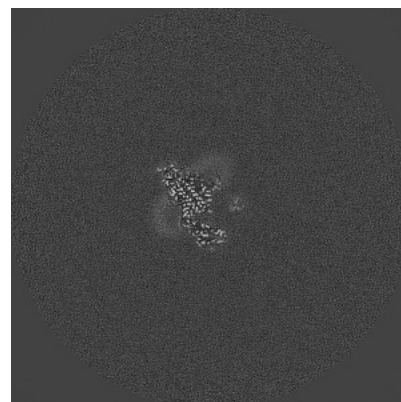
6.2.1 Primary map



X Index: 330



Y Index: 330

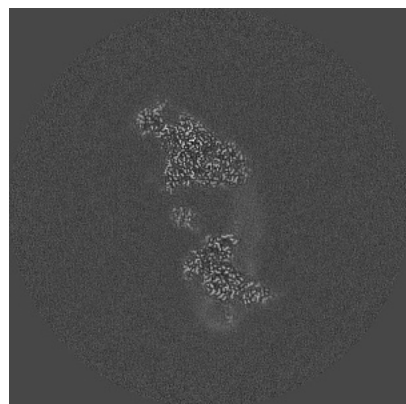


Z Index: 330

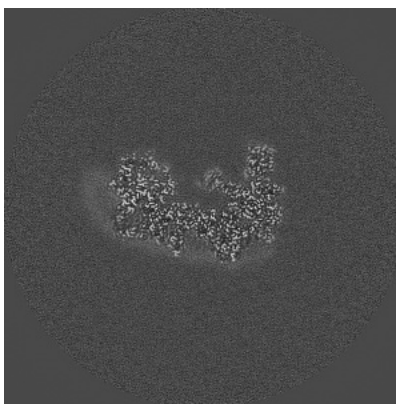
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

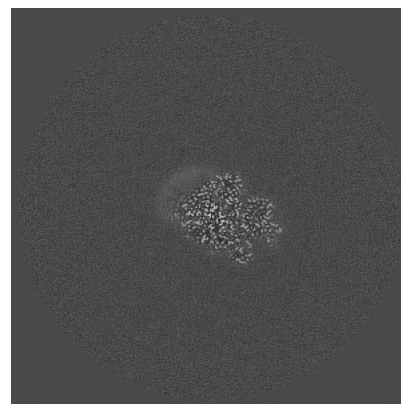
6.3.1 Primary map



X Index: 353



Y Index: 333

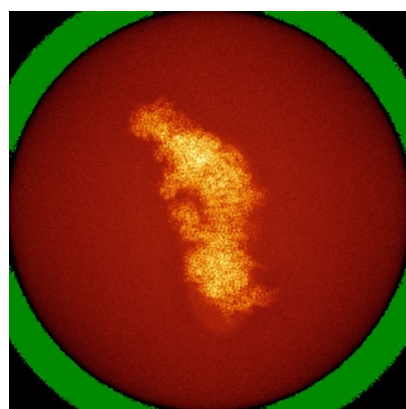


Z Index: 421

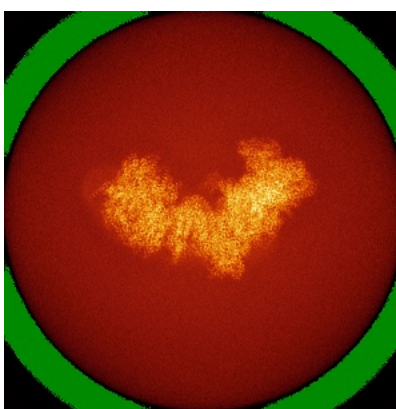
The images above show the largest variance slices of the map in three orthogonal directions.

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

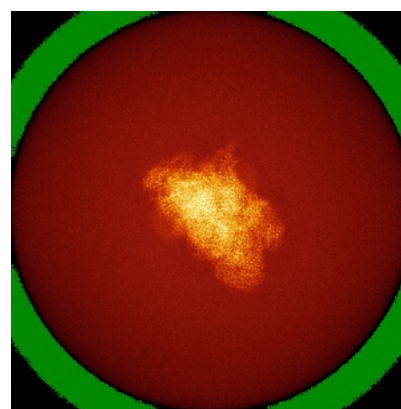
6.4.1 Primary map



X



Y

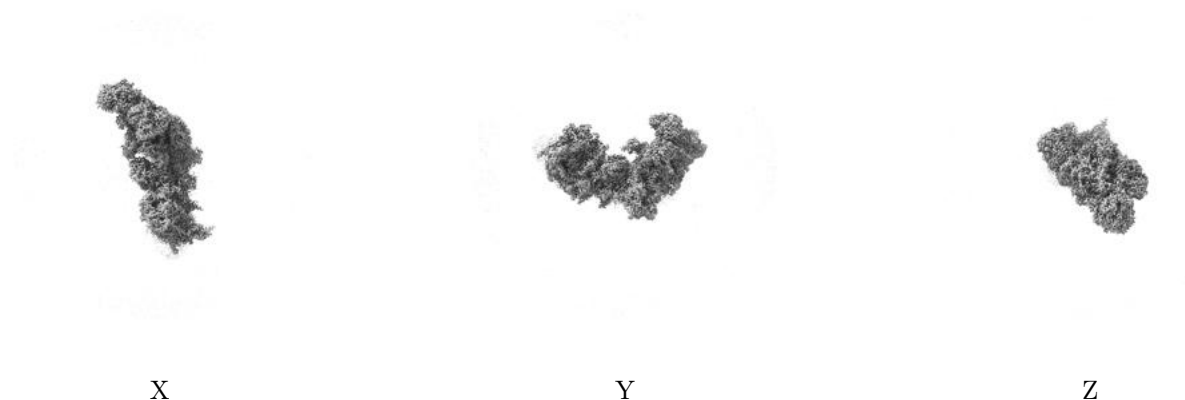


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

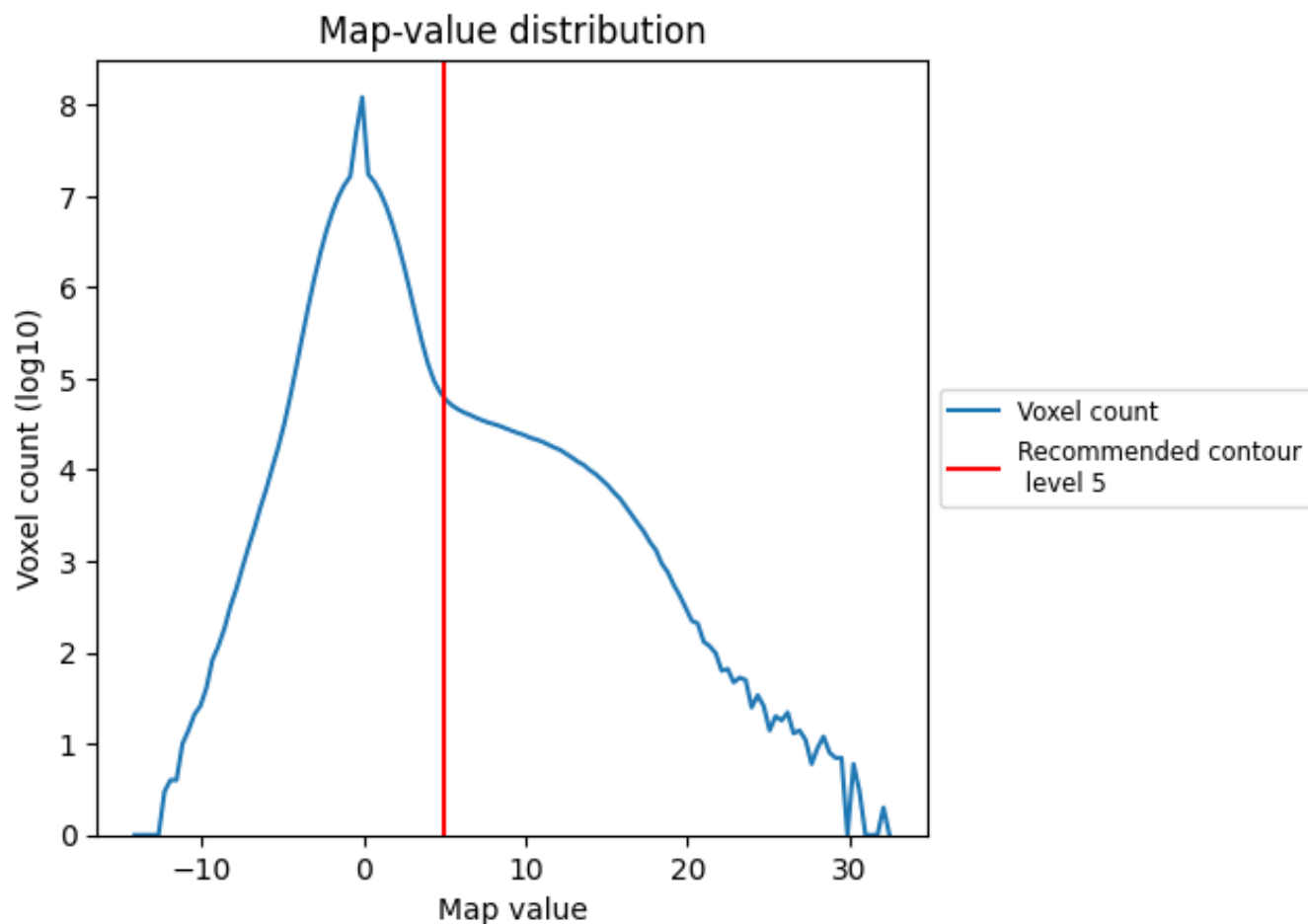
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

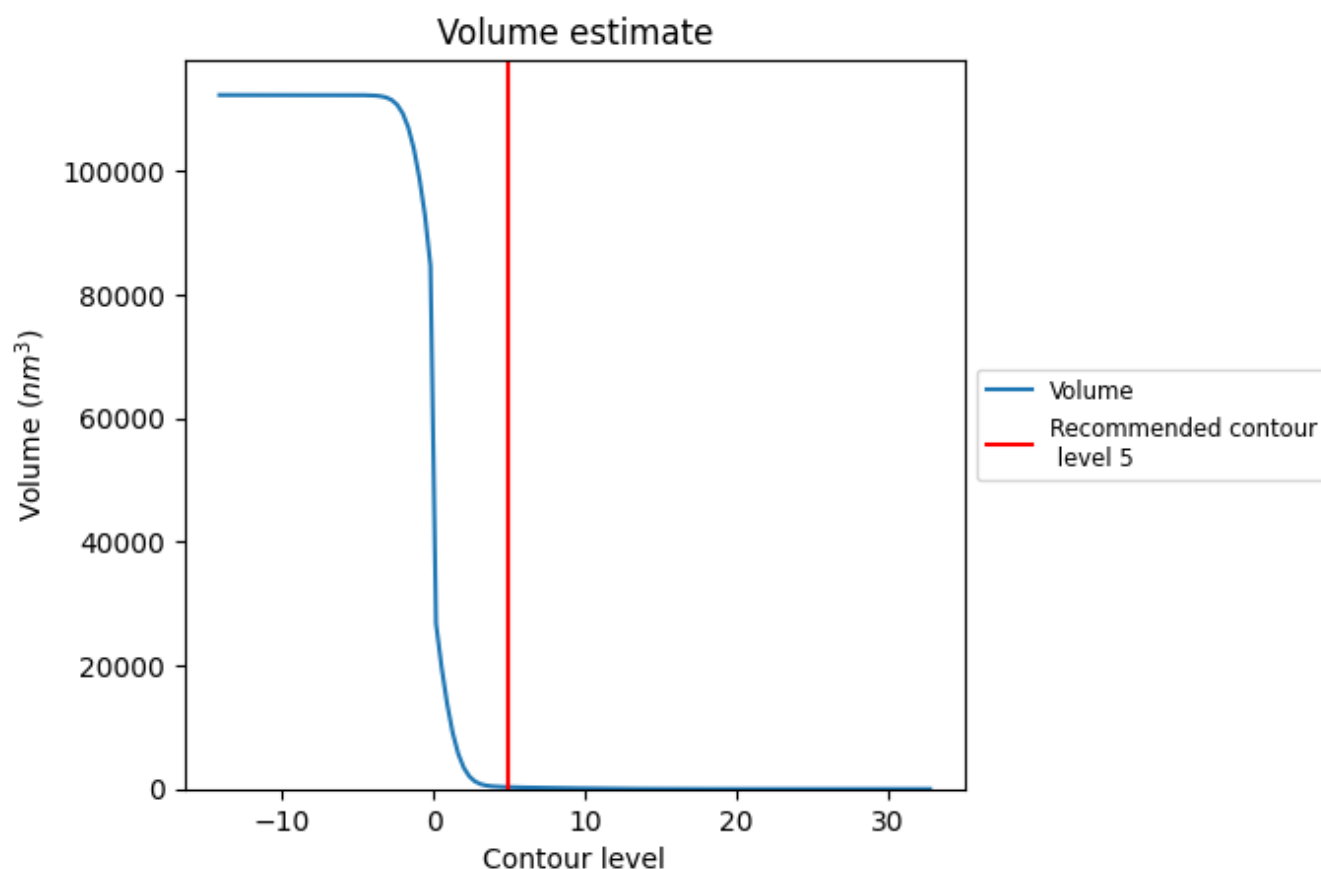
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

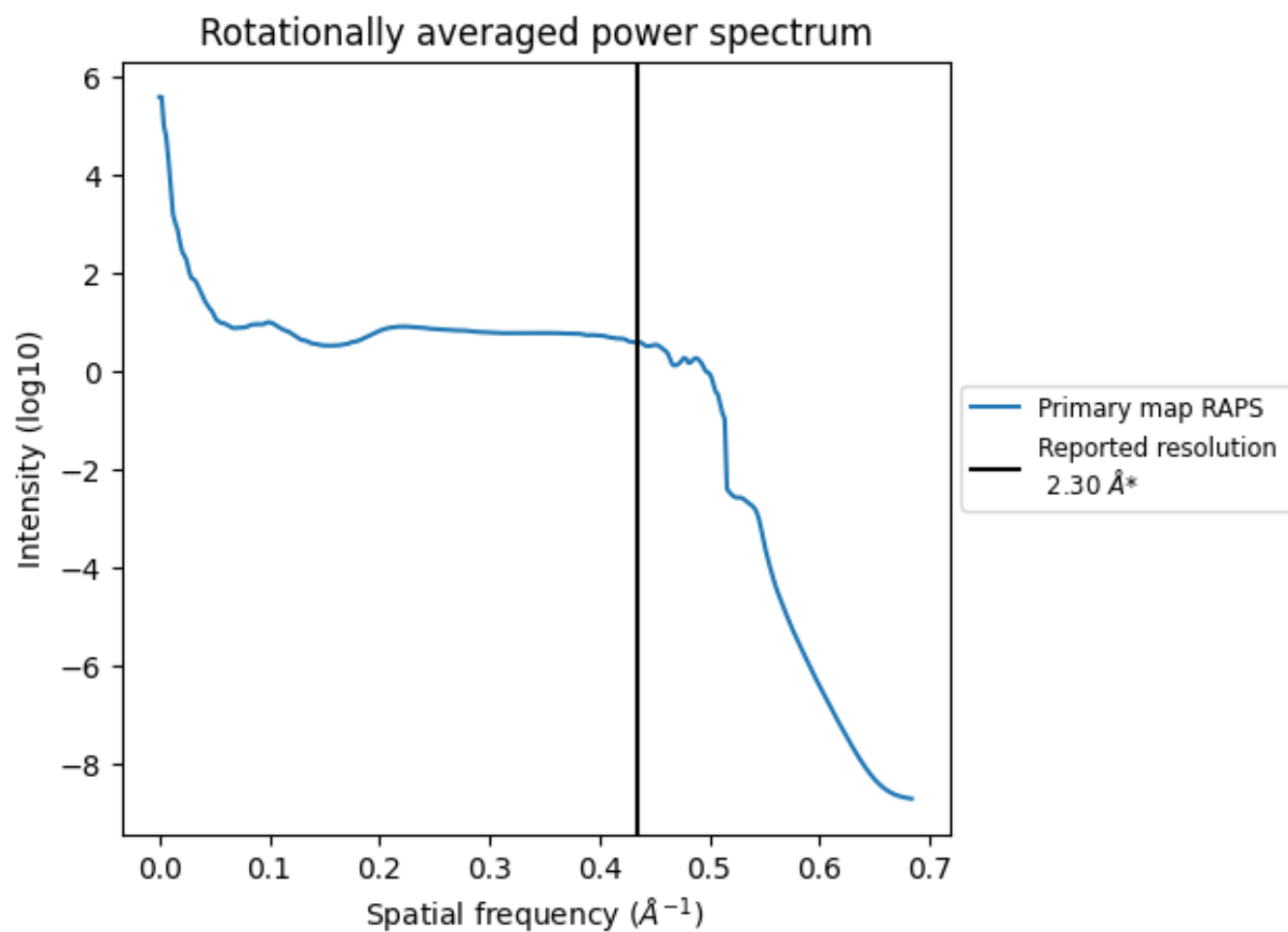
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 269 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

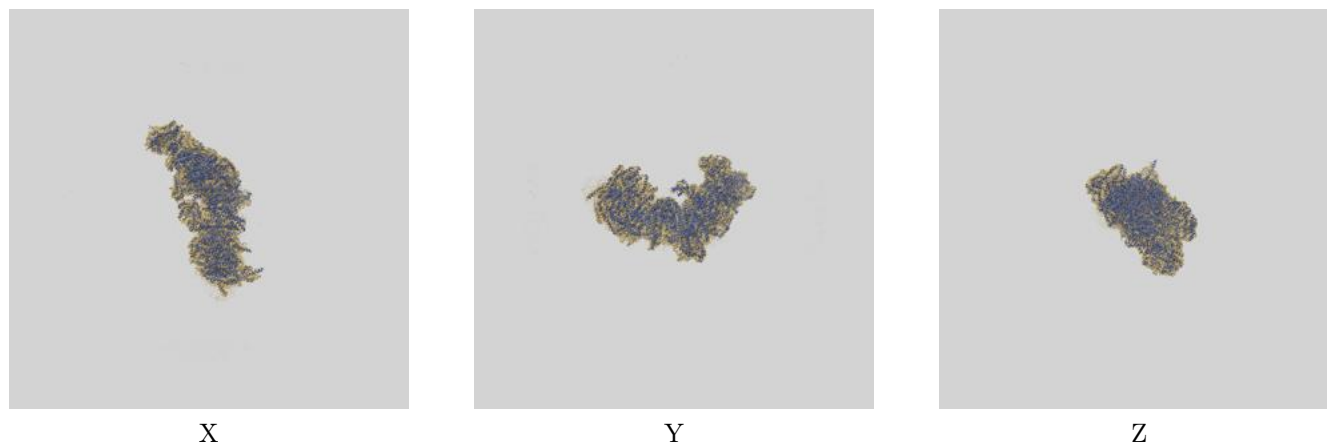
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

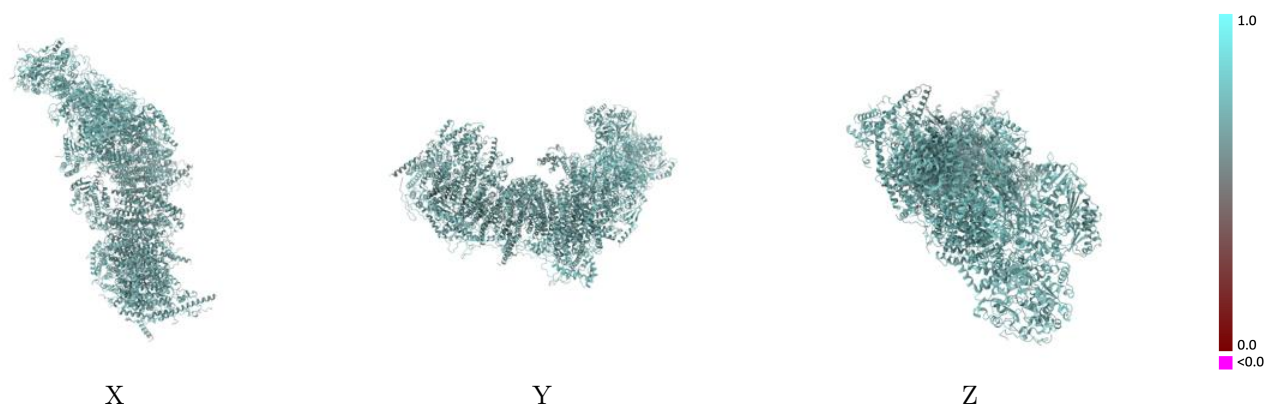
This section contains information regarding the fit between EMDB map EMD-14256 and PDB model 7R42. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



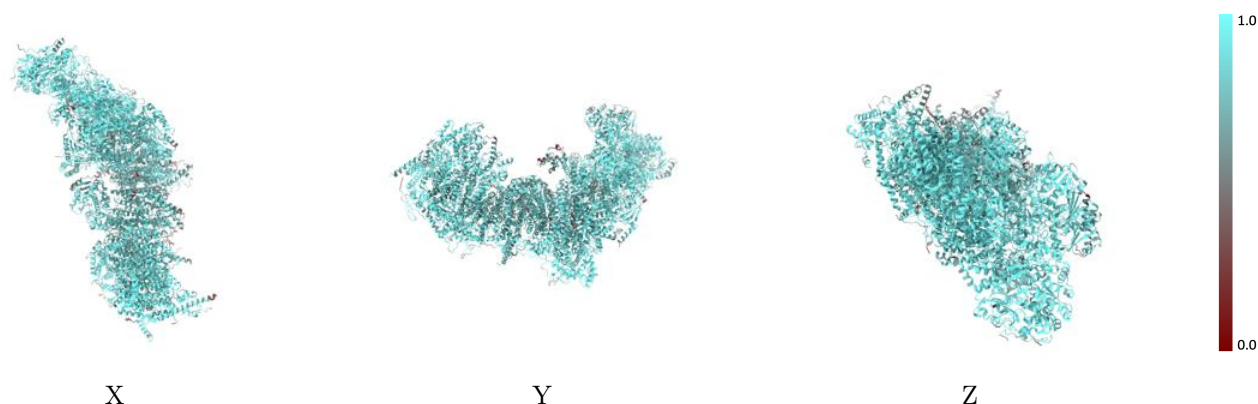
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



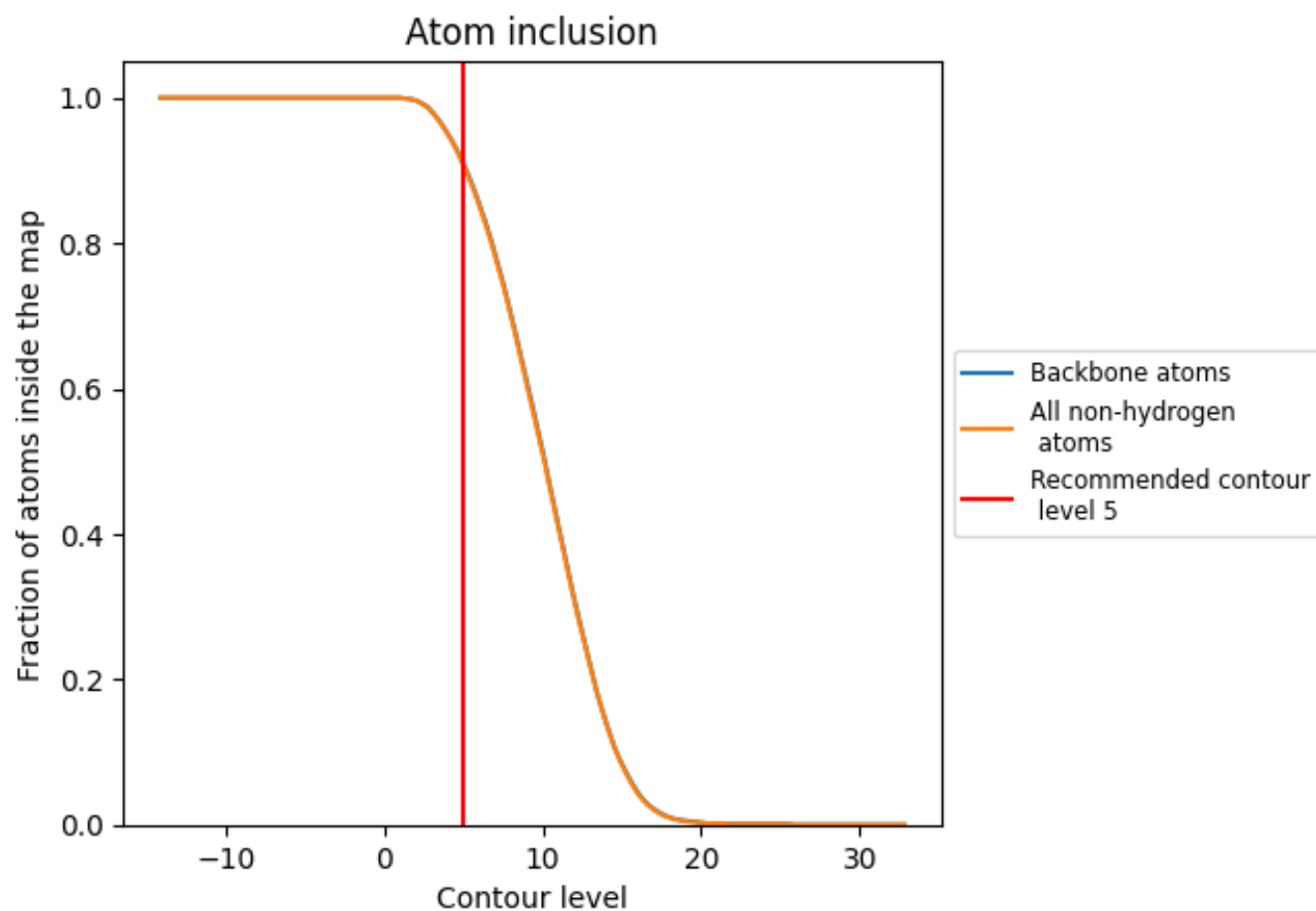
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.6970
A	 0.9030	 0.7040
B	 0.9640	 0.7340
C	 0.9610	 0.7350
D	 0.9550	 0.7320
E	 0.8870	 0.6830
F	 0.9340	 0.7000
G	 0.9170	 0.7090
H	 0.9710	 0.7220
I	 0.9740	 0.7400
J	 0.8920	 0.6930
K	 0.9050	 0.7070
L	 0.9380	 0.6860
M	 0.9570	 0.7060
N	 0.9700	 0.7160
O	 0.8990	 0.6840
P	 0.8950	 0.7030
Q	 0.9220	 0.7200
R	 0.9170	 0.7140
S	 0.8270	 0.6730
T	 0.6150	 0.6110
U	 0.9100	 0.6740
V	 0.8780	 0.7050
W	 0.8850	 0.7030
X	 0.8910	 0.6780
Y	 0.7100	 0.6520
Z	 0.8880	 0.6850
a	 0.9400	 0.7020
b	 0.8200	 0.6560
c	 0.8430	 0.6530
d	 0.8880	 0.6870
e	 0.8580	 0.6780
f	 0.8130	 0.6630
g	 0.8880	 0.6830
h	 0.9220	 0.6910



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Chain	Atom inclusion	Q-score
i	 0.8210	 0.6530
j	 0.8570	 0.6470
k	 0.8900	 0.6460
l	 0.8960	 0.6760
m	 0.8730	 0.6750
n	 0.9010	 0.6810
o	 0.8610	 0.6520
p	 0.9030	 0.6810
q	 0.9060	 0.7090
r	 0.8870	 0.7070
s	 0.8540	 0.6780