Full wwPDB EM Validation Report

Aug 27, 2026 – 03:37 am BST

PDB ID	:	9F5Z / pdb_00009f5z
EMDB ID	:	EMD-50204
Title	:	Structure of the Chlamydomonas reinhardtii respiratory complex III from respiratory supercomplex
Authors	:	Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on	:	2024-04-30
Resolution	:	2.39 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:

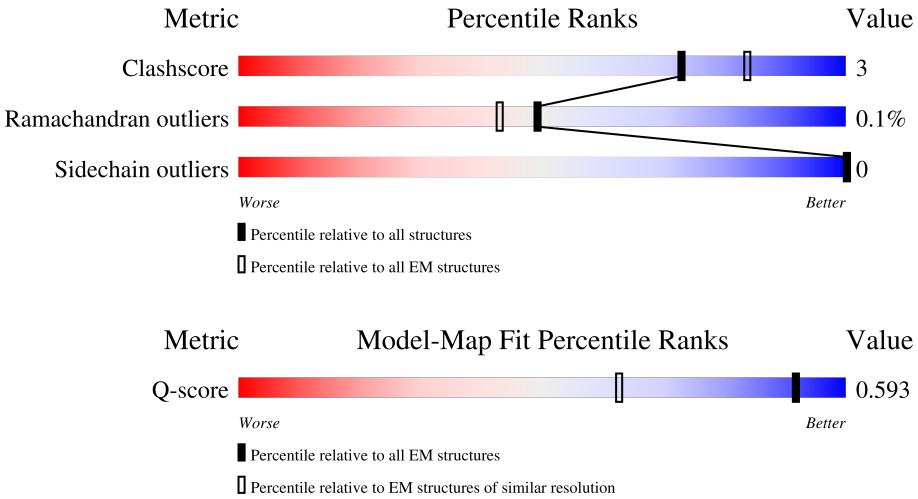
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.39 Å.

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



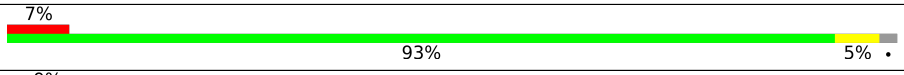
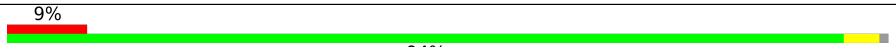
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	1A	381	93% 6%
1	1B	381	89% 10%
2	1C	262	45% 69% 10% 21%
2	1D	262	43% 69% 10% 21%

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Mol	Chain	Length	Quality of chain
3	1E	314	
3	1F	314	
4	1G	60	
4	1H	60	
5	1I	69	
5	1J	69	
6	1K	73	
6	1L	73	
7	1M	495	
7	1N	495	
8	1O	59	
8	1P	59	
9	1Q	485	
9	1S	485	
10	1R	123	
10	1T	123	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 34454 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	1B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	1D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	1F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		

- Molecule 4 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	1H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	1J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	1L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		

- Molecule 7 is a protein called MPP-Beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	1N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	1P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		

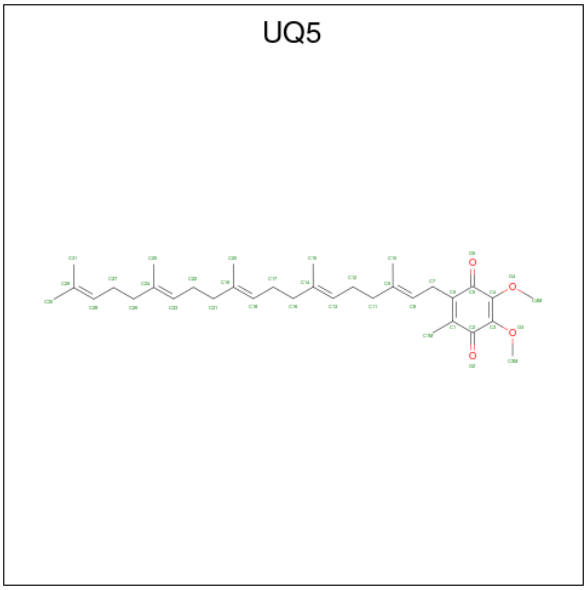
- Molecule 9 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	1S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

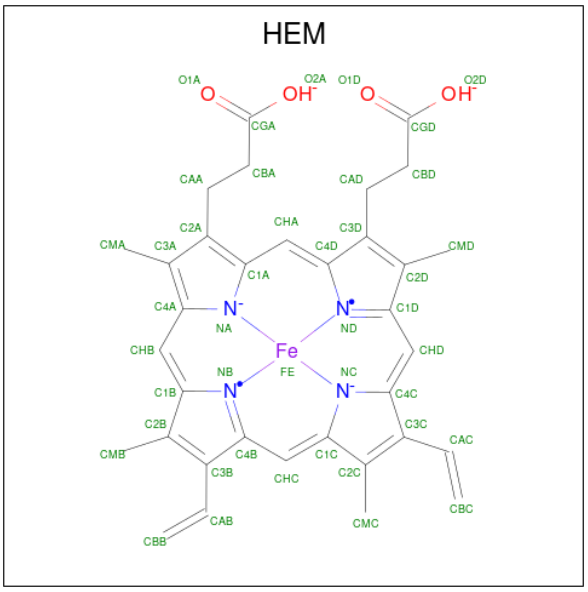
Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	1T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		

- Molecule 11 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: $C_{34}H_{50}O_4$).



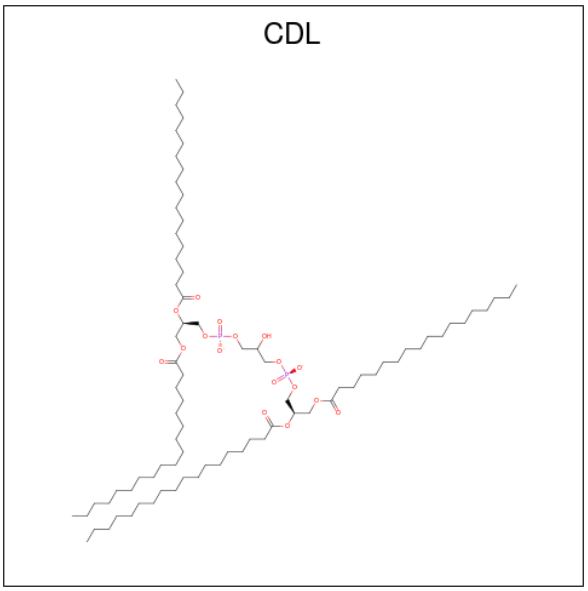
Mol	Chain	Residues	Atoms			AltConf
11	1A	1	Total	C	O	0
			38	34	4	
11	1A	1	Total	C	O	0
			38	34	4	
11	1B	1	Total	C	O	0
			38	34	4	
11	1B	1	Total	C	O	0
			38	34	4	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



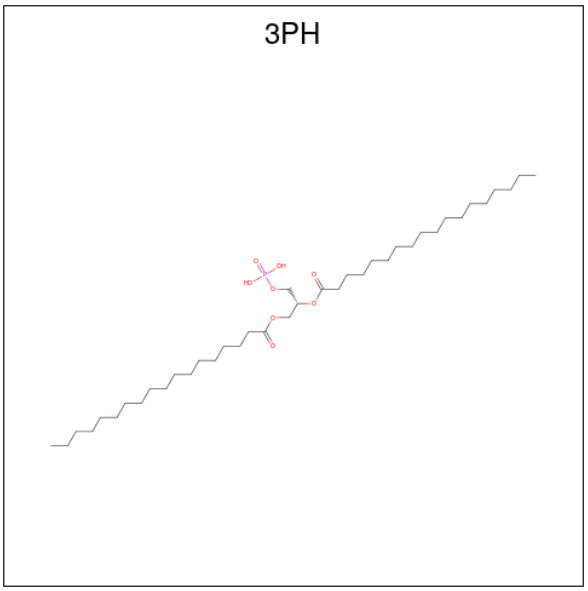
Mol	Chain	Residues	Atoms					AltConf
12	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



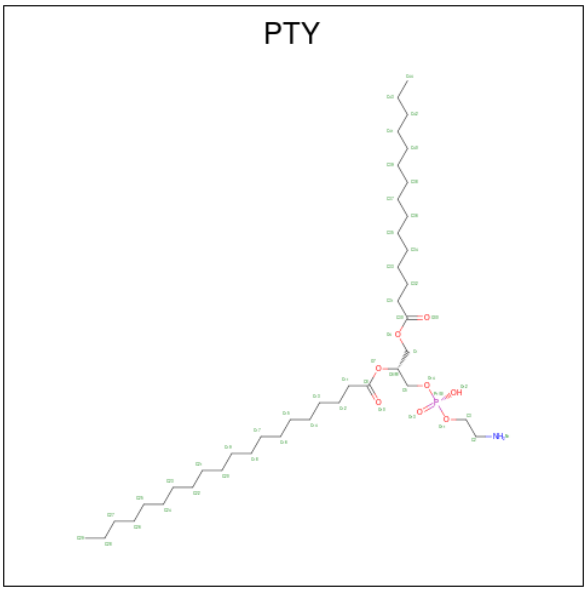
Mol	Chain	Residues	Atoms				AltConf
13	1A	1	Total 59	C 40	O 17	P 2	0
13	1B	1	Total 64	C 45	O 17	P 2	0
13	1B	1	Total 71	C 52	O 17	P 2	0
13	1E	1	Total 53	C 34	O 17	P 2	0
13	1F	1	Total 56	C 37	O 17	P 2	0
13	1K	1	Total 79	C 60	O 17	P 2	0
13	1L	1	Total 59	C 40	O 17	P 2	0
13	1M	1	Total 54	C 35	O 17	P 2	0

- Molecule 14 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



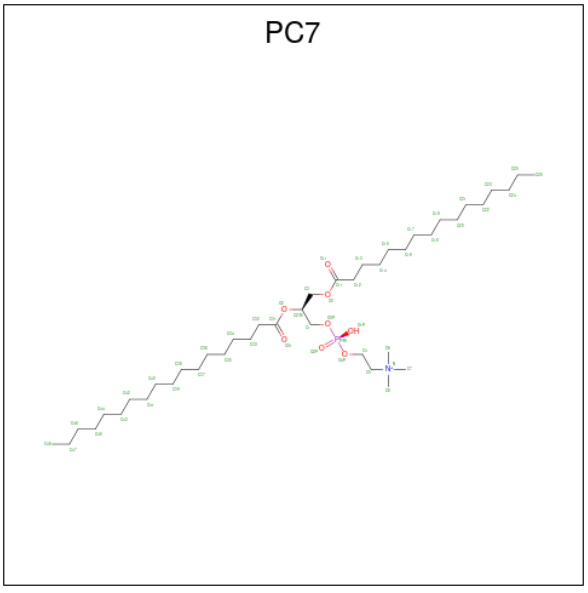
Mol	Chain	Residues	Atoms				AltConf
14	1A	1	Total	C	O	P	0
			31	22	8	1	
14	1B	1	Total	C	O	P	0
			48	39	8	1	
14	1B	1	Total	C	O	P	0
			48	39	8	1	
14	1E	1	Total	C	O	P	0
			40	31	8	1	
14	1K	1	Total	C	O	P	0
			48	39	8	1	
14	1K	1	Total	C	O	P	0
			32	23	8	1	
14	1R	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
15	1E	1	Total	C	N	O	P	0
			34	24	1	8	1	
15	1F	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 16 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
16	1G	1	Total	C	N	O	P	0
			36	26	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
16	1H	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	1M	1	Total	Zn	0
			1	1	
17	1N	1	Total	Zn	0
			1	1	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	1A	48	Total	O	0
			48	48	
18	1B	52	Total	O	0
			52	52	
18	1C	13	Total	O	0
			13	13	
18	1D	12	Total	O	0
			12	12	
18	1E	51	Total	O	0
			51	51	
18	1F	34	Total	O	0
			34	34	
18	1G	7	Total	O	0
			7	7	
18	1H	9	Total	O	0
			9	9	
18	1I	11	Total	O	0
			11	11	
18	1J	3	Total	O	0
			3	3	
18	1K	12	Total	O	0
			12	12	
18	1L	12	Total	O	0
			12	12	
18	1M	76	Total	O	0
			76	76	
18	1N	74	Total	O	0
			74	74	

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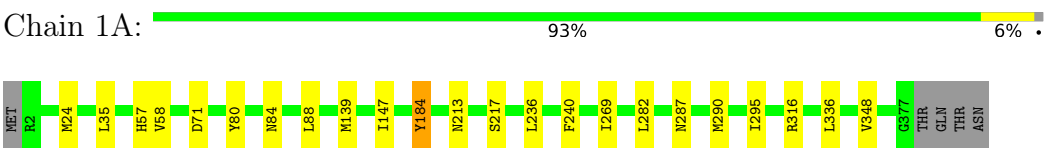
Mol	Chain	Residues	Atoms	AltConf
18	1O	4	Total O 4 4	0
18	1P	6	Total O 6 6	0
18	1Q	27	Total O 27 27	0
18	1R	32	Total O 32 32	0
18	1S	27	Total O 27 27	0
18	1T	28	Total O 28 28	0

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.

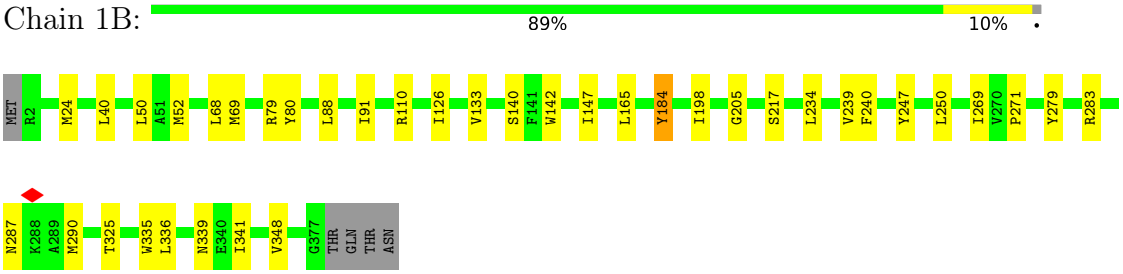
• Molecule 1: Cytochrome b

Chain 1A:



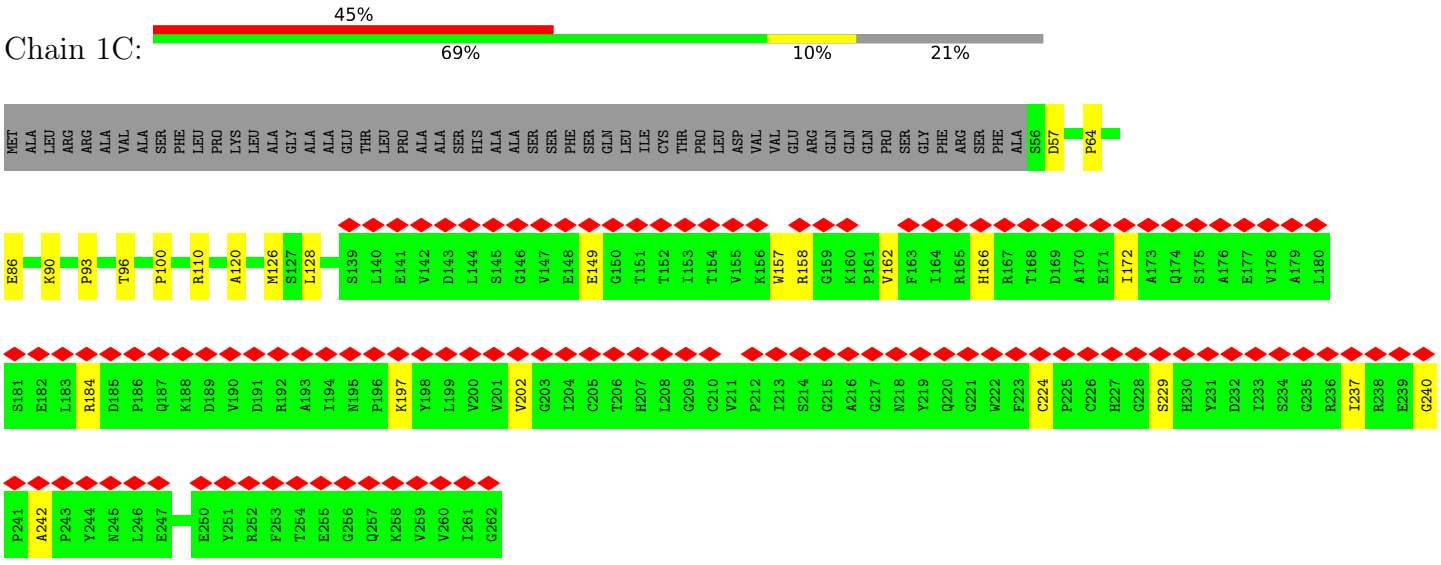
• Molecule 1: Cytochrome b

Chain 1B:



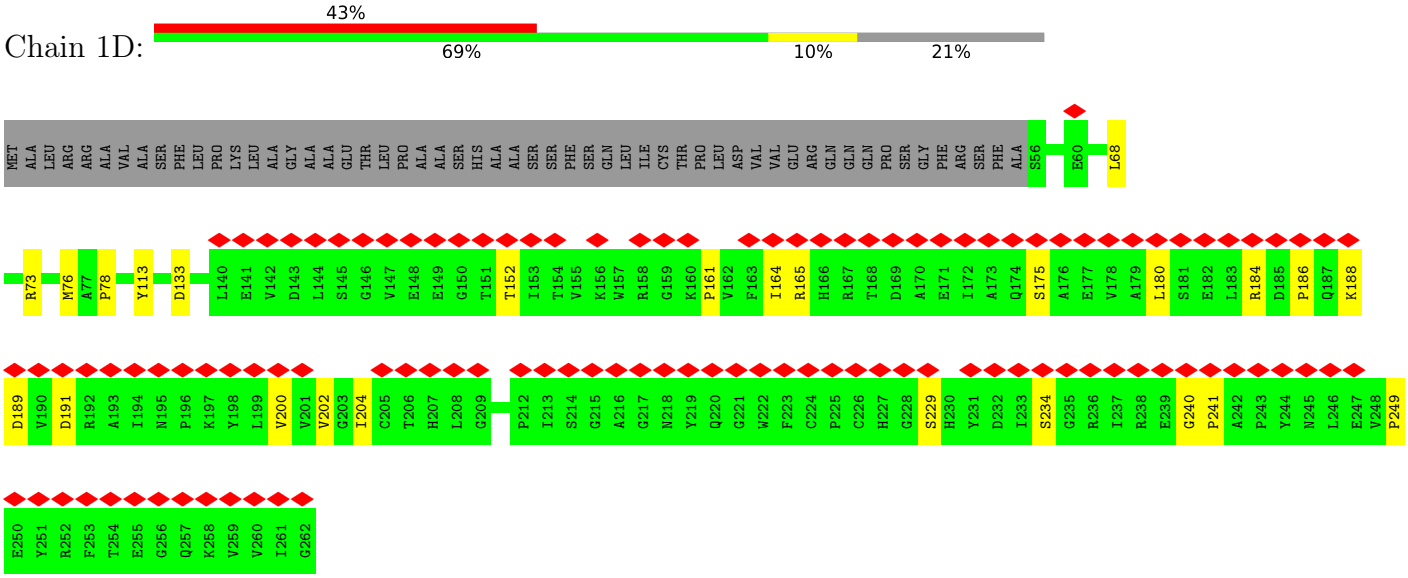
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 1C:



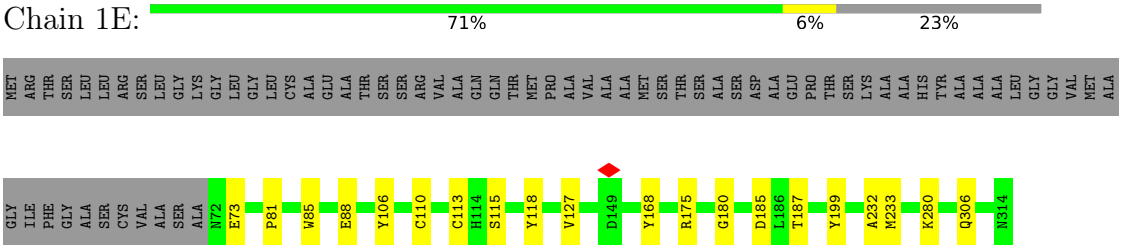
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 1D:



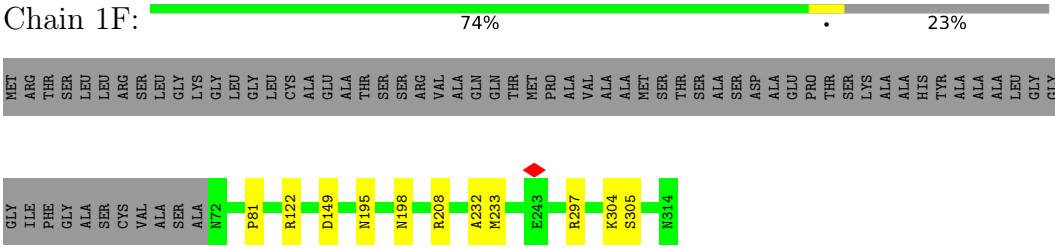
• Molecule 3: Cytochrome c1

Chain 1E:



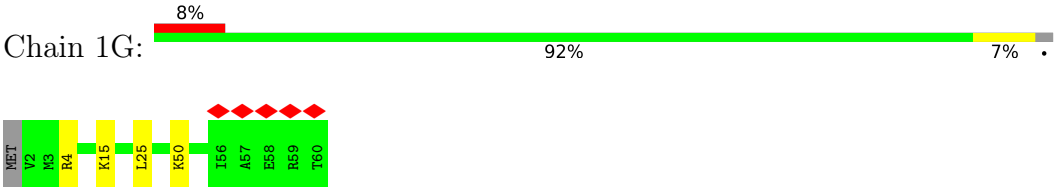
• Molecule 3: Cytochrome c1

Chain 1F:



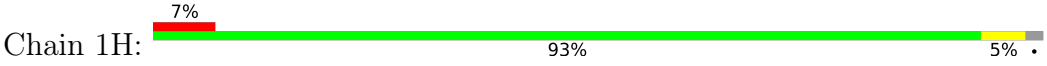
• Molecule 4: Complex III subunit 9

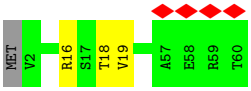
Chain 1G:



• Molecule 4: Complex III subunit 9

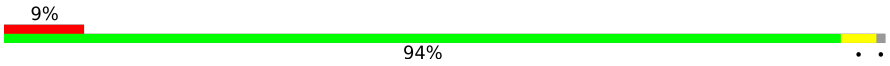
Chain 1H:

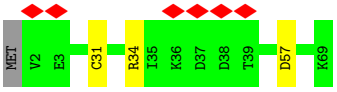




• Molecule 5: Cytochrome b-c1 complex subunit 6

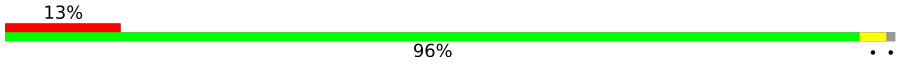
Chain 1I:

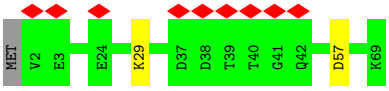




• Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1J:

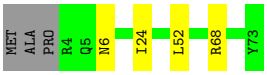




• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1K:

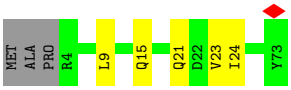




• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1L:

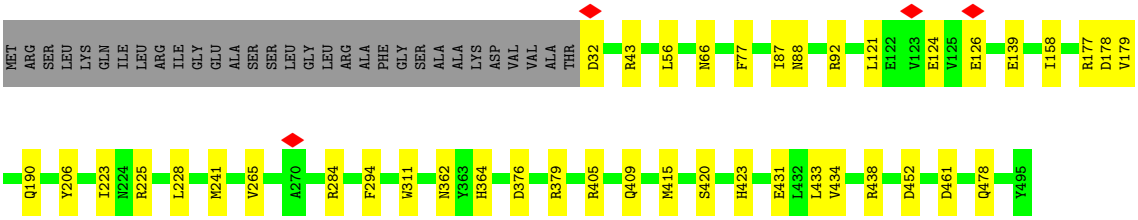




• Molecule 7: MPP-Beta

Chain 1M:

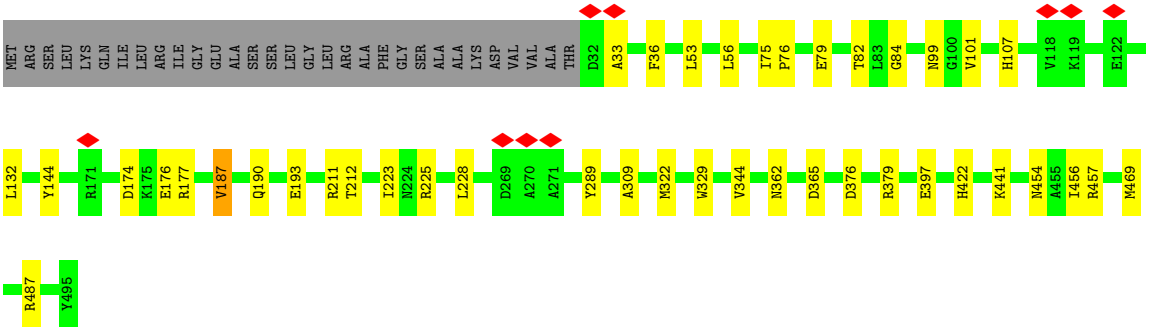




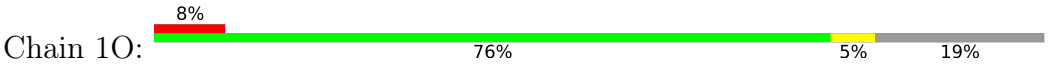
• Molecule 7: MPP-Beta

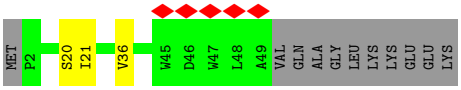
Chain 1N:





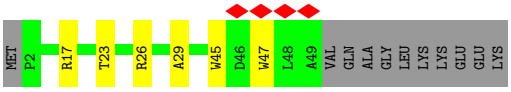
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



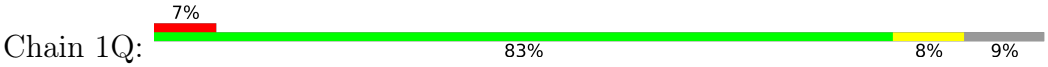


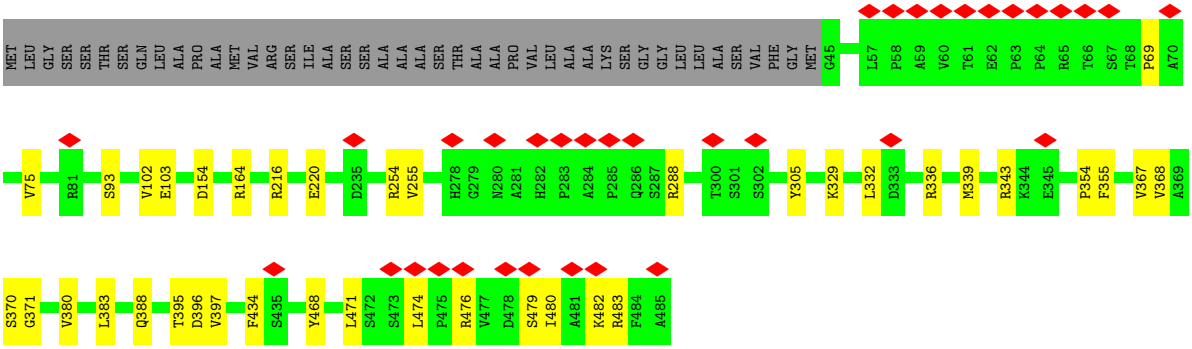
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



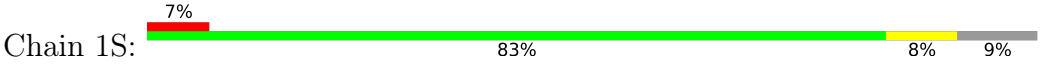


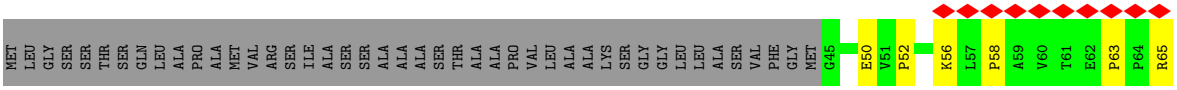
• Molecule 9: Alpha-MPP

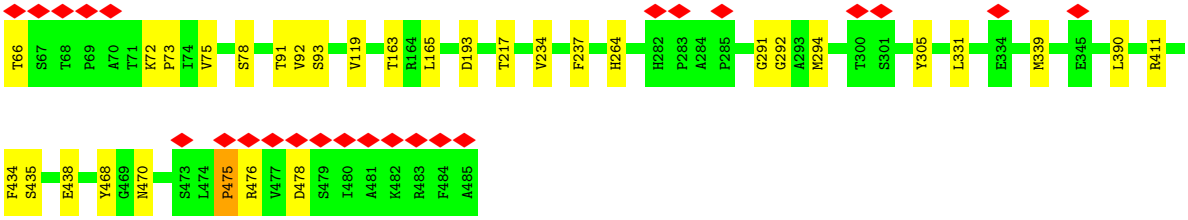




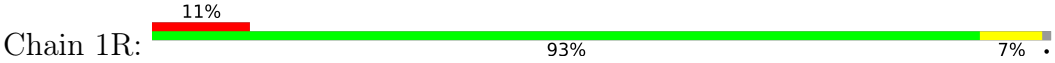
• Molecule 9: Alpha-MPP

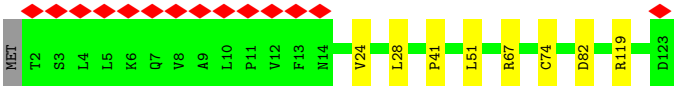




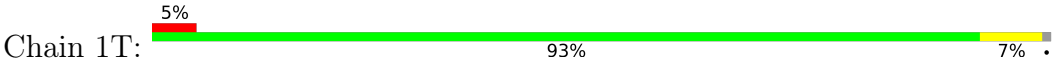


• Molecule 10: Cytochrome b-c1 complex subunit 7





• Molecule 10: Cytochrome b-c1 complex subunit 7





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.117	Depositor
Minimum map value	-0.534	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.145	Depositor
Map size (Å)	589.6, 589.6, 589.6	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0027211, 1.0027211, 1.0027211	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UQ5, 3PH, PTY, CDL, HEM, ZN, PC7

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	1A	0.25	0/3060	0.48	1/4187 (0.0%)
1	1B	0.26	0/3060	0.48	1/4187 (0.0%)
2	1C	0.18	0/1643	0.36	0/2233
2	1D	0.17	0/1643	0.33	0/2233
3	1E	0.24	0/1953	0.43	1/2654 (0.0%)
3	1F	0.22	0/1953	0.38	0/2654
4	1G	0.23	0/496	0.41	0/667
4	1H	0.22	0/496	0.39	0/667
5	1I	0.23	0/567	0.45	0/766
5	1J	0.21	0/567	0.39	0/766
6	1K	0.25	0/609	0.44	0/817
6	1L	0.22	0/609	0.42	0/817
7	1M	0.23	0/3723	0.42	0/5046
7	1N	0.22	0/3723	0.38	0/5046
8	1O	0.19	0/385	0.44	0/531
8	1P	0.21	0/385	0.52	0/531
9	1Q	0.22	0/3258	0.43	0/4439
9	1S	0.21	0/3258	0.43	1/4439 (0.0%)
10	1R	0.21	0/996	0.35	0/1349
10	1T	0.23	0/996	0.41	0/1349
All	All	0.22	0/33380	0.42	4/45378 (0.0%)

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
1	1A	0	1
1	1B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	184	TYR	N-CA-C	-5.96	104.87	111.36
3	1E	127	VAL	N-CA-C	-5.49	107.51	112.12
9	1S	234	VAL	N-CA-C	-5.43	107.08	111.91
1	1B	184	TYR	N-CA-C	-5.06	105.47	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	184	TYR	Sidechain
1	1B	184	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2958	0	2955	15	0
1	1B	2958	0	2953	25	0
2	1C	1602	0	1577	16	0
2	1D	1602	0	1577	15	0
3	1E	1898	0	1800	13	0
3	1F	1898	0	1800	10	0
4	1G	486	0	490	4	0
4	1H	486	0	490	2	0
5	1I	550	0	501	2	0
5	1J	550	0	501	2	0
6	1K	594	0	590	4	0
6	1L	594	0	590	5	0
7	1M	3646	0	3555	29	0
7	1N	3646	0	3555	28	0
8	1O	371	0	372	2	0
8	1P	371	0	372	5	0
9	1Q	3204	0	3271	26	0
9	1S	3204	0	3271	23	0
10	1R	980	0	1004	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1T	980	0	1005	6	0
11	1A	76	0	100	2	0
11	1B	76	0	100	8	0
12	1A	86	0	60	0	0
12	1B	86	0	60	2	0
12	1E	43	0	30	3	0
12	1F	43	0	30	2	0
13	1A	59	0	62	1	0
13	1B	135	0	159	6	0
13	1E	53	0	50	1	0
13	1F	56	0	56	1	0
13	1K	79	0	105	5	0
13	1L	59	0	62	0	0
13	1M	54	0	52	0	0
14	1A	31	0	35	0	0
14	1B	96	0	150	1	0
14	1E	40	0	56	1	0
14	1K	80	0	112	2	0
14	1R	37	0	50	1	0
15	1E	34	0	41	2	0
15	1F	38	0	49	0	0
16	1G	36	0	46	3	0
16	1H	39	0	52	2	0
17	1M	1	0	0	0	0
17	1N	1	0	0	0	0
18	1A	48	0	0	1	0
18	1B	52	0	0	0	0
18	1C	13	0	0	0	0
18	1D	12	0	0	0	0
18	1E	51	0	0	0	0
18	1F	34	0	0	0	0
18	1G	7	0	0	1	0
18	1H	9	0	0	0	0
18	1I	11	0	0	0	0
18	1J	3	0	0	0	0
18	1K	12	0	0	0	0
18	1L	12	0	0	0	0
18	1M	76	0	0	1	0
18	1N	74	0	0	0	0
18	1O	4	0	0	0	0
18	1P	6	0	0	0	0
18	1Q	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	1R	32	0	0	0	0
18	1S	27	0	0	0	0
18	1T	28	0	0	0	0
All	All	34454	0	33746	226	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1M:121:LEU:HB3	9:1Q:339:MET:HE1	1.74	0.67
9:1S:50:GLU:HG2	9:1S:52:PRO:HD2	1.79	0.64
9:1Q:216:ARG:HH22	9:1S:470:ASN:HB2	1.64	0.63
2:1D:180:LEU:HB3	2:1D:186:PRO:HB3	1.80	0.63
1:1A:269:ILE:HG22	11:1A:402:UQ5:H3M1	1.81	0.63
3:1E:118:TYR:HB2	3:1E:187:THR:HG21	1.80	0.62
1:1A:213:ASN:HD22	10:1R:41:PRO:HD2	1.65	0.61
7:1N:79:GLU:HG2	9:1S:411:ARG:HD3	1.82	0.61
5:1I:31:CYS:HA	5:1I:34:ARG:HE	1.66	0.60
6:1K:24:ILE:HD11	13:1K:101:CDL:H861	1.83	0.59
6:1L:15:GLN:HB2	7:1N:289:TYR:HB3	1.84	0.59
1:1A:139:MET:HE1	1:1A:269:ILE:HA	1.83	0.59
7:1N:177:ARG:NH2	7:1N:223:ILE:O	2.35	0.59
1:1A:282:LEU:HB2	1:1A:295:ILE:HD11	1.83	0.59
1:1B:50:LEU:HD22	1:1B:68:LEU:HD21	1.84	0.58
16:1G:301:PC7:H351	16:1G:301:PC7:H172	1.86	0.58
7:1M:177:ARG:NH2	7:1M:223:ILE:O	2.36	0.57
4:1H:16:ARG:HB2	4:1H:19:VAL:HG22	1.87	0.57
1:1B:110:ARG:NH1	1:1B:205:GLY:O	2.38	0.56
13:1B:405:CDL:H112	13:1B:405:CDL:H841	1.86	0.56
4:1G:15:LYS:NZ	7:1M:461:ASP:OD2	2.39	0.56
9:1Q:476:ARG:HH11	9:1S:292:GLY:HA3	1.70	0.56
16:1G:301:PC7:H121	16:1G:301:PC7:H322	1.88	0.55
3:1E:306:GLN:O	10:1T:75:LYS:NZ	2.33	0.55
2:1C:110:ARG:HG2	16:1G:301:PC7:H132	1.88	0.55
1:1A:24:MET:HE2	1:1A:217:SER:HB3	1.88	0.55
9:1S:56:LYS:HB3	9:1S:58:PRO:HD2	1.89	0.55
1:1A:71:ASP:OD2	3:1F:122:ARG:NH2	2.37	0.54
9:1Q:476:ARG:NH1	9:1S:291:GLY:O	2.40	0.54
2:1D:68:LEU:HB3	2:1D:73:ARG:HE	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1R:41:PRO:HG3	10:1R:51:LEU:HD12	1.89	0.54
1:1B:24:MET:HE3	1:1B:217:SER:HB3	1.90	0.54
1:1A:57:HIS:ND1	1:1A:58:VAL:O	2.41	0.54
1:1B:283:ARG:HH21	1:1B:341:ILE:HG12	1.71	0.53
7:1N:82:THR:HG21	7:1N:422:HIS:HA	1.89	0.53
7:1M:66:ASN:ND2	7:1M:265:VAL:O	2.31	0.53
3:1F:305:SER:OG	6:1L:21:GLN:NE2	2.42	0.53
7:1M:431:GLU:OE1	7:1M:438:ARG:NH1	2.39	0.53
7:1N:99:ASN:HD21	7:1N:211:ARG:HB3	1.74	0.53
7:1N:56:LEU:O	9:1S:65:ARG:NH1	2.42	0.53
1:1B:126:ILE:HG12	11:1B:402:UQ5:H171	1.90	0.52
7:1M:87:ILE:HG12	7:1M:241:MET:HG2	1.91	0.52
1:1B:336:LEU:HD11	1:1B:348:VAL:HG12	1.92	0.52
3:1E:115:SER:OG	3:1E:185:ASP:OD1	2.28	0.52
3:1F:304:LYS:NZ	10:1R:74:CYS:O	2.43	0.52
13:1B:405:CDL:H801	13:1K:101:CDL:H551	1.91	0.52
9:1Q:154:ASP:OD1	9:1Q:154:ASP:N	2.41	0.52
13:1E:401:CDL:H352	13:1E:401:CDL:H742	1.92	0.51
7:1M:178:ASP:OD1	7:1M:178:ASP:N	2.43	0.51
8:1P:17:ARG:NH1	10:1T:112:GLY:O	2.42	0.51
9:1S:475:PRO:O	9:1S:476:ARG:NE	2.37	0.51
9:1S:193:ASP:OD1	9:1S:193:ASP:N	2.42	0.51
9:1Q:102:VAL:HG22	9:1Q:255:VAL:HG22	1.92	0.51
1:1A:316:ARG:NH2	18:1A:505:HOH:O	2.42	0.51
2:1D:152:THR:OG1	2:1D:165:ARG:NH1	2.37	0.51
7:1M:88:ASN:HB2	7:1M:433:LEU:HD22	1.93	0.51
7:1N:107:HIS:HB3	7:1N:176:GLU:HG2	1.93	0.50
9:1Q:388:GLN:NE2	9:1Q:483:ARG:O	2.43	0.50
7:1M:420:SER:HG	7:1M:423:HIS:HD1	1.57	0.50
2:1C:86:GLU:HB3	2:1C:90:LYS:HD3	1.93	0.50
2:1D:189:ASP:OD1	2:1D:234:SER:OG	2.27	0.50
9:1Q:471:LEU:HD11	9:1Q:474:LEU:HD13	1.94	0.50
2:1D:78:PRO:HD2	7:1N:212:THR:HG21	1.94	0.50
9:1Q:395:THR:O	9:1Q:397:VAL:N	2.45	0.50
1:1B:88:LEU:HD12	1:1B:240:PHE:HD1	1.76	0.50
3:1E:175:ARG:NH1	3:1E:180:GLY:O	2.43	0.49
2:1C:93:PRO:O	2:1C:96:THR:OG1	2.25	0.49
2:1D:161:PRO:HD2	2:1D:204:ILE:HD11	1.95	0.49
1:1A:80:TYR:O	1:1A:84:ASN:ND2	2.39	0.49
9:1Q:305:TYR:HB2	9:1Q:468:TYR:HB3	1.94	0.49
3:1F:149:ASP:N	3:1F:149:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1B:405:CDL:H351	13:1B:405:CDL:H522	1.96	0.48
7:1N:376:ASP:HB2	7:1N:379:ARG:HH21	1.78	0.48
9:1Q:329:LYS:HE3	9:1Q:355:PHE:HA	1.95	0.48
2:1D:188:LYS:HG3	2:1D:191:ASP:H	1.78	0.48
3:1E:85:TRP:HB2	3:1E:88:GLU:HG3	1.96	0.48
7:1M:206:TYR:O	7:1M:284:ARG:NH2	2.41	0.48
2:1C:149:GLU:HA	2:1C:166:HIS:HB3	1.96	0.48
9:1S:91:THR:HG22	9:1S:93:SER:H	1.79	0.48
10:1T:82:ASP:OD1	10:1T:82:ASP:N	2.47	0.48
2:1C:184:ARG:NH1	2:1C:240:GLY:O	2.47	0.48
3:1E:232:ALA:HB3	12:1E:404:HEM:HBD2	1.96	0.48
7:1N:53:LEU:HB2	9:1S:63:PRO:HG3	1.95	0.48
2:1D:175:SER:HB2	2:1D:234:SER:HB2	1.96	0.48
3:1E:280:LYS:HD3	15:1E:403:PTY:HC52	1.96	0.47
3:1F:81:PRO:HG3	5:1J:57:ASP:HB3	1.95	0.47
12:1B:403:HEM:HBC2	12:1B:403:HEM:HHD	1.95	0.47
7:1N:309:ALA:O	7:1N:362:ASN:ND2	2.43	0.47
1:1A:35:LEU:HD22	1:1A:236:LEU:HD13	1.95	0.47
2:1C:224:CYS:HB2	2:1C:229:SER:HB2	1.96	0.47
9:1Q:332:LEU:HD13	9:1Q:367:VAL:HB	1.97	0.47
1:1B:79:ARG:NH1	12:1B:403:HEM:O2D	2.39	0.47
2:1C:100:PRO:HA	4:1G:4:ARG:HH11	1.80	0.47
10:1T:49:GLU:OE2	10:1T:52:ARG:NH1	2.47	0.47
1:1B:165:LEU:HD21	11:1B:402:UQ5:H222	1.96	0.46
3:1E:113:CYS:SG	3:1E:168:TYR:OH	2.73	0.46
9:1S:331:LEU:HD13	9:1S:390:LEU:HD11	1.97	0.46
1:1A:336:LEU:HD11	1:1A:348:VAL:HG12	1.97	0.46
11:1B:402:UQ5:H151	11:1B:402:UQ5:H203	1.96	0.46
2:1D:184:ARG:NH1	2:1D:240:GLY:O	2.39	0.46
9:1S:305:TYR:HB2	9:1S:468:TYR:HB3	1.97	0.46
7:1N:397:GLU:OE2	8:1P:23:THR:OG1	2.33	0.46
2:1D:76:MET:HE2	7:1N:187:VAL:HA	1.98	0.46
10:1T:57:ASP:OD1	10:1T:57:ASP:N	2.48	0.46
9:1Q:354:PRO:HA	9:1Q:367:VAL:HA	1.96	0.46
7:1M:179:VAL:HG21	9:1Q:343:ARG:HH12	1.80	0.46
9:1S:478:ASP:OD1	9:1S:478:ASP:N	2.45	0.46
7:1M:376:ASP:OD1	7:1M:376:ASP:N	2.48	0.46
13:1K:101:CDL:H761	13:1K:101:CDL:H791	1.67	0.46
6:1L:23:VAL:HG12	6:1L:24:ILE:HG23	1.98	0.46
2:1C:126:MET:HE3	2:1C:126:MET:HB3	1.81	0.45
3:1F:232:ALA:HB3	12:1F:402:HEM:HBD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1M:43:ARG:NH1	18:1M:609:HOH:O	2.43	0.45
1:1A:88:LEU:HD12	1:1A:240:PHE:HD1	1.81	0.45
2:1D:164:ILE:HG12	2:1D:200:VAL:HG22	1.96	0.45
7:1N:132:LEU:HD12	9:1S:339:MET:HG2	1.97	0.45
1:1B:40:LEU:HD23	11:1B:401:UQ5:H172	1.98	0.45
14:1K:102:3PH:H351	14:1K:102:3PH:H381	1.81	0.45
11:1B:401:UQ5:H201	11:1B:401:UQ5:H221	1.55	0.45
9:1Q:380:VAL:HG11	9:1Q:480:ILE:HD12	1.99	0.45
1:1A:287:ASN:HB3	1:1A:290:MET:HB2	1.99	0.45
9:1Q:93:SER:O	9:1Q:164:ARG:NH1	2.49	0.45
6:1K:6:ASN:OD1	7:1M:478:GLN:NE2	2.40	0.45
7:1M:376:ASP:OD1	7:1M:379:ARG:NH1	2.50	0.45
7:1N:441:LYS:HB3	7:1N:441:LYS:HE3	1.76	0.45
9:1S:78:SER:OG	9:1S:264:HIS:NE2	2.41	0.45
2:1D:133:ASP:N	2:1D:133:ASP:OD1	2.50	0.44
14:1E:402:3PH:H2B2	14:1E:402:3PH:H251	1.98	0.44
9:1S:163:THR:HG22	9:1S:165:LEU:H	1.82	0.44
3:1E:199:TYR:OH	12:1E:404:HEM:O2A	2.28	0.44
2:1C:64:PRO:HB3	7:1M:294:PHE:HE2	1.83	0.44
1:1B:198:ILE:HD12	11:1B:401:UQ5:H153	2.00	0.44
9:1Q:355:PHE:HE2	9:1Q:368:VAL:HG23	1.83	0.44
7:1M:32:ASP:OD1	7:1M:32:ASP:N	2.49	0.44
9:1Q:471:LEU:HD21	9:1Q:474:LEU:HB2	1.99	0.44
9:1S:119:VAL:HG11	9:1S:237:PHE:CE2	2.53	0.44
2:1C:120:ALA:HA	15:1E:403:PTY:H332	2.00	0.44
7:1M:364:HIS:CE1	7:1M:434:VAL:HG23	2.53	0.44
9:1S:75:VAL:HG21	9:1S:434:PHE:HD2	1.82	0.44
1:1B:271:PRO:HB3	11:1B:402:UQ5:C6	2.48	0.43
13:1F:401:CDL:H552	13:1F:401:CDL:H581	1.64	0.43
3:1E:233:MET:HB2	12:1E:404:HEM:C1D	2.54	0.43
9:1S:217:THR:HG23	9:1S:294:MET:HE3	1.99	0.43
2:1C:237:ILE:HD13	2:1C:242:ALA:HB3	2.00	0.43
13:1K:101:CDL:H521	13:1K:101:CDL:H552	1.85	0.43
10:1R:82:ASP:OD1	10:1R:82:ASP:N	2.50	0.43
4:1H:18:THR:HG21	8:1P:29:ALA:HB1	1.99	0.43
10:1R:119:ARG:HD3	14:1R:201:3PH:H11	2.00	0.43
7:1M:56:LEU:HD11	7:1M:415:MET:HE1	2.01	0.43
7:1N:454:ASN:OD1	7:1N:457:ARG:NH2	2.50	0.43
8:1P:45:TRP:HB2	8:1P:47:TRP:H	1.83	0.43
10:1R:24:VAL:O	10:1R:28:LEU:N	2.49	0.43
2:1C:57:ASP:OD1	7:1M:190:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1E:106:TYR:HA	3:1E:110:CYS:SG	2.59	0.43
7:1M:225:ARG:HA	7:1M:228:LEU:HD12	1.99	0.43
7:1N:76:PRO:HG2	9:1S:92:VAL:HG21	2.01	0.43
2:1C:162:VAL:HG22	2:1C:202:VAL:HG22	2.01	0.43
4:1G:50:LYS:NZ	18:1G:401:HOH:O	2.51	0.43
9:1S:435:SER:OG	9:1S:438:GLU:OE1	2.24	0.42
1:1B:147:ILE:HD13	1:1B:147:ILE:HA	1.81	0.42
7:1M:405:ARG:NH1	7:1M:409:GLN:OE1	2.40	0.42
9:1S:72:LYS:HD2	9:1S:73:PRO:HD2	2.00	0.42
11:1B:401:UQ5:H151	11:1B:401:UQ5:H171	1.77	0.42
3:1E:81:PRO:HG3	5:1I:57:ASP:HB3	2.00	0.42
16:1H:101:PC7:H201	16:1H:101:PC7:H362	2.01	0.42
7:1N:174:ASP:OD1	7:1N:177:ARG:NH1	2.45	0.42
1:1B:69:MET:HE1	1:1B:80:TYR:CZ	2.55	0.42
7:1M:126:GLU:OE1	9:1Q:336:ARG:NH1	2.53	0.42
9:1Q:383:LEU:HD23	9:1Q:383:LEU:HA	1.90	0.42
1:1A:88:LEU:HD23	1:1A:88:LEU:HA	1.88	0.42
7:1N:469:MET:HE1	7:1N:487:ARG:HA	2.01	0.42
13:1B:408:CDL:H141	13:1B:408:CDL:H172	1.86	0.42
6:1L:9:LEU:HD21	10:1R:67:ARG:HD3	2.01	0.42
7:1M:311:TRP:NE1	7:1M:362:ASN:O	2.53	0.42
1:1B:133:VAL:HA	1:1B:140:SER:HB3	2.02	0.42
7:1N:101:VAL:HG23	7:1N:228:LEU:HD23	2.00	0.42
4:1G:25:LEU:HD12	8:1O:36:VAL:HG12	2.02	0.42
7:1M:311:TRP:CD1	7:1M:434:VAL:HG21	2.55	0.42
7:1N:322:MET:HG3	7:1N:456:ILE:HD12	2.01	0.42
8:1P:23:THR:HA	8:1P:26:ARG:HG2	2.02	0.42
9:1Q:220:GLU:OE2	9:1Q:288:ARG:NH2	2.53	0.42
1:1B:287:ASN:HB3	1:1B:290:MET:HB2	2.01	0.42
7:1M:124:GLU:HG2	7:1M:158:ILE:HD11	2.02	0.42
13:1B:405:CDL:H522	13:1B:405:CDL:H332	2.02	0.41
13:1B:408:CDL:H152	13:1B:408:CDL:H121	1.74	0.41
7:1N:329:TRP:HB2	7:1N:344:VAL:HG13	2.02	0.41
1:1B:247:TYR:HB3	1:1B:250:LEU:HB2	2.02	0.41
7:1M:452:ASP:OD1	7:1M:452:ASP:N	2.50	0.41
8:1O:20:SER:OG	8:1O:21:ILE:N	2.53	0.41
1:1B:325:THR:HG23	6:1K:52:LEU:HD13	2.02	0.41
2:1D:229:SER:HB3	2:1D:241:PRO:HD2	2.02	0.41
11:1A:402:UQ5:H201	11:1A:402:UQ5:H222	1.80	0.41
2:1D:113:TYR:HB3	16:1H:101:PC7:H152	2.01	0.41
7:1N:190:GLN:HB2	7:1N:193:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1Q:370:SER:OG	9:1Q:371:GLY:N	2.53	0.41
2:1C:157:TRP:CE2	2:1C:158:ARG:HD3	2.55	0.41
2:1C:172:ILE:HD11	2:1C:197:LYS:HA	2.03	0.41
13:1K:101:CDL:H341	13:1K:101:CDL:H312	1.88	0.41
9:1Q:103:GLU:HB2	9:1Q:254:ARG:HB3	2.02	0.41
13:1A:405:CDL:H312	13:1A:405:CDL:H342	1.90	0.41
1:1B:142:TRP:HB3	1:1B:269:ILE:HD13	2.03	0.41
1:1B:234:LEU:HD23	1:1B:234:LEU:HA	1.87	0.41
7:1M:92:ARG:NH1	7:1M:139:GLU:OE2	2.49	0.41
7:1N:33:ALA:HB3	7:1N:36:PHE:HB2	2.03	0.41
1:1B:335:TRP:O	1:1B:339:ASN:ND2	2.54	0.41
3:1F:195:ASN:OD1	3:1F:198:ASN:ND2	2.52	0.41
3:1F:297:ARG:HD3	6:1L:24:ILE:HG22	2.02	0.41
7:1N:84:GLY:HA3	7:1N:144:TYR:HA	2.03	0.41
9:1Q:479:SER:HA	9:1Q:482:LYS:HD3	2.03	0.41
10:1T:46:ASP:OD1	10:1T:117:TYR:OH	2.36	0.41
1:1B:239:VAL:HG13	14:1B:406:3PH:H361	2.03	0.41
3:1F:208:ARG:HE	3:1F:208:ARG:HB3	1.73	0.41
2:1D:202:VAL:HG23	2:1D:249:PRO:HD3	2.03	0.40
14:1K:103:3PH:H232	14:1K:103:3PH:H332	2.03	0.40
7:1N:225:ARG:HA	7:1N:228:LEU:HD12	2.03	0.40
1:1B:279:TYR:CZ	1:1B:283:ARG:HD2	2.55	0.40
7:1N:75:ILE:HA	7:1N:76:PRO:HD3	1.96	0.40
7:1N:365:ASP:OD1	7:1N:365:ASP:N	2.53	0.40
3:1F:233:MET:HB2	12:1F:402:HEM:C1D	2.56	0.40
7:1M:77:PHE:HE2	9:1Q:69:PRO:HG2	1.86	0.40
1:1B:88:LEU:HD23	1:1B:91:ILE:HD12	2.03	0.40
3:1E:73:GLU:HG3	6:1K:68:ARG:HE	1.87	0.40
5:1J:29:LYS:HA	5:1J:29:LYS:HD2	1.83	0.40
9:1Q:75:VAL:HG21	9:1Q:434:PHE:HD2	1.86	0.40
1:1A:147:ILE:HD13	1:1A:147:ILE:HA	1.80	0.40
1:1B:52:MET:SD	2:1C:128:LEU:HD21	2.62	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	1A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	1B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
2	1C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	1D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
3	1E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	1F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
4	1G	57/60 (95%)	57 (100%)	0	0	100	100
4	1H	57/60 (95%)	57 (100%)	0	0	100	100
5	1I	66/69 (96%)	66 (100%)	0	0	100	100
5	1J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	1K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	1L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
7	1M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	1N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	58
8	1O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	1P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
9	1Q	439/485 (90%)	418 (95%)	20 (5%)	1 (0%)	43	58
9	1S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	37
10	1R	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
10	1T	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
All	All	4156/4642 (90%)	4047 (97%)	105 (2%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP
9	1S	66	THR
7	1N	187	VAL
9	1S	475	PRO

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	1A	312/317 (98%)	312 (100%)	0	100	100
1	1B	312/317 (98%)	312 (100%)	0	100	100
2	1C	171/213 (80%)	171 (100%)	0	100	100
2	1D	171/213 (80%)	171 (100%)	0	100	100
3	1E	191/238 (80%)	191 (100%)	0	100	100
3	1F	191/238 (80%)	191 (100%)	0	100	100
4	1G	52/53 (98%)	52 (100%)	0	100	100
4	1H	52/53 (98%)	52 (100%)	0	100	100
5	1I	58/59 (98%)	58 (100%)	0	100	100
5	1J	58/59 (98%)	58 (100%)	0	100	100
6	1K	62/64 (97%)	62 (100%)	0	100	100
6	1L	62/64 (97%)	62 (100%)	0	100	100
7	1M	390/413 (94%)	390 (100%)	0	100	100
7	1N	390/413 (94%)	390 (100%)	0	100	100
8	1O	38/47 (81%)	38 (100%)	0	100	100
8	1P	38/47 (81%)	38 (100%)	0	100	100
9	1Q	333/362 (92%)	333 (100%)	0	100	100
9	1S	333/362 (92%)	333 (100%)	0	100	100
10	1R	106/107 (99%)	106 (100%)	0	100	100
10	1T	106/107 (99%)	106 (100%)	0	100	100
All	All	3426/3746 (92%)	3426 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	66	GLN

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Mol	Chain	Res	Type
1	1A	213	ASN
1	1A	339	ASN
1	1A	376	HIS
1	1B	43	GLN
1	1B	67	HIS
1	1B	108	GLN
1	1B	173	ASN
1	1B	177	ASN
1	1B	215	GLN
1	1B	261	ASN
1	1B	268	HIS
1	1B	287	ASN
2	1C	72	ASN
2	1C	207	HIS
3	1E	79	HIS
3	1F	178	ASN
4	1G	11	GLN
5	1J	12	GLN
5	1J	20	HIS
6	1L	26	GLN
7	1M	190	GLN
7	1M	224	ASN
7	1M	422	HIS
7	1N	49	HIS
7	1N	99	ASN
7	1N	165	ASN
7	1N	190	GLN
7	1N	198	HIS
7	1N	291	HIS
9	1Q	166	ASN
9	1Q	211	ASN
9	1Q	225	HIS
10	1R	95	GLN
9	1S	130	ASN
9	1S	198	GLN
9	1S	202	GLN
9	1S	211	ASN
9	1S	280	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\#\|Z\| > 2$
14	3PH	1K	102	-	47,47,47	0.64	1 (2%)	51,52,52	0.60	2 (3%)
11	UQ5	1A	401	-	38,38,38	0.53	0	46,49,49	1.08	4 (8%)
13	CDL	1K	101	-	78,78,99	0.42	0	84,90,111	0.28	0
14	3PH	1E	402	-	39,39,47	0.70	1 (2%)	43,44,52	0.64	0
13	CDL	1F	401	-	55,55,99	0.42	0	61,67,111	0.27	0
16	PC7	1H	101	-	38,38,51	0.57	0	44,46,59	0.56	0
14	3PH	1A	406	-	30,30,47	0.78	1 (3%)	34,35,52	0.69	1 (2%)
13	CDL	1A	405	-	58,58,99	0.44	0	64,70,111	0.27	0
14	3PH	1K	103	-	31,31,47	0.78	1 (3%)	35,36,52	0.66	1 (2%)
14	3PH	1R	201	10	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
12	HEM	1E	404	3	50,50,50	2.14	10 (20%)	66,82,82	1.47	7 (10%)
12	HEM	1A	403	1	50,50,50	1.49	7 (14%)	66,82,82	1.38	8 (12%)
14	3PH	1B	407	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	0
15	PTY	1E	403	-	33,33,49	0.55	0	36,38,54	0.50	0
12	HEM	1A	404	1	50,50,50	1.31	7 (14%)	66,82,82	1.29	8 (12%)
13	CDL	1M	501	-	53,53,99	0.49	1 (1%)	59,65,111	0.26	0
12	HEM	1F	402	3	50,50,50	2.09	8 (16%)	66,82,82	1.52	10 (15%)
12	HEM	1B	404	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	8 (12%)
11	UQ5	1A	402	-	38,38,38	0.53	0	46,49,49	0.67	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	UQ5	1B	402	-	38,38,38	0.51	0	46,49,49	1.52	6 (13%)
13	CDL	1B	405	-	63,63,99	0.44	1 (1%)	69,75,111	0.25	0
13	CDL	1L	101	-	58,58,99	0.43	0	64,70,111	0.35	0
16	PC7	1G	301	-	35,35,51	0.61	0	41,43,59	0.60	1 (2%)
11	UQ5	1B	401	-	38,38,38	0.46	0	46,49,49	0.73	1 (2%)
14	3PH	1B	406	-	47,47,47	0.63	1 (2%)	51,52,52	0.61	1 (1%)
12	HEM	1B	403	1	50,50,50	1.42	8 (16%)	66,82,82	1.36	10 (15%)
13	CDL	1B	408	1	70,70,99	0.34	0	76,82,111	0.34	0
15	PTY	1F	403	-	37,37,49	0.51	0	40,42,54	0.44	0
13	CDL	1E	401	-	52,52,99	0.44	0	58,64,111	0.25	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
14	3PH	1K	102	-	-	15/49/49/49	-
11	UQ5	1A	401	-	-	10/33/57/57	0/1/1/1
13	CDL	1K	101	-	-	59/89/89/110	-
14	3PH	1E	402	-	-	17/41/41/49	-
13	CDL	1F	401	-	-	32/66/66/110	-
16	PC7	1H	101	-	-	19/42/42/55	-
14	3PH	1A	406	-	-	13/32/32/49	-
13	CDL	1A	405	-	-	34/69/69/110	-
14	3PH	1K	103	-	-	13/33/33/49	-
14	3PH	1R	201	10	-	13/38/38/49	-
12	HEM	1E	404	3	-	4/14/54/54	-
12	HEM	1A	403	1	-	3/14/54/54	-
14	3PH	1B	407	-	-	18/49/49/49	-
15	PTY	1E	403	-	-	15/37/37/53	-
12	HEM	1A	404	1	-	4/14/54/54	-
13	CDL	1M	501	-	-	31/64/64/110	-
12	HEM	1F	402	3	-	4/14/54/54	-
12	HEM	1B	404	1	-	4/14/54/54	-
11	UQ5	1A	402	-	-	9/33/57/57	0/1/1/1
11	UQ5	1B	402	-	-	10/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	1B	405	-	-	49/74/74/110	-
13	CDL	1L	101	-	-	43/69/69/110	-
16	PC7	1G	301	-	-	16/39/39/55	-
11	UQ5	1B	401	-	-	7/33/57/57	0/1/1/1
14	3PH	1B	406	-	-	22/49/49/49	-
12	HEM	1B	403	1	-	4/14/54/54	-
13	CDL	1B	408	1	-	45/81/81/110	-
15	PTY	1F	403	-	-	17/41/41/53	-
13	CDL	1E	401	-	-	41/63/63/110	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1E	404	HEM	C3D-C2D	7.85	1.53	1.36
12	1F	402	HEM	C3D-C2D	7.73	1.53	1.36
12	1F	402	HEM	CBC-CAC	4.94	1.54	1.30
12	1E	404	HEM	CBC-CAC	4.89	1.54	1.30
12	1F	402	HEM	FE-ND	4.88	2.10	1.94
12	1F	402	HEM	CBB-CAB	4.88	1.54	1.30
12	1E	404	HEM	CBB-CAB	4.86	1.54	1.30
12	1E	404	HEM	FE-NB	4.66	2.09	1.94
12	1F	402	HEM	FE-NB	4.65	2.09	1.94
12	1E	404	HEM	FE-ND	4.33	2.08	1.94
12	1A	403	HEM	FE-NC	4.00	2.08	1.95
12	1A	403	HEM	FE-NA	3.97	2.08	1.95
12	1E	404	HEM	FE-NC	3.62	2.07	1.95
12	1B	404	HEM	FE-NB	3.43	2.05	1.94
14	1K	103	3PH	P-O11	3.40	1.71	1.60
14	1B	407	3PH	P-O11	3.35	1.71	1.60
12	1B	403	HEM	FE-NC	3.34	2.06	1.95
14	1A	406	3PH	P-O11	3.33	1.70	1.60
12	1B	403	HEM	FE-NA	3.32	2.06	1.95
14	1K	102	3PH	P-O11	3.31	1.70	1.60
14	1E	402	3PH	P-O11	3.29	1.70	1.60
12	1A	403	HEM	FE-ND	3.27	2.05	1.94
12	1B	403	HEM	CAB-C3B	3.24	1.56	1.47
14	1B	406	3PH	P-O11	3.24	1.70	1.60
14	1R	201	3PH	P-O11	3.19	1.70	1.60
12	1F	402	HEM	CAB-C3B	3.10	1.55	1.47
12	1B	404	HEM	CAB-C3B	3.08	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1A	403	HEM	CAB-C3B	3.07	1.55	1.47
12	1E	404	HEM	FE-NA	3.07	2.05	1.95
12	1A	404	HEM	FE-ND	2.99	2.04	1.94
12	1B	404	HEM	CAC-C3C	2.98	1.55	1.47
12	1A	404	HEM	CAB-C3B	2.96	1.55	1.47
12	1B	403	HEM	CAC-C3C	2.92	1.55	1.47
12	1A	403	HEM	CAC-C3C	2.90	1.55	1.47
12	1A	404	HEM	CAC-C3C	2.89	1.55	1.47
12	1B	403	HEM	FE-ND	2.84	2.03	1.94
12	1B	404	HEM	FE-ND	2.76	2.03	1.94
12	1E	404	HEM	CAC-C3C	2.73	1.54	1.47
12	1E	404	HEM	CAB-C3B	2.72	1.54	1.47
12	1B	404	HEM	FE-NA	2.71	2.04	1.95
12	1F	402	HEM	CAC-C3C	2.66	1.54	1.47
12	1B	403	HEM	FE-NB	2.52	2.02	1.94
12	1A	404	HEM	FE-NC	2.41	2.03	1.95
13	1M	501	CDL	PB2-OB4	-2.31	1.44	1.55
12	1A	404	HEM	FE-NA	2.28	2.02	1.95
12	1B	404	HEM	FE-NC	2.27	2.02	1.95
12	1A	404	HEM	FE-NB	2.24	2.01	1.94
12	1A	403	HEM	FE-NB	2.14	2.01	1.94
12	1E	404	HEM	C2A-C3A	-2.13	1.33	1.38
12	1B	404	HEM	C2A-C3A	-2.11	1.33	1.38
12	1B	403	HEM	C3C-C2C	-2.08	1.33	1.37
12	1F	402	HEM	FE-NA	2.06	2.02	1.95
12	1B	403	HEM	C2A-C3A	-2.04	1.33	1.38
12	1A	404	HEM	C2A-C3A	-2.01	1.33	1.38
12	1A	403	HEM	C2A-C3A	-2.01	1.33	1.38
13	1B	405	CDL	PA1-OA4	-2.00	1.45	1.55

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1E	404	HEM	C4D-ND-C1D	6.28	111.56	105.07
12	1F	402	HEM	C4D-ND-C1D	5.44	110.69	105.07
11	1B	402	UQ5	C7-C6-C5	5.13	124.65	118.48
11	1B	402	UQ5	C6-C1-C2	4.44	122.69	119.18
12	1A	403	HEM	C3B-C2B-C1B	4.37	109.72	106.49
12	1A	403	HEM	CMB-C2B-C1B	-4.03	118.89	125.04
11	1B	402	UQ5	C8-C7-C6	3.61	121.78	112.05
11	1A	401	UQ5	C8-C7-C6	3.53	121.57	112.05
12	1F	402	HEM	CAA-CBA-CGA	-3.45	106.19	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	1A	401	UQ5	C7-C6-C5	3.44	122.61	118.48
12	1B	403	HEM	C3B-C2B-C1B	3.18	108.85	106.49
12	1B	403	HEM	C4C-NC-C1C	3.16	108.44	105.35
12	1A	403	HEM	CHB-C1B-NB	3.15	128.26	124.37
12	1F	402	HEM	C3B-C2B-C1B	3.12	108.80	106.49
12	1E	404	HEM	CBB-CAB-C3B	-3.07	112.35	127.62
12	1F	402	HEM	CHD-C4C-NC	2.99	127.67	124.44
12	1A	404	HEM	C4D-ND-C1D	2.95	108.12	105.07
12	1E	404	HEM	CBC-CAC-C3C	-2.94	112.97	127.62
11	1A	401	UQ5	C6-C1-C2	2.94	121.51	119.18
12	1A	403	HEM	C4D-ND-C1D	2.90	108.06	105.07
12	1B	403	HEM	C4D-ND-C1D	2.89	108.06	105.07
11	1B	402	UQ5	O5-C5-C4	-2.88	114.81	120.93
12	1F	402	HEM	CBC-CAC-C3C	-2.82	113.60	127.62
11	1A	402	UQ5	C7-C6-C5	-2.81	115.10	118.48
12	1F	402	HEM	C4A-NA-C1A	2.79	108.08	105.35
12	1E	404	HEM	CAA-CBA-CGA	-2.75	107.67	113.60
12	1A	404	HEM	CMC-C2C-C1C	-2.73	119.90	124.71
12	1B	404	HEM	C4D-ND-C1D	2.71	107.87	105.07
12	1B	404	HEM	C4A-NA-C1A	2.69	107.98	105.35
12	1B	403	HEM	CAC-C3C-C4C	2.66	131.31	124.90
12	1A	404	HEM	C4A-NA-C1A	2.64	107.94	105.35
12	1A	403	HEM	CHD-C1D-ND	2.48	127.11	124.42
11	1A	401	UQ5	C7-C8-C9	-2.45	122.71	126.79
12	1E	404	HEM	C4A-NA-C1A	2.39	107.69	105.35
11	1B	402	UQ5	C1-C6-C5	-2.38	117.34	119.58
12	1A	404	HEM	C2A-C1A-NA	-2.38	107.49	110.15
12	1B	404	HEM	C3D-C4D-ND	-2.36	107.54	110.17
12	1B	403	HEM	CHD-C4C-C3C	2.36	129.29	125.26
12	1B	403	HEM	CAC-C3C-C2C	-2.35	120.85	128.60
12	1B	404	HEM	C1B-NB-C4B	2.35	107.50	105.07
12	1A	403	HEM	C1B-NB-C4B	2.34	107.49	105.07
12	1A	403	HEM	C4C-NC-C1C	2.31	107.61	105.35
12	1E	404	HEM	CAD-CBD-CGD	-2.27	108.72	113.60
14	1R	201	3PH	O13-P-O11	-2.26	100.71	106.73
12	1B	404	HEM	C2A-C1A-NA	-2.26	107.62	110.15
12	1A	404	HEM	C3D-C4D-ND	-2.26	107.65	110.17
12	1A	404	HEM	CMB-C2B-C1B	-2.25	121.61	125.04
12	1B	404	HEM	CMC-C2C-C1C	-2.25	120.76	124.71
14	1B	406	3PH	O13-P-O11	-2.24	100.78	106.73
12	1F	402	HEM	C4C-NC-C1C	2.22	107.52	105.35
14	1K	103	3PH	O13-P-O11	-2.22	100.84	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1F	402	HEM	C1B-NB-C4B	2.20	107.35	105.07
14	1A	406	3PH	O13-P-O11	-2.19	100.90	106.73
12	1B	403	HEM	CBD-CAD-C3D	-2.19	106.56	112.63
12	1A	404	HEM	C4C-NC-C1C	2.18	107.48	105.35
12	1B	404	HEM	CBD-CAD-C3D	-2.16	106.64	112.63
12	1B	403	HEM	C4A-NA-C1A	2.15	107.46	105.35
11	1B	401	UQ5	C7-C6-C5	-2.15	115.89	118.48
11	1B	402	UQ5	O5-C5-C6	2.14	125.31	121.55
12	1B	403	HEM	C3D-C4D-ND	-2.13	107.80	110.17
12	1F	402	HEM	CAD-CBD-CGD	-2.13	109.02	113.60
14	1K	102	3PH	O13-P-O11	-2.12	101.10	106.73
12	1F	402	HEM	C2A-C1A-NA	-2.07	107.84	110.15
12	1A	404	HEM	CHB-C4A-NA	2.06	127.63	123.85
16	1G	301	PC7	C3-C2-C1	2.04	116.62	111.79
12	1E	404	HEM	CHA-C4D-ND	2.02	126.87	124.37
14	1K	102	3PH	O14-P-O13	2.02	115.35	107.64
12	1A	403	HEM	C2D-C1D-ND	-2.01	107.47	109.88
12	1B	403	HEM	CAA-CBA-CGA	-2.01	109.29	113.60
12	1B	404	HEM	CAC-C3C-C4C	-2.00	120.06	124.90

There are no chirality outliers.

All (571) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	1A	401	UQ5	C1-C6-C7-C8
11	1A	401	UQ5	C5-C6-C7-C8
11	1A	401	UQ5	C9-C11-C12-C13
11	1A	401	UQ5	C24-C26-C27-C28
11	1A	402	UQ5	C14-C16-C17-C18
11	1B	401	UQ5	C9-C11-C12-C13
11	1B	401	UQ5	C20-C19-C21-C22
11	1B	401	UQ5	C19-C21-C22-C23
11	1B	402	UQ5	C1-C6-C7-C8
11	1B	402	UQ5	C5-C6-C7-C8
11	1B	402	UQ5	C13-C14-C16-C17
11	1B	402	UQ5	C15-C14-C16-C17
11	1B	402	UQ5	C14-C16-C17-C18
11	1B	402	UQ5	C19-C21-C22-C23
11	1B	402	UQ5	C24-C26-C27-C28
12	1E	404	HEM	C2B-C3B-CAB-CBB
12	1E	404	HEM	C2C-C3C-CAC-CBC
12	1E	404	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
12	1F	402	HEM	C2B-C3B-CAB-CBB
12	1F	402	HEM	C2C-C3C-CAC-CBC
13	1A	405	CDL	O1-C1-CB2-OB2
13	1A	405	CDL	CA3-OA5-PA1-OA3
13	1A	405	CDL	CA3-OA5-PA1-OA4
13	1A	405	CDL	CB2-OB2-PB2-OB3
13	1A	405	CDL	CB2-OB2-PB2-OB4
13	1A	405	CDL	CB2-OB2-PB2-OB5
13	1A	405	CDL	CB3-OB5-PB2-OB4
13	1A	405	CDL	C51-CB5-OB6-CB4
13	1B	405	CDL	CA3-OA5-PA1-OA4
13	1B	405	CDL	C11-CA5-OA6-CA4
13	1B	405	CDL	CB3-OB5-PB2-OB3
13	1B	405	CDL	OB7-CB5-OB6-CB4
13	1B	405	CDL	C51-CB5-OB6-CB4
13	1B	408	CDL	CA2-OA2-PA1-OA3
13	1B	408	CDL	CA2-OA2-PA1-OA4
13	1B	408	CDL	CA2-OA2-PA1-OA5
13	1B	408	CDL	OA6-CA4-CA6-OA8
13	1B	408	CDL	OA7-CA5-OA6-CA4
13	1E	401	CDL	O1-C1-CB2-OB2
13	1E	401	CDL	CA2-OA2-PA1-OA3
13	1E	401	CDL	CA2-OA2-PA1-OA4
13	1E	401	CDL	CA3-OA5-PA1-OA3
13	1E	401	CDL	C11-CA5-OA6-CA4
13	1E	401	CDL	CB2-OB2-PB2-OB3
13	1E	401	CDL	CB2-OB2-PB2-OB4
13	1E	401	CDL	OB7-CB5-OB6-CB4
13	1E	401	CDL	C51-CB5-OB6-CB4
13	1F	401	CDL	CA3-OA5-PA1-OA2
13	1F	401	CDL	CA3-OA5-PA1-OA3
13	1F	401	CDL	CA3-OA5-PA1-OA4
13	1F	401	CDL	CB2-OB2-PB2-OB3
13	1F	401	CDL	CB2-OB2-PB2-OB4
13	1F	401	CDL	CB2-OB2-PB2-OB5
13	1F	401	CDL	OB5-CB3-CB4-OB6
13	1F	401	CDL	C51-CB5-OB6-CB4
13	1K	101	CDL	CA3-OA5-PA1-OA2
13	1K	101	CDL	CB2-OB2-PB2-OB3
13	1K	101	CDL	CB2-OB2-PB2-OB4
13	1K	101	CDL	CB3-OB5-PB2-OB3
13	1L	101	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
13	1L	101	CDL	CA3-OA5-PA1-OA3
13	1L	101	CDL	OA7-CA5-OA6-CA4
13	1L	101	CDL	CB2-OB2-PB2-OB3
13	1L	101	CDL	CB2-OB2-PB2-OB4
13	1L	101	CDL	CB3-OB5-PB2-OB2
13	1L	101	CDL	CB3-OB5-PB2-OB3
13	1L	101	CDL	CB3-OB5-PB2-OB4
13	1M	501	CDL	CA2-OA2-PA1-OA3
13	1M	501	CDL	CA2-OA2-PA1-OA4
13	1M	501	CDL	CA2-OA2-PA1-OA5
13	1M	501	CDL	OB6-CB4-CB6-OB8
13	1M	501	CDL	C51-CB5-OB6-CB4
14	1A	406	3PH	C22-C21-O21-C2
14	1B	406	3PH	C1-O11-P-O13
14	1B	406	3PH	C1-O11-P-O14
14	1B	406	3PH	C1-O11-P-O12
14	1B	407	3PH	C1-O11-P-O13
14	1B	407	3PH	C1-O11-P-O14
14	1B	407	3PH	C1-O11-P-O12
14	1E	402	3PH	C1-O11-P-O13
14	1E	402	3PH	C1-O11-P-O14
14	1E	402	3PH	C1-O11-P-O12
14	1E	402	3PH	O21-C2-C3-O31
14	1K	103	3PH	C1-O11-P-O13
14	1K	103	3PH	C1-O11-P-O14
14	1K	103	3PH	C1-O11-P-O12
15	1F	403	PTY	C3-O11-P1-O12
16	1G	301	PC7	C4-O4P-P-O2P
16	1H	101	PC7	C1-O3P-P-O2P
16	1H	101	PC7	C4-O4P-P-O2P
16	1H	101	PC7	O4P-C4-C5-N
13	1M	501	CDL	OA9-CA7-OA8-CA6
13	1F	401	CDL	OB9-CB7-OB8-CB6
13	1K	101	CDL	OB9-CB7-OB8-CB6
14	1B	406	3PH	O32-C31-O31-C3
14	1B	407	3PH	O32-C31-O31-C3
13	1A	405	CDL	OB7-CB5-OB6-CB4
13	1B	405	CDL	OA7-CA5-OA6-CA4
13	1E	401	CDL	OA7-CA5-OA6-CA4
13	1F	401	CDL	OB7-CB5-OB6-CB4
13	1K	101	CDL	OB7-CB5-OB6-CB4
13	1M	501	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
14	1A	406	3PH	O22-C21-O21-C2
15	1E	403	PTY	O30-C30-O4-C1
13	1E	401	CDL	C71-CB7-OB8-CB6
13	1F	401	CDL	C71-CB7-OB8-CB6
13	1M	501	CDL	C31-CA7-OA8-CA6
14	1B	407	3PH	C32-C31-O31-C3
13	1B	408	CDL	C11-CA5-OA6-CA4
13	1K	101	CDL	C51-CB5-OB6-CB4
13	1L	101	CDL	C11-CA5-OA6-CA4
11	1B	401	UQ5	C15-C14-C16-C17
11	1B	401	UQ5	C18-C19-C21-C22
13	1B	405	CDL	C31-CA7-OA8-CA6
13	1K	101	CDL	C71-CB7-OB8-CB6
14	1B	406	3PH	C32-C31-O31-C3
14	1R	201	3PH	C32-C31-O31-C3
15	1E	403	PTY	C31-C30-O4-C1
13	1E	401	CDL	OB9-CB7-OB8-CB6
13	1B	405	CDL	O1-C1-CA2-OA2
13	1F	401	CDL	O1-C1-CB2-OB2
13	1K	101	CDL	O1-C1-CA2-OA2
13	1L	101	CDL	O1-C1-CB2-OB2
14	1R	201	3PH	O32-C31-O31-C3
13	1L	101	CDL	C51-CB5-OB6-CB4
13	1B	405	CDL	OA9-CA7-OA8-CA6
16	1H	101	PC7	C12-C11-O3-C3
13	1A	405	CDL	C11-CA5-OA6-CA4
13	1F	401	CDL	CA2-C1-CB2-OB2
13	1L	101	CDL	CA2-C1-CB2-OB2
13	1L	101	CDL	OB7-CB5-OB6-CB4
13	1L	101	CDL	C31-CA7-OA8-CA6
14	1E	402	3PH	C32-C31-O31-C3
14	1K	102	3PH	C32-C31-O31-C3
16	1H	101	PC7	O11-C11-O3-C3
13	1K	101	CDL	C76-C77-C78-C79
13	1F	401	CDL	C55-C56-C57-C58
15	1E	403	PTY	C8-C11-C12-C13
16	1H	101	PC7	C31-C32-C33-C34
13	1L	101	CDL	OA9-CA7-OA8-CA6
13	1K	101	CDL	C52-C53-C54-C55
13	1B	408	CDL	CA7-C31-C32-C33
13	1E	401	CDL	CB7-C71-C72-C73
13	1B	405	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
13	1M	501	CDL	CB5-C51-C52-C53
12	1B	404	HEM	C2A-CAA-CBA-CGA
13	1K	101	CDL	C33-C34-C35-C36
11	1A	401	UQ5	C14-C16-C17-C18
11	1A	402	UQ5	C9-C11-C12-C13
13	1B	408	CDL	O1-C1-CB2-OB2
14	1K	102	3PH	O32-C31-O31-C3
14	1E	402	3PH	O32-C31-O31-C3
13	1F	401	CDL	C11-CA5-OA6-CA4
16	1G	301	PC7	C32-C31-O2-C2
13	1A	405	CDL	CA3-OA5-PA1-OA2
13	1B	405	CDL	CA3-OA5-PA1-OA2
13	1B	405	CDL	CB2-OB2-PB2-OB5
13	1B	405	CDL	CB3-OB5-PB2-OB2
13	1B	408	CDL	CA3-OA5-PA1-OA2
13	1E	401	CDL	CA2-OA2-PA1-OA5
13	1E	401	CDL	CB2-OB2-PB2-OB5
13	1E	401	CDL	CB3-OB5-PB2-OB2
13	1K	101	CDL	CB2-OB2-PB2-OB5
13	1K	101	CDL	CB3-OB5-PB2-OB2
13	1L	101	CDL	CA2-OA2-PA1-OA5
13	1L	101	CDL	CA3-OA5-PA1-OA2
13	1L	101	CDL	CB2-OB2-PB2-OB5
13	1M	501	CDL	CB3-OB5-PB2-OB2
15	1E	403	PTY	C3-O11-P1-O14
15	1F	403	PTY	C3-O11-P1-O14
16	1G	301	PC7	C4-O4P-P-O3P
16	1H	101	PC7	C4-O4P-P-O3P
13	1A	405	CDL	CA2-C1-CB2-OB2
13	1B	405	CDL	CB2-C1-CA2-OA2
13	1B	408	CDL	CA2-C1-CB2-OB2
13	1E	401	CDL	CA2-C1-CB2-OB2
13	1A	405	CDL	OA7-CA5-OA6-CA4
13	1F	401	CDL	OA7-CA5-OA6-CA4
14	1R	201	3PH	C22-C21-O21-C2
13	1B	405	CDL	C32-C33-C34-C35
13	1K	101	CDL	C81-C82-C83-C84
13	1A	405	CDL	C32-C33-C34-C35
13	1L	101	CDL	C51-C52-C53-C54
16	1G	301	PC7	O31-C31-O2-C2
13	1K	101	CDL	C57-C58-C59-C60
13	1L	101	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	1B	408	CDL	C1-CA2-OA2-PA1
13	1B	408	CDL	C51-C52-C53-C54
14	1K	102	3PH	C36-C37-C38-C39
13	1K	101	CDL	O1-C1-CB2-OB2
13	1B	408	CDL	C72-C73-C74-C75
13	1K	101	CDL	C32-C33-C34-C35
16	1H	101	PC7	C18-C19-C20-C21
11	1A	401	UQ5	C20-C19-C21-C22
11	1A	402	UQ5	C25-C24-C26-C27
11	1B	401	UQ5	C13-C14-C16-C17
13	1L	101	CDL	CA5-C11-C12-C13
13	1B	408	CDL	C32-C33-C34-C35
14	1B	406	3PH	C38-C39-C3A-C3B
14	1R	201	3PH	C33-C34-C35-C36
14	1R	201	3PH	O22-C21-O21-C2
13	1L	101	CDL	C52-C53-C54-C55
13	1A	405	CDL	CB5-C51-C52-C53
13	1B	408	CDL	C52-C53-C54-C55
13	1K	101	CDL	C72-C73-C74-C75
13	1K	101	CDL	C75-C76-C77-C78
14	1K	103	3PH	C37-C38-C39-C3A
14	1B	406	3PH	C34-C35-C36-C37
15	1E	403	PTY	N1-C2-C3-O11
13	1K	101	CDL	C11-C12-C13-C14
13	1F	401	CDL	CA5-C11-C12-C13
13	1A	405	CDL	C52-C53-C54-C55
13	1E	401	CDL	C31-CA7-OA8-CA6
13	1B	408	CDL	C73-C74-C75-C76
13	1L	101	CDL	C74-C75-C76-C77
14	1E	402	3PH	C2B-C2C-C2D-C2E
13	1B	408	CDL	C71-C72-C73-C74
13	1F	401	CDL	C51-C52-C53-C54
11	1A	401	UQ5	C18-C19-C21-C22
14	1A	406	3PH	C2A-C2B-C2C-C2D
13	1B	405	CDL	O1-C1-CB2-OB2
13	1B	408	CDL	C16-C17-C18-C19
15	1F	403	PTY	C34-C35-C36-C37
14	1B	406	3PH	C33-C34-C35-C36
13	1L	101	CDL	CB7-C71-C72-C73
13	1M	501	CDL	CA5-C11-C12-C13
14	1K	102	3PH	C23-C24-C25-C26
12	1B	403	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	1F	403	PTY	C31-C32-C33-C34
11	1A	401	UQ5	C13-C14-C16-C17
11	1A	402	UQ5	C23-C24-C26-C27
13	1E	401	CDL	OA9-CA7-OA8-CA6
14	1K	102	3PH	O22-C21-O21-C2
14	1K	103	3PH	C32-C31-O31-C3
13	1L	101	CDL	C72-C73-C74-C75
13	1M	501	CDL	C32-C33-C34-C35
13	1M	501	CDL	C33-C34-C35-C36
13	1K	101	CDL	C13-C14-C15-C16
11	1B	401	UQ5	C24-C26-C27-C28
13	1F	401	CDL	C54-C55-C56-C57
14	1B	406	3PH	C22-C21-O21-C2
14	1K	102	3PH	C22-C21-O21-C2
13	1M	501	CDL	OB5-CB3-CB4-OB6
14	1K	103	3PH	O11-C1-C2-O21
12	1E	404	HEM	C4B-C3B-CAB-CBB
12	1F	402	HEM	C4C-C3C-CAC-CBC
14	1A	406	3PH	C24-C25-C26-C27
13	1B	408	CDL	C36-C37-C38-C39
13	1F	401	CDL	C11-C12-C13-C14
13	1K	101	CDL	C78-C79-C80-C81
13	1B	408	CDL	C11-C12-C13-C14
11	1A	401	UQ5	C15-C14-C16-C17
13	1A	405	CDL	C15-C16-C17-C18
13	1A	405	CDL	C34-C35-C36-C37
14	1B	406	3PH	O22-C21-O21-C2
13	1A	405	CDL	CB3-OB5-PB2-OB2
16	1H	101	PC7	C1-O3P-P-O4P
13	1L	101	CDL	C75-C76-C77-C78
13	1B	408	CDL	CB4-CB3-OB5-PB2
14	1K	102	3PH	C27-C28-C29-C2A
16	1H	101	PC7	C12-C13-C14-C15
13	1A	405	CDL	CA5-C11-C12-C13
14	1E	402	3PH	C28-C29-C2A-C2B
13	1F	401	CDL	C12-C13-C14-C15
14	1A	406	3PH	C23-C24-C25-C26
13	1K	101	CDL	CA2-C1-CB2-OB2
13	1B	405	CDL	C52-C53-C54-C55
14	1B	407	3PH	C22-C21-O21-C2
14	1K	103	3PH	O32-C31-O31-C3
13	1B	405	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
13	1B	408	CDL	CA3-CA4-CA6-OA8
13	1K	101	CDL	CA3-CA4-CA6-OA8
13	1K	101	CDL	CB3-CB4-CB6-OB8
14	1B	406	3PH	C1-C2-C3-O31
14	1E	402	3PH	C1-C2-C3-O31
15	1E	403	PTY	O4-C1-C6-C5
13	1B	405	CDL	C11-C12-C13-C14
14	1E	402	3PH	C25-C26-C27-C28
13	1B	408	CDL	C74-C75-C76-C77
15	1F	403	PTY	C11-C12-C13-C14
14	1B	407	3PH	C21-C22-C23-C24
13	1K	101	CDL	C59-C60-C61-C62
16	1H	101	PC7	C13-C14-C15-C16
14	1A	406	3PH	C29-C2A-C2B-C2C
13	1B	405	CDL	C76-C77-C78-C79
14	1B	406	3PH	C27-C28-C29-C2A
13	1M	501	CDL	CB7-C71-C72-C73
13	1B	405	CDL	CA7-C31-C32-C33
15	1E	403	PTY	C32-C33-C34-C35
13	1K	101	CDL	C73-C74-C75-C76
13	1B	405	CDL	C84-C85-C86-C87
13	1L	101	CDL	C76-C77-C78-C79
13	1B	408	CDL	C18-C19-C20-C21
13	1E	401	CDL	C11-C12-C13-C14
13	1B	408	CDL	C37-C38-C39-C40
13	1A	405	CDL	OA5-CA3-CA4-OA6
14	1B	406	3PH	O21-C2-C3-O31
13	1M	501	CDL	C51-C52-C53-C54
14	1R	201	3PH	C2D-C2E-C2F-C2G
13	1L	101	CDL	C12-C13-C14-C15
13	1M	501	CDL	C37-C38-C39-C40
13	1M	501	CDL	C52-C53-C54-C55
13	1B	408	CDL	C12-C13-C14-C15
14	1K	102	3PH	C35-C36-C37-C38
15	1F	403	PTY	C31-C30-O4-C1
13	1F	401	CDL	C32-C33-C34-C35
13	1L	101	CDL	C32-C33-C34-C35
14	1B	407	3PH	C37-C38-C39-C3A
13	1B	405	CDL	C81-C82-C83-C84
13	1F	401	CDL	C71-C72-C73-C74
13	1B	408	CDL	OA5-CA3-CA4-CA6
13	1E	401	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
13	1F	401	CDL	OB5-CB3-CB4-CB6
13	1M	501	CDL	OA5-CA3-CA4-CA6
13	1M	501	CDL	OB5-CB3-CB4-CB6
13	1B	405	CDL	CB7-C71-C72-C73
13	1L	101	CDL	CB5-C51-C52-C53
13	1K	101	CDL	C83-C84-C85-C86
13	1E	401	CDL	O1-C1-CA2-OA2
13	1M	501	CDL	C11-CA5-OA6-CA4
13	1B	405	CDL	C71-CB7-OB8-CB6
13	1K	101	CDL	C71-C72-C73-C74
13	1L	101	CDL	C1-CB2-OB2-PB2
12	1A	403	HEM	C2A-CAA-CBA-CGA
13	1F	401	CDL	CB3-CB4-CB6-OB8
13	1L	101	CDL	CA3-CA4-CA6-OA8
14	1R	201	3PH	C1-C2-C3-O31
15	1F	403	PTY	O4-C1-C6-C5
13	1K	101	CDL	C34-C35-C36-C37
15	1E	403	PTY	C31-C32-C33-C34
13	1M	501	CDL	CA3-OA5-PA1-OA2
13	1E	401	CDL	C31-C32-C33-C34
14	1E	402	3PH	C27-C28-C29-C2A
13	1B	405	CDL	C31-C32-C33-C34
14	1B	406	3PH	O11-C1-C2-O21
16	1G	301	PC7	O3P-C1-C2-O2
13	1B	408	CDL	C17-C18-C19-C20
13	1F	401	CDL	OB6-CB4-CB6-OB8
13	1K	101	CDL	OB6-CB4-CB6-OB8
14	1B	407	3PH	O21-C2-C3-O31
16	1H	101	PC7	O2-C2-C3-O3
13	1K	101	CDL	C11-CA5-OA6-CA4
11	1A	402	UQ5	C24-C26-C27-C28
13	1K	101	CDL	CB2-C1-CA2-OA2
13	1M	501	CDL	C11-C12-C13-C14
13	1M	501	CDL	OA7-CA5-OA6-CA4
14	1A	406	3PH	C25-C26-C27-C28
14	1E	402	3PH	C32-C33-C34-C35
13	1A	405	CDL	C51-C52-C53-C54
13	1B	405	CDL	C73-C74-C75-C76
13	1A	405	CDL	C1-CA2-OA2-PA1
13	1A	405	CDL	CB4-CB3-OB5-PB2
13	1E	401	CDL	C1-CB2-OB2-PB2
13	1F	401	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
14	1K	103	3PH	C2-C1-O11-P
16	1H	101	PC7	C4-C5-N-C6
13	1F	401	CDL	C31-C32-C33-C34
13	1M	501	CDL	C34-C35-C36-C37
14	1B	407	3PH	C2D-C2E-C2F-C2G
13	1A	405	CDL	CB7-C71-C72-C73
13	1F	401	CDL	CB7-C71-C72-C73
13	1K	101	CDL	OA7-CA5-OA6-CA4
14	1B	407	3PH	O22-C21-O21-C2
13	1B	405	CDL	C75-C76-C77-C78
13	1E	401	CDL	C73-C74-C75-C76
13	1E	401	CDL	C71-C72-C73-C74
13	1K	101	CDL	OA5-CA3-CA4-CA6
14	1A	406	3PH	O11-C1-C2-C3
14	1K	102	3PH	O11-C1-C2-C3
14	1K	103	3PH	O11-C1-C2-C3
13	1L	101	CDL	O1-C1-CA2-OA2
13	1K	101	CDL	C31-CA7-OA8-CA6
11	1A	402	UQ5	C12-C11-C9-C10
14	1A	406	3PH	C27-C28-C29-C2A
13	1B	408	CDL	CA4-CA3-OA5-PA1
13	1L	101	CDL	CB4-CB3-OB5-PB2
13	1M	501	CDL	CB3-CB4-CB6-OB8
14	1B	407	3PH	C1-C2-C3-O31
16	1H	101	PC7	C1-C2-C3-O3
15	1F	403	PTY	O30-C30-O4-C1
13	1K	101	CDL	C31-C32-C33-C34
13	1B	405	CDL	OB5-CB3-CB4-OB6
13	1B	408	CDL	OA5-CA3-CA4-OA6
13	1E	401	CDL	OB5-CB3-CB4-OB6
13	1K	101	CDL	OB5-CB3-CB4-OB6
13	1M	501	CDL	OA5-CA3-CA4-OA6
14	1E	402	3PH	O11-C1-C2-O21
14	1K	102	3PH	O11-C1-C2-O21
12	1B	403	HEM	C4C-C3C-CAC-CBC
13	1K	101	CDL	OA9-CA7-OA8-CA6
13	1L	101	CDL	OA6-CA4-CA6-OA8
14	1A	406	3PH	O21-C2-C3-O31
14	1R	201	3PH	O21-C2-C3-O31
15	1E	403	PTY	O4-C1-C6-O7
13	1B	405	CDL	OB9-CB7-OB8-CB6
13	1B	405	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
13	1A	405	CDL	C31-C32-C33-C34
14	1K	102	3PH	C28-C29-C2A-C2B
13	1K	101	CDL	C37-C38-C39-C40
16	1G	301	PC7	C12-C11-O3-C3
11	1A	402	UQ5	C20-C19-C21-C22
13	1M	501	CDL	C1-CB2-OB2-PB2
14	1B	406	3PH	C2-C1-O11-P
16	1H	101	PC7	C2-C1-O3P-P
13	1A	405	CDL	CB3-OB5-PB2-OB3
13	1B	405	CDL	CA3-OA5-PA1-OA3
13	1B	405	CDL	CB2-OB2-PB2-OB3
13	1B	405	CDL	CB3-OB5-PB2-OB4
13	1B	408	CDL	CA3-OA5-PA1-OA3
13	1B	408	CDL	CA3-OA5-PA1-OA4
13	1E	401	CDL	CB3-OB5-PB2-OB3
13	1E	401	CDL	CB3-OB5-PB2-OB4
13	1K	101	CDL	CA3-OA5-PA1-OA4
13	1K	101	CDL	CB3-OB5-PB2-OB4
13	1L	101	CDL	CA2-OA2-PA1-OA3
13	1M	501	CDL	CB3-OB5-PB2-OB4
15	1E	403	PTY	C3-O11-P1-O13
16	1G	301	PC7	C4-O4P-P-O1P
16	1H	101	PC7	C1-O3P-P-O1P
16	1H	101	PC7	C4-O4P-P-O1P
13	1K	101	CDL	CA7-C31-C32-C33
13	1A	405	CDL	OA5-CA3-CA4-CA6
13	1B	405	CDL	OA5-CA3-CA4-CA6
13	1B	405	CDL	OB5-CB3-CB4-CB6
14	1B	406	3PH	O11-C1-C2-C3
14	1E	402	3PH	O11-C1-C2-C3
14	1R	201	3PH	O11-C1-C2-C3
16	1G	301	PC7	O3P-C1-C2-C3
15	1F	403	PTY	N1-C2-C3-O11
13	1B	405	CDL	C77-C78-C79-C80
13	1B	408	CDL	OB7-CB5-OB6-CB4
14	1R	201	3PH	C2F-C2G-C2H-C2I
13	1K	101	CDL	C12-C13-C14-C15
14	1K	103	3PH	C22-C21-O21-C2
13	1E	401	CDL	C51-C52-C53-C54
14	1B	406	3PH	C2E-C2F-C2G-C2H
16	1G	301	PC7	C5-C4-O4P-P
14	1B	406	3PH	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
13	1L	101	CDL	C73-C74-C75-C76
13	1K	101	CDL	C80-C81-C82-C83
13	1B	405	CDL	OA5-CA3-CA4-OA6
13	1K	101	CDL	OA5-CA3-CA4-OA6
14	1A	406	3PH	O11-C1-C2-O21
14	1B	406	3PH	C31-C32-C33-C34
14	1R	201	3PH	O11-C1-C2-O21
14	1B	407	3PH	C39-C3A-C3B-C3C
13	1A	405	CDL	CB3-CB4-CB6-OB8
16	1G	301	PC7	O4P-C4-C5-N
13	1A	405	CDL	OB6-CB4-CB6-OB8
13	1B	405	CDL	OB6-CB4-CB6-OB8
13	1E	401	CDL	OA6-CA4-CA6-OA8
13	1K	101	CDL	OA6-CA4-CA6-OA8
15	1F	403	PTY	O4-C1-C6-O7
14	1K	102	3PH	C3A-C3B-C3C-C3D
14	1K	103	3PH	C38-C39-C3A-C3B
13	1B	408	CDL	C34-C35-C36-C37
16	1G	301	PC7	O11-C11-O3-C3
15	1F	403	PTY	C32-C33-C34-C35
13	1K	101	CDL	C77-C78-C79-C80
13	1B	405	CDL	CB6-CB4-OB6-CB5
13	1L	101	CDL	CB6-CB4-OB6-CB5
13	1K	101	CDL	OB5-CB3-CB4-CB6
14	1K	103	3PH	O22-C21-O21-C2
14	1E	402	3PH	C23-C24-C25-C26
13	1B	405	CDL	C1-CA2-OA2-PA1
11	1A	402	UQ5	C12-C11-C9-C8
13	1B	408	CDL	C31-C32-C33-C34
13	1B	408	CDL	C51-CB5-OB6-CB4
13	1B	405	CDL	CA2-OA2-PA1-OA5
13	1B	408	CDL	CB2-OB2-PB2-OB5
13	1E	401	CDL	CA3-OA5-PA1-OA2
16	1G	301	PC7	C1-O3P-P-O4P
13	1A	405	CDL	C36-C37-C38-C39
14	1B	406	3PH	C25-C26-C27-C28
14	1B	407	3PH	C2C-C2D-C2E-C2F
13	1B	405	CDL	C80-C81-C82-C83
15	1E	403	PTY	C35-C36-C37-C38
16	1G	301	PC7	C2-C1-O3P-P
13	1B	405	CDL	CA2-C1-CB2-OB2
13	1E	401	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
13	1L	101	CDL	CB2-C1-CA2-OA2
13	1M	501	CDL	C36-C37-C38-C39
16	1H	101	PC7	C4-C5-N-C7
13	1L	101	CDL	OB5-CB3-CB4-OB6
14	1A	406	3PH	C28-C29-C2A-C2B
12	1F	402	HEM	C4B-C3B-CAB-CBB
16	1G	301	PC7	O2-C2-C3-O3
13	1E	401	CDL	C72-C73-C74-C75
13	1L	101	CDL	C13-C14-C15-C16
13	1K	101	CDL	C79-C80-C81-C82
15	1F	403	PTY	C35-C36-C37-C38
13	1L	101	CDL	C31-C32-C33-C34
13	1B	408	CDL	C15-C16-C17-C18
16	1H	101	PC7	C4-C5-N-C8
12	1A	404	HEM	CAD-CBD-CGD-O1D
13	1B	408	CDL	CB3-OB5-PB2-OB2
14	1B	407	3PH	C28-C29-C2A-C2B
13	1B	405	CDL	C1-CB2-OB2-PB2
13	1E	401	CDL	CB4-CB3-OB5-PB2
13	1B	408	CDL	C56-C57-C58-C59
14	1A	406	3PH	C26-C27-C28-C29
14	1K	103	3PH	C32-C33-C34-C35
13	1B	405	CDL	C71-C72-C73-C74
11	1B	402	UQ5	C12-C11-C9-C10
12	1B	404	HEM	CAA-CBA-CGA-O1A
14	1K	102	3PH	O21-C2-C3-O31
14	1B	407	3PH	C27-C28-C29-C2A
15	1E	403	PTY	C11-C12-C13-C14
12	1B	404	HEM	CAA-CBA-CGA-O2A
13	1B	408	CDL	CB7-C71-C72-C73
13	1B	408	CDL	C54-C55-C56-C57
13	1E	401	CDL	CA3-CA4-CA6-OA8
13	1K	101	CDL	CA5-C11-C12-C13
12	1A	404	HEM	CAA-CBA-CGA-O2A
12	1A	404	HEM	CAA-CBA-CGA-O1A
11	1A	402	UQ5	C18-C19-C21-C22
12	1B	403	HEM	CAD-CBD-CGD-O2D
14	1E	402	3PH	O21-C21-C22-C23
14	1B	406	3PH	C2C-C2D-C2E-C2F
12	1B	403	HEM	CAD-CBD-CGD-O1D
14	1R	201	3PH	C1-O11-P-O13
11	1B	402	UQ5	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
13	1B	408	CDL	C14-C15-C16-C17
13	1K	101	CDL	C53-C54-C55-C56
13	1F	401	CDL	O1-C1-CA2-OA2
15	1F	403	PTY	O4-C30-C31-C32
13	1E	401	CDL	CB3-CB4-OB6-CB5
13	1E	401	CDL	CB6-CB4-OB6-CB5
12	1A	403	HEM	CAD-CBD-CGD-O2D
15	1F	403	PTY	C17-C18-C19-C20
13	1B	408	CDL	CA5-C11-C12-C13
14	1K	102	3PH	O21-C21-C22-C23
12	1A	404	HEM	CAD-CBD-CGD-O2D
12	1A	403	HEM	CAD-CBD-CGD-O1D
13	1E	401	CDL	C72-C71-CB7-OB8
13	1L	101	CDL	OB5-CB3-CB4-CB6
15	1E	403	PTY	O14-C5-C6-C1
13	1K	101	CDL	C52-C51-CB5-OB6
16	1G	301	PC7	O3-C11-C12-C13
13	1K	101	CDL	C12-C11-CA5-OA6
11	1A	401	UQ5	C12-C11-C9-C10
13	1B	405	CDL	C12-C11-CA5-OA6
13	1F	401	CDL	C72-C71-CB7-OB8
14	1E	402	3PH	O22-C21-C22-C23
11	1B	402	UQ5	C11-C12-C13-C14
14	1R	201	3PH	C28-C29-C2A-C2B
13	1B	405	CDL	C12-C11-CA5-OA7
15	1F	403	PTY	O30-C30-C31-C32
13	1A	405	CDL	CA4-CA3-OA5-PA1
13	1K	101	CDL	C52-C51-CB5-OB7
13	1B	408	CDL	CB3-OB5-PB2-OB3
13	1M	501	CDL	CA3-OA5-PA1-OA3
13	1E	401	CDL	C72-C71-CB7-OB9
14	1K	102	3PH	O22-C21-C22-C23
13	1K	101	CDL	C32-C31-CA7-OA8
13	1B	405	CDL	C82-C83-C84-C85
15	1F	403	PTY	C15-C16-C17-C18
13	1E	401	CDL	C52-C51-CB5-OB6
15	1F	403	PTY	C2-C3-O11-P1
13	1A	405	CDL	C32-C31-CA7-OA8
16	1G	301	PC7	O11-C11-C12-C13
14	1B	406	3PH	C2B-C2C-C2D-C2E
12	1B	404	HEM	CAD-CBD-CGD-O1D
13	1A	405	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
15	1E	403	PTY	C12-C11-C8-O7
15	1E	403	PTY	O14-C5-C6-O7
13	1F	401	CDL	C72-C71-CB7-OB9
13	1K	101	CDL	C12-C11-CA5-OA7
14	1B	407	3PH	C34-C35-C36-C37
13	1K	101	CDL	C32-C31-CA7-OA9
14	1B	407	3PH	C26-C27-C28-C29

There are no ring outliers.

20 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1K	102	3PH	1	0
13	1K	101	CDL	5	0
14	1E	402	3PH	1	0
13	1F	401	CDL	1	0
16	1H	101	PC7	2	0
13	1A	405	CDL	1	0
14	1K	103	3PH	1	0
14	1R	201	3PH	1	0
12	1E	404	HEM	3	0
15	1E	403	PTY	2	0
12	1F	402	HEM	2	0
11	1A	402	UQ5	2	0
11	1B	402	UQ5	4	0
13	1B	405	CDL	4	0
16	1G	301	PC7	3	0
11	1B	401	UQ5	4	0
14	1B	406	3PH	1	0
12	1B	403	HEM	2	0
13	1B	408	CDL	2	0
13	1E	401	CDL	1	0

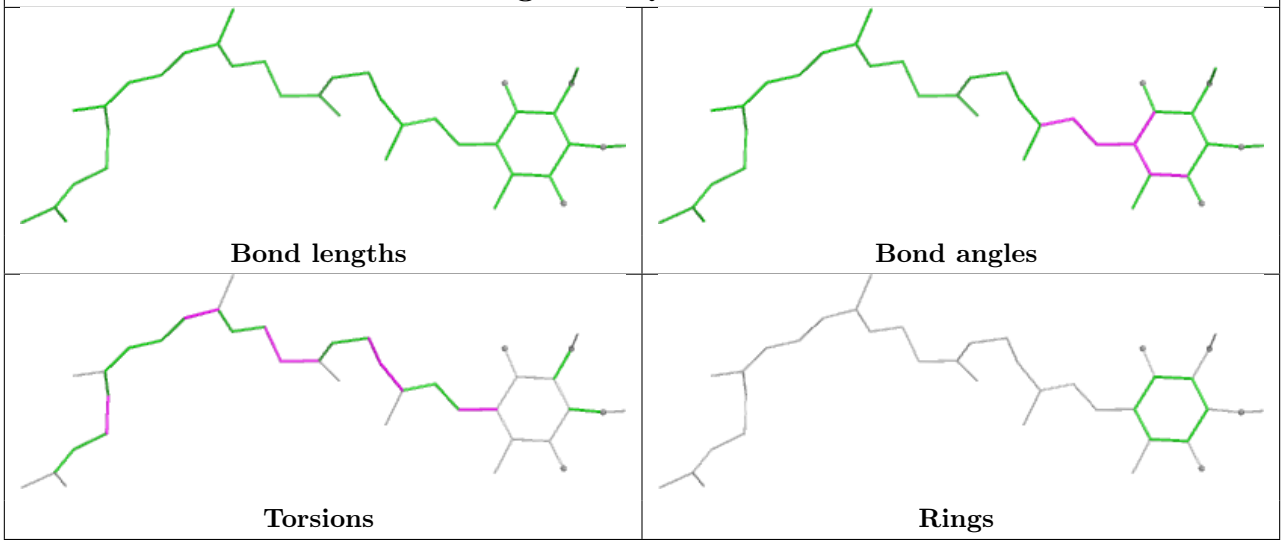
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

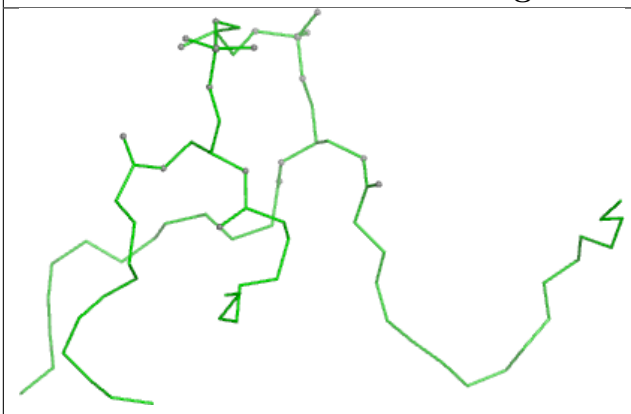
Ligand 3PH 1K 102



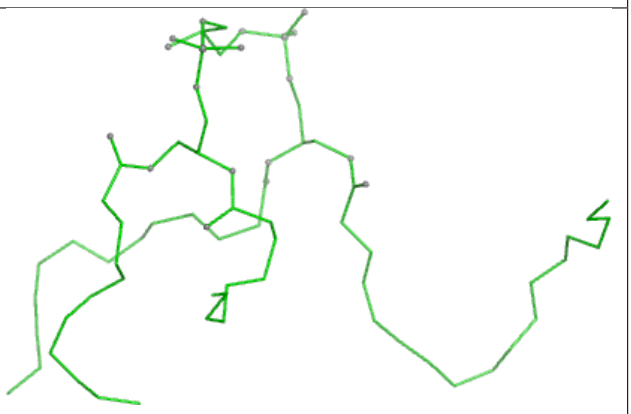
Ligand UQ5 1A 401



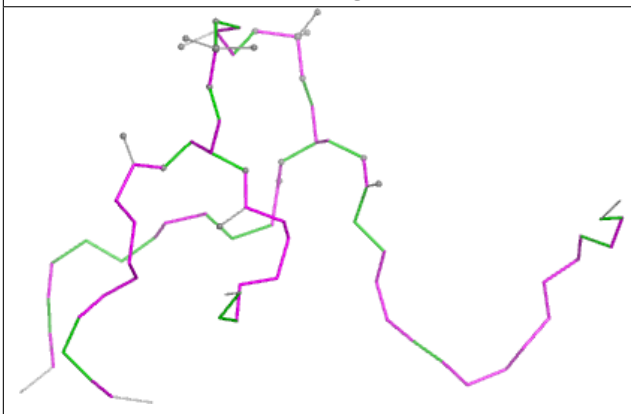
Ligand CDL 1K 101



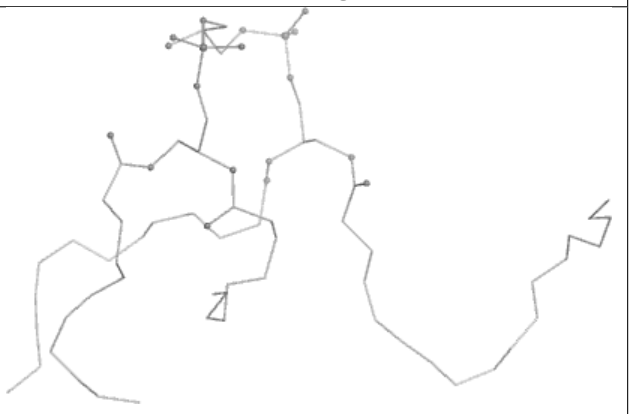
Bond lengths



Bond angles

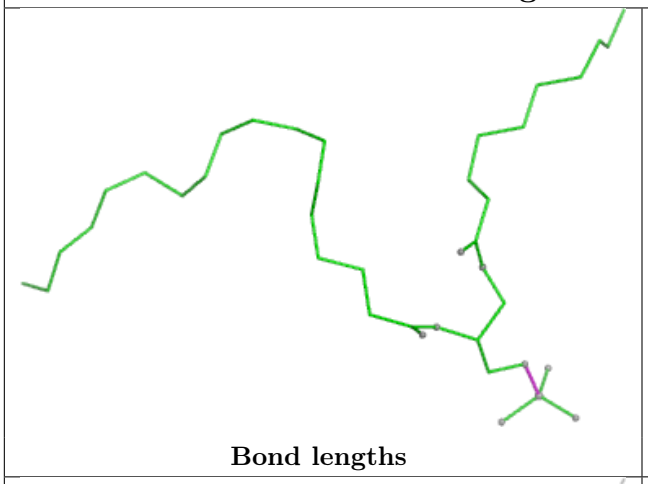


Torsions

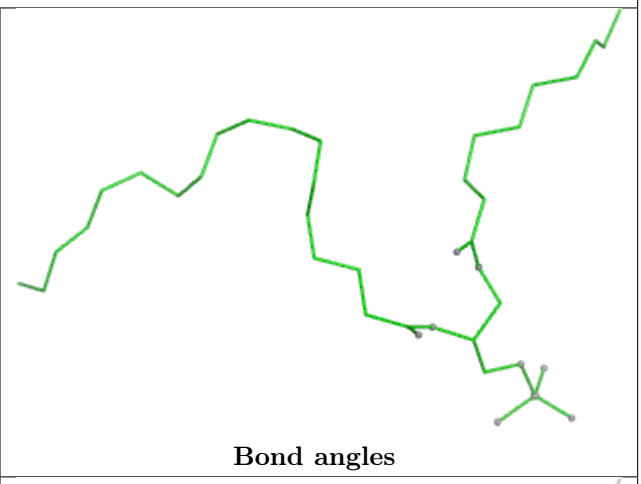


Rings

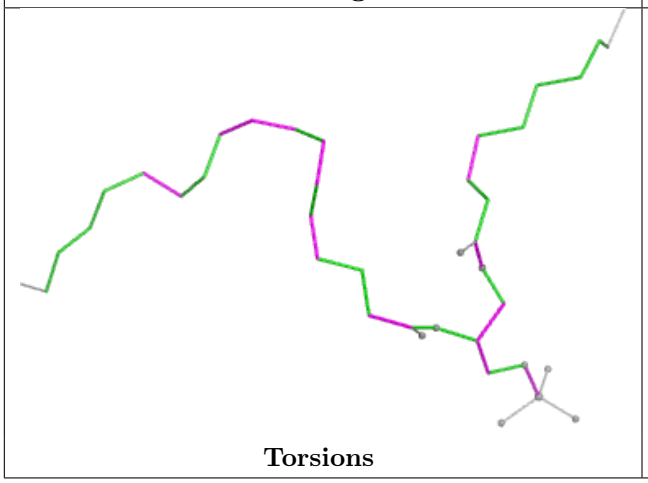
Ligand 3PH 1E 402



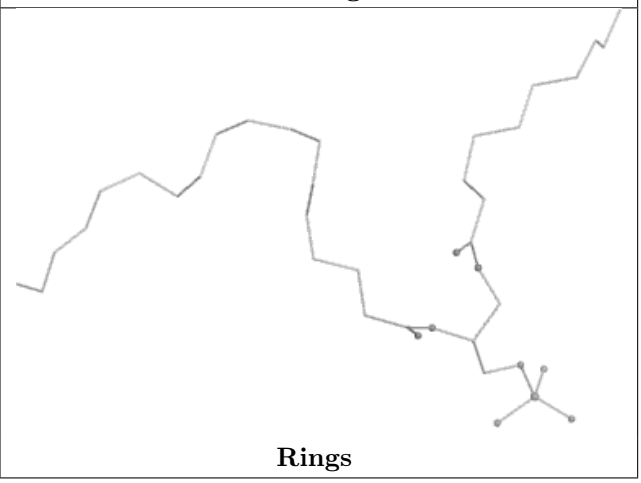
Bond lengths



Bond angles

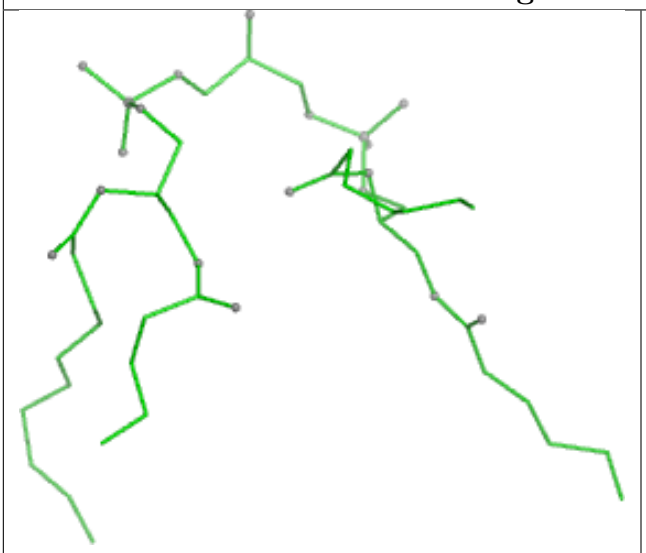


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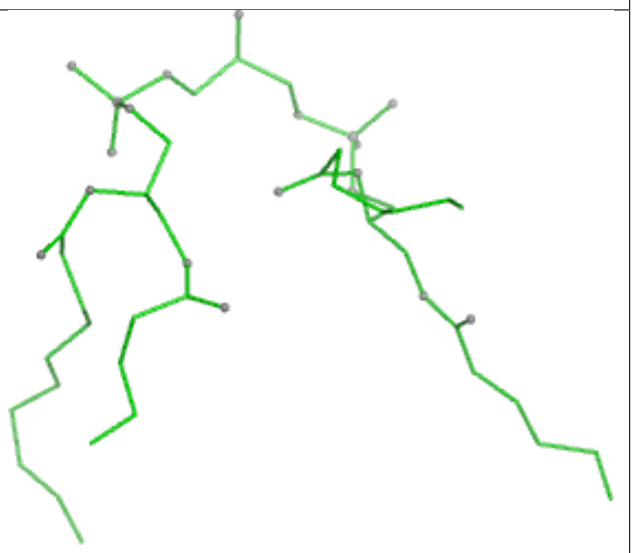


Rings

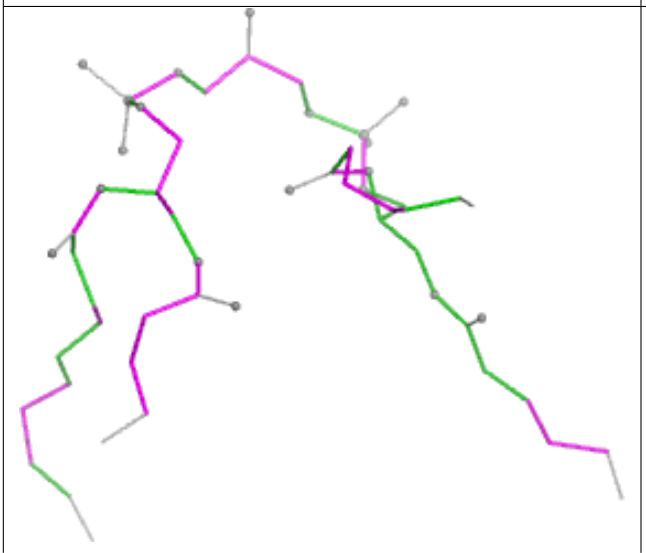
Ligand CDL 1F 401



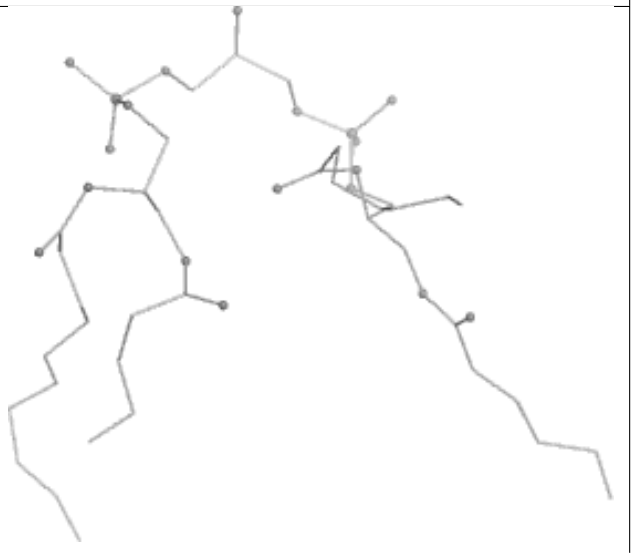
Bond lengths



Bond angles

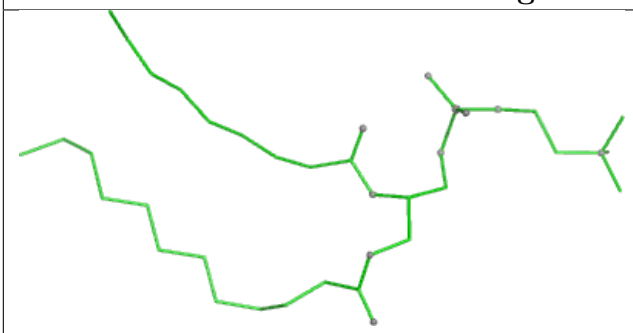


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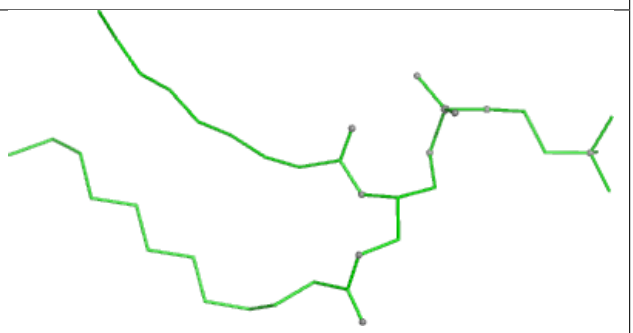


Rings

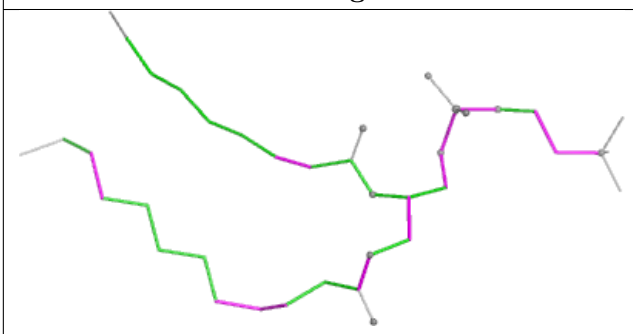
Ligand PC7 1H 101



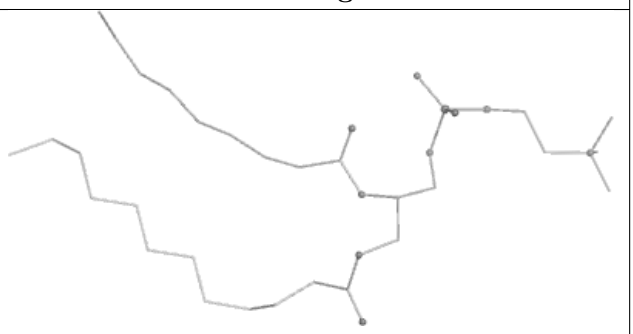
Bond lengths



Bond angles

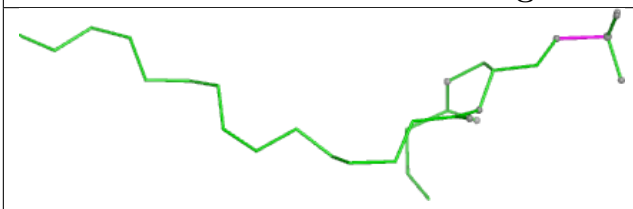


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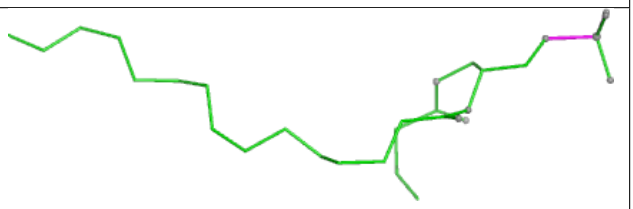


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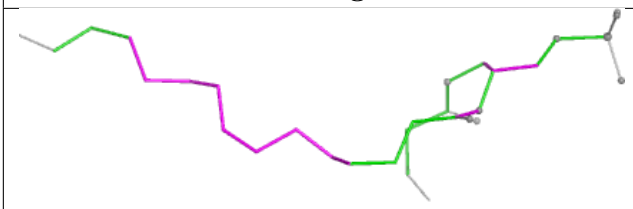
Ligand 3PH 1A 406



Bond lengths



Bond angles



Torsions



Rings

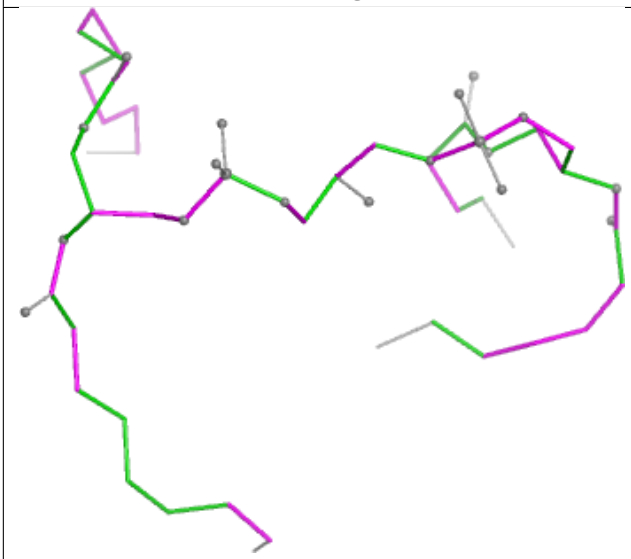
Ligand CDL 1A 405



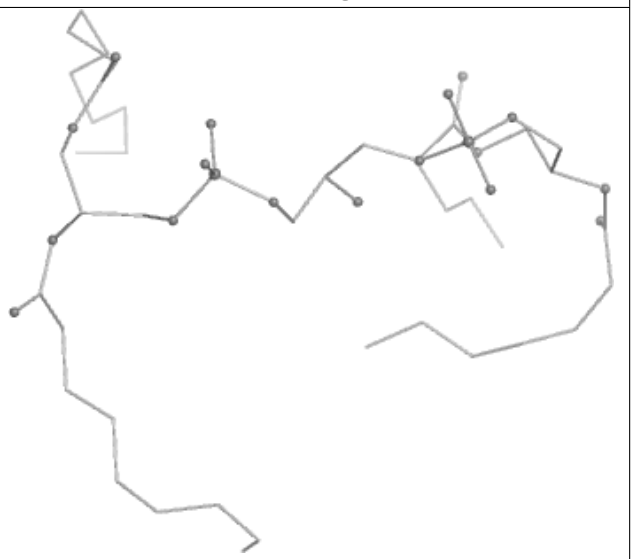
Bond lengths



Bond angles

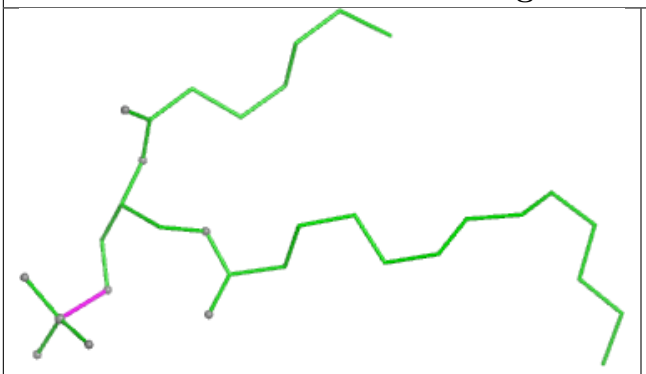


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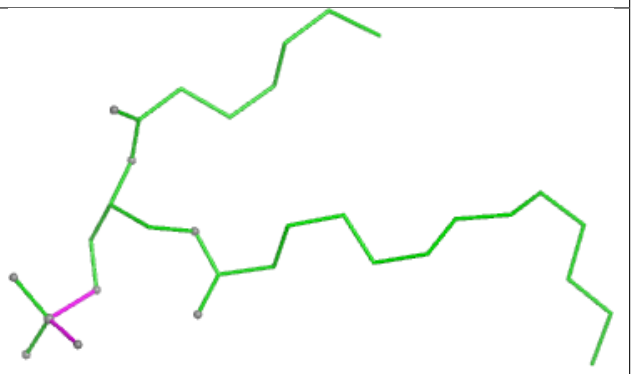


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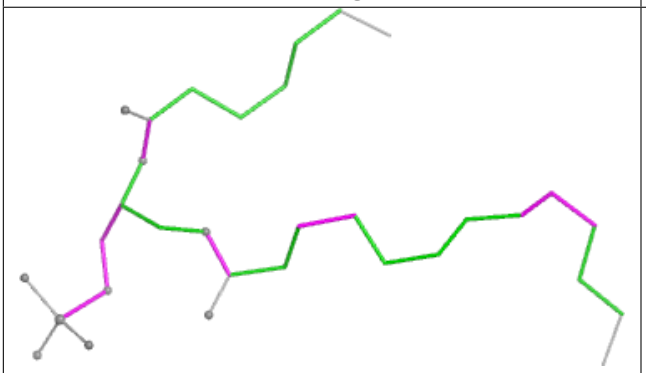
Ligand 3PH 1K 103



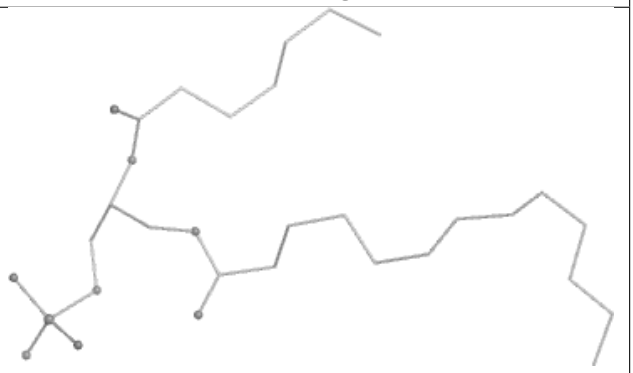
Bond lengths



Bond angles

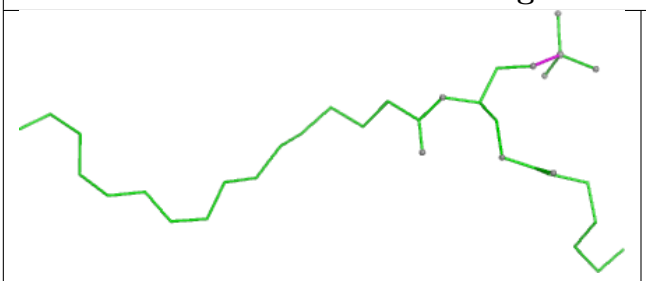


Torsions



Rings

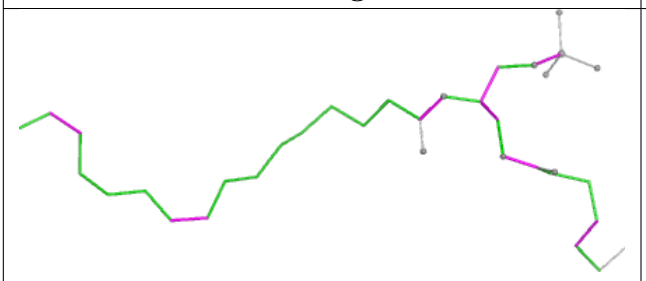
Ligand 3PH 1R 201



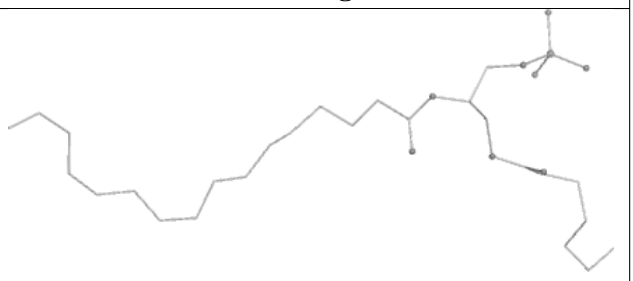
Bond lengths



Bond angles

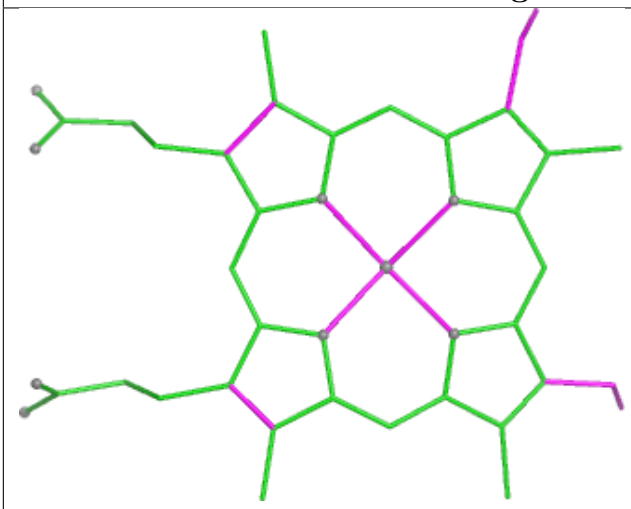


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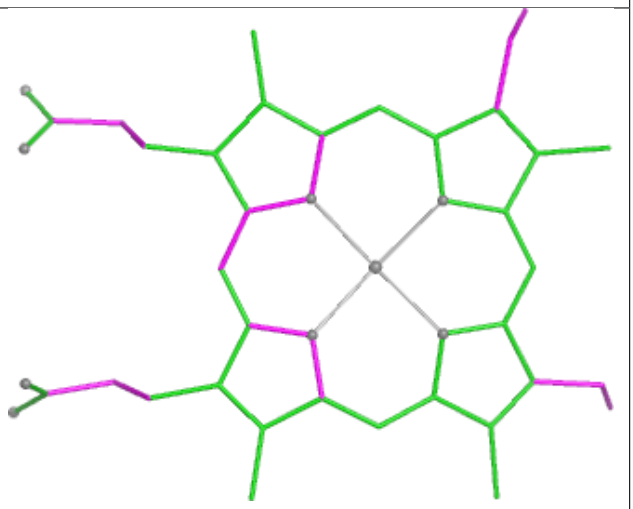


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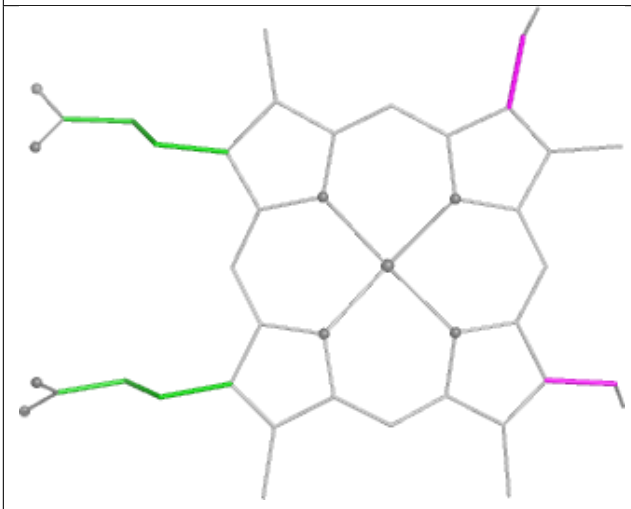
Ligand HEM 1E 404



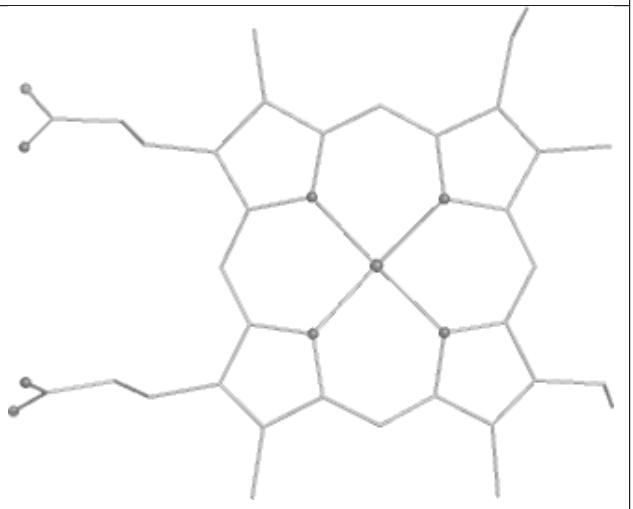
Bond lengths



Bond angles

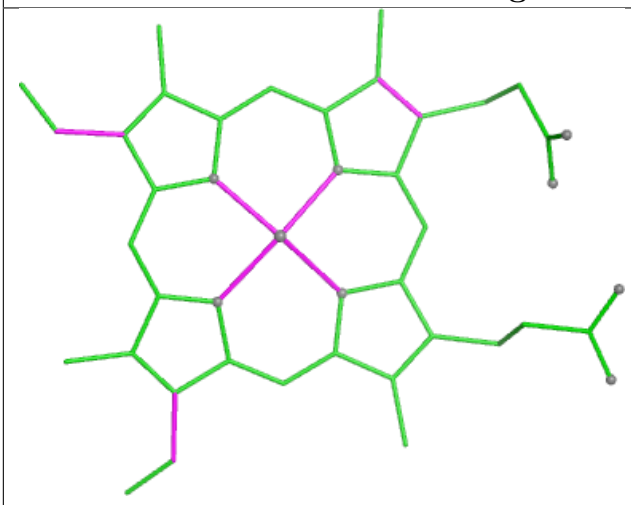


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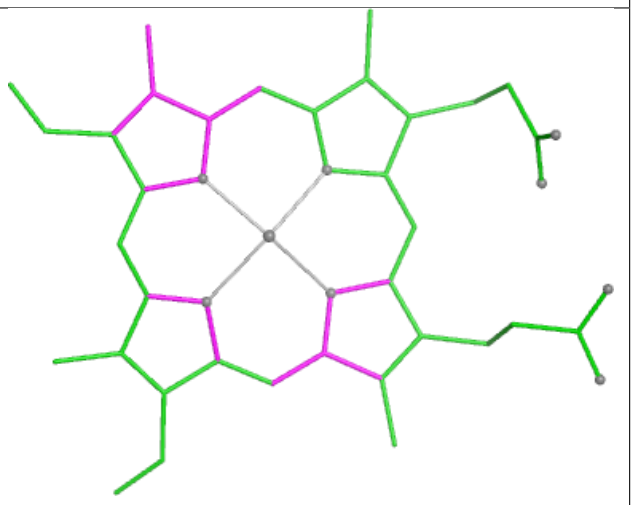


Rings

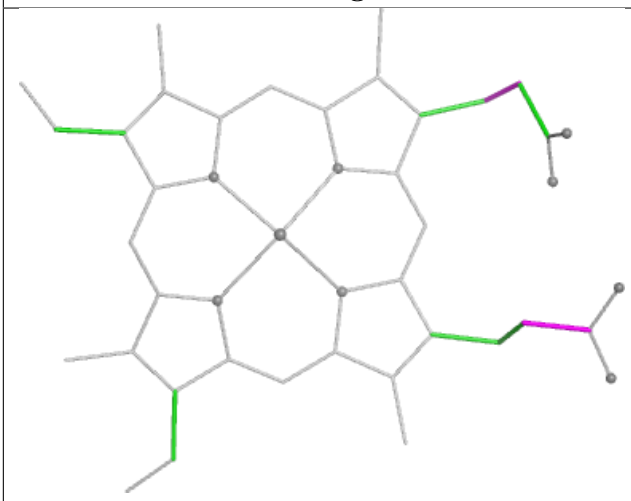
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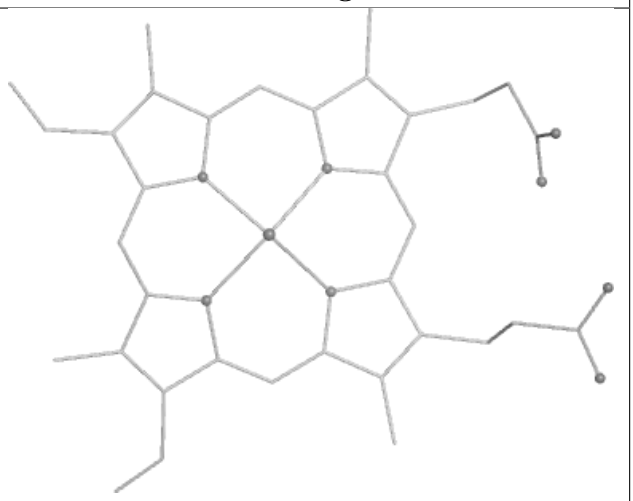
Bond lengths



Bond angles

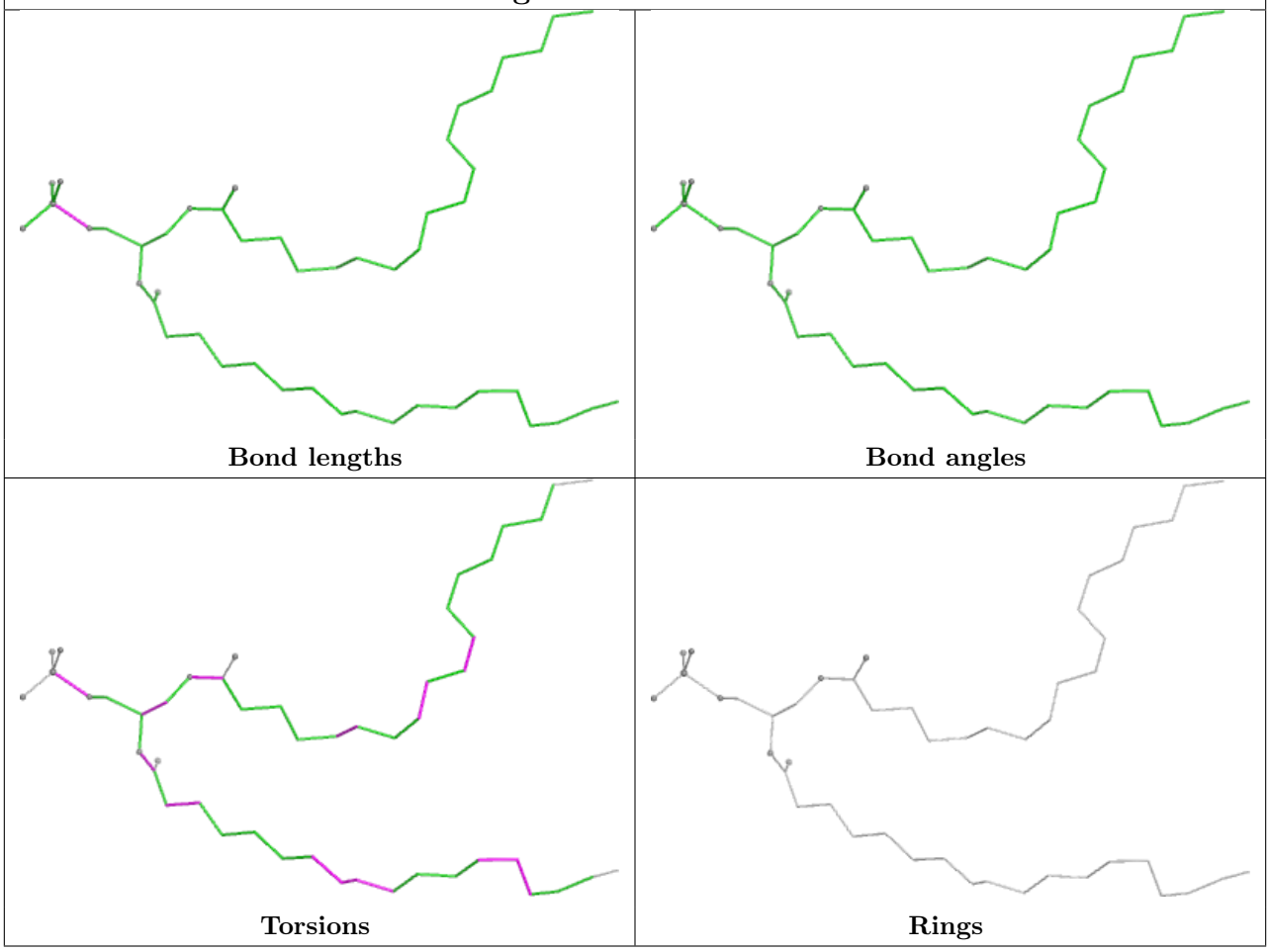


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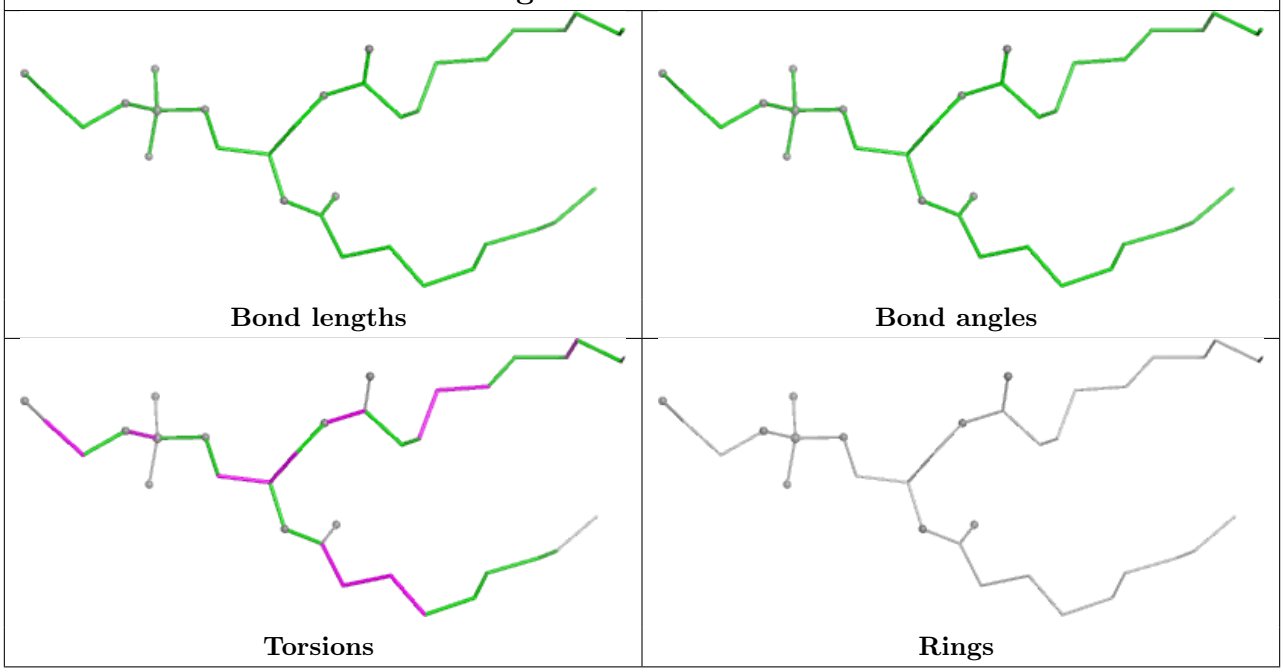


Rings

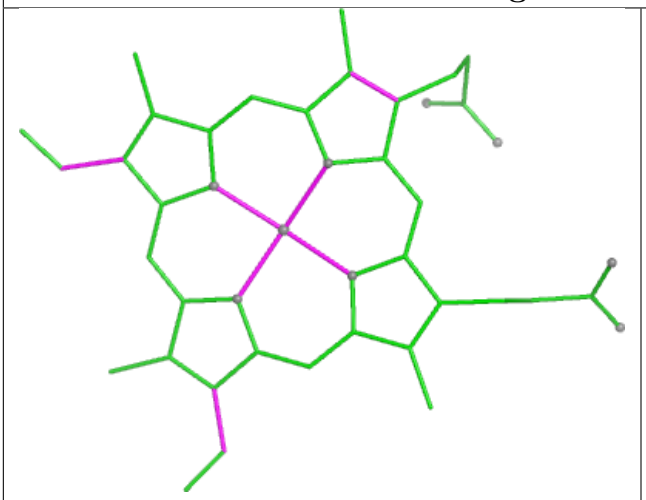
Ligand 3PH 1B 407



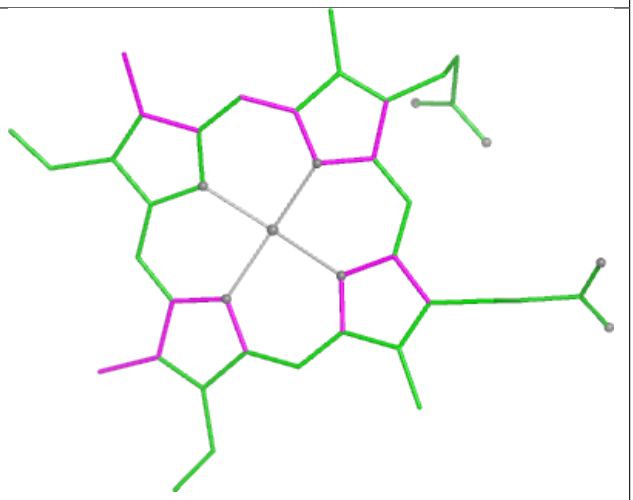
Ligand PTY 1E 403



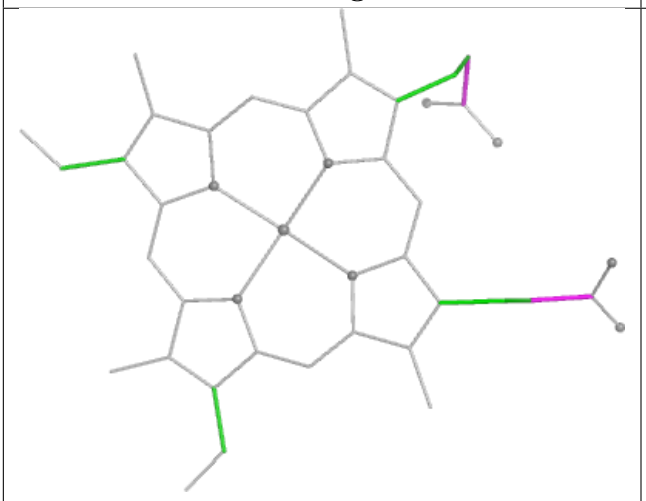
Ligand HEM 1A 404



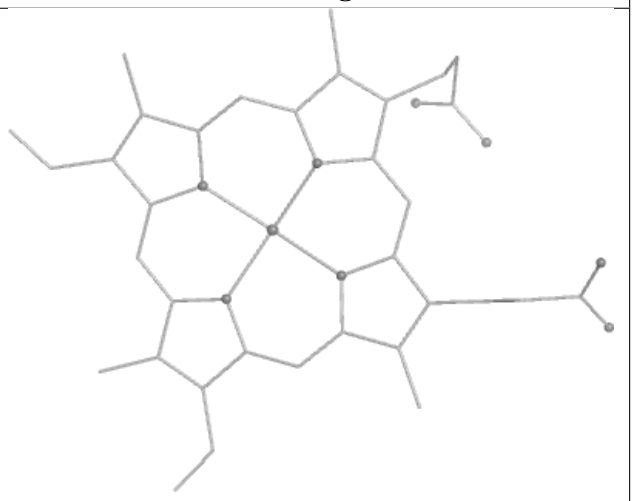
Bond lengths



Bond angles

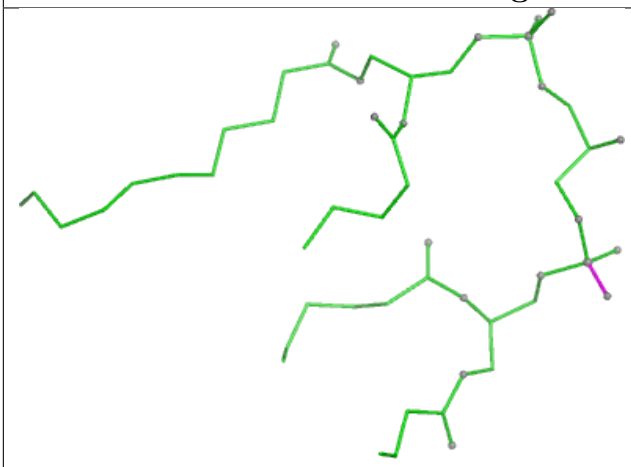


Torsions

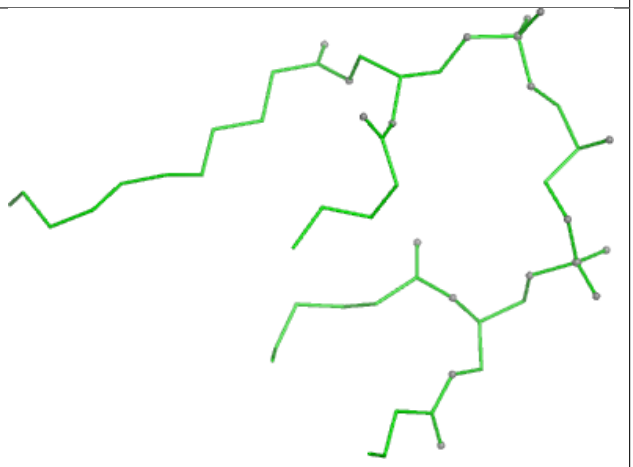


Rings

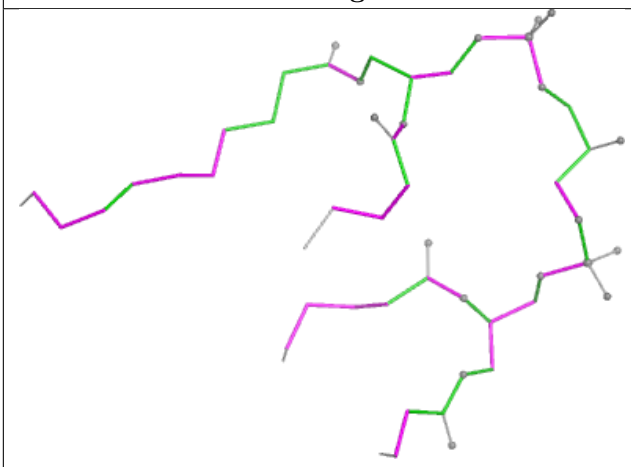
Ligand CDL 1M 501



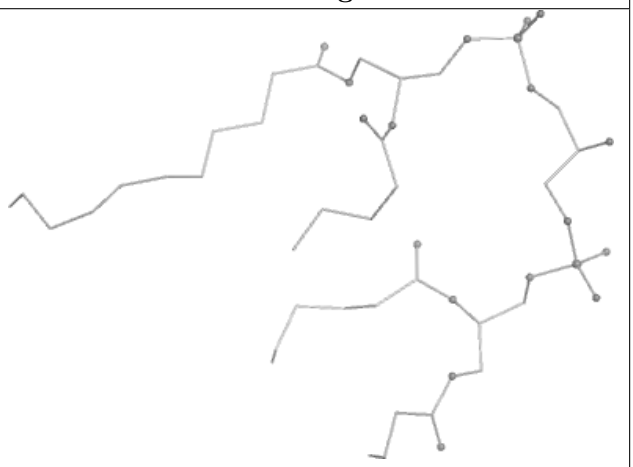
Bond lengths



Bond angles

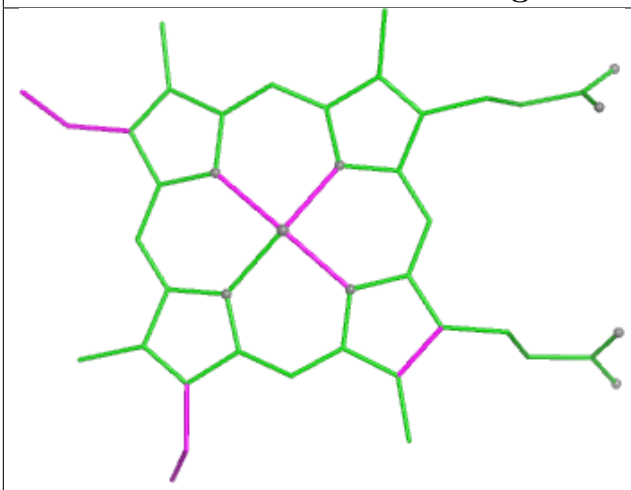


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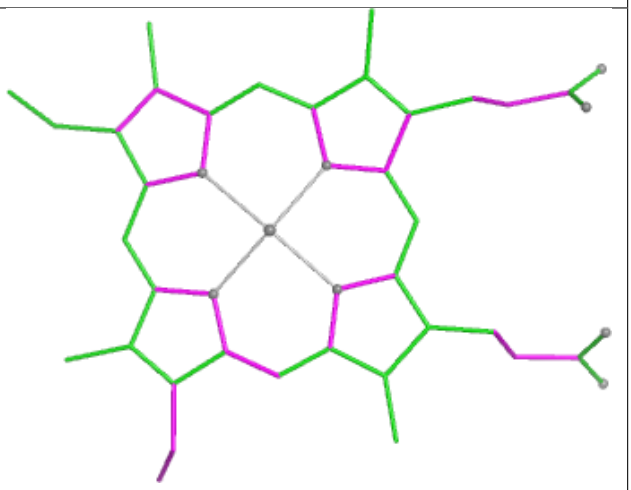


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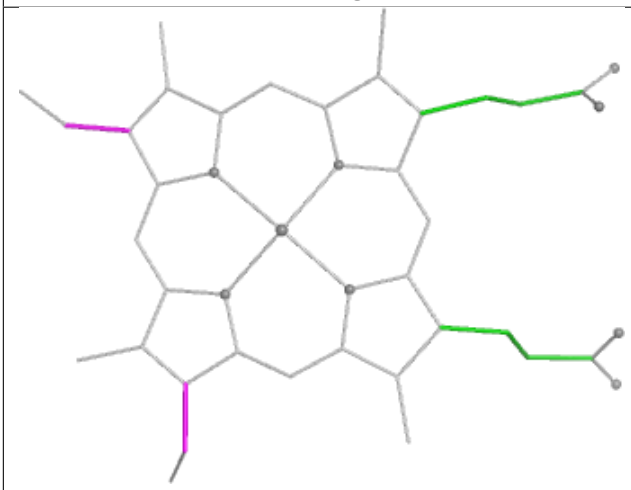
Ligand HEM 1F 402



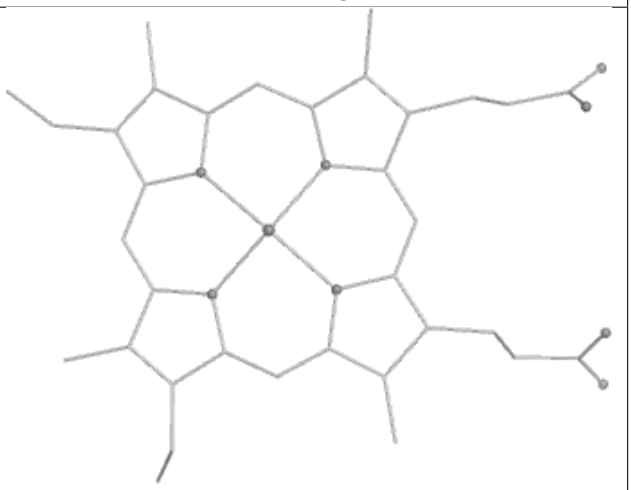
Bond lengths



Bond angles

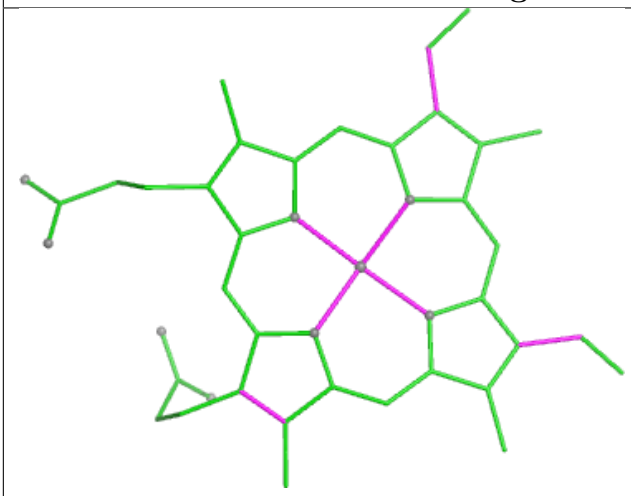


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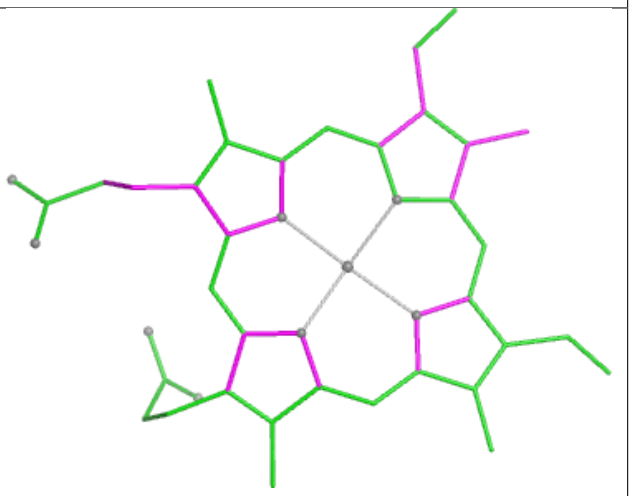


Rings

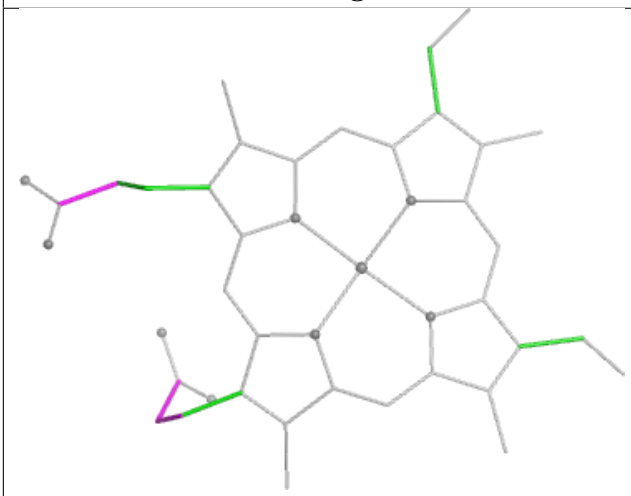
Ligand HEM 1B 404



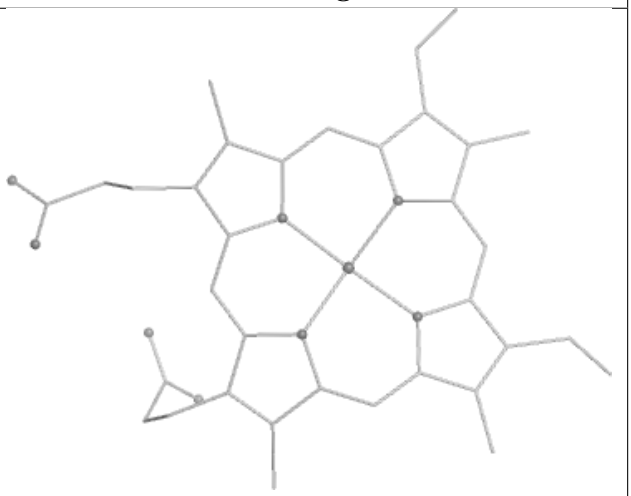
Bond lengths



Bond angles

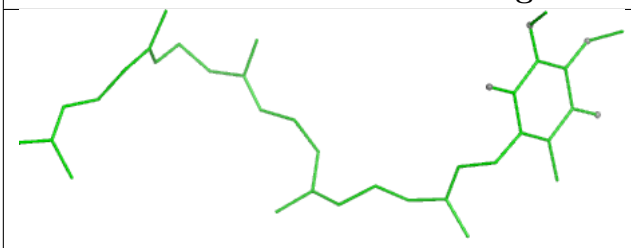


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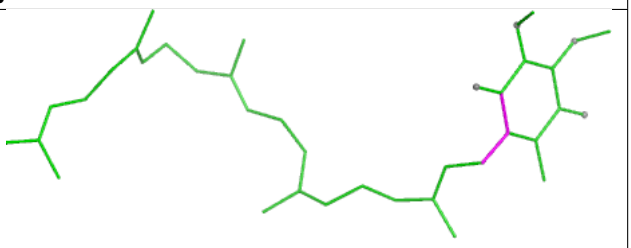


Rings

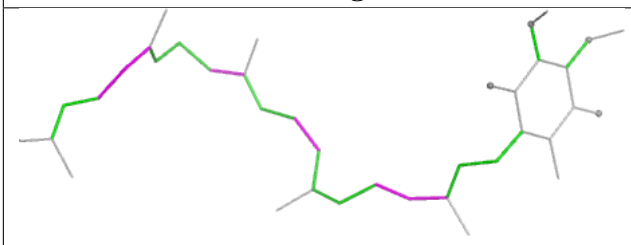
Ligand UQ5 1A 402



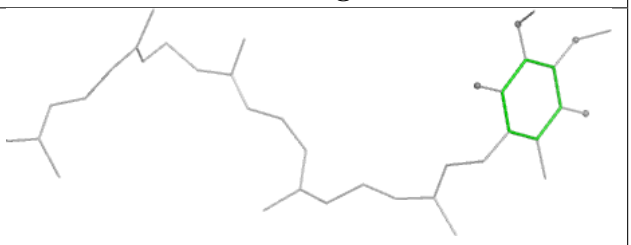
Bond lengths



Bond angles

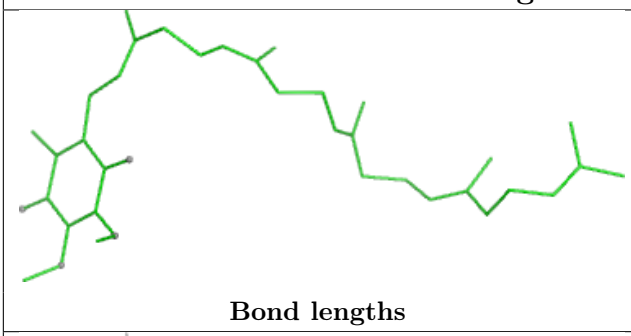


Torsions

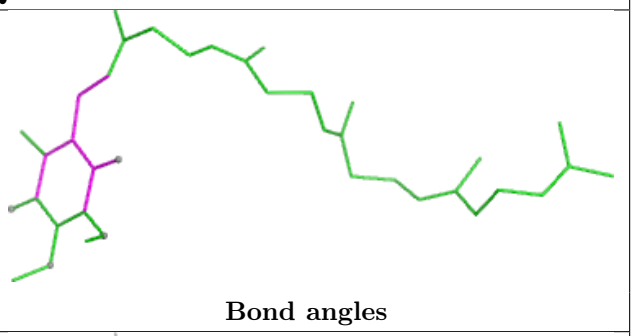


Rings

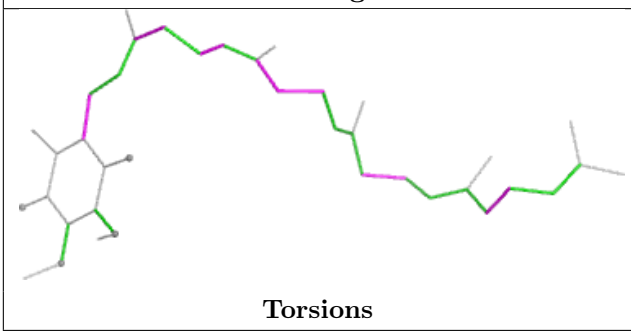
Ligand UQ5 1B 402



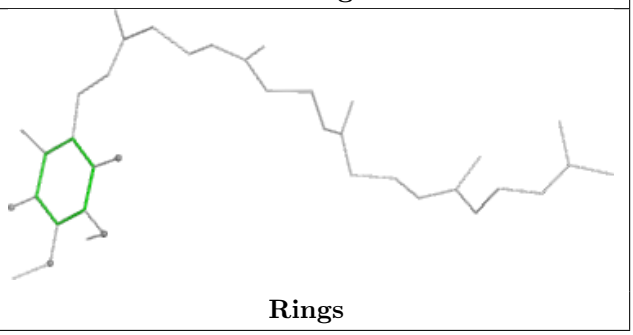
Bond lengths



Bond angles

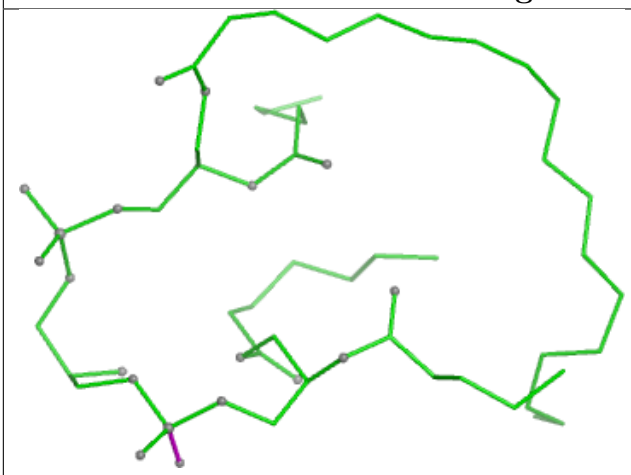


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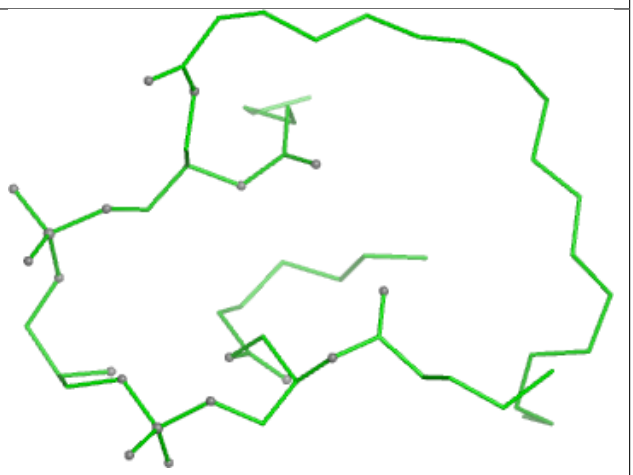


Rings

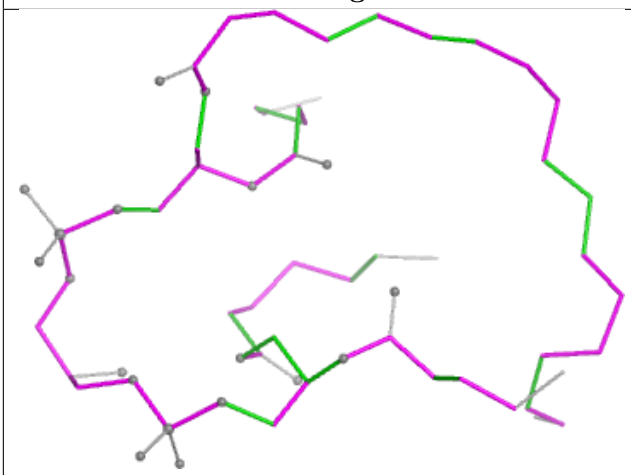
Ligand CDL 1B 405



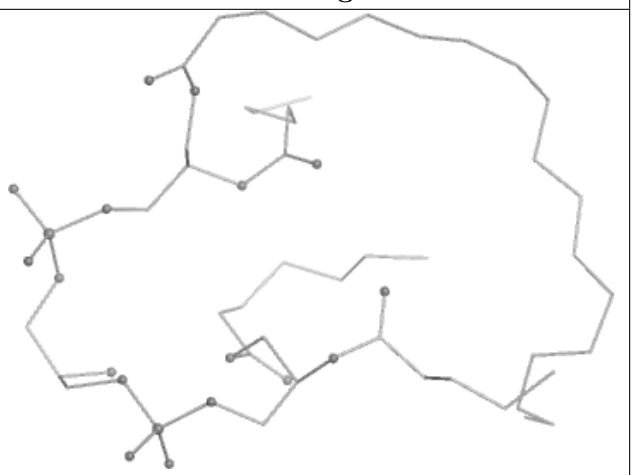
Bond lengths



Bond angles

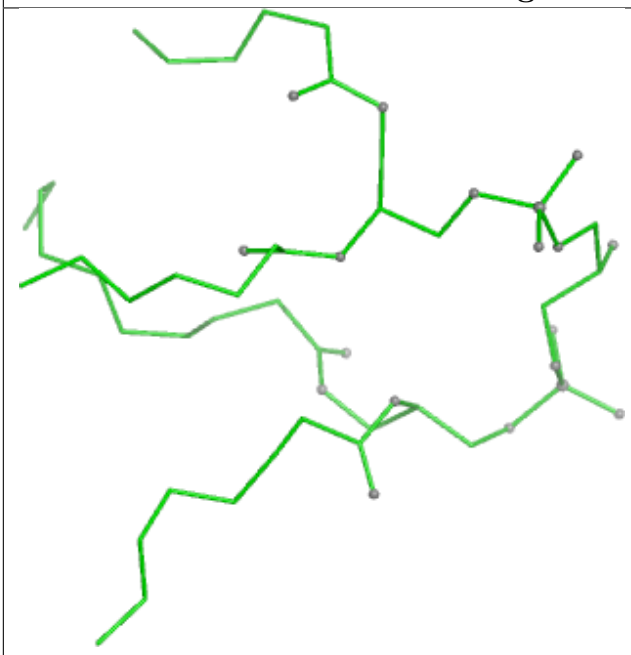


Torsions

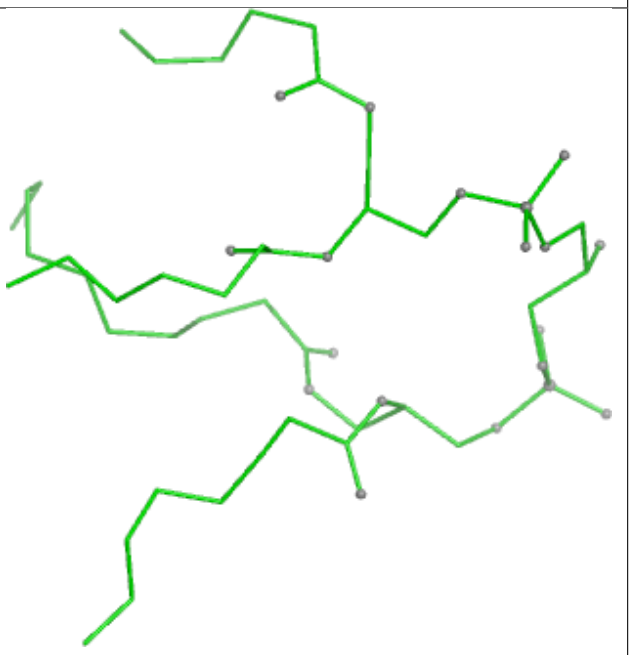


Rings

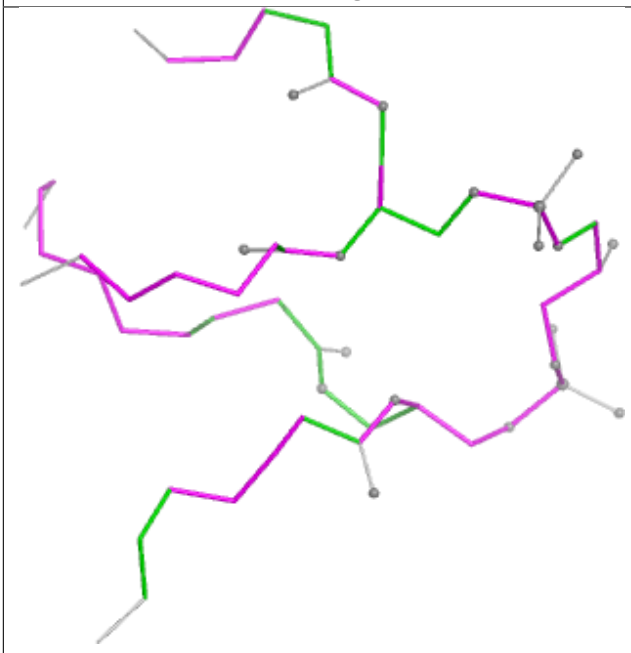
Ligand CDL 1L 101



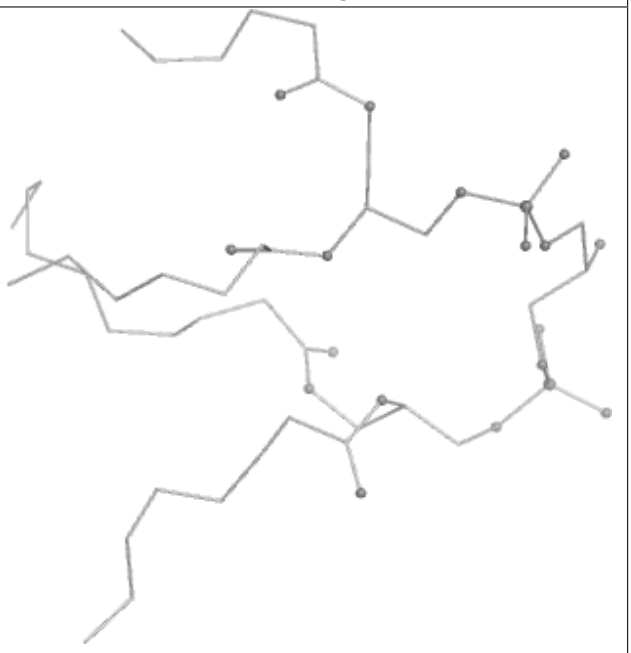
Bond lengths



Bond angles

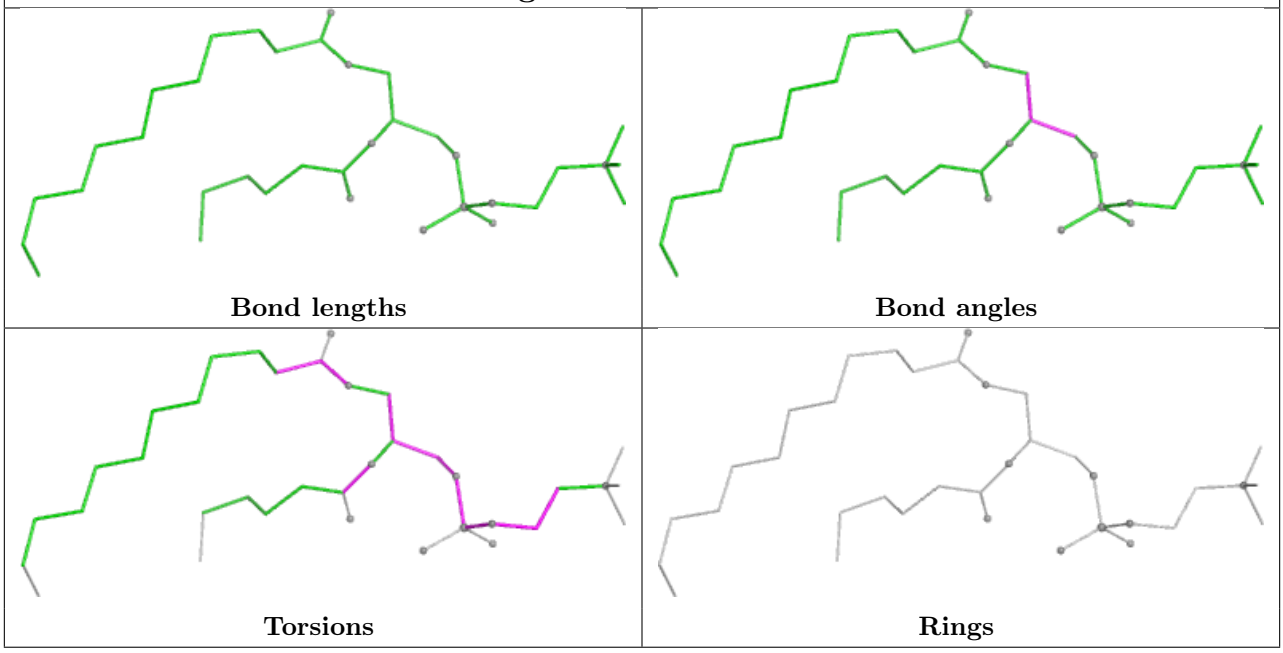


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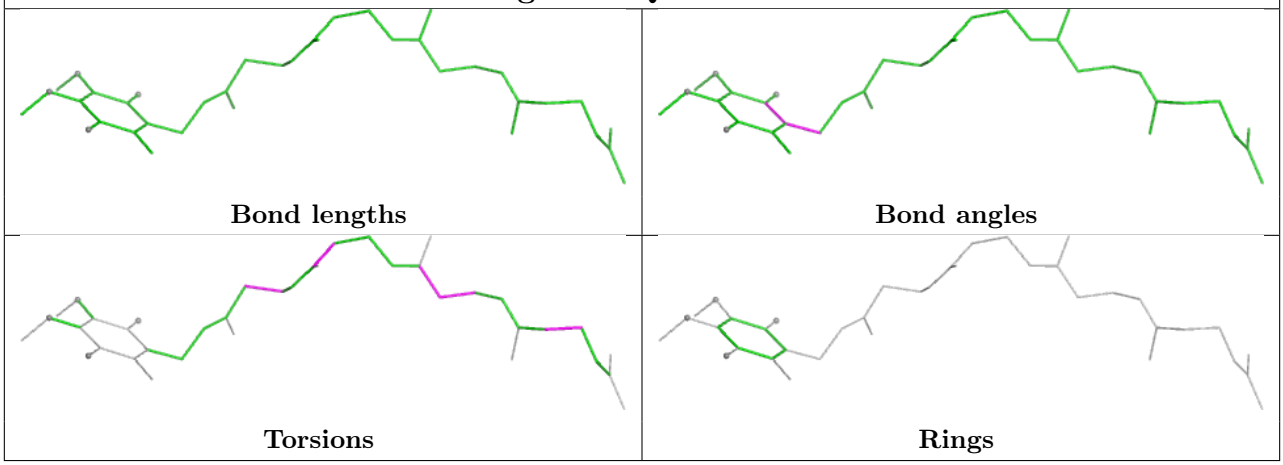


Rings

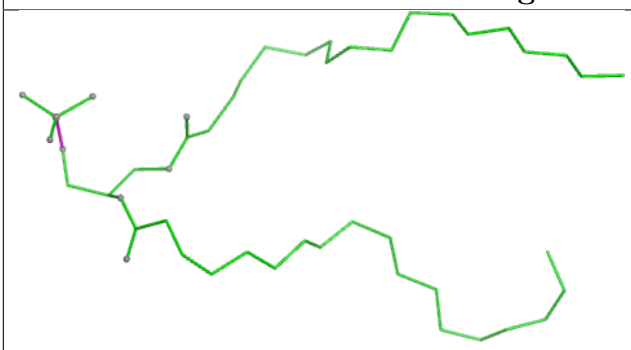
Ligand PC7 1G 301



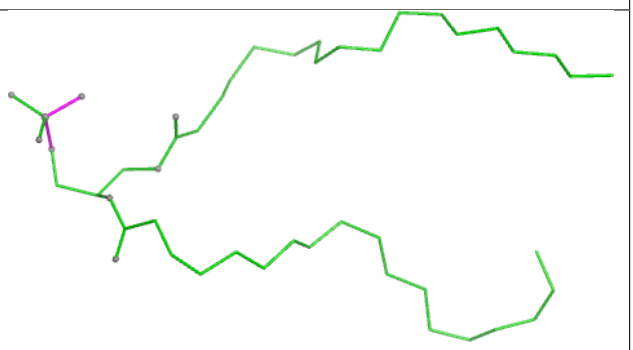
Ligand UQ5 1B 401



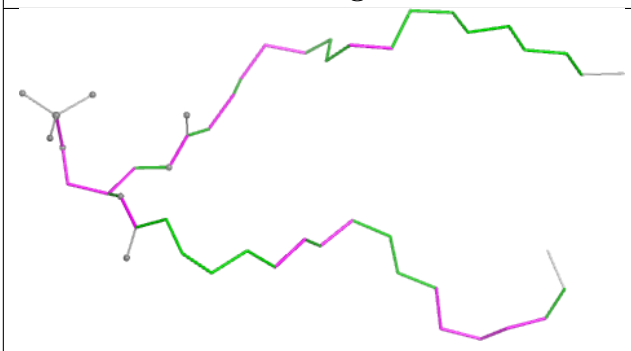
Ligand 3PH 1B 406



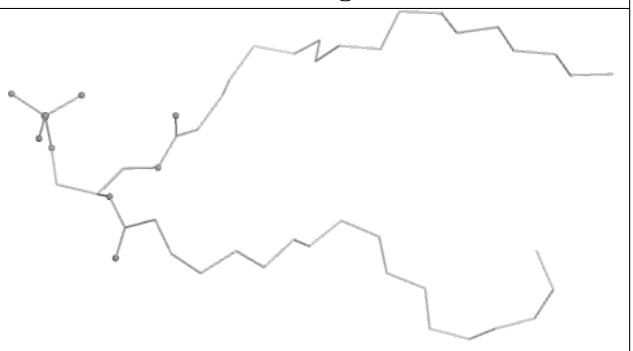
Bond lengths



Bond angles

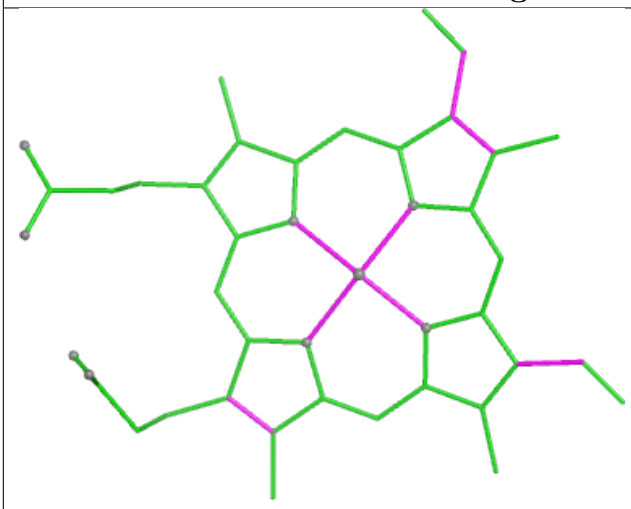


Torsions

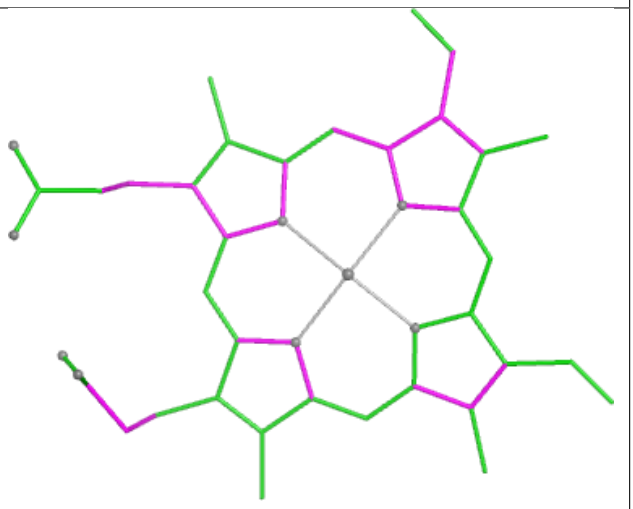


Rings

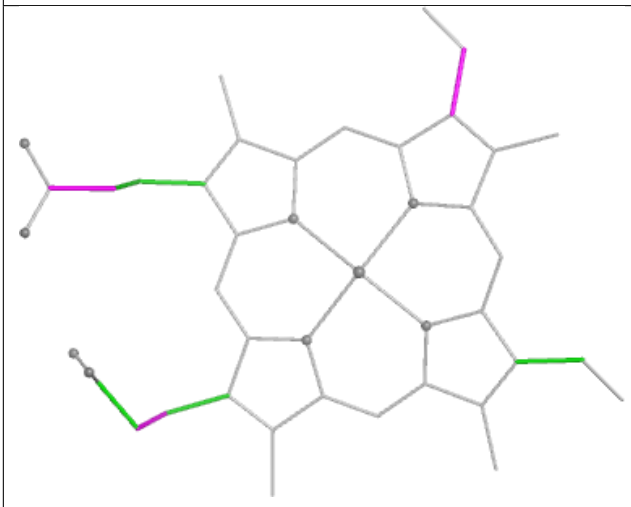
Ligand HEM 1B 403



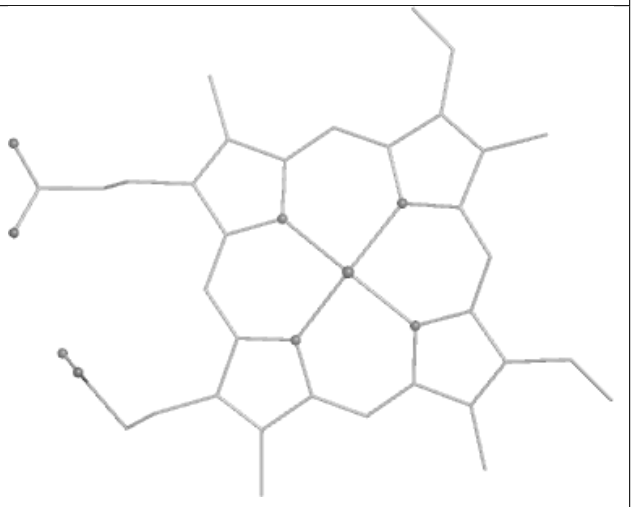
Bond lengths



Bond angles

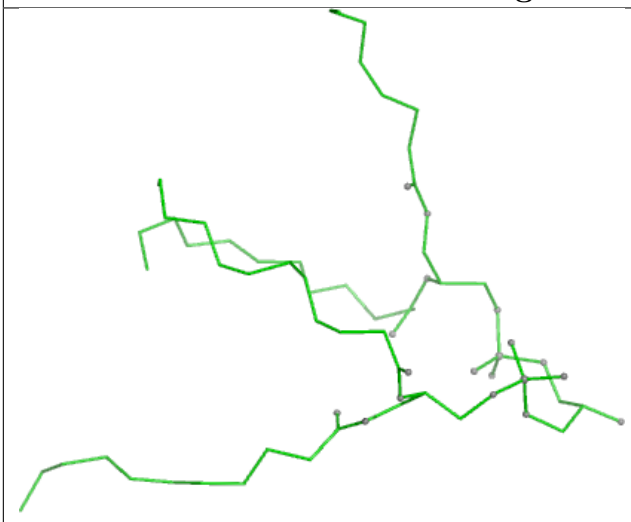


Torsions

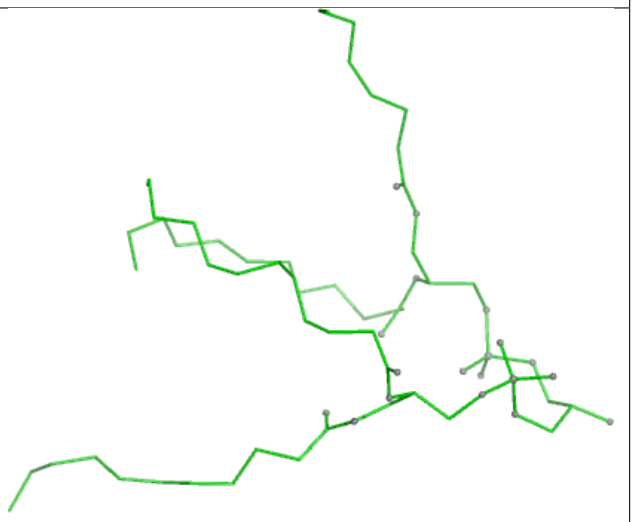


Rings

Ligand CDL 1B 408



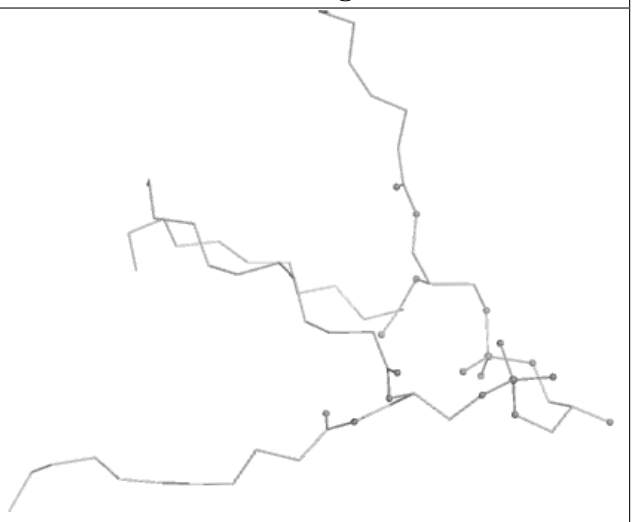
Bond lengths



Bond angles

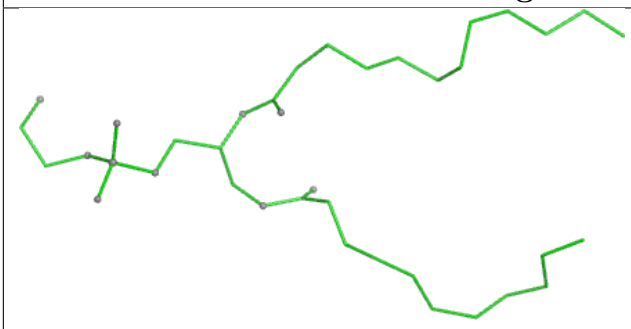


Torsions

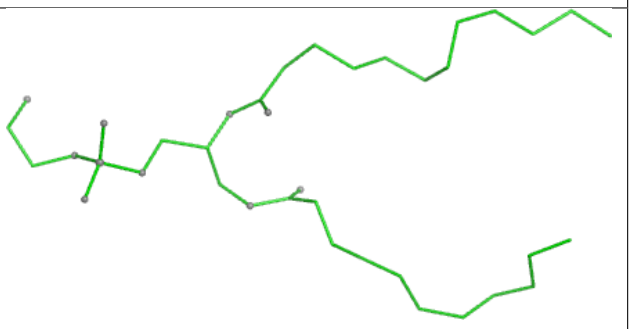


Rings

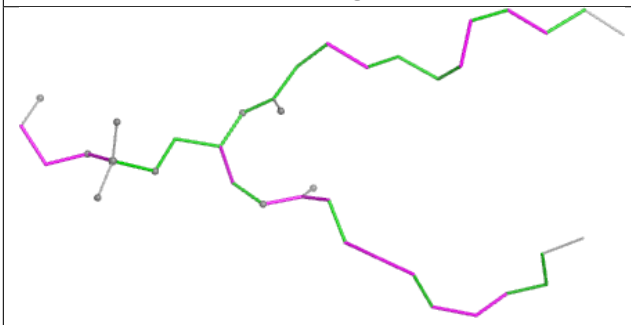
Ligand PTY 1F 403



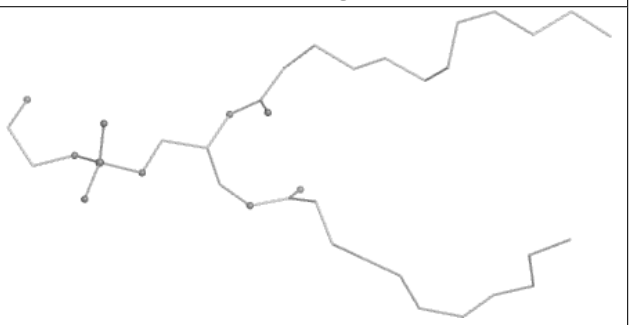
Bond lengths



Bond angles

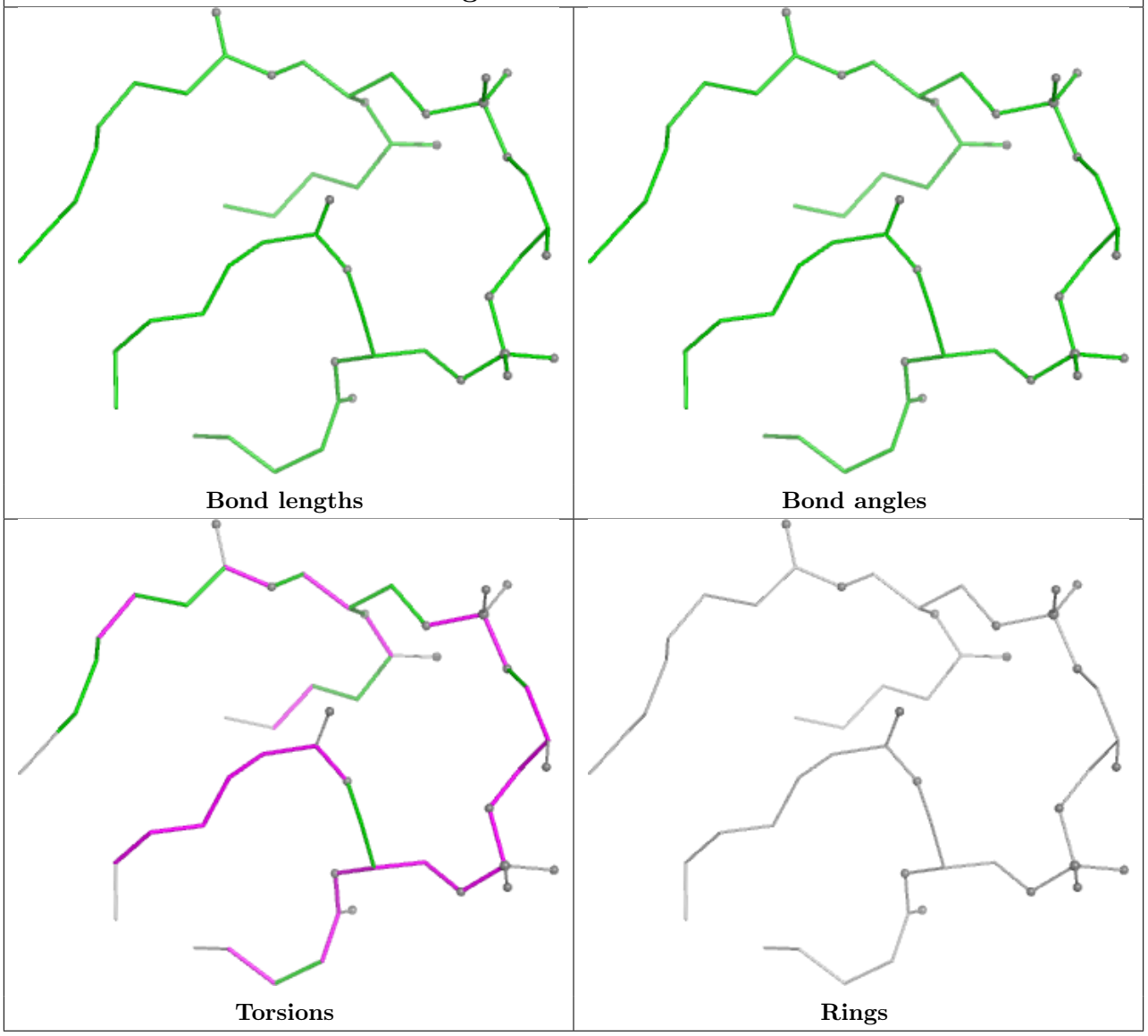


Torsions



Rings

Ligand CDL 1E 401



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-50204. These allow visual inspection of the internal detail of the map and identification of artifacts.

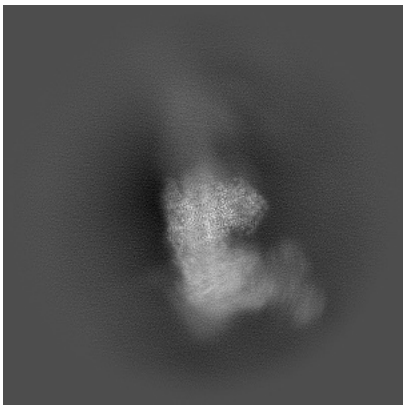
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

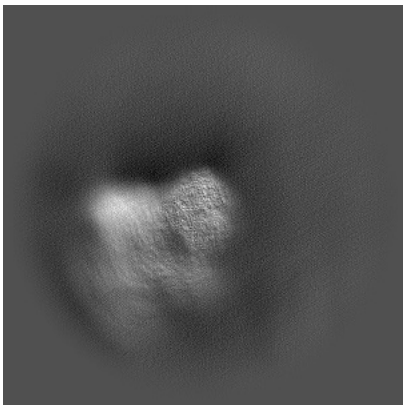
6.1.1 Primary map



X

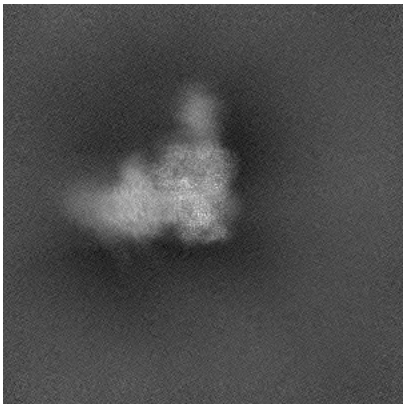


Y

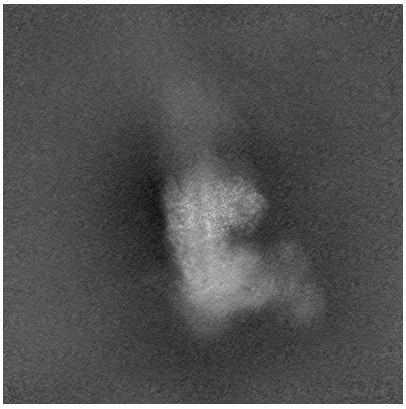


Z

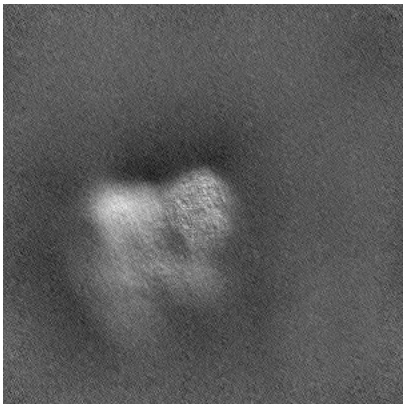
6.1.2 Raw map



X



Y

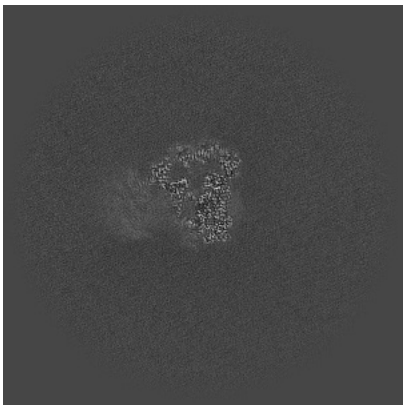


Z

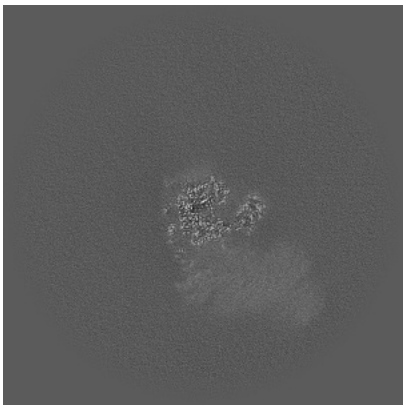
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

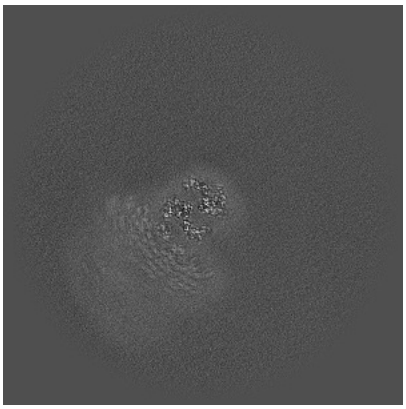
6.2.1 Primary map



X Index: 294

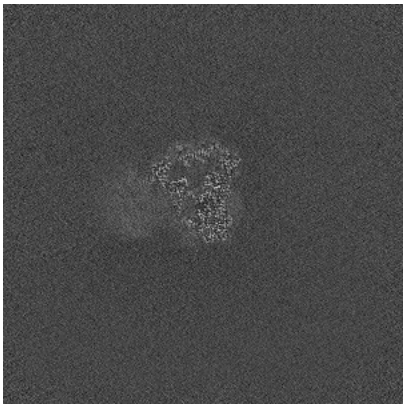


Y Index: 294



Z Index: 294

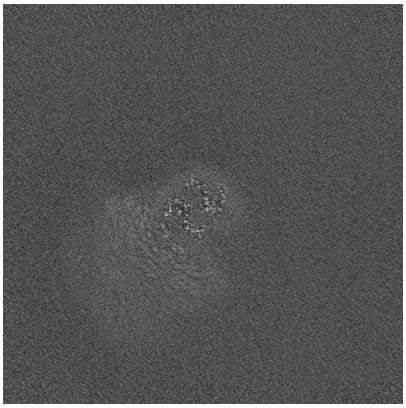
6.2.2 Raw map



X Index: 294



Y Index: 294

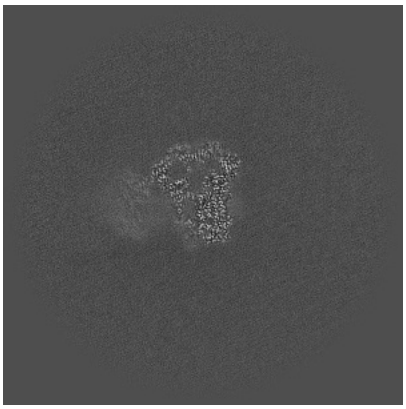


Z Index: 294

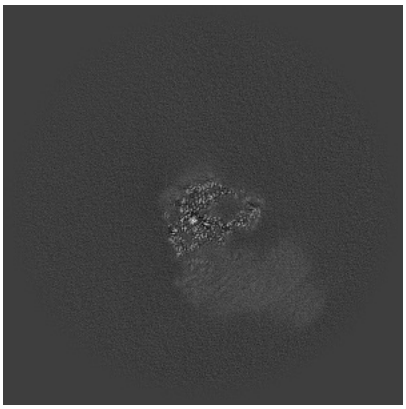
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

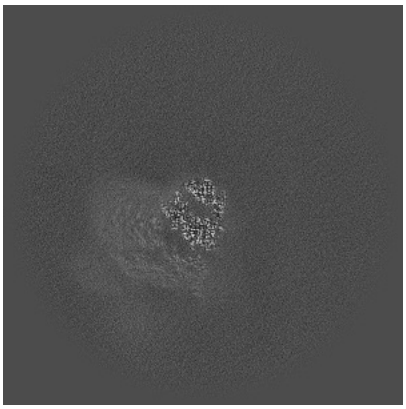
6.3.1 Primary map



X Index: 295

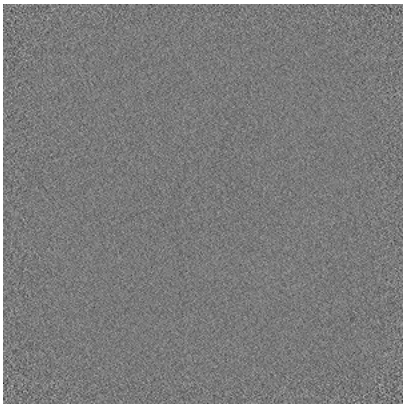


Y Index: 286

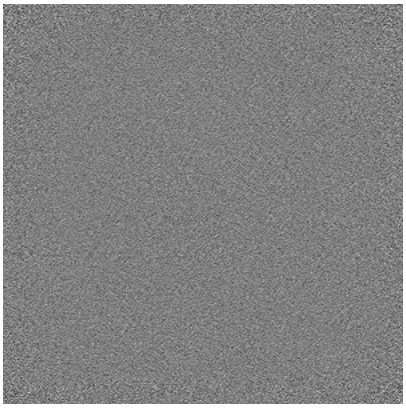


Z Index: 322

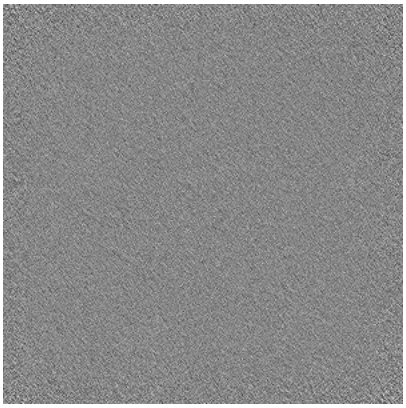
6.3.2 Raw map



X Index: 0



Y Index: 0

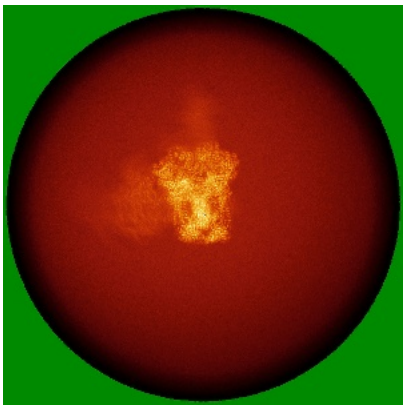


Z Index: 0

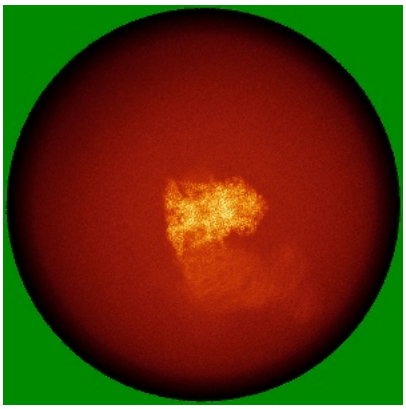
The images above show the largest variance slices of the map in three orthogonal directions.

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

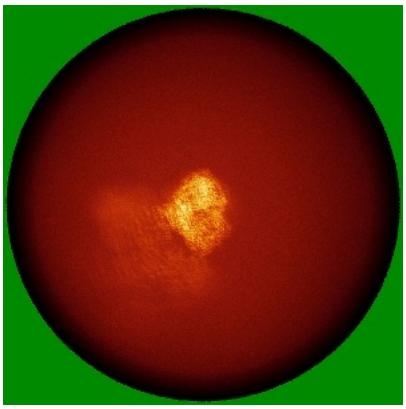
6.4.1 Primary map



X

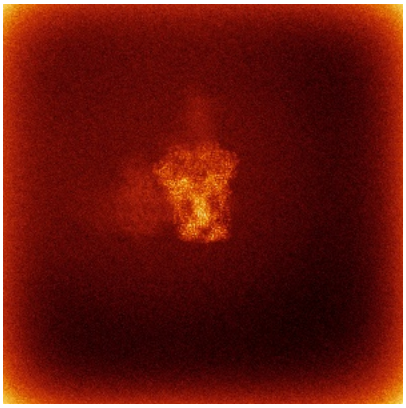


Y

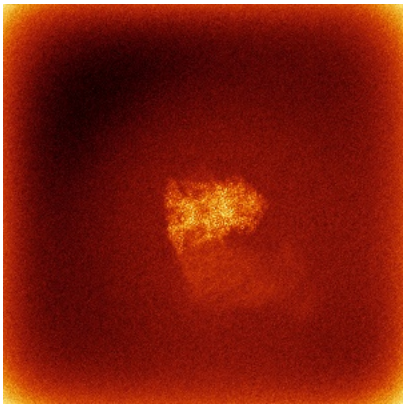


Z

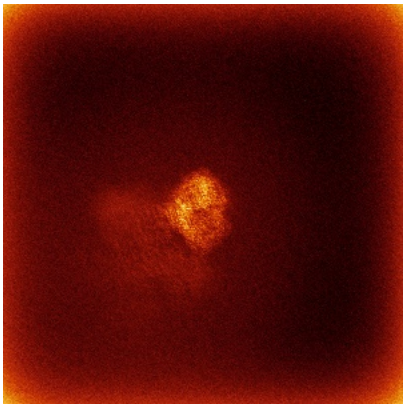
6.4.2 Raw map



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 0.145. 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.

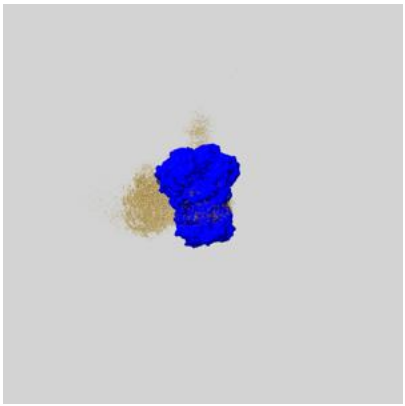
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

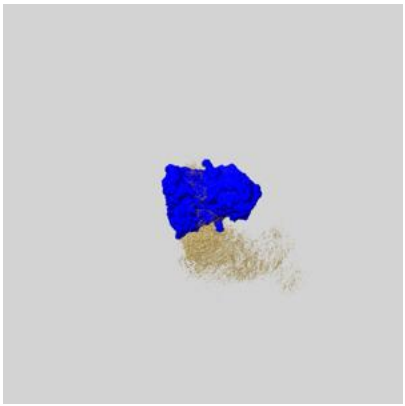
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

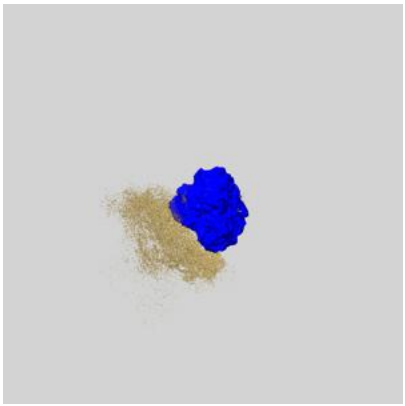
6.6.1 emd_50204_msk_1.map (i)



X



Y

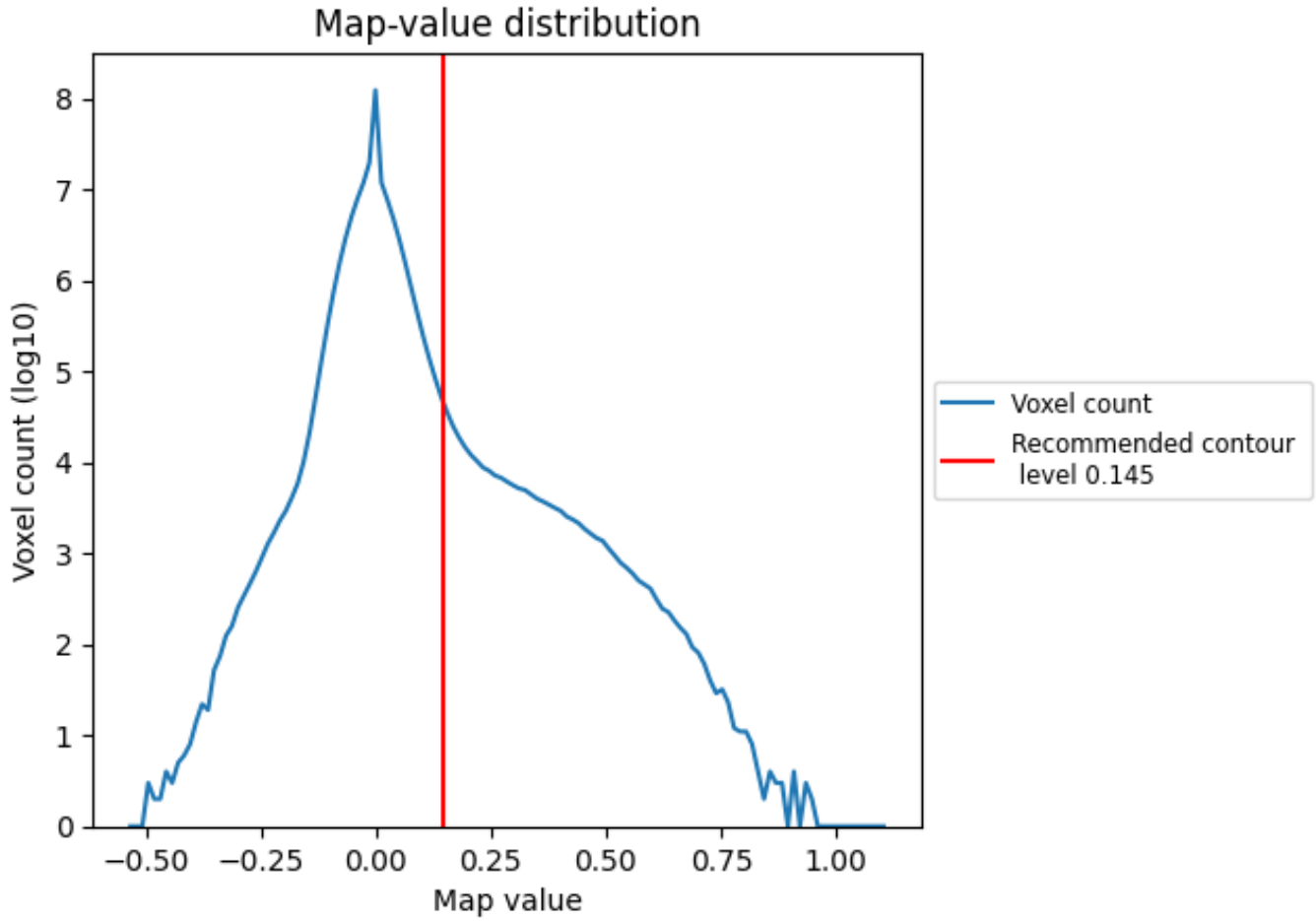


Z

7 Map analysis

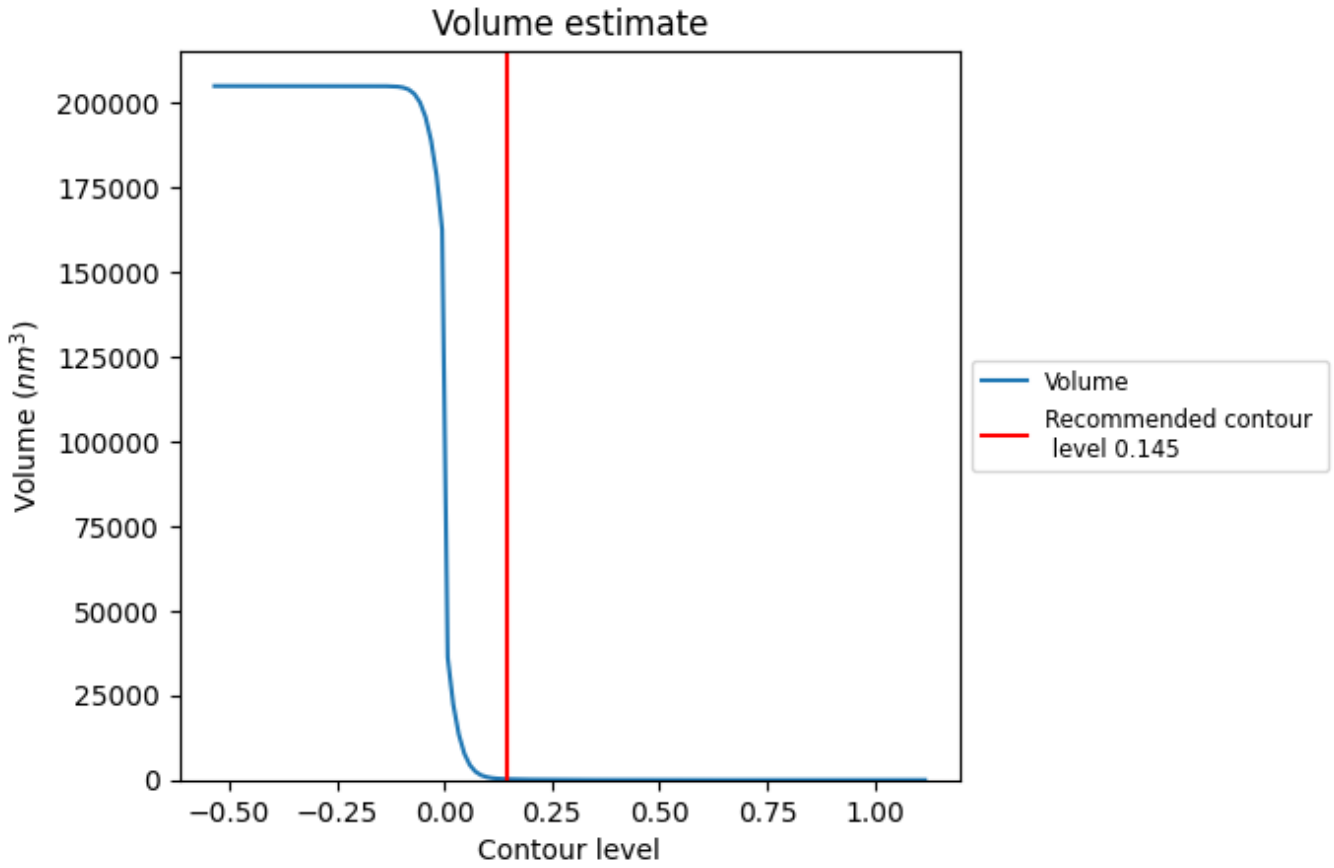
This section contains the results of statistical analysis of the map.

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.

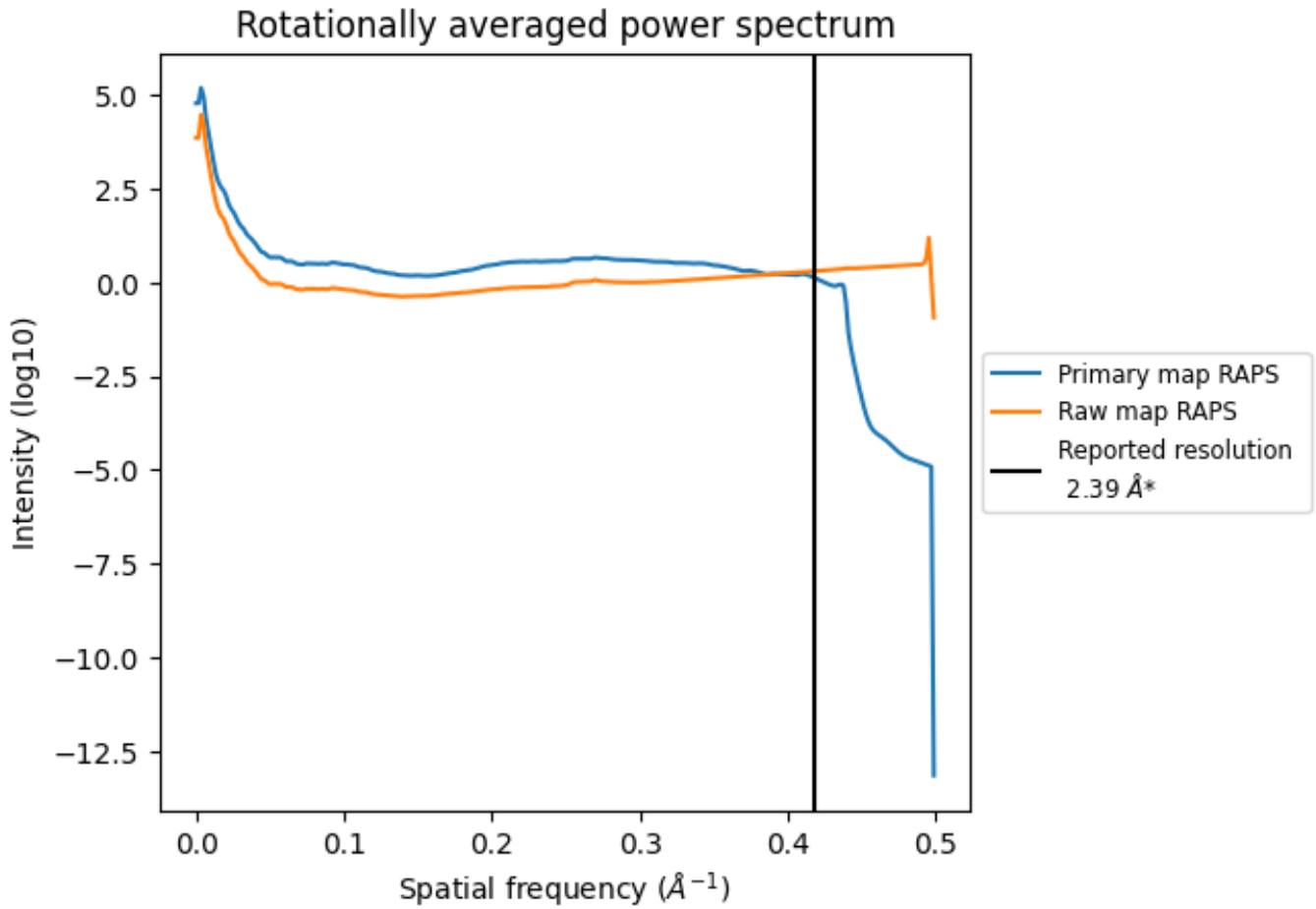
7.2 Volume estimate



The volume at the recommended contour level is 254 nm^3; this corresponds to an approximate mass of 230 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 (i)

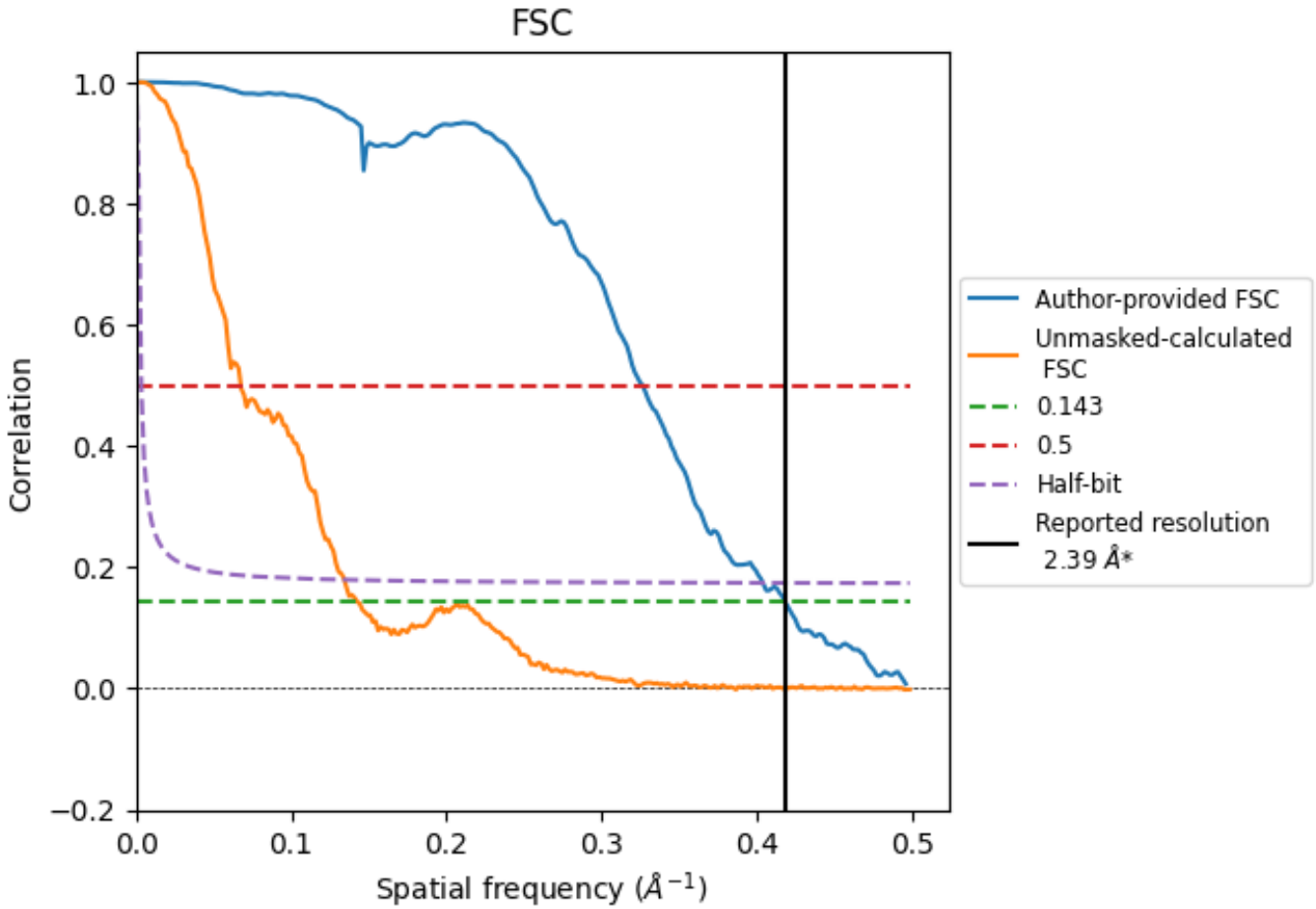


*Reported resolution corresponds to spatial frequency of 0.418 $Å^{-1}$

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 0.418 Å^{-1}

8.2 Resolution estimates (i)

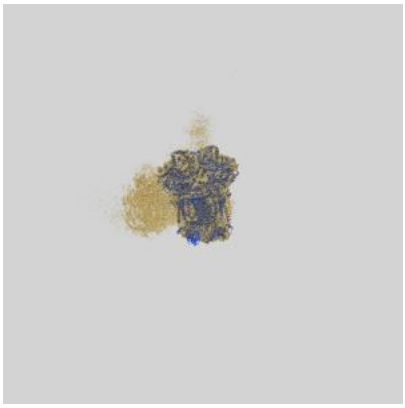
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	3.06	2.48
Unmasked-calculated*	7.02	14.81	7.45

*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 7.02 differs from the reported value 2.39 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50204 and PDB model 9F5Z. Per-residue inclusion information can be found in section 3 on page 13.

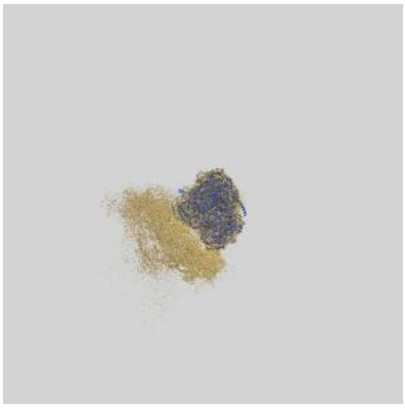
9.1 Map-model overlay



X



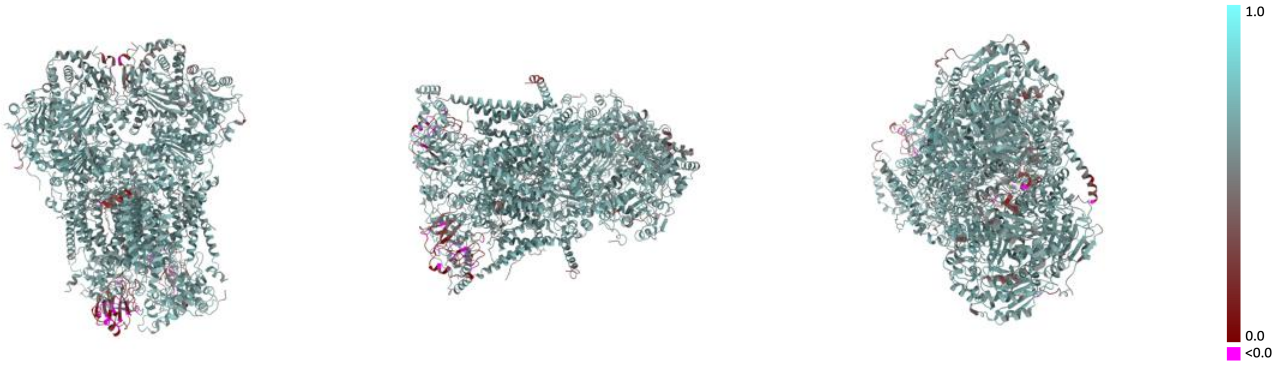
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.145 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.

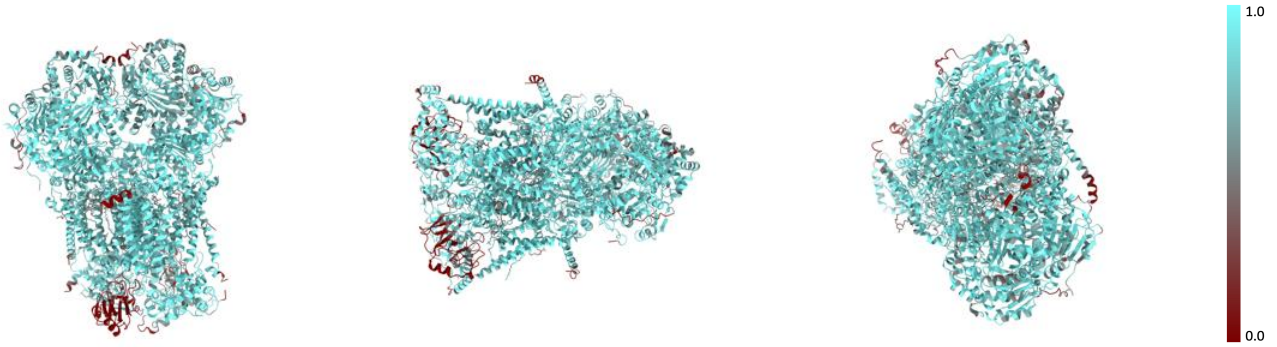
9.2 Q-score mapped to coordinate model (i)



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.

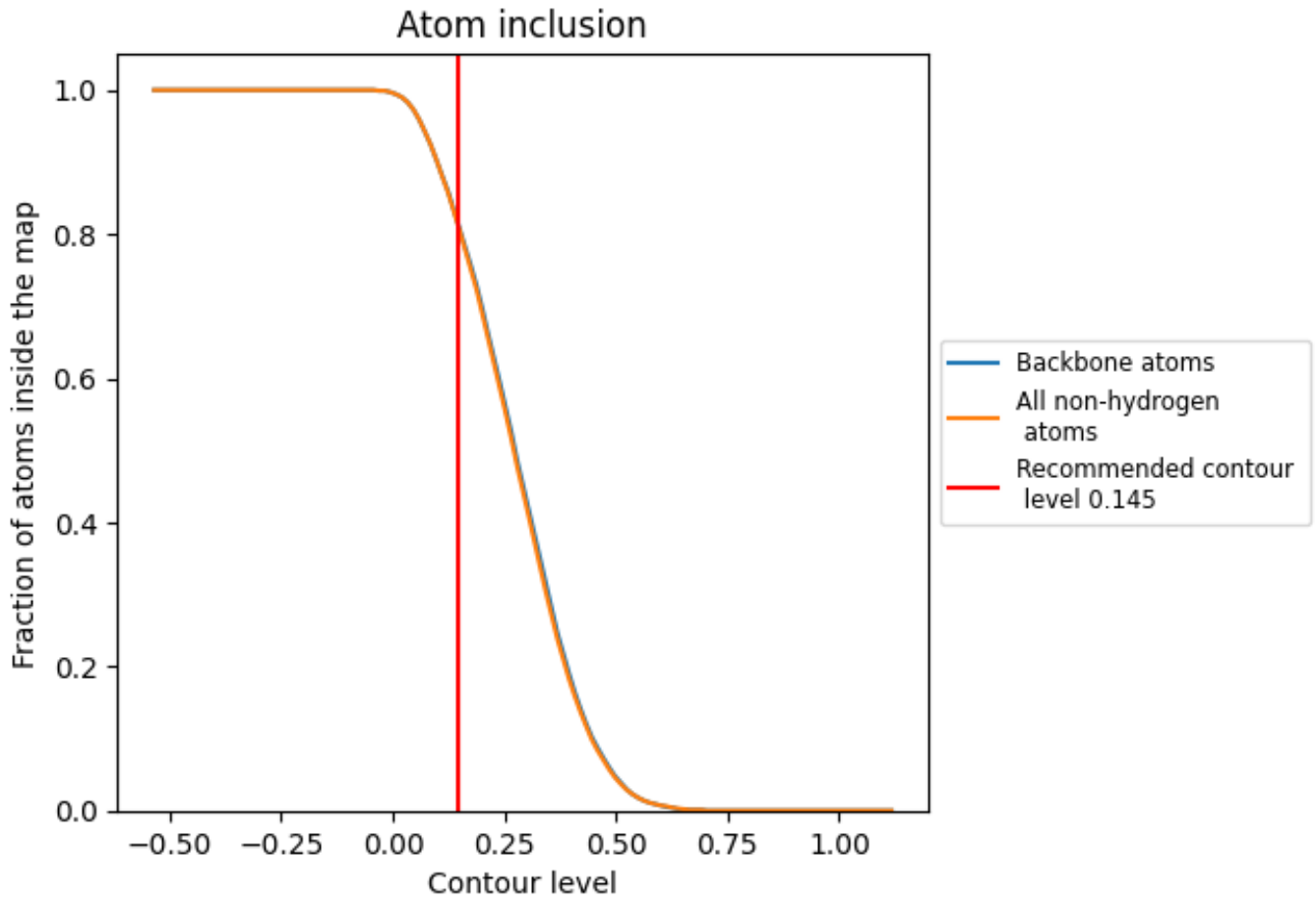
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.145).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5930
1A	0.9220	0.6410
1B	0.9120	0.6450
1C	0.4250	0.3640
1D	0.4290	0.3780
1E	0.9040	0.6430
1F	0.8880	0.6290
1G	0.8350	0.6150
1H	0.8340	0.6170
1I	0.8160	0.6070
1J	0.7270	0.5830
1K	0.8440	0.6140
1L	0.8400	0.6020
1M	0.8880	0.6310
1N	0.8760	0.6220
1O	0.7760	0.5900
1P	0.7920	0.5700
1Q	0.7930	0.5750
1R	0.8120	0.5980
1S	0.7770	0.5730
1T	0.8680	0.6350

