



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:26 PM UTC

PDB ID : 7R44 / pdb_00007r44
EMDB ID : EMD-14266
Title : Bovine complex I in the presence of IM1761092, active class iv (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

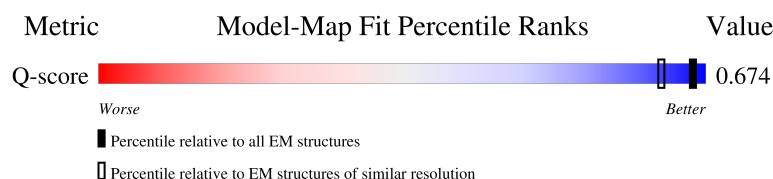
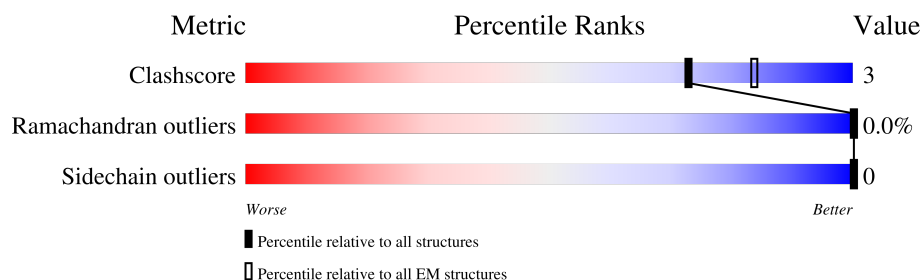
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



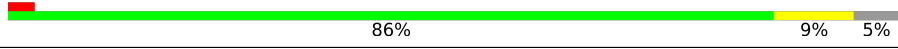
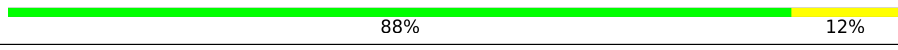
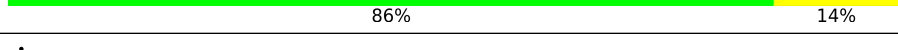
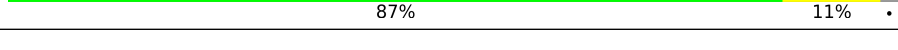
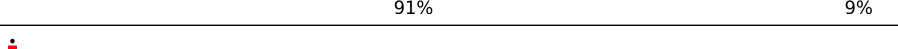
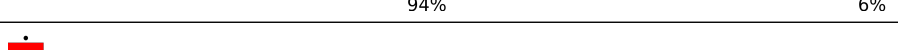
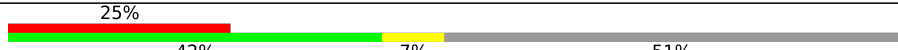
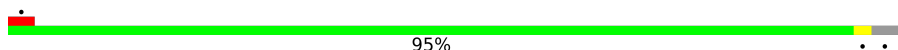
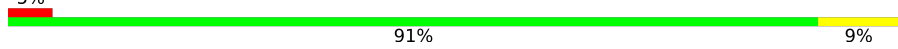
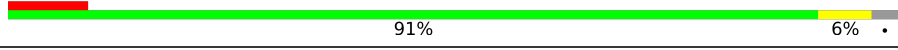
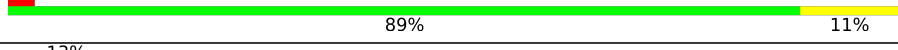
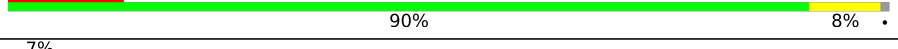
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A	115	 87% 12%
2	B	216	 67% 5% 28%
3	C	266	 74% 22%
4	D	463	 83% 9% 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 68213 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	595	Total	C	N	O	S	0	0
			4692	3119	723	807	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	82	Total	C	N	O	S	0	0
			663	416	124	121	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	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	112	Total	C	N	O	S	0	0
			911	589	154	165	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	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	102	Total	C	N	O	S	0	0
			876	575	151	149	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
			647	424	109	112	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	113	Total	C	N	O	S	0	0
			954	613	167	174			

- 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	170	Total	C	N	O	S	0	0
			1435	900	265	262	8		

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

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

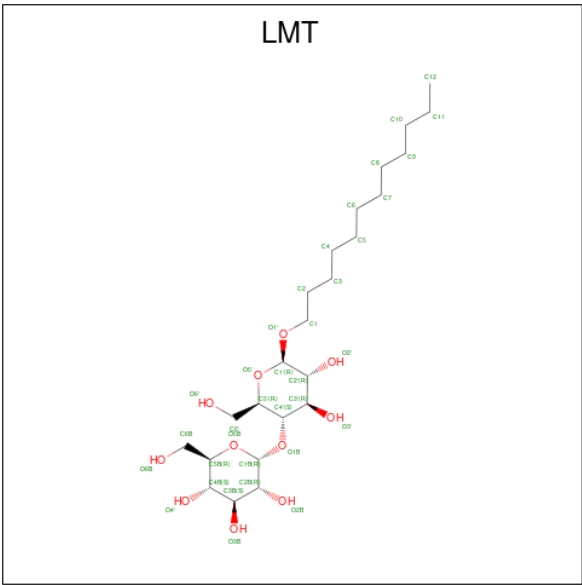
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	42	Total	C	N	O	S	0	0
			353	219	64	69	1		

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



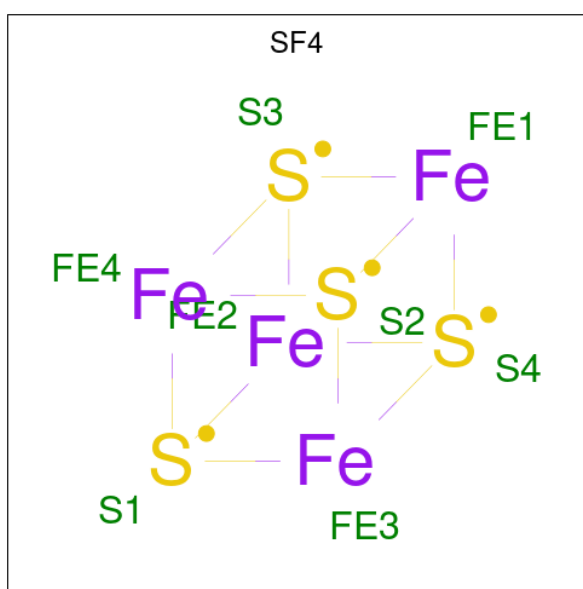
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	A	1	Total	C	O	0
			35	24	11	
45	L	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	M	1	Total	C	O	0
			35	24	11	
45	Y	1	Total	C	O	0
			35	24	11	
45	Z	1	Total	C	O	0
			35	24	11	

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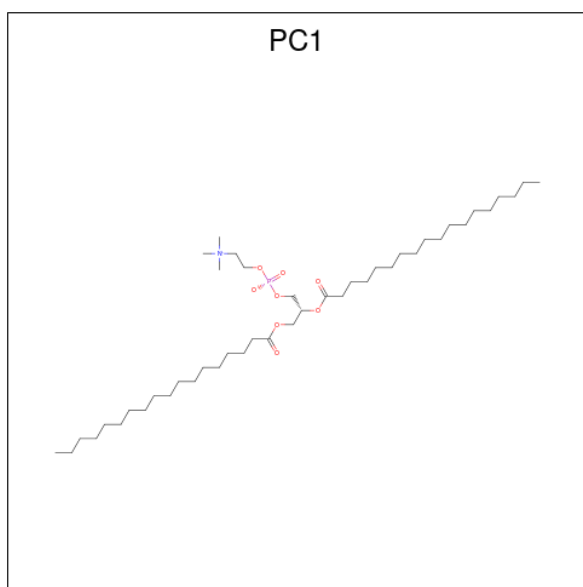
Mol	Chain	Residues	Atoms			AltConf
45	e	1	Total	C	O	0
			35	24	11	
45	h	1	Total	C	O	0
			35	24	11	
45	k	1	Total	C	O	0
			35	24	11	
45	l	1	Total	C	O	0
			35	24	11	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



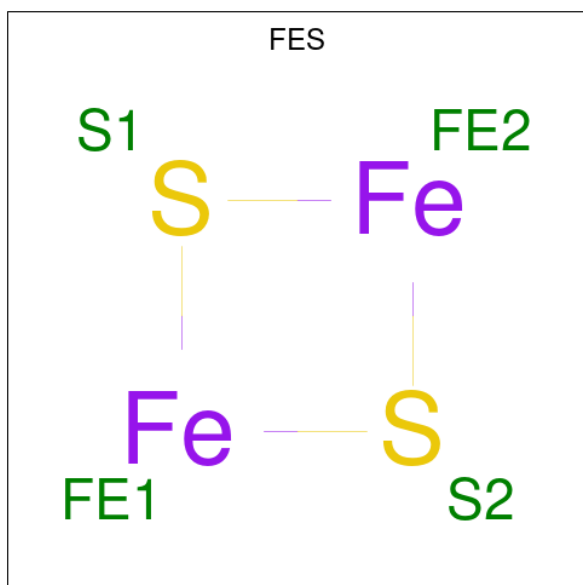
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$).



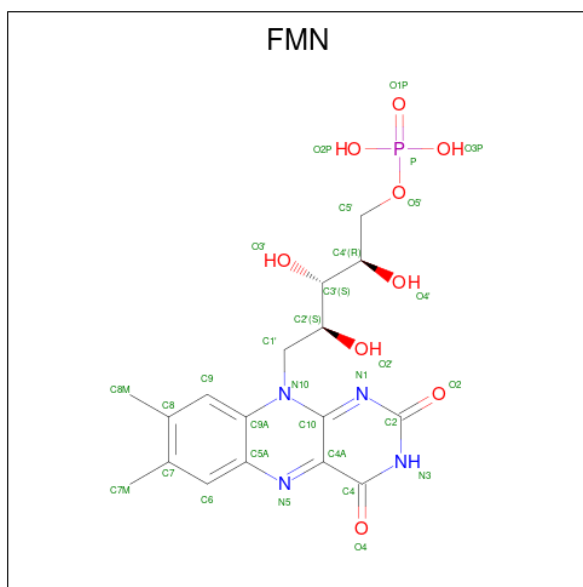
Mol	Chain	Residues	Atoms					AltConf
47	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
47	P	1	Total	C	N	O	P	0
			21	11	1	8	1	

- 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: $C_{17}H_{21}N_4O_9P$).

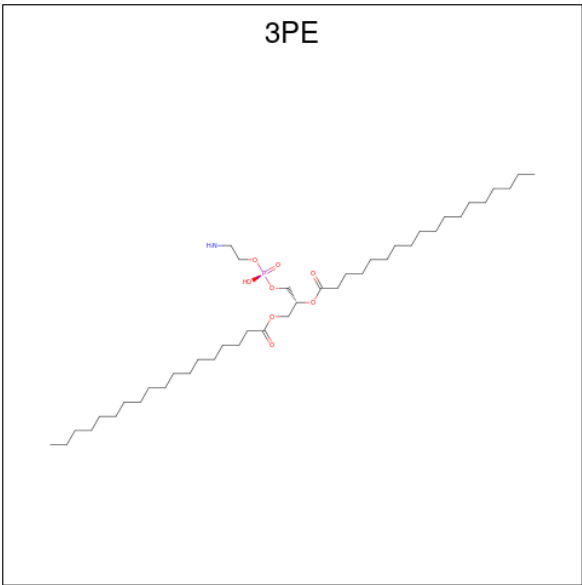


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

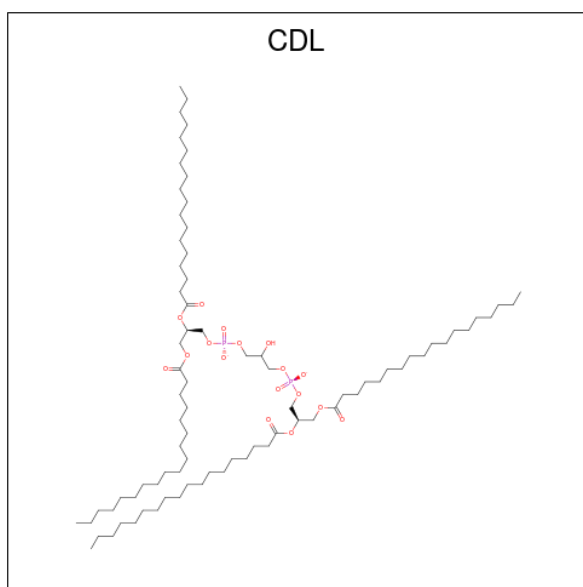
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



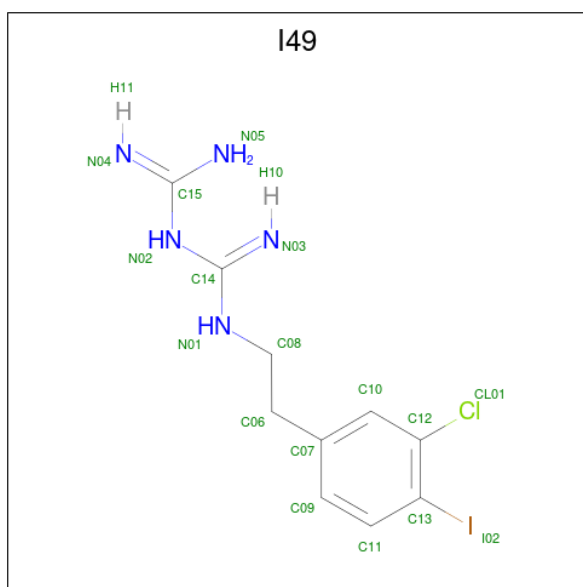
Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
51	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
51	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
51	M	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	M	1	Total	C	N	O	P	0
			51	41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

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



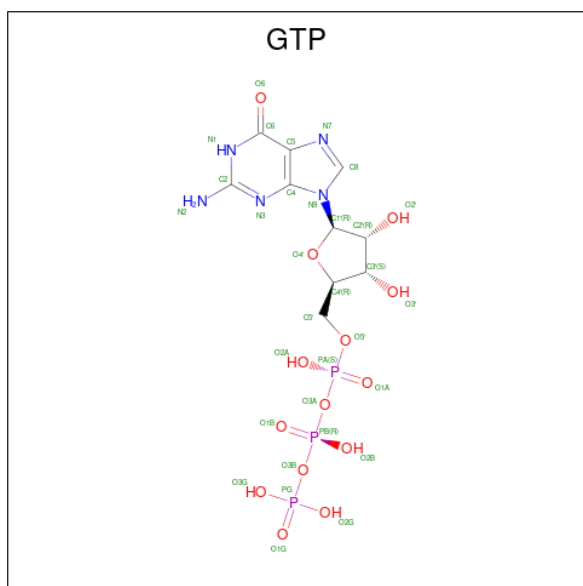
Mol	Chain	Residues	Atoms				AltConf
52	J	1	Total	C	O	P	0
			62	43	17	2	
52	K	1	Total	C	O	P	0
			71	52	17	2	
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	a	1	Total	C	O	P	0
			76	57	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	

- 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: $C_{10}H_{16}N_5O_{14}P_3$).

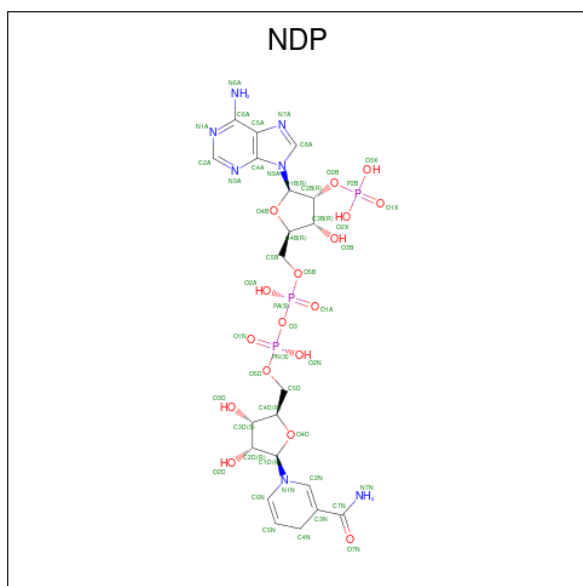


Mol	Chain	Residues	Atoms					AltConf
54	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

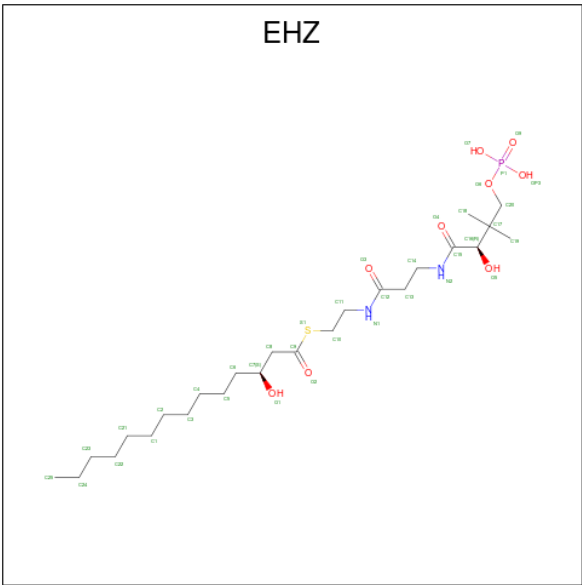


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

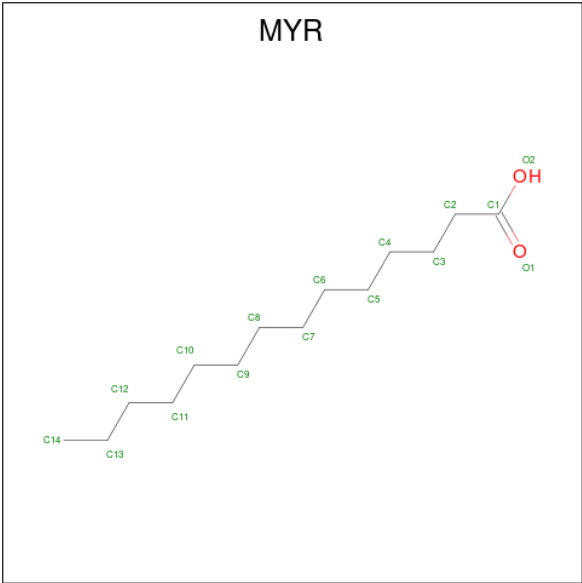
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- 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
			7	6	1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	16	Total O 16 16	0
60	B	48	Total O 48 48	0
60	C	61	Total O 61 61	0
60	D	123	Total O 123 123	0
60	E	7	Total O 7 7	0
60	F	36	Total O 36 36	0
60	G	132	Total O 132 132	0
60	H	42	Total O 42 42	0
60	I	76	Total O 76 76	0
60	J	10	Total O 10 10	0
60	K	11	Total O 11 11	0
60	L	23	Total O 23 23	0
60	M	28	Total O 28 28	0
60	N	30	Total O 30 30	0
60	O	10	Total O 10 10	0
60	P	35	Total O 35 35	0
60	Q	45	Total O 45 45	0
60	R	20	Total O 20 20	0
60	S	1	Total O 1 1	0
60	V	10	Total O 10 10	0
60	W	3	Total O 3 3	0
60	X	14	Total O 14 14	0

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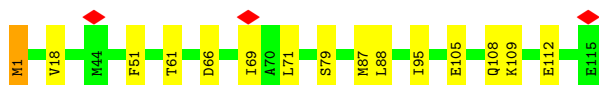
Mol	Chain	Residues	Atoms		AltConf
60	Y	1	Total 1	O 1	0
60	Z	13	Total 13	O 13	0
60	a	6	Total 6	O 6	0
60	d	8	Total 8	O 8	0
60	e	10	Total 10	O 10	0
60	f	1	Total 1	O 1	0
60	g	2	Total 2	O 2	0
60	h	8	Total 8	O 8	0
60	i	1	Total 1	O 1	0
60	j	1	Total 1	O 1	0
60	k	2	Total 2	O 2	0
60	l	7	Total 7	O 7	0
60	m	4	Total 4	O 4	0
60	n	10	Total 10	O 10	0
60	o	1	Total 1	O 1	0
60	p	10	Total 10	O 10	0
60	q	22	Total 22	O 22	0
60	r	15	Total 15	O 15	0
60	s	2	Total 2	O 2	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.

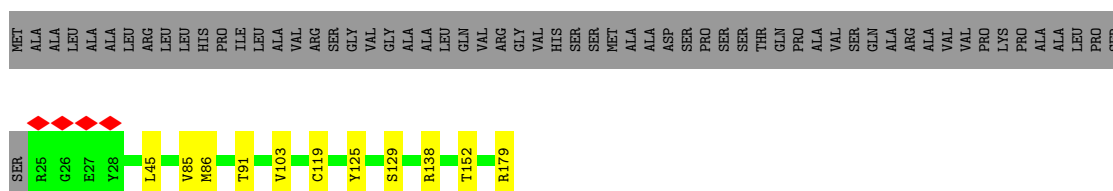
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



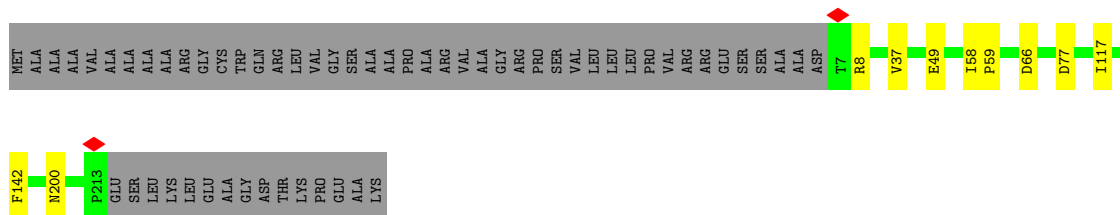
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



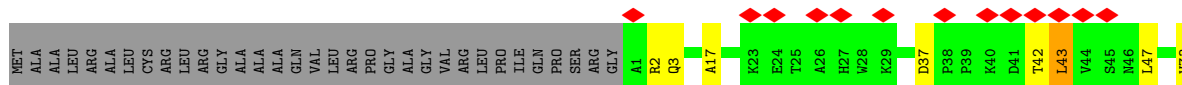
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



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

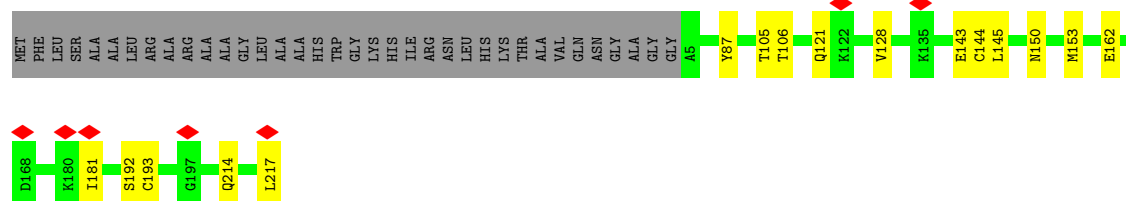
Chain D: 





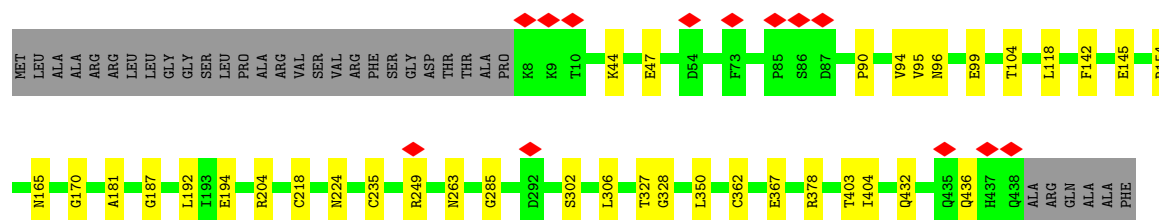
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 79% 6% 14%



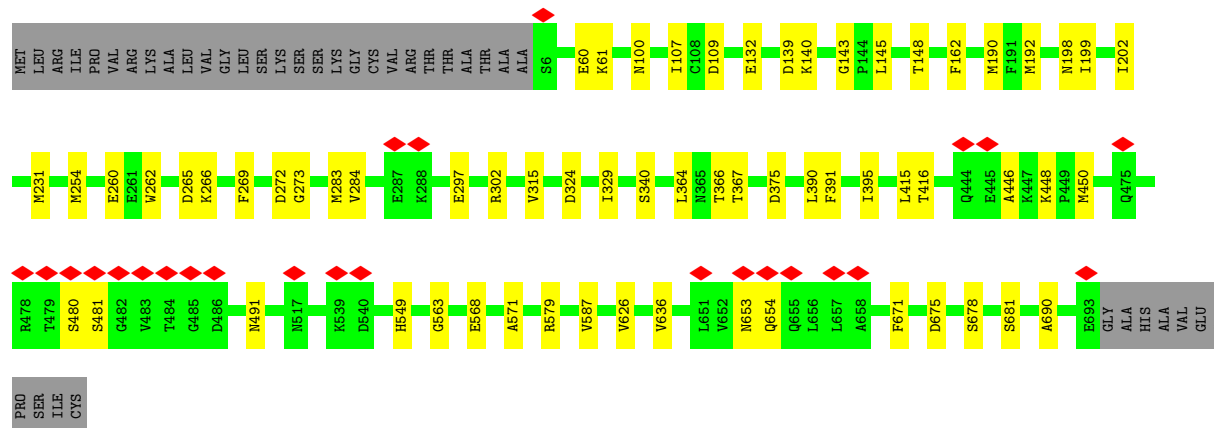
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 85% 8% 7%



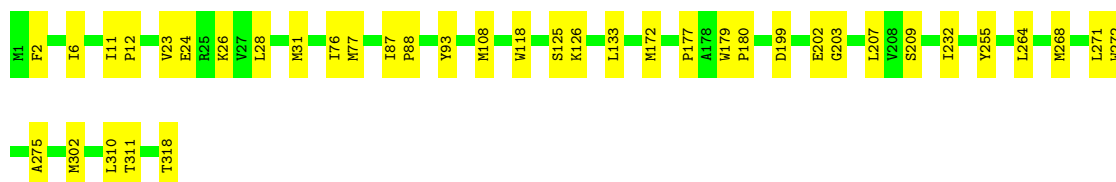
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 86% 9% 5%

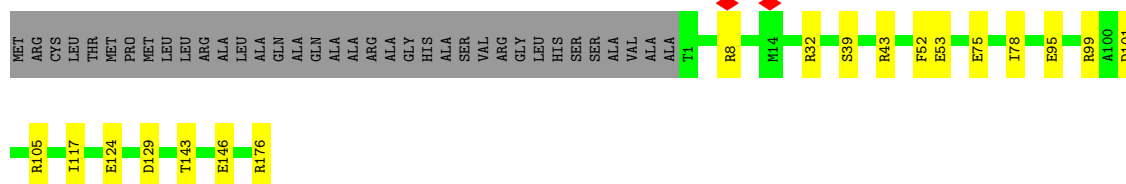


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

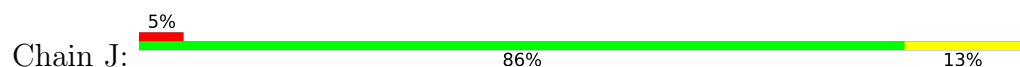
Chain H: 88% 12%



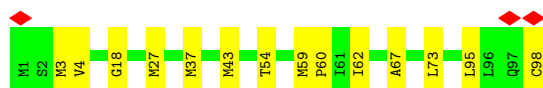
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



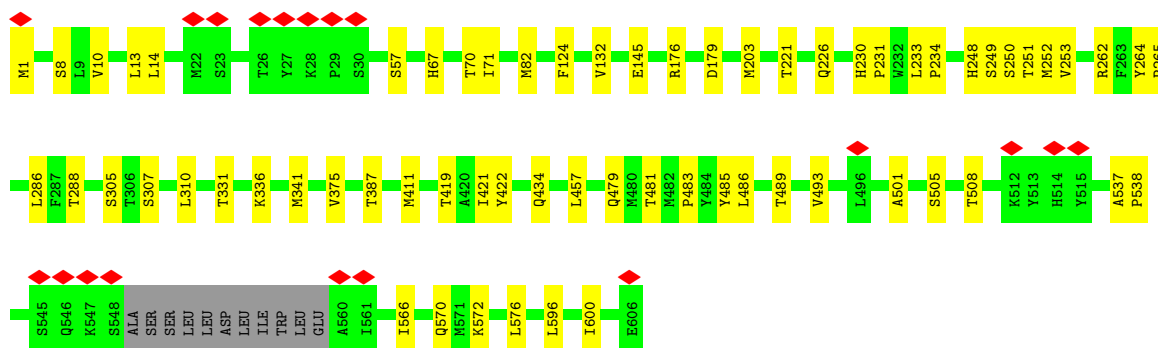
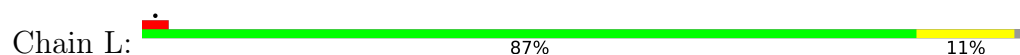
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

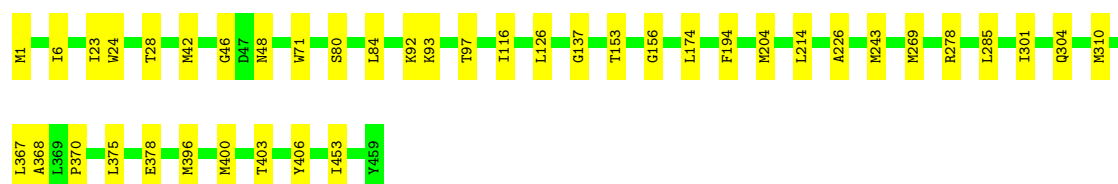


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

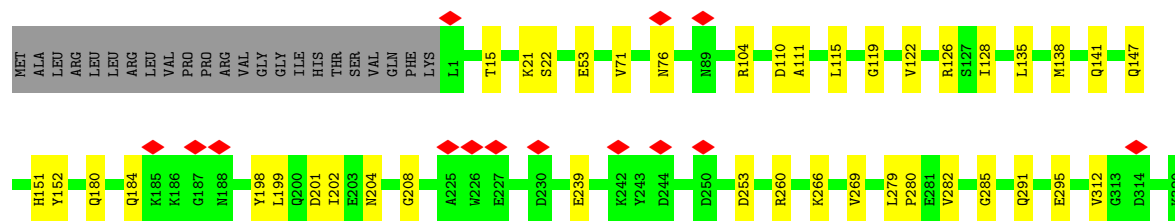
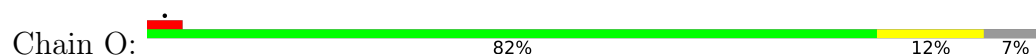




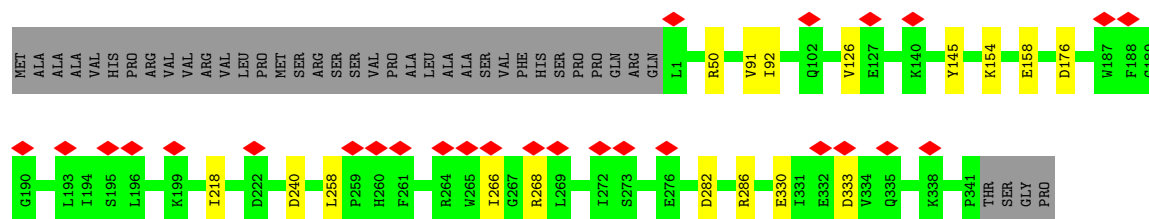
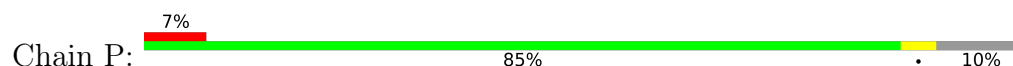
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



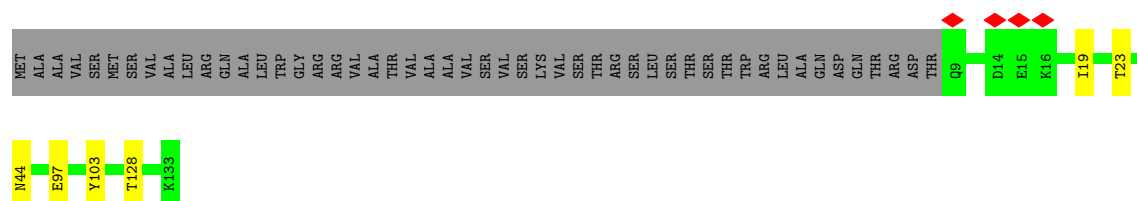
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



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

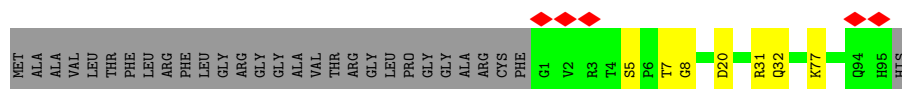


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



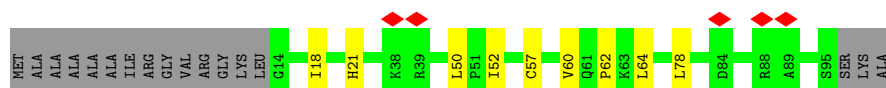
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  71% 6% 23%

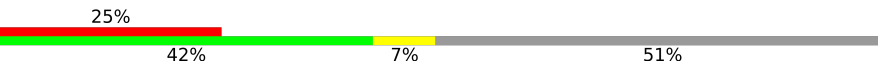


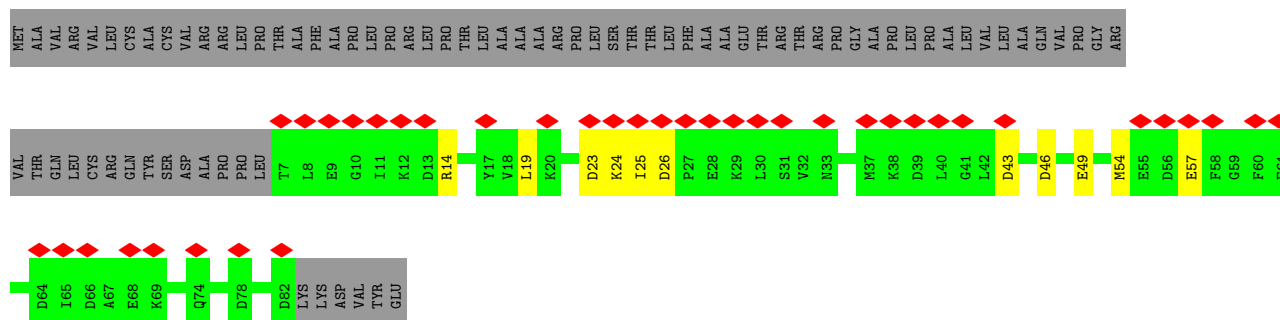
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:  5% 74% 9% 17%



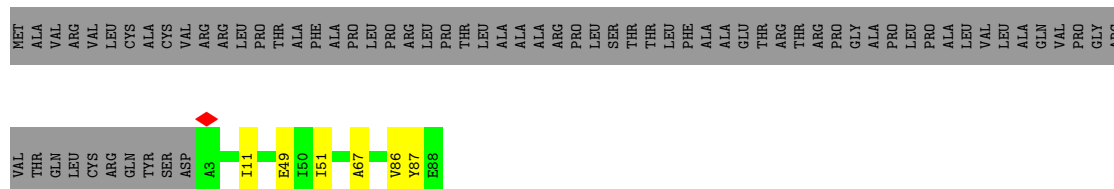
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  25% 42% 7% 51%

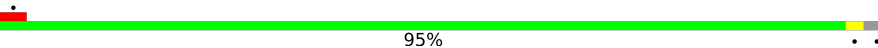


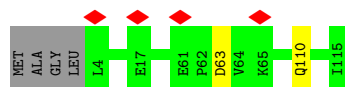
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  51% 45%



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

Chain V:  95%

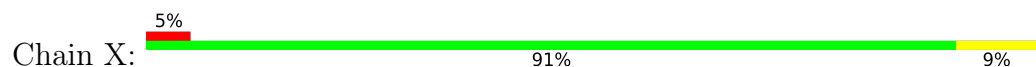


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

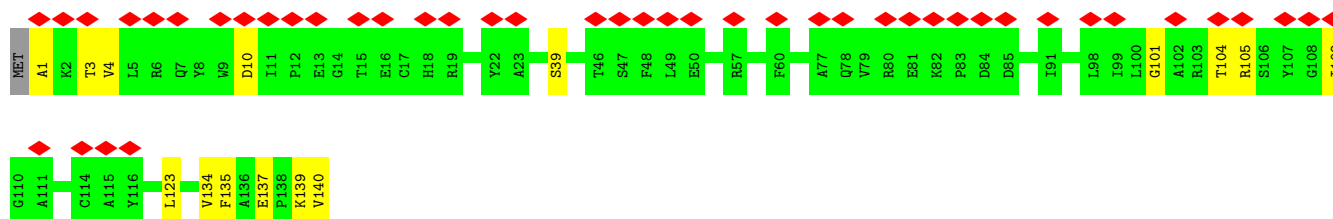
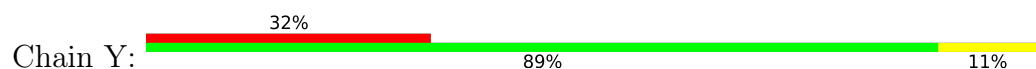
Chain W:  5% 87% 11%



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



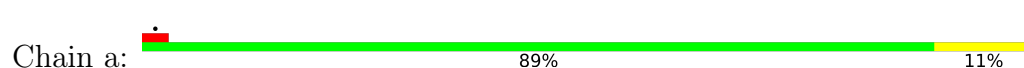
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



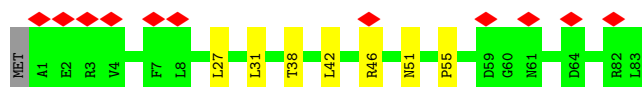
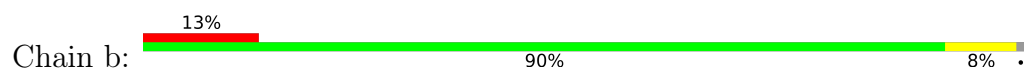
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

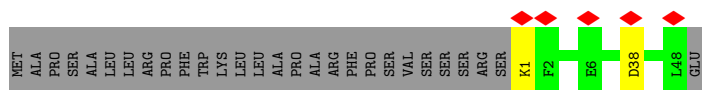


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

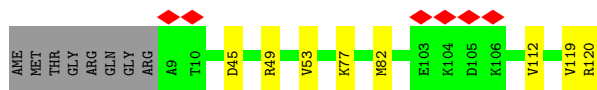
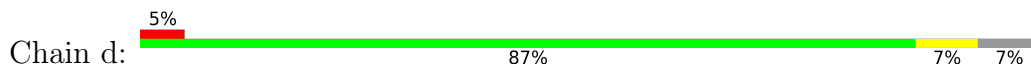


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

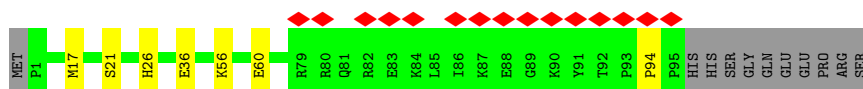
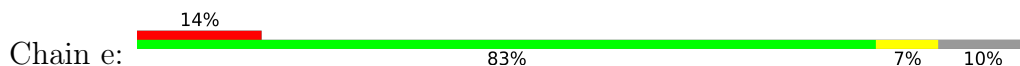




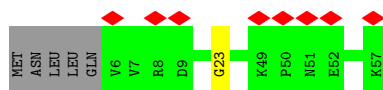
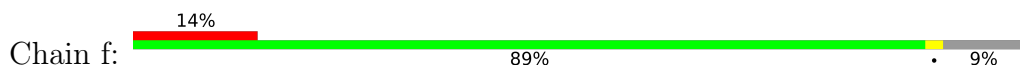
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



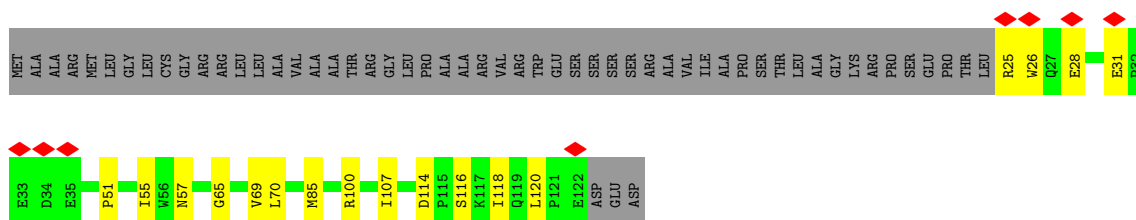
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



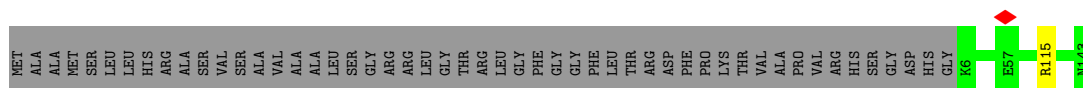
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

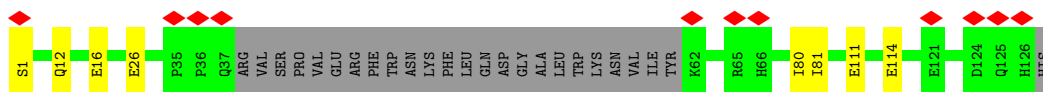


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

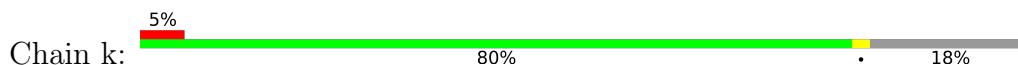




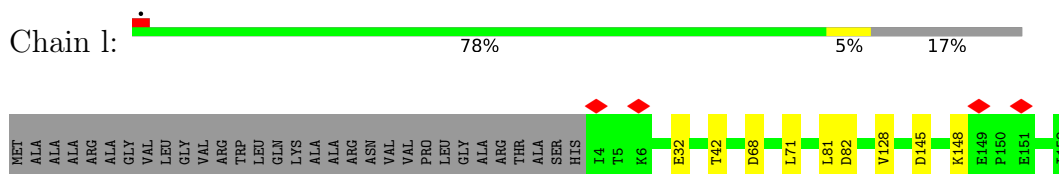
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



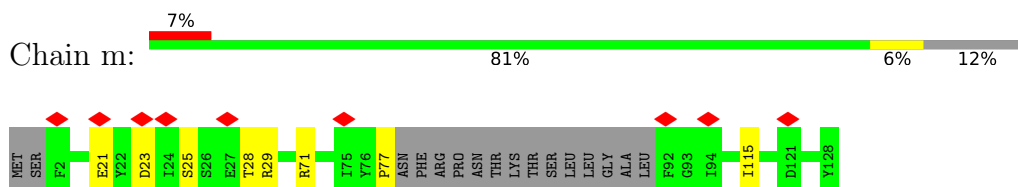
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



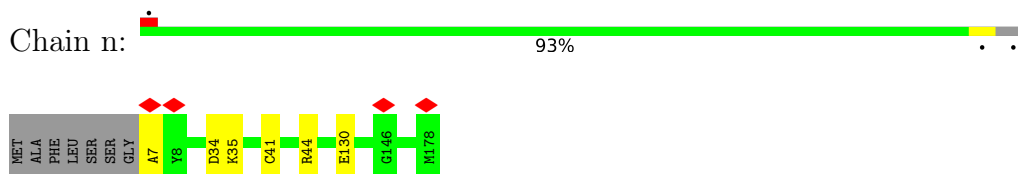
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



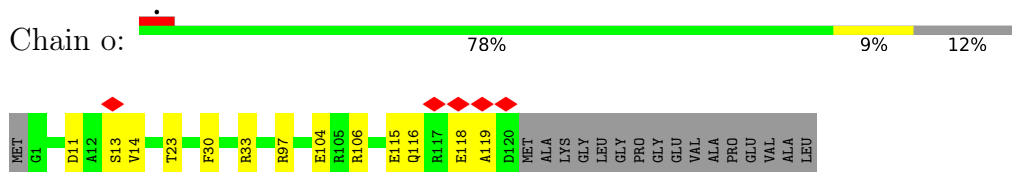
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



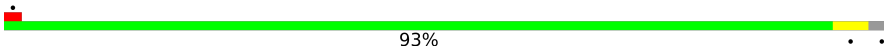
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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

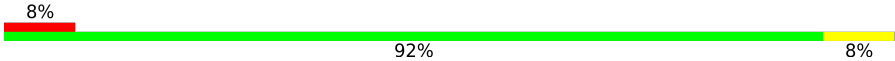


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p: 



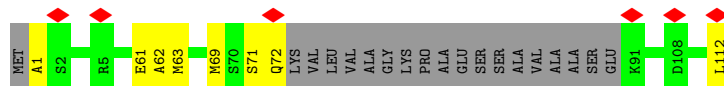
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 



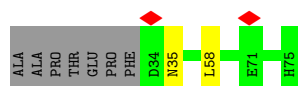
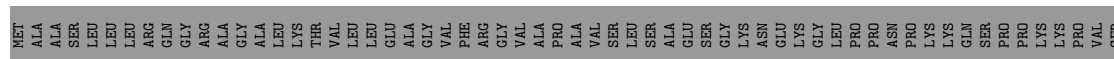
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 



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

Chain s: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31957	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	30.444	Depositor
Minimum map value	-11.792	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.039	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/1272	0.41	0/1720
3	C	0.25	0/1772	0.32	0/2413
4	D	0.25	0/3537	0.33	0/4794
5	E	0.23	0/1695	0.31	0/2307
6	F	0.23	0/3393	0.31	0/4584
7	G	0.24	0/5367	0.32	0/7274
8	H	0.26	0/2571	0.34	0/3513
9	I	0.27	0/1445	0.36	0/1956
10	J	0.22	0/1362	0.30	0/1848
11	K	0.25	0/745	0.35	0/1008
12	L	0.25	0/4805	0.30	0/6536
13	M	0.26	0/3738	0.30	0/5097
14	N	0.25	0/2792	0.30	0/3800
15	O	0.23	0/2651	0.28	0/3587
16	P	0.22	0/2824	0.33	0/3831
17	Q	0.24	0/1039	0.30	0/1404
18	R	0.25	0/742	0.30	0/999
19	S	0.21	0/674	0.31	0/908
20	T	0.19	0/621	0.36	0/837
20	U	0.29	0/705	0.33	0/952
21	V	0.21	0/931	0.27	0/1261
22	W	0.23	0/995	0.30	0/1337
23	X	0.23	0/1439	0.32	0/1942
24	Y	0.17	0/1042	0.26	0/1414
25	Z	0.22	0/1175	0.28	0/1584
26	a	0.24	0/584	0.30	0/786
27	b	0.21	0/672	0.30	0/923
28	c	0.20	0/418	0.27	0/567
29	d	0.23	0/964	0.29	0/1305
30	e	0.23	0/818	0.33	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.21	0/464	0.29	0/626
32	g	0.24	0/850	0.31	0/1154
33	h	0.24	0/1188	0.28	0/1607
34	i	0.26	0/896	0.33	0/1218
35	j	0.27	0/607	0.26	0/833
36	k	0.24	0/666	0.29	0/898
37	l	0.26	0/1358	0.29	0/1858
38	m	0.25	0/978	0.30	0/1321
39	n	0.27	0/1545	0.30	0/2092
40	o	0.29	0/1060	0.33	0/1420
41	p	0.25	0/1468	0.28	0/1979
42	q	0.22	0/1242	0.30	0/1688
43	r	0.24	0/780	0.33	0/1056
44	s	0.20	0/363	0.30	0/491
All	All	0.24	0/67189	0.31	0/91102

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	12	0
2	B	1241	0	1251	11	0
3	C	1721	0	1675	9	0
4	D	3459	0	3404	35	0
5	E	1655	0	1661	11	0
6	F	3319	0	3274	25	0
7	G	5279	0	5301	46	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	16	0
10	J	1337	0	1346	23	0
11	K	745	0	785	21	0
12	L	4692	0	4835	43	0
13	M	3654	0	3852	30	0
14	N	2733	0	2912	17	0
15	O	2589	0	2566	29	0
16	P	2747	0	2766	11	0
17	Q	1016	0	1014	4	0
18	R	730	0	707	5	0
19	S	663	0	672	5	0
20	T	612	0	604	9	0
20	U	693	0	688	4	0
21	V	911	0	950	2	0
22	W	971	0	989	4	0
23	X	1402	0	1385	11	0
24	Y	1030	0	1039	10	0
25	Z	1146	0	1146	7	0
26	a	569	0	568	7	0
27	b	651	0	662	5	0
28	c	405	0	409	2	0
29	d	934	0	919	7	0
30	e	799	0	807	5	0
31	f	451	0	453	1	0
32	g	824	0	772	13	0
33	h	1154	0	1168	1	0
34	i	876	0	891	9	0
35	j	580	0	519	3	0
36	k	647	0	634	2	0
37	l	1304	0	1203	7	0
38	m	954	0	944	8	0
39	n	1492	0	1438	6	0
40	o	1035	0	1004	9	0
41	p	1435	0	1411	9	0
42	q	1201	0	1170	9	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	353	0	327	2	0
45	A	70	0	92	1	0
45	L	35	0	46	1	0
45	M	70	0	92	1	0
45	Y	35	0	46	0	0
45	Z	35	0	46	0	0
45	e	35	0	46	1	0
45	h	35	0	46	0	0
45	k	35	0	46	1	0
45	l	35	0	46	0	0
46	B	8	0	0	0	0
46	F	8	0	0	1	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	B	77	0	105	3	0
47	M	49	0	75	2	0
47	P	21	0	18	1	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	78	0	112	2	0
51	I	51	0	82	0	0
51	L	94	0	142	2	0
51	M	97	0	151	1	0
51	N	92	0	138	1	0
51	X	45	0	67	0	0
51	Y	35	0	44	1	0
51	d	51	0	82	1	0
52	J	62	0	68	2	0
52	K	71	0	86	0	0
52	L	69	0	82	0	0
52	a	76	0	96	0	0
52	h	67	0	81	1	0
53	N	17	0	0	1	0
54	O	32	0	12	3	0
55	O	1	0	0	0	0
56	P	48	0	26	2	0
57	R	1	0	0	0	0
58	T	37	0	0	0	0
58	U	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	o	7	0	8	0	0
60	A	16	0	0	1	0
60	B	48	0	0	1	0
60	C	61	0	0	4	0
60	D	123	0	0	9	0
60	E	7	0	0	0	0
60	F	36	0	0	1	0
60	G	132	0	0	4	0
60	H	42	0	0	3	0
60	I	76	0	0	2	0
60	J	10	0	0	0	0
60	K	11	0	0	1	0
60	L	23	0	0	1	0
60	M	28	0	0	2	0
60	N	30	0	0	0	0
60	O	10	0	0	3	0
60	P	35	0	0	2	0
60	Q	45	0	0	1	0
60	R	20	0	0	0	0
60	S	1	0	0	0	0
60	V	10	0	0	1	0
60	W	3	0	0	0	0
60	X	14	0	0	2	0
60	Y	1	0	0	0	0
60	Z	13	0	0	1	0
60	a	6	0	0	0	0
60	d	8	0	0	0	0
60	e	10	0	0	0	0
60	f	1	0	0	0	0
60	g	2	0	0	0	0
60	h	8	0	0	0	0
60	i	1	0	0	0	0
60	j	1	0	0	0	0
60	k	2	0	0	0	0
60	l	7	0	0	0	0
60	m	4	0	0	0	0
60	n	10	0	0	1	0
60	o	1	0	0	0	0
60	p	10	0	0	1	0
60	q	22	0	0	1	0
60	r	15	0	0	0	0
60	s	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	68213	0	67840	450	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 (450) 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)
45:k:101:LMT:H3O2	45:k:101:LMT:H2O1	0.93	0.91
34:i:12:GLN:NE2	34:i:16:GLU:OE1	2.06	0.89
1:A:112:GLU:OE1	60:A:401:HOH:O	1.91	0.89
3:C:200:ASN:ND2	60:C:304:HOH:O	2.05	0.88
4:D:337:GLU:OE1	60:D:501:HOH:O	1.93	0.85
13:M:84:LEU:O	13:M:92:LYS:NZ	2.09	0.85
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.60	0.83
34:i:114:GLU:OE1	41:p:15:ARG:NH1	2.11	0.83
51:H:401:3PE:O14	60:H:502:HOH:O	1.97	0.82
12:L:479:GLN:NE2	12:L:481:THR:O	2.12	0.82
8:H:125:SER:OG	60:H:501:HOH:O	1.97	0.82
7:G:260:GLU:OE2	60:G:901:HOH:O	1.97	0.81
3:C:49:GLU:OE1	60:C:302:HOH:O	1.98	0.81
7:G:675:ASP:OD1	7:G:678:SER:OG	1.97	0.81
3:C:77:ASP:OD2	60:C:301:HOH:O	1.97	0.81
11:K:37:MET:SD	14:N:68:MET:HE1	2.21	0.80
12:L:566:ILE:O	12:L:570:GLN:NE2	2.14	0.80
21:V:110:GLN:OE1	60:V:201:HOH:O	1.97	0.80
41:p:15:ARG:O	60:p:201:HOH:O	1.97	0.80
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.15	0.79
15:O:128:ILE:O	60:O:501:HOH:O	2.01	0.78
9:I:124:GLU:OE2	60:I:301:HOH:O	2.04	0.76
9:I:143:THR:OG1	9:I:146:GLU:OE2	2.02	0.76
20:U:87:TYR:OH	34:i:26:GLU:OE2	2.02	0.76
7:G:109:ASP:OD2	60:G:902:HOH:O	2.04	0.76
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.20	0.75
3:C:66:ASP:OD2	60:C:303:HOH:O	2.03	0.74
12:L:505:SER:O	12:L:508:THR:OG1	2.03	0.74
56:P:501:NDP:O1X	60:P:601:HOH:O	2.04	0.73
45:A:301:LMT:O6B	27:b:38:THR:O	2.07	0.73
4:D:333:PRO:O	60:D:502:HOH:O	2.06	0.73
12:L:10:VAL:HG12	34:i:81:ILE:HD12	1.70	0.73
3:C:8:ARG:NH2	43:r:61:GLU:OE1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:366:THR:O	7:G:367:THR:OG1	2.06	0.72
15:O:291:GLN:NE2	15:O:295:GLU:OE2	2.22	0.71
15:O:53:GLU:OE1	15:O:126:ARG:NH1	2.23	0.71
18:R:7:THR:OG1	18:R:20:ASP:OD1	2.09	0.71
32:g:114:ASP:OD2	32:g:116:SER:OG	2.07	0.71
4:D:172:GLU:OE2	60:D:503:HOH:O	2.09	0.70
8:H:318:THR:HG21	10:J:135:PHE:CZ	2.27	0.70
4:D:368:GLU:OE2	60:D:504:HOH:O	2.11	0.69
20:T:19:LEU:HD12	20:T:25:ILE:HD13	1.75	0.68
11:K:54:THR:OG1	60:K:501:HOH:O	2.12	0.68
42:q:32:ASP:OD2	60:q:201:HOH:O	2.11	0.68
23:X:169:TRP:O	60:X:501:HOH:O	2.12	0.68
4:D:266:GLN:OE1	60:D:505:HOH:O	2.12	0.67
15:O:269:VAL:O	60:O:502:HOH:O	2.10	0.67
39:n:130:GLU:O	60:n:201:HOH:O	2.11	0.67
22:W:96:VAL:HG12	22:W:96:VAL:O	1.94	0.67
13:M:204:MET:SD	13:M:243:MET:HE1	2.35	0.66
6:F:306:LEU:O	60:F:601:HOH:O	2.13	0.66
15:O:22:SER:OG	15:O:119:GLY:O	2.12	0.66
29:d:45:ASP:OD2	29:d:49:ARG:NH1	2.28	0.66
10:J:141:MET:HA	10:J:141:MET:HE2	1.75	0.66
2:B:138:ARG:NH1	60:B:301:HOH:O	2.25	0.66
40:o:115:GLU:O	40:o:119:ALA:N	2.28	0.66
17:Q:44:ASN:ND2	17:Q:44:ASN:O	2.30	0.65
12:L:286:LEU:HD22	12:L:411:MET:SD	2.36	0.65
4:D:37:ASP:OD2	11:K:95:LEU:HD13	1.96	0.65
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.32	0.65
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.78	0.65
1:A:87:MET:SD	1:A:88:LEU:N	2.69	0.65
20:T:23:ASP:OD2	20:T:24:LYS:N	2.30	0.65
8:H:23:VAL:HG11	8:H:268:MET:HE1	1.78	0.65
17:Q:128:THR:O	60:Q:201:HOH:O	2.14	0.64
2:B:125:TYR:HB2	9:I:117:ILE:CG2	2.28	0.64
23:X:162:HIS:O	60:X:502:HOH:O	2.15	0.64
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.33	0.64
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.29	0.64
17:Q:19:ILE:O	17:Q:23:THR:HG23	1.98	0.64
13:M:48:ASN:OD1	60:M:701:HOH:O	2.15	0.63
27:b:51:ASN:ND2	30:e:26:HIS:O	2.25	0.63
13:M:278:ARG:O	38:m:71:ARG:NH1	2.31	0.63
5:E:121:GLN:OE1	5:E:128:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:341:MET:CE	12:L:457:LEU:HD12	2.29	0.63
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.34	0.63
6:F:224:ASN:ND2	49:F:501:FMN:O2	2.29	0.62
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.81	0.62
7:G:143:GLY:HA2	7:G:190:MET:HE3	1.80	0.62
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.80	0.62
15:O:147:GLN:N	15:O:147:GLN:OE1	2.33	0.62
7:G:563:GLY:O	60:G:903:HOH:O	2.16	0.61
37:l:71:LEU:HD11	37:l:81:LEU:HD11	1.80	0.61
39:n:34:ASP:OD1	39:n:35:LYS:N	2.34	0.61
1:A:71:LEU:O	10:J:147:TYR:OH	2.17	0.61
12:L:331:THR:HB	12:L:387:THR:HG22	1.83	0.61
16:P:240:ASP:OD2	60:P:602:HOH:O	2.16	0.61
24:Y:39:SER:OG	51:Y:802:3PE:O12	2.14	0.60
4:D:42:THR:O	4:D:43:LEU:HB2	2.01	0.60
7:G:231:MET:HE2	7:G:231:MET:HA	1.82	0.60
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.83	0.60
9:I:8:ARG:NH1	43:r:112:LEU:O	2.35	0.60
7:G:265:ASP:OD2	60:G:904:HOH:O	2.17	0.59
13:M:378:GLU:OE1	13:M:400:MET:HE3	2.02	0.59
11:K:43:MET:HE1	14:N:72:MET:SD	2.42	0.59
1:A:61:THR:HG21	1:A:105:GLU:OE1	2.02	0.59
13:M:370:PRO:HB3	13:M:375:LEU:HD13	1.83	0.59
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.83	0.59
4:D:182:GLU:OE1	60:D:506:HOH:O	2.17	0.59
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.85	0.59
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.84	0.59
14:N:214:THR:HG22	14:N:218:MET:HE2	1.85	0.58
30:e:21:SER:OG	30:e:36:GLU:OE1	2.12	0.58
12:L:8:SER:HB2	12:L:82:MET:HE2	1.86	0.58
42:q:67:GLU:OE2	42:q:70:GLY:N	2.34	0.58
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.37	0.58
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.38	0.58
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.37	0.58
13:M:368:ALA:O	13:M:375:LEU:HD12	2.05	0.57
10:J:84:LEU:HD13	52:J:701:CDL:OB9	2.03	0.57
8:H:318:THR:HG21	10:J:135:PHE:HZ	1.67	0.57
14:N:270:MET:HE1	14:N:282:MET:SD	2.45	0.56
12:L:13:LEU:HD23	34:i:81:ILE:HD11	1.87	0.56
20:T:14:ARG:NE	20:T:57:GLU:OE1	2.38	0.56
4:D:123:GLU:OE1	4:D:138:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:371:LYS:HE2	4:D:424:VAL:HG23	1.88	0.56
11:K:59:MET:HE3	14:N:84:TRP:CH2	2.41	0.56
12:L:483:PRO:HD2	12:L:486:LEU:HD12	1.88	0.56
7:G:190:MET:HE1	7:G:690:ALA:CB	2.33	0.56
5:E:214:GLN:NE2	6:F:235:CYS:O	2.39	0.56
8:H:26:LYS:NZ	60:H:504:HOH:O	2.31	0.56
6:F:47:GLU:N	6:F:47:GLU:OE1	2.39	0.56
34:i:111:GLU:OE1	41:p:16:THR:HG22	2.06	0.56
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.36	0.55
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.87	0.55
13:M:269:MET:HE1	13:M:396:MET:HE2	1.88	0.55
40:o:30:PHE:HB3	40:o:33:ARG:HG3	1.89	0.55
15:O:21:LYS:NZ	15:O:239:GLU:OE2	2.39	0.55
1:A:51:PHE:CD1	8:H:133:LEU:HD13	2.41	0.55
16:P:154:LYS:O	16:P:158:GLU:OE1	2.25	0.55
6:F:378:ARG:NH2	7:G:132:GLU:OE2	2.40	0.55
9:I:176:ARG:NH2	60:I:304:HOH:O	2.37	0.55
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.88	0.55
24:Y:137:GLU:O	24:Y:139:LYS:NZ	2.30	0.55
5:E:192:SER:OG	5:E:193:CYS:N	2.38	0.55
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.38	0.54
7:G:375:ASP:OD2	7:G:448:LYS:N	2.40	0.54
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.39	0.54
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.88	0.54
23:X:79:GLU:O	23:X:83:GLU:OE1	2.25	0.54
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.38	0.53
32:g:65:GLY:O	32:g:70:LEU:HD13	2.09	0.53
7:G:415:LEU:O	7:G:416:THR:OG1	2.21	0.53
51:L:704:3PE:N	47:M:605:PC1:O14	2.42	0.53
7:G:139:ASP:O	18:R:77:LYS:NZ	2.28	0.53
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.90	0.53
32:g:57:ASN:ND2	32:g:57:ASN:O	2.42	0.53
15:O:71:VAL:HG22	15:O:76:ASN:HA	1.90	0.53
5:E:181:ILE:HG23	5:E:181:ILE:O	2.10	0.52
13:M:304:GLN:O	29:d:119:VAL:HG11	2.08	0.52
15:O:180:GLN:NE2	15:O:199:LEU:HD12	2.24	0.52
2:B:179:ARG:NE	47:B:202:PC1:O12	2.35	0.52
4:D:42:THR:O	4:D:42:THR:HG22	2.08	0.52
32:g:100:ARG:NH1	32:g:107:ILE:O	2.40	0.52
4:D:128:ILE:HD13	4:D:330:VAL:HG11	1.90	0.52
6:F:99:GLU:OE2	6:F:104:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:ARG:N	32:g:31:GLU:OE2	2.38	0.52
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.91	0.52
8:H:28:LEU:HD13	8:H:275:ALA:HB2	1.91	0.52
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.91	0.52
47:M:605:PC1:H142	52:h:1001:CDL:OA3	2.09	0.52
12:L:176:ARG:HH22	13:M:367:LEU:HD13	1.74	0.52
12:L:132:VAL:O	12:L:262:ARG:NH1	2.40	0.52
4:D:3:GLN:NE2	13:M:137:GLY:O	2.43	0.52
9:I:99:ARG:O	9:I:101:ASP:O	2.27	0.52
11:K:43:MET:HE1	14:N:72:MET:HE1	1.92	0.52
7:G:140:LYS:O	7:G:148:THR:OG1	2.22	0.52
12:L:249:SER:OG	12:L:250:SER:N	2.43	0.52
12:L:264:TYR:N	12:L:265:PRO:CD	2.73	0.52
18:R:5:SER:O	18:R:8:GLY:N	2.39	0.52
37:l:42:THR:O	37:l:42:THR:HG22	2.09	0.52
13:M:370:PRO:CB	13:M:375:LEU:HD13	2.40	0.51
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.91	0.51
38:m:29:ARG:NH2	39:n:7:ALA:O	2.43	0.51
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.91	0.51
12:L:57:SER:O	60:L:801:HOH:O	2.19	0.51
26:a:58:ASN:O	26:a:59:ARG:NE	2.43	0.51
2:B:125:TYR:HB2	9:I:117:ILE:HG21	1.91	0.51
13:M:156:GLY:O	60:M:702:HOH:O	2.19	0.51
12:L:124:PHE:CE2	12:L:251:THR:HG21	2.46	0.51
5:E:150:ASN:HB3	5:E:162:GLU:HB3	1.92	0.51
9:I:95:GLU:OE2	42:q:130:THR:HG21	2.11	0.51
6:F:194:GLU:OE1	6:F:204:ARG:NE	2.32	0.50
5:E:105:THR:HG22	5:E:106:THR:H	1.76	0.50
8:H:310:LEU:HD12	8:H:311:THR:HG23	1.93	0.50
15:O:204:ASN:O	15:O:208:GLY:N	2.44	0.50
14:N:242:VAL:HG11	51:N:1301:3PE:H332	1.93	0.50
25:Z:143:TYR:CZ	26:a:48:MET:HE1	2.46	0.50
16:P:258:LEU:HD21	16:P:266:ILE:HD12	1.94	0.50
40:o:23:THR:OG1	40:o:104:GLU:OE2	2.18	0.50
6:F:263:ASN:ND2	6:F:285:GLY:O	2.45	0.50
7:G:366:THR:HB	7:G:450:MET:HE3	1.94	0.50
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.94	0.49
24:Y:101:GLY:O	24:Y:105:ARG:N	2.45	0.49
7:G:284:VAL:HG11	7:G:302:ARG:HD2	1.93	0.49
2:B:129:SER:OG	4:D:85:2MR:O	2.29	0.49
41:p:103:ASN:O	41:p:107:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:35:ASN:CG	44:s:35:ASN:O	2.55	0.49
11:K:37:MET:HE2	11:K:67:ALA:HB2	1.94	0.49
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.94	0.49
4:D:201:GLN:NE2	60:D:512:HOH:O	2.32	0.49
7:G:190:MET:HE2	7:G:192:MET:HG3	1.95	0.49
10:J:124:ASP:OD2	11:K:4:VAL:HB	2.13	0.49
15:O:110:ASP:OD1	15:O:266:LYS:NZ	2.32	0.49
25:Z:120:MET:HG2	25:Z:123:GLU:HG3	1.95	0.49
13:M:214:LEU:HD21	38:m:77:PRO:HG2	1.95	0.48
14:N:146:PHE:HA	14:N:149:ILE:HD12	1.95	0.48
35:j:70:ASP:OD1	35:j:71:GLU:N	2.46	0.48
37:l:68:ASP:N	37:l:68:ASP:OD1	2.46	0.48
17:Q:97:GLU:OE2	17:Q:103:TYR:OH	2.14	0.48
7:G:199:ILE:HA	7:G:202:ILE:HG12	1.96	0.48
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.95	0.48
37:l:32:GLU:OE2	37:l:32:GLU:N	2.44	0.48
10:J:153:LEU:O	10:J:157:THR:HG23	2.13	0.48
25:Z:125:TYR:HB3	25:Z:133:VAL:HG22	1.95	0.48
4:D:271:LYS:NZ	4:D:283:PHE:O	2.38	0.48
4:D:385:ARG:NH1	60:D:517:HOH:O	2.37	0.48
12:L:251:THR:HG22	12:L:252:MET:N	2.28	0.48
13:M:403:THR:HA	13:M:406:TYR:CE1	2.49	0.48
2:B:91:THR:HA	2:B:119:CYS:HB3	1.95	0.48
19:S:50:LEU:O	19:S:52:ILE:HD12	2.14	0.48
20:T:26:ASP:OD1	20:T:26:ASP:O	2.32	0.48
23:X:70:PHE:HB3	26:a:69:ILE:HD13	1.95	0.48
24:Y:3:THR:HG23	24:Y:4:VAL:N	2.29	0.48
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.96	0.47
40:o:11:ASP:OD1	40:o:13:SER:OG	2.31	0.47
40:o:116:GLN:N	40:o:116:GLN:OE1	2.47	0.47
2:B:45:LEU:HD22	2:B:85:VAL:CG2	2.43	0.47
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.96	0.47
12:L:230:HIS:N	12:L:231:PRO:CD	2.77	0.47
23:X:45:CYS:HG	23:X:55:CYS:HG	1.61	0.47
37:l:128:VAL:HG22	40:o:97:ARG:HB3	1.95	0.47
4:D:164:MET:HE3	8:H:28:LEU:HD12	1.97	0.47
5:E:217:LEU:HD22	6:F:44:LYS:CE	2.44	0.47
6:F:165:ASN:OD1	6:F:170:GLY:N	2.41	0.47
9:I:39:SER:O	9:I:43:ARG:HG3	2.15	0.47
12:L:305:SER:OG	12:L:336:LYS:NZ	2.43	0.47
13:M:42:MET:HE1	13:M:453:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:190:MET:HE2	7:G:192:MET:CG	2.45	0.47
24:Y:104:THR:HG22	24:Y:104:THR:O	2.14	0.47
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.97	0.47
16:P:268:ARG:O	16:P:268:ARG:HD3	2.15	0.47
42:q:6:VAL:HG22	42:q:9:ARG:NH2	2.30	0.47
5:E:145:LEU:HD12	5:E:153:MET:SD	2.55	0.47
11:K:59:MET:HE2	14:N:27:LEU:HD13	1.97	0.47
12:L:485:TYR:O	12:L:489:THR:OG1	2.34	0.47
45:L:702:LMT:O5B	45:L:702:LMT:O6'	2.32	0.47
15:O:15:THR:HG23	15:O:253:ASP:OD1	2.15	0.47
38:m:25:SER:O	38:m:28:THR:N	2.48	0.47
15:O:138:MET:CE	54:O:401:GTP:HN21	2.27	0.46
38:m:23:ASP:O	38:m:23:ASP:OD1	2.33	0.46
47:B:202:PC1:O22	47:P:502:PC1:H151	2.15	0.46
37:l:82:ASP:OD1	38:m:71:ARG:NH2	2.48	0.46
29:d:120:ARG:HD2	38:m:115:ILE:HD13	1.97	0.46
35:j:61:ASP:OD1	40:o:106:ARG:NH2	2.49	0.46
2:B:86:MET:CE	2:B:103:VAL:HG23	2.46	0.46
7:G:579:ARG:HB2	7:G:636:VAL:HG22	1.96	0.46
4:D:165:THR:OG1	8:H:275:ALA:O	2.28	0.46
6:F:362:CYS:HB3	6:F:404:ILE:HD12	1.97	0.46
8:H:172:MET:HE3	8:H:177:PRO:HD3	1.97	0.46
10:J:120:ASN:O	11:K:3:MET:HB3	2.16	0.46
12:L:233:LEU:HD11	12:L:248:HIS:NE2	2.31	0.46
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.50	0.46
12:L:419:THR:HA	12:L:422:TYR:CE1	2.51	0.46
30:e:17:MET:O	30:e:17:MET:HG2	2.15	0.46
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.23	0.46
7:G:254:MET:HA	7:G:260:GLU:O	2.15	0.46
8:H:179:TRP:N	8:H:180:PRO:CD	2.79	0.46
11:K:73:LEU:HD21	14:N:41:ILE:HG13	1.98	0.46
16:P:176:ASP:OD1	16:P:176:ASP:C	2.58	0.46
8:H:199:ASP:HB2	8:H:202:GLU:OE2	2.16	0.45
4:D:219:SER:OG	60:D:507:HOH:O	2.21	0.45
10:J:70:TYR:HB3	11:K:27:MET:HE1	1.97	0.45
15:O:285:GLY:HA3	32:g:28:GLU:OE1	2.17	0.45
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.45
10:J:93:PHE:CE2	10:J:97:LEU:HD11	2.52	0.45
18:R:31:ARG:HA	42:q:121:PRO:O	2.16	0.45
8:H:232:ILE:HG21	26:a:16:LEU:HD21	1.98	0.45
11:K:37:MET:SD	14:N:68:MET:CE	3.01	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.98	0.45
7:G:315:VAL:O	7:G:340:SER:OG	2.31	0.45
25:Z:68:ARG:NH1	60:Z:401:HOH:O	2.35	0.45
8:H:87:ILE:N	8:H:88:PRO:CD	2.79	0.45
12:L:13:LEU:CD2	34:i:81:ILE:HD11	2.47	0.45
12:L:572:LYS:NZ	12:L:576:LEU:HD11	2.32	0.45
10:J:23:LYS:NZ	11:K:18:GLY:O	2.48	0.45
20:T:49:GLU:OE2	22:W:36:TYR:OH	2.32	0.45
51:d:301:3PE:H3E2	51:d:301:3PE:H3I3	1.98	0.45
13:M:116:ILE:HG12	13:M:174:LEU:HD13	1.99	0.45
15:O:279:LEU:HB2	15:O:282:VAL:HG22	1.97	0.45
23:X:44:LEU:HD22	23:X:130:VAL:HB	1.99	0.45
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.98	0.44
6:F:403:THR:HB	46:F:502:SF4:S4	2.57	0.44
7:G:190:MET:CE	7:G:690:ALA:HB1	2.41	0.44
53:N:1303:I49:I02	29:d:82:MET:O	3.05	0.44
16:P:330:GLU:HG2	16:P:333:ASP:OD1	2.17	0.44
4:D:47:LEU:HD21	8:H:126:LYS:HD3	1.99	0.44
7:G:266:LYS:HE2	7:G:671:PHE:O	2.16	0.44
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.99	0.44
18:R:32:GLN:HG2	42:q:122:GLN:HA	2.00	0.44
7:G:273:GLY:O	7:G:549:HIS:NE2	2.48	0.44
11:K:59:MET:N	11:K:60:PRO:CD	2.81	0.44
13:M:367:LEU:C	13:M:367:LEU:HD12	2.42	0.44
15:O:151:HIS:HB2	15:O:279:LEU:HD11	1.98	0.44
20:T:43:ASP:OD1	20:T:46:ASP:OD2	2.35	0.44
11:K:59:MET:HG3	11:K:60:PRO:HD3	2.00	0.44
15:O:104:ARG:NH2	54:O:401:GTP:O6	2.42	0.44
15:O:138:MET:HE3	54:O:401:GTP:HN21	1.82	0.44
3:C:37:VAL:HG12	43:r:69:MET:CE	2.47	0.44
12:L:203:MET:HG2	41:p:109:LEU:HD11	2.00	0.44
19:S:57:CYS:O	19:S:60:VAL:HG22	2.18	0.44
25:Z:93:GLU:OE2	30:e:94:PRO:HG3	2.17	0.44
37:l:145:ASP:OD2	37:l:148:LYS:NZ	2.49	0.44
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.57	0.44
5:E:87:TYR:HB3	6:F:181:ALA:O	2.18	0.44
10:J:7:PHE:CE1	11:K:3:MET:HE2	2.53	0.44
13:M:24:TRP:O	13:M:28:THR:OG1	2.30	0.44
15:O:151:HIS:CB	15:O:279:LEU:HD11	2.48	0.44
3:C:117:ILE:O	3:C:142:PHE:HA	2.17	0.43
30:e:56:LYS:O	30:e:60:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:306:LEU:C	6:F:306:LEU:HD12	2.43	0.43
12:L:375:VAL:HG22	35:j:32:MET:SD	2.59	0.43
12:L:489:THR:O	12:L:493:VAL:HG22	2.18	0.43
13:M:46:GLY:HA3	32:g:85:MET:HG2	2.00	0.43
24:Y:10:ASP:OD1	24:Y:10:ASP:O	2.36	0.43
1:A:1:FME:SD	10:J:2:MET:HE2	2.59	0.43
4:D:155:THR:HB	4:D:167:PHE:HA	1.99	0.43
6:F:96:ASN:ND2	6:F:187:GLY:O	2.40	0.43
8:H:207:LEU:O	8:H:209:SER:N	2.51	0.43
12:L:230:HIS:N	12:L:231:PRO:HD3	2.34	0.43
20:T:19:LEU:CD2	20:T:54:MET:HE1	2.48	0.43
20:U:51:ILE:HG21	20:U:67:ALA:HB1	2.00	0.43
10:J:135:PHE:CD2	10:J:135:PHE:O	2.72	0.43
22:W:68:LYS:HE2	22:W:68:LYS:HA	2.00	0.43
23:X:152:GLU:O	23:X:154:GLU:OE1	2.36	0.43
34:i:111:GLU:CD	41:p:16:THR:HG22	2.43	0.43
38:m:21:GLU:OE2	39:n:7:ALA:HB2	2.19	0.43
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.00	0.43
4:D:112:MET:HG3	4:D:181:TYR:CZ	2.54	0.43
7:G:391:PHE:CE2	7:G:395:ILE:HD11	2.53	0.43
8:H:202:GLU:O	8:H:203:GLY:C	2.61	0.43
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.99	0.43
15:O:312:VAL:HG11	28:c:1:LYS:HA	2.01	0.43
45:e:501:LMT:O5B	45:e:501:LMT:O3'	2.33	0.43
47:B:203:PC1:O13	47:B:203:PC1:H133	2.18	0.43
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.53	0.43
8:H:255:TYR:CD1	8:H:255:TYR:C	2.97	0.43
13:M:126:LEU:HD21	13:M:153:THR:HG21	2.00	0.43
13:M:194:PHE:CZ	24:Y:123:LEU:HD21	2.54	0.43
14:N:30:TRP:O	14:N:34:GLU:HG2	2.19	0.43
43:r:62:ALA:O	43:r:63:MET:HE2	2.18	0.43
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.25	0.42
29:d:112:VAL:O	41:p:159:LYS:NZ	2.51	0.42
43:r:71:SER:O	43:r:72:GLN:C	2.62	0.42
7:G:297:GLU:H	7:G:297:GLU:CD	2.27	0.42
12:L:421:ILE:HA	12:L:501:ALA:HB2	2.01	0.42
1:A:66:ASP:O	1:A:69:ILE:HG12	2.20	0.42
7:G:568:GLU:HA	7:G:587:VAL:O	2.19	0.42
8:H:318:THR:HG21	10:J:135:PHE:CE2	2.54	0.42
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.47	0.42
20:T:43:ASP:OD1	20:T:43:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:96:VAL:O	22:W:96:VAL:CG1	2.65	0.42
8:H:264:LEU:O	8:H:268:MET:HG2	2.19	0.42
16:P:282:ASP:OD2	16:P:286:ARG:NE	2.48	0.42
16:P:50:ARG:NH1	56:P:501:NDP:O2X	2.44	0.42
16:P:91:VAL:HG23	16:P:126:VAL:HG11	2.01	0.42
23:X:43:MET:HE3	25:Z:73:PRO:HA	2.01	0.42
24:Y:104:THR:HG21	24:Y:109:ILE:HD13	2.02	0.42
7:G:329:ILE:HD11	7:G:626:VAL:HG21	2.01	0.42
13:M:80:SER:OG	13:M:226:ALA:HB2	2.19	0.42
2:B:86:MET:HE1	2:B:103:VAL:HG23	2.02	0.42
26:a:66:LEU:O	26:a:69:ILE:HG12	2.20	0.42
27:b:42:LEU:HD21	27:b:46:ARG:NH1	2.35	0.42
1:A:108:GLN:O	1:A:109:LYS:HB2	2.20	0.42
7:G:272:ASP:OD1	7:G:681:SER:OG	2.38	0.42
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.02	0.42
10:J:103:MET:HG2	10:J:115:VAL:HG21	2.02	0.42
6:F:432:GLN:O	6:F:436:GLN:HG3	2.20	0.42
7:G:60:GLU:O	7:G:61:LYS:HG2	2.20	0.42
12:L:124:PHE:CZ	12:L:251:THR:HG21	2.55	0.42
12:L:434:GLN:HG3	36:k:52:TYR:CE1	2.55	0.42
15:O:280:PRO:HB3	32:g:25:ARG:HG3	2.01	0.42
19:S:64:LEU:HB2	19:S:78:LEU:HD11	2.02	0.42
21:V:63:ASP:OD1	21:V:63:ASP:C	2.63	0.41
40:o:14:VAL:O	40:o:14:VAL:HG23	2.20	0.41
8:H:77:MET:HE1	8:H:118:TRP:CZ3	2.55	0.41
8:H:108:MET:HE1	51:H:401:3PE:H391	2.02	0.41
20:U:49:GLU:OE1	39:n:44:ARG:NH1	2.52	0.41
7:G:145:LEU:HD22	7:G:269:PHE:CD2	2.54	0.41
12:L:145:GLU:OE1	12:L:179:ASP:OD1	2.38	0.41
19:S:21:HIS:O	19:S:62:PRO:HA	2.20	0.41
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.50	0.41
6:F:142:PHE:HB3	6:F:145:GLU:HB2	2.02	0.41
6:F:249:ARG:NH2	6:F:249:ARG:HB2	2.35	0.41
7:G:162:PHE:CZ	7:G:198:ASN:HB2	2.56	0.41
12:L:288:THR:HG21	12:L:307:SER:OG	2.20	0.41
13:M:285:LEU:HD23	13:M:285:LEU:C	2.46	0.41
20:U:11:ILE:HD11	20:U:86:VAL:HG21	2.02	0.41
32:g:51:PRO:O	32:g:55:ILE:HG12	2.21	0.41
1:A:18:VAL:HG21	8:H:76:ILE:HG13	2.02	0.41
2:B:125:TYR:CE2	4:D:102:TYR:CD1	3.08	0.41
12:L:253:VAL:HB	12:L:310:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:596:LEU:O	12:L:600:ILE:HG12	2.20	0.41
51:L:704:3PE:H291	34:i:80:ILE:HG23	2.02	0.41
23:X:130:VAL:HG23	27:b:55:PRO:HB2	2.01	0.41
24:Y:134:VAL:HG12	24:Y:135:PHE:CD1	2.55	0.41
36:k:42:ASP:OD1	39:n:41:CYS:SG	2.78	0.41
9:I:32:ARG:NH2	25:Z:26:PRO:O	2.54	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.35	0.41
11:K:43:MET:HE1	14:N:72:MET:CE	2.50	0.41
45:M:603:LMT:O2'	45:M:603:LMT:H11	2.21	0.41
15:O:180:GLN:O	15:O:184:GLN:OE1	2.38	0.41
23:X:14:VAL:HG22	23:X:15:GLN:N	2.35	0.41
27:b:27:LEU:HD22	27:b:31:LEU:HD11	2.02	0.41
6:F:90:PRO:O	6:F:218:CYS:HB3	2.21	0.41
12:L:10:VAL:O	12:L:14:LEU:HB2	2.19	0.41
13:M:93:LYS:O	13:M:97:THR:OG1	2.32	0.41
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.02	0.41
40:o:115:GLU:O	40:o:118:GLU:N	2.54	0.41
4:D:411:LEU:C	4:D:411:LEU:HD23	2.46	0.41
4:D:417:ILE:O	4:D:420:THR:HG22	2.21	0.41
5:E:143:GLU:O	5:E:144:CYS:C	2.64	0.41
7:G:329:ILE:CD1	7:G:626:VAL:HG21	2.50	0.41
7:G:375:ASP:OD1	7:G:446:ALA:HB1	2.21	0.41
7:G:480:SER:O	7:G:481:SER:OG	2.30	0.41
10:J:7:PHE:CD1	11:K:3:MET:HE2	2.56	0.41
10:J:170:GLU:OE2	10:J:173:ARG:NH1	2.54	0.41
12:L:71:ILE:HG23	13:M:310:MET:HE1	2.03	0.41
15:O:260:ARG:NH1	60:O:504:HOH:O	2.41	0.41
20:T:14:ARG:HE	20:T:57:GLU:CD	2.28	0.41
32:g:25:ARG:N	32:g:26:TRP:CE3	2.89	0.41
9:I:52:PHE:CZ	42:q:30:ALA:HA	2.56	0.41
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.50	0.41
19:S:18:ILE:HD12	19:S:50:LEU:HD21	2.03	0.40
28:c:38:ASP:OD2	29:d:77:LYS:NZ	2.41	0.40
7:G:653:ASN:OD1	7:G:654:GLN:N	2.54	0.40
9:I:75:GLU:O	9:I:105:ARG:NH1	2.54	0.40
15:O:198:TYR:CE2	15:O:202:ILE:HD11	2.56	0.40
16:P:145:TYR:CD2	16:P:286:ARG:HD3	2.57	0.40
12:L:14:LEU:O	12:L:14:LEU:HD23	2.21	0.40
13:M:23:ILE:HG13	13:M:24:TRP:N	2.36	0.40
51:M:604:3PE:H321	29:d:53:VAL:HG11	2.03	0.40
1:A:79:SER:HA	1:A:87:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:THR:HG22	5:E:106:THR:N	2.36	0.40
10:J:84:LEU:HD13	52:J:701:CDL:CB7	2.50	0.40
14:N:269:GLU:OE2	14:N:269:GLU:HA	2.22	0.40
32:g:118:ILE:HG21	41:p:162:MET:HE1	2.03	0.40
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.03	0.40
4:D:161:ILE:O	4:D:161:ILE:HG22	2.22	0.40
32:g:120:LEU:HD21	41:p:162:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	153/216 (71%)	147 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	411 (96%)	15 (4%)	1 (0%)	43	58
5	E	211/249 (85%)	205 (97%)	6 (3%)	0	100	100
6	F	429/464 (92%)	420 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	668 (97%)	18 (3%)	0	100	100
8	H	316/318 (99%)	304 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	172/175 (98%)	162 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	591/606 (98%)	568 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	339/380 (89%)	335 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
18	R	93/124 (75%)	89 (96%)	4 (4%)	0	100	100
19	S	80/99 (81%)	77 (96%)	3 (4%)	0	100	100
20	T	74/156 (47%)	73 (99%)	1 (1%)	0	100	100
20	U	84/156 (54%)	84 (100%)	0	0	100	100
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
25	Z	138/144 (96%)	134 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	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	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	91 (98%)	2 (2%)	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	98/127 (77%)	94 (96%)	4 (4%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100
36	k	78/98 (80%)	76 (97%)	2 (3%)	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
38	m	109/129 (84%)	105 (96%)	4 (4%)	0	100	100
39	n	170/179 (95%)	168 (99%)	2 (1%)	0	100	100
40	o	118/137 (86%)	113 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	167 (99%)	1 (1%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	40/109 (37%)	39 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8064/9212 (88%)	7860 (98%)	203 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	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%)	131 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	518/533 (97%)	518 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	119/121 (98%)	119 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100
31	f	49/54 (91%)	49 (100%)	0	100	100
32	g	89/131 (68%)	89 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	97/120 (81%)	97 (100%)	0	100	100
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	101/115 (88%)	101 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	84 (100%)	0	100	100
44	s	41/92 (45%)	41 (100%)	0	100	100
All	All	7114/7892 (90%)	7114 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	160	HIS
3	C	200	ASN
4	D	13	GLN
4	D	150	HIS
4	D	201	GLN
5	E	37	ASN
5	E	42	HIS
6	F	148	ASN
6	F	200	GLN
6	F	421	HIS
6	F	435	GLN
7	G	392	ASN
7	G	441	GLN
7	G	517	ASN
7	G	535	GLN
7	G	629	ASN
11	K	52	HIS
12	L	200	GLN
12	L	541	ASN
12	L	570	GLN
13	M	304	GLN
13	M	338	HIS
13	M	415	GLN
14	N	172	GLN
14	N	274	ASN
14	N	289	ASN
15	O	76	ASN
15	O	251	GLN
15	O	287	HIS
16	P	103	ASN
16	P	250	HIS
17	Q	44	ASN
18	R	90	GLN
19	S	30	GLN
19	S	61	GLN
19	S	85	GLN
20	T	33	ASN
21	V	72	GLN
21	V	82	GLN
22	W	70	ASN
29	d	97	HIS
29	d	117	HIS
30	e	69	GLN

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Mol	Chain	Res	Type
31	f	30	ASN
33	h	63	HIS
34	i	88	HIS
39	n	52	ASN
39	n	140	GLN
40	o	54	GLN
41	p	122	GLN
42	q	91	HIS
42	q	112	ASN
43	r	24	GLN
44	s	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FME	J	1	10	8,9,10	0.98	0	8,9,11	1.17	1 (12%)
24	AYA	Y	1	24	6,7,8	1.85	1 (16%)	6,8,10	1.38	1 (16%)
13	FME	M	1	13	8,9,10	1.05	1 (12%)	8,9,11	0.95	0
8	FME	H	1	8	8,9,10	1.00	0	8,9,11	0.94	0
34	SAC	i	1	34	7,8,9	0.98	0	7,9,11	1.55	2 (28%)
14	FME	N	1	14	8,9,10	0.92	0	8,9,11	1.05	1 (12%)
12	FME	L	1	12	8,9,10	1.06	1 (12%)	8,9,11	0.80	0
4	2MR	D	85	4	10,12,13	2.76	3 (30%)	5,13,15	1.14	1 (20%)
11	FME	K	1	11	8,9,10	0.96	0	8,9,11	0.79	0
43	AYA	r	1	43	6,7,8	1.88	2 (33%)	6,8,10	1.22	1 (16%)
1	FME	A	1	1	8,9,10	0.99	1 (12%)	8,9,11	0.85	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	-
24	AYA	Y	1	24	-	0/5/6/8	-
13	FME	M	1	13	-	0/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
12	FME	L	1	12	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	1/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
1	FME	A	1	1	-	2/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.26	1.44	1.33
4	D	85	2MR	CZ-NE	4.78	1.44	1.34
4	D	85	2MR	O-C	4.12	1.35	1.20
24	Y	1	AYA	CT-N	3.48	1.45	1.34
43	r	1	AYA	CT-N	3.41	1.45	1.34
12	L	1	FME	CA-N	-2.24	1.43	1.46
13	M	1	FME	CA-N	-2.20	1.43	1.46
43	r	1	AYA	OT-CT	-2.13	1.18	1.23
1	A	1	FME	CA-N	-2.00	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C-CA-N	2.77	114.85	109.50
10	J	1	FME	C-CA-N	2.46	114.25	109.50
24	Y	1	AYA	CM-CT-N	2.45	120.18	116.12
34	i	1	SAC	OG-CB-CA	-2.22	105.02	111.13
43	r	1	AYA	CM-CT-N	2.21	119.78	116.12
4	D	85	2MR	NE-CZ-NH2	-2.17	117.49	119.48
14	N	1	FME	C-CA-N	2.09	113.54	109.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	85	2MR	1	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	SF4	B	201	2	0,12,12	-	-	-		
51	3PE	Y	802	-	34,34,50	1.05	4 (11%)	37,39,55	1.22	2 (5%)
45	LMT	Y	801	-	36,36,36	1.20	3 (8%)	47,47,47	1.20	4 (8%)
47	PC1	B	203	-	34,34,53	1.18	4 (11%)	40,42,61	1.12	2 (5%)
47	PC1	P	502	-	20,20,53	1.76	3 (15%)	24,27,61	1.17	1 (4%)
52	CDL	a	101	-	75,75,99	1.01	6 (8%)	81,87,111	1.13	5 (6%)
45	LMT	l	201	-	36,36,36	1.21	3 (8%)	47,47,47	1.10	4 (8%)
45	LMT	k	101	-	36,36,36	1.19	3 (8%)	47,47,47	1.01	3 (6%)
45	LMT	L	702	-	36,36,36	1.16	3 (8%)	47,47,47	0.83	0
52	CDL	J	701	-	61,61,99	1.09	6 (9%)	67,73,111	1.26	4 (5%)
51	3PE	X	401	-	44,44,50	0.92	4 (9%)	47,49,55	1.16	2 (4%)
45	LMT	M	603	-	36,36,36	1.22	5 (13%)	47,47,47	1.24	4 (8%)
56	NDP	P	501	-	51,52,52	2.23	4 (7%)	71,80,80	1.51	15 (21%)
49	FMN	F	501	-	33,33,33	1.06	2 (6%)	48,50,50	1.27	6 (12%)
54	GTP	O	401	55	33,34,34	3.26	15 (45%)	50,54,54	1.85	13 (26%)
51	3PE	M	604	-	50,50,50	0.86	3 (6%)	53,55,55	1.09	2 (3%)
45	LMT	h	1002	-	36,36,36	1.12	2 (5%)	47,47,47	1.22	4 (8%)
45	LMT	A	302	-	36,36,36	1.18	3 (8%)	47,47,47	1.41	3 (6%)
48	FES	E	301	5	0,4,4	-	-	-		
51	3PE	I	201	-	50,50,50	0.88	4 (8%)	53,55,55	0.98	2 (3%)
51	3PE	L	704	-	44,44,50	0.93	4 (9%)	47,49,55	1.16	2 (4%)
45	LMT	M	602	-	36,36,36	1.21	3 (8%)	47,47,47	0.94	1 (2%)
51	3PE	d	301	-	50,50,50	0.85	4 (8%)	53,55,55	1.17	3 (5%)
51	3PE	N	1301	-	50,50,50	0.89	4 (8%)	53,55,55	1.11	2 (3%)
47	PC1	M	605	-	48,48,53	0.99	4 (8%)	54,56,61	1.08	2 (3%)
52	CDL	L	703	-	68,68,99	1.05	6 (8%)	74,80,111	1.13	4 (5%)
51	3PE	H	401	-	43,43,50	0.94	3 (6%)	46,48,55	1.14	2 (4%)
46	SF4	G	802	7	0,12,12	-	-	-		
45	LMT	e	501	-	36,36,36	1.21	3 (8%)	47,47,47	1.05	2 (4%)
59	MYR	o	201	40	5,6,15	1.02	0	4,5,15	0.79	0
46	SF4	G	801	7	0,12,12	-	-	-		
48	FES	G	803	7	0,4,4	-	-	-		
47	PC1	B	202	-	41,41,53	1.06	3 (7%)	47,49,61	1.05	2 (4%)
46	SF4	I	202	9	0,12,12	-	-	-		
51	3PE	N	1302	-	40,40,50	0.98	4 (10%)	43,45,55	1.01	2 (4%)
46	SF4	I	203	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	LMT	Z	301	-	36,36,36	1.27	3 (8%)	47,47,47	1.35	5 (10%)
51	3PE	H	402	-	33,33,50	1.30	4 (12%)	34,37,55	1.24	2 (5%)
51	3PE	L	701	-	48,48,50	0.91	3 (6%)	51,53,55	1.10	2 (3%)
58	EHZ	U	101	20	31,36,37	1.53	5 (16%)	36,44,47	1.67	4 (11%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
53	I49	N	1303	-	15,17,17	0.86	1 (6%)	17,22,22	1.60	2 (11%)
51	3PE	M	601	-	45,45,50	0.92	3 (6%)	48,50,55	1.04	2 (4%)
52	CDL	K	401	-	70,70,99	1.04	7 (10%)	76,82,111	1.11	4 (5%)
52	CDL	h	1001	-	66,66,99	1.06	7 (10%)	72,78,111	1.21	4 (5%)
45	LMT	A	301	-	36,36,36	1.16	2 (5%)	47,47,47	0.98	3 (6%)
58	EHZ	T	101	20	31,36,37	1.55	5 (16%)	36,44,47	1.72	7 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SF4	B	201	2	-	-	0/6/5/5
51	3PE	Y	802	-	-	16/38/38/54	-
45	LMT	Y	801	-	-	10/21/61/61	0/2/2/2
47	PC1	B	203	-	-	17/38/38/57	-
47	PC1	P	502	-	-	8/22/22/57	-
52	CDL	a	101	-	-	34/86/86/110	-
45	LMT	l	201	-	-	4/21/61/61	0/2/2/2
45	LMT	k	101	-	-	4/21/61/61	0/2/2/2
45	LMT	L	702	-	-	9/21/61/61	0/2/2/2
52	CDL	J	701	-	-	28/71/71/110	-
51	3PE	X	401	-	-	20/48/48/54	-
45	LMT	M	603	-	-	8/21/61/61	0/2/2/2
56	NDP	P	501	-	-	6/34/77/77	0/5/5/5
49	FMN	F	501	-	-	1/18/18/18	0/3/3/3
54	GTP	O	401	55	-	7/22/38/38	0/3/3/3
51	3PE	M	604	-	-	29/54/54/54	-
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
45	LMT	A	302	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	I	201	-	-	24/54/54/54	-
51	3PE	L	704	-	-	20/48/48/54	-
48	FES	E	301	5	-	-	0/1/1/1
45	LMT	M	602	-	-	9/21/61/61	0/2/2/2
51	3PE	d	301	-	-	16/54/54/54	-
51	3PE	N	1301	-	-	21/54/54/54	-
47	PC1	M	605	-	-	23/52/52/57	-
52	CDL	L	703	-	-	33/79/79/110	-
51	3PE	H	401	-	-	15/47/47/54	-
46	SF4	G	802	7	-	-	0/6/5/5
45	LMT	e	501	-	-	11/21/61/61	0/2/2/2
59	MYR	o	201	40	-	3/4/4/13	-
46	SF4	G	801	7	-	-	0/6/5/5
48	FES	G	803	7	-	-	0/1/1/1
47	PC1	B	202	-	-	13/45/45/57	-
46	SF4	I	202	9	-	-	0/6/5/5
51	3PE	N	1302	-	-	20/44/44/54	-
46	SF4	I	203	9	-	-	0/6/5/5
45	LMT	Z	301	-	-	8/21/61/61	0/2/2/2
51	3PE	H	402	-	-	18/36/36/54	-
51	3PE	L	701	-	-	26/52/52/54	-
58	EHZ	U	101	20	-	7/42/44/45	-
46	SF4	F	502	6	-	-	0/6/5/5
53	I49	N	1303	-	-	3/10/10/10	0/1/1/1
51	3PE	M	601	-	-	20/49/49/54	-
52	CDL	K	401	-	-	37/81/81/110	-
52	CDL	h	1001	-	-	34/77/77/110	-
45	LMT	A	301	-	-	7/21/61/61	0/2/2/2
58	EHZ	T	101	20	-	15/42/44/45	-

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	12.76	1.81	1.59
54	O	401	GTP	O6-C6	8.50	1.39	1.23
54	O	401	GTP	C5-N7	6.66	1.52	1.39
54	O	401	GTP	PA-O3A	5.26	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	O	401	GTP	PB-O3A	5.03	1.64	1.59
47	P	502	PC1	O21-C2	-4.95	1.40	1.46
58	T	101	EHZ	C12-N1	4.91	1.45	1.33
58	T	101	EHZ	C15-N2	4.89	1.45	1.33
58	U	101	EHZ	C15-N2	4.86	1.45	1.33
54	O	401	GTP	C2-N1	4.84	1.49	1.37
58	U	101	EHZ	C12-N1	4.71	1.44	1.33
54	O	401	GTP	C2-N3	4.64	1.44	1.33
54	O	401	GTP	C8-N9	-4.53	1.27	1.37
54	O	401	GTP	C2-N2	4.52	1.44	1.34
51	H	402	3PE	O21-C2	-4.45	1.40	1.46
54	O	401	GTP	PB-O3B	4.42	1.64	1.59
56	P	501	NDP	PA-O3	3.98	1.63	1.59
54	O	401	GTP	C4-N9	-3.71	1.28	1.38
45	Z	301	LMT	O5B-C1B	3.57	1.51	1.41
45	M	602	LMT	O5B-C1B	3.49	1.50	1.41
45	e	501	LMT	O5B-C1B	3.48	1.50	1.41
56	P	501	NDP	PN-O5D	3.47	1.73	1.59
45	Z	301	LMT	O5'-C1'	3.42	1.50	1.41
45	M	603	LMT	O5B-C1B	3.38	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.37	1.32	1.44
45	k	101	LMT	O5B-C1B	3.36	1.50	1.41
45	A	302	LMT	O5B-C1B	3.35	1.50	1.41
45	l	201	LMT	O5B-C1B	3.31	1.50	1.41
45	L	702	LMT	O5B-C1B	3.29	1.50	1.41
45	A	301	LMT	O5B-C1B	3.28	1.50	1.41
45	l	201	LMT	O5'-C1'	3.28	1.50	1.41
45	e	501	LMT	O5'-C1'	3.22	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.21	1.50	1.41
51	H	402	3PE	O21-C21	3.18	1.40	1.33
45	Y	801	LMT	O5B-C1B	3.18	1.50	1.41
45	A	302	LMT	O5'-C1'	3.11	1.49	1.41
49	F	501	FMN	C4A-N5	3.09	1.37	1.30
47	P	502	PC1	O21-C21	3.09	1.40	1.33
45	M	602	LMT	O5'-C1'	3.06	1.49	1.41
45	M	603	LMT	O5'-C1'	3.05	1.49	1.41
51	L	701	3PE	O21-C2	-3.02	1.39	1.46
45	Y	801	LMT	O5'-C1'	3.02	1.49	1.41
45	A	301	LMT	O5'-C1'	3.00	1.49	1.41
45	k	101	LMT	O5'-C1'	3.00	1.49	1.41
51	M	601	3PE	O21-C2	-2.96	1.39	1.46
51	N	1301	3PE	O21-C2	-2.94	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	K	401	CDL	OA6-CA4	-2.92	1.39	1.46
45	L	702	LMT	O5'-C1'	2.90	1.49	1.41
54	O	401	GTP	O4'-C1'	2.89	1.48	1.42
51	H	401	3PE	O21-C2	-2.89	1.39	1.46
45	h	1002	LMT	O5'-C1'	2.87	1.49	1.41
52	a	101	CDL	OB6-CB4	-2.85	1.39	1.46
52	h	1001	CDL	OA6-CA4	-2.84	1.39	1.46
51	N	1302	3PE	O21-C2	-2.82	1.40	1.46
52	L	703	CDL	OB6-CB4	-2.81	1.40	1.46
52	J	701	CDL	OB6-CB4	-2.80	1.40	1.46
52	L	703	CDL	OA6-CA4	-2.77	1.40	1.46
52	a	101	CDL	OA6-CA4	-2.75	1.40	1.46
47	B	202	PC1	O21-C2	-2.74	1.40	1.46
51	X	401	3PE	O21-C2	-2.73	1.40	1.46
52	K	401	CDL	OB6-CB4	-2.70	1.40	1.46
51	Y	802	3PE	O21-C2	-2.70	1.40	1.46
52	a	101	CDL	OA8-CA6	-2.68	1.39	1.45
47	B	203	PC1	O21-C2	-2.65	1.40	1.46
52	h	1001	CDL	OB6-CB4	-2.63	1.40	1.46
51	L	704	3PE	O21-C2	-2.63	1.40	1.46
51	H	402	3PE	O31-C31	2.60	1.40	1.33
58	U	101	EHZ	O4-C15	-2.60	1.18	1.23
52	J	701	CDL	OA6-CA5	2.59	1.40	1.35
52	K	401	CDL	OA8-CA6	-2.58	1.39	1.45
51	I	201	3PE	O21-C2	-2.58	1.40	1.46
51	L	701	3PE	O31-C3	-2.55	1.39	1.45
51	M	604	3PE	O31-C31	2.53	1.40	1.33
51	I	201	3PE	O31-C3	-2.53	1.39	1.45
51	H	401	3PE	O31-C3	-2.51	1.39	1.45
58	T	101	EHZ	O4-C15	-2.51	1.18	1.23
51	M	601	3PE	O31-C3	-2.50	1.39	1.45
47	M	605	PC1	O21-C2	-2.50	1.40	1.46
52	J	701	CDL	OA8-CA7	2.50	1.40	1.33
51	L	704	3PE	O31-C3	-2.47	1.39	1.45
51	N	1301	3PE	O31-C3	-2.46	1.39	1.45
52	L	703	CDL	OB8-CB7	2.45	1.40	1.33
54	O	401	GTP	PG-O3G	-2.40	1.45	1.54
51	N	1302	3PE	O31-C31	2.40	1.40	1.33
53	N	1303	I49	C15-N02	-2.38	1.31	1.36
54	O	401	GTP	PG-O2G	-2.37	1.46	1.54
51	d	301	3PE	O31-C3	-2.37	1.39	1.45
51	Y	802	3PE	O31-C31	2.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	101	CDL	OB8-CB7	2.34	1.40	1.33
51	Y	802	3PE	O31-C3	-2.33	1.40	1.45
52	L	703	CDL	OA8-CA6	-2.33	1.40	1.45
54	O	401	GTP	C2'-C3'	-2.33	1.47	1.53
58	T	101	EHZ	O3-C12	-2.33	1.18	1.23
58	U	101	EHZ	O3-C12	-2.32	1.18	1.23
47	M	605	PC1	O31-C3	-2.32	1.40	1.45
47	B	203	PC1	O31-C31	2.32	1.40	1.33
52	L	703	CDL	OA8-CA7	2.32	1.40	1.33
51	X	401	3PE	O31-C3	-2.31	1.40	1.45
52	J	701	CDL	OB8-CB6	-2.31	1.40	1.45
52	h	1001	CDL	OA8-CA6	-2.29	1.40	1.45
52	h	1001	CDL	OA8-CA7	2.28	1.40	1.33
51	M	604	3PE	O21-C2	-2.27	1.41	1.46
45	Z	301	LMT	O5'-C5'	2.27	1.49	1.44
47	B	202	PC1	O31-C3	-2.26	1.40	1.45
52	a	101	CDL	OB8-CB6	-2.25	1.40	1.45
52	h	1001	CDL	OB8-CB6	-2.25	1.40	1.45
52	K	401	CDL	OB8-CB6	-2.25	1.40	1.45
52	h	1001	CDL	OB8-CB7	2.25	1.39	1.33
52	J	701	CDL	OA6-CA4	-2.25	1.41	1.46
51	d	301	3PE	O21-C2	-2.24	1.41	1.46
52	K	401	CDL	OB8-CB7	2.24	1.39	1.33
51	I	201	3PE	O21-C21	2.23	1.40	1.34
51	M	604	3PE	O21-C21	2.22	1.40	1.34
51	H	401	3PE	O31-C31	2.22	1.39	1.33
47	M	605	PC1	O31-C31	2.21	1.39	1.33
47	B	202	PC1	O31-C31	2.21	1.39	1.33
45	A	302	LMT	O1B-C4'	2.20	1.49	1.43
51	L	704	3PE	O31-C31	2.20	1.39	1.33
51	X	401	3PE	O31-C31	2.18	1.39	1.33
52	K	401	CDL	OB6-CB5	2.17	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.17	1.40	1.34
47	B	203	PC1	O21-C21	2.16	1.40	1.34
51	d	301	3PE	O21-C21	2.15	1.40	1.34
47	M	605	PC1	O21-C21	2.15	1.40	1.34
51	X	401	3PE	O21-C21	2.14	1.40	1.34
52	J	701	CDL	OB8-CB7	2.13	1.39	1.33
45	M	603	LMT	O5B-C5B	2.13	1.49	1.44
45	M	603	LMT	O5'-C5'	2.13	1.49	1.44
45	e	501	LMT	O5B-C5B	2.13	1.49	1.44
52	a	101	CDL	OA6-CA5	2.13	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	M	601	3PE	O31-C31	2.12	1.39	1.33
51	N	1302	3PE	O21-C21	2.11	1.40	1.34
51	d	301	3PE	O31-C31	2.11	1.39	1.33
51	I	201	3PE	O31-C31	2.11	1.39	1.33
47	P	502	PC1	O31-C3	-2.11	1.40	1.45
47	B	203	PC1	O31-C3	-2.10	1.40	1.45
51	H	402	3PE	O31-C3	-2.10	1.40	1.45
51	Y	802	3PE	O21-C21	2.10	1.40	1.34
51	N	1302	3PE	O31-C3	-2.09	1.40	1.45
45	l	201	LMT	O5B-C5B	2.09	1.49	1.44
51	N	1301	3PE	O31-C31	2.09	1.39	1.33
51	L	701	3PE	O31-C31	2.09	1.39	1.33
45	L	702	LMT	O5B-C5B	2.08	1.49	1.44
45	k	101	LMT	O5B-C5B	2.07	1.49	1.44
51	L	704	3PE	O21-C21	2.06	1.40	1.34
58	T	101	EHZ	C9-S1	2.04	1.81	1.76
51	N	1301	3PE	O21-C21	2.04	1.40	1.34
52	K	401	CDL	OA8-CA7	2.04	1.39	1.33
54	O	401	GTP	PA-O2A	-2.02	1.46	1.55
45	M	602	LMT	O5B-C5B	2.02	1.49	1.44
49	F	501	FMN	C10-N1	2.01	1.37	1.33
45	M	603	LMT	O1B-C4'	2.01	1.49	1.43
58	U	101	EHZ	C9-S1	2.01	1.81	1.76
52	L	703	CDL	OB8-CB6	-2.00	1.40	1.45
45	Y	801	LMT	O5'-C5'	2.00	1.49	1.44

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	O	401	GTP	C8-N9-C4	7.46	120.00	106.03
58	U	101	EHZ	C8-C9-S1	6.63	121.92	113.56
58	T	101	EHZ	C8-C9-S1	6.37	121.59	113.56
45	A	302	LMT	C1-O1'-C1'	5.08	122.36	113.68
52	J	701	CDL	OA6-CA5-C11	4.75	119.57	111.09
51	d	301	3PE	O21-C21-C22	4.63	121.50	111.48
47	P	502	PC1	O21-C21-O22	-4.61	119.78	125.70
52	J	701	CDL	OB6-CB5-C51	4.50	121.22	111.48
51	H	402	3PE	O21-C21-O22	-4.41	120.04	125.70
51	L	704	3PE	O21-C21-C22	4.37	120.93	111.48
52	h	1001	CDL	OB6-CB5-C51	4.32	120.82	111.48
51	X	401	3PE	O21-C21-C22	4.27	120.71	111.48
47	M	605	PC1	O21-C21-C22	4.26	120.69	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	M	604	3PE	O21-C21-C22	4.24	120.65	111.48
47	B	203	PC1	O21-C21-C22	4.23	120.63	111.48
45	A	302	LMT	O1'-C1'-C2'	4.18	114.63	108.27
51	Y	802	3PE	O21-C21-C22	4.17	120.51	111.48
47	B	202	PC1	O21-C21-C22	4.14	120.43	111.48
52	a	101	CDL	OA6-CA5-C11	4.08	120.31	111.48
52	h	1001	CDL	OA6-CA5-C11	4.01	120.15	111.48
51	L	701	3PE	O21-C21-C22	4.01	120.15	111.48
52	L	703	CDL	OA6-CA5-C11	3.91	119.93	111.48
56	P	501	NDP	O2B-P2B-O1X	-3.88	95.51	109.33
52	a	101	CDL	OB6-CB5-C51	3.84	119.78	111.48
52	K	401	CDL	OA6-CA5-C11	3.82	119.74	111.48
51	N	1301	3PE	O21-C21-C22	3.80	119.71	111.48
45	M	603	LMT	O5'-C5'-C4'	3.69	117.36	109.72
51	I	201	3PE	O21-C21-C22	3.66	119.39	111.48
52	K	401	CDL	OB6-CB5-C51	3.64	119.36	111.48
51	N	1302	3PE	O21-C21-C22	3.64	119.35	111.48
56	P	501	NDP	P2B-O2B-C2B	-3.64	113.72	123.43
51	H	401	3PE	O21-C21-C22	3.56	119.17	111.48
45	Z	301	LMT	O5B-C1B-C2B	3.54	117.64	110.37
52	L	703	CDL	OB6-CB5-C51	3.49	119.03	111.48
51	H	402	3PE	O31-C31-C32	3.49	122.47	111.83
45	Z	301	LMT	C1B-C2B-C3B	3.46	117.28	110.01
49	F	501	FMN	C4-N3-C2	-3.45	119.51	125.64
51	M	601	3PE	O21-C21-C22	3.42	118.88	111.48
53	N	1303	I49	N01-C14-N03	3.40	126.53	120.26
54	O	401	GTP	C2-N1-C6	-3.32	119.09	125.11
56	P	501	NDP	O3-PA-O1A	-3.31	100.75	110.70
58	U	101	EHZ	O2-C9-C8	-3.19	118.72	123.74
51	H	401	3PE	O31-C31-C32	3.19	121.55	111.83
51	M	604	3PE	O31-C31-C32	3.18	121.54	111.83
45	Z	301	LMT	O5'-C5'-C4'	3.12	116.16	109.72
51	Y	802	3PE	O31-C31-C32	3.04	121.09	111.83
49	F	501	FMN	C4A-C10-N10	3.02	120.80	116.48
51	N	1301	3PE	O31-C31-C32	3.00	120.97	111.83
52	J	701	CDL	OA8-CA7-C31	2.99	120.94	111.83
45	Y	801	LMT	O5'-C5'-C4'	2.95	115.82	109.72
47	B	203	PC1	O31-C31-C32	2.94	120.81	111.83
58	U	101	EHZ	C10-S1-C9	2.94	110.53	101.84
58	T	101	EHZ	C10-S1-C9	2.93	110.52	101.84
54	O	401	GTP	C1'-N9-C8	-2.93	118.42	126.73
58	T	101	EHZ	O2-C9-S1	-2.92	118.97	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	h	1001	CDL	OB8-CB7-C71	2.91	120.71	111.83
54	O	401	GTP	O2G-PG-O3B	2.90	114.36	104.64
56	P	501	NDP	PA-O5B-C5B	-2.86	104.96	121.35
51	X	401	3PE	O31-C31-C32	2.86	120.55	111.83
52	h	1001	CDL	OA8-CA7-C31	2.85	120.54	111.83
45	h	1002	LMT	C1B-C2B-C3B	2.84	115.98	110.01
52	K	401	CDL	OB8-CB7-C71	2.83	120.47	111.83
47	B	202	PC1	O31-C31-C32	2.81	120.42	111.83
45	h	1002	LMT	C4B-C3B-C2B	2.81	115.77	110.83
45	Y	801	LMT	C3B-C4B-C5B	2.81	115.32	110.23
53	N	1303	I49	N05-C15-N04	-2.78	112.15	120.07
52	L	703	CDL	OB8-CB7-C71	2.74	120.20	111.83
58	T	101	EHZ	O2-C9-C8	-2.74	119.43	123.74
45	M	603	LMT	C3'-C4'-C5'	2.73	116.99	110.93
45	Z	301	LMT	C1'-O5'-C5'	2.72	119.03	113.72
47	M	605	PC1	O31-C31-C32	2.72	120.12	111.83
52	J	701	CDL	OB8-CB7-C71	2.70	120.06	111.83
51	L	704	3PE	O31-C31-C32	2.69	120.04	111.83
45	l	201	LMT	O5B-C5B-C4B	2.68	114.52	109.70
56	P	501	NDP	O4B-C4B-C3B	2.67	110.45	105.15
45	A	302	LMT	C1B-C2B-C3B	2.67	115.62	110.01
56	P	501	NDP	O2N-PN-O3	2.66	114.47	107.27
52	a	101	CDL	OB8-CB7-C71	2.66	119.95	111.83
56	P	501	NDP	PN-O5D-C5D	-2.66	106.13	121.35
49	F	501	FMN	C4A-C4-N3	2.65	119.99	113.25
51	L	701	3PE	O31-C31-C32	2.65	119.90	111.83
58	T	101	EHZ	C13-C14-N2	-2.65	106.37	112.00
51	d	301	3PE	O31-C31-C32	2.64	119.89	111.83
51	M	601	3PE	O31-C31-C32	2.64	119.87	111.83
52	L	703	CDL	OA8-CA7-C31	2.63	119.85	111.83
58	U	101	EHZ	O2-C9-S1	-2.61	119.36	122.68
58	T	101	EHZ	C13-C12-N1	2.60	121.07	116.34
54	O	401	GTP	O2A-PA-O1A	-2.58	100.43	112.44
51	N	1302	3PE	O31-C31-C32	2.57	119.67	111.83
56	P	501	NDP	O3X-P2B-O2X	2.56	117.40	107.80
51	I	201	3PE	O31-C31-C32	2.52	119.53	111.83
49	F	501	FMN	O4-C4-C4A	-2.52	119.89	126.53
54	O	401	GTP	O3G-PG-O3B	2.49	113.00	104.64
54	O	401	GTP	C3'-C2'-C1'	2.49	106.18	101.46
54	O	401	GTP	C5-C6-N1	2.48	119.56	113.25
54	O	401	GTP	C2'-C3'-C4'	2.47	107.39	102.61
52	a	101	CDL	OA8-CA7-C31	2.44	119.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	101	LMT	O5B-C5B-C4B	2.43	114.08	109.70
56	P	501	NDP	O2N-PN-O1N	2.42	123.72	112.44
56	P	501	NDP	O5D-PN-O1N	-2.41	99.39	108.94
45	M	603	LMT	C6'-C5'-C4'	-2.39	106.67	113.38
52	K	401	CDL	OA8-CA7-C31	2.36	119.03	111.83
56	P	501	NDP	N3A-C4A-N9A	2.35	131.17	127.17
56	P	501	NDP	C5B-C4B-C3B	-2.32	106.86	115.21
56	P	501	NDP	C2A-N1A-C6A	-2.32	114.92	118.73
54	O	401	GTP	O6-C6-C5	-2.30	120.46	126.53
45	l	201	LMT	C3B-C4B-C5B	2.29	114.39	110.23
54	O	401	GTP	C5-C4-N9	-2.29	101.56	105.66
49	F	501	FMN	C10-C4A-N5	-2.28	120.15	124.81
54	O	401	GTP	O2B-PB-O1B	-2.27	101.90	112.44
45	l	201	LMT	O5'-C1'-C2'	2.26	115.02	110.37
45	Z	301	LMT	C1B-O1B-C4'	-2.22	112.72	117.98
45	M	603	LMT	C1-O1'-C1'	2.18	117.41	113.68
45	e	501	LMT	O5B-C5B-C4B	2.18	113.62	109.70
45	A	301	LMT	C1B-O1B-C4'	-2.17	112.84	117.98
51	d	301	3PE	O21-C21-O22	-2.17	118.64	123.70
56	P	501	NDP	C5A-C4A-N3A	-2.12	123.80	126.72
45	Y	801	LMT	O5B-C5B-C4B	2.11	113.50	109.70
45	h	1002	LMT	C1B-O5B-C5B	-2.10	109.61	113.72
52	a	101	CDL	CA6-CA4-CA3	-2.10	106.88	111.78
45	Y	801	LMT	C1'-O5'-C5'	2.10	117.81	113.72
45	l	201	LMT	C4B-C3B-C2B	2.09	114.50	110.83
45	e	501	LMT	O5'-C5'-C4'	2.09	114.04	109.72
49	F	501	FMN	C4A-C10-N1	-2.08	119.48	124.59
58	T	101	EHZ	C19-C17-C16	2.08	112.31	108.77
45	k	101	LMT	C1B-O1B-C4'	-2.07	113.08	117.98
45	h	1002	LMT	C3B-C4B-C5B	2.07	113.98	110.23
54	O	401	GTP	N9-C8-N7	-2.06	109.58	113.40
45	A	301	LMT	O1'-C1'-C2'	2.04	111.37	108.27
56	P	501	NDP	O7N-C7N-C3N	2.04	124.74	120.90
45	A	301	LMT	C1B-O5B-C5B	-2.02	109.77	113.72
45	M	602	LMT	O1'-C1'-C2'	2.01	111.33	108.27
45	k	101	LMT	C2'-C3'-C4'	2.01	114.23	109.68

There are no chirality outliers.

All (605) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	302	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
45	L	702	LMT	C2'-C1'-O1'-C1
45	M	603	LMT	O5'-C1'-O1'-C1
45	Z	301	LMT	O5'-C1'-O1'-C1
45	Z	301	LMT	C2-C1-O1'-C1'
47	B	203	PC1	C11-O13-P-O14
47	M	605	PC1	C11-O13-P-O12
47	M	605	PC1	C11-O13-P-O14
47	M	605	PC1	C11-O13-P-O11
47	M	605	PC1	C22-C21-O21-C2
47	P	502	PC1	C11-O13-P-O12
47	P	502	PC1	C11-O13-P-O14
47	P	502	PC1	C11-O13-P-O11
47	P	502	PC1	C1-O11-P-O13
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	O13-C11-C12-N
51	H	402	3PE	C1-C2-O21-C21
51	H	402	3PE	O22-C21-O21-C2
51	I	201	3PE	O11-C1-C2-O21
51	L	701	3PE	C1-O11-P-O13
51	L	701	3PE	C1-O11-P-O14
51	L	701	3PE	C11-O13-P-O11
51	L	701	3PE	C11-O13-P-O14
51	L	701	3PE	O13-C11-C12-N
51	L	701	3PE	C22-C21-O21-C2
51	L	704	3PE	C1-O11-P-O12
51	L	704	3PE	C11-O13-P-O11
51	L	704	3PE	C11-O13-P-O14
51	M	601	3PE	C11-O13-P-O11
51	M	601	3PE	C11-O13-P-O12
51	M	601	3PE	O13-C11-C12-N
51	M	604	3PE	O13-C11-C12-N
51	M	604	3PE	O32-C31-O31-C3
51	M	604	3PE	C32-C31-O31-C3
51	N	1301	3PE	C1-O11-P-O13
51	N	1301	3PE	C1-O11-P-O14
51	N	1301	3PE	O13-C11-C12-N
51	N	1301	3PE	O21-C2-C3-O31
51	N	1302	3PE	O13-C11-C12-N
51	X	401	3PE	C1-O11-P-O12
51	X	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
51	X	401	3PE	C1-O11-P-O14
51	X	401	3PE	C12-C11-O13-P
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	C1-O11-P-O14
51	Y	802	3PE	C11-O13-P-O14
51	Y	802	3PE	C22-C21-O21-C2
51	d	301	3PE	O22-C21-O21-C2
52	J	701	CDL	CA2-OA2-PA1-OA3
52	J	701	CDL	CA2-OA2-PA1-OA5
52	J	701	CDL	OB7-CB5-OB6-CB4
52	J	701	CDL	C51-CB5-OB6-CB4
52	K	401	CDL	CA2-C1-CB2-OB2
52	K	401	CDL	CA3-OA5-PA1-OA2
52	K	401	CDL	CA3-OA5-PA1-OA3
52	K	401	CDL	CB2-OB2-PB2-OB3
52	K	401	CDL	CB2-OB2-PB2-OB4
52	K	401	CDL	CB2-OB2-PB2-OB5
52	L	703	CDL	CA2-OA2-PA1-OA3
52	L	703	CDL	CB3-OB5-PB2-OB2
52	L	703	CDL	CB3-OB5-PB2-OB4
52	a	101	CDL	CA2-OA2-PA1-OA3
52	a	101	CDL	CA2-OA2-PA1-OA5
52	a	101	CDL	CA3-OA5-PA1-OA2
52	a	101	CDL	CA3-OA5-PA1-OA4
52	a	101	CDL	CB2-OB2-PB2-OB3
52	a	101	CDL	CB2-OB2-PB2-OB4
52	a	101	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	C51-CB5-OB6-CB4
53	N	1303	I49	N01-C14-N02-C15
53	N	1303	I49	N03-C14-N02-C15
54	O	401	GTP	PB-O3B-PG-O2G
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5

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Mol	Chain	Res	Type	Atoms
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	C5-C6-C7-C8
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
51	H	402	3PE	O32-C31-O31-C3
52	J	701	CDL	C11-CA5-OA6-CA4
51	H	402	3PE	C32-C31-O31-C3
51	H	401	3PE	O32-C31-O31-C3
45	k	101	LMT	O5B-C1B-O1B-C4'
45	A	302	LMT	C5'-C4'-O1B-C1B
45	e	501	LMT	O5B-C1B-O1B-C4'
47	M	605	PC1	O22-C21-O21-C2
51	X	401	3PE	O22-C21-O21-C2
51	Y	802	3PE	O22-C21-O21-C2
52	h	1001	CDL	OB7-CB5-OB6-CB4
51	H	401	3PE	C32-C31-O31-C3
51	N	1301	3PE	C32-C31-O31-C3
51	d	301	3PE	C22-C21-O21-C2
52	L	703	CDL	OA9-CA7-OA8-CA6
45	M	602	LMT	O5'-C5'-C6'-O6'
52	K	401	CDL	C71-CB7-OB8-CB6
52	a	101	CDL	C31-CA7-OA8-CA6
45	A	301	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	k	101	LMT	C2B-C1B-O1B-C4'
51	N	1301	3PE	O32-C31-O31-C3
51	Y	802	3PE	O32-C31-O31-C3
51	L	701	3PE	O22-C21-O21-C2
52	J	701	CDL	OA7-CA5-OA6-CA4
47	P	502	PC1	C32-C31-O31-C3
45	e	501	LMT	C3'-C4'-O1B-C1B
52	J	701	CDL	CA4-CA6-OA8-CA7
52	K	401	CDL	O1-C1-CB2-OB2
51	Y	802	3PE	C32-C31-O31-C3
52	J	701	CDL	C31-CA7-OA8-CA6
52	L	703	CDL	C31-CA7-OA8-CA6
45	M	602	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
45	Y	801	LMT	O5B-C5B-C6B-O6B
45	e	501	LMT	O5B-C5B-C6B-O6B
52	a	101	CDL	OA9-CA7-OA8-CA6
45	h	1002	LMT	C4'-C5'-C6'-O6'
52	J	701	CDL	OA9-CA7-OA8-CA6
45	M	602	LMT	C4'-C5'-C6'-O6'
45	e	501	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	C4'-C5'-C6'-O6'
45	Y	801	LMT	C4'-C5'-C6'-O6'
52	K	401	CDL	OB9-CB7-OB8-CB6
45	L	702	LMT	O5'-C1'-O1'-C1
45	e	501	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	O5'-C1'-O1'-C1
45	A	302	LMT	O5'-C5'-C6'-O6'
45	Y	801	LMT	O5'-C5'-C6'-O6'
52	a	101	CDL	C11-CA5-OA6-CA4
47	B	203	PC1	C32-C31-O31-C3
47	M	605	PC1	C32-C31-O31-C3
51	L	701	3PE	C32-C31-O31-C3
45	M	602	LMT	C4B-C5B-C6B-O6B
45	M	603	LMT	C4B-C5B-C6B-O6B
52	L	703	CDL	CB4-CB6-OB8-CB7
45	e	501	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	C2'-C1'-O1'-C1
51	N	1301	3PE	C31-C32-C33-C34
52	J	701	CDL	O1-C1-CA2-OA2
52	h	1001	CDL	O1-C1-CB2-OB2
45	A	301	LMT	O5B-C5B-C6B-O6B
47	M	605	PC1	O32-C31-O31-C3
51	L	701	3PE	O32-C31-O31-C3
51	M	604	3PE	C22-C21-O21-C2
53	N	1303	I49	C07-C06-C08-N01
52	K	401	CDL	CA5-C11-C12-C13
51	M	604	3PE	O22-C21-O21-C2
47	B	202	PC1	C31-C32-C33-C34
47	B	203	PC1	O32-C31-O31-C3
47	P	502	PC1	O32-C31-O31-C3
51	L	704	3PE	C21-C22-C23-C24
51	d	301	3PE	C31-C32-C33-C34
52	L	703	CDL	CA5-C11-C12-C13
52	L	703	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
45	e	501	LMT	C4B-C5B-C6B-O6B
47	B	203	PC1	C21-C22-C23-C24
52	a	101	CDL	OA7-CA5-OA6-CA4
45	Y	801	LMT	C4B-C5B-C6B-O6B
45	L	702	LMT	O5B-C5B-C6B-O6B
52	h	1001	CDL	C31-CA7-OA8-CA6
45	M	603	LMT	O5B-C5B-C6B-O6B
45	e	501	LMT	C5'-C4'-O1B-C1B
52	K	401	CDL	C51-CB5-OB6-CB4
45	M	603	LMT	C2'-C1'-O1'-C1
45	Y	801	LMT	C2'-C1'-O1'-C1
52	K	401	CDL	OB7-CB5-OB6-CB4
45	A	301	LMT	O5'-C1'-O1'-C1
45	Y	801	LMT	O5'-C1'-O1'-C1
52	L	703	CDL	C11-CA5-OA6-CA4
45	M	603	LMT	C3'-C4'-O1B-C1B
47	M	605	PC1	C2D-C2E-C2F-C2G
52	h	1001	CDL	OA9-CA7-OA8-CA6
45	L	702	LMT	C5-C6-C7-C8
51	M	604	3PE	C29-C2A-C2B-C2C
51	N	1301	3PE	C2D-C2E-C2F-C2G
52	L	703	CDL	OA7-CA5-OA6-CA4
45	L	702	LMT	C2-C1-O1'-C1'
45	M	603	LMT	C5'-C4'-O1B-C1B
51	I	201	3PE	C2B-C2C-C2D-C2E
51	M	604	3PE	C3E-C3F-C3G-C3H
51	X	401	3PE	C28-C29-C2A-C2B
52	L	703	CDL	C38-C39-C40-C41
52	h	1001	CDL	C22-C23-C24-C25
47	M	605	PC1	C24-C25-C26-C27
51	L	704	3PE	C34-C35-C36-C37
51	X	401	3PE	C36-C37-C38-C39
45	A	302	LMT	O5B-C5B-C6B-O6B
45	A	302	LMT	C4B-C5B-C6B-O6B
51	N	1301	3PE	C22-C21-O21-C2
51	X	401	3PE	C23-C24-C25-C26
51	L	704	3PE	C36-C37-C38-C39
52	h	1001	CDL	C72-C73-C74-C75
52	K	401	CDL	CB7-C71-C72-C73
51	M	601	3PE	C33-C34-C35-C36
45	M	603	LMT	O1'-C1-C2-C3
45	Z	301	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
51	I	201	3PE	C33-C34-C35-C36
51	L	704	3PE	C3C-C3D-C3E-C3F
52	J	701	CDL	C73-C74-C75-C76
52	L	703	CDL	CA3-CA4-CA6-OA8
51	L	701	3PE	C2D-C2E-C2F-C2G
51	X	401	3PE	C32-C33-C34-C35
51	X	401	3PE	C38-C39-C3A-C3B
51	d	301	3PE	C24-C25-C26-C27
52	J	701	CDL	C76-C77-C78-C79
52	a	101	CDL	C58-C59-C60-C61
58	U	101	EHZ	C21-C1-C2-C3
51	L	701	3PE	C33-C34-C35-C36
51	M	604	3PE	C34-C35-C36-C37
52	a	101	CDL	C11-C12-C13-C14
51	d	301	3PE	C32-C33-C34-C35
51	M	601	3PE	C31-C32-C33-C34
52	K	401	CDL	C40-C41-C42-C43
47	B	203	PC1	C22-C21-O21-C2
51	N	1302	3PE	C22-C21-O21-C2
51	M	601	3PE	C38-C39-C3A-C3B
51	d	301	3PE	C27-C28-C29-C2A
52	h	1001	CDL	C14-C15-C16-C17
47	B	203	PC1	C23-C24-C25-C26
45	Z	301	LMT	C2-C3-C4-C5
45	A	302	LMT	C11-C10-C9-C8
47	B	203	PC1	C32-C33-C34-C35
51	M	601	3PE	C37-C38-C39-C3A
51	N	1302	3PE	C32-C33-C34-C35
52	a	101	CDL	C51-C52-C53-C54
47	B	203	PC1	C31-C32-C33-C34
51	L	701	3PE	C28-C29-C2A-C2B
52	a	101	CDL	O1-C1-CB2-OB2
45	A	302	LMT	C7-C8-C9-C10
47	M	605	PC1	C2B-C2C-C2D-C2E
51	d	301	3PE	C26-C27-C28-C29
52	K	401	CDL	C11-C12-C13-C14
59	o	201	MYR	C2-C3-C4-C5
51	L	704	3PE	C22-C21-O21-C2
52	K	401	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C11-CA5-OA6-CA4
52	J	701	CDL	C77-C78-C79-C80
51	L	704	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
51	M	601	3PE	C35-C36-C37-C38
52	h	1001	CDL	C13-C14-C15-C16
45	A	301	LMT	C4B-C5B-C6B-O6B
51	X	401	3PE	C3C-C3D-C3E-C3F
51	d	301	3PE	C3E-C3F-C3G-C3H
51	N	1301	3PE	O22-C21-O21-C2
52	J	701	CDL	C72-C73-C74-C75
51	N	1301	3PE	C35-C36-C37-C38
51	M	604	3PE	C21-C22-C23-C24
52	a	101	CDL	C39-C40-C41-C42
52	L	703	CDL	OA6-CA4-CA6-OA8
52	L	703	CDL	C71-CB7-OB8-CB6
51	M	604	3PE	C2B-C2C-C2D-C2E
47	M	605	PC1	C26-C27-C28-C29
51	M	604	3PE	C32-C33-C34-C35
45	L	702	LMT	O5'-C5'-C6'-O6'
45	Z	301	LMT	O5'-C5'-C6'-O6'
51	I	201	3PE	C3B-C3C-C3D-C3E
51	N	1302	3PE	C36-C37-C38-C39
52	J	701	CDL	C78-C79-C80-C81
52	K	401	CDL	OA7-CA5-OA6-CA4
58	T	101	EHZ	O4-C15-C16-O5
52	K	401	CDL	C36-C37-C38-C39
45	A	302	LMT	O1'-C1-C2-C3
51	I	201	3PE	O11-C1-C2-C3
51	N	1302	3PE	O22-C21-O21-C2
52	h	1001	CDL	OA7-CA5-OA6-CA4
51	d	301	3PE	C23-C24-C25-C26
47	M	605	PC1	C29-C2A-C2B-C2C
51	d	301	3PE	C35-C36-C37-C38
51	M	604	3PE	C2D-C2E-C2F-C2G
51	Y	802	3PE	C37-C38-C39-C3A
58	U	101	EHZ	C2-C3-C4-C5
45	M	602	LMT	C9-C10-C11-C12
52	L	703	CDL	C31-C32-C33-C34
47	B	203	PC1	O22-C21-O21-C2
51	L	701	3PE	C23-C24-C25-C26
51	I	201	3PE	C21-C22-C23-C24
51	L	704	3PE	C1-C2-C3-O31
45	M	603	LMT	C2-C3-C4-C5
47	M	605	PC1	C27-C28-C29-C2A
51	d	301	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
45	Z	301	LMT	C5-C6-C7-C8
52	J	701	CDL	C74-C75-C76-C77
51	I	201	3PE	C32-C31-O31-C3
51	N	1301	3PE	C36-C37-C38-C39
51	N	1302	3PE	C35-C36-C37-C38
51	L	704	3PE	C38-C39-C3A-C3B
58	U	101	EHZ	C21-C22-C23-C24
47	M	605	PC1	C1-C2-O21-C21
51	M	601	3PE	C26-C27-C28-C29
51	N	1302	3PE	C23-C24-C25-C26
51	L	704	3PE	C33-C34-C35-C36
52	a	101	CDL	CA2-C1-CB2-OB2
52	h	1001	CDL	C52-C53-C54-C55
52	K	401	CDL	C16-C17-C18-C19
51	N	1301	3PE	C26-C27-C28-C29
47	M	605	PC1	C23-C24-C25-C26
51	L	701	3PE	C3B-C3C-C3D-C3E
52	a	101	CDL	OA6-CA4-CA6-OA8
51	M	601	3PE	C22-C23-C24-C25
52	L	703	CDL	C13-C14-C15-C16
51	N	1301	3PE	C3D-C3E-C3F-C3G
51	N	1301	3PE	C23-C24-C25-C26
56	P	501	NDP	PN-O3-PA-O1A
52	K	401	CDL	C31-CA7-OA8-CA6
47	M	605	PC1	C39-C3A-C3B-C3C
58	T	101	EHZ	C21-C22-C23-C24
52	L	703	CDL	C51-CB5-OB6-CB4
58	T	101	EHZ	C2-C1-C21-C22
52	L	703	CDL	OB9-CB7-OB8-CB6
52	a	101	CDL	C56-C57-C58-C59
51	L	701	3PE	C2F-C2G-C2H-C2I
51	Y	802	3PE	C3B-C3C-C3D-C3E
51	H	401	3PE	C31-C32-C33-C34
51	X	401	3PE	C3F-C3G-C3H-C3I
51	M	601	3PE	C32-C31-O31-C3
52	h	1001	CDL	C71-CB7-OB8-CB6
47	B	202	PC1	C35-C36-C37-C38
45	Y	801	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	C2-C1-O1'-C1'
47	M	605	PC1	C37-C38-C39-C3A
52	a	101	CDL	C1-CB2-OB2-PB2
51	I	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
51	H	401	3PE	C23-C24-C25-C26
45	M	602	LMT	C2'-C1'-O1'-C1
45	h	1002	LMT	C4B-C5B-C6B-O6B
52	K	401	CDL	OB5-CB3-CB4-CB6
47	B	203	PC1	C36-C37-C38-C39
45	L	702	LMT	C6-C7-C8-C9
52	L	703	CDL	C34-C35-C36-C37
51	L	701	3PE	C29-C2A-C2B-C2C
51	M	604	3PE	C2F-C2G-C2H-C2I
52	L	703	CDL	C54-C55-C56-C57
45	M	602	LMT	C6-C7-C8-C9
47	B	203	PC1	C24-C25-C26-C27
51	M	601	3PE	C34-C35-C36-C37
52	h	1001	CDL	C11-C12-C13-C14
51	X	401	3PE	C3E-C3F-C3G-C3H
47	P	502	PC1	C1-C2-C3-O31
51	H	401	3PE	C1-C2-C3-O31
51	H	402	3PE	C1-C2-C3-O31
51	M	604	3PE	C1-C2-C3-O31
52	J	701	CDL	CA3-CA4-CA6-OA8
52	J	701	CDL	CB3-CB4-CB6-OB8
52	L	703	CDL	CB3-CB4-CB6-OB8
52	a	101	CDL	CA3-CA4-CA6-OA8
52	L	703	CDL	C71-C72-C73-C74
52	h	1001	CDL	C16-C17-C18-C19
52	K	401	CDL	CB4-CB3-OB5-PB2
51	M	604	3PE	C23-C24-C25-C26
51	H	402	3PE	C33-C34-C35-C36
47	P	502	PC1	O21-C2-C3-O31
51	H	401	3PE	O21-C2-C3-O31
51	H	402	3PE	O21-C2-C3-O31
45	e	501	LMT	C4'-C5'-C6'-O6'
52	h	1001	CDL	CB7-C71-C72-C73
51	L	701	3PE	C25-C26-C27-C28
52	K	401	CDL	C41-C42-C43-C44
47	B	202	PC1	C33-C34-C35-C36
45	h	1002	LMT	C7-C8-C9-C10
45	l	201	LMT	O1'-C1-C2-C3
51	X	401	3PE	C31-C32-C33-C34
51	H	402	3PE	C3B-C3C-C3D-C3E
51	Y	802	3PE	C32-C33-C34-C35
51	Y	802	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	OB5-CB3-CB4-CB6
51	N	1301	3PE	C3B-C3C-C3D-C3E
52	L	703	CDL	C58-C59-C60-C61
52	L	703	CDL	C35-C36-C37-C38
52	L	703	CDL	OB7-CB5-OB6-CB4
51	M	601	3PE	O32-C31-O31-C3
52	h	1001	CDL	OB9-CB7-OB8-CB6
51	N	1302	3PE	C21-C22-C23-C24
51	d	301	3PE	C1-C2-O21-C21
45	A	302	LMT	C3-C4-C5-C6
51	I	201	3PE	C3C-C3D-C3E-C3F
52	K	401	CDL	OA9-CA7-OA8-CA6
51	M	601	3PE	O11-C1-C2-O21
51	L	704	3PE	C3A-C3B-C3C-C3D
45	A	302	LMT	O5'-C1'-O1'-C1
47	B	202	PC1	C1-C2-C3-O31
47	B	203	PC1	C1-C2-C3-O31
47	M	605	PC1	C1-C2-C3-O31
51	N	1301	3PE	C1-C2-C3-O31
51	Y	802	3PE	C1-C2-C3-O31
51	L	701	3PE	C21-C22-C23-C24
47	B	202	PC1	C23-C24-C25-C26
51	M	604	3PE	O21-C21-C22-C23
51	M	601	3PE	C12-C11-O13-P
51	N	1301	3PE	C12-C11-O13-P
51	N	1302	3PE	C12-C11-O13-P
47	B	202	PC1	O21-C2-C3-O31
51	N	1302	3PE	O21-C2-C3-O31
51	Y	802	3PE	O21-C2-C3-O31
52	J	701	CDL	OA6-CA4-CA6-OA8
52	J	701	CDL	OB6-CB4-CB6-OB8
52	L	703	CDL	OB6-CB4-CB6-OB8
52	h	1001	CDL	OA6-CA4-CA6-OA8
51	N	1301	3PE	C3A-C3B-C3C-C3D
51	I	201	3PE	C38-C39-C3A-C3B
51	L	701	3PE	C34-C35-C36-C37
52	K	401	CDL	C1-CB2-OB2-PB2
51	H	402	3PE	C3C-C3D-C3E-C3F
51	H	402	3PE	C31-C32-C33-C34
59	o	201	MYR	C1-C2-C3-C4
51	I	201	3PE	C2E-C2F-C2G-C2H
45	l	201	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
52	L	703	CDL	C11-C12-C13-C14
51	L	701	3PE	O11-C1-C2-C3
51	M	601	3PE	O11-C1-C2-C3
51	H	401	3PE	C3D-C3E-C3F-C3G
51	M	604	3PE	C38-C39-C3A-C3B
52	L	703	CDL	C52-C53-C54-C55
45	M	602	LMT	O1'-C1-C2-C3
52	J	701	CDL	C71-C72-C73-C74
51	H	402	3PE	C2-C1-O11-P
51	M	604	3PE	C28-C29-C2A-C2B
51	L	701	3PE	O11-C1-C2-O21
52	K	401	CDL	OB5-CB3-CB4-OB6
52	h	1001	CDL	OB5-CB3-CB4-OB6
52	a	101	CDL	C57-C58-C59-C60
47	B	203	PC1	O21-C2-C3-O31
51	M	604	3PE	O21-C2-C3-O31
51	d	301	3PE	O21-C2-C3-O31
52	a	101	CDL	OB6-CB4-CB6-OB8
51	N	1302	3PE	C33-C34-C35-C36
51	d	301	3PE	C1-C2-C3-O31
52	h	1001	CDL	CA3-CA4-CA6-OA8
51	d	301	3PE	C25-C26-C27-C28
52	K	401	CDL	C15-C16-C17-C18
47	B	202	PC1	C11-O13-P-O14
51	I	201	3PE	C1-O11-P-O12
51	I	201	3PE	C1-O11-P-O13
51	I	201	3PE	C1-O11-P-O14
51	I	201	3PE	C11-O13-P-O11
51	I	201	3PE	C11-O13-P-O12
51	L	701	3PE	C1-O11-P-O12
51	L	704	3PE	C1-O11-P-O13
51	L	704	3PE	C1-O11-P-O14
51	L	704	3PE	C11-O13-P-O12
51	M	601	3PE	C1-O11-P-O14
51	M	604	3PE	C1-O11-P-O12
51	M	604	3PE	C1-O11-P-O13
51	M	604	3PE	C1-O11-P-O14
51	M	604	3PE	C11-O13-P-O11
51	M	604	3PE	C11-O13-P-O12
51	N	1301	3PE	C1-O11-P-O12
51	X	401	3PE	C11-O13-P-O11
51	X	401	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
51	Y	802	3PE	C11-O13-P-O11
51	Y	802	3PE	C11-O13-P-O12
52	J	701	CDL	CA2-OA2-PA1-OA4
52	K	401	CDL	CB3-OB5-PB2-OB3
52	a	101	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CB2-OB2-PB2-OB3
52	h	1001	CDL	CB2-OB2-PB2-OB4
52	h	1001	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	CB3-OB5-PB2-OB4
47	M	605	PC1	C35-C36-C37-C38
47	M	605	PC1	C2-C1-O11-P
51	M	604	3PE	C2-C1-O11-P
52	a	101	CDL	C33-C34-C35-C36
51	d	301	3PE	C3B-C3C-C3D-C3E
52	K	401	CDL	C71-C72-C73-C74
52	J	701	CDL	CA3-CA4-OA6-CA5
52	K	401	CDL	CB5-C51-C52-C53
51	L	704	3PE	O21-C2-C3-O31
58	T	101	EHZ	C12-C13-C14-N2
51	I	201	3PE	C29-C2A-C2B-C2C
56	P	501	NDP	PN-O3-PA-O2A
52	L	703	CDL	C53-C54-C55-C56
47	M	605	PC1	C34-C35-C36-C37
45	L	702	LMT	C4B-C5B-C6B-O6B
51	I	201	3PE	C39-C3A-C3B-C3C
45	A	302	LMT	C2-C1-O1'-C1'
45	k	101	LMT	C2-C1-O1'-C1'
52	J	701	CDL	CB2-C1-CA2-OA2
52	h	1001	CDL	CA2-C1-CB2-OB2
56	P	501	NDP	C2B-O2B-P2B-O3X
52	J	701	CDL	C72-C71-CB7-OB8
52	K	401	CDL	C31-C32-C33-C34
56	P	501	NDP	O4D-C1D-N1N-C6N
51	I	201	3PE	C3A-C3B-C3C-C3D
52	a	101	CDL	C13-C14-C15-C16
45	A	301	LMT	C4-C5-C6-C7
51	N	1302	3PE	C2-C1-O11-P
52	a	101	CDL	CA4-CA3-OA5-PA1
51	M	604	3PE	C1-C2-O21-C21
45	Y	801	LMT	C5'-C4'-O1B-C1B
51	N	1302	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
51	H	401	3PE	C37-C38-C39-C3A
51	H	401	3PE	O11-C1-C2-C3
45	k	101	LMT	C4-C5-C6-C7
52	a	101	CDL	C38-C39-C40-C41
52	a	101	CDL	C32-C33-C34-C35
56	P	501	NDP	O4D-C4D-C5D-O5D
51	L	704	3PE	C27-C28-C29-C2A
51	L	701	3PE	C3A-C3B-C3C-C3D
51	M	604	3PE	C2E-C2F-C2G-C2H
45	e	501	LMT	C7-C8-C9-C10
52	L	703	CDL	C55-C56-C57-C58
52	a	101	CDL	C35-C36-C37-C38
51	H	402	3PE	C32-C33-C34-C35
51	H	402	3PE	C3E-C3F-C3G-C3H
54	O	401	GTP	C4'-C5'-O5'-PA
45	e	501	LMT	C4-C5-C6-C7
52	a	101	CDL	CB3-CB4-CB6-OB8
58	T	101	EHZ	C6-C7-C8-C9
51	L	701	3PE	C2E-C2F-C2G-C2H
47	M	605	PC1	C2F-C2G-C2H-C2I
45	M	602	LMT	C2-C1-O1'-C1'
51	H	401	3PE	O11-C1-C2-O21
45	A	301	LMT	C2-C3-C4-C5
52	J	701	CDL	C75-C76-C77-C78
52	J	701	CDL	CA7-C31-C32-C33
51	N	1301	3PE	C27-C28-C29-C2A
51	N	1302	3PE	O11-C1-C2-C3
52	L	703	CDL	CA7-C31-C32-C33
51	N	1302	3PE	C27-C28-C29-C2A
45	Y	801	LMT	C3'-C4'-O1B-C1B
59	o	201	MYR	C3-C4-C5-C6
51	L	701	3PE	C36-C37-C38-C39
45	A	302	LMT	C3'-C4'-O1B-C1B
45	Z	301	LMT	C4B-C5B-C6B-O6B
52	a	101	CDL	CA5-C11-C12-C13
51	N	1302	3PE	O31-C31-C32-C33
52	K	401	CDL	C14-C15-C16-C17
52	h	1001	CDL	C31-C32-C33-C34
45	Y	801	LMT	C4-C5-C6-C7
58	T	101	EHZ	C3-C4-C5-C6
51	I	201	3PE	C22-C23-C24-C25
51	H	402	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
52	K	401	CDL	CB2-C1-CA2-OA2
51	N	1302	3PE	O11-C1-C2-O21
47	B	202	PC1	C32-C31-O31-C3
51	N	1302	3PE	C1-C2-C3-O31
47	B	202	PC1	O32-C31-O31-C3
52	K	401	CDL	C53-C54-C55-C56
51	I	201	3PE	C34-C35-C36-C37
45	h	1002	LMT	C4-C5-C6-C7
51	N	1302	3PE	C29-C2A-C2B-C2C
52	a	101	CDL	C34-C35-C36-C37
45	h	1002	LMT	C11-C10-C9-C8
51	X	401	3PE	O21-C21-C22-C23
51	I	201	3PE	C2F-C2G-C2H-C2I
45	h	1002	LMT	O5B-C5B-C6B-O6B
51	L	701	3PE	C3C-C3D-C3E-C3F
47	B	202	PC1	C22-C23-C24-C25
52	J	701	CDL	C33-C34-C35-C36
54	O	401	GTP	PG-O3B-PB-O2B
45	L	702	LMT	C1-C2-C3-C4
51	X	401	3PE	C21-C22-C23-C24
51	H	401	3PE	O21-C21-C22-C23
51	I	201	3PE	C26-C27-C28-C29
58	T	101	EHZ	O4-C15-C16-C17
52	K	401	CDL	C33-C34-C35-C36
52	h	1001	CDL	C12-C13-C14-C15
51	M	604	3PE	C37-C38-C39-C3A
51	H	401	3PE	C32-C33-C34-C35
51	N	1302	3PE	C3A-C3B-C3C-C3D
52	L	703	CDL	C12-C11-CA5-OA6
47	B	203	PC1	O21-C21-C22-C23
51	M	601	3PE	O21-C2-C3-O31
52	K	401	CDL	OB6-CB4-CB6-OB8
47	B	203	PC1	C2-C3-O31-C31
52	a	101	CDL	C52-C53-C54-C55
47	B	202	PC1	O31-C31-C32-C33
51	M	601	3PE	C21-C22-C23-C24
49	F	501	FMN	N10-C1'-C2'-O2'
47	B	202	PC1	C34-C35-C36-C37
47	M	605	PC1	C33-C34-C35-C36
58	T	101	EHZ	N2-C15-C16-C17
51	H	401	3PE	O22-C21-C22-C23
51	M	604	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	C71-C72-C73-C74
52	L	703	CDL	C12-C11-CA5-OA7
51	H	401	3PE	C36-C37-C38-C39
51	L	704	3PE	C28-C29-C2A-C2B
51	X	401	3PE	O22-C21-C22-C23
45	Z	301	LMT	C5'-C4'-O1B-C1B
51	L	704	3PE	O31-C31-C32-C33
51	I	201	3PE	C24-C25-C26-C27
47	B	203	PC1	O22-C21-C22-C23
47	B	203	PC1	C2-C1-O11-P
47	B	202	PC1	O32-C31-C32-C33
56	P	501	NDP	C2D-C1D-N1N-C6N
52	K	401	CDL	C35-C36-C37-C38
51	M	601	3PE	O21-C21-C22-C23
51	H	402	3PE	C3A-C3B-C3C-C3D
54	O	401	GTP	PB-O3A-PA-O2A

There are no ring outliers.

22 monomers are involved in 27 short contacts:

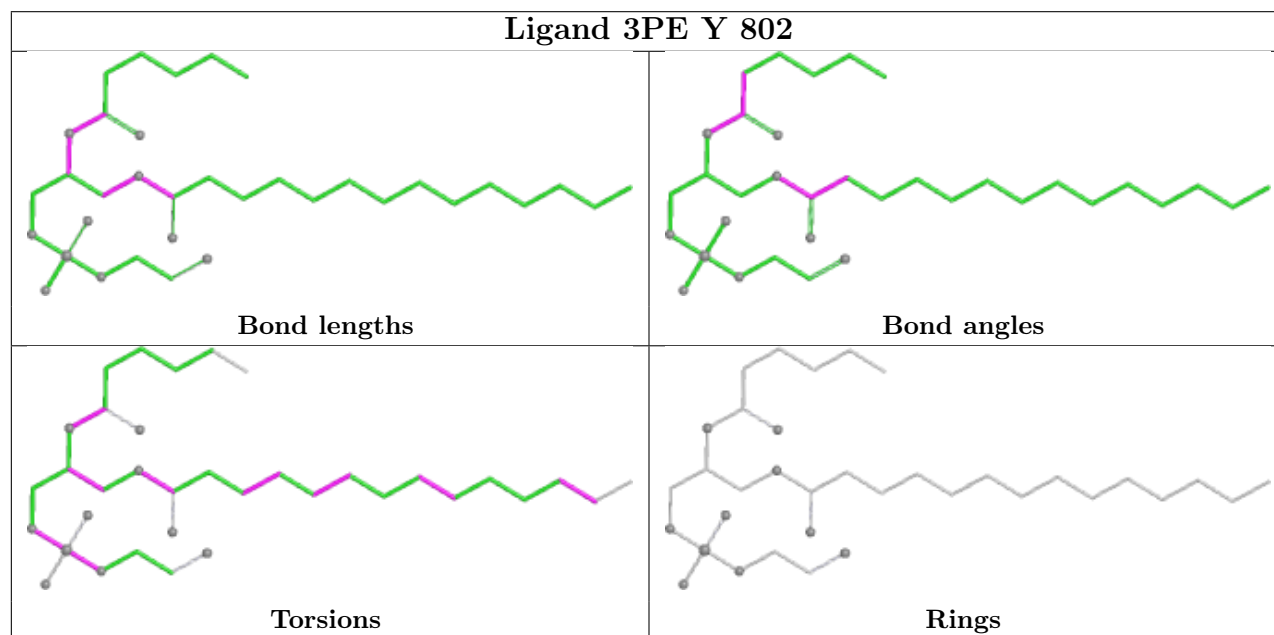
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	Y	802	3PE	1	0
47	B	203	PC1	1	0
47	P	502	PC1	1	0
45	k	101	LMT	1	0
45	L	702	LMT	1	0
52	J	701	CDL	2	0
45	M	603	LMT	1	0
56	P	501	NDP	2	0
49	F	501	FMN	1	0
54	O	401	GTP	3	0
51	M	604	3PE	1	0
51	L	704	3PE	2	0
51	d	301	3PE	1	0
51	N	1301	3PE	1	0
47	M	605	PC1	2	0
51	H	401	3PE	2	0
45	e	501	LMT	1	0
47	B	202	PC1	2	0
46	F	502	SF4	1	0
53	N	1303	I49	1	0
52	h	1001	CDL	1	0

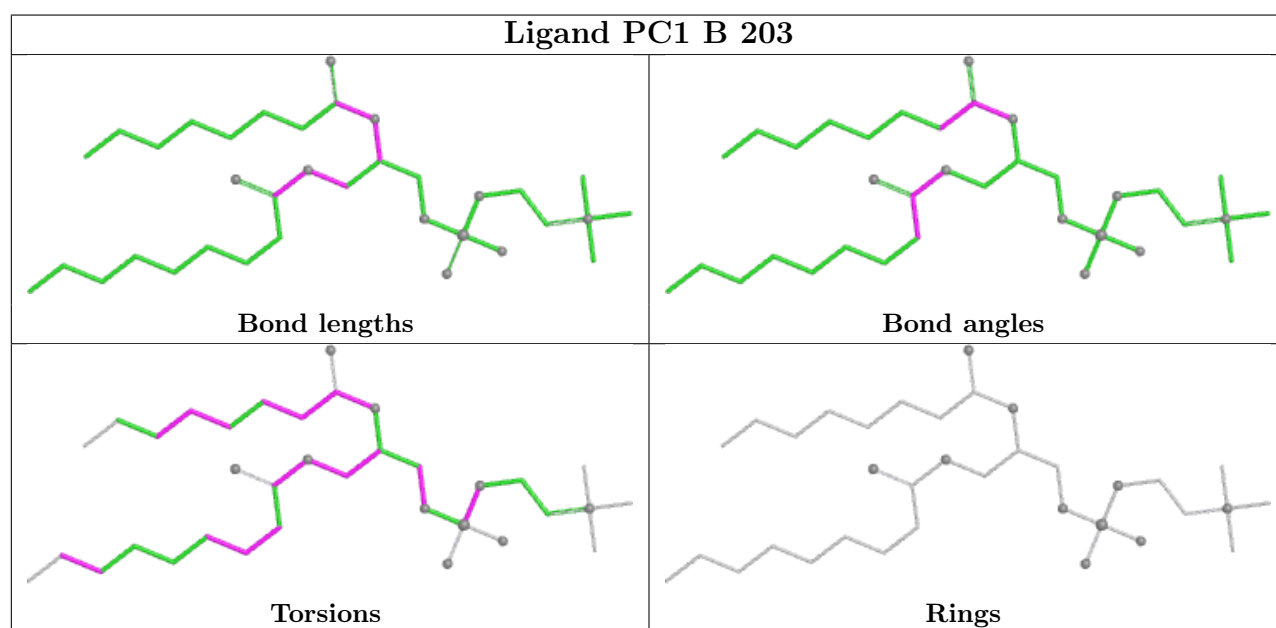
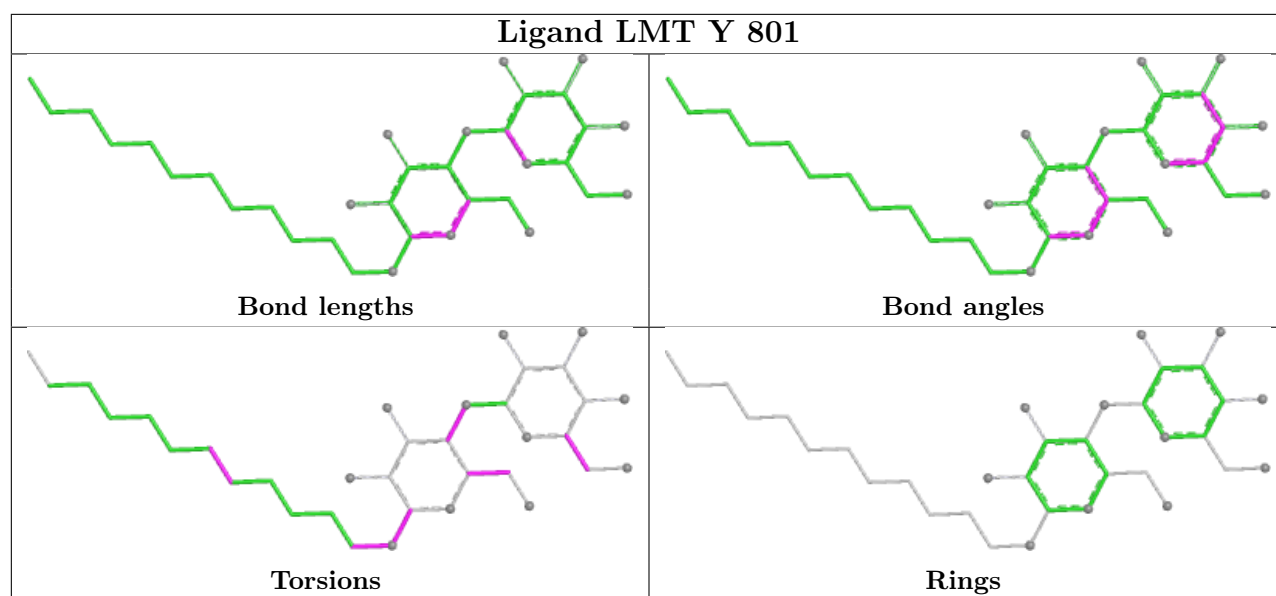
Continued on next page...

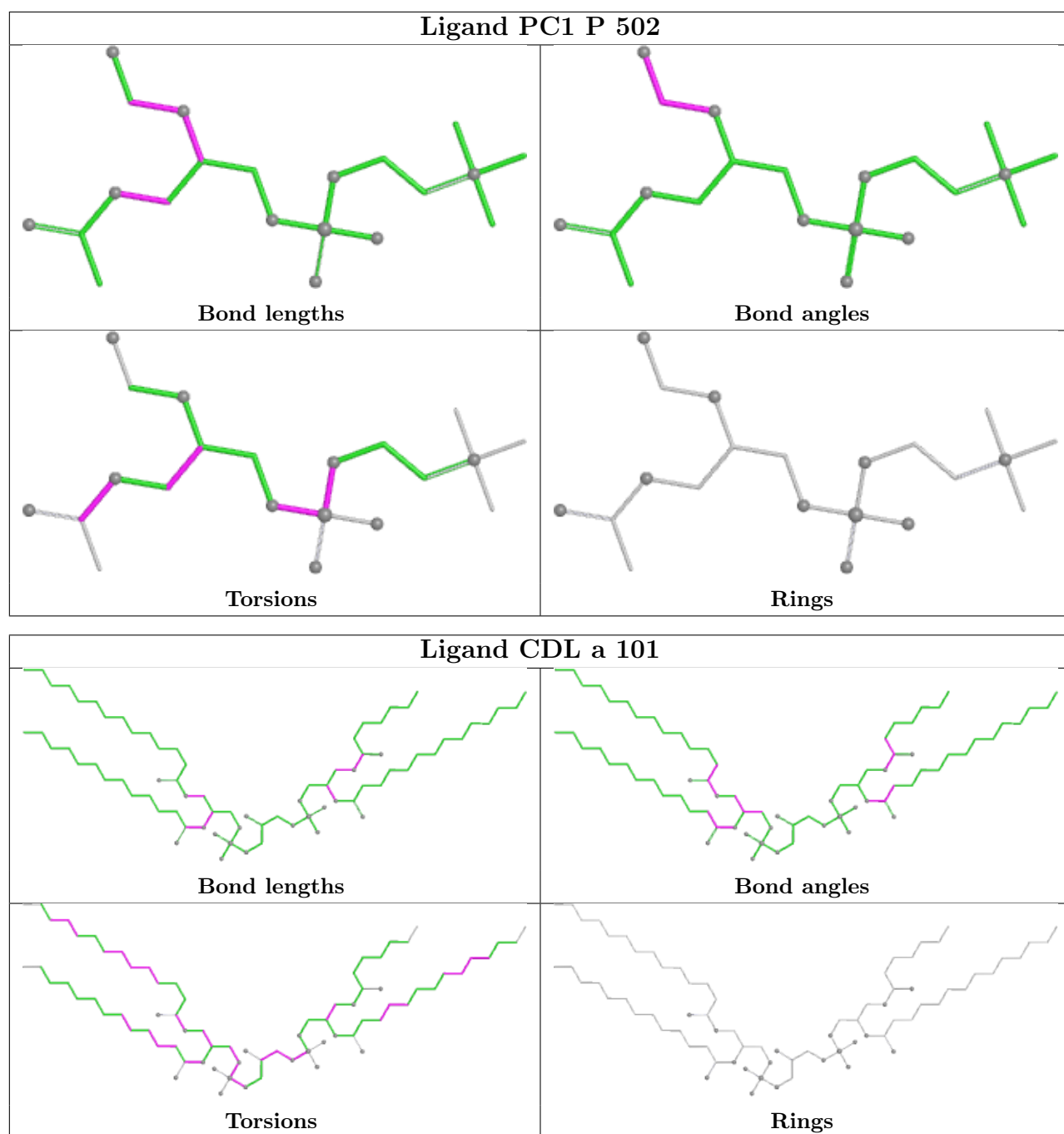
Continued from previous page...

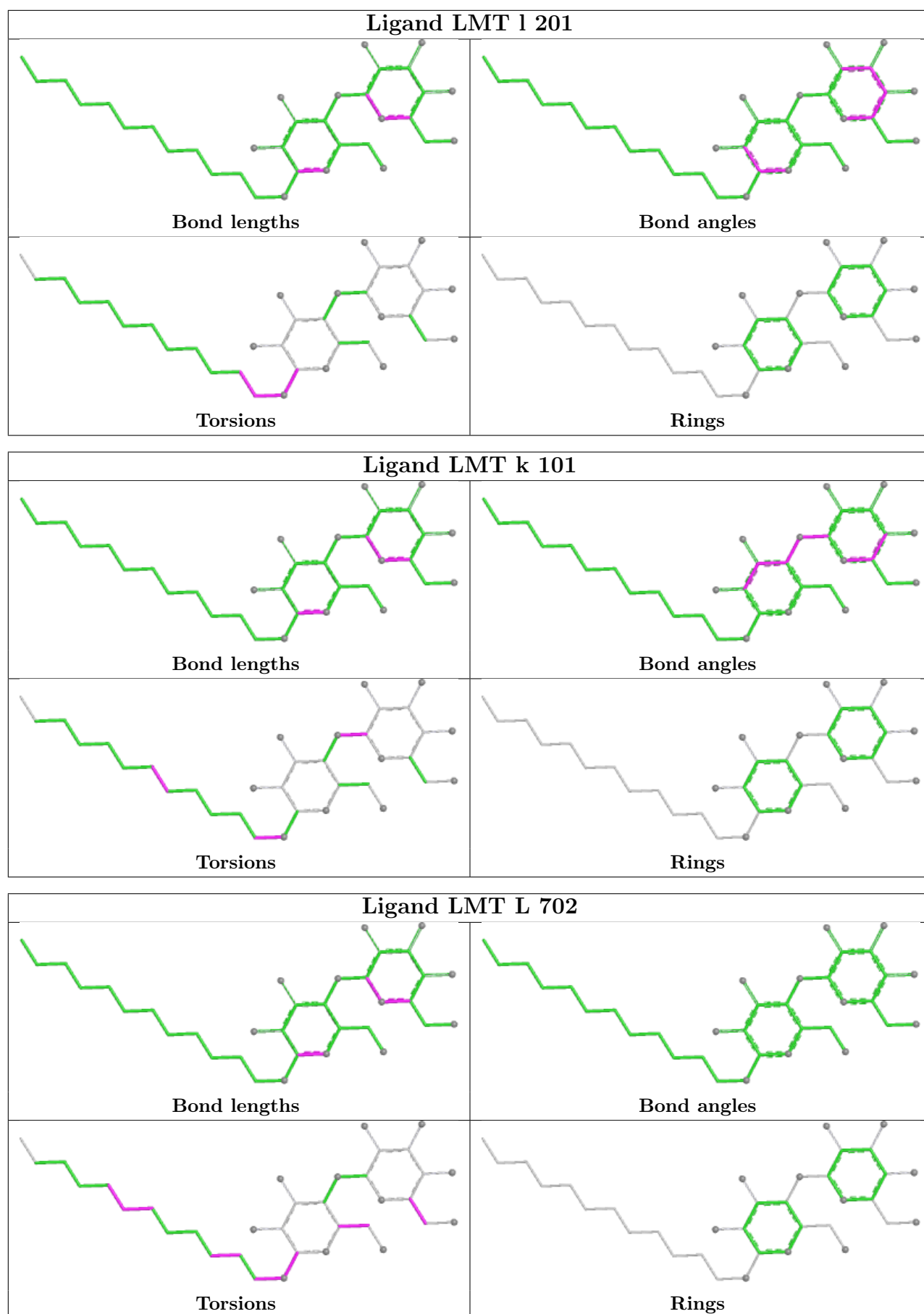
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	301	LMT	1	0

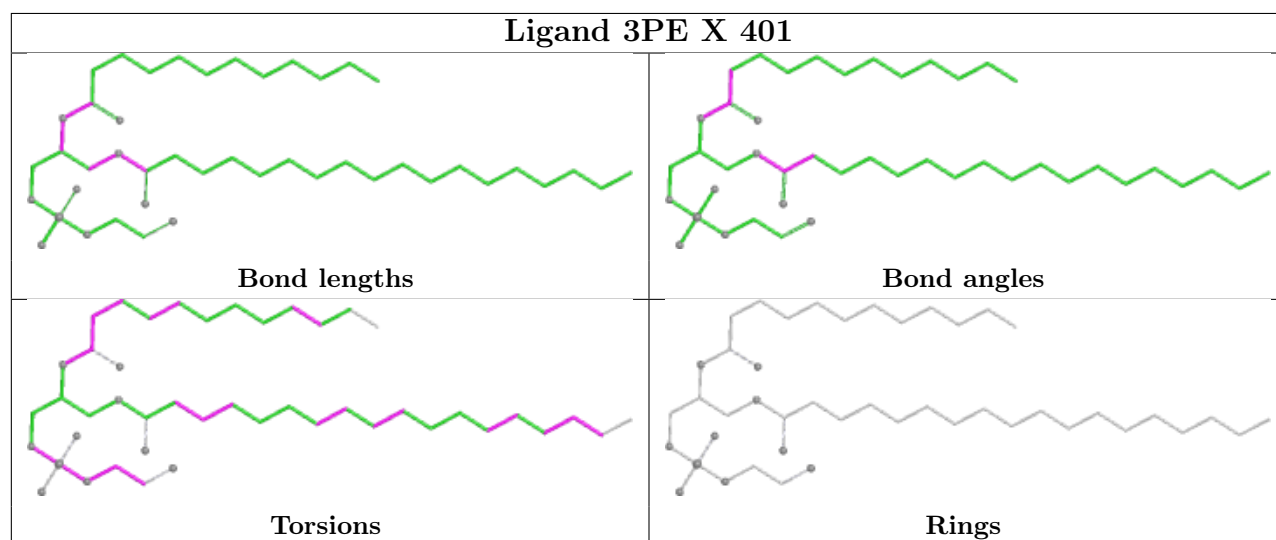
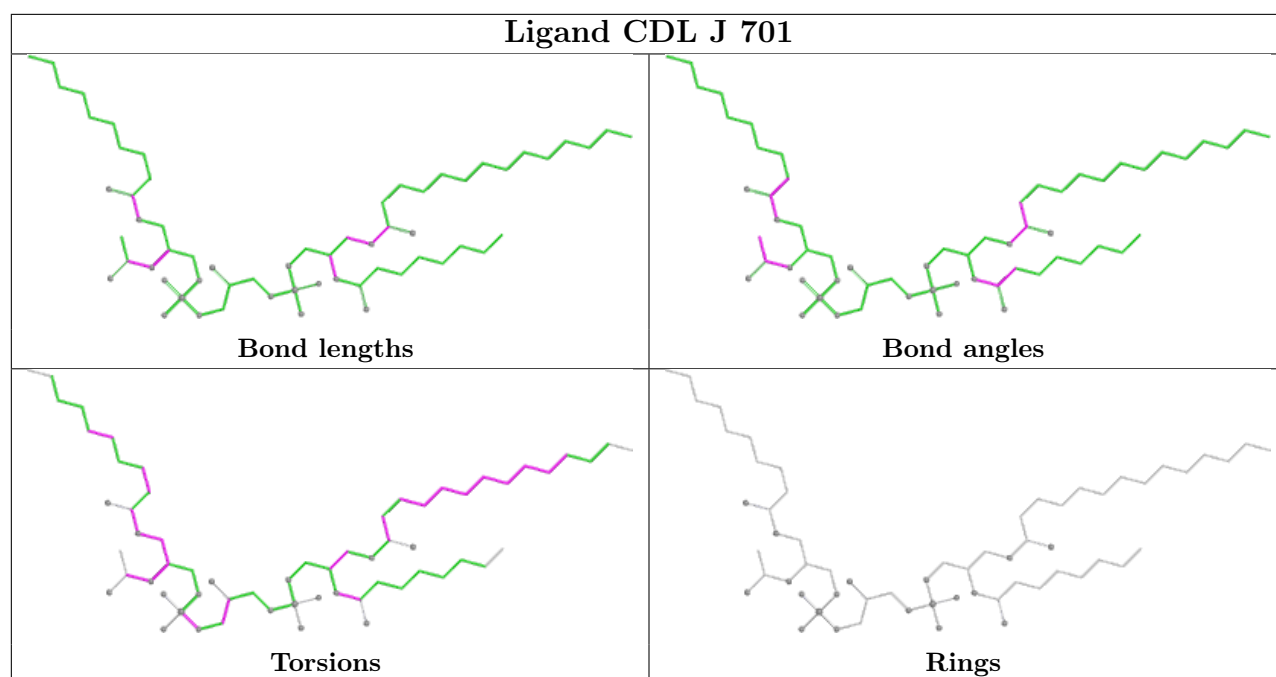
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

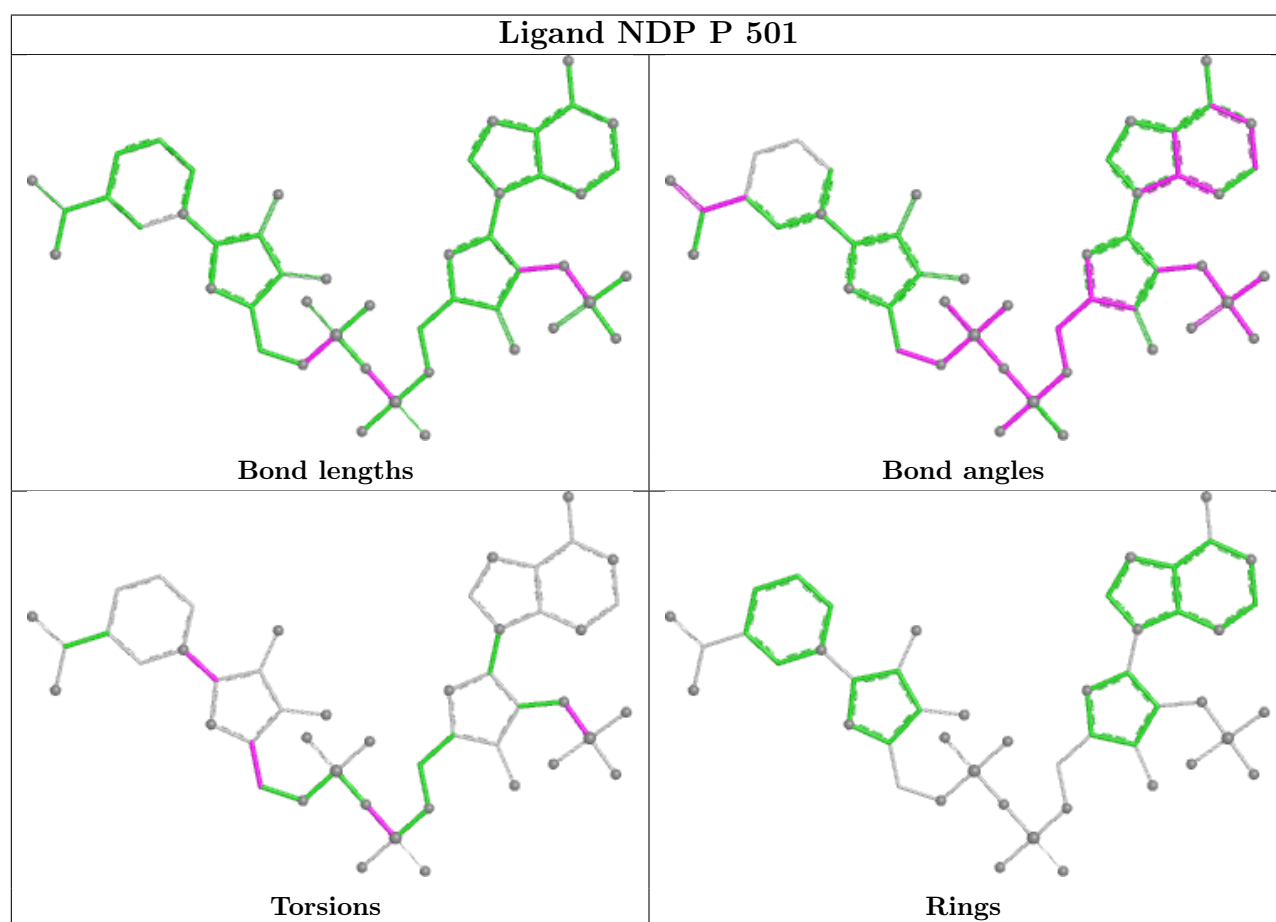
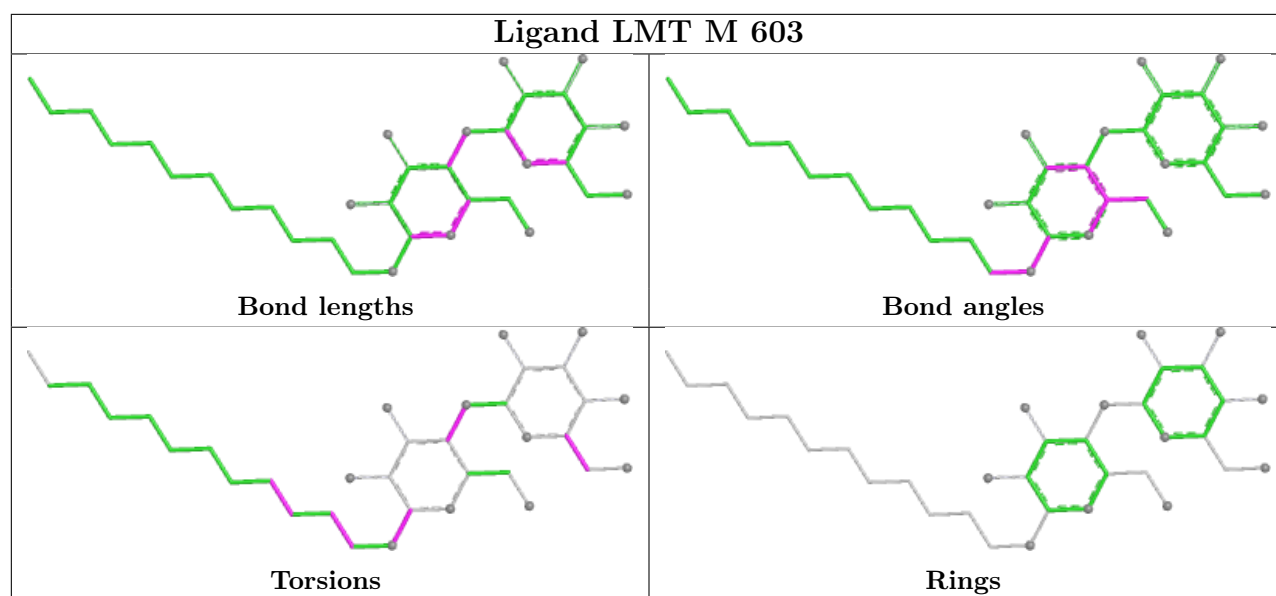


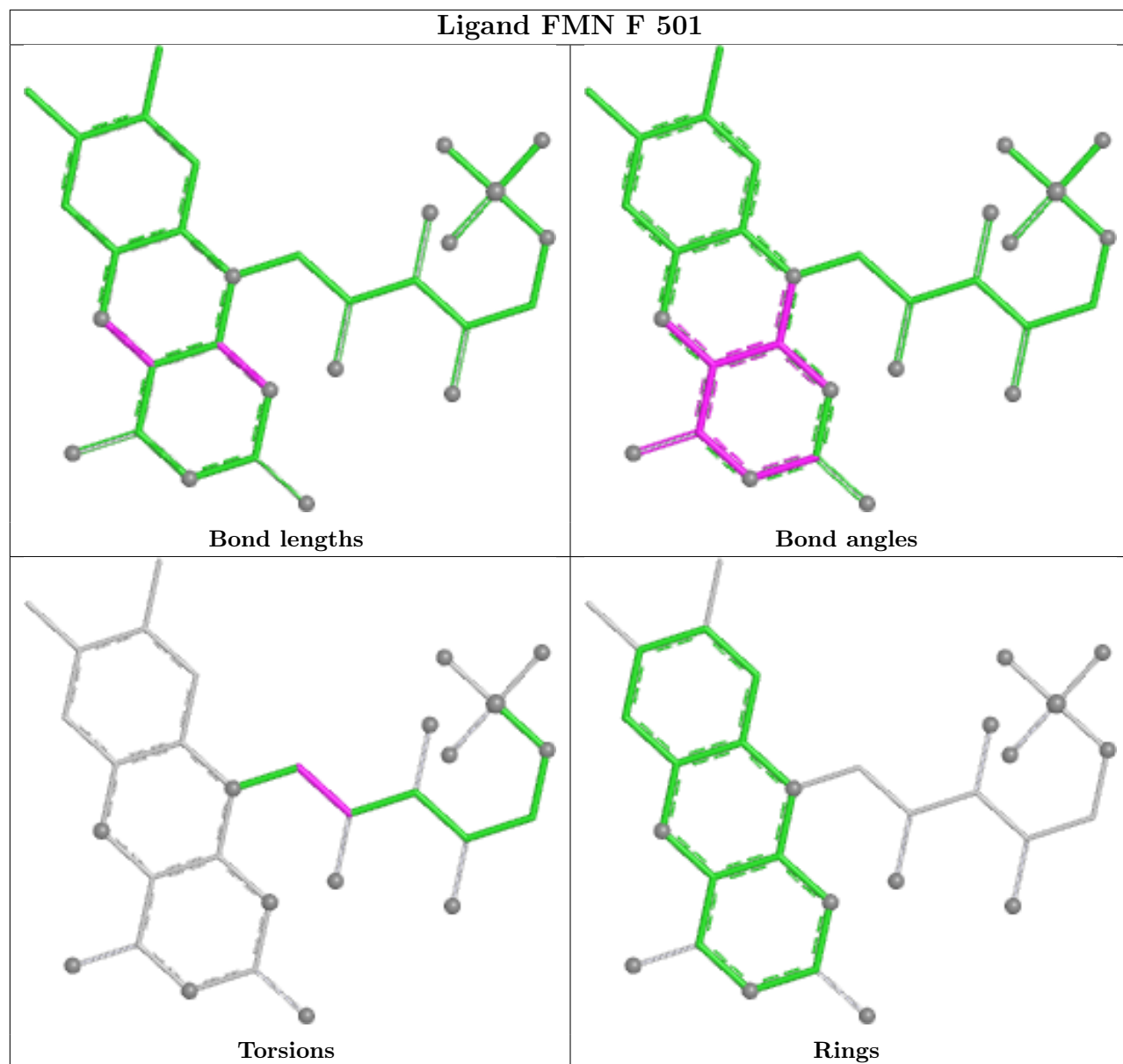


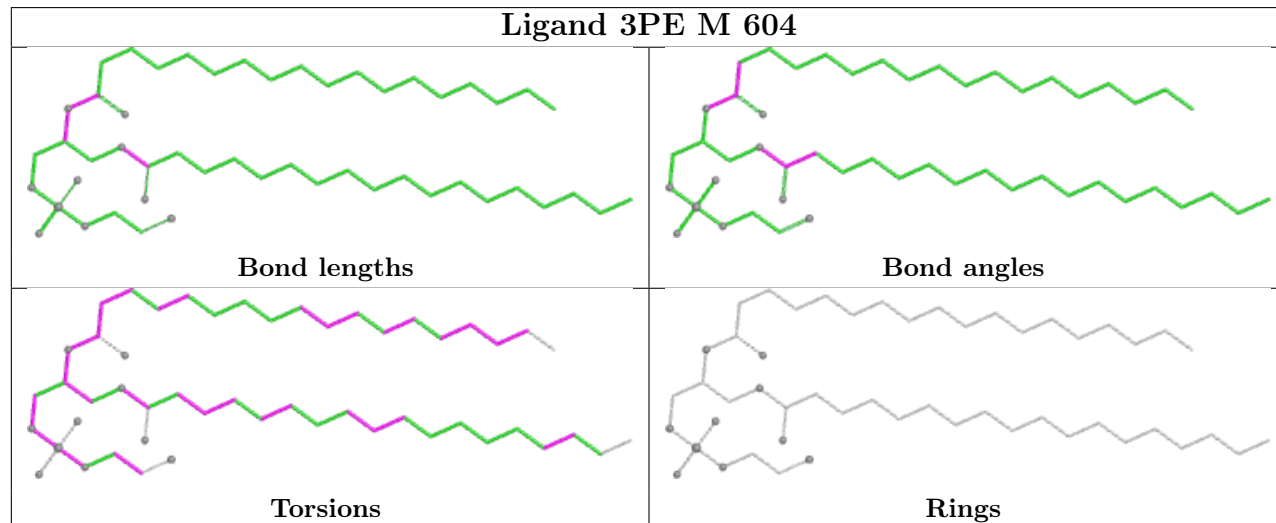
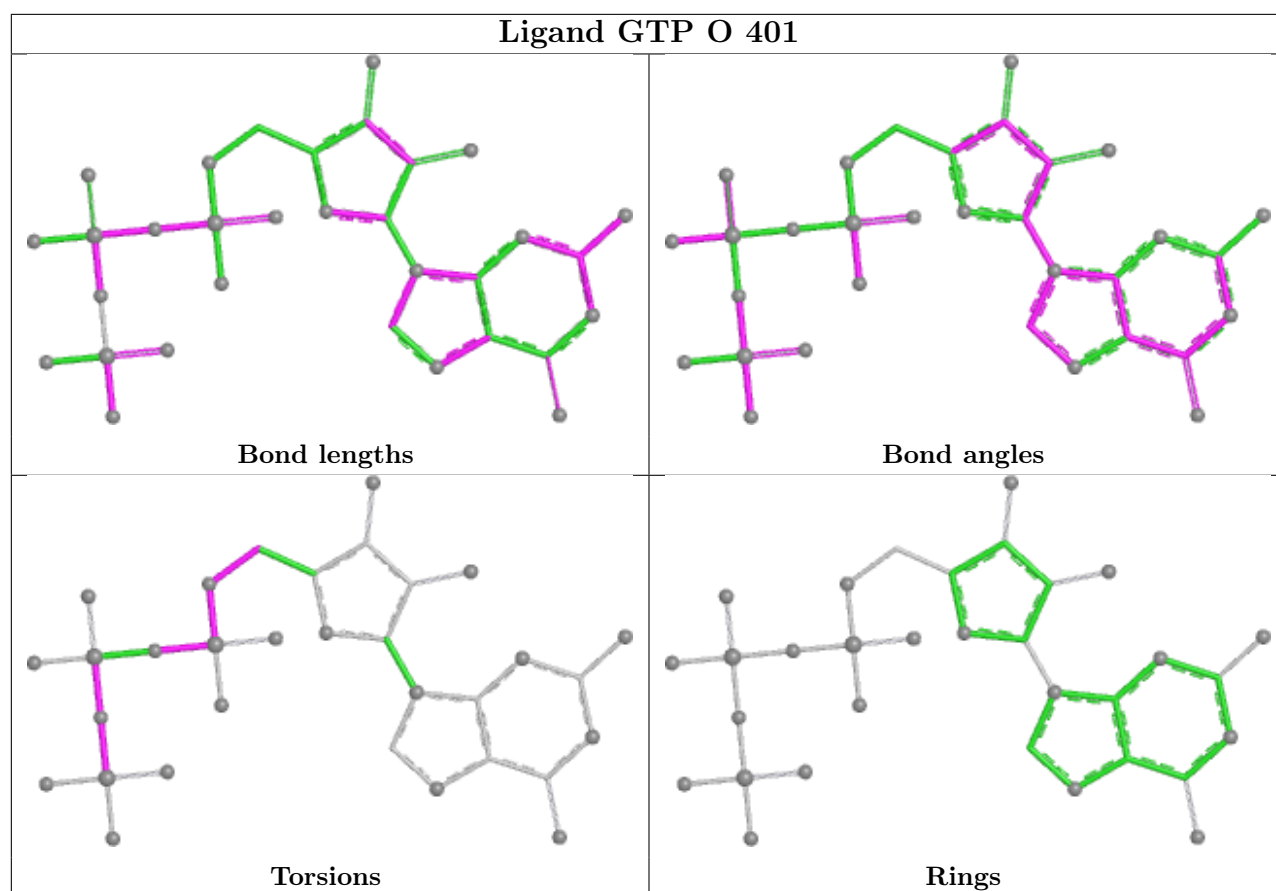


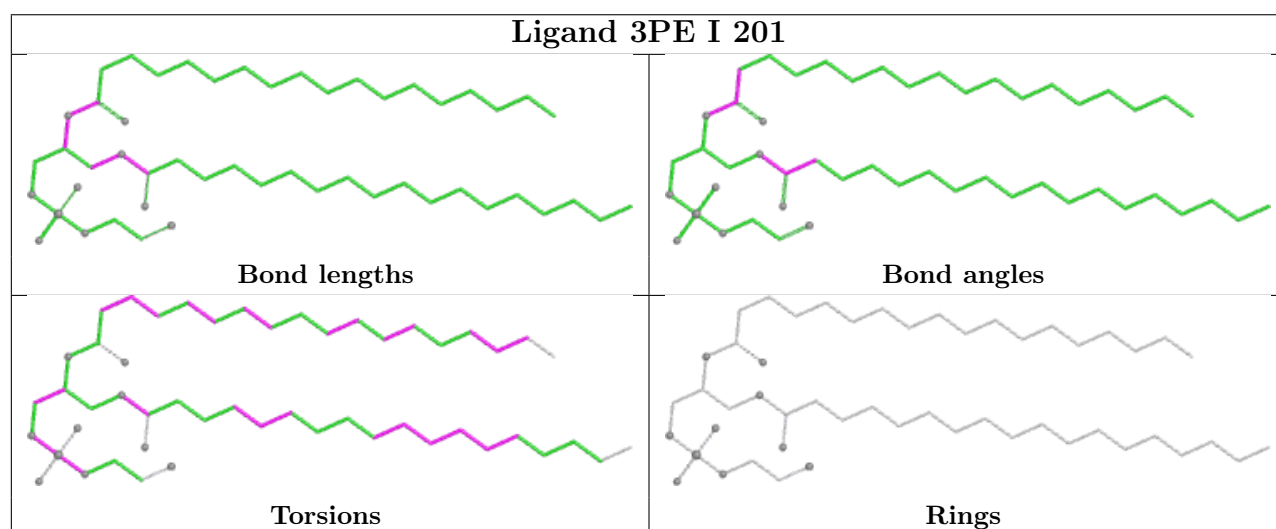
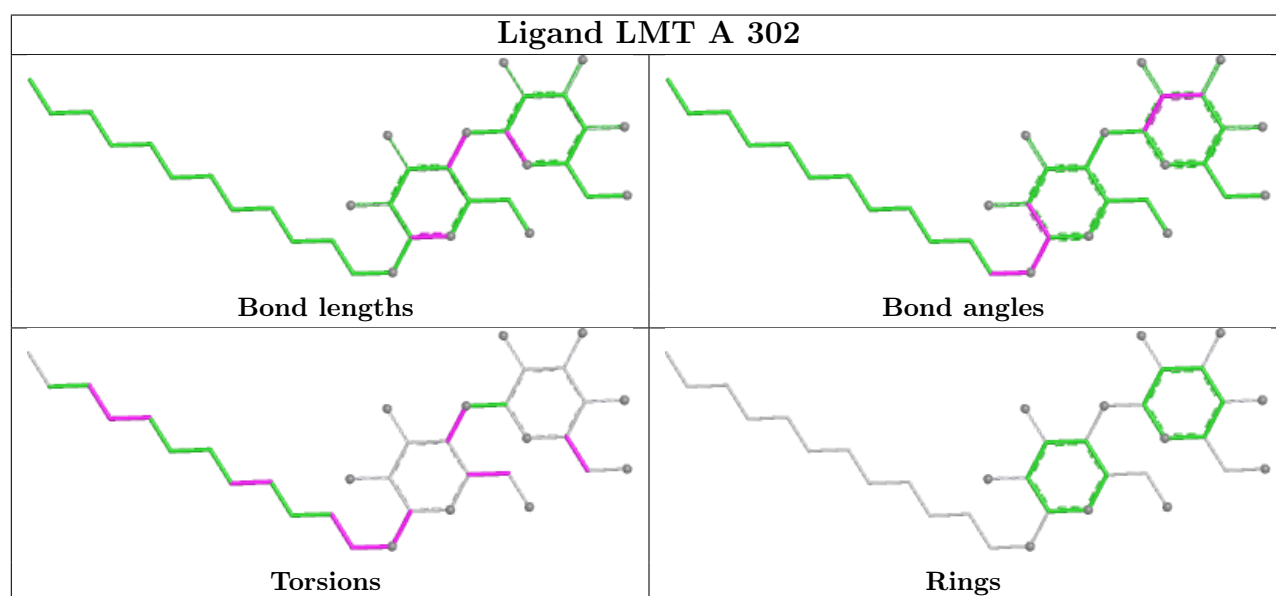
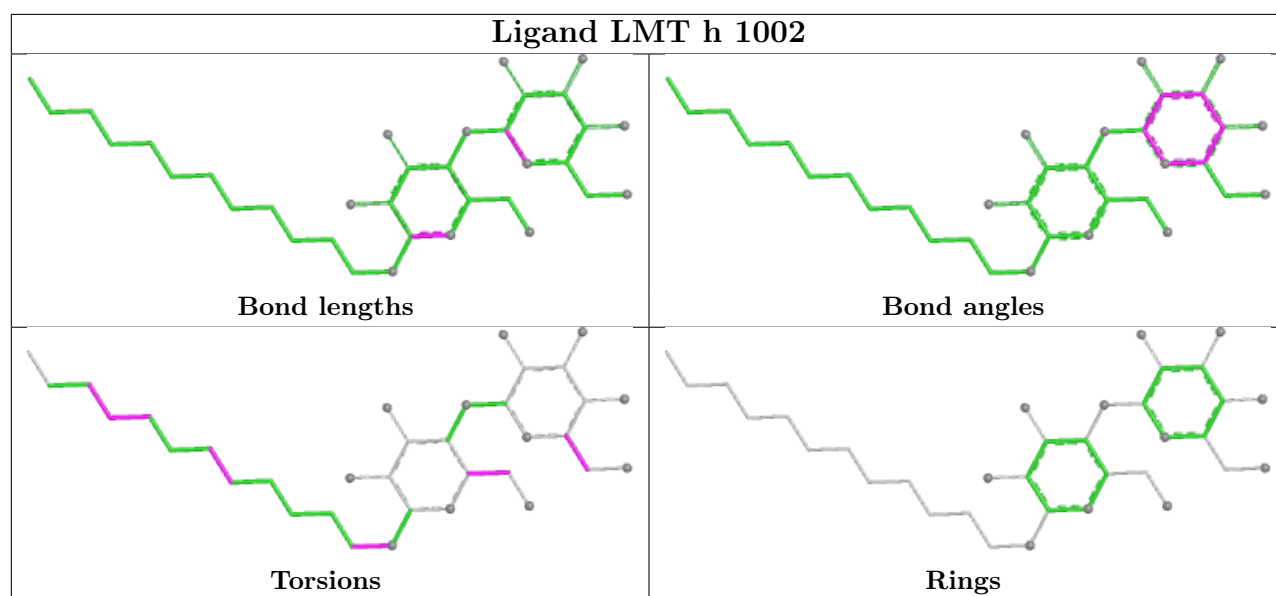


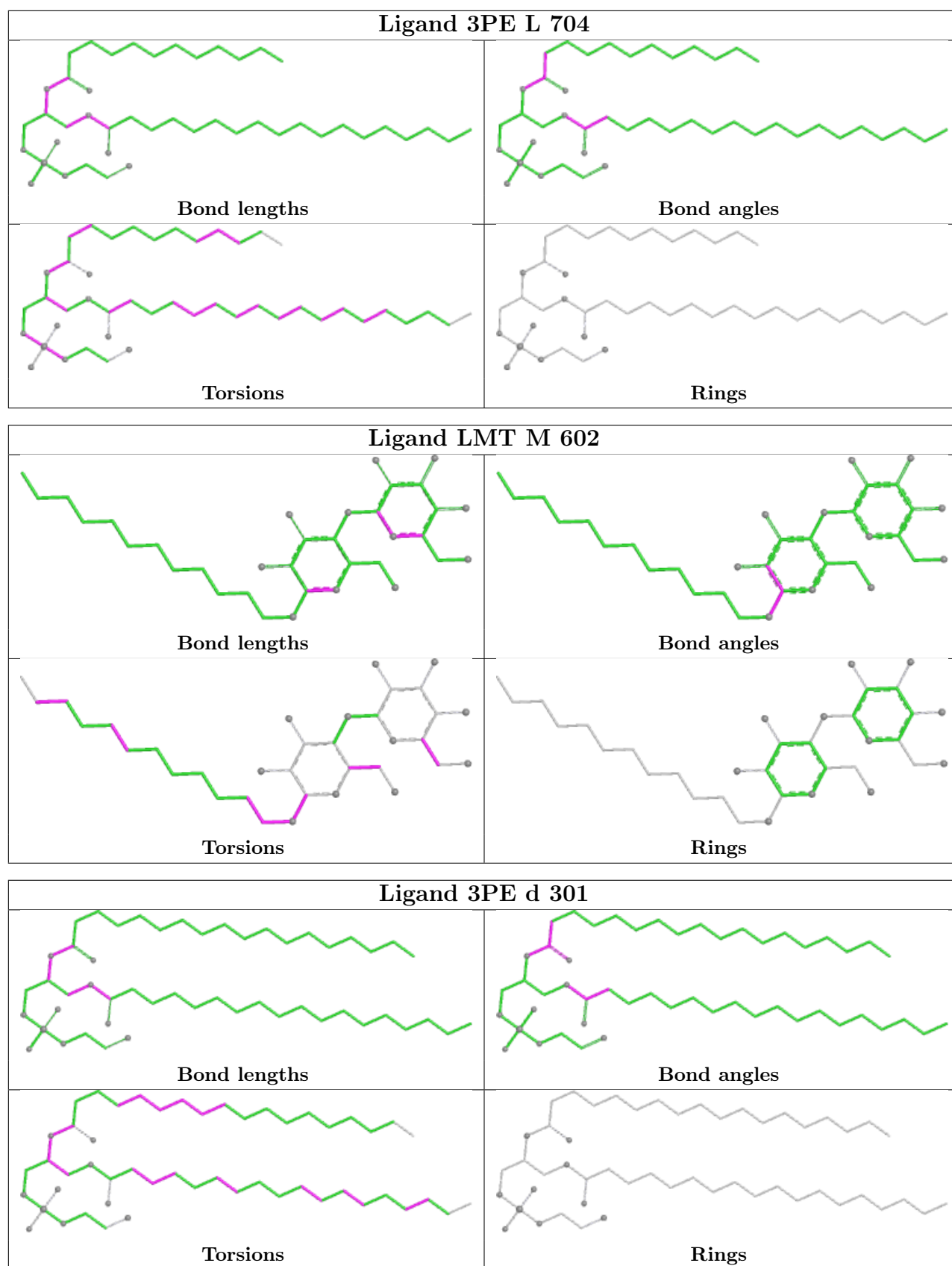


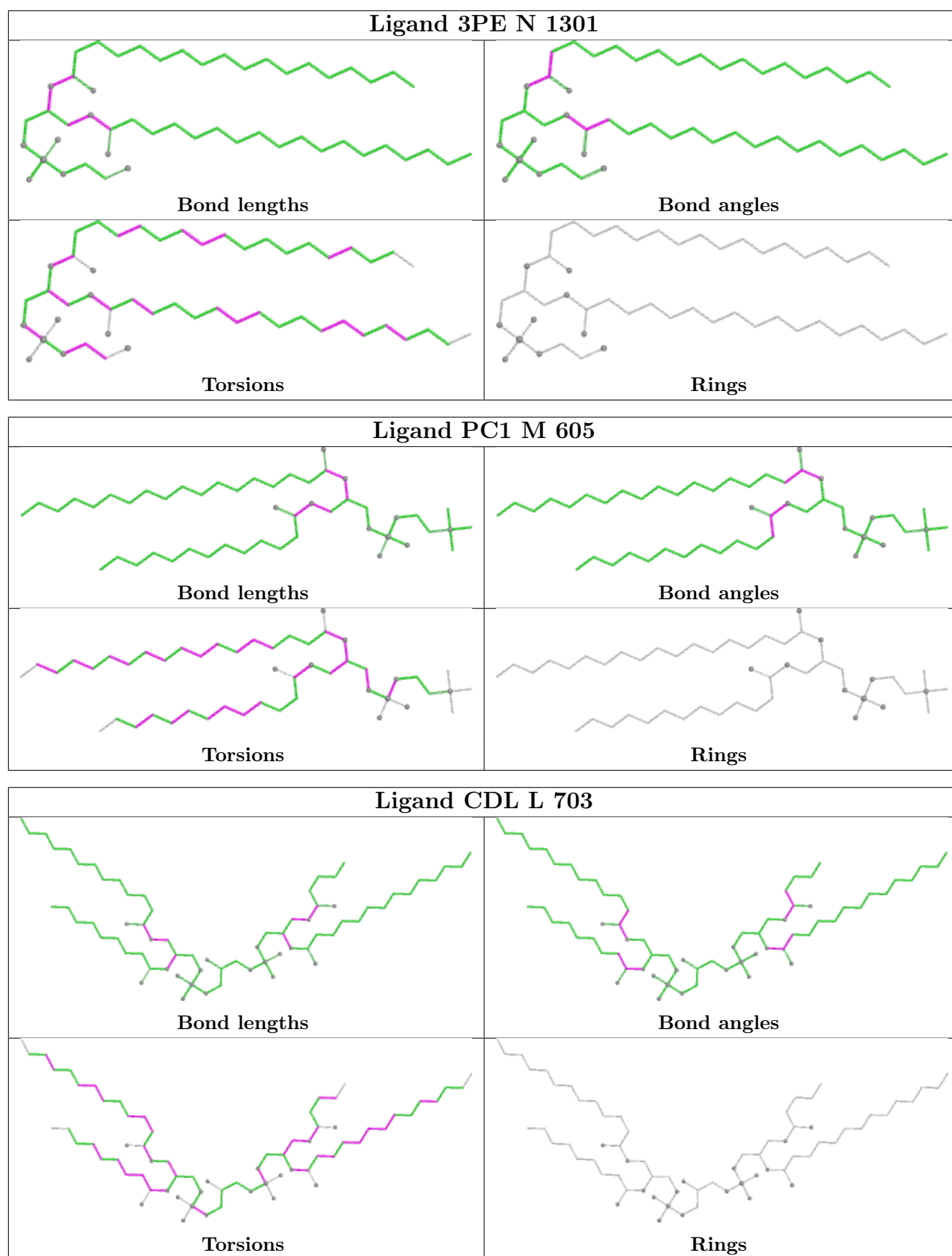


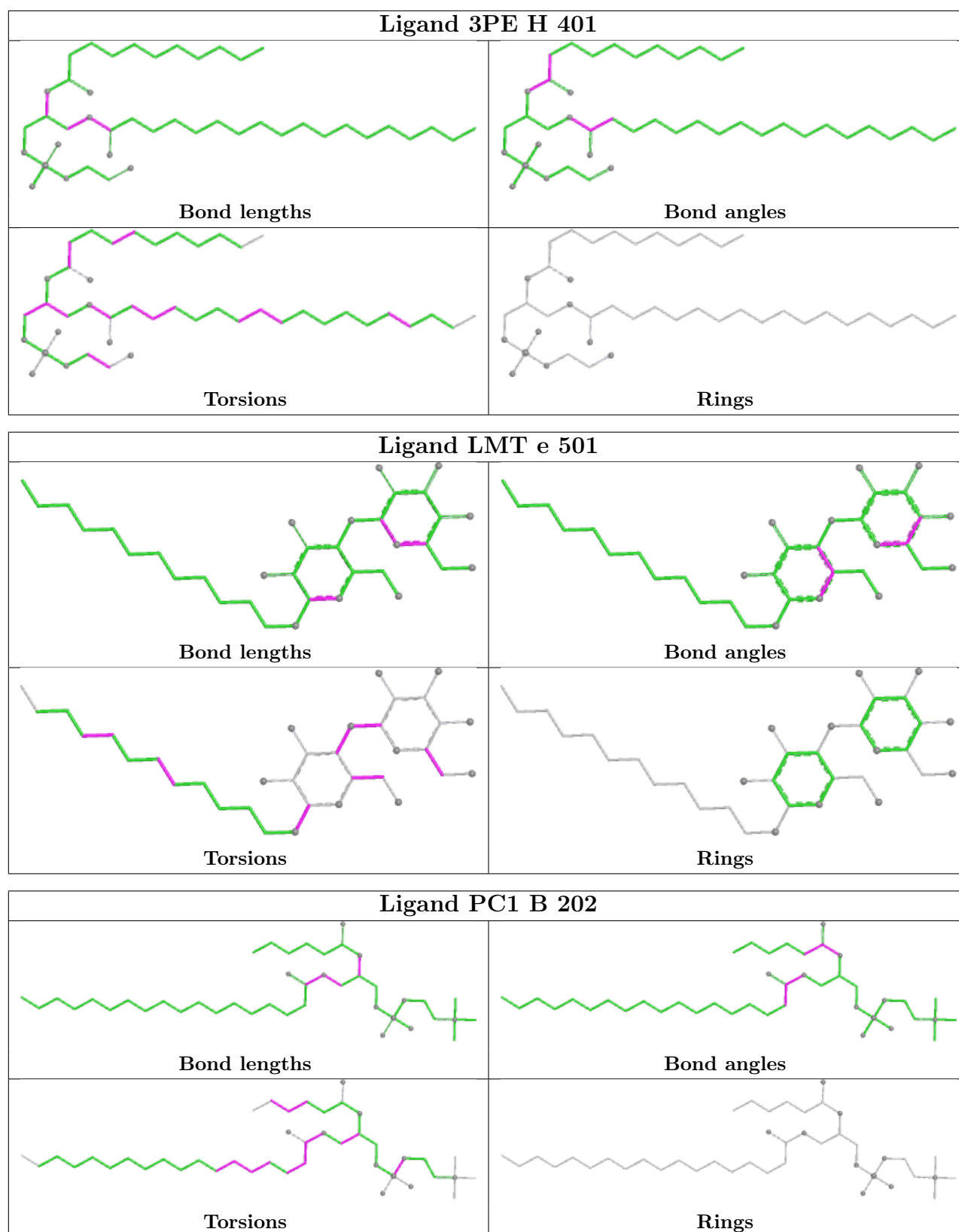


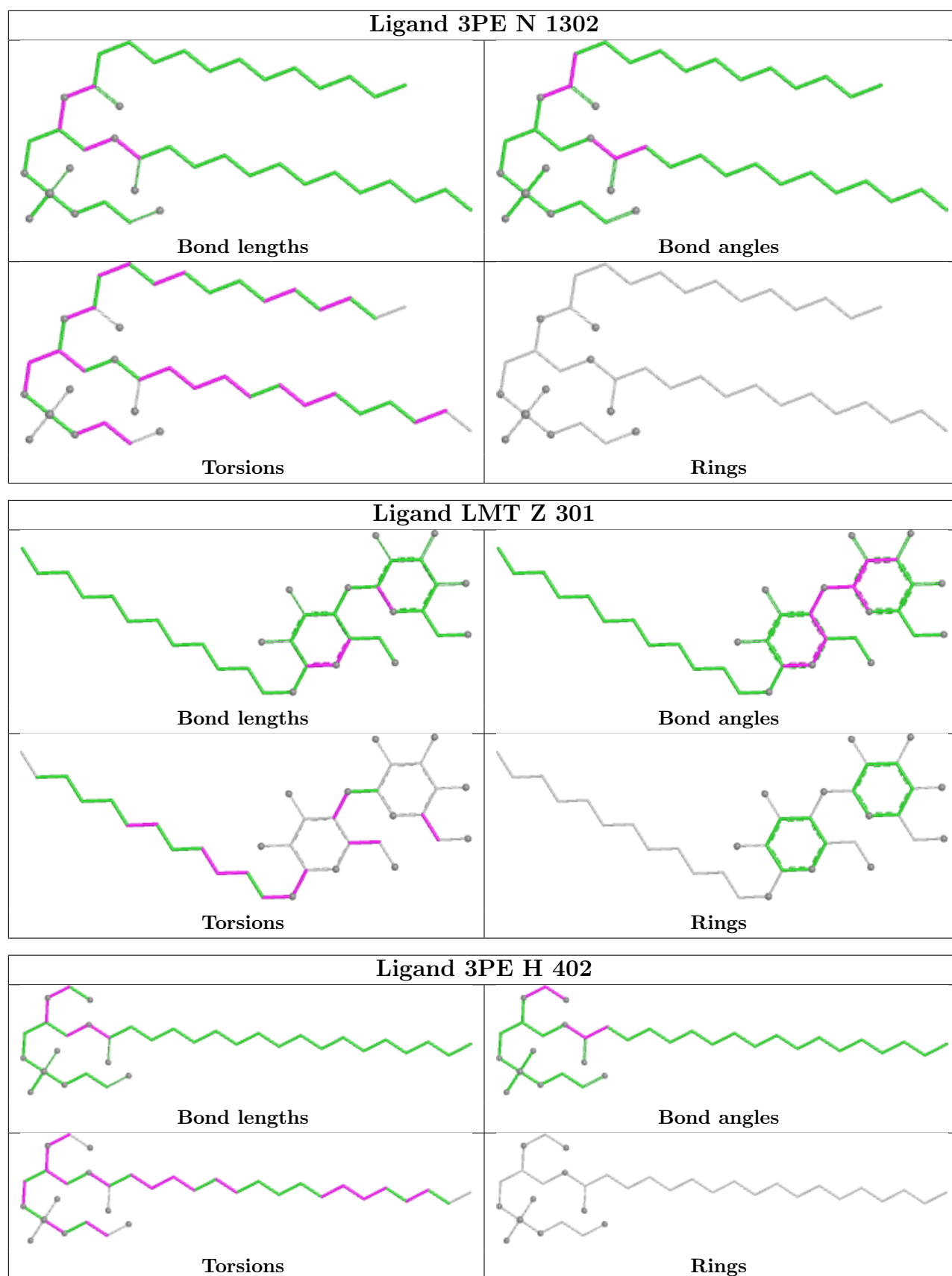


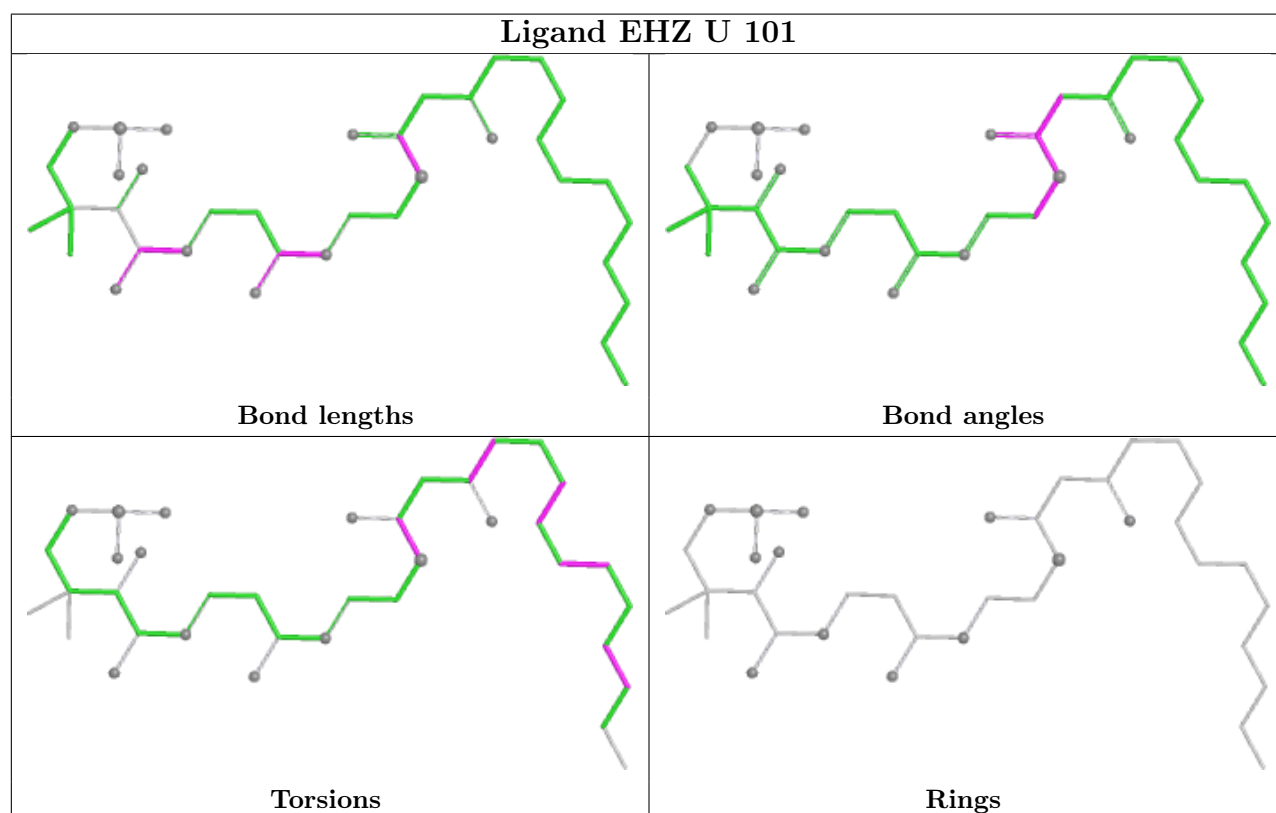
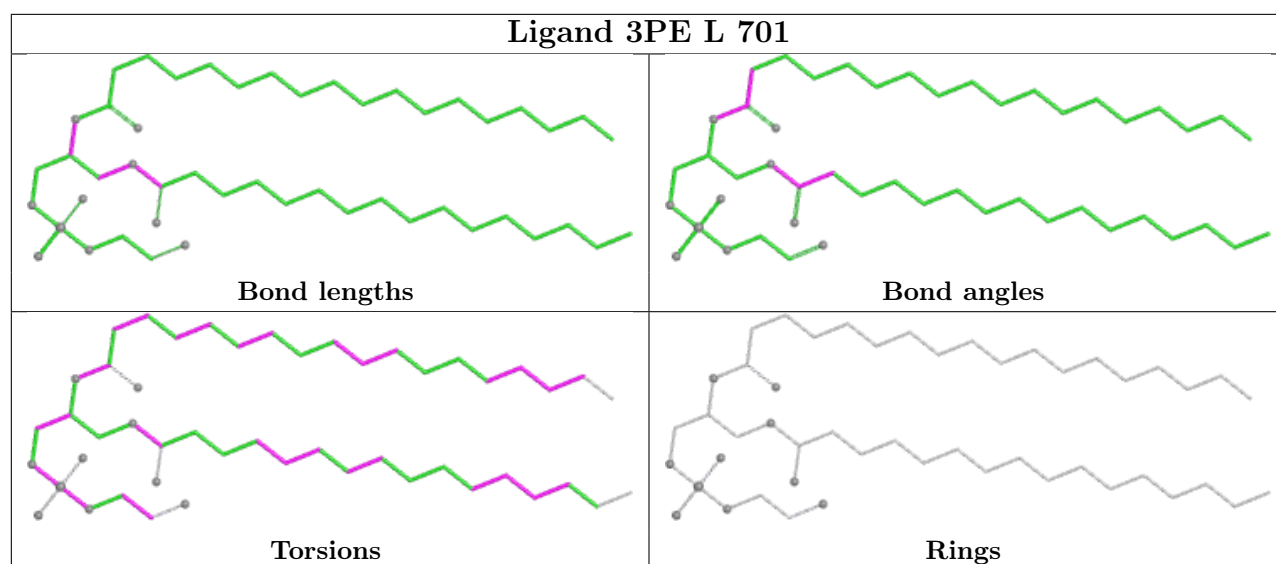




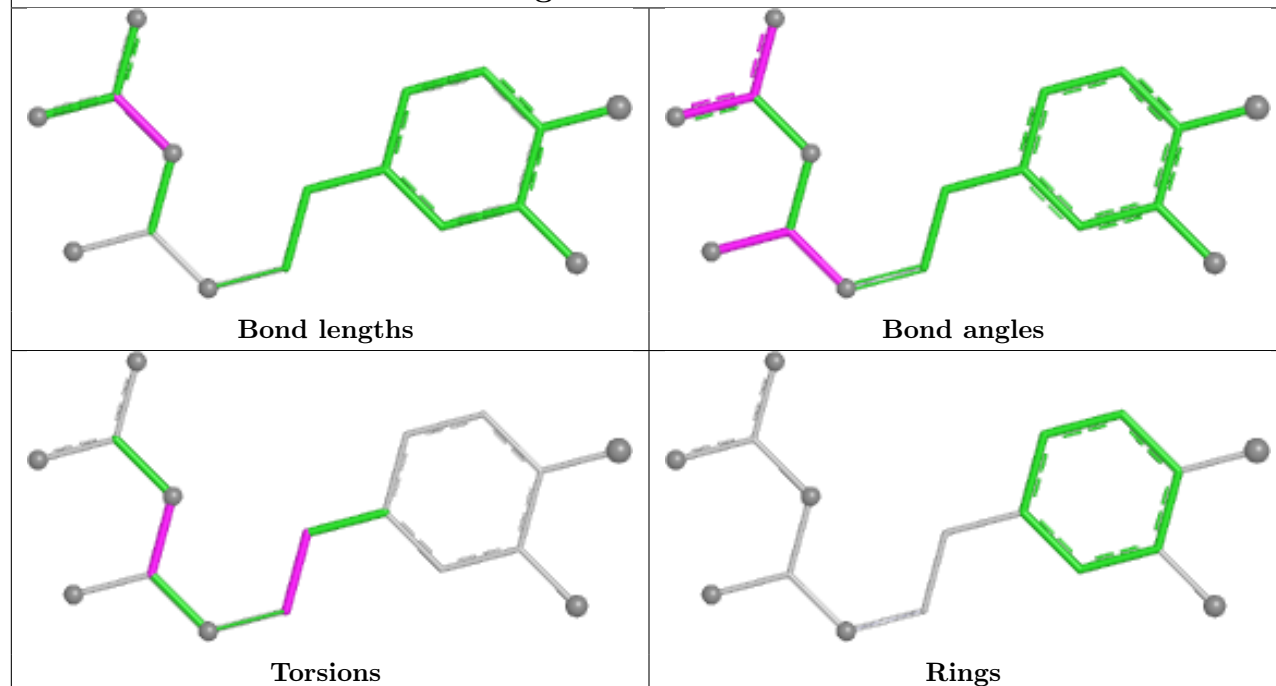




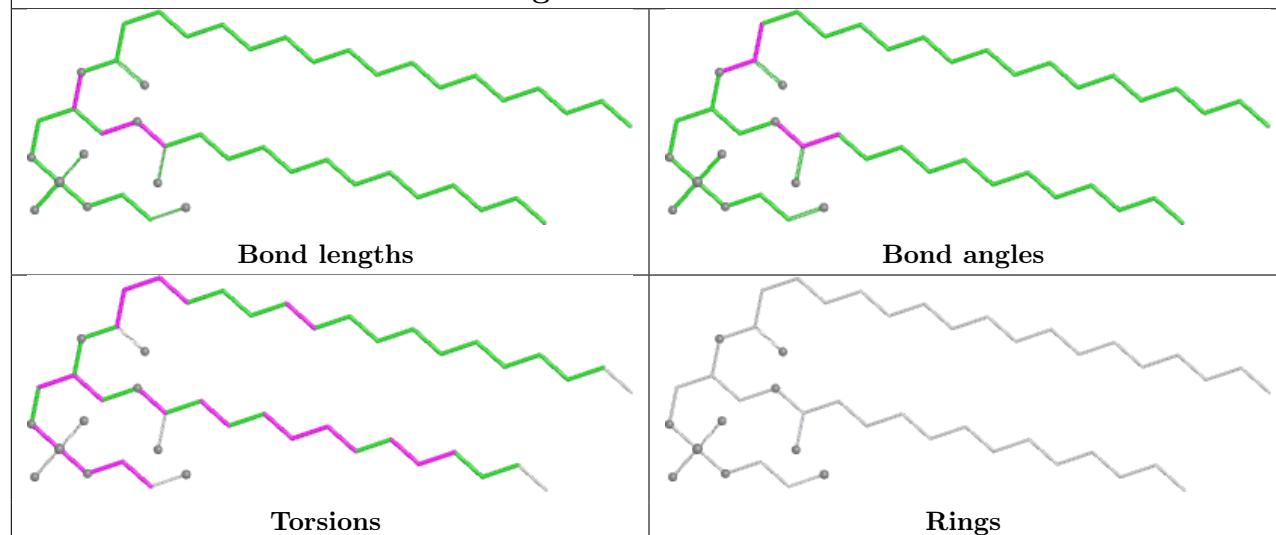


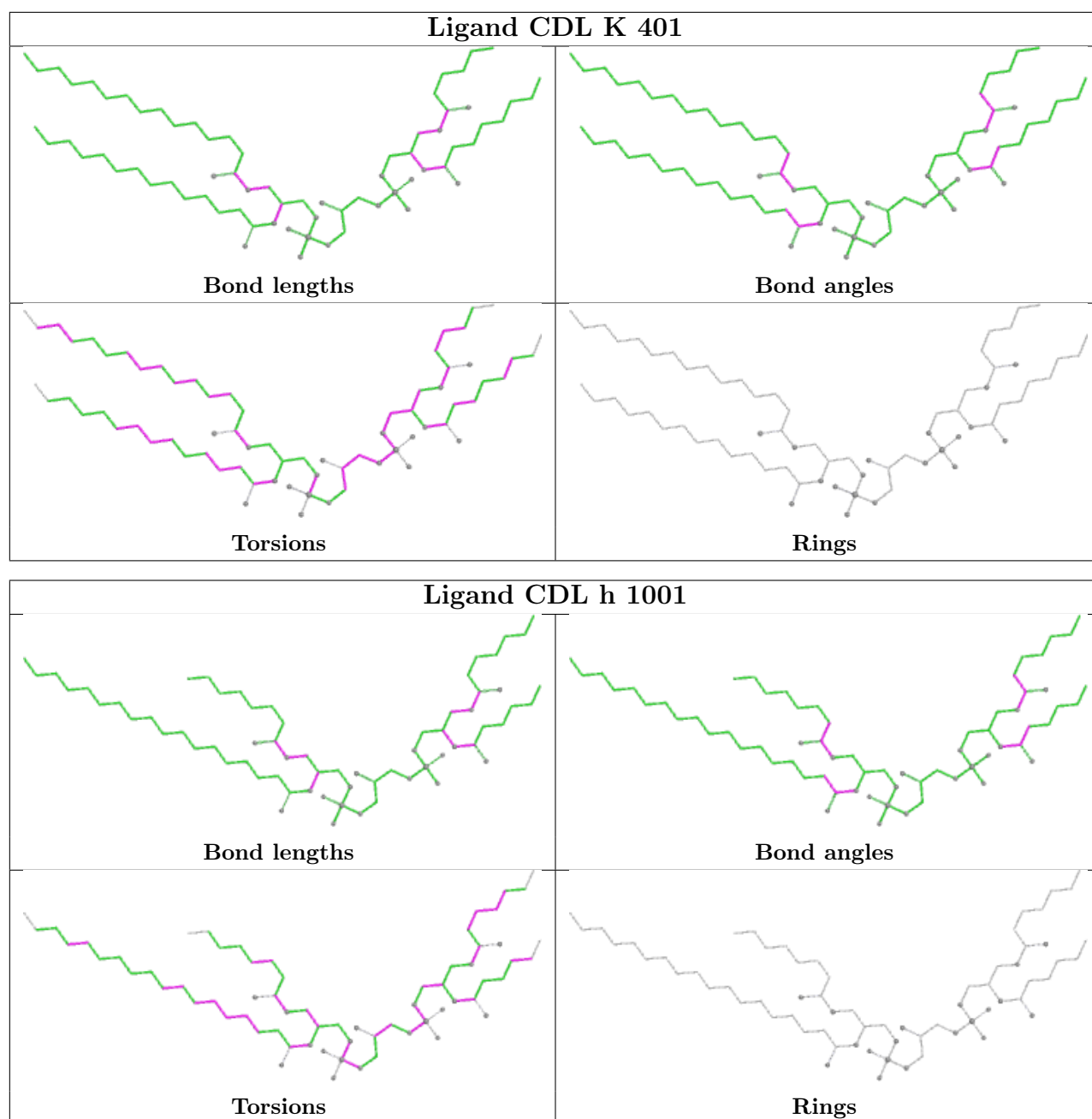


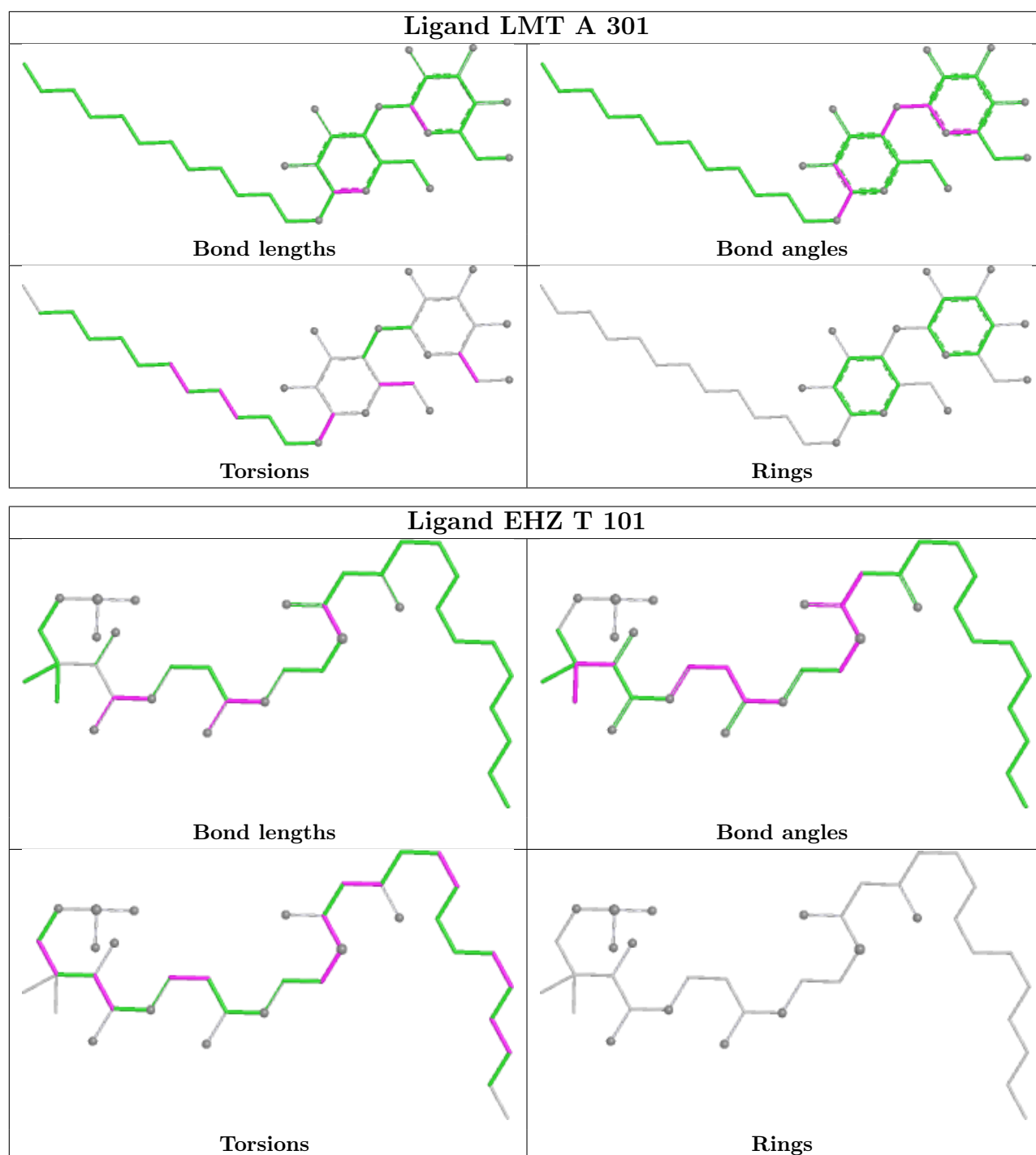
Ligand I49 N 1303



Ligand 3PE M 601







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.

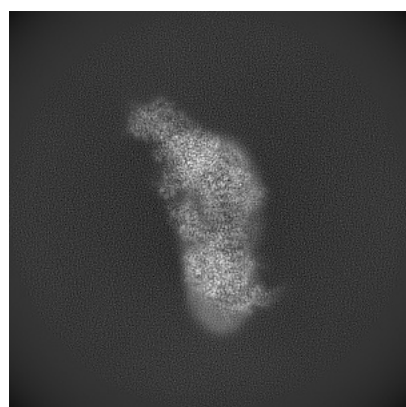
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14266. These allow visual inspection of the internal detail of the map and identification of artifacts.

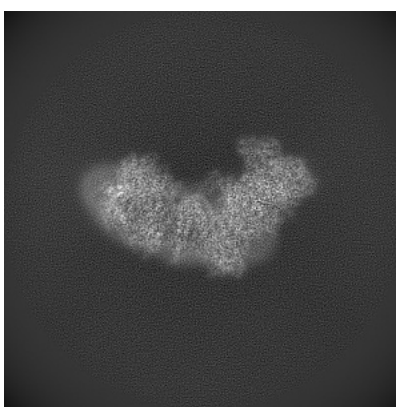
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

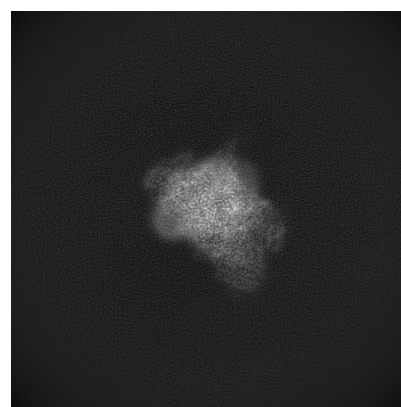
6.1.1 Primary map



X



Y

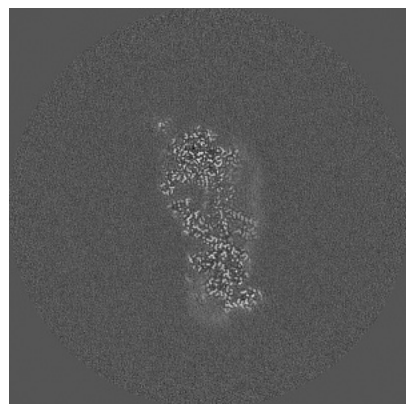


Z

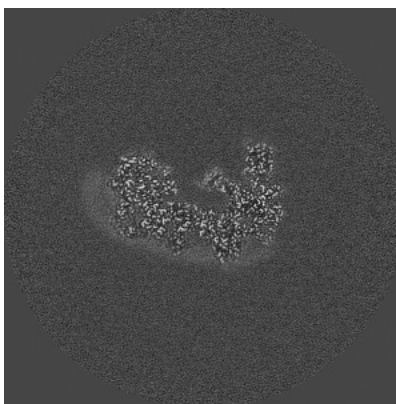
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

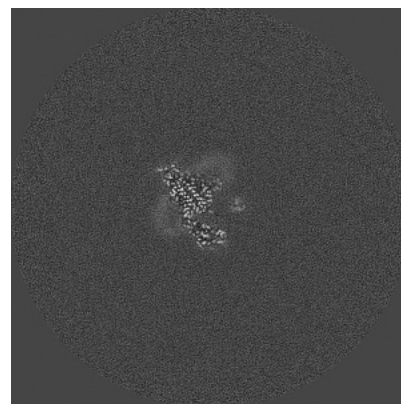
6.2.1 Primary map



X Index: 330



Y Index: 330

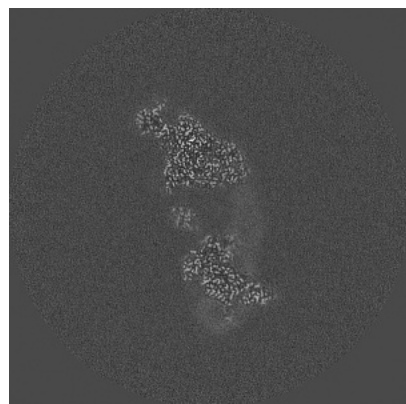


Z Index: 330

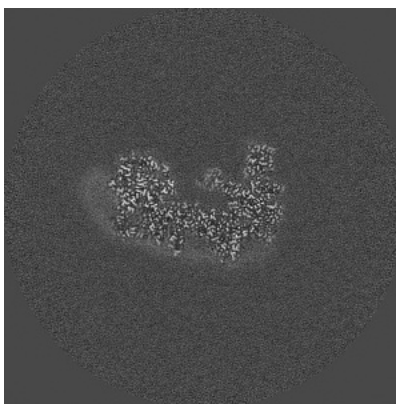
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

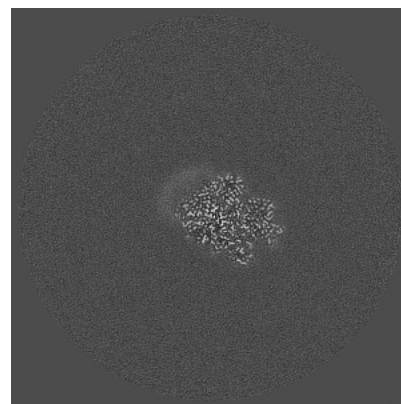
6.3.1 Primary map



X Index: 354



Y Index: 332

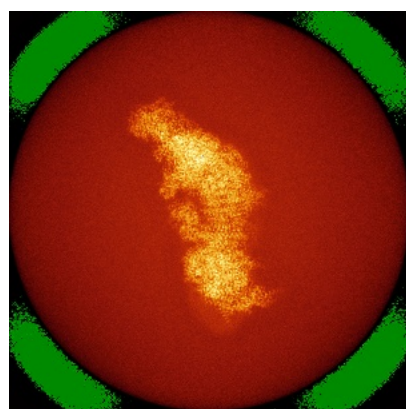


Z Index: 421

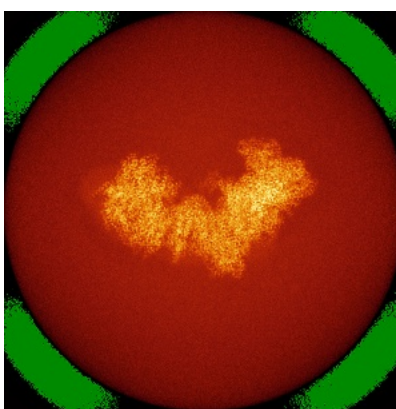
The images above show the largest variance slices of the map in three orthogonal directions.

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

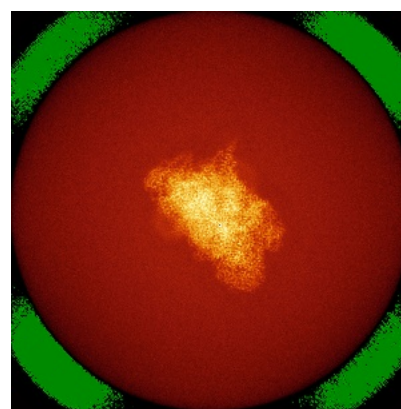
6.4.1 Primary map



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



X



Y



Z

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

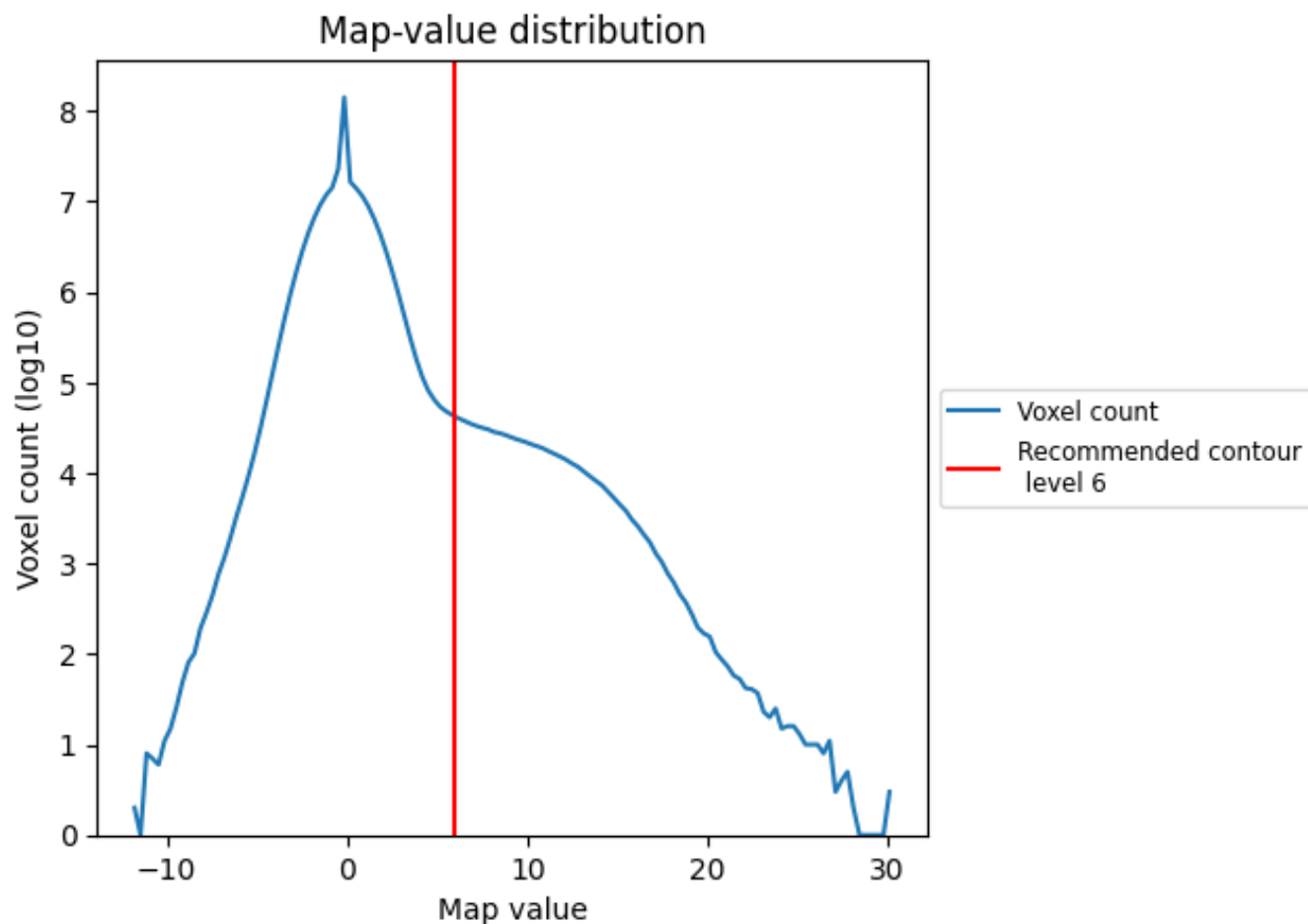
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

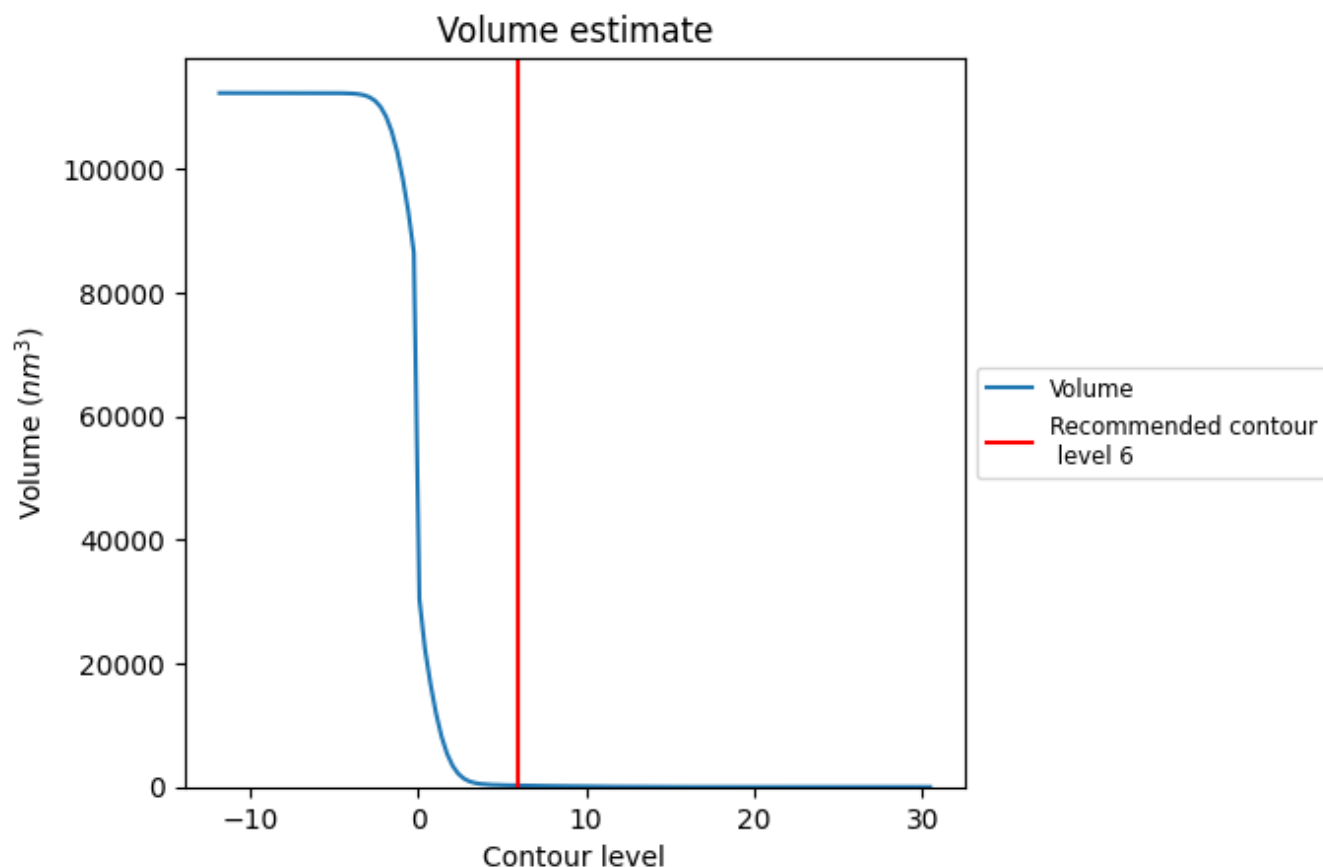
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

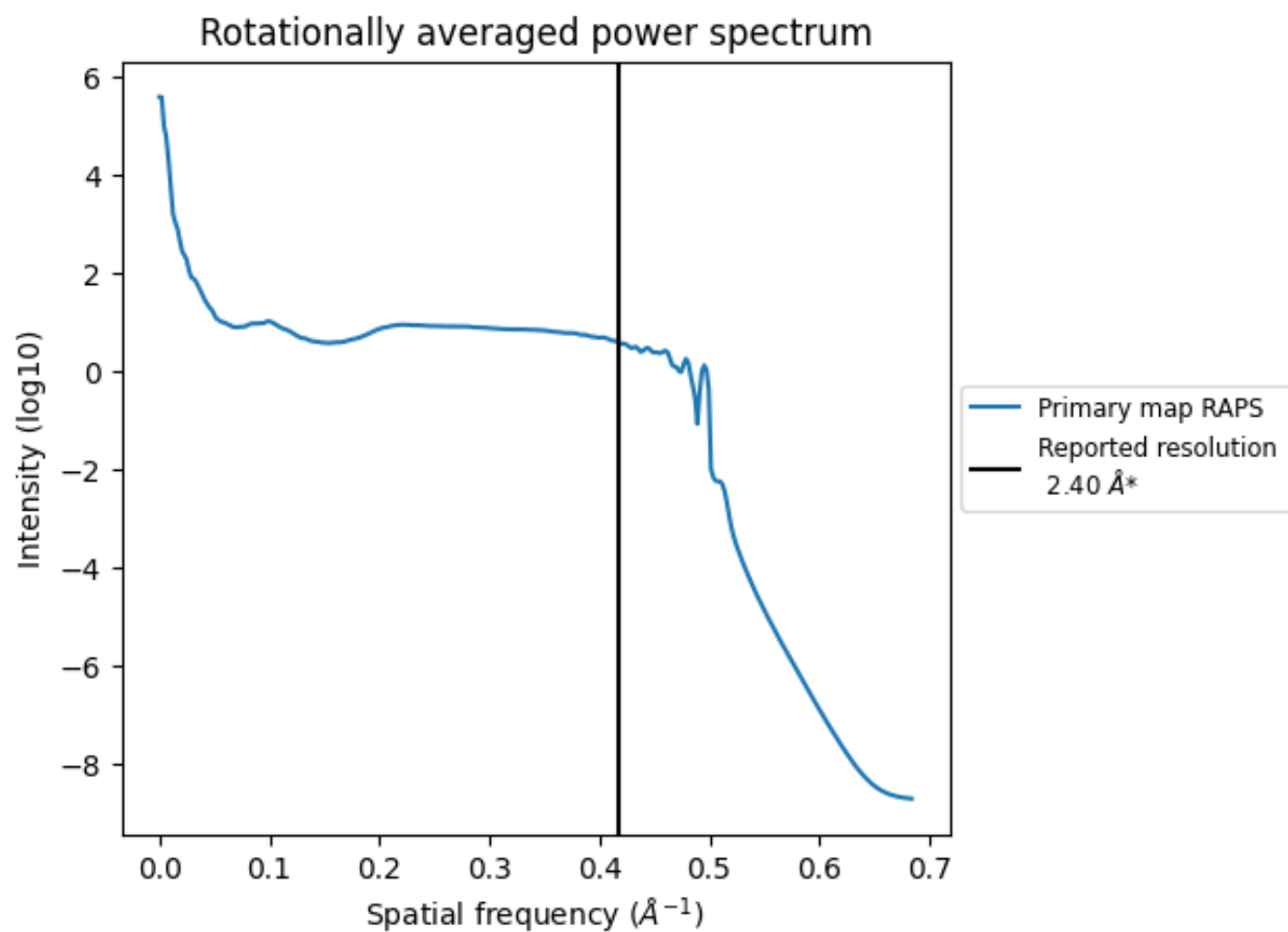
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm^3 ; this corresponds to an approximate mass of 212 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

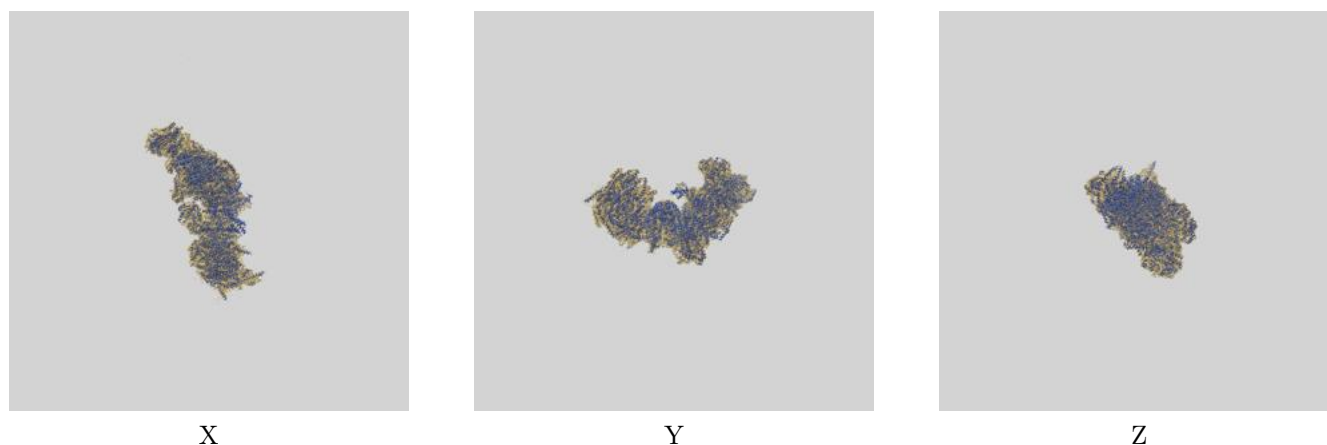
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

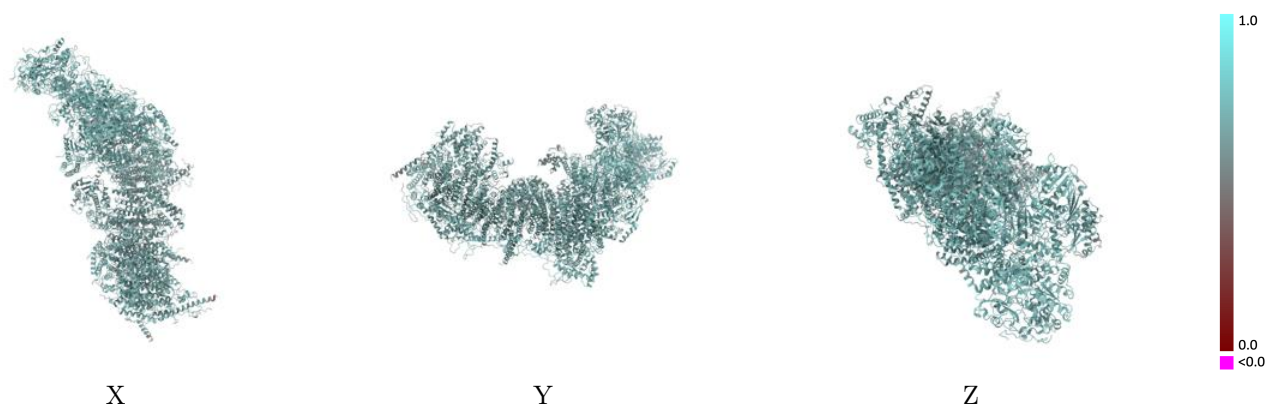
This section contains information regarding the fit between EMDB map EMD-14266 and PDB model 7R44. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



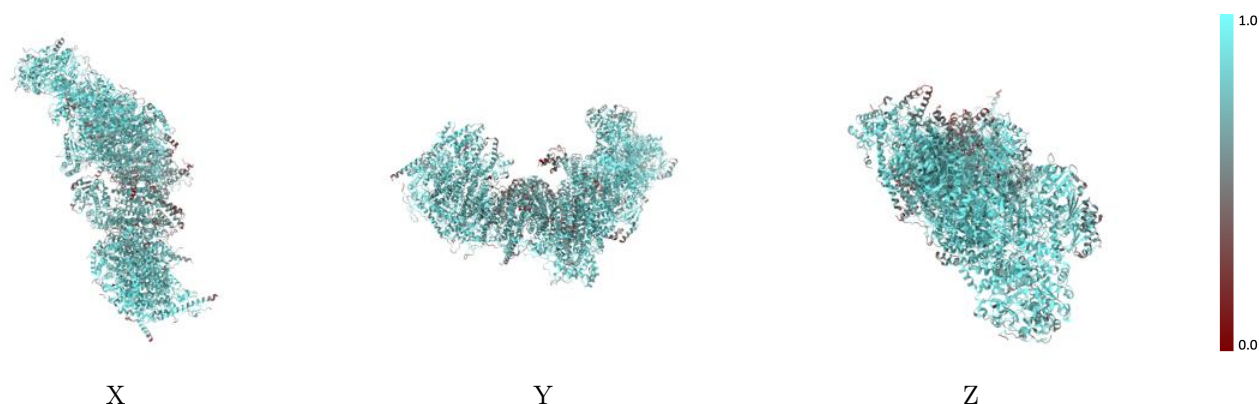
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



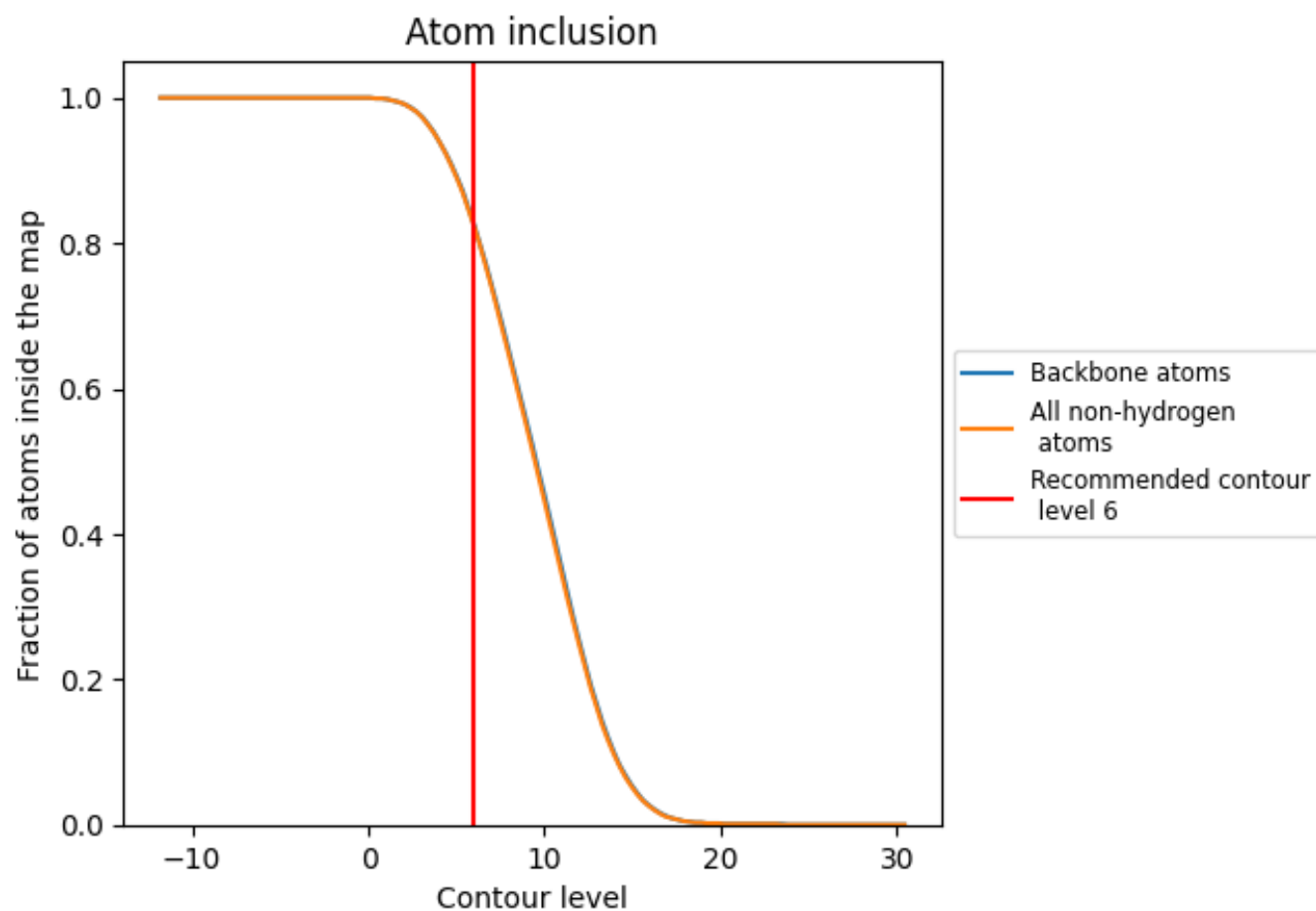
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.8240	 0.6740
A	 0.8010	 0.6780
B	 0.8980	 0.7130
C	 0.9300	 0.7160
D	 0.9030	 0.7120
E	 0.8110	 0.6700
F	 0.8500	 0.6840
G	 0.8590	 0.6910
H	 0.9160	 0.7000
I	 0.9280	 0.7170
J	 0.7790	 0.6650
K	 0.8360	 0.6880
L	 0.8540	 0.6600
M	 0.8840	 0.6800
N	 0.9090	 0.6940
O	 0.7870	 0.6560
P	 0.7930	 0.6810
Q	 0.8570	 0.7030
R	 0.8390	 0.6890
S	 0.7210	 0.6580
T	 0.4500	 0.5760
U	 0.8590	 0.6510
V	 0.7970	 0.6830
W	 0.7950	 0.6810
X	 0.7810	 0.6520
Y	 0.5000	 0.6180
Z	 0.7510	 0.6580
a	 0.7740	 0.6690
b	 0.7240	 0.6390
c	 0.6590	 0.6390
d	 0.7900	 0.6640
e	 0.7120	 0.6450
f	 0.6870	 0.6400
g	 0.7720	 0.6460
h	 0.8130	 0.6680



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Chain	Atom inclusion	Q-score
i	 0.7720	 0.6280
j	 0.8270	 0.6320
k	 0.7480	 0.6170
l	 0.8400	 0.6500
m	 0.7720	 0.6360
n	 0.8670	 0.6590
o	 0.8290	 0.6310
p	 0.8290	 0.6520
q	 0.8210	 0.6900
r	 0.7950	 0.6920
s	 0.7850	 0.6750