Full wwPDB EM Validation Report ⓘ

Feb 1, 2023 – 01:29 pm GMT

PDB ID	:	7R4F
EMDB ID	:	EMD-14302
Title	:	Bovine complex I in the presence of IM1761092, slack class i (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:

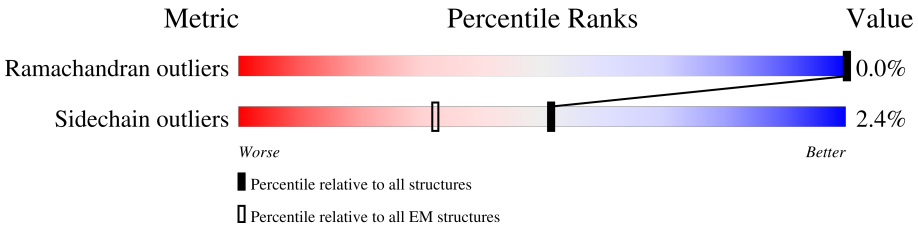
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	81% · 17%
2	B	216	69% · 29%
3	C	266	77% 23%
4	D	463	82% · 17%
5	E	249	84% · 14%
6	F	464	91% · 8%
7	G	727	92% · 5%
8	H	318	99% ·
9	I	212	83% 17%

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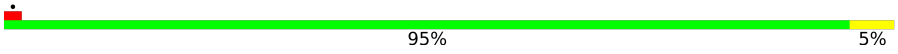
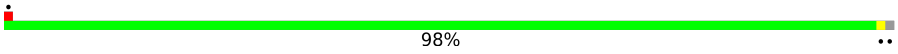
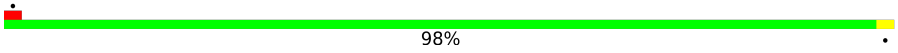
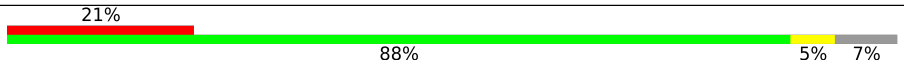
Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 65494 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
			Total	C	N	O	S		
1	A	95	769	529	109	126	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	386	3095	1973	536	562	24	0	0

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	429	Total	C	N	O	S	0	0
			3301	2080	589	612	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	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	119	Total	C	N	O	S	0	0
			877	592	126	150	9		

- 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	547	Total	C	N	O	S	0	0
			4312	2863	665	743	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	453	Total	C	N	O	S	0	0
			3606	2408	560	599	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	288	Total	C	N	O	S	0	0
			2289	1464	413	407	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			720	442	134	141	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 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	72	Total	C	N	O	S	0	0
			584	376	86	117	5		
20	U	84	Total	C	N	O	S	0	0
			681	439	100	137	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	111	Total	C	N	O	S	0	0
			903	583	153	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 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 subunit 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 subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	S	0	0
			154	102	25	26	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	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	88	Total	C	N	O	S	0	0
			733	474	122	133	4		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	108	Total	C	N	O	0	0
			908	580	161	167		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	119	Total	C	N	O	S	0	0
			1027	641	198	180	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	143	Total	C	N	O	S	0	0
			1192	768	214	206	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	43	Total	C	N	O	S	0	0
			364	228	65	70	1		

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

  Image for chem-comp LMT is not available.

Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	O	0
			35	24	11	
45	J	1	Total	C	O	0
			35	24	11	
45	K	1	Total	C	O	0
			35	24	11	
45	f	1	Total	C	O	0
			35	24	11	
45	h	1	Total	C	O	0
			35	24	11	
45	l	1	Total	C	O	0
			35	24	11	
45	p	1	Total	C	O	0
			35	24	11	

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

  Image for chem-comp PC1 is not available.

Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
46	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

  Image for chem-comp SF4 is not available.

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

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

  Image for chem-comp FES is not available.

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 (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

  Image for chem-comp FMN is not available.

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

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

  Image for chem-comp 3PE is not available.

Mol	Chain	Residues	Atoms					AltConf
51	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
51	H	1	Total	C	N	O	P	0
			25	15	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
			33	23	1	8	1	
51	Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	Z	1	Total	C	N	O	P	0
			33	23	1	8	1	
51	d	1	Total	C	N	O	P	0
			51	41	1	8	1	

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

  Image for chem-comp CDL is not available.

Mol	Chain	Residues	Atoms				AltConf
52	L	1	Total	C	O	P	0
			69	50	17	2	
52	N	1	Total	C	O	P	0
			61	42	17	2	
52	X	1	Total	C	O	P	0
			52	33	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	h	1	Total	C	O	P	0
			67	48	17	2	
52	r	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).

  Image for chem-comp I49 is not available.

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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

  Image for chem-comp GTP is not available.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: 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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

  Image for chem-comp NDP is not available.

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

- Molecule 57 is ZINC ION (three-letter code: 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 (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

  Image for chem-comp EHZ is not available.

Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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

  Image for chem-comp MYR is not available.

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	9	Total	O	0
			9	9	
60	B	60	Total	O	0
			60	60	
60	C	99	Total	O	0
			99	99	
60	D	160	Total	O	0
			160	160	
60	E	19	Total	O	0
			19	19	
60	F	73	Total	O	0
			73	73	
60	G	221	Total	O	0
			221	221	
60	H	54	Total	O	0
			54	54	
60	I	104	Total	O	0
			104	104	
60	J	2	Total	O	0
			2	2	
60	K	2	Total	O	0
			2	2	
60	L	38	Total	O	0
			38	38	
60	M	53	Total	O	0
			53	53	
60	N	17	Total	O	0
			17	17	
60	P	42	Total	O	0
			42	42	
60	Q	73	Total	O	0
			73	73	
60	R	40	Total	O	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
60	S	1	Total O 1 1	0
60	U	15	Total O 15 15	0
60	V	11	Total O 11 11	0
60	W	17	Total O 17 17	0
60	X	24	Total O 24 24	0
60	Y	2	Total O 2 2	0
60	Z	18	Total O 18 18	0
60	a	12	Total O 12 12	0
60	b	9	Total O 9 9	0
60	d	6	Total O 6 6	0
60	e	13	Total O 13 13	0
60	f	4	Total O 4 4	0
60	g	11	Total O 11 11	0
60	h	21	Total O 21 21	0
60	i	7	Total O 7 7	0
60	j	4	Total O 4 4	0
60	k	8	Total O 8 8	0
60	l	16	Total O 16 16	0
60	m	9	Total O 9 9	0
60	n	26	Total O 26 26	0
60	o	9	Total O 9 9	0

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Mol	Chain	Residues	Atoms	AltConf
60	p	26	Total O 26 26	0
60	q	42	Total O 42 42	0
60	r	30	Total O 30 30	0
60	s	8	Total O 8 8	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89435	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 ($e^-/Å^2$)	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	41.163	Depositor
Minimum map value	-17.328	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.086	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

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

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	0.29	0/779	0.43	0/1067
2	B	0.36	0/1261	0.46	0/1706
3	C	0.35	0/1765	0.45	0/2403
4	D	0.33	0/3155	0.46	0/4264
5	E	0.31	0/1695	0.44	0/2307
6	F	0.31	0/3375	0.45	0/4561
7	G	0.30	0/5367	0.46	0/7274
8	H	0.32	0/2571	0.43	0/3513
9	I	0.34	0/1445	0.48	0/1956
10	J	0.34	0/897	0.42	0/1213
11	K	0.29	0/745	0.41	0/1008
12	L	0.35	0/4419	0.43	0/6016
13	M	0.32	0/3689	0.42	0/5029
14	N	0.29	0/2792	0.43	0/3800
15	O	0.29	0/2651	0.40	0/3587
16	P	0.30	0/2339	0.44	0/3159
17	Q	0.30	0/1039	0.45	0/1404
18	R	0.34	0/731	0.48	0/984
19	S	0.29	0/674	0.44	0/908
20	T	0.28	0/593	0.39	0/799
20	U	0.37	0/692	0.41	0/932
21	V	0.28	0/923	0.37	0/1250
22	W	0.29	0/995	0.41	0/1337
23	X	0.31	0/1439	0.41	0/1942
24	Y	0.25	0/157	0.38	0/211
25	Z	0.31	0/1181	0.43	0/1592
26	a	0.34	0/576	0.42	0/775
27	b	0.31	0/672	0.41	0/923
28	c	0.29	0/418	0.37	0/567
29	d	0.34	0/964	0.42	0/1305
30	e	0.30	0/818	0.44	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	f	0.32	0/464	0.42	0/626
32	g	0.37	0/755	0.41	0/1023
33	h	0.33	0/1188	0.41	0/1607
34	i	0.37	0/904	0.42	0/1230
35	j	0.37	0/607	0.38	0/833
36	k	0.35	0/657	0.42	0/887
37	l	0.37	0/1358	0.42	0/1858
38	m	0.36	0/929	0.43	0/1252
39	n	0.38	0/1540	0.41	0/2085
40	o	0.35	0/1052	0.40	0/1409
41	p	0.36	0/1468	0.42	0/1979
42	q	0.31	0/1233	0.44	0/1676
43	r	0.31	0/780	0.45	0/1056
44	s	0.30	0/375	0.42	0/507
All	All	0.32	0/64127	0.43	0/86913

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

4.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 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	91/115 (79%)	90 (99%)	1 (1%)	0	100	100
2	B	152/216 (70%)	145 (95%)	7 (5%)	0	100	100
3	C	204/266 (77%)	199 (98%)	5 (2%)	0	100	100
4	D	383/463 (83%)	372 (97%)	11 (3%)	0	100	100
5	E	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
6	F	427/464 (92%)	418 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	665 (97%)	21 (3%)	0	100	100
8	H	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	115/175 (66%)	108 (94%)	7 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	545/606 (90%)	525 (96%)	19 (4%)	1 (0%)	47	62
13	M	449/459 (98%)	442 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
15	O	318/343 (93%)	302 (95%)	16 (5%)	0	100	100
16	P	280/380 (74%)	276 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	123 (100%)	0	0	100	100
18	R	92/124 (74%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99 (81%)	78 (98%)	2 (2%)	0	100	100
20	T	70/156 (45%)	69 (99%)	1 (1%)	0	100	100
20	U	82/156 (53%)	81 (99%)	1 (1%)	0	100	100
21	V	109/116 (94%)	109 (100%)	0	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	18/141 (13%)	16 (89%)	2 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
26	a	67/70 (96%)	67 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	110/120 (92%)	110 (100%)	0	0	100	100
30	e	93/106 (88%)	92 (99%)	1 (1%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	86/154 (56%)	80 (93%)	6 (7%)	0	100	100
33	h	136/189 (72%)	136 (100%)	0	0	100	100
34	i	99/127 (78%)	96 (97%)	3 (3%)	0	100	100
35	j	65/108 (60%)	65 (100%)	0	0	100	100
36	k	77/98 (79%)	74 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
38	m	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	117/137 (85%)	112 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	168 (100%)	0	0	100	100
42	q	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
43	r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	s	41/109 (38%)	40 (98%)	1 (2%)	0	100	100
All	All	7679/9212 (83%)	7489 (98%)	189 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	252	MET

4.3.2 Protein sidechains (i)

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	83/100 (83%)	81 (98%)	2 (2%)	49 68
2	B	130/175 (74%)	125 (96%)	5 (4%)	33 51
3	C	187/228 (82%)	187 (100%)	0	100 100
4	D	332/392 (85%)	327 (98%)	5 (2%)	65 80
5	E	183/205 (89%)	179 (98%)	4 (2%)	52 71
6	F	343/368 (93%)	334 (97%)	9 (3%)	46 66
7	G	578/608 (95%)	561 (97%)	17 (3%)	42 62
8	H	274/274 (100%)	271 (99%)	3 (1%)	73 87
9	I	151/175 (86%)	150 (99%)	1 (1%)	84 92
10	J	92/141 (65%)	89 (97%)	3 (3%)	38 57
11	K	85/85 (100%)	81 (95%)	4 (5%)	26 42
12	L	474/533 (89%)	463 (98%)	11 (2%)	50 70
13	M	407/412 (99%)	403 (99%)	4 (1%)	76 88
14	N	315/315 (100%)	309 (98%)	6 (2%)	57 75
15	O	283/303 (93%)	265 (94%)	18 (6%)	17 28
16	P	247/327 (76%)	243 (98%)	4 (2%)	62 79
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78 90
18	R	77/97 (79%)	75 (97%)	2 (3%)	46 66
19	S	73/82 (89%)	71 (97%)	2 (3%)	44 65
20	T	67/135 (50%)	62 (92%)	5 (8%)	13 21
20	U	78/135 (58%)	78 (100%)	0	100 100
21	V	99/102 (97%)	97 (98%)	2 (2%)	55 74
22	W	107/114 (94%)	105 (98%)	2 (2%)	57 75
23	X	154/155 (99%)	150 (97%)	4 (3%)	46 66
24	Y	15/102 (15%)	13 (87%)	2 (13%)	4 4
25	Z	120/121 (99%)	117 (98%)	3 (2%)	47 67
26	a	58/59 (98%)	57 (98%)	1 (2%)	60 78
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%)	83 (96%)	3 (4%)	36 55
31	f	49/54 (91%)	45 (92%)	4 (8%)	11 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	g	79/131 (60%)	75 (95%)	4 (5%)	24 39
33	h	121/158 (77%)	121 (100%)	0	100 100
34	i	98/120 (82%)	96 (98%)	2 (2%)	55 74
35	j	61/84 (73%)	59 (97%)	2 (3%)	38 57
36	k	61/76 (80%)	61 (100%)	0	100 100
37	l	139/159 (87%)	136 (98%)	3 (2%)	52 71
38	m	96/115 (84%)	94 (98%)	2 (2%)	53 72
39	n	156/161 (97%)	154 (99%)	2 (1%)	69 84
40	o	108/120 (90%)	102 (94%)	6 (6%)	21 34
41	p	154/157 (98%)	150 (97%)	4 (3%)	46 66
42	q	129/131 (98%)	125 (97%)	4 (3%)	40 60
43	r	84/97 (87%)	81 (96%)	3 (4%)	35 54
44	s	42/92 (46%)	41 (98%)	1 (2%)	49 68
All	All	6802/7892 (86%)	6642 (98%)	160 (2%)	51 68

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	87	MET
2	B	50	PHE
2	B	54	CYS
2	B	59	MET
2	B	81	ARG
2	B	125	TYR
4	D	49	LEU
4	D	75	LYS
4	D	111	MET
4	D	331	SER
4	D	341	SER
5	E	118	GLU
5	E	123	LYS
5	E	162	GLU
5	E	163	ASP
6	F	28	ARG
6	F	84	LYS
6	F	99	GLU

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Mol	Chain	Res	Type
6	F	105	CYS
6	F	150	GLN
6	F	164	LYS
6	F	310	SER
6	F	359	CYS
6	F	405	CYS
7	G	17	SER
7	G	35	MET
7	G	39	ARG
7	G	137	VAL
7	G	188	GLU
7	G	193	SER
7	G	237	ASN
7	G	309	SER
7	G	337	ARG
7	G	405	LYS
7	G	480	SER
7	G	484	THR
7	G	512	GLU
7	G	516	LYS
7	G	596	ASP
7	G	646	SER
7	G	657	LEU
8	H	54	LYS
8	H	121	TRP
8	H	259	PHE
9	I	15	LYS
10	J	3	LEU
10	J	20	PHE
10	J	168	ILE
11	K	10	MET
11	K	53	PHE
11	K	97	GLN
11	K	98	CYS
12	L	6	SER
12	L	22	MET
12	L	79	SER
12	L	124	PHE
12	L	197	ASP
12	L	262	ARG
12	L	393	ASP
12	L	461	SER

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Mol	Chain	Res	Type
12	L	512	LYS
12	L	514	HIS
12	L	515	TYR
13	M	116	ILE
13	M	168	GLN
13	M	189	SER
13	M	387	SER
14	N	37	MET
14	N	237	THR
14	N	291	TYR
14	N	305	PHE
14	N	307	SER
14	N	324	THR
15	O	1	LEU
15	O	19	THR
15	O	21	LYS
15	O	26	THR
15	O	30	ASN
15	O	60	ASP
15	O	92	ASN
15	O	135	LEU
15	O	140	ARG
15	O	146	LYS
15	O	194	ILE
15	O	206	TYR
15	O	215	SER
15	O	250	ASP
15	O	269	VAL
15	O	282	VAL
15	O	295	GLU
15	O	302	ARG
16	P	199	LYS
16	P	234	SER
16	P	240	ASP
16	P	281	ARG
17	Q	14	ASP
18	R	4	THR
18	R	20	ASP
19	S	22	LEU
19	S	82	SER
20	T	12	LYS
20	T	31	SER

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Mol	Chain	Res	Type
20	T	39	ASP
20	T	44(A)	SER
20	T	72	CYS
21	V	17	GLU
21	V	75	GLN
22	W	22	SER
22	W	95	LYS
23	X	14	VAL
23	X	47	TRP
23	X	101	LYS
23	X	109	CYS
24	Y	125	LYS
24	Y	128	GLN
25	Z	82	ARG
25	Z	105	LYS
25	Z	128	ARG
26	a	12	MET
30	e	56	LYS
30	e	90	LYS
30	e	92	THR
31	f	6	VAL
31	f	29	LYS
31	f	47	GLU
31	f	57	LYS
32	g	57	ASN
32	g	110	SER
32	g	112	CYS
32	g	122	GLU
34	i	65	ARG
34	i	78	VAL
35	j	19	ARG
35	j	70	ASP
37	l	18	GLU
37	l	42	THR
37	l	56	GLN
38	m	29	ARG
38	m	92	PHE
39	n	8	TYR
39	n	159	GLN
40	o	30	PHE
40	o	33	ARG
40	o	34	LYS

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Mol	Chain	Res	Type
40	o	77	LEU
40	o	111	LYS
40	o	112	LYS
41	p	3	SER
41	p	16	THR
41	p	167	LYS
41	p	171	GLU
42	q	15	SER
42	q	133	LYS
42	q	144	TYR
42	q	145	LYS
43	r	5	ARG
43	r	24	GLN
43	r	72	GLN
44	s	59	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
4	D	55	HIS
4	D	157	HIS
8	H	317	GLN
35	j	24	GLN
39	n	159	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

9 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	$\#\|Z\|>2$
43	AYA	r	1	43	6,7,8	1.76	2 (33%)	5,8,10	1.40	1 (20%)
11	FME	K	1	11	8,9,10	0.88	0	7,9,11	1.17	1 (14%)
34	SAC	i	1	34	7,8,9	1.83	1 (14%)	8,9,11	2.03	2 (25%)
4	2MR	D	85	4	10,12,13	2.66	3 (30%)	5,13,15	1.20	1 (20%)
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	1.08	1 (14%)
1	FME	A	1	1	8,9,10	0.92	0	7,9,11	0.78	0
12	FME	L	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.88	0
8	FME	H	1	8	8,9,10	0.99	0	7,9,11	0.88	0
14	FME	N	1	14	8,9,10	0.97	0	7,9,11	0.84	0

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.00	1.44	1.33
4	D	85	2MR	CZ-NE	4.71	1.44	1.34
34	i	1	SAC	O-C	4.15	1.36	1.19
4	D	85	2MR	O-C	3.94	1.35	1.19
43	r	1	AYA	CT-N	3.17	1.45	1.34
12	L	1	FME	CA-N	-2.10	1.43	1.46
43	r	1	AYA	OT-CT	-2.07	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	i	1	SAC	O-C-CA	-4.66	112.56	124.78
43	r	1	AYA	CM-CT-N	2.51	120.36	116.10
4	D	85	2MR	NE-CZ-NH2	-2.44	117.24	119.48
13	M	1	FME	C-CA-N	2.41	114.08	109.73
11	K	1	FME	C-CA-N	2.22	113.73	109.73
34	i	1	SAC	OG-CB-CA	-2.18	105.41	110.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	CB-CA-N-CN
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
14	N	1	FME	O1-CN-N-CA
34	i	1	SAC	C-CA-CB-OG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
11	K	1	FME	N-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
12	L	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
14	N	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 3 are monoatomic - leaving 41 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	$\#\|Z\| > 2$
52	CDL	h	1001	-	66,66,99	1.06	7 (10%)	72,78,111	1.22	5 (6%)
52	CDL	L	702	-	68,68,99	1.04	7 (10%)	74,80,111	1.10	4 (5%)
52	CDL	d	1202	-	64,64,99	1.07	7 (10%)	70,76,111	1.12	4 (5%)
52	CDL	r	201	-	75,75,99	0.99	7 (9%)	81,87,111	1.12	5 (6%)
46	PC1	M	1302	-	39,39,53	1.10	3 (7%)	45,47,61	1.05	2 (4%)
52	CDL	X	201	-	51,51,99	1.19	8 (15%)	57,63,111	1.28	4 (7%)
59	MYR	o	201	40	14,14,15	0.85	0	13,13,15	0.66	0
51	3PE	I	201	-	50,50,50	0.86	3 (6%)	53,55,55	1.02	2 (3%)
51	3PE	d	1201	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
45	LMT	f	1101	-	36,36,36	1.17	3 (8%)	47,47,47	0.88	0
45	LMT	A	301	-	36,36,36	1.19	2 (5%)	47,47,47	0.86	0
45	LMT	h	1002	-	36,36,36	1.20	3 (8%)	47,47,47	1.18	4 (8%)
52	CDL	N	1101	-	60,60,99	1.11	7 (11%)	66,72,111	1.15	4 (6%)
48	FES	G	803	7	0,4,4	-	-	-		
47	SF4	B	201	2	0,12,12	-	-	-		
47	SF4	G	801	7	0,12,12	-	-	-		
53	I49	N	1102	-	15,17,17	1.50	2 (13%)	21,22,22	1.76	6 (28%)
47	SF4	G	802	7	0,12,12	-	-	-		
47	SF4	I	203	9	0,12,12	-	-	-		
51	3PE	H	902	-	24,24,50	1.23	4 (16%)	27,29,55	1.18	2 (7%)
51	3PE	H	903	-	33,33,50	1.36	3 (9%)	34,37,55	1.18	2 (5%)
45	LMT	K	901	-	36,36,36	1.19	3 (8%)	47,47,47	0.97	1 (2%)
51	3PE	L	701	-	48,48,50	0.87	3 (6%)	51,53,55	1.13	3 (5%)
51	3PE	M	1301	-	32,32,50	1.07	4 (12%)	35,37,55	1.18	3 (8%)
45	LMT	p	201	-	36,36,36	1.17	3 (8%)	47,47,47	1.17	4 (8%)
58	EHZ	T	101	20	29,36,37	1.76	5 (17%)	35,44,47	1.66	6 (17%)
49	FMN	F	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.29	6 (12%)
46	PC1	B	202	-	34,34,53	1.16	4 (11%)	40,42,61	1.10	2 (5%)
47	SF4	I	202	9	0,12,12	-	-	-		
51	3PE	Y	601	-	34,34,50	1.01	4 (11%)	37,39,55	1.07	2 (5%)
45	LMT	l	201	-	36,36,36	1.21	3 (8%)	47,47,47	1.01	1 (2%)
45	LMT	J	201	-	36,36,36	1.20	2 (5%)	47,47,47	0.81	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
51	3PE	H	901	-	47,47,50	0.89	4 (8%)	50,52,55	1.06	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-		
46	PC1	A	302	-	51,51,53	0.95	4 (7%)	57,59,61	1.08	2 (3%)
51	3PE	L	703	-	44,44,50	0.90	4 (9%)	47,49,55	1.27	3 (6%)
54	GTP	O	401	55	26,34,34	2.93	10 (38%)	32,54,54	1.70	10 (31%)
51	3PE	Z	301	-	32,32,50	1.06	4 (12%)	35,37,55	1.09	2 (5%)
47	SF4	F	502	6	0,12,12	-	-	-		
58	EHZ	U	101	20	29,36,37	1.62	5 (17%)	35,44,47	1.43	2 (5%)
56	NDP	P	501	-	45,52,52	2.17	4 (8%)	53,80,80	1.67	11 (20%)

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
52	CDL	h	1001	-	-	28/77/77/110	-
52	CDL	L	702	-	-	28/79/79/110	-
52	CDL	d	1202	-	-	32/75/75/110	-
52	CDL	r	201	-	-	34/86/86/110	-
46	PC1	M	1302	-	-	27/43/43/57	-
52	CDL	X	201	-	-	29/61/61/110	-
59	MYR	o	201	40	-	8/11/12/13	-
51	3PE	I	201	-	-	18/54/54/54	-
51	3PE	d	1201	-	-	23/54/54/54	-
45	LMT	f	1101	-	-	7/21/61/61	0/2/2/2
45	LMT	A	301	-	-	8/21/61/61	0/2/2/2
45	LMT	h	1002	-	-	10/21/61/61	0/2/2/2
52	CDL	N	1101	-	-	27/71/71/110	-
48	FES	G	803	7	-	-	0/1/1/1
47	SF4	B	201	2	-	-	0/6/5/5
53	I49	N	1102	-	-	5/10/10/10	0/1/1/1
47	SF4	G	801	7	-	-	0/6/5/5
51	3PE	H	902	-	-	13/28/28/54	-
51	3PE	H	903	-	-	16/36/36/54	-
51	3PE	M	1301	-	-	15/36/36/54	-
51	3PE	L	701	-	-	20/52/52/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	LMT	K	901	-	-	8/21/61/61	0/2/2/2
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	I	203	9	-	-	0/6/5/5
45	LMT	p	201	-	-	11/21/61/61	0/2/2/2
58	EHZ	T	101	20	-	17/42/44/45	-
49	FMN	F	501	-	-	2/18/18/18	0/3/3/3
46	PC1	B	202	-	-	20/38/38/57	-
47	SF4	I	202	9	-	-	0/6/5/5
51	3PE	Y	601	-	-	20/38/38/54	-
45	LMT	l	201	-	-	8/21/61/61	0/2/2/2
45	LMT	J	201	-	-	8/21/61/61	0/2/2/2
51	3PE	H	901	-	-	29/51/51/54	-
51	3PE	L	703	-	-	17/48/48/54	-
46	PC1	A	302	-	-	16/55/55/57	-
54	GTP	O	401	55	-	4/18/38/38	0/3/3/3
48	FES	E	301	5	-	-	0/1/1/1
51	3PE	Z	301	-	-	16/36/36/54	-
58	EHZ	U	101	20	-	13/42/44/45	-
47	SF4	F	502	6	-	-	0/6/5/5
56	NDP	P	501	-	-	6/30/77/77	0/5/5/5

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.98	1.81	1.59
54	O	401	GTP	O6-C6	8.32	1.40	1.23
58	T	101	EHZ	C15-N2	5.98	1.46	1.33
54	O	401	GTP	O4'-C1'	5.49	1.48	1.41
58	T	101	EHZ	C12-N1	5.22	1.45	1.33
51	H	903	3PE	O21-C2	-5.12	1.40	1.46
58	U	101	EHZ	C15-N2	5.05	1.44	1.33
54	O	401	GTP	C2-N1	4.94	1.49	1.37
58	U	101	EHZ	C12-N1	4.92	1.44	1.33
54	O	401	GTP	C2-N3	4.65	1.44	1.33
54	O	401	GTP	C2-N2	4.53	1.45	1.34
53	N	1102	I49	C15-N02	-4.52	1.31	1.37
45	l	201	LMT	O5B-C1B	3.69	1.51	1.41
45	h	1002	LMT	O5B-C1B	3.55	1.50	1.41
56	P	501	NDP	PN-O5D	3.52	1.73	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	F	501	FMN	C4A-N5	3.50	1.37	1.30
45	p	201	LMT	O5B-C1B	3.46	1.50	1.41
45	f	1101	LMT	O5B-C1B	3.43	1.50	1.41
45	A	301	LMT	O5B-C1B	3.42	1.50	1.41
45	J	201	LMT	O5B-C1B	3.37	1.50	1.41
51	H	903	3PE	O21-C21	3.19	1.40	1.33
45	K	901	LMT	O5B-C1B	3.18	1.49	1.41
56	P	501	NDP	O2B-C2B	-3.16	1.32	1.44
45	A	301	LMT	O5'-C1'	3.15	1.49	1.41
45	J	201	LMT	O5'-C1'	3.13	1.49	1.41
54	O	401	GTP	C5-C6	-3.08	1.41	1.47
53	N	1102	I49	C14-N03	3.04	1.38	1.29
45	f	1101	LMT	O5'-C1'	3.02	1.49	1.41
45	l	201	LMT	O5'-C1'	3.02	1.49	1.41
45	K	901	LMT	O5'-C1'	3.01	1.49	1.41
54	O	401	GTP	C2'-C1'	-2.95	1.49	1.53
45	h	1002	LMT	O5'-C1'	2.90	1.49	1.41
45	p	201	LMT	O5'-C1'	2.80	1.49	1.41
51	L	701	3PE	O21-C2	-2.80	1.39	1.46
52	h	1001	CDL	OA6-CA4	-2.79	1.39	1.46
52	X	201	CDL	OB6-CB4	-2.70	1.39	1.46
51	M	1301	3PE	O21-C2	-2.67	1.39	1.46
52	N	1101	CDL	OB6-CB4	-2.66	1.39	1.46
46	M	1302	PC1	O21-C2	-2.66	1.39	1.46
52	h	1001	CDL	OB6-CB4	-2.63	1.40	1.46
51	I	201	3PE	O21-C2	-2.63	1.40	1.46
52	h	1001	CDL	OB8-CB6	-2.62	1.39	1.45
52	L	702	CDL	OA6-CA4	-2.62	1.40	1.46
52	r	201	CDL	OB6-CB4	-2.62	1.40	1.46
51	Z	301	3PE	O21-C2	-2.61	1.40	1.46
52	d	1202	CDL	OB8-CB7	2.61	1.41	1.33
51	H	903	3PE	O31-C31	2.59	1.40	1.33
51	H	901	3PE	O31-C31	2.58	1.40	1.33
52	r	201	CDL	OA6-CA4	-2.58	1.40	1.46
52	L	702	CDL	OB6-CB4	-2.57	1.40	1.46
51	I	201	3PE	O31-C3	-2.57	1.39	1.45
52	N	1101	CDL	OA6-CA4	-2.56	1.40	1.46
58	U	101	EHZ	O4-C15	-2.54	1.18	1.23
52	r	201	CDL	OA8-CA6	-2.53	1.39	1.45
51	d	1201	3PE	O21-C2	-2.52	1.40	1.46
58	T	101	EHZ	O4-C15	-2.51	1.18	1.23
52	X	201	CDL	OA6-CA4	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	r	201	CDL	OB8-CB7	2.51	1.40	1.33
46	B	202	PC1	O21-C2	-2.51	1.40	1.46
52	d	1202	CDL	OA6-CA4	-2.49	1.40	1.46
58	U	101	EHZ	O3-C12	-2.48	1.18	1.23
51	Y	601	3PE	O21-C2	-2.47	1.40	1.46
52	N	1101	CDL	OB8-CB7	2.45	1.40	1.33
58	T	101	EHZ	O3-C12	-2.44	1.18	1.23
52	X	201	CDL	OA8-CA7	2.43	1.40	1.33
52	d	1202	CDL	OB6-CB4	-2.42	1.40	1.46
52	X	201	CDL	OB8-CB7	2.41	1.40	1.33
51	L	703	3PE	O21-C2	-2.41	1.40	1.46
51	Z	301	3PE	O31-C31	2.41	1.40	1.33
51	L	703	3PE	O31-C31	2.40	1.40	1.33
52	h	1001	CDL	OA8-CA6	-2.38	1.39	1.45
46	A	302	PC1	O31-C31	2.38	1.40	1.33
52	L	702	CDL	OA8-CA7	2.38	1.40	1.33
52	L	702	CDL	OB8-CB7	2.37	1.40	1.33
54	O	401	GTP	C2'-C3'	-2.36	1.46	1.53
52	d	1202	CDL	OA8-CA7	2.35	1.40	1.33
51	M	1301	3PE	O31-C31	2.33	1.40	1.33
46	M	1302	PC1	O31-C31	2.33	1.40	1.33
51	H	902	3PE	O21-C21	2.33	1.40	1.34
45	l	201	LMT	O5B-C5B	2.32	1.50	1.44
46	M	1302	PC1	O31-C3	-2.32	1.39	1.45
52	N	1101	CDL	OA8-CA7	2.28	1.40	1.33
51	L	701	3PE	O31-C31	2.28	1.40	1.33
51	d	1201	3PE	O31-C3	-2.27	1.40	1.45
51	d	1201	3PE	O31-C31	2.26	1.39	1.33
51	H	902	3PE	O21-C2	-2.26	1.40	1.46
52	X	201	CDL	OB8-CB6	-2.26	1.40	1.45
51	H	902	3PE	O31-C3	-2.26	1.40	1.45
54	O	401	GTP	PG-O3G	-2.26	1.46	1.54
51	Y	601	3PE	O31-C3	-2.25	1.40	1.45
46	A	302	PC1	O21-C21	2.25	1.40	1.34
46	B	202	PC1	O31-C31	2.25	1.39	1.33
45	p	201	LMT	O5B-C5B	2.24	1.49	1.44
46	B	202	PC1	O31-C3	-2.24	1.40	1.45
51	L	701	3PE	O31-C3	-2.24	1.40	1.45
52	d	1202	CDL	OB6-CB5	2.24	1.40	1.34
46	B	202	PC1	O21-C21	2.24	1.40	1.34
46	A	302	PC1	O31-C3	-2.23	1.40	1.45
46	A	302	PC1	O21-C2	-2.23	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	H	902	3PE	O31-C31	2.22	1.39	1.33
51	Y	601	3PE	O31-C31	2.22	1.39	1.33
52	L	702	CDL	OB8-CB6	-2.21	1.40	1.45
54	O	401	GTP	PG-O2G	-2.20	1.46	1.54
52	N	1101	CDL	OA8-CA6	-2.19	1.40	1.45
58	T	101	EHZ	C9-S1	2.19	1.81	1.76
52	h	1001	CDL	OA8-CA7	2.19	1.39	1.33
52	d	1202	CDL	OA8-CA6	-2.18	1.40	1.45
51	H	901	3PE	O21-C2	-2.18	1.41	1.46
51	M	1301	3PE	O31-C3	-2.17	1.40	1.45
52	X	201	CDL	OA6-CA5	2.17	1.40	1.35
52	X	201	CDL	OA8-CA6	-2.16	1.40	1.45
51	I	201	3PE	O31-C31	2.16	1.39	1.33
52	h	1001	CDL	OB8-CB7	2.15	1.39	1.33
52	L	702	CDL	OA8-CA6	-2.15	1.40	1.45
45	K	901	LMT	O5B-C5B	2.15	1.49	1.44
52	h	1001	CDL	OB6-CB5	2.13	1.40	1.34
51	H	901	3PE	O21-C21	2.13	1.40	1.34
52	N	1101	CDL	OB8-CB6	-2.12	1.40	1.45
51	d	1201	3PE	O21-C21	2.12	1.40	1.34
52	r	201	CDL	OB6-CB5	2.12	1.40	1.34
51	L	703	3PE	O31-C3	-2.12	1.40	1.45
52	N	1101	CDL	OA6-CA5	2.12	1.40	1.34
52	d	1202	CDL	OA6-CA5	2.11	1.40	1.34
52	r	201	CDL	OA6-CA5	2.10	1.40	1.34
45	h	1002	LMT	O5B-C5B	2.10	1.49	1.44
56	P	501	NDP	O5D-C5D	-2.09	1.36	1.44
52	r	201	CDL	OB8-CB6	-2.09	1.40	1.45
51	Z	301	3PE	O21-C21	2.08	1.40	1.34
45	f	1101	LMT	O5B-C5B	2.08	1.49	1.44
51	Z	301	3PE	O31-C3	-2.07	1.40	1.45
51	H	901	3PE	O31-C3	-2.07	1.40	1.45
49	F	501	FMN	C10-N1	2.05	1.37	1.33
51	L	703	3PE	O21-C21	2.04	1.40	1.34
51	Y	601	3PE	O21-C21	2.03	1.40	1.34
52	L	702	CDL	OB6-CB5	2.02	1.40	1.34
52	X	201	CDL	OB6-CB5	2.02	1.40	1.34
58	U	101	EHZ	O6-C20	-2.01	1.39	1.44
51	M	1301	3PE	O21-C21	2.00	1.40	1.34

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	P	501	NDP	PN-O3-PA	-6.72	109.76	132.83
58	U	101	EHZ	C8-C9-S1	5.68	120.65	113.63
58	T	101	EHZ	C8-C9-S1	5.34	120.24	113.63
51	L	703	3PE	O21-C21-C22	5.04	122.36	111.50
52	X	201	CDL	OA6-CA5-C11	5.00	120.28	111.09
52	h	1001	CDL	OB6-CB5-C51	4.97	122.22	111.50
58	T	101	EHZ	C16-C15-N2	4.57	125.68	116.58
51	H	903	3PE	O21-C21-O22	-4.52	119.82	125.57
46	A	302	PC1	O21-C21-C22	4.49	121.17	111.50
53	N	1102	I49	N01-C14-N03	4.32	128.36	120.26
46	B	202	PC1	O21-C21-C22	4.26	120.68	111.50
51	d	1201	3PE	O21-C21-C22	4.17	120.49	111.50
52	X	201	CDL	OB6-CB5-C51	4.13	120.40	111.50
51	L	701	3PE	O21-C21-C22	4.07	120.27	111.50
52	r	201	CDL	OA6-CA5-C11	4.06	120.26	111.50
51	H	901	3PE	O21-C21-C22	3.96	120.04	111.50
51	M	1301	3PE	O21-C21-C22	3.95	120.02	111.50
52	h	1001	CDL	OA6-CA5-C11	3.91	119.93	111.50
52	N	1101	CDL	OB6-CB5-C51	3.89	119.88	111.50
52	d	1202	CDL	OA6-CA5-C11	3.88	119.87	111.50
53	N	1102	I49	C14-N02-C15	-3.88	118.74	125.21
52	N	1101	CDL	OA6-CA5-C11	3.85	119.80	111.50
52	L	702	CDL	OA6-CA5-C11	3.83	119.76	111.50
51	Y	601	3PE	O21-C21-C22	3.82	119.74	111.50
46	M	1302	PC1	O21-C21-C22	3.82	119.72	111.50
51	Z	301	3PE	O21-C21-C22	3.77	119.62	111.50
51	H	902	3PE	O21-C21-C22	3.70	119.48	111.50
45	h	1002	LMT	C1B-O1B-C4'	-3.70	108.82	117.96
52	L	702	CDL	OB6-CB5-C51	3.67	119.40	111.50
52	r	201	CDL	OB6-CB5-C51	3.64	119.36	111.50
51	I	201	3PE	O21-C21-C22	3.58	119.21	111.50
58	T	101	EHZ	O4-C15-N2	-3.46	115.57	122.99
49	F	501	FMN	C4-N3-C2	-3.33	119.49	125.64
52	d	1202	CDL	OB8-CB7-C71	3.33	122.35	111.91
56	P	501	NDP	O2B-P2B-O1X	-3.26	96.82	109.39
54	O	401	GTP	C2-N1-C6	-3.19	119.22	125.10
52	d	1202	CDL	OB6-CB5-C51	3.11	119.47	110.80
54	O	401	GTP	PB-O3B-PG	-3.11	122.16	132.83
49	F	501	FMN	C4A-C10-N10	3.08	120.98	116.48
45	h	1002	LMT	C3'-C4'-C5'	3.06	117.95	110.93
54	O	401	GTP	C5-C6-N1	3.05	119.33	113.95
54	O	401	GTP	O3G-PG-O3B	2.97	114.59	104.64
45	h	1002	LMT	O5'-C5'-C4'	2.95	115.98	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	L	701	3PE	O31-C31-C32	2.93	121.09	111.91
54	O	401	GTP	O2G-PG-O3B	2.82	114.09	104.64
51	H	903	3PE	O31-C31-C32	2.82	120.75	111.91
51	L	703	3PE	O31-C31-C32	2.81	120.72	111.91
56	P	501	NDP	PA-O5B-C5B	-2.80	105.26	121.68
51	H	902	3PE	O31-C31-C32	2.77	120.61	111.91
52	X	201	CDL	OA8-CA7-C31	2.76	120.56	111.91
51	Z	301	3PE	O31-C31-C32	2.73	120.48	111.91
54	O	401	GTP	PA-O3A-PB	-2.73	123.45	132.83
56	P	501	NDP	PN-O5D-C5D	-2.71	105.80	121.68
53	N	1102	I49	N05-C15-N04	-2.68	112.01	120.26
49	F	501	FMN	C4A-C4-N3	2.68	120.00	113.19
52	L	702	CDL	OA8-CA7-C31	2.67	120.28	111.91
46	B	202	PC1	O31-C31-C32	2.67	120.28	111.91
45	l	201	LMT	C2'-C3'-C4'	2.66	115.75	109.68
51	M	1301	3PE	O31-C31-C32	2.65	120.22	111.91
52	N	1101	CDL	OB8-CB7-C71	2.65	120.21	111.91
52	h	1001	CDL	OB8-CB7-C71	2.64	120.20	111.91
52	r	201	CDL	OB8-CB7-C71	2.62	120.14	111.91
52	N	1101	CDL	OA8-CA7-C31	2.59	120.03	111.91
52	h	1001	CDL	OA8-CA7-C31	2.59	120.02	111.91
46	A	302	PC1	O31-C31-C32	2.58	120.01	111.91
51	H	901	3PE	O31-C31-C32	2.56	119.94	111.91
52	L	702	CDL	OB8-CB7-C71	2.55	119.92	111.91
51	Y	601	3PE	O31-C31-C32	2.55	119.92	111.91
56	P	501	NDP	O3X-P2B-O2X	2.55	117.38	107.64
46	M	1302	PC1	O31-C31-C32	2.55	119.90	111.91
52	r	201	CDL	OA8-CA7-C31	2.54	119.87	111.91
51	d	1201	3PE	O31-C31-C32	2.53	119.84	111.91
52	X	201	CDL	OB8-CB7-C71	2.53	119.83	111.91
56	P	501	NDP	O4B-C4B-C3B	2.48	110.02	105.11
45	J	201	LMT	C1B-O1B-C4'	-2.47	111.86	117.96
45	K	901	LMT	O5B-C5B-C4B	2.44	114.13	109.69
52	d	1202	CDL	OA8-CA7-C31	2.43	119.55	111.91
45	p	201	LMT	O1'-C1'-C2'	2.41	112.06	108.30
56	P	501	NDP	C2A-N1A-C6A	-2.40	114.65	118.75
56	P	501	NDP	O5D-PN-O1N	-2.38	99.77	109.07
45	p	201	LMT	C1'-O5'-C5'	-2.37	109.04	113.69
54	O	401	GTP	C3'-C2'-C1'	2.37	104.54	100.98
49	F	501	FMN	O4-C4-C4A	-2.36	120.33	126.60
54	O	401	GTP	O2A-PA-O1A	-2.34	100.65	112.24
49	F	501	FMN	C10-C4A-N5	-2.34	119.88	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	N	1102	I49	N05-C15-N02	2.29	126.87	117.44
58	T	101	EHZ	C10-S1-C9	2.26	108.92	101.87
45	p	201	LMT	C3B-C4B-C5B	2.26	114.27	110.24
56	P	501	NDP	O2N-PN-O1N	2.26	123.40	112.24
51	I	201	3PE	O31-C31-C32	2.25	118.98	111.91
49	F	501	FMN	C4A-C10-N1	-2.25	119.51	124.73
58	U	101	EHZ	O2-C9-S1	-2.25	119.69	122.61
52	r	201	CDL	CA6-CA4-CA3	-2.22	106.54	111.79
56	P	501	NDP	O7N-C7N-N7N	-2.20	117.74	122.88
45	p	201	LMT	O5'-C5'-C4'	2.17	114.33	109.75
54	O	401	GTP	O2B-PB-O1B	-2.17	101.53	112.24
45	h	1002	LMT	C2'-C3'-C4'	2.16	114.62	109.68
58	T	101	EHZ	C13-C12-N1	2.16	120.05	116.42
56	P	501	NDP	C5B-C4B-C3B	-2.15	107.11	115.18
54	O	401	GTP	O6-C6-C5	-2.14	120.19	124.37
52	h	1001	CDL	CB6-CB4-CB3	-2.12	106.78	111.79
51	L	701	3PE	C2-O21-C21	-2.11	112.60	117.79
51	L	703	3PE	C2-O21-C21	-2.07	112.71	117.79
58	T	101	EHZ	O2-C9-S1	-2.03	119.98	122.61
53	N	1102	I49	C09-C07-C10	2.03	121.38	118.54
51	M	1301	3PE	C2-O21-C21	-2.02	112.82	117.79
53	N	1102	I49	C08-N01-C14	-2.00	119.85	123.50

There are no chirality outliers.

All (543) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	301	LMT	C2'-C1'-O1'-C1
45	A	301	LMT	O5'-C1'-O1'-C1
45	K	901	LMT	C2-C1-O1'-C1'
45	h	1002	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	O5B-C1B-O1B-C4'
45	l	201	LMT	C2'-C1'-O1'-C1
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C22-C21-O21-C2
46	M	1302	PC1	C1-O11-P-O12
46	M	1302	PC1	C1-O11-P-O14
46	M	1302	PC1	O13-C11-C12-N
51	H	901	3PE	O13-C11-C12-N
51	H	901	3PE	O22-C21-O21-C2
51	H	902	3PE	C11-O13-P-O11
51	H	902	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
51	H	902	3PE	C11-O13-P-O14
51	H	902	3PE	O13-C11-C12-N
51	H	903	3PE	C11-O13-P-O12
51	H	903	3PE	C11-O13-P-O14
51	H	903	3PE	O13-C11-C12-N
51	H	903	3PE	C1-C2-O21-C21
51	H	903	3PE	O22-C21-O21-C2
51	L	703	3PE	C1-O11-P-O13
51	L	703	3PE	C1-O11-P-O14
51	L	703	3PE	C11-O13-P-O11
51	M	1301	3PE	O13-C11-C12-N
51	M	1301	3PE	C22-C21-O21-C2
51	Y	601	3PE	C11-O13-P-O12
51	Z	301	3PE	C1-O11-P-O14
51	d	1201	3PE	C1-O11-P-O12
51	d	1201	3PE	C1-O11-P-O13
51	d	1201	3PE	C1-O11-P-O14
51	d	1201	3PE	C11-O13-P-O14
51	d	1201	3PE	O22-C21-O21-C2
52	L	702	CDL	CA3-OA5-PA1-OA3
52	L	702	CDL	CB2-OB2-PB2-OB3
52	L	702	CDL	CB2-OB2-PB2-OB5
52	L	702	CDL	CB3-OB5-PB2-OB2
52	L	702	CDL	CB3-OB5-PB2-OB3
52	L	702	CDL	CB3-OB5-PB2-OB4
52	N	1101	CDL	OA5-CA3-CA4-OA6
52	X	201	CDL	CA2-OA2-PA1-OA3
52	X	201	CDL	CA2-OA2-PA1-OA4
52	X	201	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	C11-CA5-OA6-CA4
52	X	201	CDL	CB3-OB5-PB2-OB3
52	X	201	CDL	CB3-OB5-PB2-OB4
52	d	1202	CDL	CA3-OA5-PA1-OA2
52	d	1202	CDL	CA3-OA5-PA1-OA3
52	d	1202	CDL	CB2-OB2-PB2-OB3
52	d	1202	CDL	CB2-OB2-PB2-OB4
52	d	1202	CDL	OB6-CB4-CB6-OB8
52	d	1202	CDL	OB9-CB7-OB8-CB6
52	d	1202	CDL	C71-CB7-OB8-CB6
52	h	1001	CDL	CB2-OB2-PB2-OB3
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	CB2-C1-CA2-OA2
52	r	201	CDL	CB2-OB2-PB2-OB3
53	N	1102	I49	N04-C15-N02-C14
53	N	1102	I49	N05-C15-N02-C14
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O2A
56	P	501	NDP	C2B-O2B-P2B-O1X
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C12-C13-C14-N2
58	T	101	EHZ	C16-C15-N2-C14
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
51	H	902	3PE	O32-C31-O31-C3
51	H	903	3PE	O32-C31-O31-C3
51	d	1201	3PE	O32-C31-O31-C3
51	H	902	3PE	C32-C31-O31-C3
51	H	903	3PE	C32-C31-O31-C3
51	d	1201	3PE	C32-C31-O31-C3
52	X	201	CDL	OA9-CA7-OA8-CA6
52	h	1001	CDL	OB9-CB7-OB8-CB6
46	B	202	PC1	O22-C21-O21-C2
52	r	201	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	C31-CA7-OA8-CA6
45	K	901	LMT	O5B-C5B-C6B-O6B
51	H	901	3PE	C22-C21-O21-C2
51	d	1201	3PE	C22-C21-O21-C2
52	h	1001	CDL	C51-CB5-OB6-CB4
52	r	201	CDL	C11-CA5-OA6-CA4
45	J	201	LMT	O5'-C5'-C6'-O6'
45	K	901	LMT	O5'-C5'-C6'-O6'
45	A	301	LMT	O5'-C5'-C6'-O6'
45	p	201	LMT	C3'-C4'-O1B-C1B
52	h	1001	CDL	C31-CA7-OA8-CA6
52	h	1001	CDL	C71-CB7-OB8-CB6
45	J	201	LMT	O5B-C1B-O1B-C4'
51	M	1301	3PE	O22-C21-O21-C2
52	N	1101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	OA9-CA7-OA8-CA6
45	J	201	LMT	C2B-C1B-O1B-C4'
52	X	201	CDL	O1-C1-CB2-OB2
52	r	201	CDL	O1-C1-CA2-OA2
52	L	702	CDL	C71-CB7-OB8-CB6
45	A	301	LMT	C3'-C4'-O1B-C1B
46	A	302	PC1	O32-C31-O31-C3
45	f	1101	LMT	O5'-C5'-C6'-O6'
45	l	201	LMT	O5'-C5'-C6'-O6'
58	T	101	EHZ	O4-C15-N2-C14
52	d	1202	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C11-CA5-OA6-CA4
45	K	901	LMT	C4B-C5B-C6B-O6B
45	h	1002	LMT	O5'-C5'-C6'-O6'
56	P	501	NDP	O4D-C4D-C5D-O5D
56	P	501	NDP	C3D-C4D-C5D-O5D
46	A	302	PC1	C32-C31-O31-C3
52	N	1101	CDL	C71-CB7-OB8-CB6
45	p	201	LMT	O5B-C5B-C6B-O6B
51	H	903	3PE	C2-C1-O11-P
52	N	1101	CDL	CA4-CA3-OA5-PA1
53	N	1102	I49	C07-C06-C08-N01
45	A	301	LMT	C4'-C5'-C6'-O6'
45	f	1101	LMT	C4'-C5'-C6'-O6'
52	L	702	CDL	OB9-CB7-OB8-CB6
45	J	201	LMT	C4'-C5'-C6'-O6'
45	K	901	LMT	C4'-C5'-C6'-O6'
45	l	201	LMT	O5'-C1'-O1'-C1
52	N	1101	CDL	C31-CA7-OA8-CA6
45	l	201	LMT	C4'-C5'-C6'-O6'
52	h	1001	CDL	OA7-CA5-OA6-CA4
52	N	1101	CDL	OA9-CA7-OA8-CA6
52	r	201	CDL	OA9-CA7-OA8-CA6
46	M	1302	PC1	C32-C31-O31-C3
51	L	701	3PE	C32-C31-O31-C3
51	Z	301	3PE	C32-C31-O31-C3
52	r	201	CDL	C31-CA7-OA8-CA6
45	J	201	LMT	O5B-C5B-C6B-O6B
45	f	1101	LMT	C3'-C4'-O1B-C1B
45	h	1002	LMT	C2'-C1'-O1'-C1
51	H	901	3PE	O21-C2-C3-O31
51	L	701	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	J	201	LMT	C4B-C5B-C6B-O6B
45	p	201	LMT	C4B-C5B-C6B-O6B
51	Z	301	3PE	O32-C31-O31-C3
51	M	1301	3PE	C32-C31-O31-C3
52	X	201	CDL	C71-CB7-OB8-CB6
46	M	1302	PC1	C21-C22-C23-C24
52	X	201	CDL	CA7-C31-C32-C33
46	B	202	PC1	C21-C22-C23-C24
45	K	901	LMT	O1'-C1-C2-C3
52	d	1202	CDL	OA7-CA5-OA6-CA4
52	L	702	CDL	CA5-C11-C12-C13
52	h	1001	CDL	CA7-C31-C32-C33
46	M	1302	PC1	O32-C31-O31-C3
51	M	1301	3PE	C21-C22-C23-C24
52	X	201	CDL	OB9-CB7-OB8-CB6
51	Z	301	3PE	C31-C32-C33-C34
51	M	1301	3PE	O32-C31-O31-C3
46	A	302	PC1	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O11
46	M	1302	PC1	C1-O11-P-O13
51	H	903	3PE	C11-O13-P-O11
51	I	201	3PE	C11-O13-P-O11
51	M	1301	3PE	C1-O11-P-O13
51	M	1301	3PE	C11-O13-P-O11
51	Y	601	3PE	C11-O13-P-O11
51	d	1201	3PE	C11-O13-P-O11
52	X	201	CDL	CA2-OA2-PA1-OA5
52	X	201	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	CB3-OB5-PB2-OB2
46	B	202	PC1	C32-C31-O31-C3
46	A	302	PC1	O22-C21-O21-C2
51	Y	601	3PE	C32-C31-O31-C3
45	p	201	LMT	C5-C6-C7-C8
45	p	201	LMT	C4-C5-C6-C7
51	H	901	3PE	C35-C36-C37-C38
51	L	701	3PE	C38-C39-C3A-C3B
52	L	702	CDL	C52-C53-C54-C55
45	h	1002	LMT	C4'-C5'-C6'-O6'
58	T	101	EHZ	C19-C17-C20-O6
51	H	901	3PE	C1-C2-O21-C21
52	L	702	CDL	OA7-CA5-OA6-CA4
51	H	901	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
45	K	901	LMT	C11-C10-C9-C8
51	L	703	3PE	C26-C27-C28-C29
52	L	702	CDL	C12-C13-C14-C15
46	M	1302	PC1	C25-C26-C27-C28
52	r	201	CDL	C59-C60-C61-C62
51	H	901	3PE	C27-C28-C29-C2A
46	M	1302	PC1	C26-C27-C28-C29
51	H	901	3PE	C3C-C3D-C3E-C3F
51	I	201	3PE	C33-C34-C35-C36
46	B	202	PC1	O32-C31-O31-C3
51	Y	601	3PE	O32-C31-O31-C3
51	L	701	3PE	C27-C28-C29-C2A
51	L	701	3PE	C39-C3A-C3B-C3C
59	o	201	MYR	C2-C3-C4-C5
51	I	201	3PE	C29-C2A-C2B-C2C
58	U	101	EHZ	C2-C3-C4-C5
52	L	702	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	C51-C52-C53-C54
52	r	201	CDL	C57-C58-C59-C60
52	X	201	CDL	C53-C54-C55-C56
52	d	1202	CDL	C72-C73-C74-C75
59	o	201	MYR	C5-C6-C7-C8
51	d	1201	3PE	C32-C33-C34-C35
51	d	1201	3PE	C2C-C2D-C2E-C2F
52	L	702	CDL	C59-C60-C61-C62
51	L	701	3PE	O13-C11-C12-N
51	H	903	3PE	C32-C33-C34-C35
51	H	903	3PE	C3C-C3D-C3E-C3F
52	h	1001	CDL	CA5-C11-C12-C13
52	d	1202	CDL	C33-C34-C35-C36
45	h	1002	LMT	C2-C1-O1'-C1'
59	o	201	MYR	C3-C4-C5-C6
45	h	1002	LMT	C6-C7-C8-C9
46	B	202	PC1	C24-C25-C26-C27
51	H	901	3PE	C21-C22-C23-C24
51	d	1201	3PE	C31-C32-C33-C34
46	M	1302	PC1	C2B-C2C-C2D-C2E
51	L	701	3PE	C22-C21-O21-C2
51	Z	301	3PE	C22-C21-O21-C2
51	H	901	3PE	C33-C34-C35-C36
46	M	1302	PC1	C31-C32-C33-C34
51	H	901	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	L	703	3PE	C38-C39-C3A-C3B
52	N	1101	CDL	O1-C1-CB2-OB2
51	Y	601	3PE	C27-C28-C29-C2A
59	o	201	MYR	C9-C10-C11-C12
52	N	1101	CDL	C76-C77-C78-C79
51	Z	301	3PE	O22-C21-O21-C2
52	h	1001	CDL	C20-C21-C22-C23
52	r	201	CDL	C16-C17-C18-C19
51	d	1201	3PE	C29-C2A-C2B-C2C
52	d	1202	CDL	C76-C77-C78-C79
52	r	201	CDL	C71-CB7-OB8-CB6
45	A	301	LMT	C1-C2-C3-C4
52	N	1101	CDL	C74-C75-C76-C77
52	r	201	CDL	OB9-CB7-OB8-CB6
51	L	703	3PE	C33-C34-C35-C36
52	d	1202	CDL	CA5-C11-C12-C13
52	L	702	CDL	C31-CA7-OA8-CA6
51	L	703	3PE	C35-C36-C37-C38
51	M	1301	3PE	C35-C36-C37-C38
58	U	101	EHZ	C5-C6-C7-C8
52	N	1101	CDL	CB7-C71-C72-C73
51	Y	601	3PE	C23-C24-C25-C26
58	U	101	EHZ	C1-C2-C3-C4
51	d	1201	3PE	C35-C36-C37-C38
52	N	1101	CDL	C72-C73-C74-C75
51	I	201	3PE	C21-C22-C23-C24
52	L	702	CDL	C51-CB5-OB6-CB4
51	Z	301	3PE	O11-C1-C2-O21
51	d	1201	3PE	C3A-C3B-C3C-C3D
52	d	1202	CDL	C40-C41-C42-C43
51	L	701	3PE	O22-C21-O21-C2
52	L	702	CDL	OB7-CB5-OB6-CB4
52	L	702	CDL	OA6-CA4-CA6-OA8
52	N	1101	CDL	OB6-CB4-CB6-OB8
51	L	701	3PE	C2D-C2E-C2F-C2G
59	o	201	MYR	C4-C5-C6-C7
45	l	201	LMT	C5'-C4'-O1B-C1B
51	H	901	3PE	C24-C25-C26-C27
51	H	903	3PE	C33-C34-C35-C36
51	H	901	3PE	C1-O11-P-O13
52	N	1101	CDL	CA3-OA5-PA1-OA2
52	d	1202	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
52	h	1001	CDL	CB2-OB2-PB2-OB5
52	r	201	CDL	CB2-OB2-PB2-OB5
52	L	702	CDL	OA9-CA7-OA8-CA6
45	l	201	LMT	C3'-C4'-O1B-C1B
45	p	201	LMT	C5'-C4'-O1B-C1B
51	I	201	3PE	C26-C27-C28-C29
51	H	903	3PE	C34-C35-C36-C37
52	r	201	CDL	C38-C39-C40-C41
46	A	302	PC1	C33-C34-C35-C36
51	H	901	3PE	C36-C37-C38-C39
52	N	1101	CDL	C71-C72-C73-C74
52	X	201	CDL	C31-C32-C33-C34
51	H	901	3PE	C1-C2-C3-O31
52	d	1202	CDL	CB3-CB4-CB6-OB8
52	h	1001	CDL	CB3-CB4-CB6-OB8
51	d	1201	3PE	C2A-C2B-C2C-C2D
51	Z	301	3PE	C32-C33-C34-C35
51	H	903	3PE	C3F-C3G-C3H-C3I
51	d	1201	3PE	C25-C26-C27-C28
58	U	101	EHZ	C21-C1-C2-C3
45	h	1002	LMT	O5B-C5B-C6B-O6B
58	T	101	EHZ	C5-C6-C7-O1
51	L	701	3PE	C3B-C3C-C3D-C3E
58	T	101	EHZ	C1-C21-C22-C23
45	p	201	LMT	O5'-C5'-C6'-O6'
45	p	201	LMT	O1'-C1-C2-C3
51	L	701	3PE	C2F-C2G-C2H-C2I
52	h	1001	CDL	C12-C13-C14-C15
51	H	901	3PE	C32-C31-O31-C3
51	Y	601	3PE	O11-C1-C2-O21
51	L	701	3PE	C23-C24-C25-C26
58	U	101	EHZ	C21-C22-C23-C24
51	L	703	3PE	C32-C33-C34-C35
52	h	1001	CDL	OB6-CB4-CB6-OB8
45	h	1002	LMT	O5B-C1B-O1B-C4'
51	L	701	3PE	C2A-C2B-C2C-C2D
45	f	1101	LMT	C5'-C4'-O1B-C1B
51	Y	601	3PE	C2C-C2D-C2E-C2F
58	T	101	EHZ	C5-C6-C7-C8
51	I	201	3PE	C3E-C3F-C3G-C3H
51	L	701	3PE	C36-C37-C38-C39
52	L	702	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	C31-C32-C33-C34
51	Z	301	3PE	O11-C1-C2-C3
52	X	201	CDL	OA5-CA3-CA4-CA6
52	d	1202	CDL	OB5-CB3-CB4-CB6
51	I	201	3PE	C36-C37-C38-C39
46	A	302	PC1	C3B-C3C-C3D-C3E
51	L	703	3PE	C32-C31-O31-C3
45	f	1101	LMT	O1'-C1-C2-C3
52	N	1101	CDL	C53-C54-C55-C56
46	M	1302	PC1	C22-C21-O21-C2
52	r	201	CDL	C1-CB2-OB2-PB2
52	L	702	CDL	C53-C54-C55-C56
56	P	501	NDP	O4D-C1D-N1N-C6N
52	r	201	CDL	C37-C38-C39-C40
51	H	903	3PE	C1-C2-C3-O31
52	L	702	CDL	CA3-CA4-CA6-OA8
52	N	1101	CDL	CB3-CB4-CB6-OB8
45	A	301	LMT	C5'-C4'-O1B-C1B
46	M	1302	PC1	C22-C23-C24-C25
52	r	201	CDL	C15-C16-C17-C18
51	H	901	3PE	C37-C38-C39-C3A
46	A	302	PC1	C3A-C3B-C3C-C3D
52	d	1202	CDL	C38-C39-C40-C41
46	B	202	PC1	O11-C1-C2-O21
51	H	901	3PE	O32-C31-O31-C3
51	Y	601	3PE	O21-C21-C22-C23
51	H	903	3PE	O21-C2-C3-O31
52	X	201	CDL	CA2-C1-CB2-OB2
58	T	101	EHZ	C1-C2-C3-C4
51	d	1201	3PE	C2-C1-O11-P
52	N	1101	CDL	CB4-CB3-OB5-PB2
59	o	201	MYR	C10-C11-C12-C13
51	I	201	3PE	C2B-C2C-C2D-C2E
51	Z	301	3PE	C34-C35-C36-C37
59	o	201	MYR	C11-C12-C13-C14
46	B	202	PC1	C34-C35-C36-C37
51	L	701	3PE	O11-C1-C2-C3
51	Y	601	3PE	O11-C1-C2-C3
52	N	1101	CDL	OA5-CA3-CA4-CA6
51	H	901	3PE	C38-C39-C3A-C3B
51	I	201	3PE	C32-C31-O31-C3
51	L	701	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
51	L	703	3PE	C3C-C3D-C3E-C3F
59	o	201	MYR	C7-C8-C9-C10
51	I	201	3PE	C24-C25-C26-C27
46	A	302	PC1	C3-C2-O21-C21
51	H	902	3PE	C1-C2-O21-C21
58	U	101	EHZ	C12-C13-C14-N2
45	h	1002	LMT	C11-C10-C9-C8
46	M	1302	PC1	C1-C2-C3-O31
52	d	1202	CDL	C1-CB2-OB2-PB2
52	d	1202	CDL	CB4-CB3-OB5-PB2
53	N	1102	I49	N01-C14-N02-C15
52	N	1101	CDL	C51-CB5-OB6-CB4
51	L	701	3PE	O11-C1-C2-O21
52	X	201	CDL	OA5-CA3-CA4-OA6
52	d	1202	CDL	C77-C78-C79-C80
58	T	101	EHZ	C3-C4-C5-C6
45	l	201	LMT	C3-C4-C5-C6
52	L	702	CDL	C15-C16-C17-C18
51	L	703	3PE	O32-C31-O31-C3
46	M	1302	PC1	O21-C2-C3-O31
51	H	902	3PE	O21-C2-C3-O31
56	P	501	NDP	C2B-O2B-P2B-O3X
52	N	1101	CDL	C57-C58-C59-C60
46	M	1302	PC1	C2E-C2F-C2G-C2H
52	r	201	CDL	C72-C73-C74-C75
46	M	1302	PC1	O22-C21-O21-C2
52	N	1101	CDL	OB7-CB5-OB6-CB4
51	I	201	3PE	O32-C31-O31-C3
53	N	1102	I49	N03-C14-N02-C15
46	B	202	PC1	C1-O11-P-O13
51	Z	301	3PE	C1-O11-P-O13
52	h	1001	CDL	CA2-OA2-PA1-OA5
46	M	1302	PC1	C2-C1-O11-P
51	L	703	3PE	C22-C23-C24-C25
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
51	H	901	3PE	C1-O11-P-O12
51	I	201	3PE	C11-O13-P-O14
51	M	1301	3PE	C1-O11-P-O12
51	M	1301	3PE	C11-O13-P-O12
51	Y	601	3PE	C11-O13-P-O14
51	Z	301	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
52	N	1101	CDL	CA3-OA5-PA1-OA4
52	r	201	CDL	CB2-OB2-PB2-OB4
54	O	401	GTP	C5'-O5'-PA-O1A
46	B	202	PC1	O11-C1-C2-C3
46	A	302	PC1	C23-C24-C25-C26
52	h	1001	CDL	C52-C53-C54-C55
51	M	1301	3PE	C12-C11-O13-P
51	Z	301	3PE	C12-C11-O13-P
52	X	201	CDL	CB5-C51-C52-C53
45	J	201	LMT	C5-C6-C7-C8
52	d	1202	CDL	OB5-CB3-CB4-OB6
51	Y	601	3PE	C31-C32-C33-C34
46	M	1302	PC1	C11-C12-N-C15
51	H	902	3PE	C33-C34-C35-C36
52	h	1001	CDL	CA3-CA4-CA6-OA8
46	A	302	PC1	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
52	h	1001	CDL	OA6-CA4-CA6-OA8
45	p	201	LMT	C2-C3-C4-C5
52	h	1001	CDL	C33-C34-C35-C36
52	r	201	CDL	C33-C34-C35-C36
51	I	201	3PE	C22-C23-C24-C25
46	M	1302	PC1	C11-C12-N-C14
51	Z	301	3PE	C27-C28-C29-C2A
52	d	1202	CDL	C31-C32-C33-C34
49	F	501	FMN	C4'-C5'-O5'-P
52	X	201	CDL	CB4-CB3-OB5-PB2
51	d	1201	3PE	C38-C39-C3A-C3B
52	N	1101	CDL	C55-C56-C57-C58
52	r	201	CDL	C11-C12-C13-C14
45	A	301	LMT	O5B-C5B-C6B-O6B
52	N	1101	CDL	C51-C52-C53-C54
52	r	201	CDL	OB6-CB4-CB6-OB8
52	X	201	CDL	CA3-OA5-PA1-OA2
52	r	201	CDL	CA3-OA5-PA1-OA2
51	H	901	3PE	C2C-C2D-C2E-C2F
45	h	1002	LMT	C2B-C1B-O1B-C4'
54	O	401	GTP	PB-O3A-PA-O2A
51	Y	601	3PE	C2-C1-O11-P
51	I	201	3PE	O22-C21-O21-C2
46	M	1302	PC1	C2C-C2D-C2E-C2F
52	L	702	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
52	N	1101	CDL	C54-C55-C56-C57
51	L	703	3PE	C23-C24-C25-C26
51	Y	601	3PE	C28-C29-C2A-C2B
58	T	101	EHZ	O4-C15-C16-C17
46	M	1302	PC1	C28-C29-C2A-C2B
51	L	701	3PE	C35-C36-C37-C38
52	N	1101	CDL	C56-C57-C58-C59
51	H	902	3PE	C2-C1-O11-P
52	h	1001	CDL	C16-C17-C18-C19
52	L	702	CDL	C56-C57-C58-C59
52	d	1202	CDL	C32-C33-C34-C35
52	r	201	CDL	CB3-CB4-CB6-OB8
51	d	1201	3PE	C33-C34-C35-C36
58	T	101	EHZ	C2-C3-C4-C5
51	Z	301	3PE	C24-C25-C26-C27
58	T	101	EHZ	N2-C15-C16-C17
45	K	901	LMT	C2-C3-C4-C5
52	X	201	CDL	CA6-CA4-OA6-CA5
52	h	1001	CDL	CB3-CB4-OB6-CB5
46	M	1302	PC1	C11-C12-N-C13
51	I	201	3PE	C32-C33-C34-C35
51	I	201	3PE	C22-C21-O21-C2
46	M	1302	PC1	C29-C2A-C2B-C2C
58	U	101	EHZ	C11-C10-S1-C9
51	d	1201	3PE	C37-C38-C39-C3A
52	X	201	CDL	OB6-CB4-CB6-OB8
51	L	703	3PE	C39-C3A-C3B-C3C
52	d	1202	CDL	C42-C43-C44-C45
51	H	901	3PE	C28-C29-C2A-C2B
51	M	1301	3PE	C22-C23-C24-C25
46	A	302	PC1	C28-C29-C2A-C2B
52	L	702	CDL	C55-C56-C57-C58
51	H	901	3PE	O11-C1-C2-O21
52	r	201	CDL	OB5-CB3-CB4-OB6
46	A	302	PC1	C27-C28-C29-C2A
52	d	1202	CDL	CB2-C1-CA2-OA2
51	L	701	3PE	O21-C21-C22-C23
51	M	1301	3PE	C36-C37-C38-C39
52	h	1001	CDL	CB6-CB4-OB6-CB5
52	r	201	CDL	C40-C41-C42-C43
51	I	201	3PE	C3B-C3C-C3D-C3E
58	T	101	EHZ	C10-C11-N1-C12

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Mol	Chain	Res	Type	Atoms
51	H	902	3PE	O31-C31-C32-C33
51	I	201	3PE	C2A-C2B-C2C-C2D
46	A	302	PC1	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
51	H	902	3PE	C1-C2-C3-O31
52	X	201	CDL	C74-C75-C76-C77
52	d	1202	CDL	OA9-CA7-OA8-CA6
52	d	1202	CDL	C74-C75-C76-C77
46	B	202	PC1	O21-C21-C22-C23
51	L	701	3PE	C2B-C2C-C2D-C2E
51	Y	601	3PE	O22-C21-C22-C23
51	d	1201	3PE	C2E-C2F-C2G-C2H
52	d	1202	CDL	CA2-C1-CB2-OB2
58	T	101	EHZ	O1-C7-C8-C9
52	r	201	CDL	C39-C40-C41-C42
52	r	201	CDL	C71-C72-C73-C74
51	H	901	3PE	O11-C1-C2-C3
52	L	702	CDL	C72-C71-CB7-OB8
52	r	201	CDL	C32-C31-CA7-OA8
51	Y	601	3PE	C26-C27-C28-C29
52	r	201	CDL	C13-C14-C15-C16
45	p	201	LMT	C6-C7-C8-C9
46	A	302	PC1	C2A-C2B-C2C-C2D
51	M	1301	3PE	C32-C33-C34-C35
52	d	1202	CDL	C44-C45-C46-C47
51	L	703	3PE	C25-C26-C27-C28
51	d	1201	3PE	C3D-C3E-C3F-C3G
51	Z	301	3PE	C23-C24-C25-C26
56	P	501	NDP	O4B-C4B-C5B-O5B
52	h	1001	CDL	C52-C51-CB5-OB6
46	B	202	PC1	O22-C21-C22-C23
51	H	901	3PE	C2B-C2C-C2D-C2E
52	d	1202	CDL	C31-CA7-OA8-CA6
52	X	201	CDL	C52-C53-C54-C55
52	d	1202	CDL	CB4-CB6-OB8-CB7
52	X	201	CDL	CB3-CB4-CB6-OB8
51	H	901	3PE	C39-C3A-C3B-C3C
45	f	1101	LMT	C4B-C5B-C6B-O6B
46	B	202	PC1	C2-C1-O11-P
52	X	201	CDL	CA4-CA3-OA5-PA1
46	B	202	PC1	C11-C12-N-C14
51	H	901	3PE	C11-O13-P-O14

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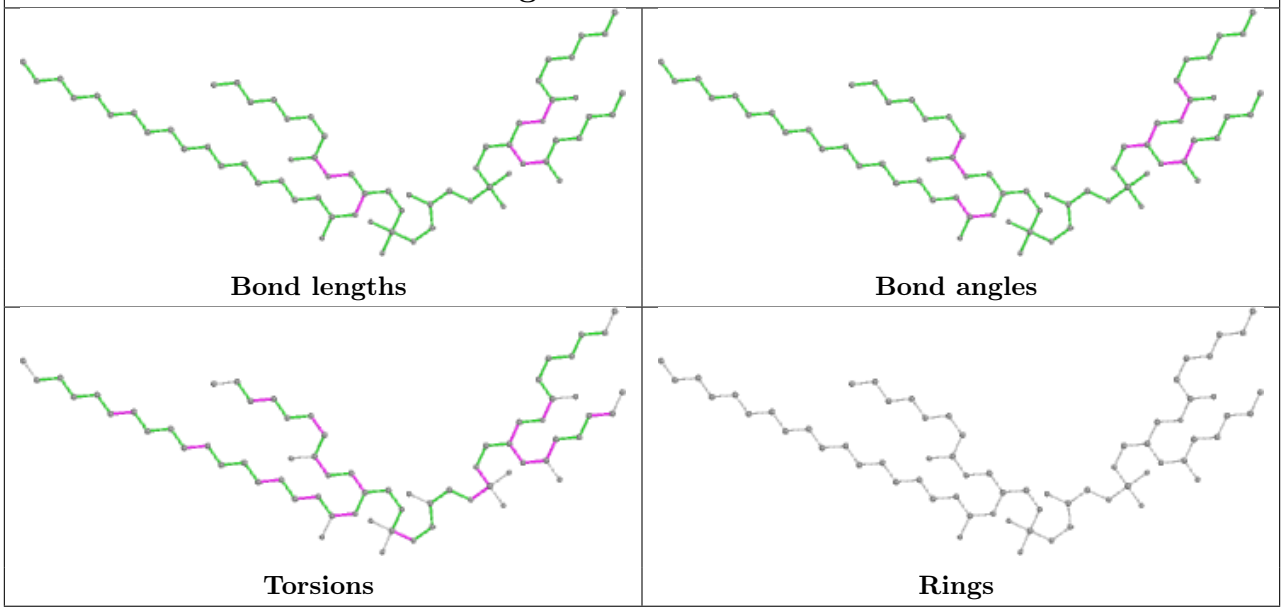
Mol	Chain	Res	Type	Atoms
51	Y	601	3PE	C1-O11-P-O14
52	r	201	CDL	CA3-OA5-PA1-OA3
46	M	1302	PC1	O21-C21-C22-C23
45	f	1101	LMT	C2-C3-C4-C5
46	A	302	PC1	C37-C38-C39-C3A
52	r	201	CDL	C32-C31-CA7-OA9
51	H	901	3PE	C12-C11-O13-P
51	L	703	3PE	C12-C11-O13-P
51	Y	601	3PE	C12-C11-O13-P
51	Y	601	3PE	C1-C2-O21-C21
51	H	902	3PE	O32-C31-C32-C33
52	L	702	CDL	C72-C71-CB7-OB9
46	A	302	PC1	O31-C31-C32-C33
49	F	501	FMN	N10-C1'-C2'-O2'
46	M	1302	PC1	O32-C31-C32-C33
52	h	1001	CDL	C52-C51-CB5-OB7
45	p	201	LMT	O5B-C1B-O1B-C4'
46	M	1302	PC1	O31-C31-C32-C33
45	J	201	LMT	C2-C1-O1'-C1'
52	N	1101	CDL	C72-C71-CB7-OB8
58	U	101	EHZ	C22-C23-C24-C25
51	Y	601	3PE	C29-C2A-C2B-C2C
52	X	201	CDL	C32-C31-CA7-OA8
51	L	703	3PE	C27-C28-C29-C2A

There are no ring outliers.

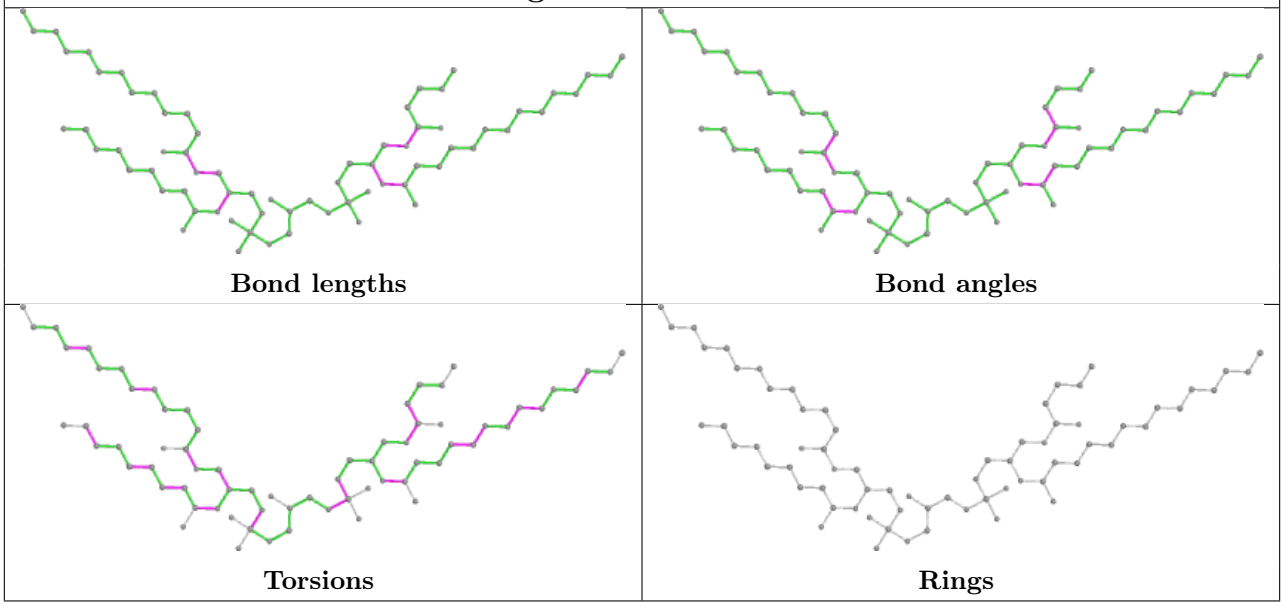
No monomer is involved in short contacts.

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 then 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.

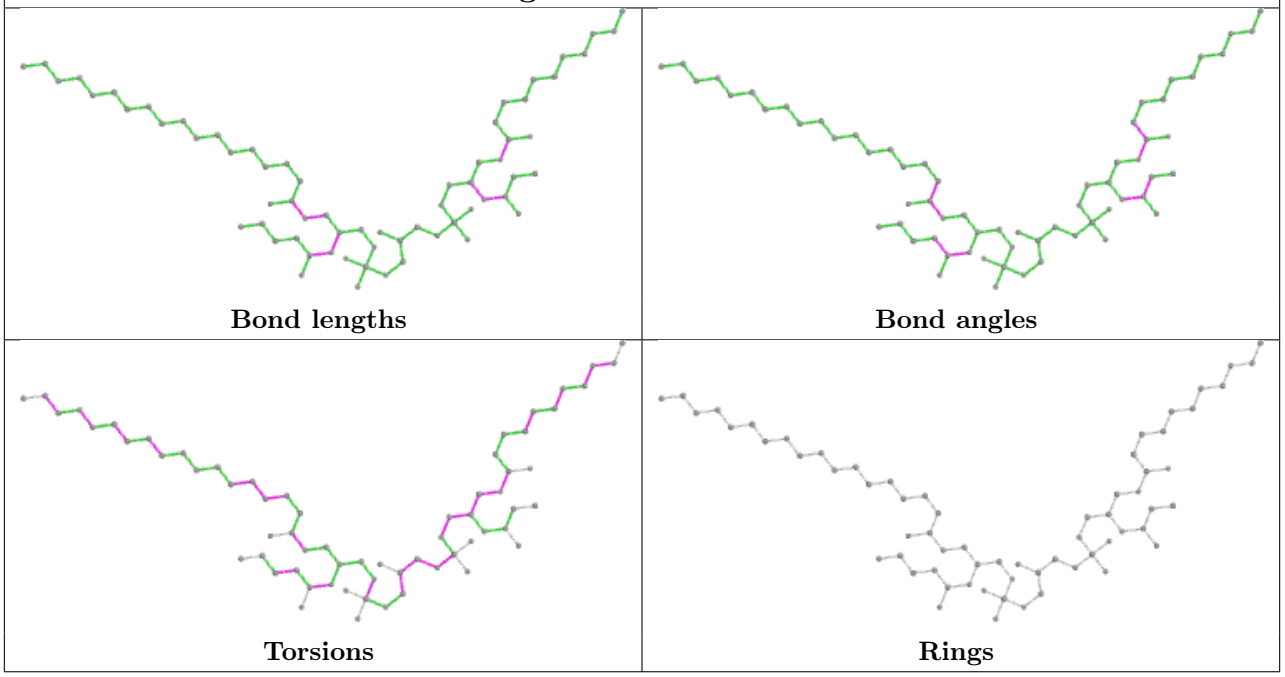
Ligand CDL h 1001



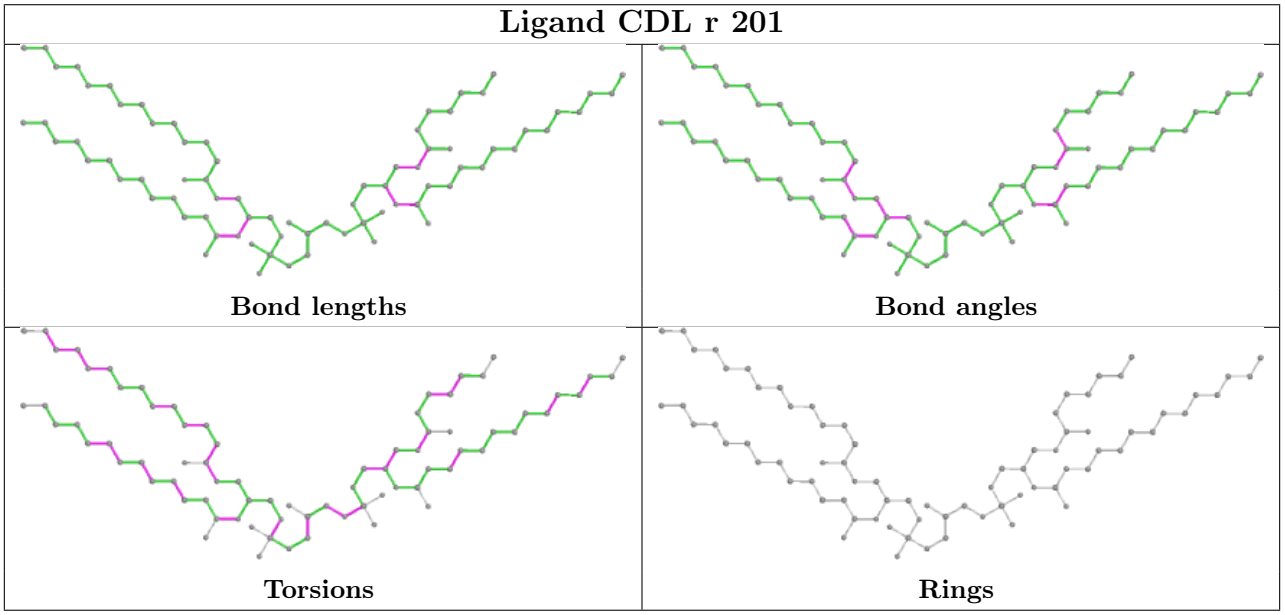
Ligand CDL L 702



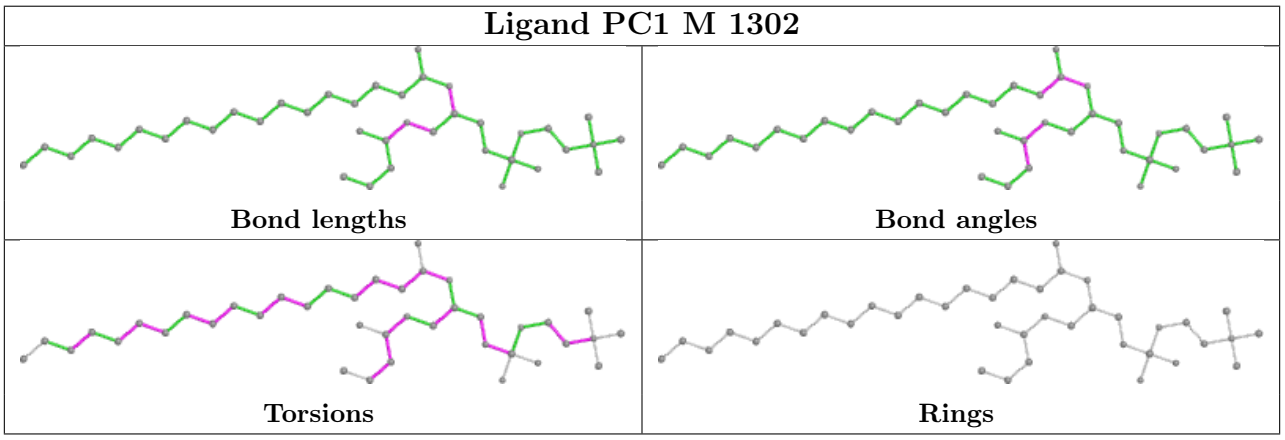
Ligand CDL d 1202



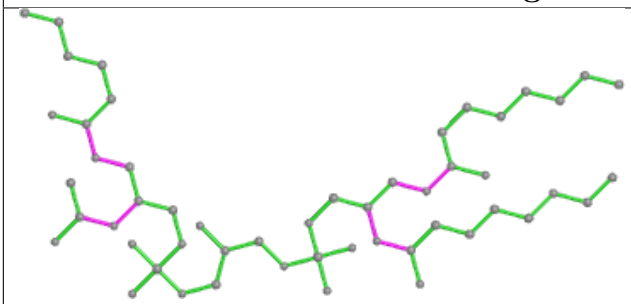
Ligand CDL r 201



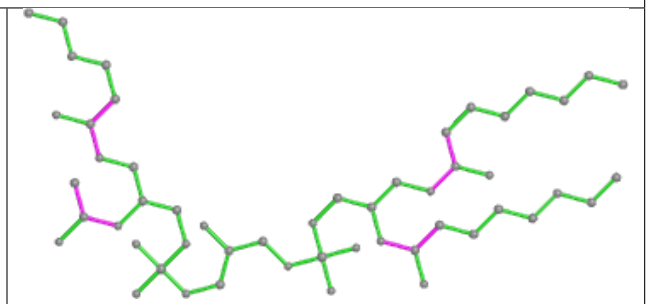
Ligand PC1 M 1302



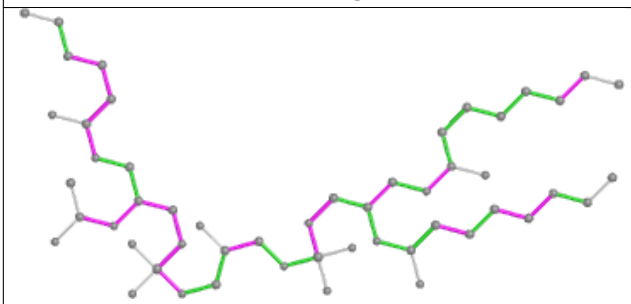
Ligand CDL X 201



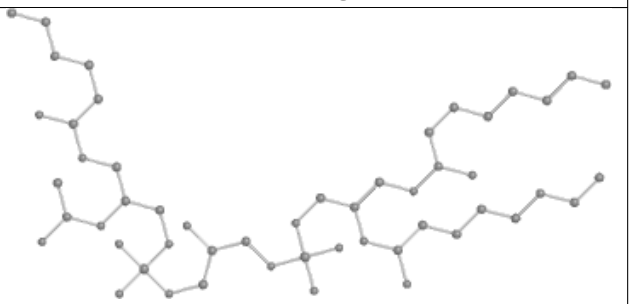
Bond lengths



Bond angles

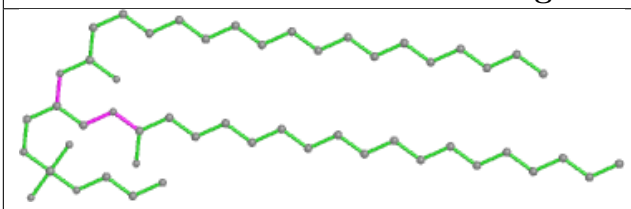


Torsions



Rings

Ligand 3PE I 201



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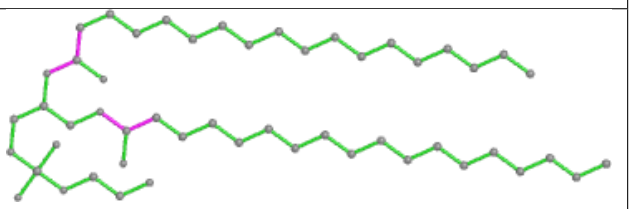
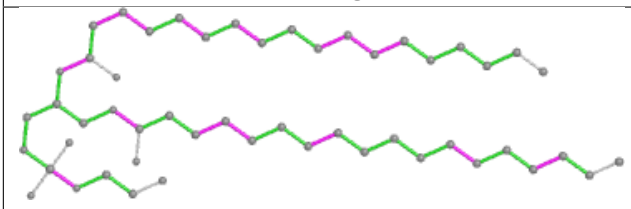


Bond angles



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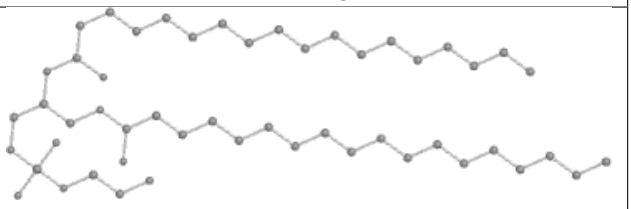
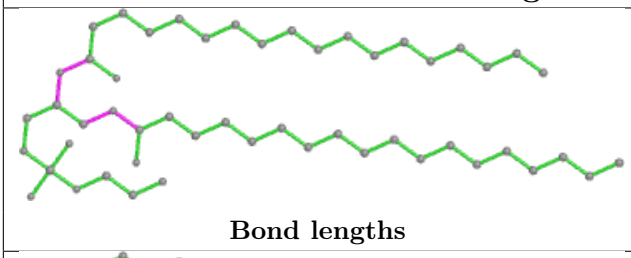


Rings

Ligand 3PE d 1201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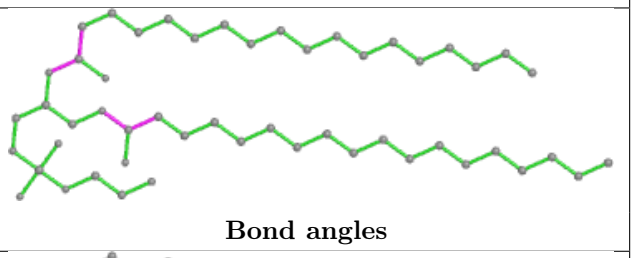
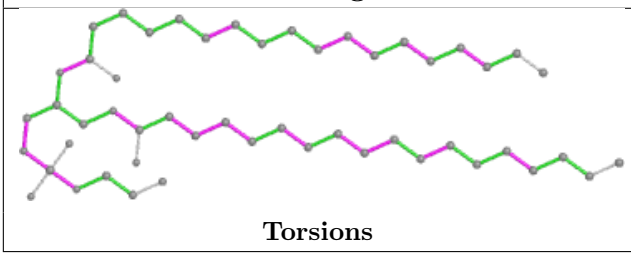
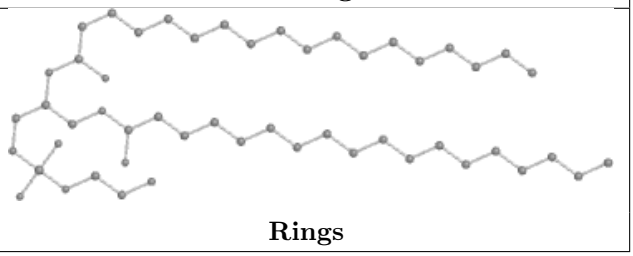
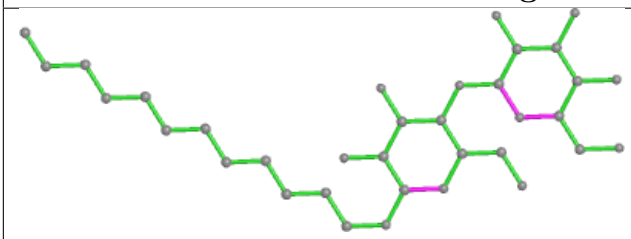

Bond angles


Torsions


Rings

Ligand LMT f 1101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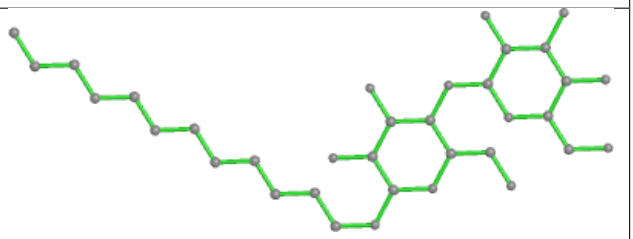
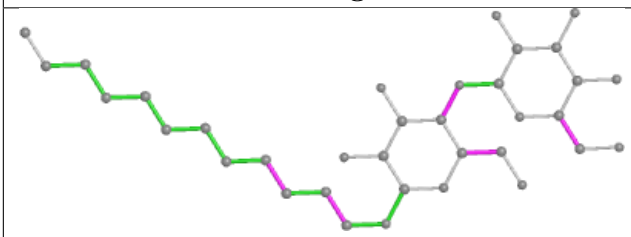

Bond angles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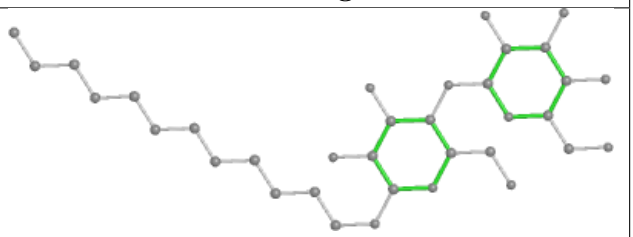
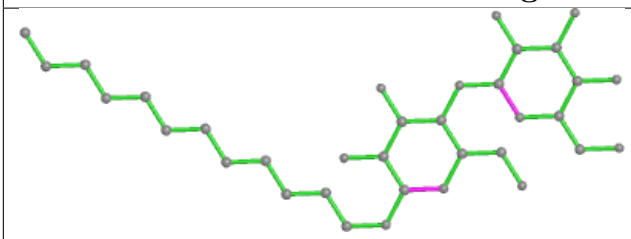

Rings

Ligand LMT A 301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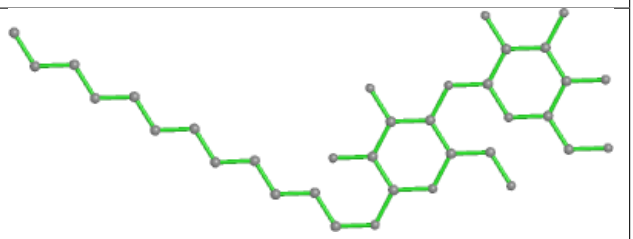
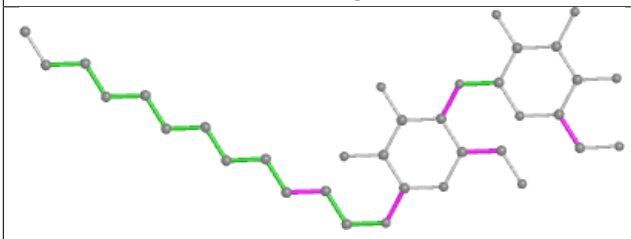

Bond angles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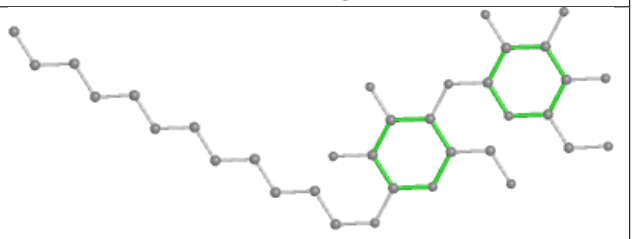
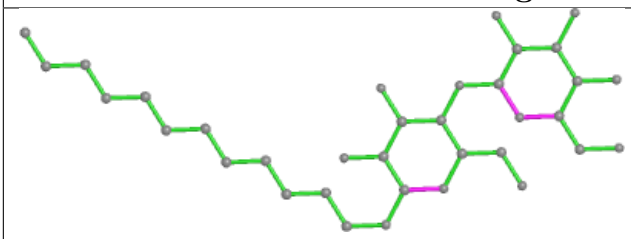

Rings

Ligand LMT h 1002



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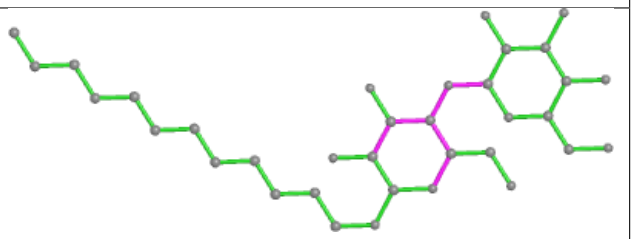
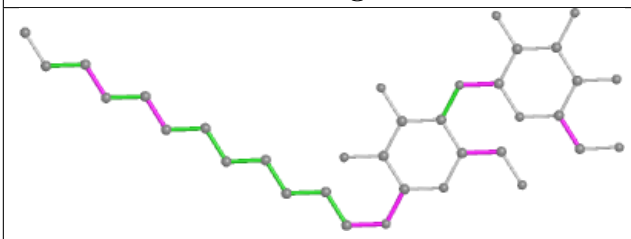


Bond angles



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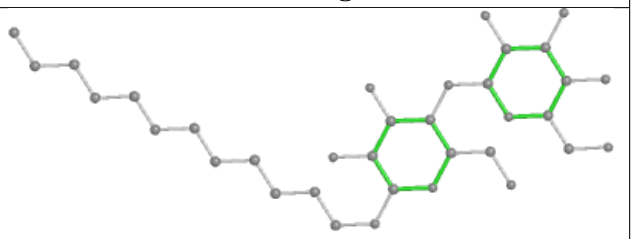
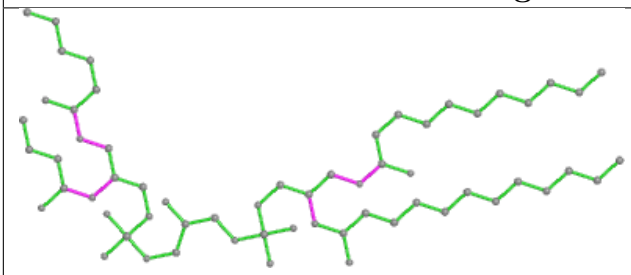


Rings

Ligand CDL N 1101



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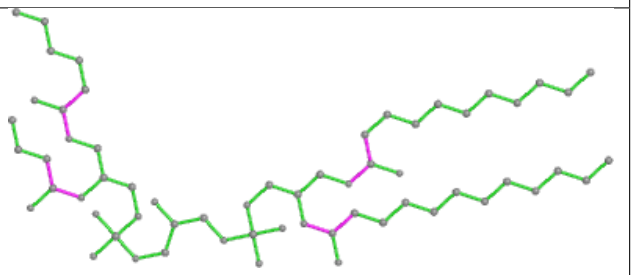
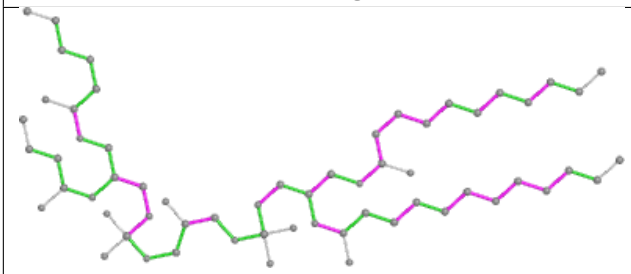


Bond angles



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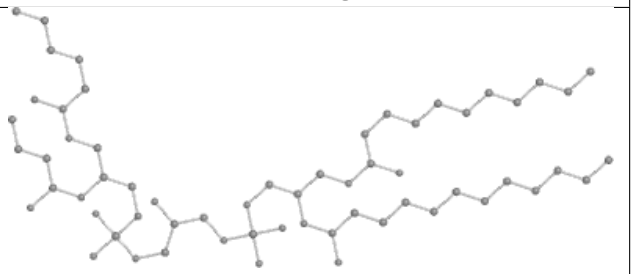
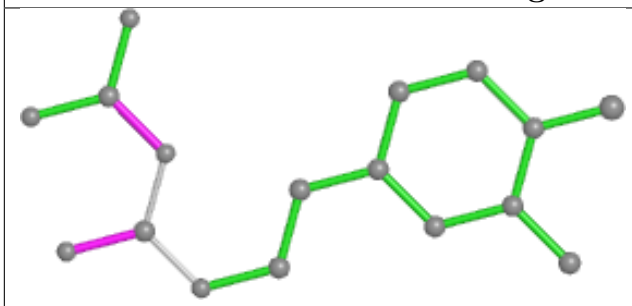


Rings

Ligand I49 N 1102



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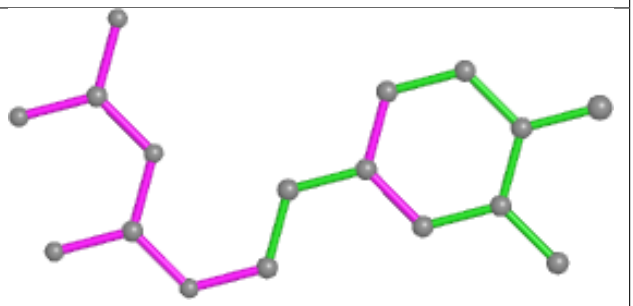
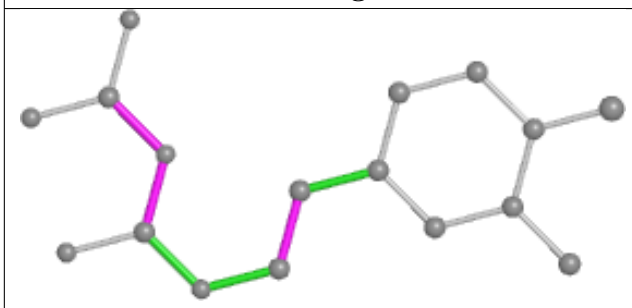
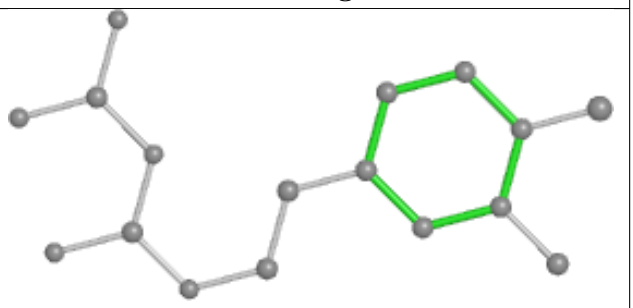


Bond angles

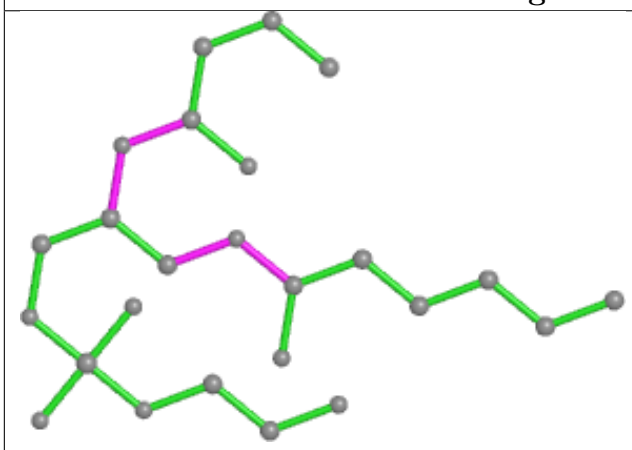


Torsions



Rings

Ligand 3PE H 902



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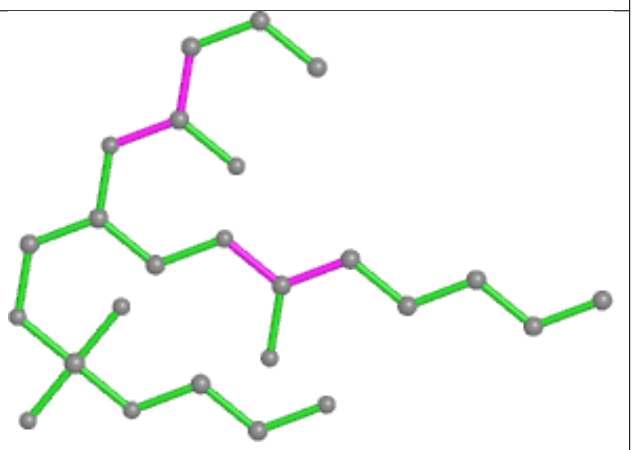
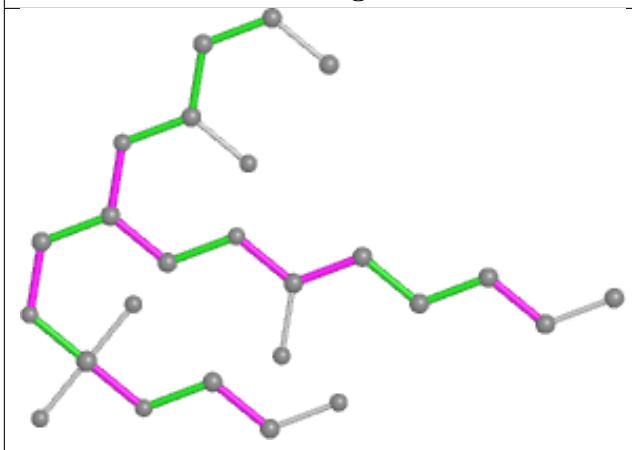
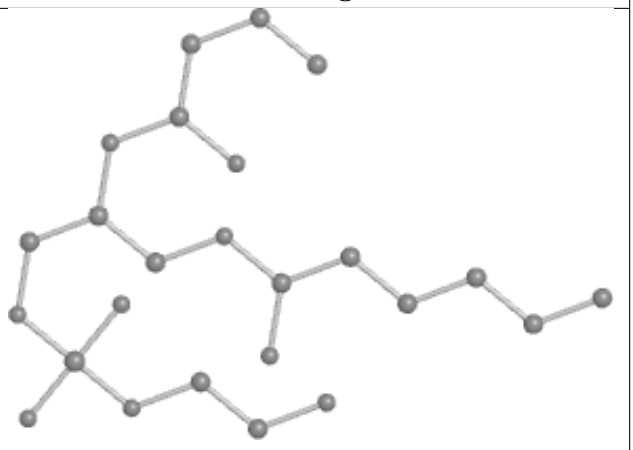


Bond angles

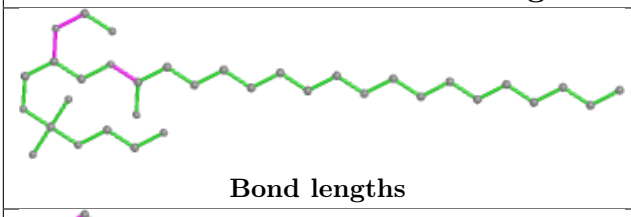


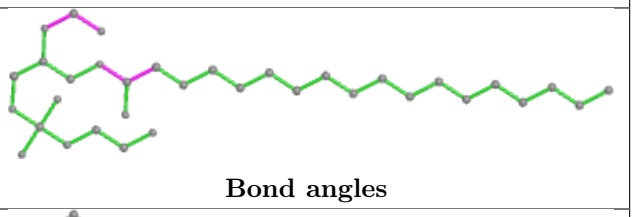
Torsions

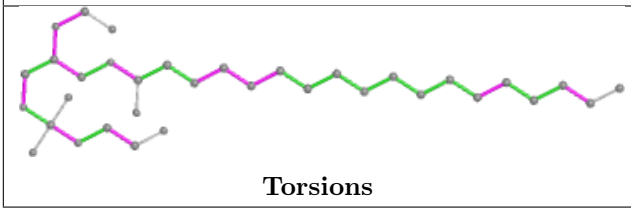


Rings

Ligand 3PE H 903


Bond lengths


Bond angles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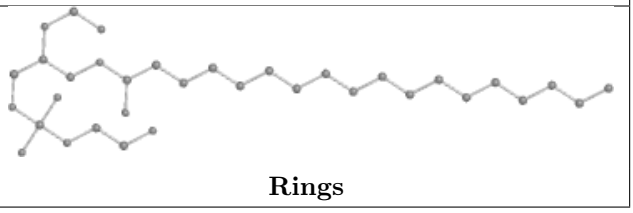
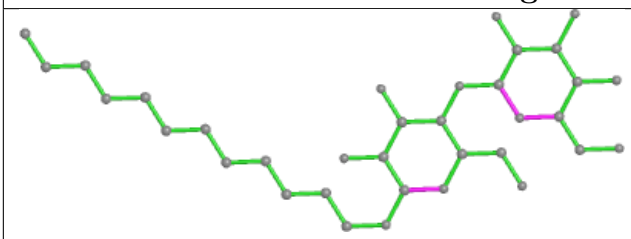

Rings

Ligand LMT K 901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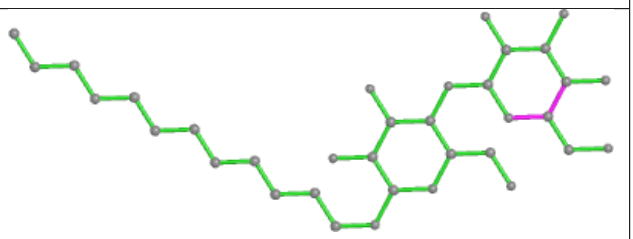
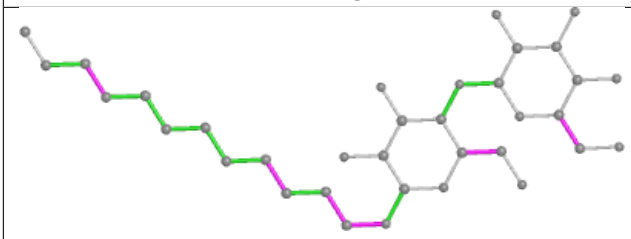

Bond angles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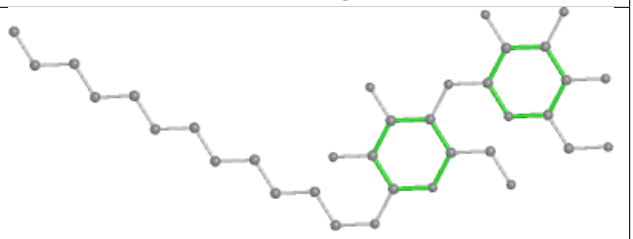
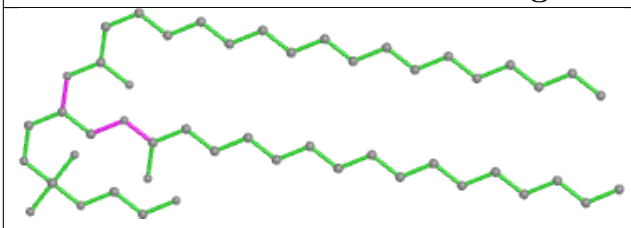

Rings

Ligand 3PE L 701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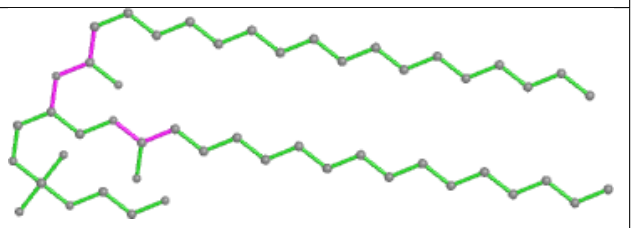
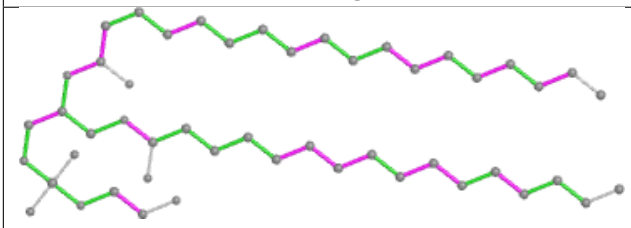

Bond angles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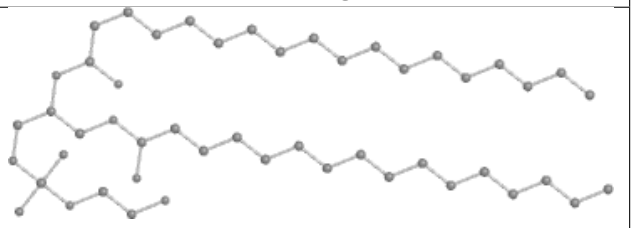
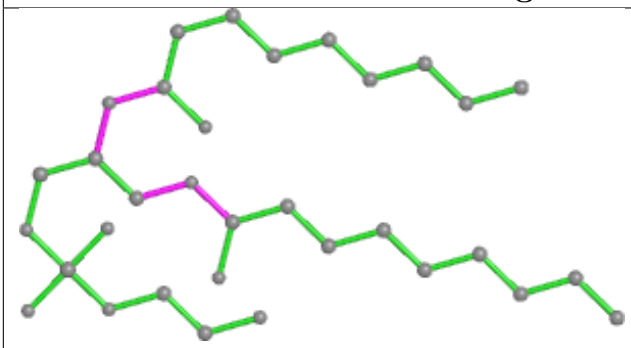

Rings

Ligand 3PE M 1301



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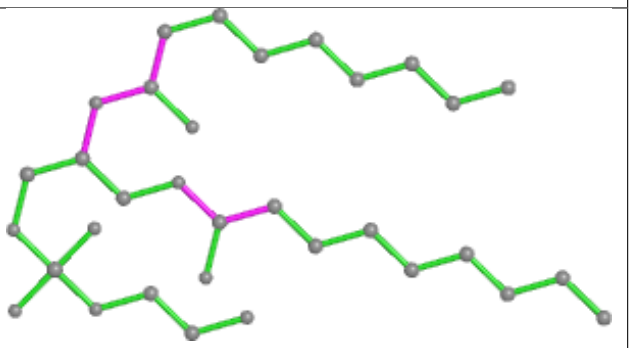
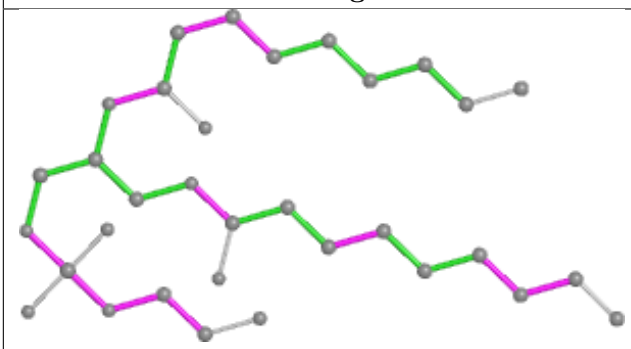
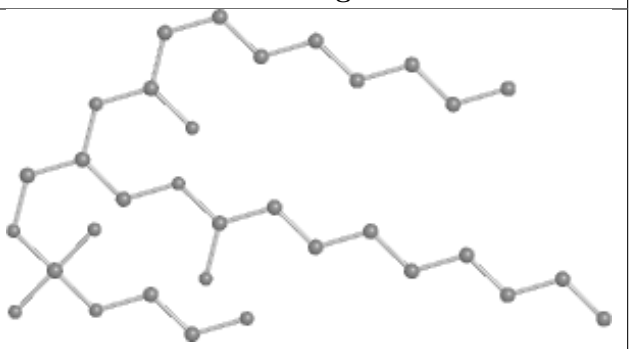


Bond angles

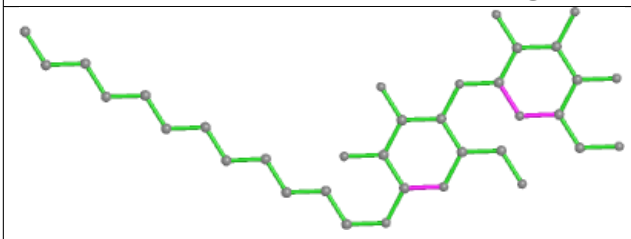


Torsions



Rings

Ligand LMT p 201



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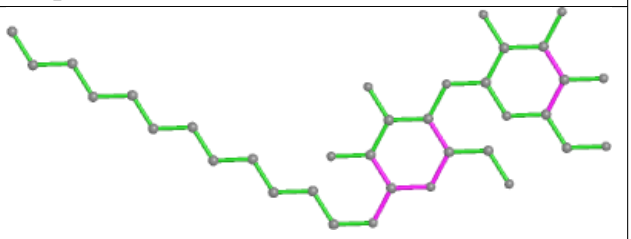
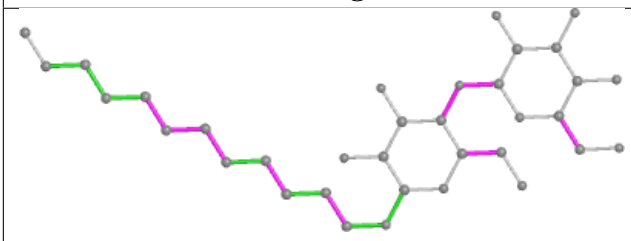
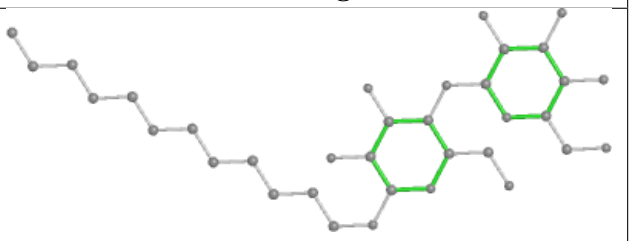


Bond angles

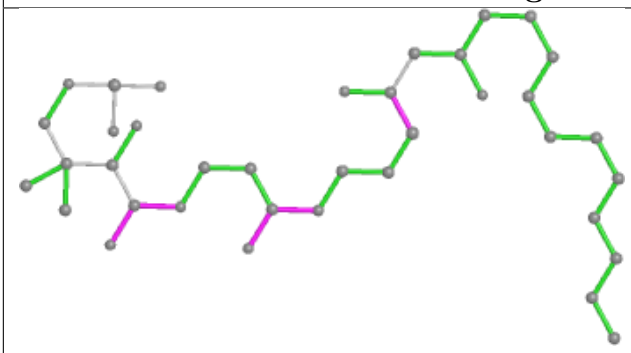


Torsions

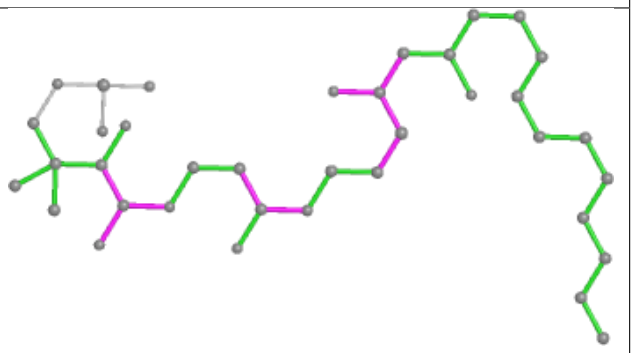


Rings

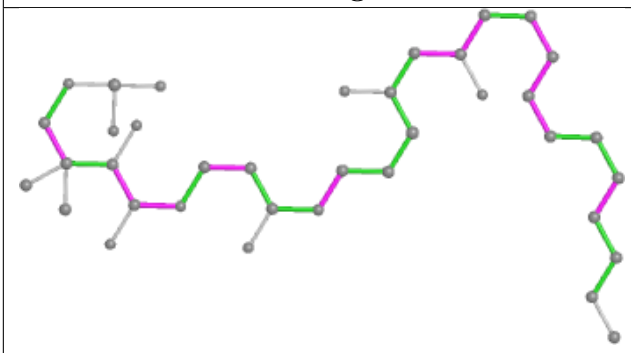
Ligand EHZ T 101



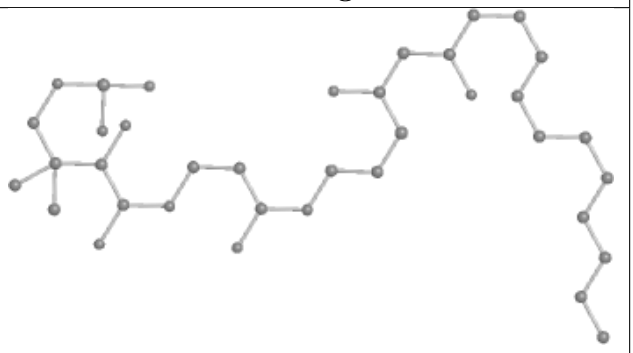
Bond lengths



Bond angles

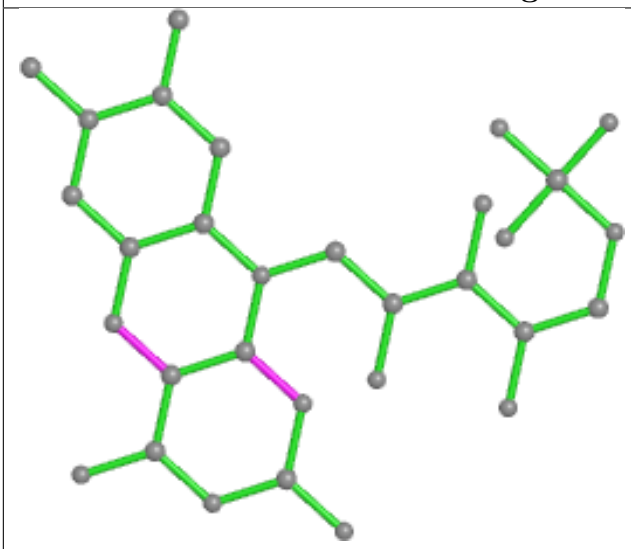


Torsions

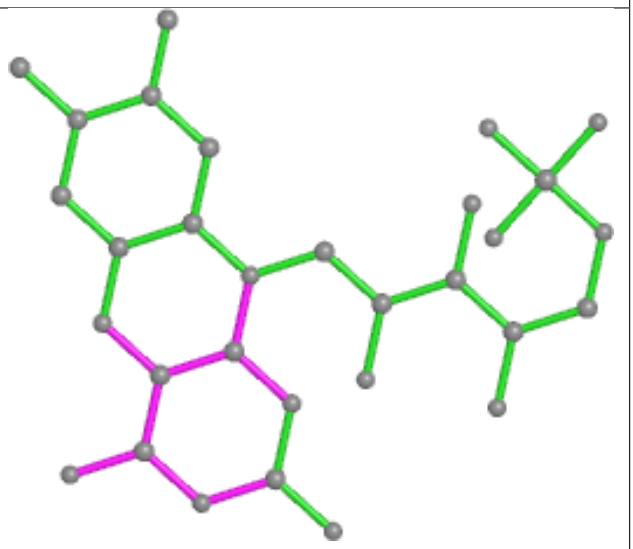


Rings

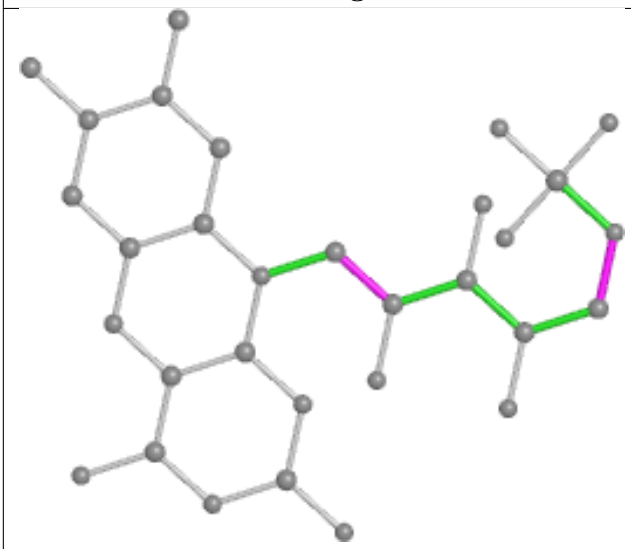
Ligand FMN F 501



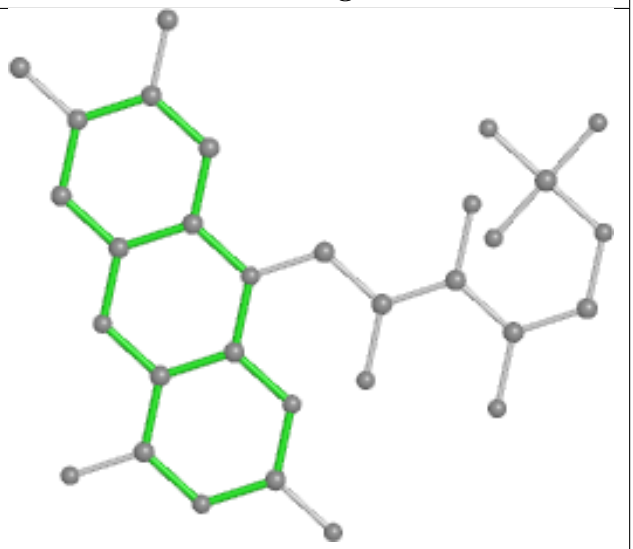
Bond lengths



Bond angles

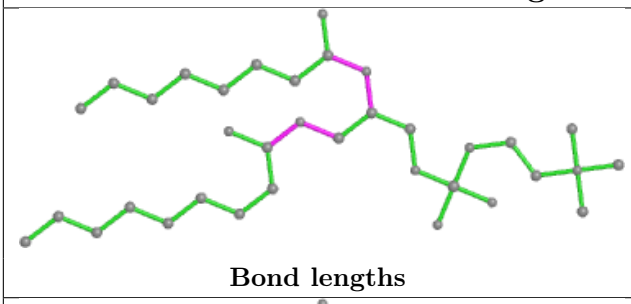


Torsions

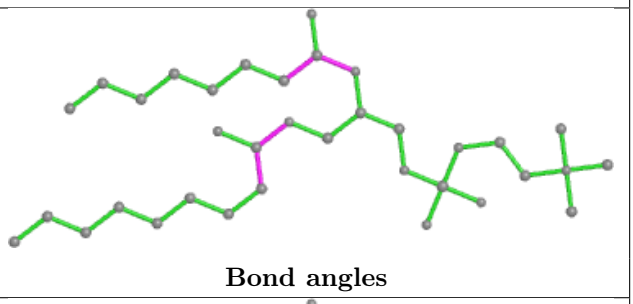


Rings

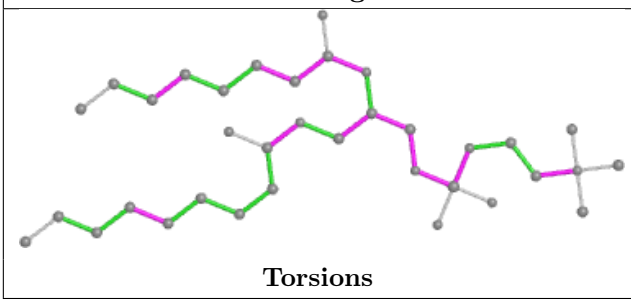
Ligand PC1 B 202



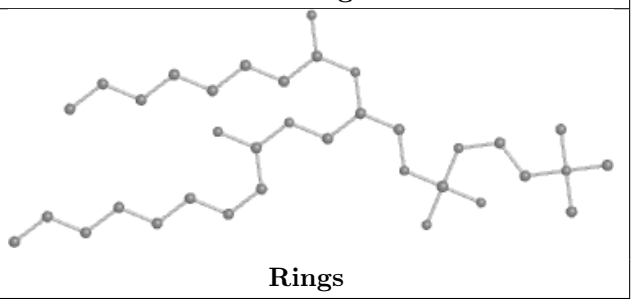
Bond lengths



Bond angles

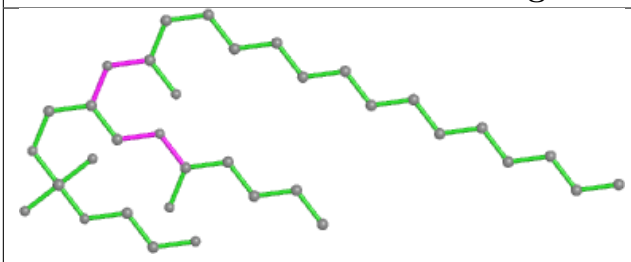


Torsions

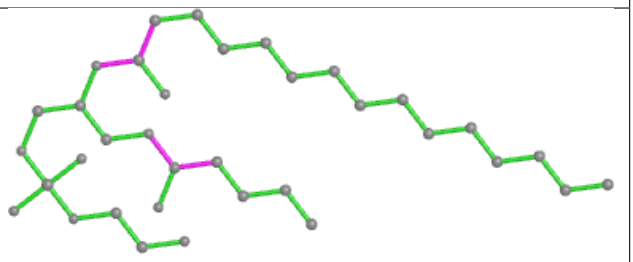


Rings

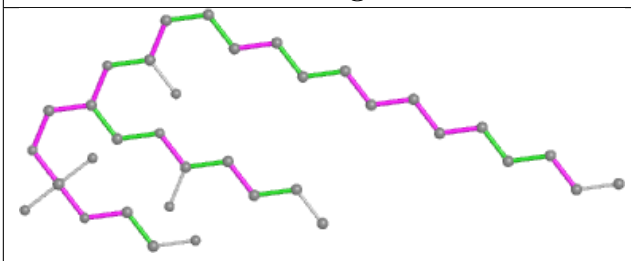
Ligand 3PE Y 601



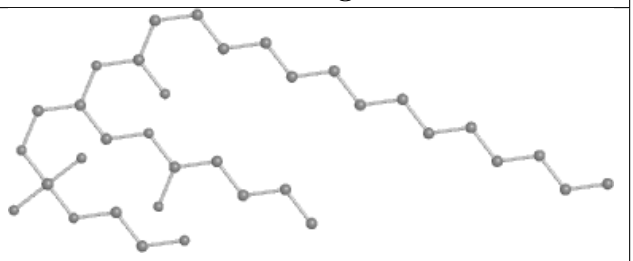
Bond lengths



Bond angles

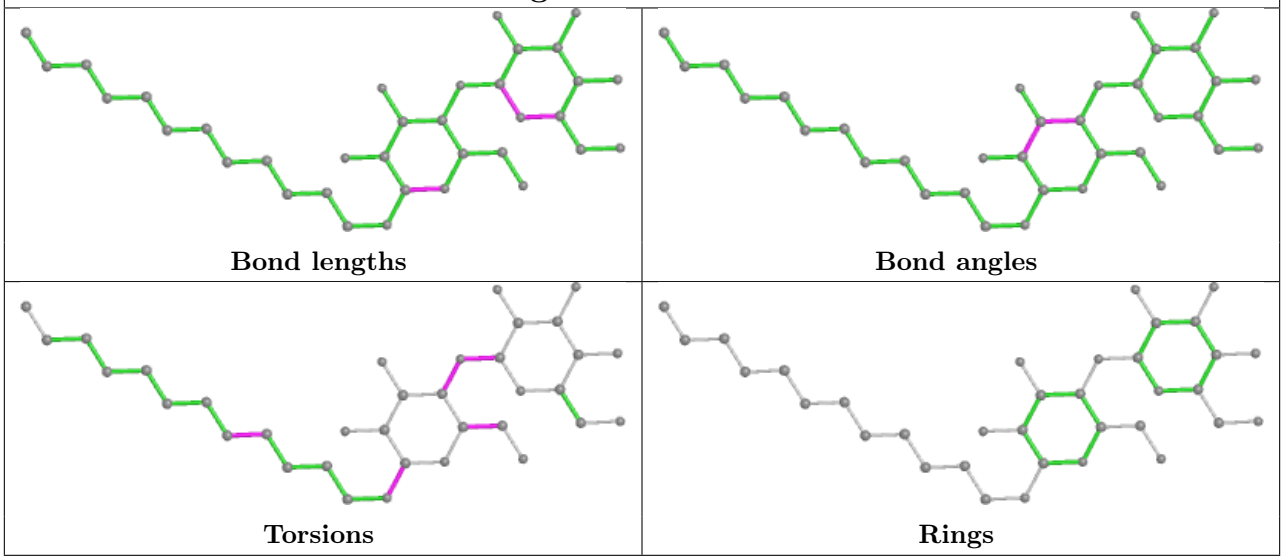


Torsions

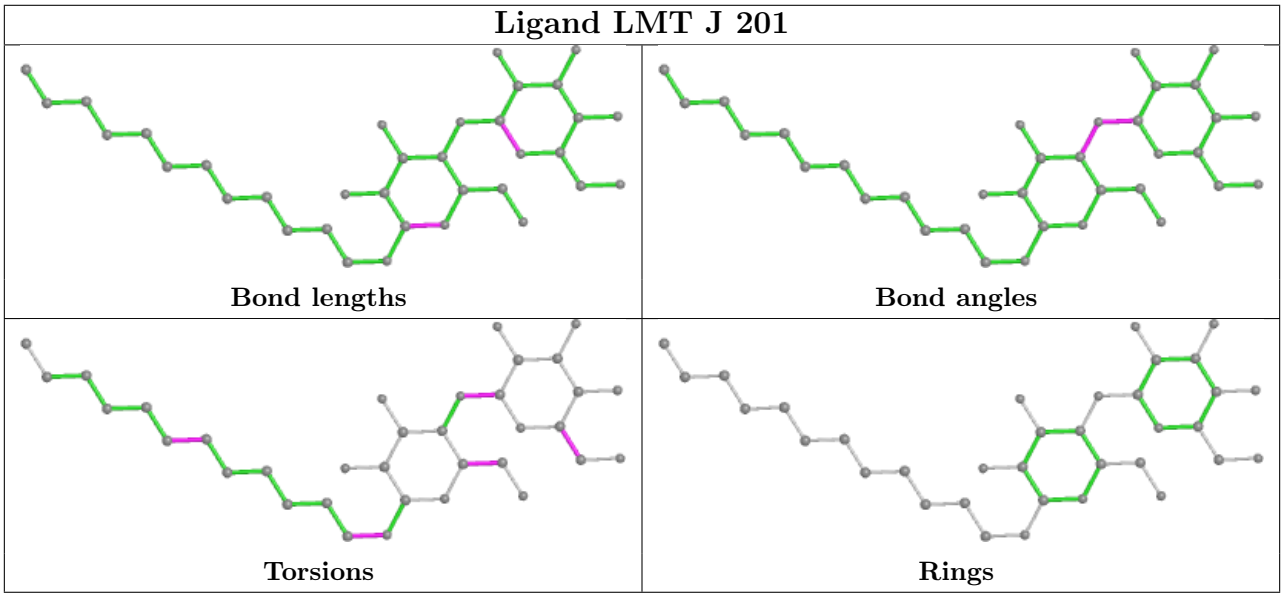


Rings

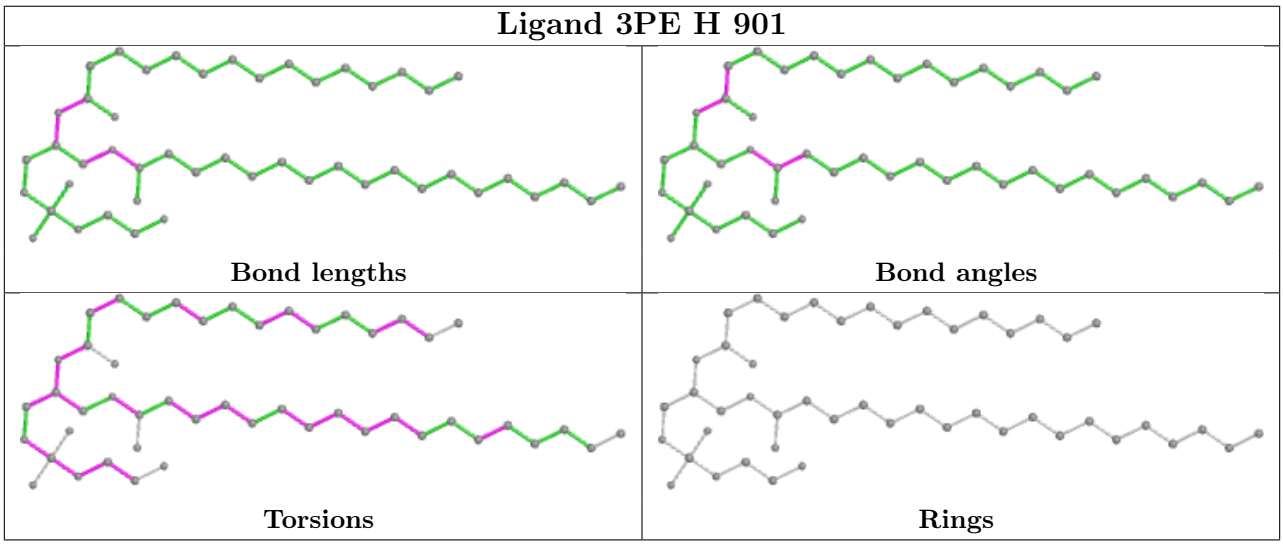
Ligand LMT l 201



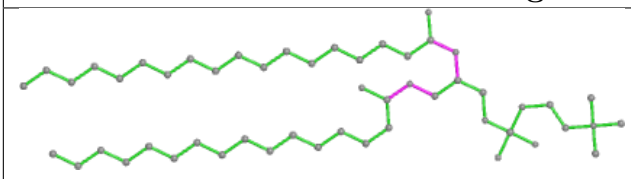
Ligand LMT J 201



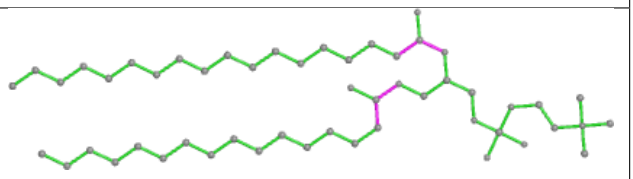
Ligand 3PE H 901



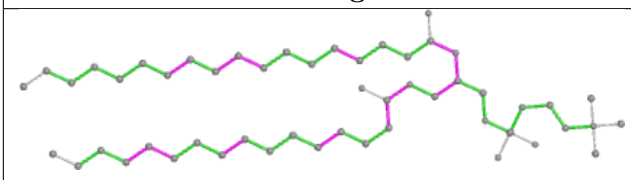
Ligand PC1 A 302



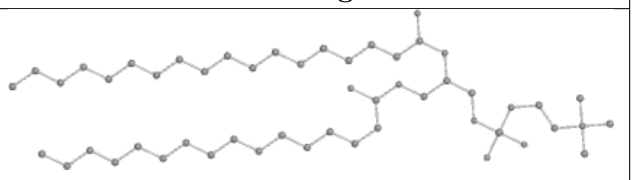
Bond lengths



Bond angles

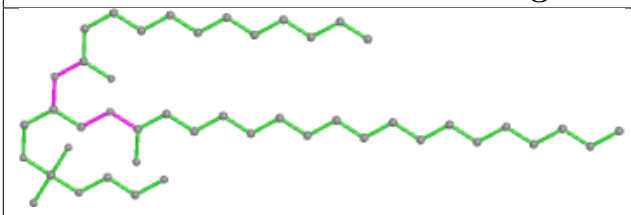


Torsions

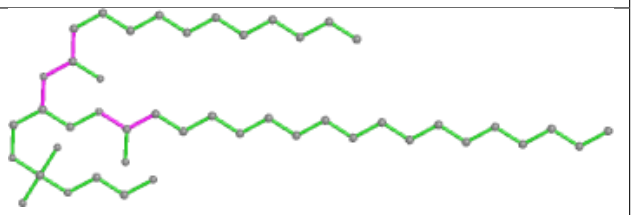


Rings

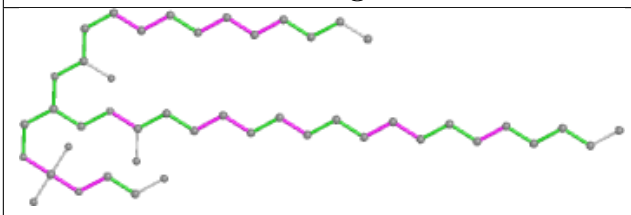
Ligand 3PE L 703



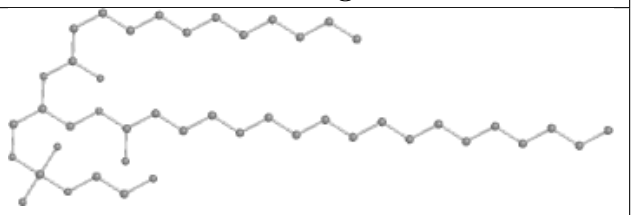
Bond lengths



Bond angles

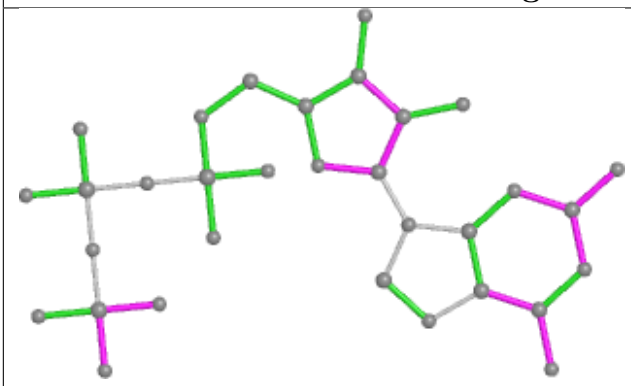


Torsions

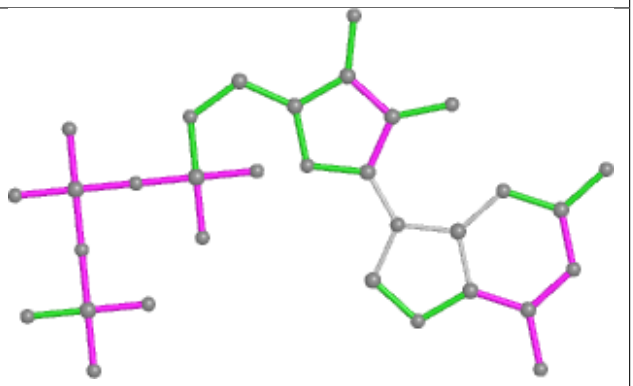


Rings

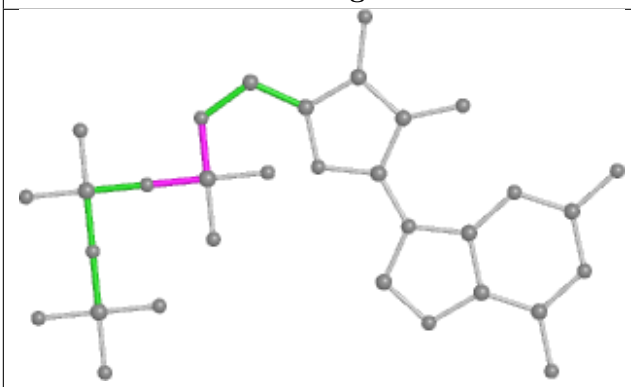
Ligand GTP O 401



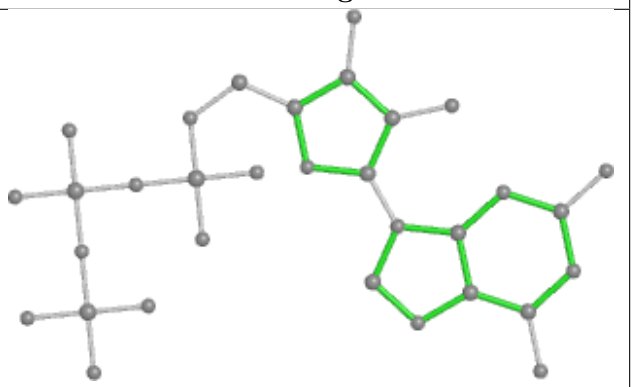
Bond lengths



Bond angles

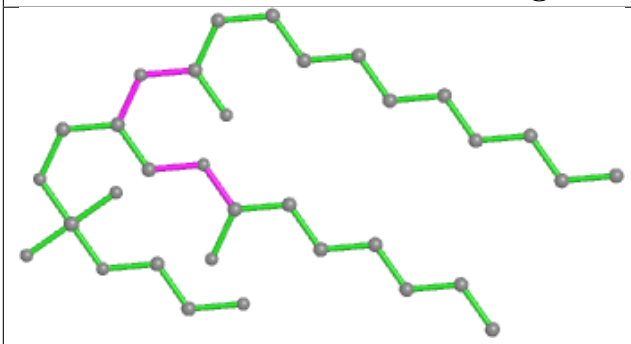


Torsions

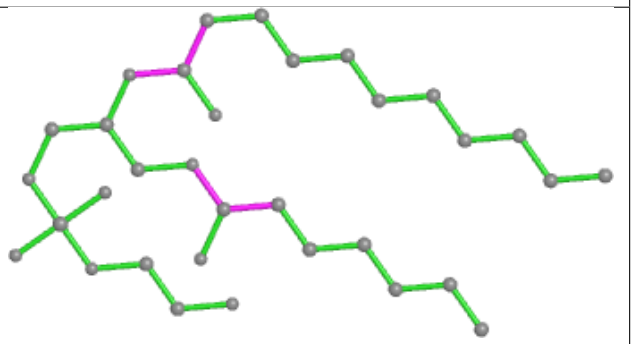


Rings

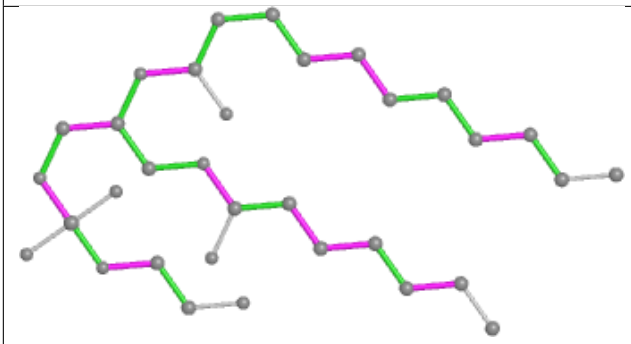
Ligand 3PE Z 301



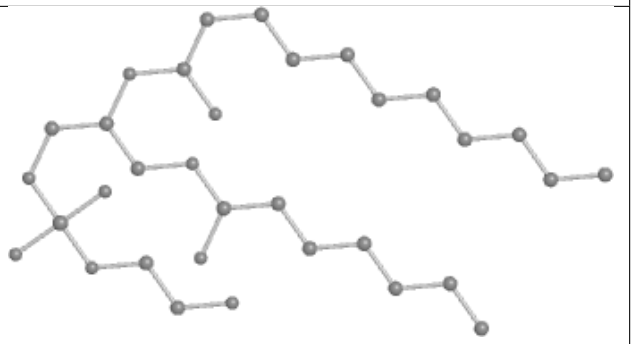
Bond lengths



Bond angles

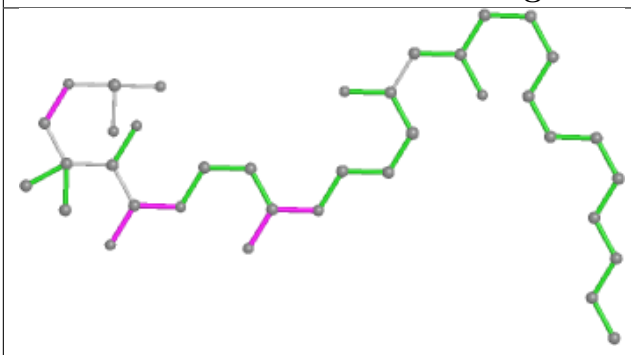


Torsions

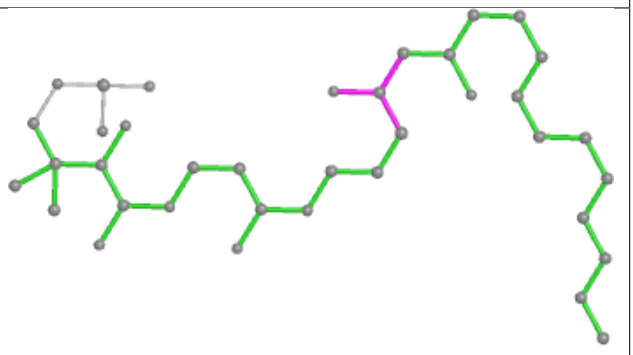


Rings

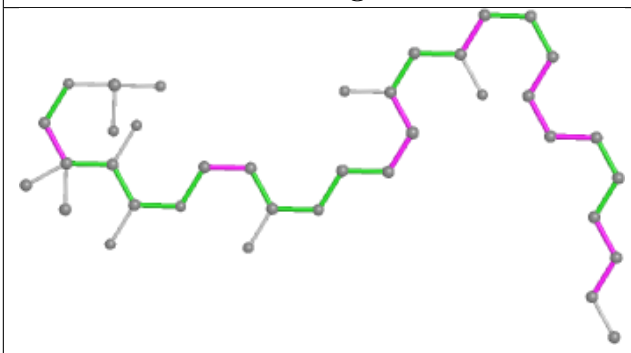
Ligand EHZ U 101



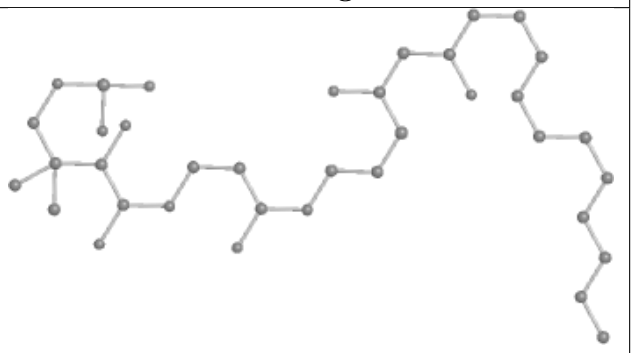
Bond lengths



Bond angles

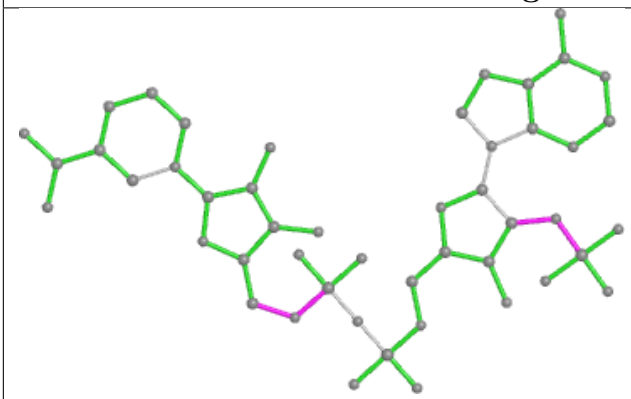


Torsions

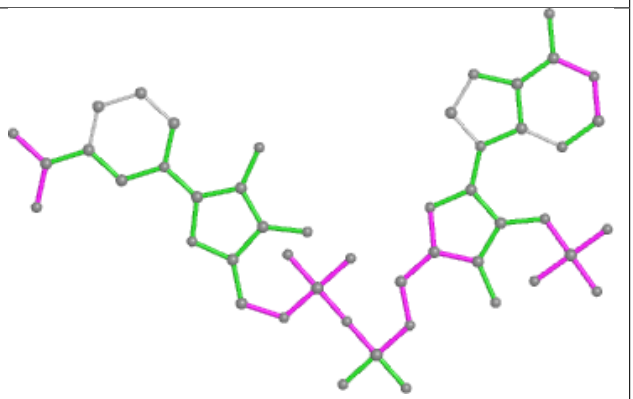


Rings

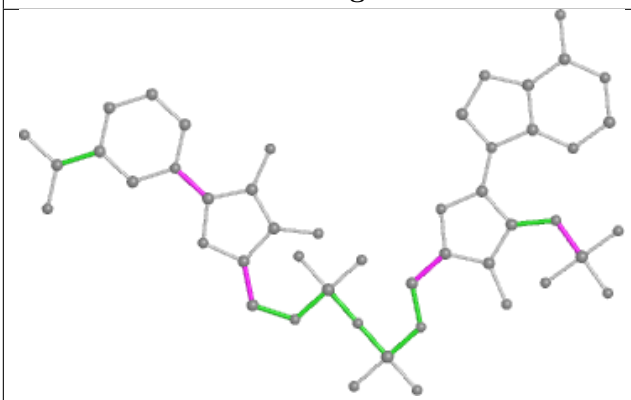
Ligand NDP P 501



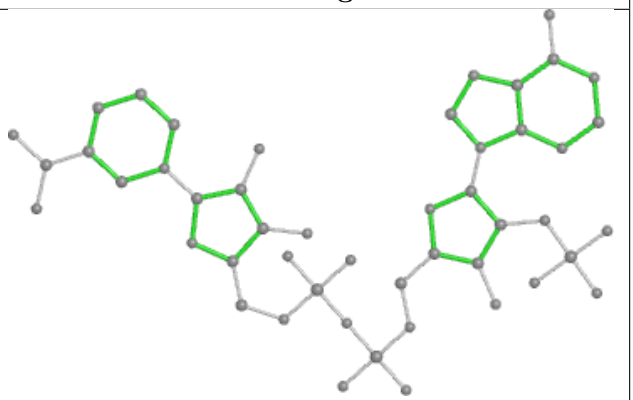
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

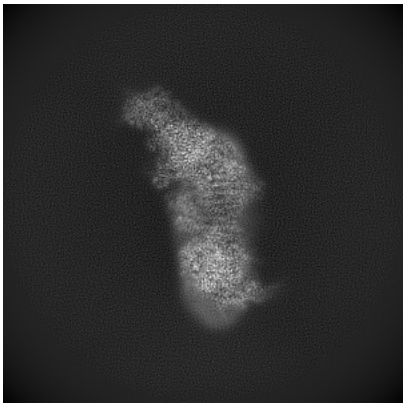
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-14302. These allow visual inspection of the internal detail of the map and identification of artifacts.

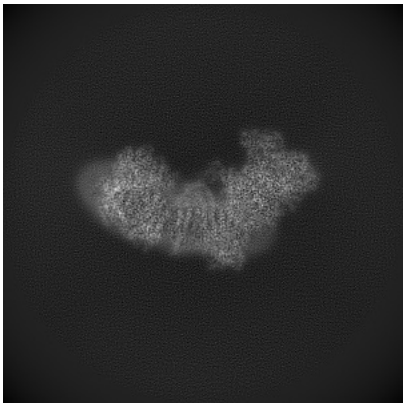
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

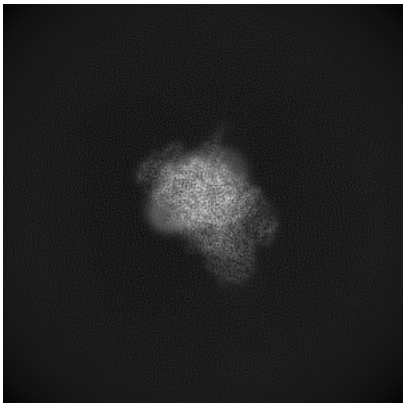
5.1.1 Primary map



X



Y

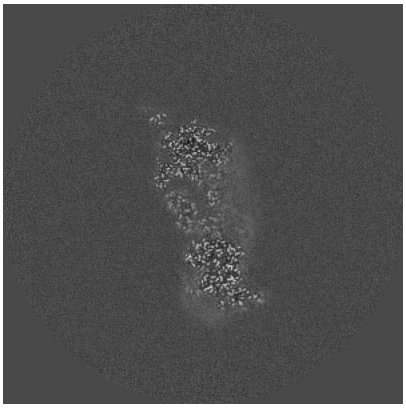


Z

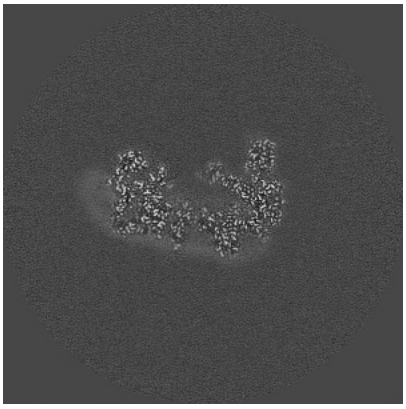
The images above show the map projected in three orthogonal directions.

5.2 Central slices

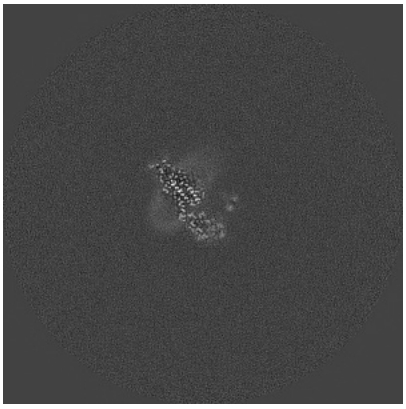
5.2.1 Primary map



X Index: 330



Y Index: 330

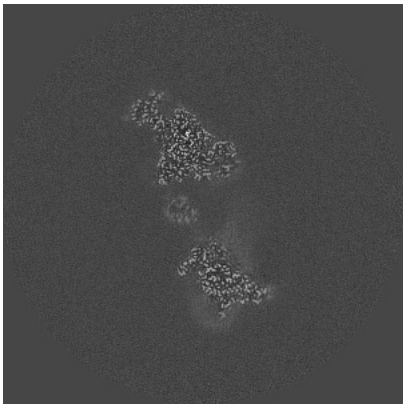


Z Index: 330

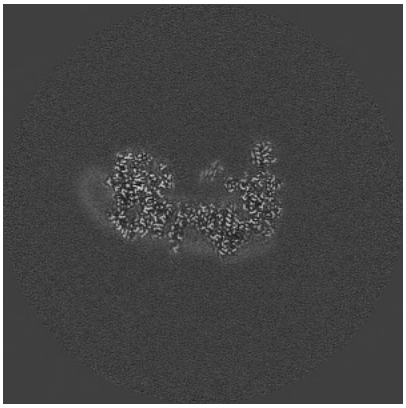
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

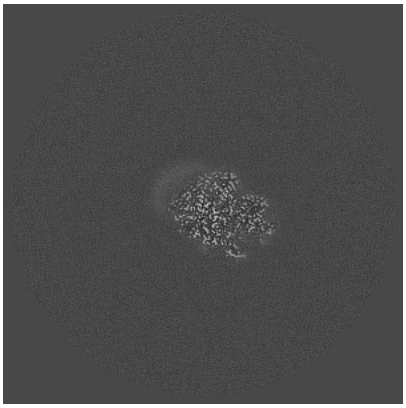
5.3.1 Primary map



X Index: 353



Y Index: 337



Z Index: 424

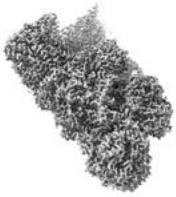
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal surface views (i)

5.4.1 Primary map

X

Y



Z

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

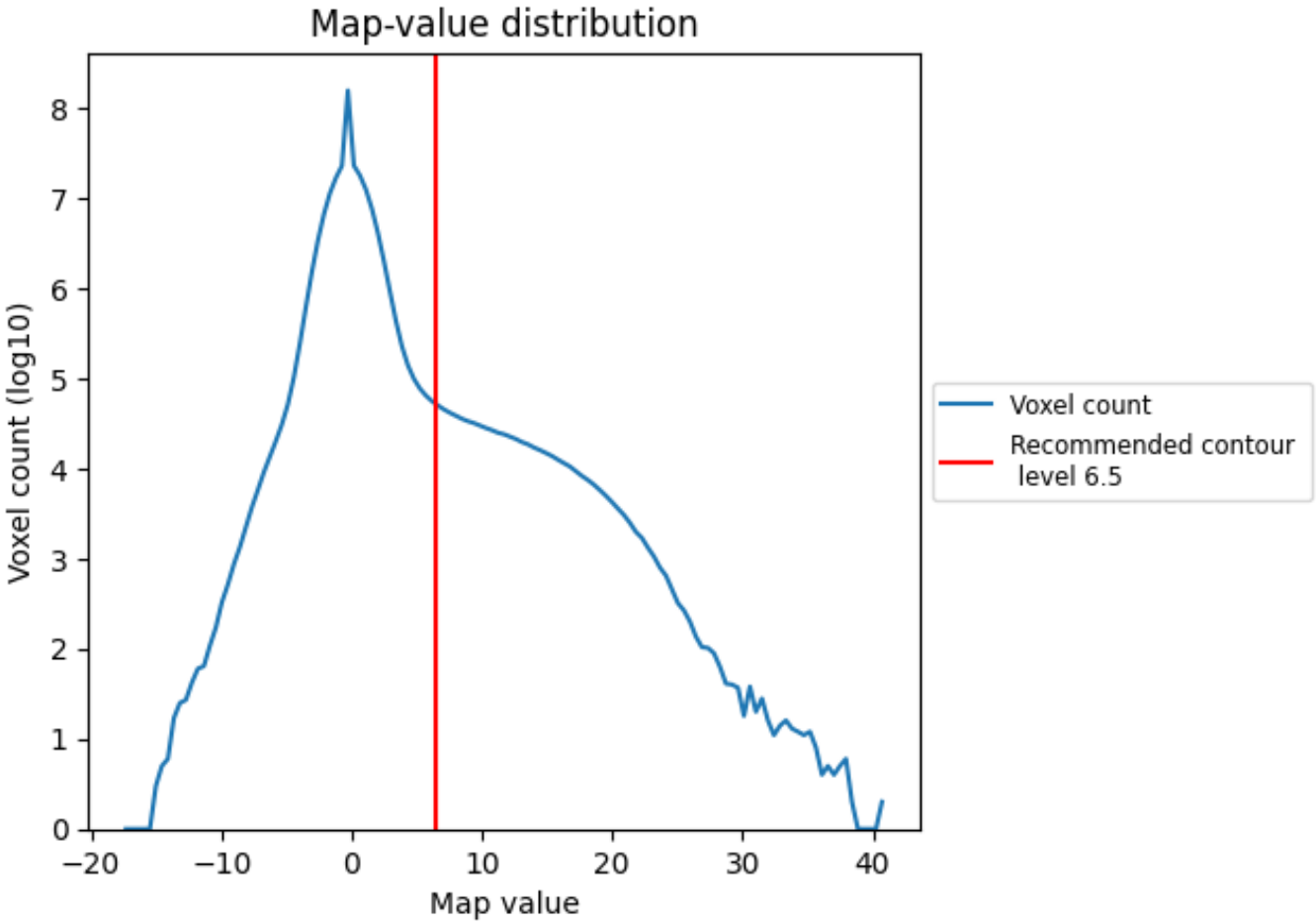
5.5 Mask visualisation (i)

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

6 Map analysis

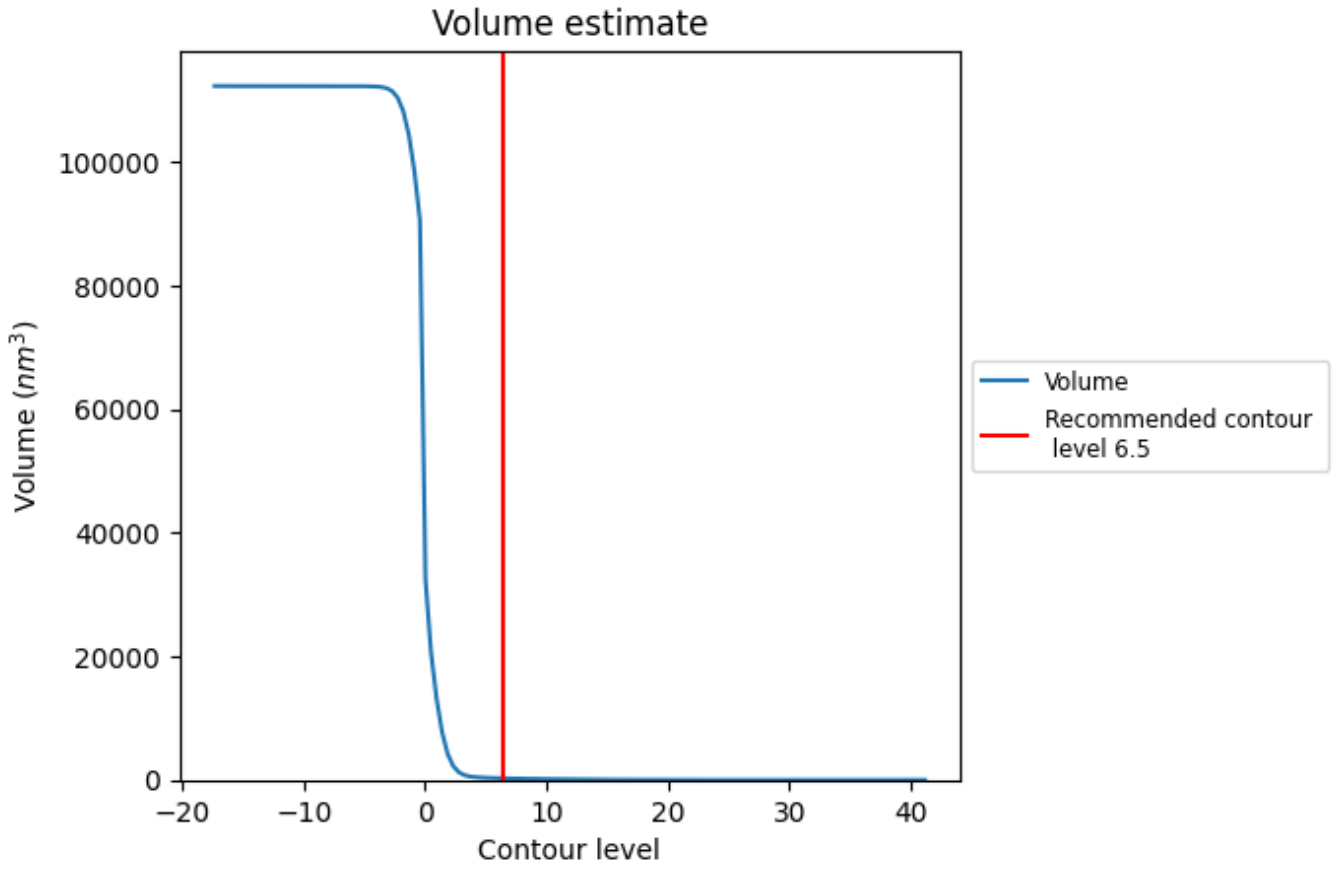
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



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.

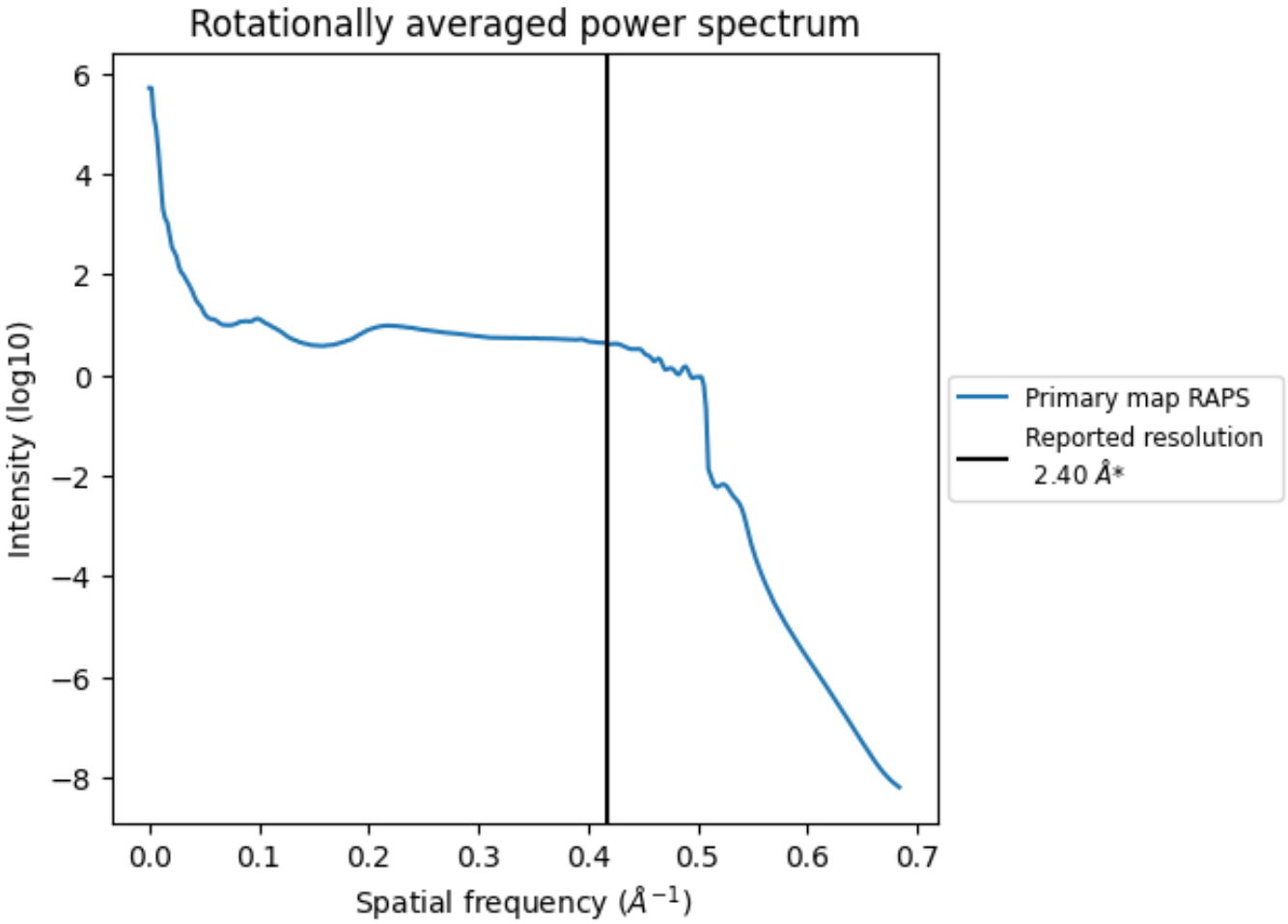
6.2 Volume estimate



The volume at the recommended contour level is 260 nm^3; this corresponds to an approximate mass of 235 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.

6.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

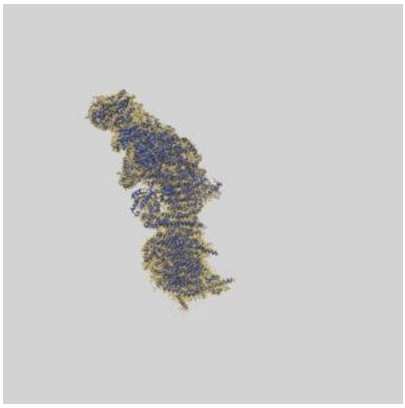
7 Fourier-Shell correlation (i)

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

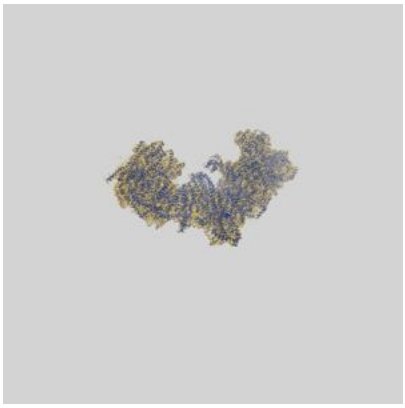
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14302 and PDB model 7R4F. Per-residue inclusion information can be found in section ?? on page ??.

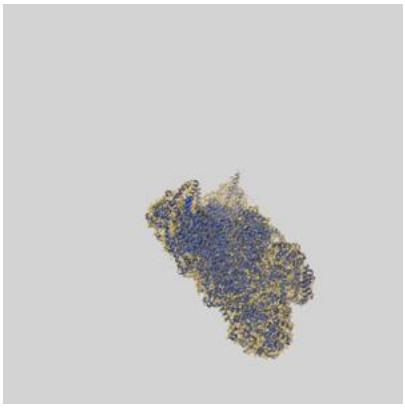
8.1 Map-model overlay



X



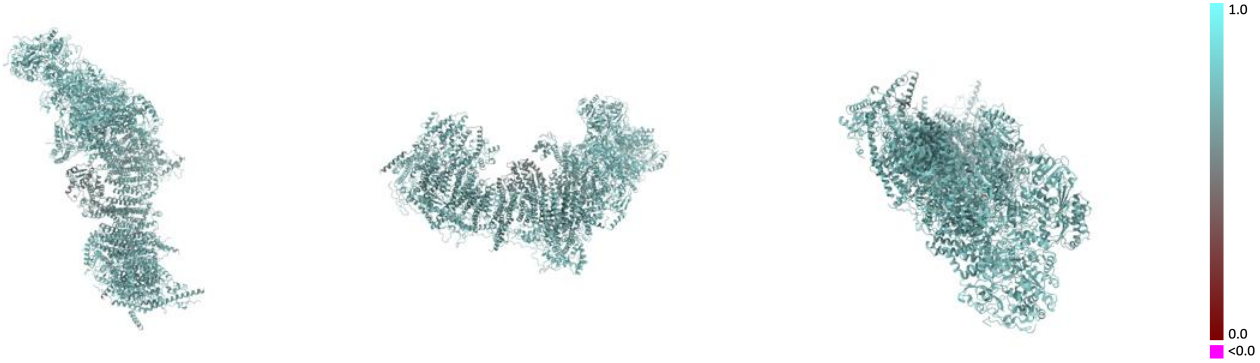
Y



Z

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

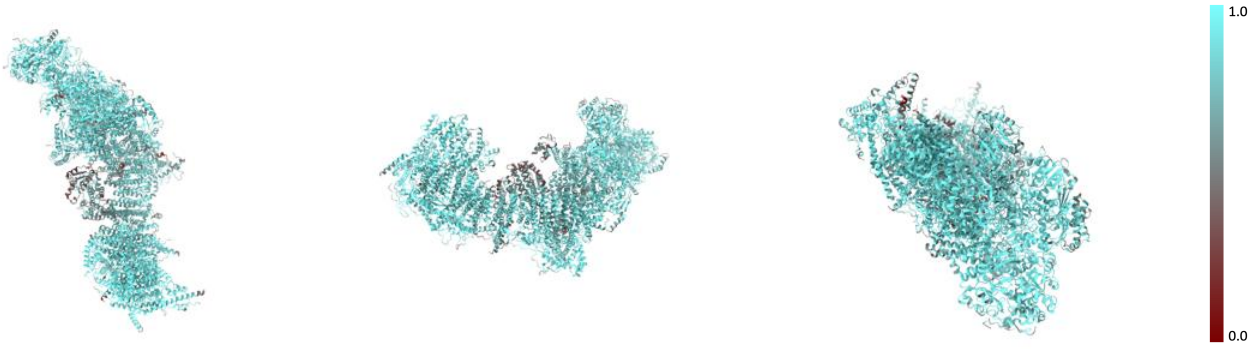
8.2 Q-score mapped to coordinate model (i)



X Y Z

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.

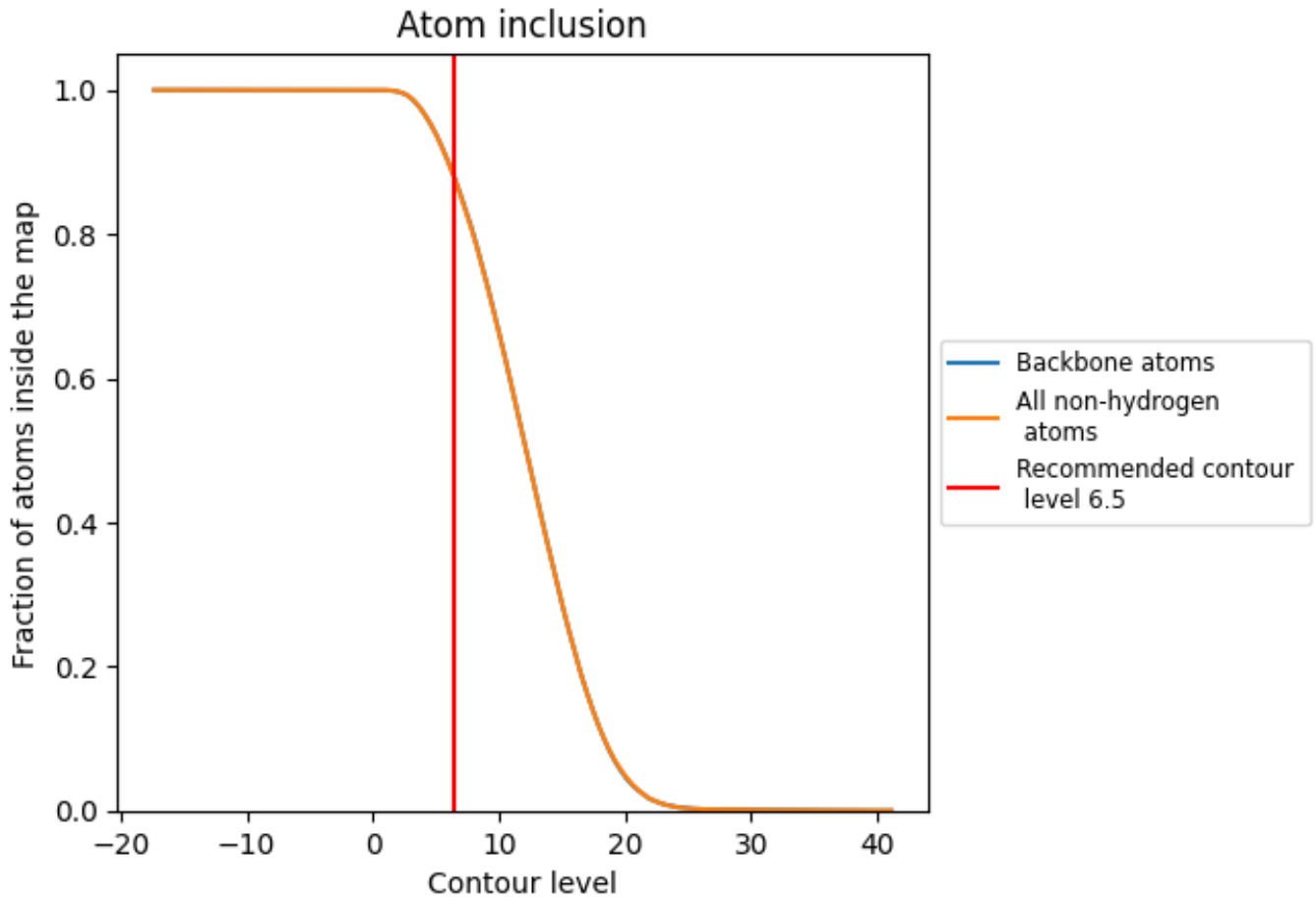
8.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.5).

8.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8777	0.6930
A	0.7974	0.6740
B	0.9276	0.7280
C	0.9580	0.7390
D	0.9593	0.7390
E	0.8770	0.6950
F	0.9219	0.7120
G	0.9104	0.7170
H	0.9116	0.7060
I	0.9659	0.7430
J	0.8592	0.6850
K	0.8695	0.6930
L	0.9491	0.6870
M	0.9532	0.7010
N	0.8794	0.6870
O	0.5875	0.5880
P	0.8535	0.6980
Q	0.9033	0.7260
R	0.8990	0.7200
S	0.8276	0.6890
T	0.5341	0.6140
U	0.9298	0.6800
V	0.8502	0.7060
W	0.8524	0.7080
X	0.8526	0.6810
Y	0.5532	0.6550
Z	0.7934	0.6810
a	0.9464	0.7010
b	0.8352	0.6800
c	0.7121	0.6240
d	0.7642	0.6640
e	0.8183	0.6740
f	0.7822	0.6570
g	0.9272	0.6900
h	0.8939	0.6880

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Chain	Atom inclusion	Q-score
i	0.8778	0.6610
j	0.8991	0.6620
k	0.8842	0.6500
l	0.8956	0.6680
m	0.8703	0.6670
n	0.9260	0.6840
o	0.8981	0.6650
p	0.9073	0.6780
q	0.8782	0.7200
r	0.8435	0.7130
s	0.8563	0.6970