Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 04:29 PM EDT

PDB ID	:	7N9Z / pdb_00007n9z
EMDB ID	:	EMD-24265
Title	:	E. coli cytochrome bo3 in MSP nanodisc
Authors	:	Vallese, F.; Clarke, O.B.
Deposited on	:	2021-06-19
Resolution	:	2.19 Å(reported)
Based on initial model	:	1FFT

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:

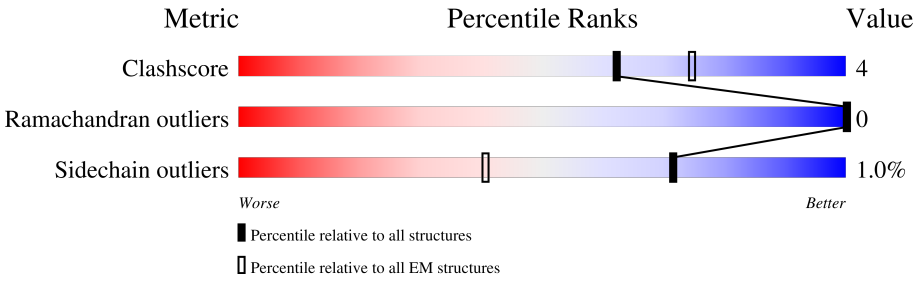
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.19 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	663	87% 11%
2	G	315	78% 5% 17%
3	H	204	85% 10%
4	I	109	75% 15% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	HEO	F	710	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 20938 atoms, of which 10465 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 Cytochrome o ubiquinol oxidase, subunit I.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	F	658	10454	3517	5215	834	851	37	7	0

- Molecule 2 is a protein called Ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	G	262	3982	1316	1972	326	357	11	0	0

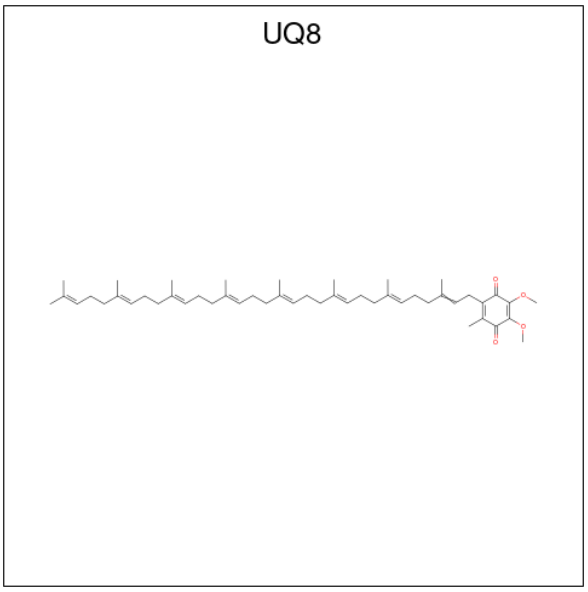
- Molecule 3 is a protein called Cytochrome o ubiquinol oxidase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	H	184	2847	959	1415	225	235	13	0	0

- Molecule 4 is a protein called Cytochrome o ubiquinol oxidase, subunit IV.

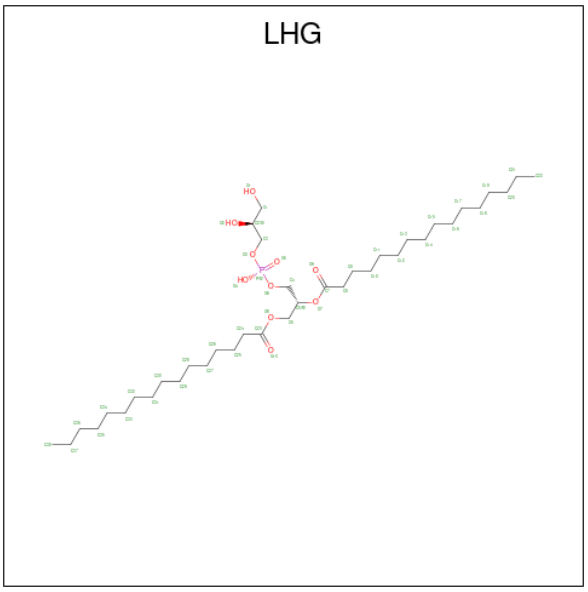
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	I	98	1554	512	787	119	125	11	2	0

- Molecule 5 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	F	1	Total	C	H	O	P	0
			93	30	52	10	1	
6	F	1	Total	C	H	O	P	0
			102	32	59	10	1	

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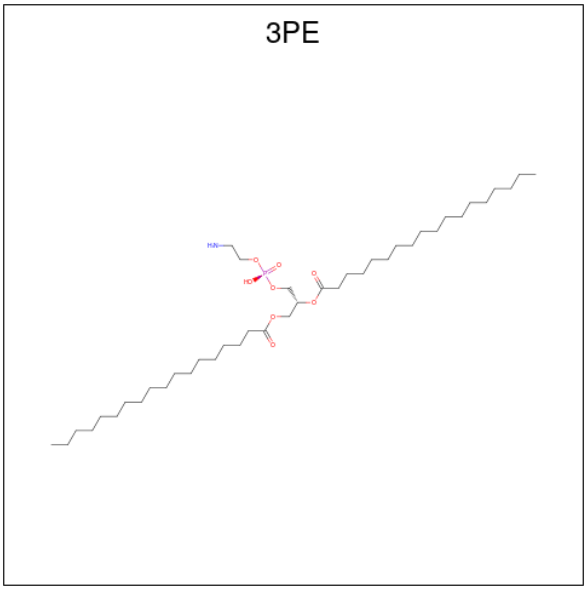
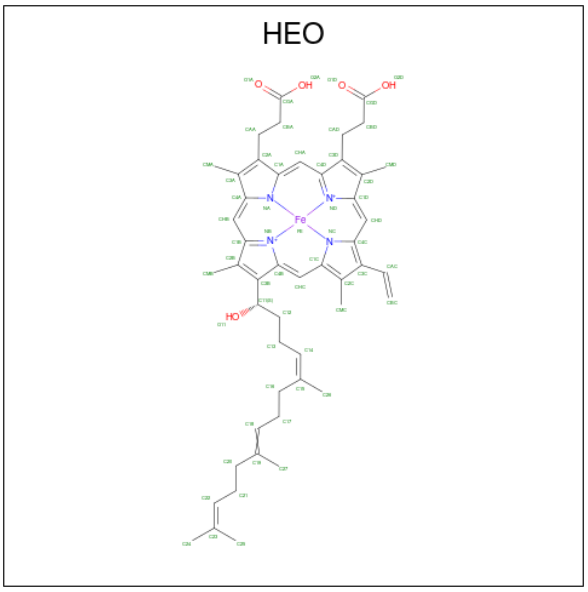
Mol	Chain	Residues	Atoms					AltConf
6	F	1	Total	C	H	O	P	0
			123	38	74	10	1	
6	F	1	Total	C	H	O	P	0
			123	38	74	10	1	
6	F	1	Total	C	H	O	P	0
			102	32	59	10	1	
6	F	1	Total	C	H	O	P	0
			123	38	74	10	1	
6	F	1	Total	C	H	O	P	0
			123	38	74	10	1	
6	H	1	Total	C	H	O	P	0
			123	38	74	10	1	
6	H	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 7 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



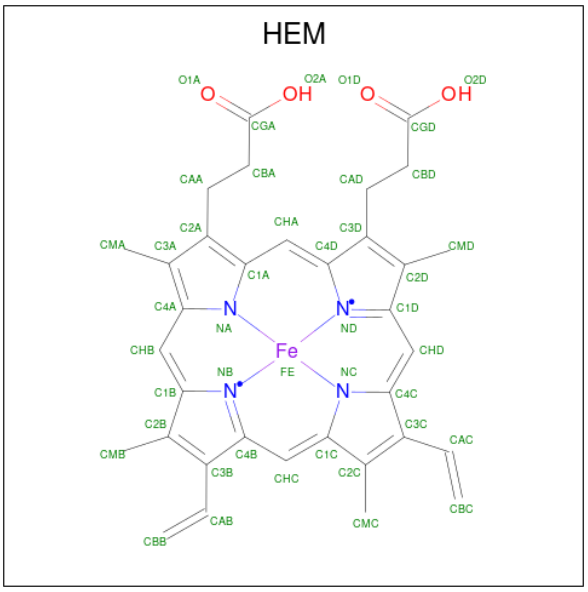
Mol	Chain	Residues	Atoms						AltConf
7	F	1	Total	C	H	N	O	P	0
			111	36	65	1	8	1	
7	H	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

- Molecule 8 is HEME O (CCD ID: HEO) (formula: $C_{49}H_{58}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).



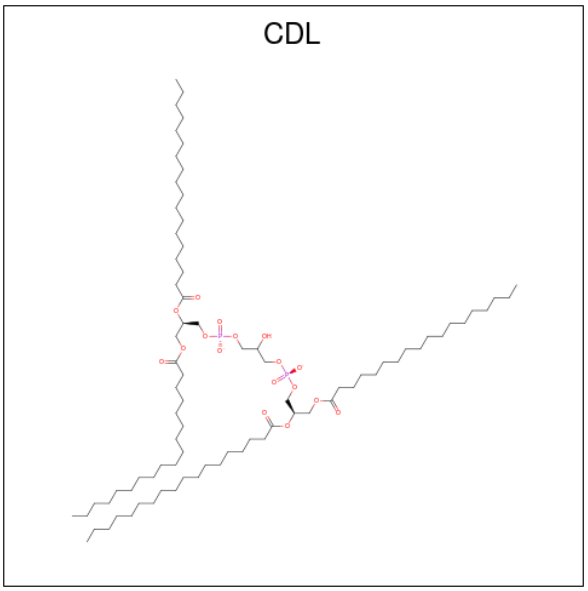
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
8	F	1	115	49	1	56	4	5	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
9	F	1	73	34	1	30	4	4	0

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	F	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 11 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	F	1	Total	Cu	0
			1	1	

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	G	1	Total	Zn	0
			1	1	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	F	150	Total	O	0
			150	150	
13	G	65	Total	O	0
			65	65	
13	H	26	Total	O	0
			26	26	

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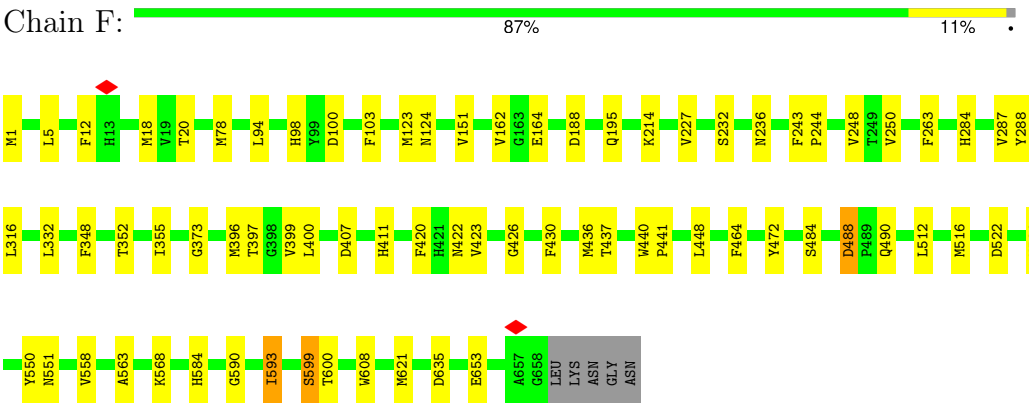
Mol	Chain	Residues	Atoms	AltConf
13	I	9	Total O 9 9	0

3 Residue-property plots (i)

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

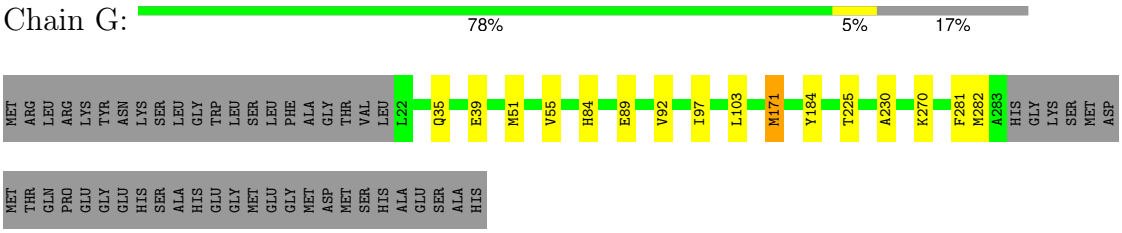
• Molecule 1: Cytochrome o ubiquinol oxidase, subunit I

Chain F:



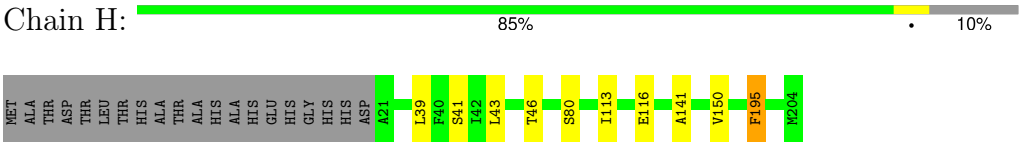
• Molecule 2: Ubiquinol oxidase subunit 2

Chain G:



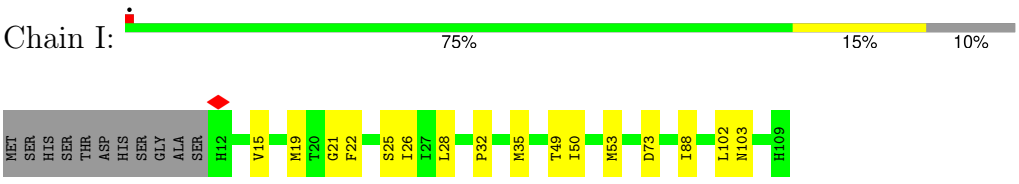
• Molecule 3: Cytochrome o ubiquinol oxidase

Chain H:



• Molecule 4: Cytochrome o ubiquinol oxidase, subunit IV

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.415	Depositor
Minimum map value	-2.982	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.49	Depositor
Map size (Å)	184.16325, 156.02145, 168.43695	wwPDB
Map dimensions	445, 377, 407	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.41385, 0.41385, 0.41385	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, UQ8, ZN, LHG, 3PE, HEO, CU, HEM

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	F	0.18	0/5443	0.34	0/7423
2	G	0.17	0/2069	0.31	0/2825
3	H	0.17	0/1473	0.31	0/2000
4	I	0.15	0/795	0.28	0/1086
All	All	0.18	0/9780	0.32	0/13334

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5239	5215	5218	61	0
2	G	2010	1972	1976	11	0
3	H	1432	1415	1431	8	0
4	I	767	787	781	11	0
5	F	53	74	74	7	0
6	F	323	466	466	1	0
6	H	98	148	148	0	0
7	F	46	65	66	2	0
7	H	51	81	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	59	56	56	3	0
9	F	43	30	30	0	0
10	F	100	156	156	1	0
11	F	1	0	0	0	0
12	G	1	0	0	0	0
13	F	150	0	0	7	0
13	G	65	0	0	0	0
13	H	26	0	0	2	0
13	I	9	0	0	1	0
All	All	10473	10465	10484	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:MET:SD	13:F:819:HOH:O	2.25	0.94
1:F:164:GLU:OE2	13:F:801:HOH:O	1.94	0.85
5:F:701:UQ8:H3MB	5:F:701:UQ8:H4MA	1.58	0.84
1:F:188:ASP:OD2	13:F:802:HOH:O	1.99	0.80
1:F:528:ASP:OD1	13:F:803:HOH:O	2.01	0.79
1:F:373:GLY:O	13:F:804:HOH:O	2.02	0.76
1:F:1:MET:HA	1:F:1:MET:HE2	1.72	0.70
1:F:5:LEU:O	13:F:805:HOH:O	2.10	0.69
3:H:116:GLU:OE1	13:H:401:HOH:O	2.12	0.67
4:I:28:LEU:HD23	4:I:53:MET:HE2	1.77	0.65
1:F:98[B]:HIS:NE2	5:F:701:UQ8:O2	2.31	0.63
1:F:20:THR:HG21	5:F:701:UQ8:H8	1.83	0.60
4:I:103:ASN:OD1	13:I:201:HOH:O	2.17	0.58
1:F:20:THR:OG1	5:F:701:UQ8:H1MA	2.03	0.58
3:H:43:LEU:HD21	7:H:303:3PE:H3I1	1.88	0.54
1:F:227:VAL:HG21	1:F:310:LEU:CD2	2.38	0.54
1:F:98[B]:HIS:CD2	5:F:701:UQ8:H3MA	2.44	0.53
1:F:512:LEU:HD11	1:F:516:MET:HE2	1.89	0.53
4:I:22:PHE:CE1	4:I:26:ILE:HD11	2.44	0.52
1:F:653:GLU:OE1	1:F:653:GLU:HA	2.08	0.52
1:F:12:PHE:CD1	1:F:18:MET:HE2	2.45	0.52
1:F:232:SER:O	1:F:236:ASN:ND2	2.41	0.52
1:F:397:THR:HG21	1:F:472:TYR:CZ	2.45	0.52
1:F:420:PHE:HA	1:F:423:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:VAL:HG13	1:F:563:ALA:HB2	1.92	0.51
1:F:584:HIS:NE2	1:F:635:ASP:OD2	2.43	0.51
1:F:214:LYS:NZ	4:I:73:ASP:OD2	2.38	0.51
8:F:710:HEO:H272	2:G:55:VAL:HG22	1.94	0.50
3:H:113:ILE:HD11	3:H:150:VAL:HB	1.93	0.50
4:I:35:MET:SD	4:I:49:THR:HG21	2.52	0.50
1:F:397:THR:HG21	1:F:472:TYR:CE1	2.46	0.50
4:I:32:PRO:HB3	4:I:50:ILE:HG22	1.94	0.49
1:F:407:ASP:OD1	8:F:710:HEO:O2A	2.30	0.49
1:F:423:VAL:HG21	8:F:710:HEO:C4C	2.43	0.49
1:F:151:VAL:HG22	1:F:600:THR:OG1	2.14	0.48
4:I:21:GLY:O	4:I:25:SER:OG	2.26	0.48
1:F:352:THR:O	1:F:355:ILE:HG22	2.14	0.48
1:F:310:LEU:HD21	1:F:316:LEU:CD1	2.44	0.47
1:F:288:TYR:HA	1:F:291:ILE:HG22	1.96	0.47
1:F:100:ASP:HA	1:F:103:PHE:CE2	2.49	0.47
3:H:46:THR:HG23	13:H:426:HOH:O	2.13	0.47
1:F:599:SER:HB2	1:F:621:MET:HE3	1.96	0.47
1:F:248:VAL:CG2	3:H:39:LEU:HG	2.45	0.47
1:F:12:PHE:HD1	1:F:18:MET:HE2	1.79	0.46
1:F:243:PHE:N	1:F:244:PRO:HD2	2.31	0.46
1:F:621:MET:HE1	7:F:709:3PE:H2C1	1.97	0.46
3:H:41:SER:HB2	4:I:88:ILE:HG23	1.97	0.46
2:G:225:THR:HB	2:G:230:ALA:HB3	1.96	0.46
1:F:164:GLU:N	1:F:164:GLU:OE1	2.49	0.46
1:F:411:HIS:NE2	2:G:184:TYR:OH	2.34	0.45
1:F:162:VAL:HG12	1:F:608:TRP:CZ2	2.51	0.45
1:F:195:GLN:HG2	1:F:250:VAL:HG11	1.97	0.45
2:G:89:GLU:HA	2:G:92:VAL:HG22	1.99	0.44
1:F:263:PHE:HZ	3:H:141:ALA:HB2	1.83	0.44
1:F:396:MET:HG3	2:G:51:MET:HB3	2.00	0.44
1:F:355:ILE:HG12	1:F:355:ILE:O	2.18	0.43
1:F:590:GLY:O	1:F:593:ILE:HG22	2.18	0.43
1:F:284:HIS:O	1:F:287:VAL:HG22	2.18	0.43
1:F:98[B]:HIS:NE2	5:F:701:UQ8:H3MA	2.34	0.43
1:F:332:LEU:HB3	1:F:348:PHE:CG	2.54	0.43
1:F:20:THR:CG2	5:F:701:UQ8:H8	2.49	0.43
2:G:171:MET:HE1	2:G:184:TYR:CE2	2.54	0.42
3:H:195:PHE:C	3:H:195:PHE:CD1	2.97	0.42
2:G:35:GLN:O	2:G:39:GLU:HG3	2.20	0.42
1:F:522:ASP:O	1:F:526:ASN:ND2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:15:VAL:O	4:I:19:MET:HG2	2.19	0.42
1:F:399:VAL:HB	2:G:51:MET:SD	2.60	0.41
1:F:400:LEU:HB2	2:G:51:MET:HE1	2.02	0.41
1:F:440:TRP:CD2	1:F:448:LEU:HD21	2.54	0.41
2:G:281:PHE:O	2:G:282:MET:HE2	2.19	0.41
1:F:488:ASP:OD2	1:F:490:GLN:CG	2.68	0.41
1:F:426:GLY:O	1:F:430:PHE:HB2	2.20	0.41
10:F:712:CDL:H392	2:G:97:ILE:HD11	2.02	0.41
1:F:440:TRP:N	1:F:441:PRO:HD2	2.35	0.41
1:F:488:ASP:OD2	1:F:490:GLN:HG2	2.21	0.41
6:F:706:LHG:H222	7:F:709:3PE:H2F2	2.03	0.41
1:F:436:MET:HE3	13:F:935:HOH:O	2.22	0.40
1:F:422:ASN:HA	1:F:464:PHE:CE1	2.56	0.40
1:F:550:TYR:O	1:F:551:ASN:HB2	2.21	0.40
4:I:19:MET:HE3	4:I:19:MET:HA	2.03	0.40
1:F:78:MET:HE2	1:F:94:LEU:HD21	2.02	0.40
1:F:536:GLY:O	1:F:568:LYS:NZ	2.51	0.40
1:F:437:THR:HA	1:F:448:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	663/663 (100%)	654 (99%)	9 (1%)	0	100	100
2	G	260/315 (82%)	255 (98%)	5 (2%)	0	100	100
3	H	182/204 (89%)	180 (99%)	2 (1%)	0	100	100
4	I	98/109 (90%)	98 (100%)	0	0	100	100
All	All	1203/1291 (93%)	1187 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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	F	543/547 (99%)	539 (99%)	4 (1%)	81 90
2	G	208/262 (79%)	204 (98%)	4 (2%)	52 67
3	H	148/166 (89%)	146 (99%)	2 (1%)	62 77
4	I	86/94 (92%)	86 (100%)	0	100 100
All	All	985/1069 (92%)	975 (99%)	10 (1%)	71 84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	124	ASN
1	F	488	ASP
1	F	593	ILE
1	F	599	SER
2	G	84	HIS
2	G	103	LEU
2	G	171	MET
2	G	270	LYS
3	H	80	SER
3	H	195	PHE

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

Mol	Chain	Res	Type
1	F	378	HIS
1	F	557	HIS
2	G	35	GLN
2	G	268	ASN
3	H	126	ASN
4	I	77	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
7	3PE	H	303	-	50,50,50	0.93	4 (8%)	53,55,55	1.08	3 (5%)
6	LHG	H	301	-	48,48,48	0.28	0	51,54,54	0.44	0
6	LHG	F	705	-	48,48,48	0.31	0	51,54,54	0.38	0
6	LHG	F	703	-	42,42,48	0.31	0	45,48,54	0.32	0
6	LHG	F	704	-	48,48,48	0.28	0	51,54,54	0.45	0
8	HEO	F	710	13,1	63,66,66	1.60	12 (19%)	73,102,102	2.05	18 (24%)
6	LHG	F	706	-	42,42,48	0.31	0	45,48,54	0.34	0
10	CDL	F	712	-	99,99,99	1.32	11 (11%)	105,111,111	1.14	6 (5%)
9	HEM	F	711	1	42,50,50	2.01	12 (28%)	46,82,82	2.27	15 (32%)
7	3PE	F	709	-	45,45,50	0.98	4 (8%)	48,50,55	1.13	3 (6%)
6	LHG	F	702	-	40,40,48	1.23	4 (10%)	43,46,54	1.17	3 (6%)
6	LHG	F	707	-	48,48,48	0.30	0	51,54,54	0.48	0
5	UQ8	F	701	-	53,53,53	3.51	13 (24%)	66,67,67	2.65	24 (36%)
6	LHG	H	302	-	48,48,48	0.27	0	51,54,54	0.33	0
6	LHG	F	708	-	48,48,48	0.28	0	51,54,54	0.41	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
7	3PE	H	303	-	-	20/54/54/54	-
6	LHG	H	301	-	-	24/53/53/53	-
6	LHG	F	705	-	-	18/53/53/53	-
6	LHG	F	703	-	-	21/47/47/53	-
6	LHG	F	704	-	-	25/53/53/53	-
8	HEO	F	710	13,1	3/3/25/25	7/32/114/114	-
6	LHG	F	706	-	-	20/47/47/53	-
10	CDL	F	712	-	-	65/110/110/110	-
9	HEM	F	711	1	-	4/12/54/54	-
7	3PE	F	709	-	-	23/49/49/54	-
6	LHG	F	702	-	-	17/45/45/53	-
6	LHG	F	707	-	-	21/53/53/53	-
5	UQ8	F	701	-	-	28/51/75/75	0/1/1/1
6	LHG	H	302	-	-	28/53/53/53	-
6	LHG	F	708	-	-	23/53/53/53	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	701	UQ8	C8-C9	8.83	1.53	1.33
5	F	701	UQ8	C38-C39	8.82	1.53	1.33
5	F	701	UQ8	C33-C34	8.78	1.53	1.33
5	F	701	UQ8	C13-C14	8.75	1.53	1.33
5	F	701	UQ8	C28-C29	8.75	1.53	1.33
5	F	701	UQ8	C23-C24	8.73	1.53	1.33
5	F	701	UQ8	C18-C19	8.65	1.53	1.33
5	F	701	UQ8	C43-C44	6.98	1.53	1.32
9	F	711	HEM	C1B-NB	-5.61	1.30	1.40
8	F	710	HEO	C4C-NC	4.69	1.45	1.36
8	F	710	HEO	FE-NA	4.63	2.13	1.95
8	F	710	HEO	C1B-NB	4.56	1.47	1.38
9	F	711	HEM	O2D-CGD	-4.34	1.16	1.30
9	F	711	HEM	C4D-ND	-4.18	1.33	1.40
9	F	711	HEM	C1D-ND	-3.92	1.31	1.38
8	F	710	HEO	C1C-NC	3.83	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	711	HEM	O2A-CGA	-3.83	1.18	1.30
8	F	710	HEO	C1A-NA	3.52	1.46	1.39
10	F	712	CDL	OA8-CA7	3.35	1.43	1.33
8	F	710	HEO	C4A-NA	3.29	1.45	1.39
8	F	710	HEO	C1D-ND	3.21	1.45	1.40
10	F	712	CDL	OB6-CB5	3.15	1.43	1.34
10	F	712	CDL	OA6-CA5	3.12	1.43	1.34
10	F	712	CDL	OB8-CB7	3.00	1.42	1.33
8	F	710	HEO	FE-NB	2.98	2.15	1.98
9	F	711	HEM	C3C-C4C	-2.85	1.37	1.41
9	F	711	HEM	C4B-NB	-2.73	1.33	1.38
8	F	710	HEO	FE-ND	2.73	2.14	1.98
7	F	709	3PE	O21-C2	-2.64	1.40	1.46
9	F	711	HEM	FE-NB	2.63	2.12	1.98
6	F	702	LHG	O7-C7	2.63	1.41	1.34
9	F	711	HEM	C1B-C2B	-2.56	1.39	1.44
7	H	303	3PE	O21-C2	-2.53	1.40	1.46
10	F	712	CDL	OA6-CA4	-2.52	1.40	1.46
8	F	710	HEO	C4B-C3B	2.48	1.49	1.44
5	F	701	UQ8	O4-C4M	-2.46	1.39	1.45
10	F	712	CDL	OB6-CB4	-2.45	1.40	1.46
7	H	303	3PE	O31-C3	-2.39	1.39	1.45
7	F	709	3PE	O31-C3	-2.37	1.39	1.45
8	F	710	HEO	C4D-ND	2.36	1.43	1.38
7	H	303	3PE	O31-C31	2.33	1.40	1.33
6	F	702	LHG	O7-C5	-2.32	1.41	1.46
5	F	701	UQ8	O3-C3M	-2.29	1.40	1.45
6	F	702	LHG	O8-C23	2.26	1.39	1.33
7	F	709	3PE	O31-C31	2.26	1.39	1.33
9	F	711	HEM	C3D-C2D	-2.22	1.32	1.36
5	F	701	UQ8	C6-C5	2.22	1.52	1.46
9	F	711	HEM	C2C-C1C	-2.20	1.37	1.42
10	F	712	CDL	PA1-OA5	2.18	1.67	1.59
10	F	712	CDL	PB2-OB5	2.15	1.67	1.59
10	F	712	CDL	PB2-OB2	2.14	1.67	1.59
5	F	701	UQ8	O2-C2	-2.14	1.18	1.23
10	F	712	CDL	PA1-OA2	2.13	1.67	1.59
6	F	702	LHG	O8-C6	-2.12	1.40	1.45
7	H	303	3PE	O21-C21	2.12	1.40	1.34
9	F	711	HEM	CBD-CGD	-2.06	1.45	1.50
8	F	710	HEO	FE-NC	2.05	2.13	1.96
7	F	709	3PE	P-O12	-2.04	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	701	UQ8	O5-C5	-2.02	1.18	1.23
10	F	712	CDL	PA1-OA4	-2.01	1.46	1.55

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	701	UQ8	C7-C8-C9	-7.61	113.71	126.83
8	F	710	HEO	C3B-C4B-NB	-7.06	101.73	109.84
5	F	701	UQ8	C17-C18-C19	-6.78	112.09	127.62
8	F	710	HEO	C2A-C1A-NA	-6.66	103.90	110.32
5	F	701	UQ8	C12-C13-C14	-6.52	112.70	127.62
5	F	701	UQ8	C32-C33-C34	-6.26	113.30	127.62
5	F	701	UQ8	C22-C23-C24	-6.24	113.33	127.62
5	F	701	UQ8	C27-C28-C29	-6.15	113.55	127.62
5	F	701	UQ8	C37-C38-C39	-5.90	114.11	127.62
9	F	711	HEM	C3B-C4B-NB	-5.90	105.23	109.47
9	F	711	HEM	C1B-NB-C4B	5.27	111.45	105.21
8	F	710	HEO	C3C-C4C-NC	-4.73	103.10	109.21
9	F	711	HEM	CBA-CAA-C2A	-4.69	104.65	112.54
8	F	710	HEO	CHA-C1A-NA	4.64	129.51	124.45
8	F	710	HEO	C4B-NB-C1B	4.52	110.55	105.21
9	F	711	HEM	O2D-CGD-O1D	-4.44	111.92	123.33
5	F	701	UQ8	C42-C43-C44	-4.35	113.14	127.64
9	F	711	HEM	CHC-C4B-NB	4.34	129.10	124.44
6	F	702	LHG	O7-C7-C8	4.28	120.74	111.48
8	F	710	HEO	C3D-C4D-ND	-4.09	106.40	110.35
7	F	709	3PE	O21-C21-C22	4.05	120.24	111.48
10	F	712	CDL	OA6-CA5-C11	3.97	120.07	111.48
10	F	712	CDL	OB6-CB5-C51	3.89	119.91	111.48
8	F	710	HEO	C4B-C3B-C2B	3.83	113.87	107.44
9	F	711	HEM	O2A-CGA-O1A	-3.79	113.59	123.33
7	H	303	3PE	O21-C21-C22	3.69	119.45	111.48
5	F	701	UQ8	C35-C34-C33	-3.54	114.53	123.63
8	F	710	HEO	C2D-C1D-ND	-3.37	105.97	109.84
9	F	711	HEM	CHB-C1B-NB	3.23	128.38	124.37
5	F	701	UQ8	C25-C24-C23	-3.11	115.64	123.63
9	F	711	HEM	CHA-C4D-ND	3.10	128.22	124.37
9	F	711	HEM	CMA-C3A-C4A	-3.07	123.95	128.46
5	F	701	UQ8	C15-C14-C13	-3.01	115.89	123.63
5	F	701	UQ8	C40-C39-C38	-3.00	115.93	123.63
5	F	701	UQ8	C30-C29-C28	-2.99	115.95	123.63
8	F	710	HEO	C4A-NA-C1A	2.97	110.67	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	701	UQ8	C36-C34-C33	-2.96	114.51	121.17
8	F	710	HEO	C1A-C2A-C3A	2.94	110.98	107.11
8	F	710	HEO	C1D-ND-C4D	2.90	108.64	105.21
8	F	710	HEO	C2B-C1B-NB	-2.83	106.63	109.90
8	F	710	HEO	C3A-C4A-NA	-2.81	104.44	109.64
9	F	711	HEM	CHD-C1D-ND	2.67	127.30	124.44
7	F	709	3PE	O31-C31-C32	2.65	119.93	111.83
6	F	702	LHG	O8-C23-C24	2.57	119.69	111.83
10	F	712	CDL	OA8-CA7-C31	2.57	119.68	111.83
8	F	710	HEO	CHC-C4B-NB	2.56	127.55	124.37
10	F	712	CDL	OB8-CB7-C71	2.56	119.63	111.83
8	F	710	HEO	C1D-C2D-C3D	2.54	109.65	106.98
5	F	701	UQ8	C10-C9-C8	-2.52	117.15	123.63
7	H	303	3PE	O12-P-O14	-2.51	100.77	112.44
5	F	701	UQ8	C20-C19-C18	-2.49	117.23	123.63
7	H	303	3PE	O31-C31-C32	2.45	119.30	111.83
9	F	711	HEM	CAD-CBD-CGD	-2.41	107.27	113.67
6	F	702	LHG	O4-P-O5	-2.40	101.28	112.44
7	F	709	3PE	O12-P-O14	-2.37	101.44	112.44
5	F	701	UQ8	C41-C39-C38	-2.36	115.86	121.17
10	F	712	CDL	OB4-PB2-OB3	-2.35	101.52	112.44
10	F	712	CDL	OA4-PA1-OA3	-2.35	101.53	112.44
5	F	701	UQ8	C45-C44-C43	-2.30	115.75	122.66
9	F	711	HEM	O2D-CGD-CBD	2.29	121.24	114.00
5	F	701	UQ8	C46-C44-C43	-2.29	115.79	122.66
8	F	710	HEO	O11-C11-C12	-2.27	103.11	109.14
5	F	701	UQ8	C16-C14-C13	-2.25	116.12	121.17
5	F	701	UQ8	C10-C9-C11	2.25	119.12	115.23
5	F	701	UQ8	C4-C3-C2	-2.24	116.58	120.69
5	F	701	UQ8	C26-C24-C23	-2.24	116.14	121.17
9	F	711	HEM	O2A-CGA-CBA	2.19	120.92	114.00
9	F	711	HEM	CMC-C2C-C3C	2.12	128.93	124.68
8	F	710	HEO	CHB-C4A-NA	2.11	126.75	124.45
5	F	701	UQ8	C31-C29-C28	-2.06	116.54	121.17
8	F	710	HEO	C4A-C3A-C2A	2.04	110.00	106.97
9	F	711	HEM	CHD-C1D-C2D	-2.03	121.82	125.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	710	HEO	NA
8	F	710	HEO	NB

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Mol	Chain	Res	Type	Atom
8	F	710	HEO	ND

All (344) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	701	UQ8	C42-C43-C44-C45
5	F	701	UQ8	C37-C38-C39-C40
5	F	701	UQ8	C29-C31-C32-C33
5	F	701	UQ8	C17-C18-C19-C20
5	F	701	UQ8	C12-C13-C14-C16
5	F	701	UQ8	C12-C13-C14-C15
5	F	701	UQ8	C7-C8-C9-C10
6	F	702	LHG	C3-O3-P-O4
6	F	702	LHG	C3-O3-P-O5
6	F	702	LHG	C3-O3-P-O6
6	F	702	LHG	C8-C7-O7-C5
6	F	703	LHG	C1-C2-C3-O3
6	F	703	LHG	C4-O6-P-O3
6	F	703	LHG	C4-O6-P-O4
6	F	704	LHG	C3-O3-P-O4
6	F	704	LHG	C3-O3-P-O6
6	F	704	LHG	O7-C5-C6-O8
6	F	705	LHG	C8-C7-O7-C5
6	F	707	LHG	O1-C1-C2-C3
6	H	301	LHG	O1-C1-C2-C3
6	H	301	LHG	C3-O3-P-O4
6	H	301	LHG	C3-O3-P-O6
6	H	301	LHG	C8-C7-O7-C5
6	H	302	LHG	C3-O3-P-O4
6	H	302	LHG	C3-O3-P-O6
6	H	302	LHG	C4-O6-P-O5
7	F	709	3PE	C11-O13-P-O14
10	F	712	CDL	O1-C1-CB2-OB2
10	F	712	CDL	CA3-OA5-PA1-OA2
10	F	712	CDL	CA3-OA5-PA1-OA4
10	F	712	CDL	CA6-CA4-OA6-CA5
10	F	712	CDL	C11-CA5-OA6-CA4
10	F	712	CDL	CB2-OB2-PB2-OB3
10	F	712	CDL	C71-CB7-OB8-CB6
6	F	708	LHG	O10-C23-O8-C6
10	F	712	CDL	OA9-CA7-OA8-CA6
10	F	712	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
6	F	702	LHG	O9-C7-O7-C5
6	F	705	LHG	O9-C7-O7-C5
6	F	706	LHG	O9-C7-O7-C5
6	H	301	LHG	O9-C7-O7-C5
10	F	712	CDL	OA7-CA5-OA6-CA4
6	F	704	LHG	C24-C23-O8-C6
6	F	706	LHG	C24-C23-O8-C6
6	F	708	LHG	C24-C23-O8-C6
6	F	706	LHG	C8-C7-O7-C5
5	F	701	UQ8	C12-C11-C9-C10
6	F	705	LHG	O10-C23-O8-C6
6	F	707	LHG	C24-C23-O8-C6
10	F	712	CDL	C31-CA7-OA8-CA6
5	F	701	UQ8	C32-C33-C34-C35
5	F	701	UQ8	C27-C28-C29-C30
5	F	701	UQ8	C22-C23-C24-C25
5	F	701	UQ8	C17-C18-C19-C21
5	F	701	UQ8	C7-C8-C9-C11
6	F	707	LHG	O10-C23-O8-C6
6	F	703	LHG	O2-C2-C3-O3
6	F	705	LHG	C24-C23-O8-C6
6	F	704	LHG	O10-C23-O8-C6
6	F	706	LHG	O10-C23-O8-C6
6	F	703	LHG	C8-C7-O7-C5
10	F	712	CDL	C51-CB5-OB6-CB4
5	F	701	UQ8	C33-C34-C36-C37
5	F	701	UQ8	C34-C36-C37-C38
5	F	701	UQ8	C24-C26-C27-C28
5	F	701	UQ8	C14-C16-C17-C18
6	F	703	LHG	C24-C23-O8-C6
6	H	302	LHG	C24-C23-O8-C6
7	H	303	3PE	C32-C31-O31-C3
6	H	302	LHG	O10-C23-O8-C6
6	F	703	LHG	O9-C7-O7-C5
10	F	712	CDL	CA2-C1-CB2-OB2
6	H	301	LHG	C24-C23-O8-C6
6	H	301	LHG	O10-C23-O8-C6
6	F	704	LHG	C8-C7-O7-C5
6	F	707	LHG	O1-C1-C2-O2
10	F	712	CDL	OB7-CB5-OB6-CB4
6	F	707	LHG	C23-C24-C25-C26
6	F	708	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
10	F	712	CDL	CA7-C31-C32-C33
6	F	703	LHG	O10-C23-O8-C6
7	H	303	3PE	O32-C31-O31-C3
6	F	704	LHG	O9-C7-O7-C5
6	F	702	LHG	C24-C23-O8-C6
7	F	709	3PE	C32-C31-O31-C3
6	F	704	LHG	O2-C2-C3-O3
6	H	302	LHG	C7-C8-C9-C10
10	F	712	CDL	C78-C79-C80-C81
6	F	702	LHG	C11-C12-C13-C14
6	F	704	LHG	C12-C13-C14-C15
6	F	704	LHG	C16-C17-C18-C19
10	F	712	CDL	C51-C52-C53-C54
6	F	702	LHG	O10-C23-O8-C6
6	F	706	LHG	C11-C12-C13-C14
6	H	301	LHG	O1-C1-C2-O2
10	F	712	CDL	C15-C16-C17-C18
6	F	708	LHG	C8-C7-O7-C5
6	F	704	LHG	C31-C32-C33-C34
6	F	708	LHG	C18-C19-C20-C21
7	F	709	3PE	O32-C31-O31-C3
10	F	712	CDL	C60-C61-C62-C63
7	F	709	3PE	C38-C39-C3A-C3B
7	F	709	3PE	C29-C2A-C2B-C2C
6	F	704	LHG	C1-C2-C3-O3
6	F	708	LHG	C10-C11-C12-C13
6	F	702	LHG	C12-C13-C14-C15
7	F	709	3PE	C31-C32-C33-C34
6	H	302	LHG	C31-C32-C33-C34
6	F	706	LHG	C26-C27-C28-C29
7	F	709	3PE	C27-C28-C29-C2A
6	F	707	LHG	O9-C7-O7-C5
6	F	708	LHG	O9-C7-O7-C5
6	F	703	LHG	C15-C16-C17-C18
6	H	301	LHG	C30-C31-C32-C33
5	F	701	UQ8	C37-C38-C39-C41
6	F	708	LHG	C34-C35-C36-C37
6	F	708	LHG	C28-C29-C30-C31
5	F	701	UQ8	C42-C43-C44-C46
6	F	707	LHG	C8-C7-O7-C5
6	H	302	LHG	C8-C7-O7-C5
10	F	712	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
6	H	302	LHG	O9-C7-O7-C5
6	H	301	LHG	C26-C27-C28-C29
7	H	303	3PE	C32-C33-C34-C35
7	F	709	3PE	C26-C27-C28-C29
7	F	709	3PE	C2B-C2C-C2D-C2E
6	H	301	LHG	C7-C8-C9-C10
6	F	703	LHG	C10-C11-C12-C13
6	F	704	LHG	C10-C11-C12-C13
6	F	706	LHG	C16-C17-C18-C19
6	F	703	LHG	C28-C29-C30-C31
6	F	702	LHG	C13-C14-C15-C16
6	F	705	LHG	C27-C28-C29-C30
6	H	302	LHG	C30-C31-C32-C33
6	F	708	LHG	C16-C17-C18-C19
6	F	706	LHG	C13-C14-C15-C16
7	F	709	3PE	C22-C23-C24-C25
6	F	705	LHG	O6-C4-C5-C6
6	F	704	LHG	C28-C29-C30-C31
5	F	701	UQ8	C38-C39-C41-C42
6	H	301	LHG	C33-C34-C35-C36
6	H	302	LHG	C27-C28-C29-C30
6	F	705	LHG	C25-C26-C27-C28
6	H	302	LHG	C4-C5-C6-O8
6	F	703	LHG	C24-C25-C26-C27
10	F	712	CDL	C12-C13-C14-C15
10	F	712	CDL	C62-C63-C64-C65
6	F	708	LHG	C24-C25-C26-C27
6	F	702	LHG	C27-C28-C29-C30
6	F	702	LHG	O6-C4-C5-O7
6	H	302	LHG	C16-C17-C18-C19
6	F	708	LHG	C11-C12-C13-C14
10	F	712	CDL	C36-C37-C38-C39
6	H	301	LHG	C24-C25-C26-C27
10	F	712	CDL	C76-C77-C78-C79
6	H	302	LHG	C18-C19-C20-C21
7	H	303	3PE	C2C-C2D-C2E-C2F
10	F	712	CDL	C81-C82-C83-C84
10	F	712	CDL	C16-C17-C18-C19
6	F	703	LHG	C7-C8-C9-C10
7	F	709	3PE	C23-C24-C25-C26
6	F	707	LHG	C32-C33-C34-C35
6	H	302	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
8	F	710	HEO	C17-C18-C19-C20
10	F	712	CDL	C41-C42-C43-C44
10	F	712	CDL	OB5-CB3-CB4-CB6
6	F	706	LHG	C24-C25-C26-C27
6	F	703	LHG	C4-C5-C6-O8
6	F	704	LHG	C7-C8-C9-C10
8	F	710	HEO	C27-C19-C20-C21
6	H	301	LHG	C28-C29-C30-C31
6	H	302	LHG	C11-C12-C13-C14
6	F	705	LHG	C13-C14-C15-C16
10	F	712	CDL	C14-C15-C16-C17
10	F	712	CDL	C44-C45-C46-C47
6	F	707	LHG	C7-C8-C9-C10
10	F	712	CDL	C56-C57-C58-C59
6	F	703	LHG	C12-C13-C14-C15
6	F	708	LHG	C15-C16-C17-C18
7	F	709	3PE	C22-C21-O21-C2
6	F	702	LHG	C9-C10-C11-C12
6	F	705	LHG	C14-C15-C16-C17
6	H	302	LHG	C28-C29-C30-C31
7	H	303	3PE	C36-C37-C38-C39
6	H	301	LHG	C1-C2-C3-O3
6	H	302	LHG	C34-C35-C36-C37
6	F	708	LHG	O6-C4-C5-C6
10	F	712	CDL	OA5-CA3-CA4-CA6
10	F	712	CDL	C13-C14-C15-C16
10	F	712	CDL	C72-C73-C74-C75
7	H	303	3PE	C3E-C3F-C3G-C3H
6	F	705	LHG	C19-C20-C21-C22
7	H	303	3PE	C26-C27-C28-C29
6	F	707	LHG	C26-C27-C28-C29
6	F	707	LHG	O6-C4-C5-O7
6	F	708	LHG	O6-C4-C5-O7
10	F	712	CDL	OA5-CA3-CA4-OA6
10	F	712	CDL	OB5-CB3-CB4-OB6
6	F	707	LHG	C15-C16-C17-C18
6	F	704	LHG	C4-C5-C6-O8
7	F	709	3PE	C1-C2-C3-O31
10	F	712	CDL	C55-C56-C57-C58
6	F	707	LHG	C14-C15-C16-C17
6	H	302	LHG	O7-C5-C6-O8
7	F	709	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
7	F	709	3PE	C35-C36-C37-C38
10	F	712	CDL	C22-C23-C24-C25
7	H	303	3PE	C29-C2A-C2B-C2C
8	F	710	HEO	C18-C19-C20-C21
10	F	712	CDL	C34-C35-C36-C37
7	F	709	3PE	O22-C21-O21-C2
6	F	708	LHG	C31-C32-C33-C34
7	F	709	3PE	C2C-C2D-C2E-C2F
6	F	704	LHG	C24-C25-C26-C27
10	F	712	CDL	C43-C44-C45-C46
10	F	712	CDL	C54-C55-C56-C57
6	F	705	LHG	O6-C4-C5-O7
6	F	703	LHG	C13-C14-C15-C16
6	F	703	LHG	O7-C5-C6-O8
6	F	708	LHG	O7-C5-C6-O8
10	F	712	CDL	C18-C19-C20-C21
6	F	704	LHG	C19-C20-C21-C22
6	H	302	LHG	C32-C33-C34-C35
6	F	704	LHG	C11-C10-C9-C8
6	H	301	LHG	C15-C16-C17-C18
7	F	709	3PE	C32-C33-C34-C35
6	F	702	LHG	C4-O6-P-O5
6	F	704	LHG	C3-O3-P-O5
6	F	705	LHG	C3-O3-P-O5
6	H	301	LHG	C3-O3-P-O5
6	H	302	LHG	C4-O6-P-O3
7	H	303	3PE	C11-O13-P-O12
10	F	712	CDL	CA3-OA5-PA1-OA3
10	F	712	CDL	CB3-OB5-PB2-OB2
10	F	712	CDL	CB3-OB5-PB2-OB4
6	F	702	LHG	C16-C17-C18-C19
7	F	709	3PE	C37-C38-C39-C3A
6	F	707	LHG	C4-C5-O7-C7
6	F	702	LHG	O6-C4-C5-C6
6	H	302	LHG	C26-C27-C28-C29
8	F	710	HEO	C4D-C3D-CAD-CBD
6	F	707	LHG	C18-C19-C20-C21
6	F	705	LHG	C16-C17-C18-C19
5	F	701	UQ8	C23-C24-C26-C27
6	F	703	LHG	C29-C30-C31-C32
6	F	704	LHG	C23-C24-C25-C26
6	F	706	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
10	F	712	CDL	C58-C59-C60-C61
10	F	712	CDL	C83-C84-C85-C86
6	F	708	LHG	C4-C5-C6-O8
6	F	705	LHG	C35-C36-C37-C38
10	F	712	CDL	C53-C54-C55-C56
6	F	703	LHG	C23-C24-C25-C26
7	H	303	3PE	C2-C1-O11-P
7	H	303	3PE	O11-C1-C2-O21
6	F	706	LHG	C12-C13-C14-C15
6	F	706	LHG	C10-C11-C12-C13
7	F	709	3PE	C2D-C2E-C2F-C2G
10	F	712	CDL	C35-C36-C37-C38
6	F	703	LHG	C25-C26-C27-C28
10	F	712	CDL	C57-C58-C59-C60
6	F	707	LHG	C30-C31-C32-C33
6	H	301	LHG	C5-C4-O6-P
10	F	712	CDL	C37-C38-C39-C40
5	F	701	UQ8	C30-C29-C31-C32
6	F	706	LHG	C9-C10-C11-C12
9	F	711	HEM	CAA-CBA-CGA-O1A
10	F	712	CDL	C31-C32-C33-C34
5	F	701	UQ8	C15-C14-C16-C17
5	F	701	UQ8	C3-C4-O4-C4M
6	F	707	LHG	C34-C35-C36-C37
7	H	303	3PE	C2D-C2E-C2F-C2G
7	H	303	3PE	C38-C39-C3A-C3B
6	F	707	LHG	C12-C13-C14-C15
8	F	710	HEO	CAD-CBD-CGD-O1D
6	H	301	LHG	C10-C11-C12-C13
6	F	704	LHG	C26-C27-C28-C29
6	H	301	LHG	C11-C12-C13-C14
9	F	711	HEM	CAA-CBA-CGA-O2A
8	F	710	HEO	CAD-CBD-CGD-O2D
6	F	702	LHG	C15-C16-C17-C18
6	F	707	LHG	C11-C12-C13-C14
6	H	302	LHG	O6-C4-C5-O7
6	F	708	LHG	C17-C18-C19-C20
10	F	712	CDL	C79-C80-C81-C82
5	F	701	UQ8	C2-C3-O3-C3M
5	F	701	UQ8	C5-C4-O4-C4M
10	F	712	CDL	C77-C78-C79-C80
6	H	302	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	F	706	LHG	C29-C30-C31-C32
7	H	303	3PE	C39-C3A-C3B-C3C
9	F	711	HEM	CAD-CBD-CGD-O2D
9	F	711	HEM	CAD-CBD-CGD-O1D
6	F	706	LHG	C23-C24-C25-C26
6	F	704	LHG	C33-C34-C35-C36
7	H	303	3PE	C27-C28-C29-C2A
6	F	705	LHG	C29-C30-C31-C32
6	F	706	LHG	C18-C19-C20-C21
6	F	707	LHG	O6-C4-C5-C6
6	H	302	LHG	C11-C10-C9-C8
6	F	704	LHG	C27-C28-C29-C30
10	F	712	CDL	C21-C22-C23-C24
6	F	708	LHG	O8-C23-C24-C25
6	H	301	LHG	O2-C2-C3-O3
10	F	712	CDL	C73-C74-C75-C76
6	F	706	LHG	O8-C23-C24-C25
10	F	712	CDL	C17-C18-C19-C20
10	F	712	CDL	C64-C65-C66-C67
6	F	703	LHG	C11-C12-C13-C14
6	F	706	LHG	O7-C7-C8-C9
7	H	303	3PE	O31-C31-C32-C33
6	H	302	LHG	C10-C11-C12-C13
10	F	712	CDL	C19-C20-C21-C22
6	F	705	LHG	C11-C10-C9-C8
7	H	303	3PE	C23-C24-C25-C26
10	F	712	CDL	C52-C51-CB5-OB6
10	F	712	CDL	C82-C83-C84-C85
10	F	712	CDL	OB6-CB4-CB6-OB8
8	F	710	HEO	C20-C21-C22-C23
6	F	705	LHG	C24-C25-C26-C27
6	F	705	LHG	C7-C8-C9-C10
7	H	303	3PE	O21-C21-C22-C23
7	F	709	3PE	C39-C3A-C3B-C3C
5	F	701	UQ8	C21-C22-C23-C24
6	H	301	LHG	C23-C24-C25-C26
6	F	708	LHG	C29-C30-C31-C32
6	H	301	LHG	C13-C14-C15-C16
5	F	701	UQ8	C6-C7-C8-C9
7	F	709	3PE	C21-C22-C23-C24
7	F	709	3PE	C2-C1-O11-P
6	F	708	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	F	708	LHG	O10-C23-C24-C25
6	H	301	LHG	C17-C18-C19-C20
6	F	706	LHG	O9-C7-C8-C9
7	H	303	3PE	O32-C31-C32-C33
10	F	712	CDL	C52-C51-CB5-OB7
6	F	704	LHG	C13-C14-C15-C16
7	H	303	3PE	O22-C21-C22-C23
6	F	706	LHG	O10-C23-C24-C25
10	F	712	CDL	C32-C31-CA7-OA8
10	F	712	CDL	C63-C64-C65-C66
6	F	707	LHG	C25-C26-C27-C28
6	H	302	LHG	O7-C7-C8-C9
6	H	302	LHG	C17-C18-C19-C20

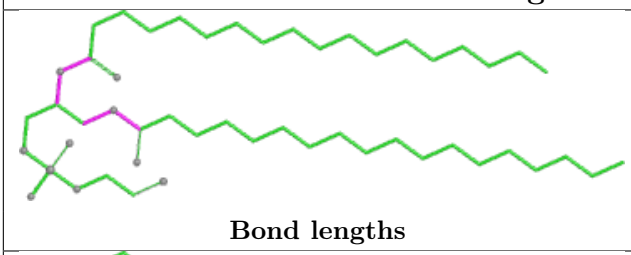
There are no ring outliers.

6 monomers are involved in 14 short contacts:

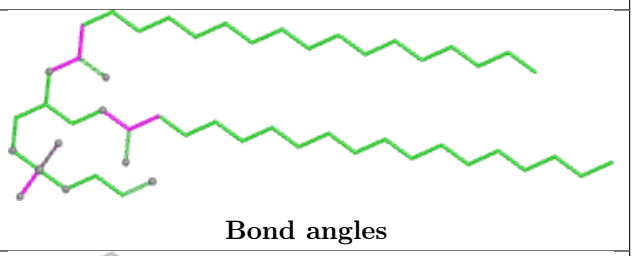
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	303	3PE	1	0
8	F	710	HEO	3	0
6	F	706	LHG	1	0
10	F	712	CDL	1	0
7	F	709	3PE	2	0
5	F	701	UQ8	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

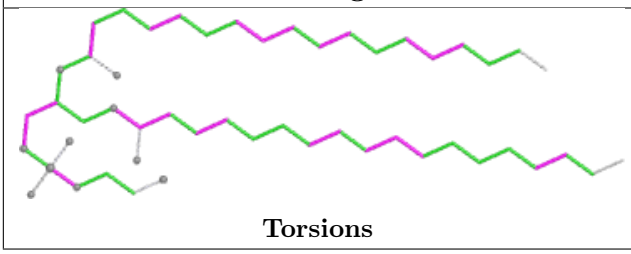
Ligand 3PE H 303



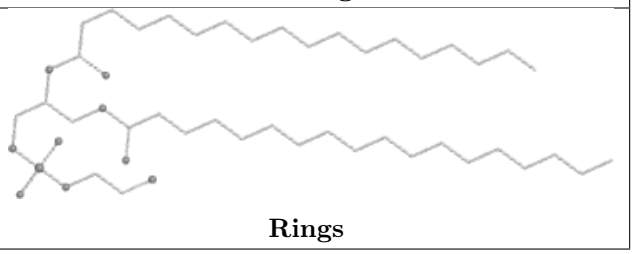
Bond lengths



Bond angles

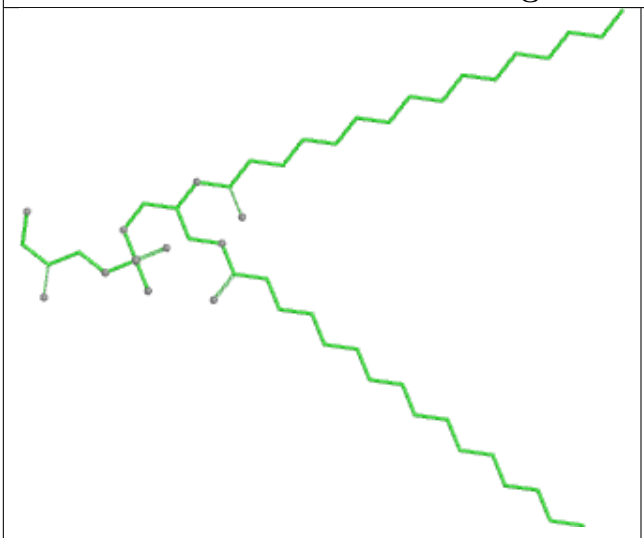


Torsions

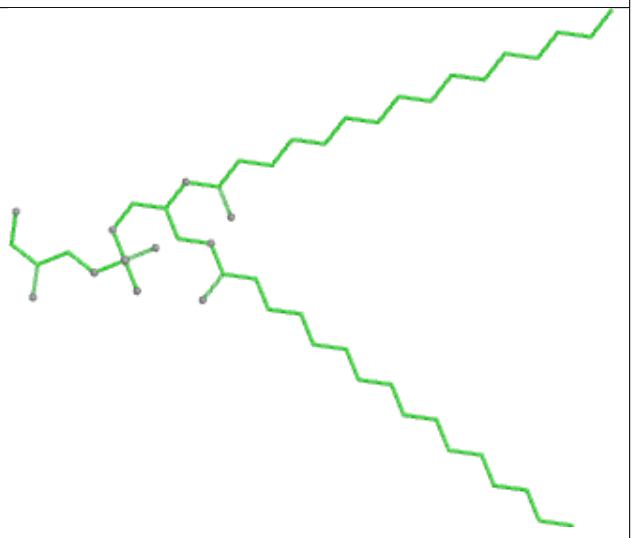


Rings

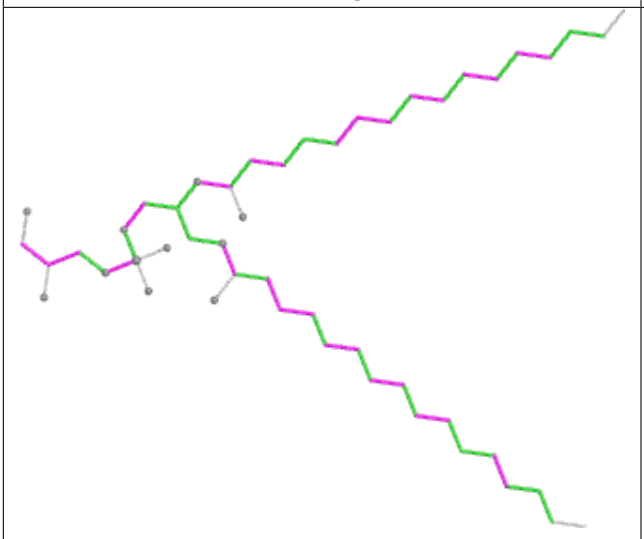
Ligand LHG H 301



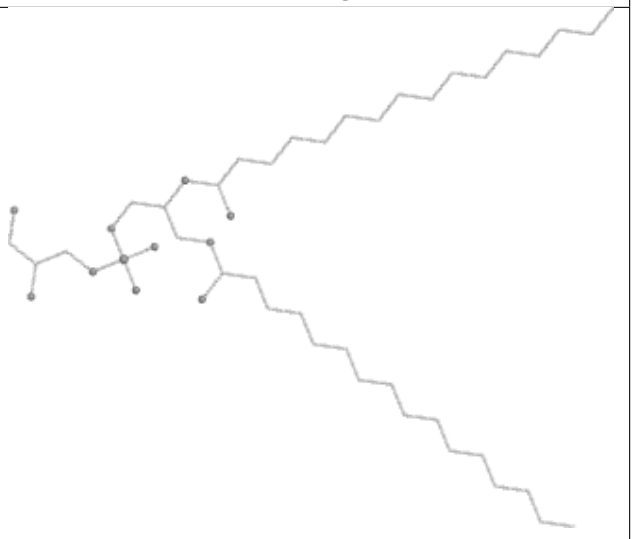
Bond lengths



Bond angles

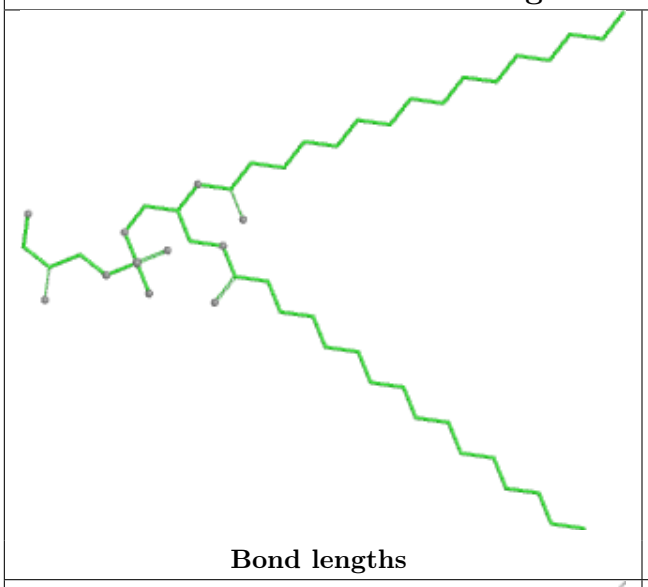


Torsions

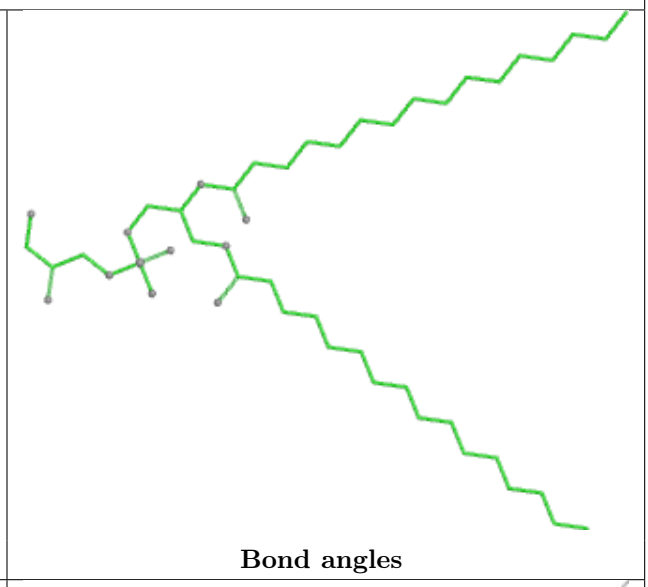


Rings

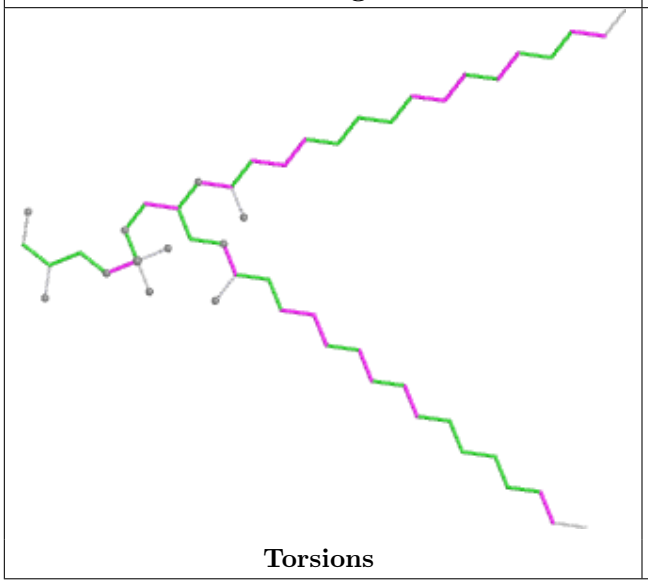
Ligand LHG F 705



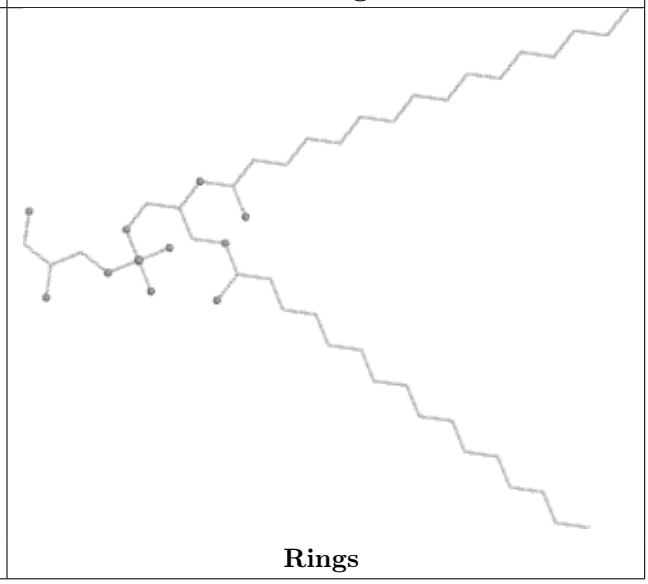
Bond lengths



Bond angles

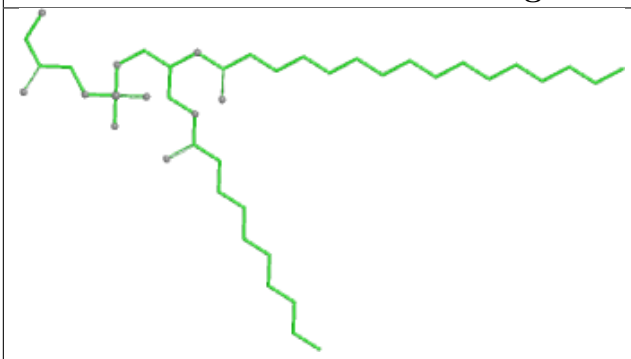


Torsions

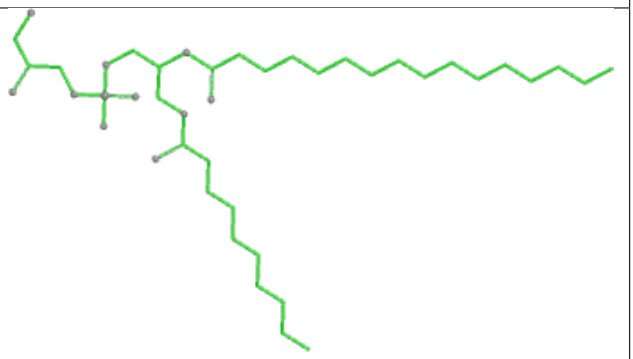


Rings

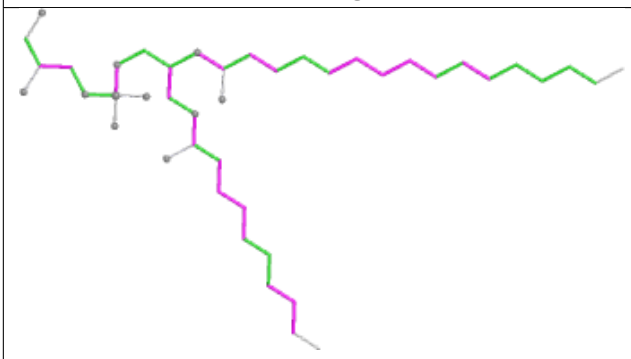
Ligand LHG F 703



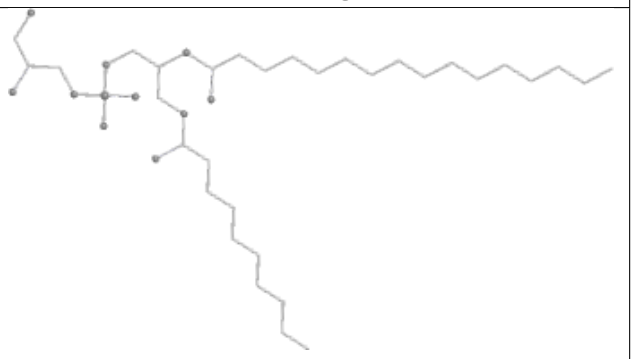
Bond lengths



Bond angles

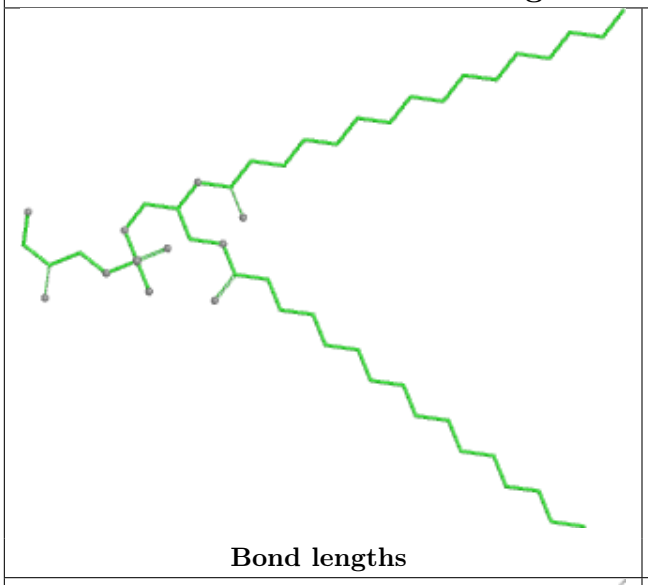


Torsions

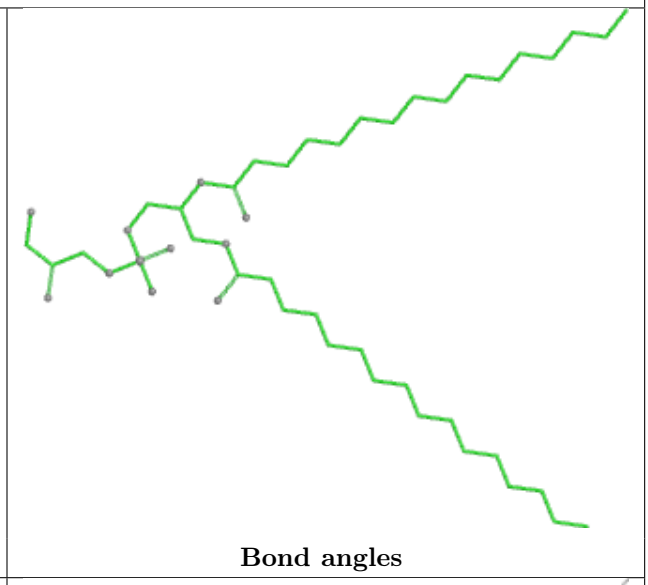


Rings

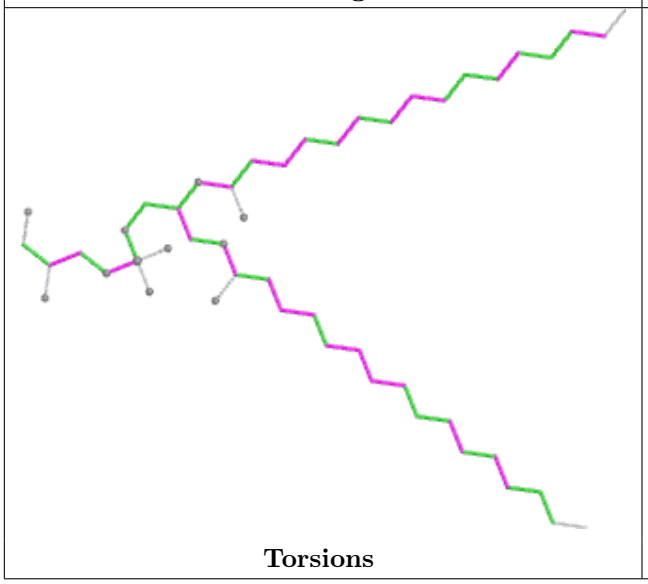
Ligand LHG F 704



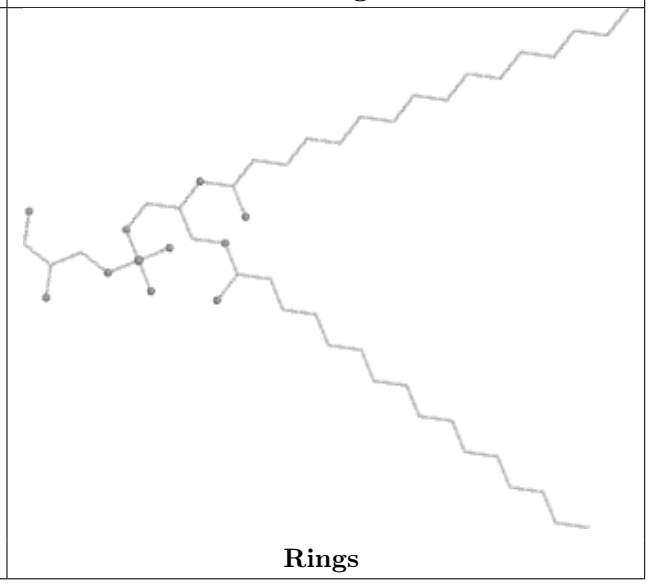
Bond lengths



Bond angles

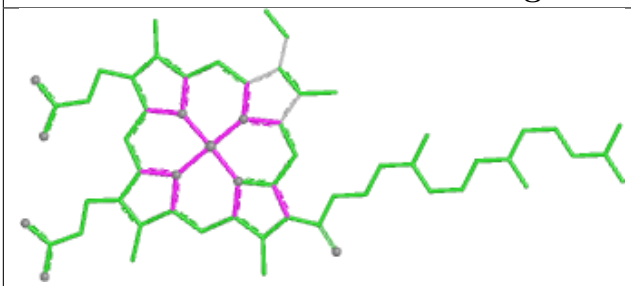


Torsions



Rings

Ligand HEO F 710



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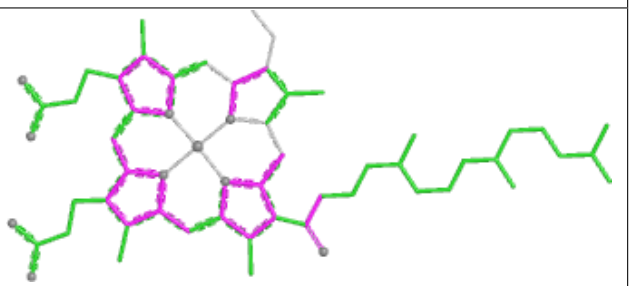
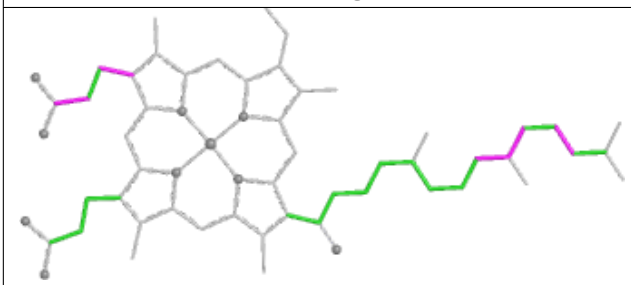
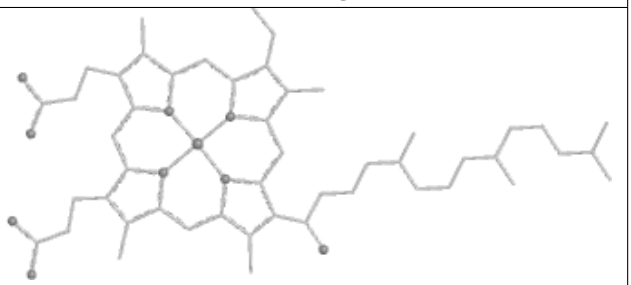


Bond angles

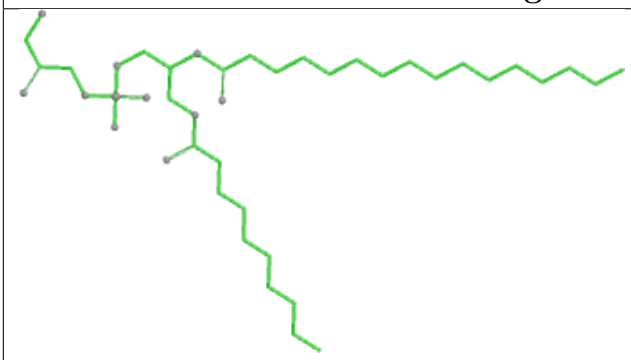


Torsions

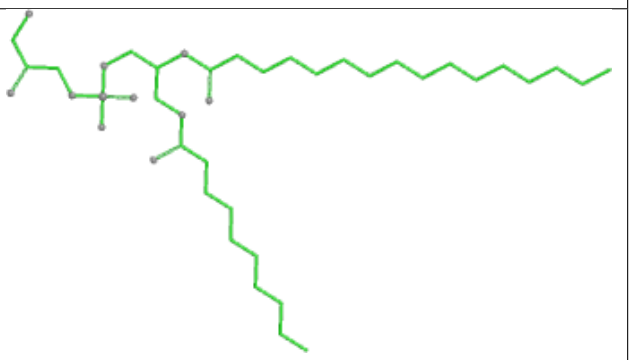


Rings

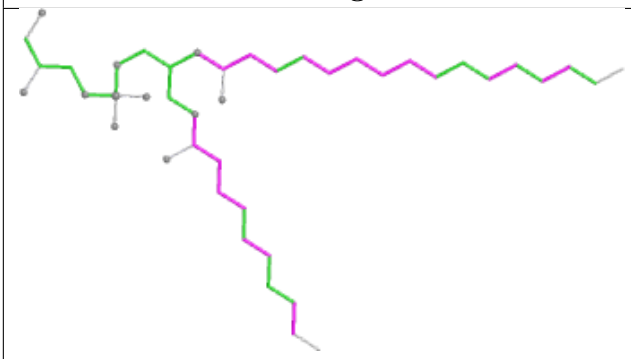
Ligand LHG F 706



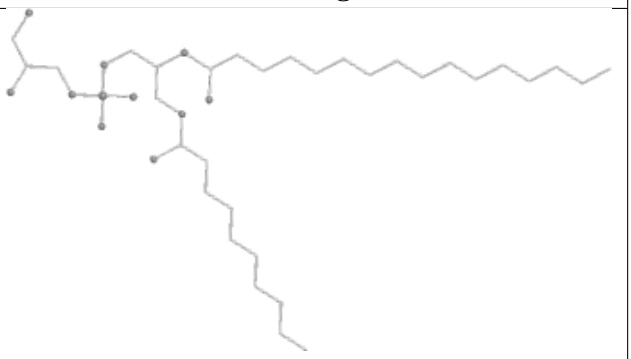
Bond lengths



Bond angles

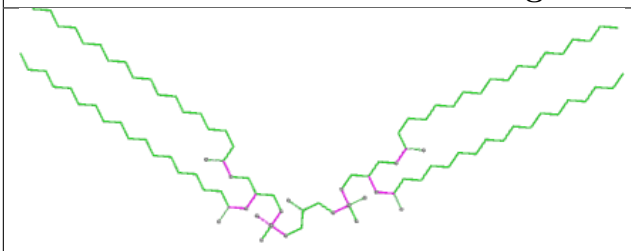


Torsions

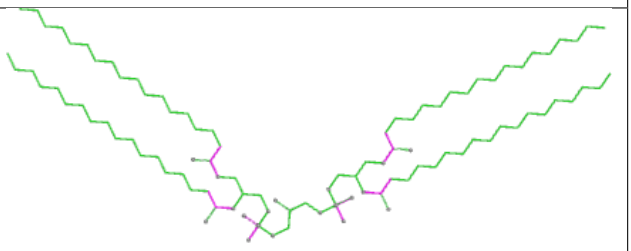


Rings

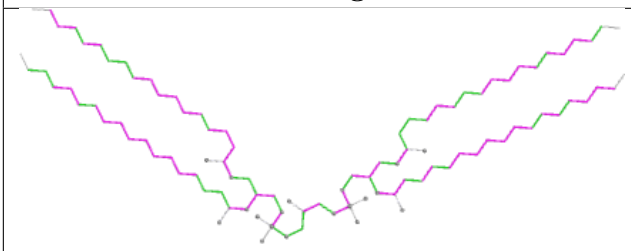
Ligand CDL F 712



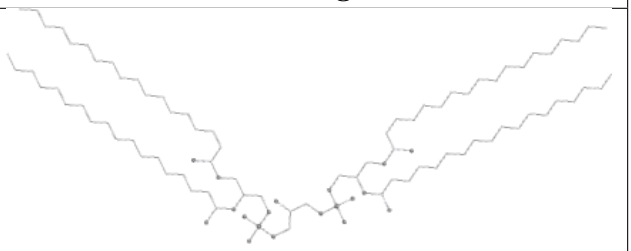
Bond lengths



Bond angles

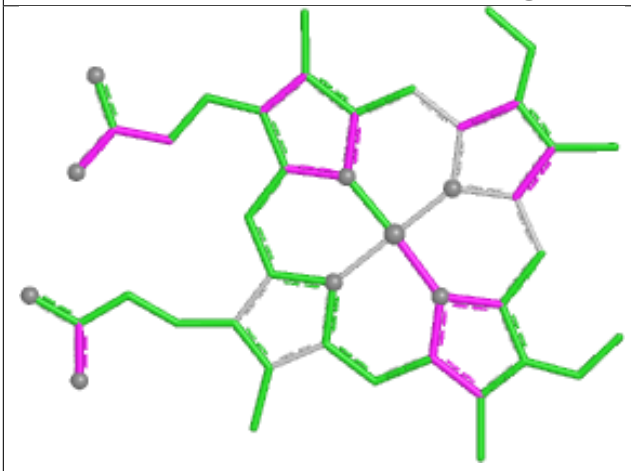


Torsions

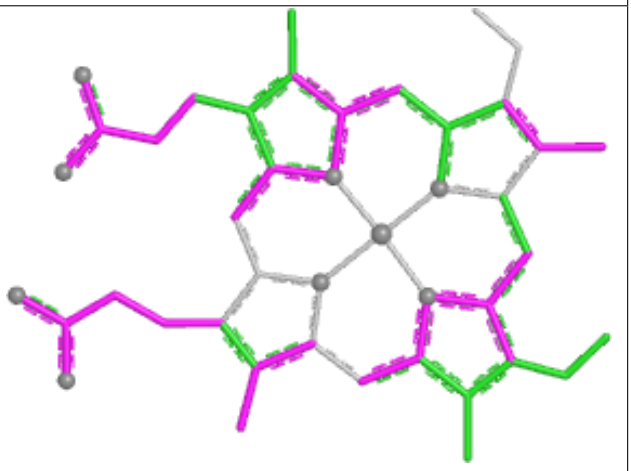


Rings

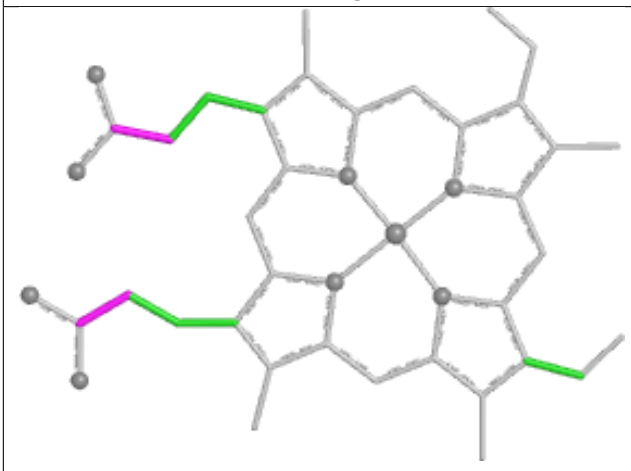
Ligand HEM F 711



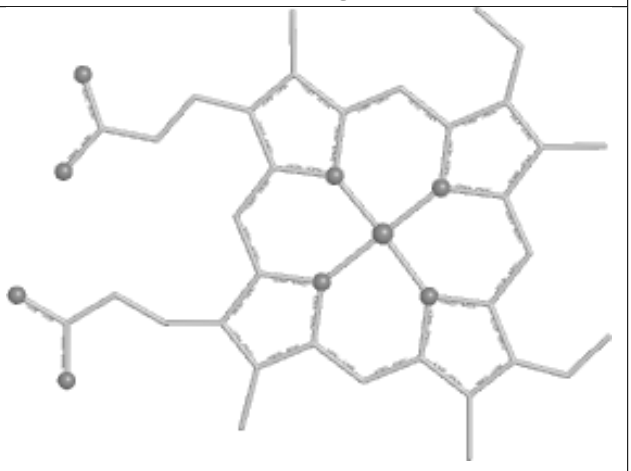
Bond lengths



Bond angles

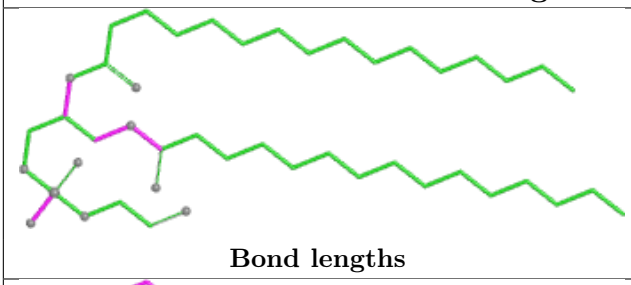


Torsions

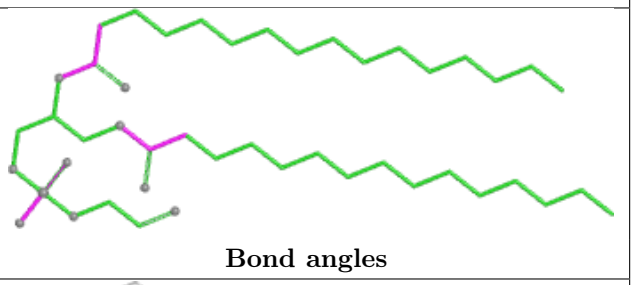


Rings

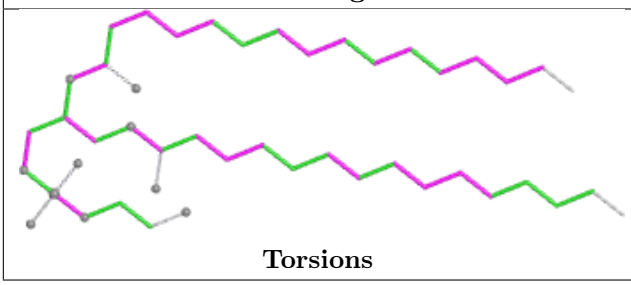
Ligand 3PE F 709



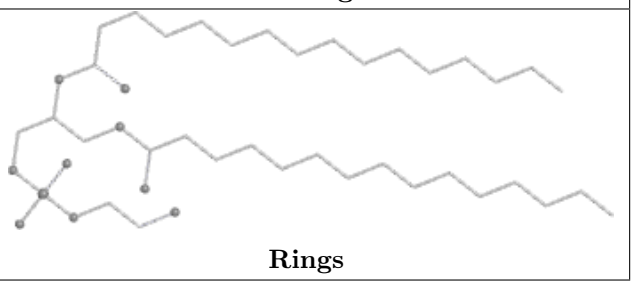
Bond lengths



Bond angles

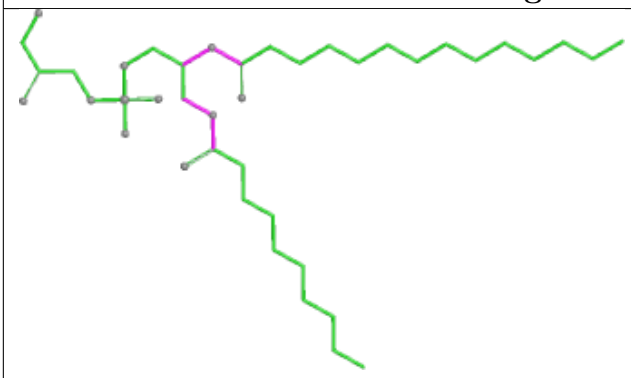


Torsions

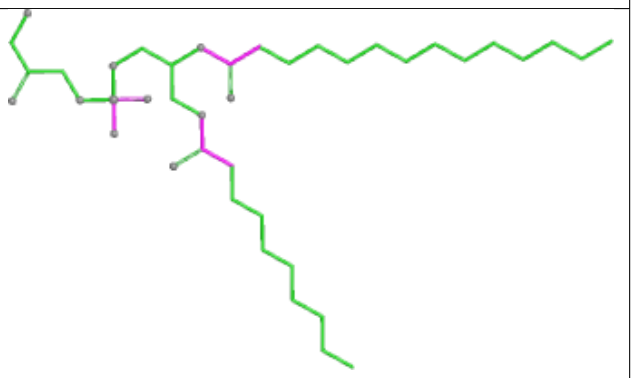


Rings

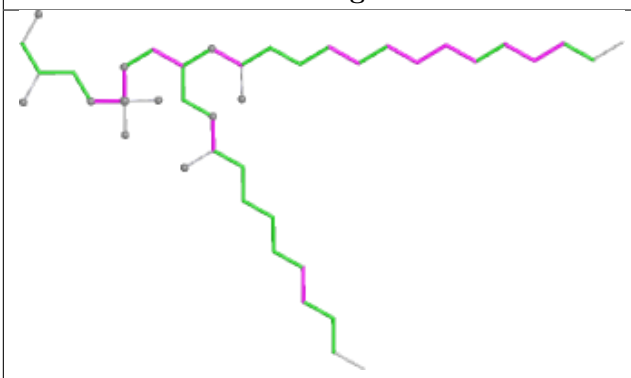
Ligand LHG F 702



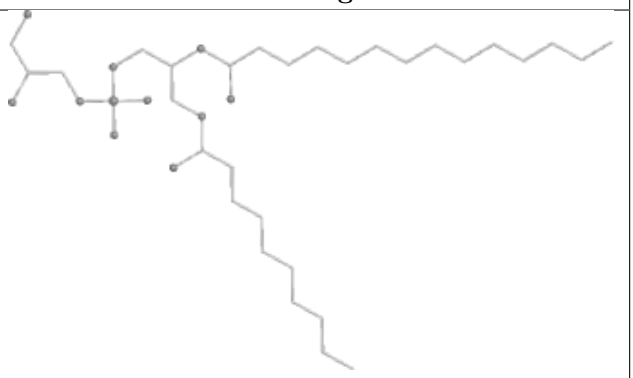
Bond lengths



Bond angles

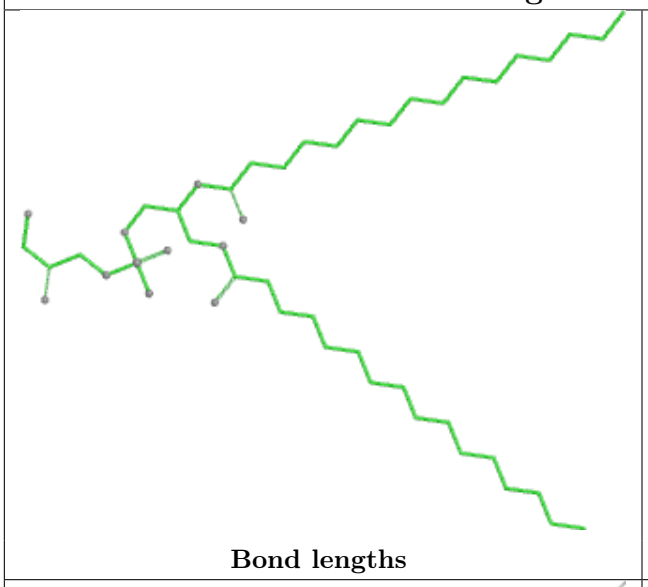


Torsions

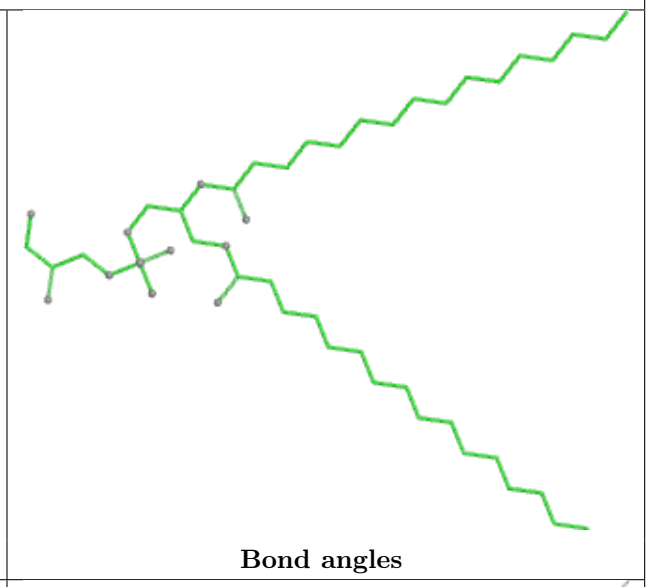


Rings

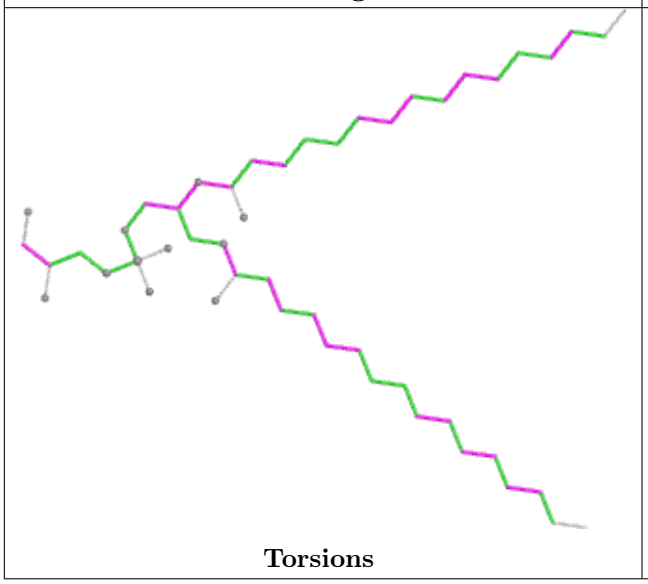
Ligand LHG F 707



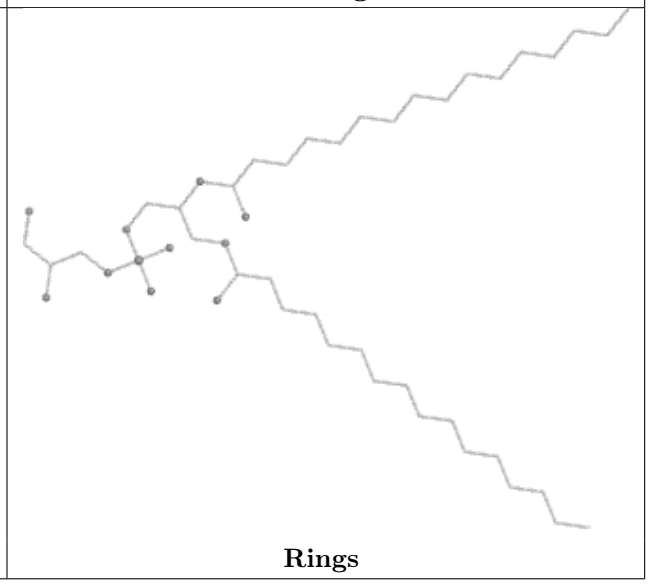
Bond lengths



Bond angles

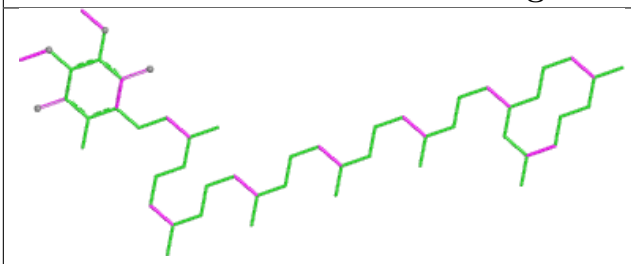


Torsions

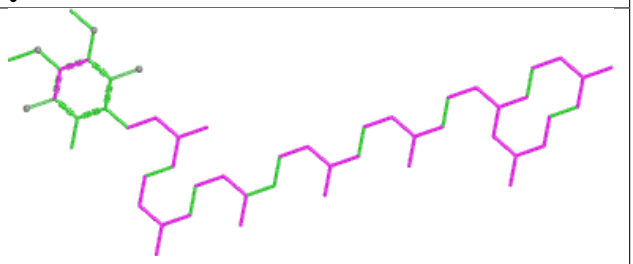


Rings

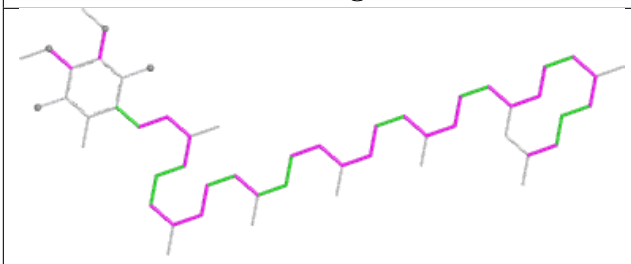
Ligand UQ8 F 701



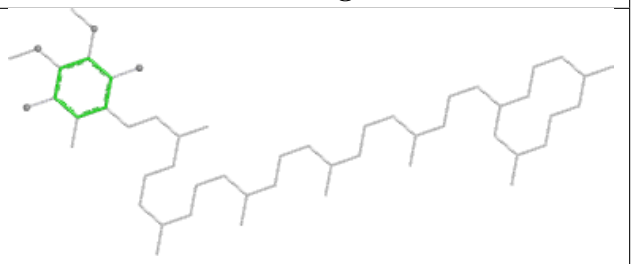
Bond lengths



Bond angles

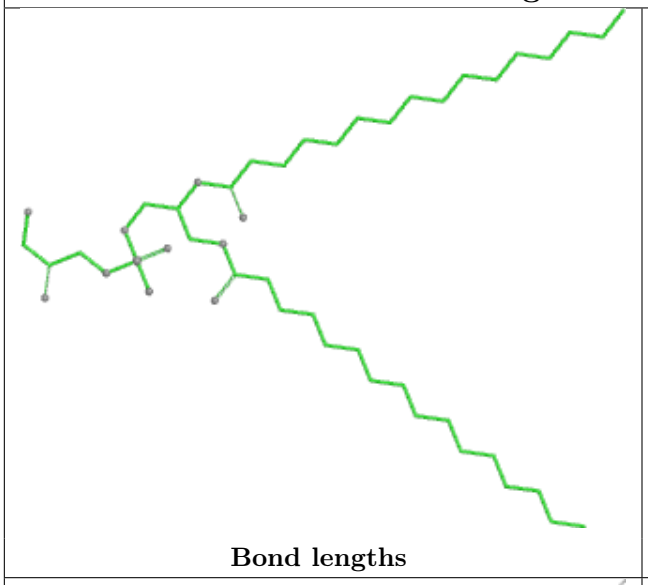


Torsions

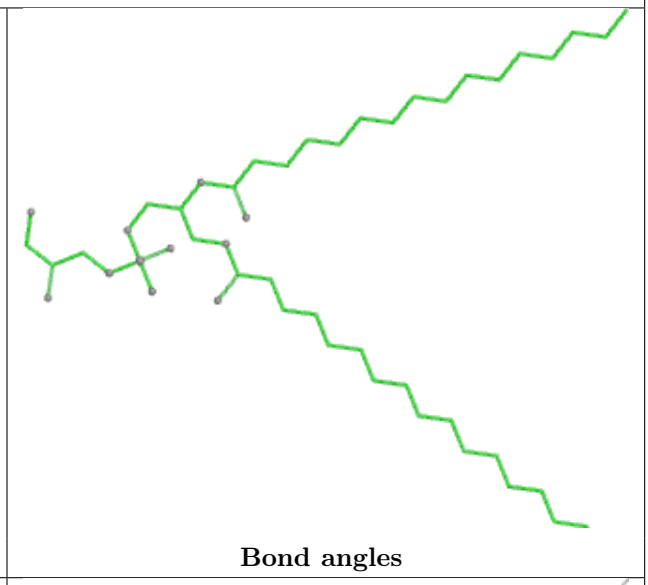


Rings

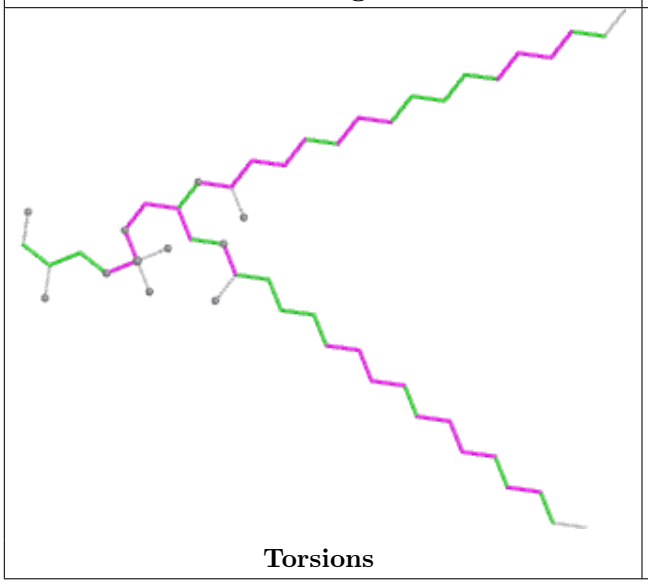
Ligand LHG H 302



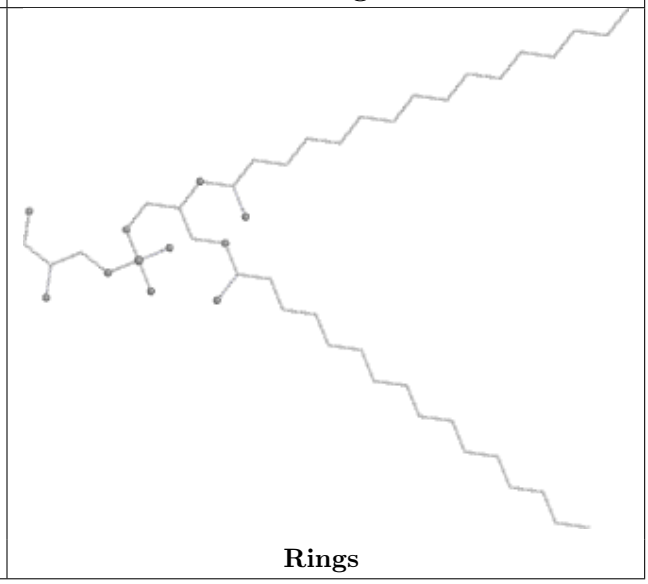
Bond lengths



Bond angles

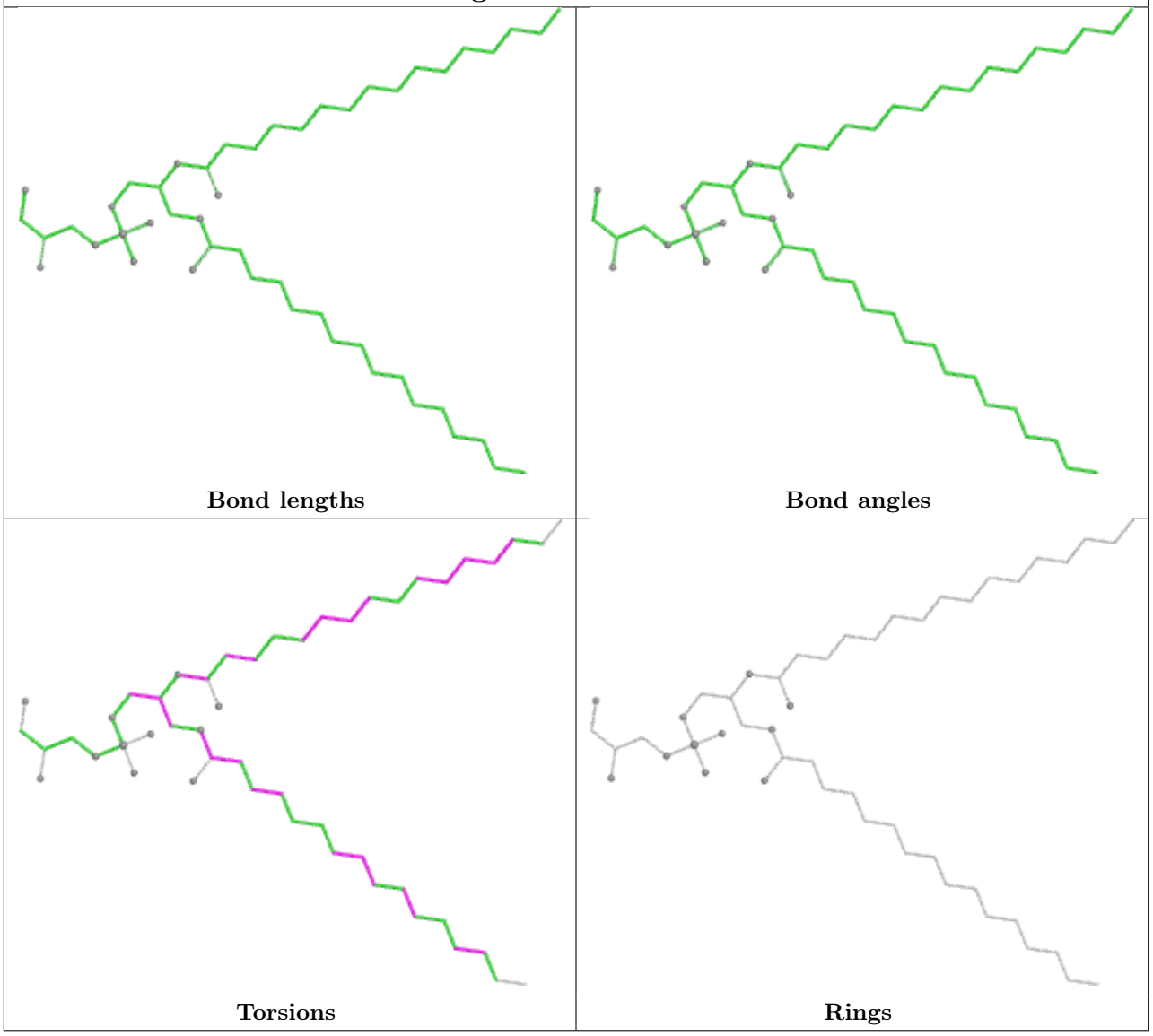


Torsions



Rings

Ligand LHG F 708



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

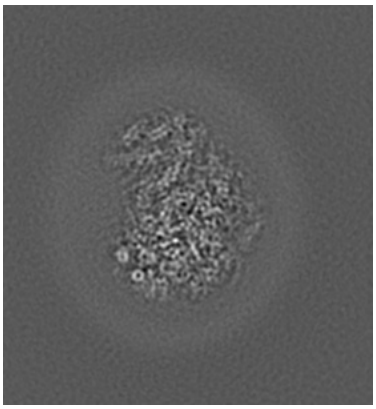
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24265. These allow visual inspection of the internal detail of the map and identification of artifacts.

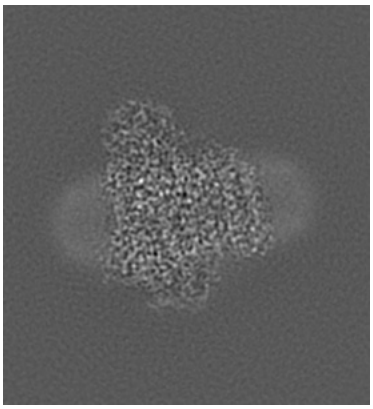
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

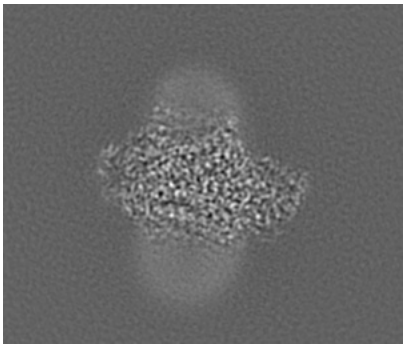
6.1.1 Primary map



X

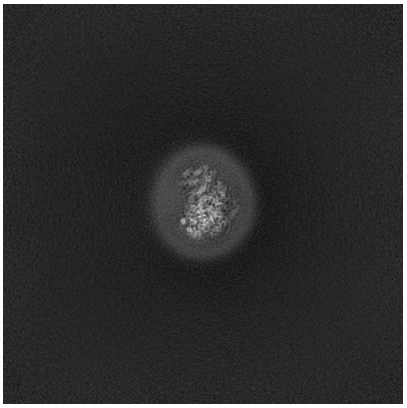


Y

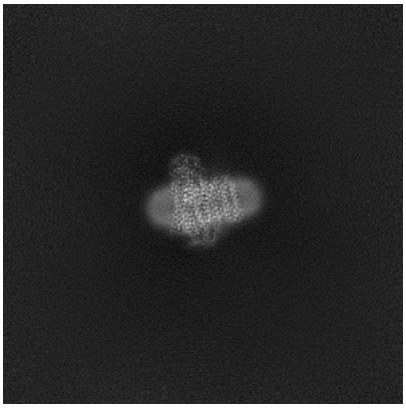


Z

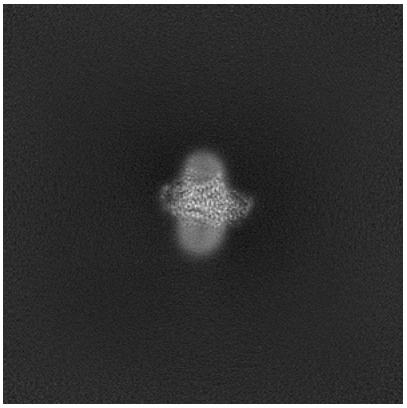
6.1.2 Raw map



X



Y

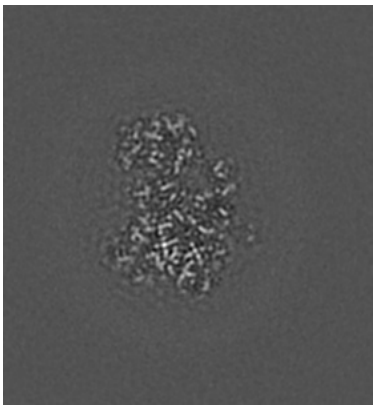


Z

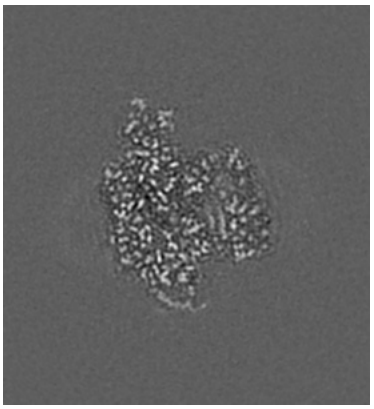
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

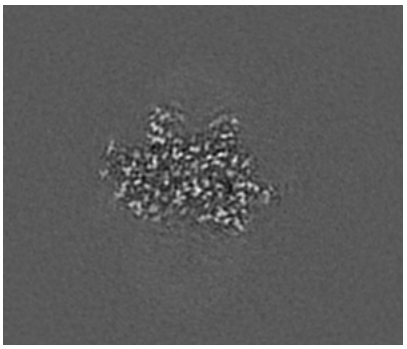
6.2.1 Primary map



X Index: 222

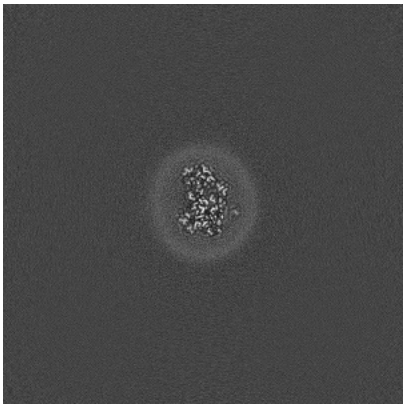


Y Index: 188

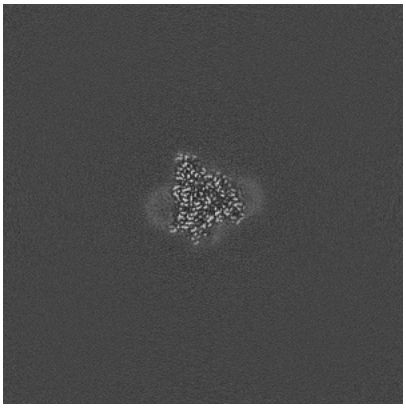


Z Index: 203

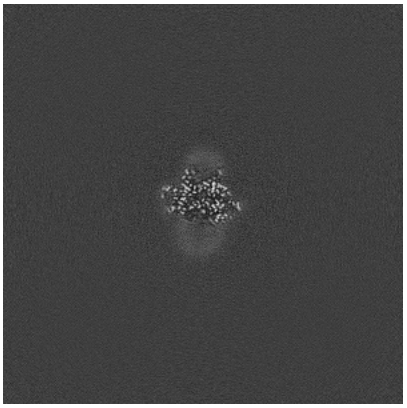
6.2.2 Raw map



X Index: 256



Y Index: 256

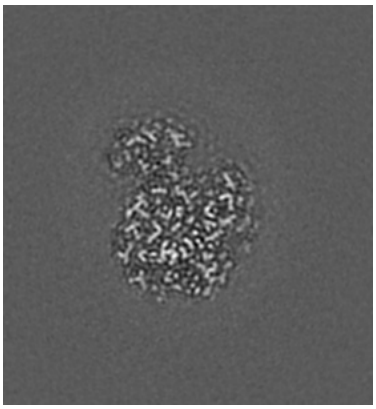


Z Index: 256

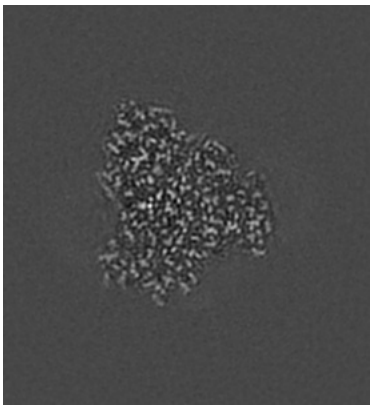
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

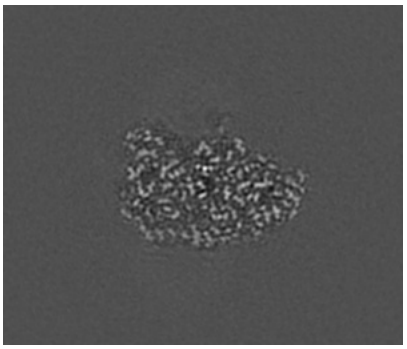
6.3.1 Primary map



X Index: 248

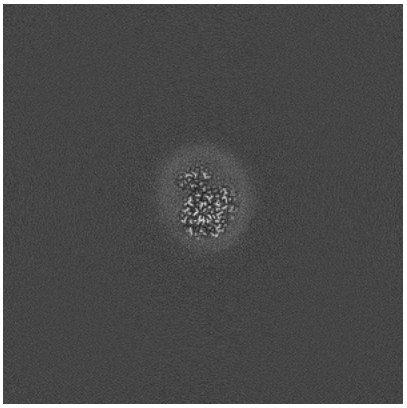


Y Index: 165

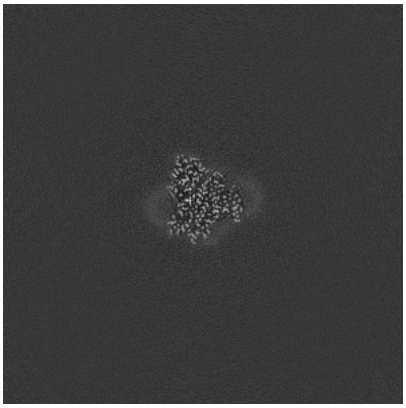


Z Index: 155

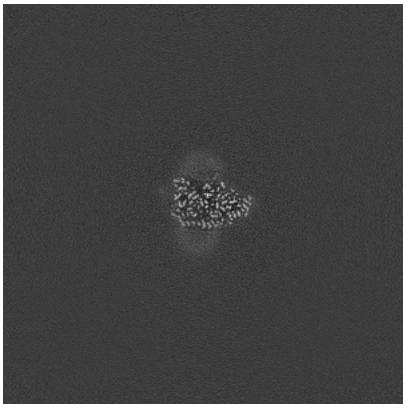
6.3.2 Raw map



X Index: 274



Y Index: 252

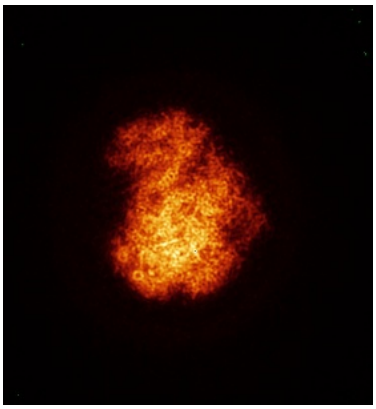


Z Index: 235

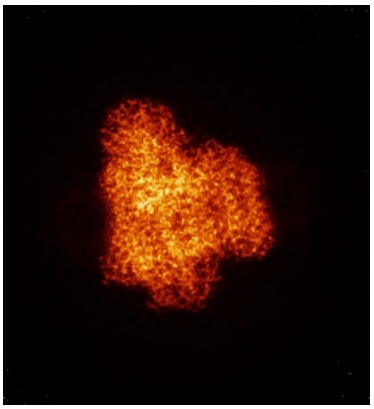
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

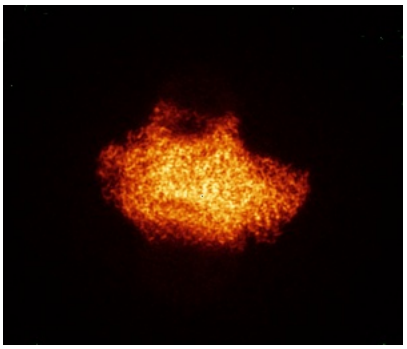
6.4.1 Primary map



X

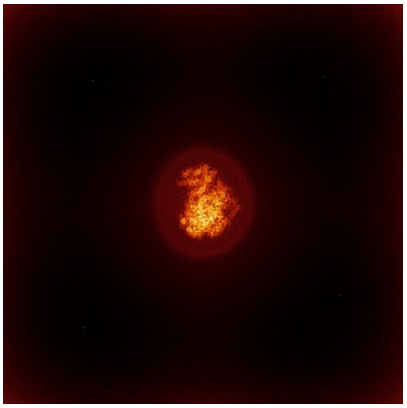


Y

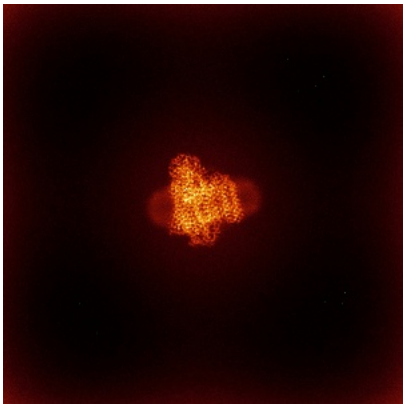


Z

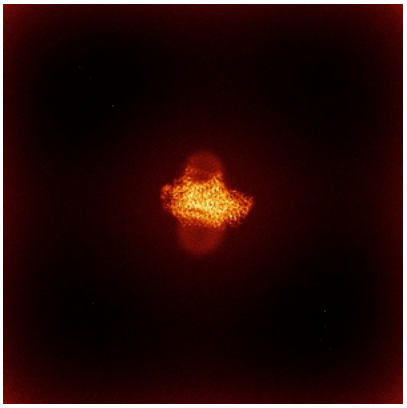
6.4.2 Raw map



X



Y

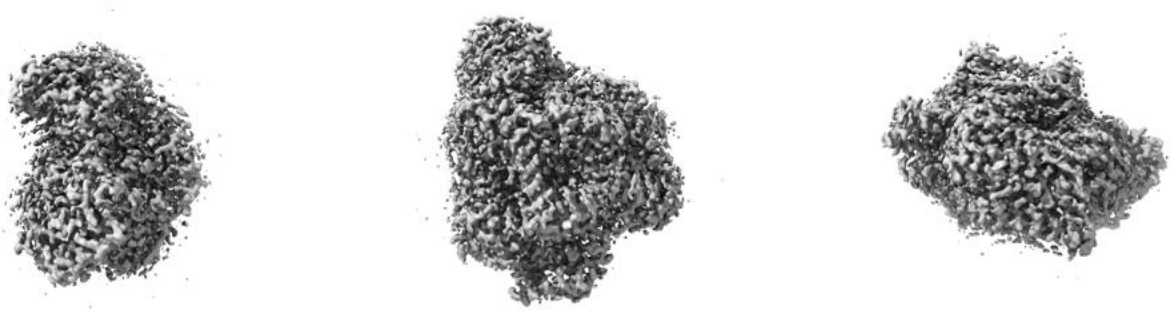


Z

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

6.5 Orthogonal surface views (i)

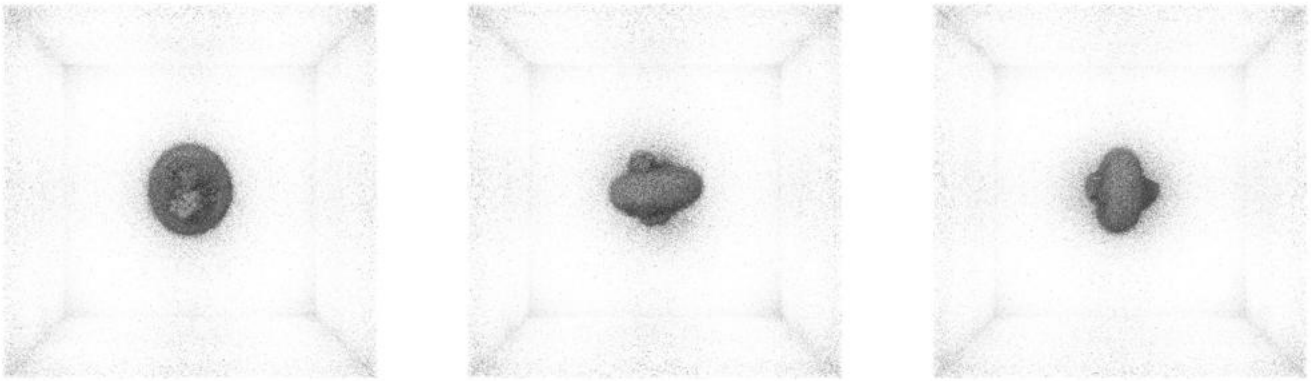
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.49. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

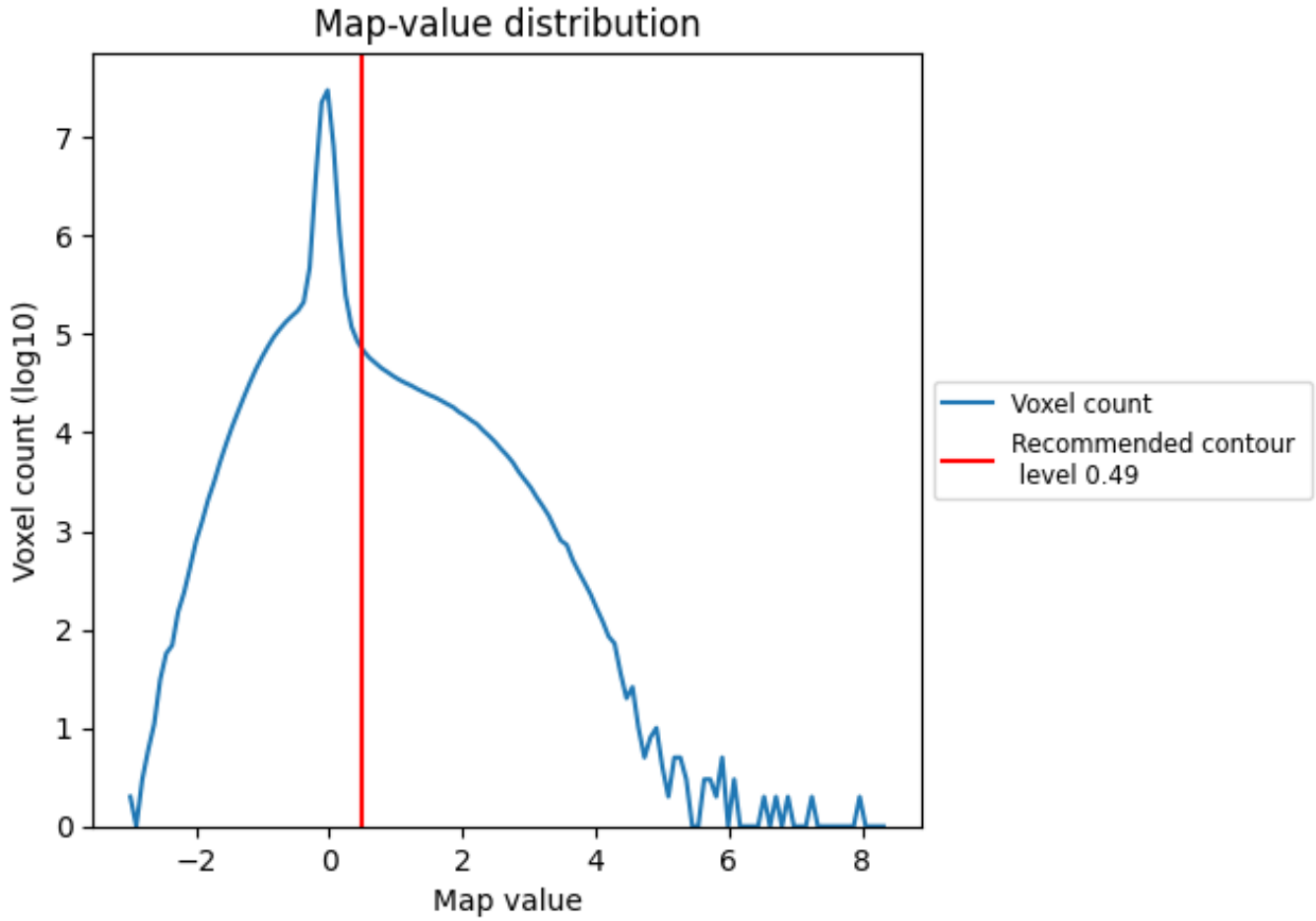
6.6 Mask visualisation (i)

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

7 Map analysis

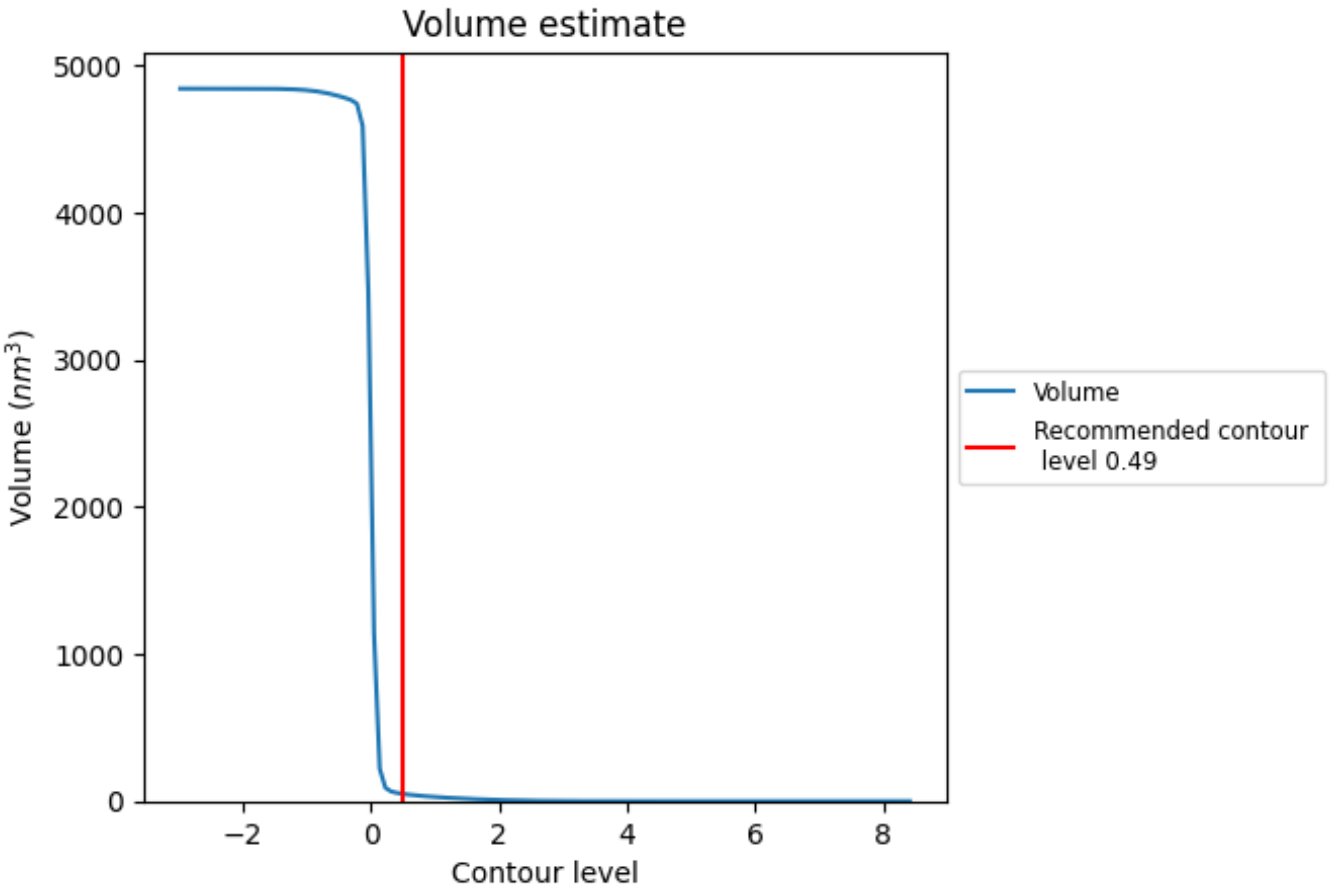
This section contains the results of statistical analysis of the map.

7.1 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.

7.2 Volume estimate



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 kDa.

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

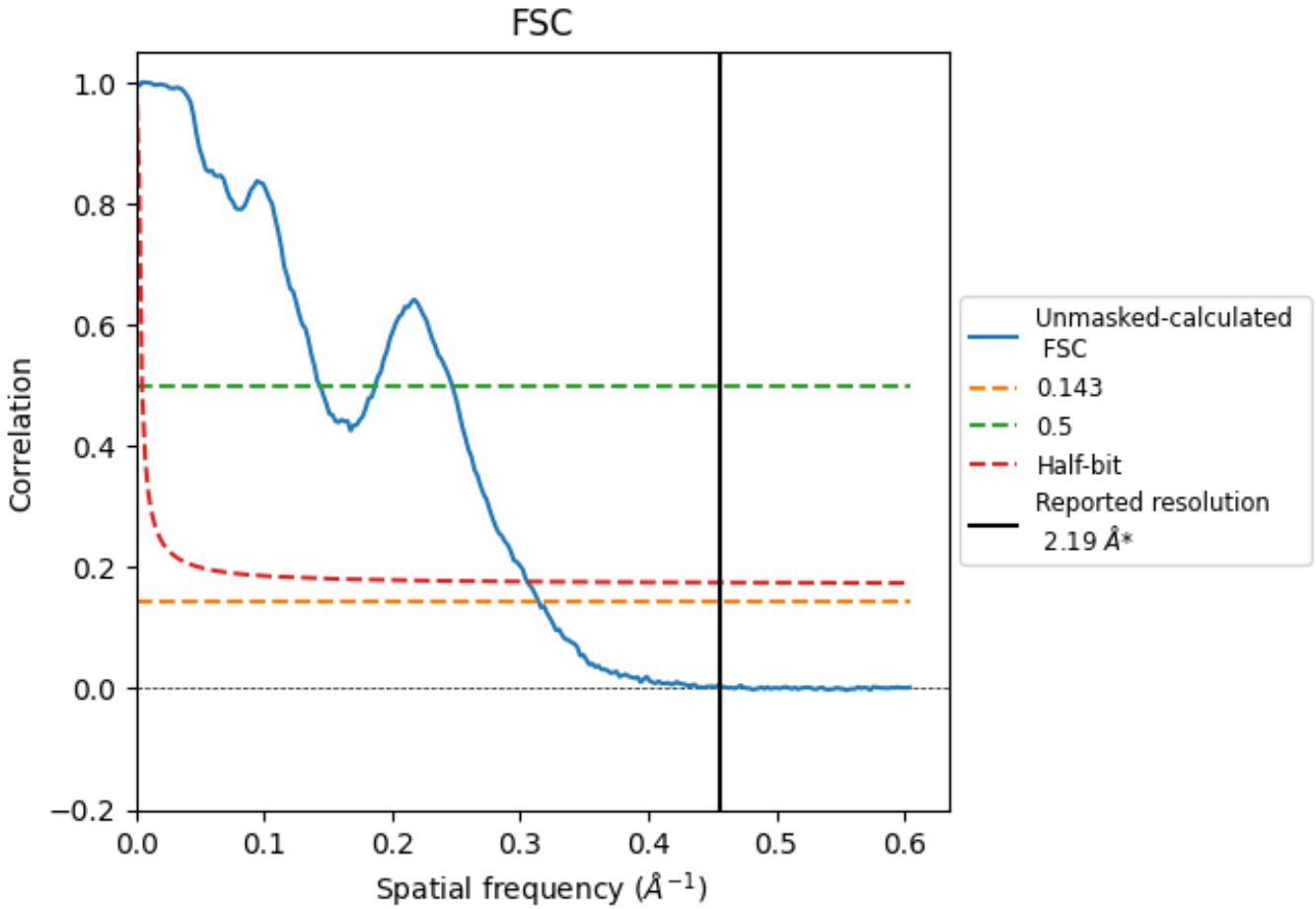
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.457 Å^{-1}

8.2 Resolution estimates (i)

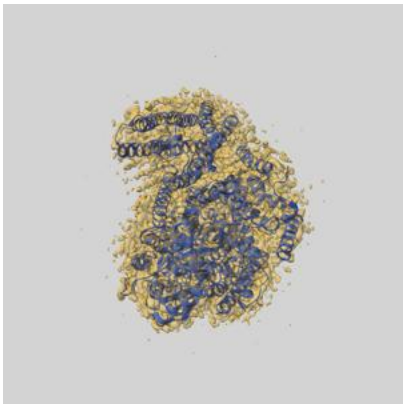
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	6.96	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.19 by more than 10 %

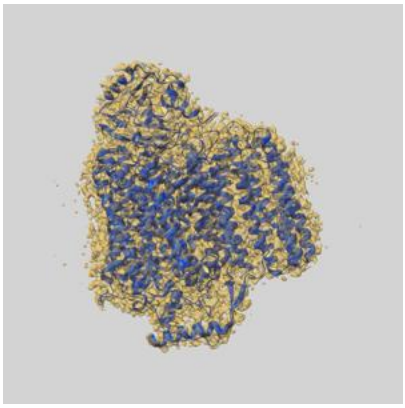
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24265 and PDB model 7N9Z. Per-residue inclusion information can be found in section 3 on page 9.

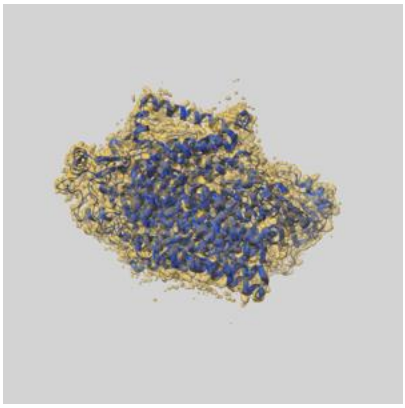
9.1 Map-model overlay



X



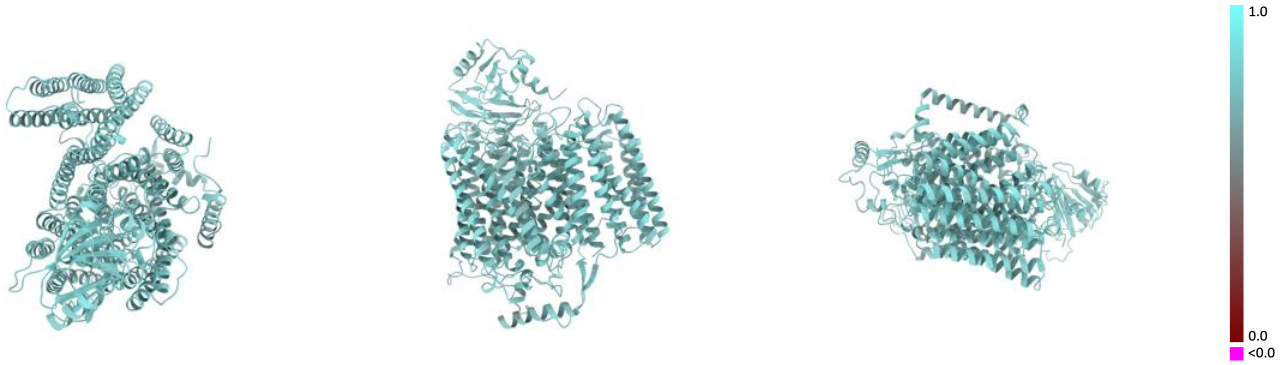
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.49 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

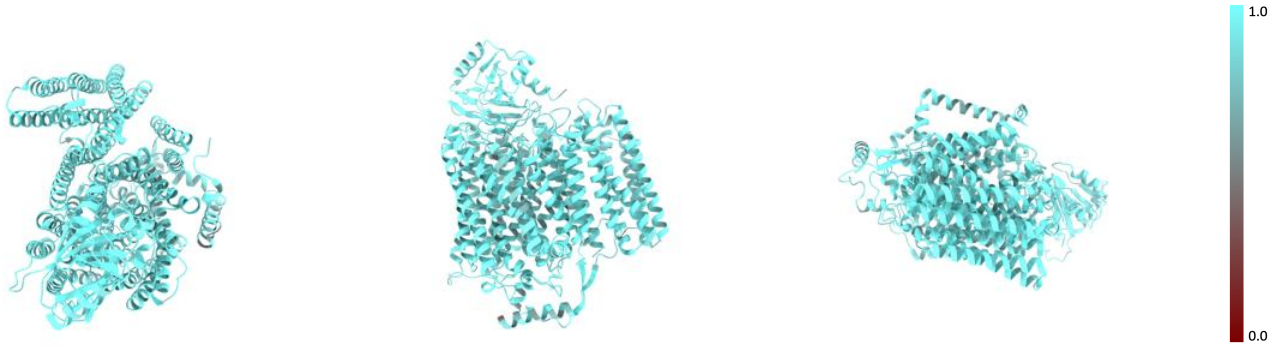
9.2 Q-score mapped to coordinate model (i)



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.

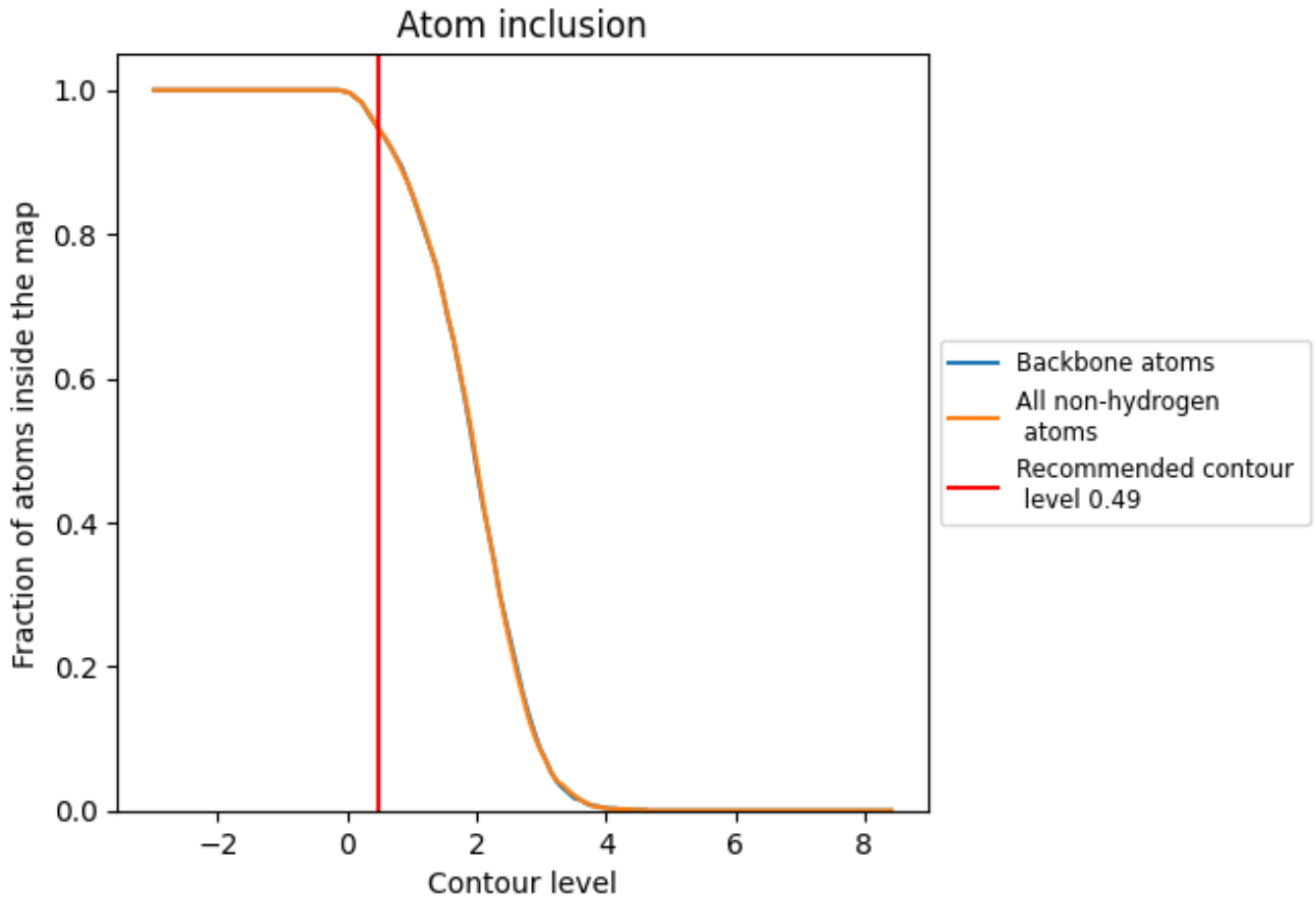
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.49).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.49) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.7340
F	0.9360	0.7320
G	0.9730	0.7400
H	0.9530	0.7350
I	0.9600	0.7240