wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 05:42 PM EST

PDB ID	:	6WTI
EMDB ID	:	EMD-21897
Title	:	The Cryo-EM structure of the ubiquinol oxidase from Escherichia coli
Authors	:	Su, C.-C.
Deposited on	:	2020-05-02
Resolution	:	2.38 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

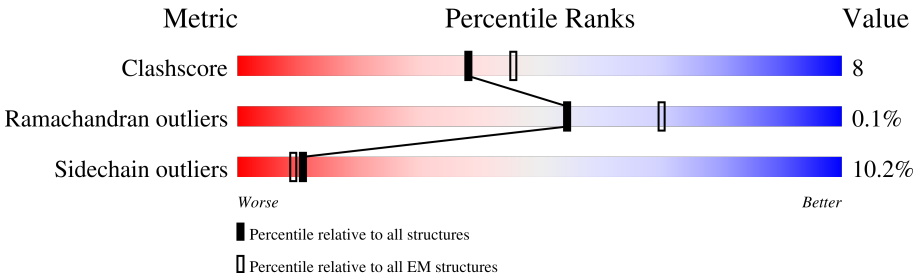
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	663	75% 22%
2	B	315	65% 17% 17%
3	C	204	72% 18% 9%
4	D	109	68% 20% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HEO	A	1002	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 9980 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 o ubiquinol oxidase, subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	660	5240	3516	829	858	37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	262	2047	1337	332	367	11	0	0

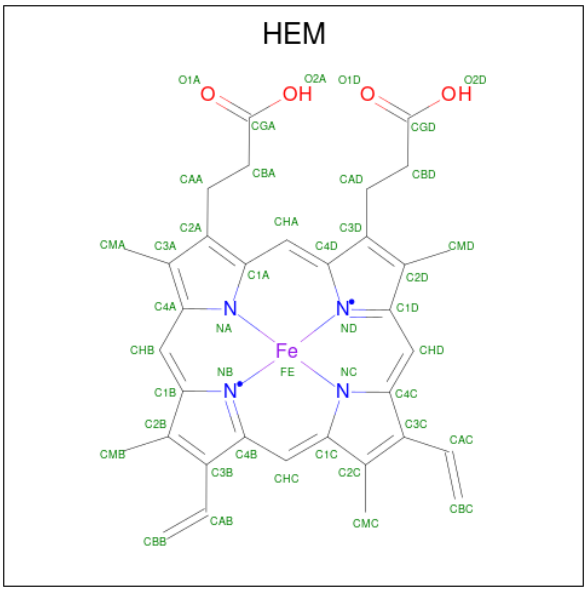
- Molecule 3 is a protein called Cytochrome o ubiquinol oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	186	1459	975	230	241	13	0	0

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

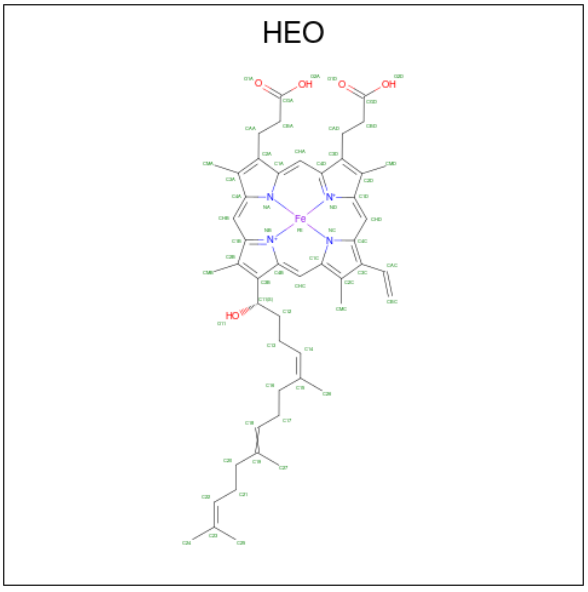
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	99	769	514	119	125	11	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 6 is HEME O (three-letter code: HEO) (formula: $C_{49}H_{58}FeN_4O_5$).

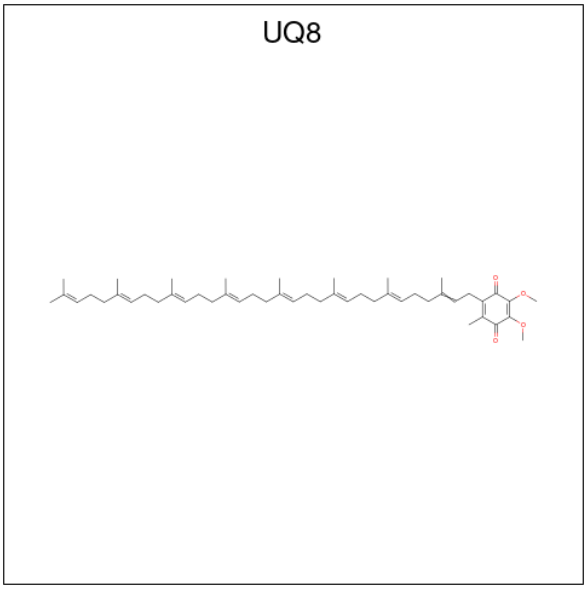


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			59	49	1	4	5	

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

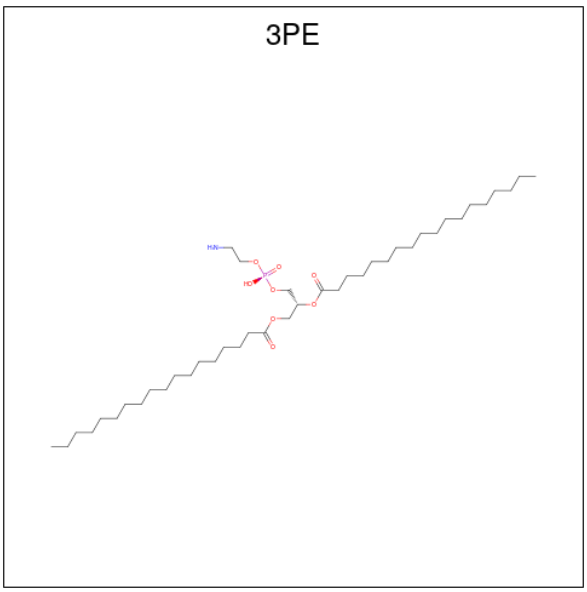
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
7	A	1	1	1	0

- Molecule 8 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



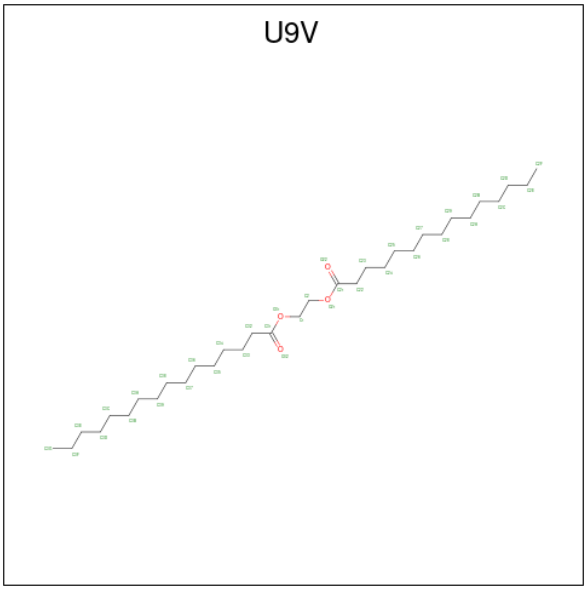
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	53	49	4	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O P 47 37 1 8 1	0
9	A	1	Total C O 28 24 4	0
9	A	1	Total C 10 10	0
9	A	1	Total C O P 26 18 7 1	0
9	B	1	Total C O 14 12 2	0
9	C	1	Total C N O P 47 37 1 8 1	0
9	C	1	Total C N O P 40 30 1 8 1	0
9	D	1	Total C N O P 45 35 1 8 1	0
9	D	1	Total C 17 17	0

- Molecule 10 is pentadecyl(tetradecyl)peroxyanhydride (three-letter code: U9V) (formula: $C_{33}H_{64}O_4$).



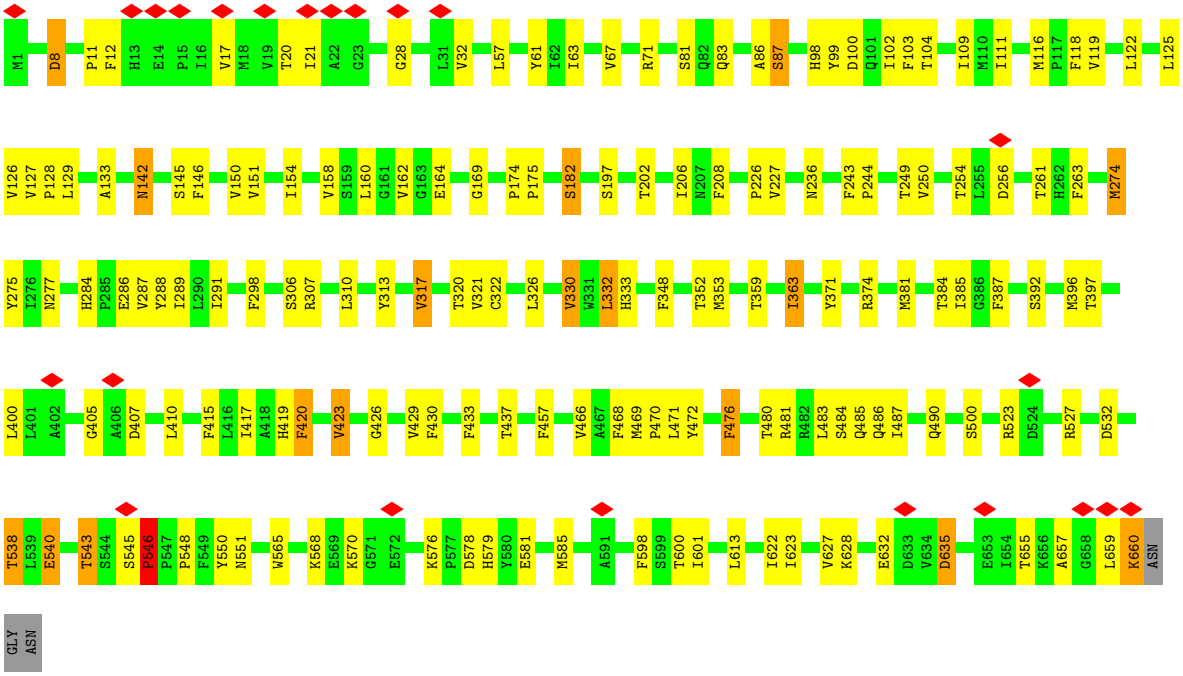
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 35 31 4	0

3 Residue-property plots (i)

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

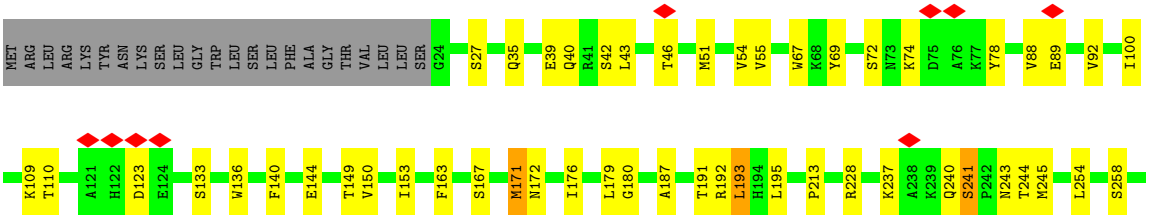
• Molecule 1: Cytochrome o ubiquinol oxidase, subunit I

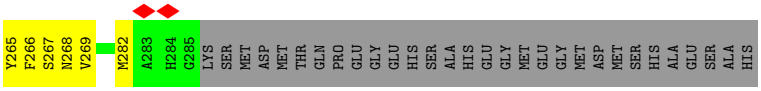
Chain A:



• Molecule 2: Ubiquinol oxidase subunit 2

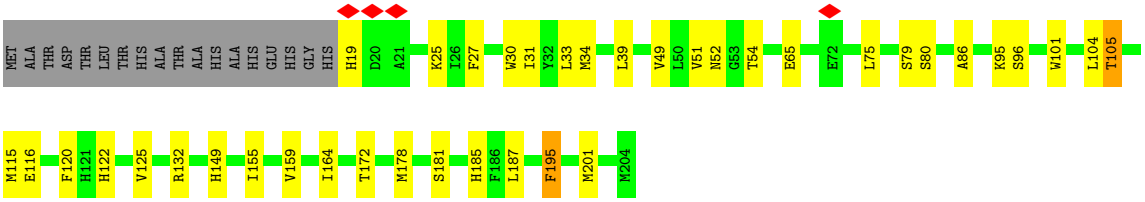
Chain B:





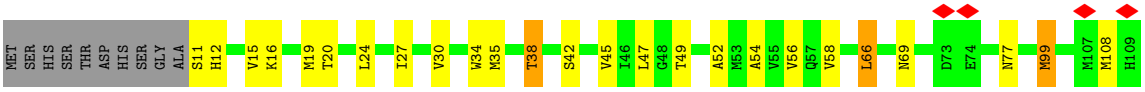
• Molecule 3: Cytochrome o ubiquinol oxidase

Chain C:



• Molecule 4: Cytochrome o ubiquinol oxidase, subunit IV

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.271	Depositor
Minimum map value	-3.624	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.410	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	114.48, 91.8, 104.76	wwPDB
Map dimensions	97, 85, 106	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEO, UQ8, 3PE, U9V, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/5417	0.54	1/7385 (0.0%)
2	B	0.45	0/2107	0.60	0/2869
3	C	0.41	0/1502	0.51	0/2040
4	D	0.38	0/789	0.48	0/1077
All	All	0.43	0/9815	0.54	1/13371 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	546	PRO	N-CA-C	-5.67	97.36	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5240	0	5247	104	0
2	B	2047	0	2040	35	0
3	C	1459	0	1467	17	0
4	D	769	0	800	8	0
5	A	43	0	30	9	0
6	A	59	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
8	A	53	0	74	8	0
9	A	111	0	148	1	0
9	B	14	0	18	0	0
9	C	87	0	122	1	0
9	D	62	0	94	0	0
10	A	35	0	0	0	0
All	All	9980	0	10096	161	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 8.

The worst 5 of 161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:SER:HB2	1:A:546:PRO:CD	1.57	1.33
1:A:545:SER:CB	1:A:546:PRO:HD3	1.65	1.26
1:A:208:PHE:HB2	1:A:236:ASN:OD1	1.51	1.08
1:A:284:HIS:HD2	1:A:330:VAL:HG23	1.27	0.97
1:A:284:HIS:CD2	1:A:330:VAL:HG23	2.00	0.96

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	658/663 (99%)	630 (96%)	27 (4%)	1 (0%)	47 61
2	B	260/315 (82%)	246 (95%)	14 (5%)	0	100 100
3	C	184/204 (90%)	179 (97%)	5 (3%)	0	100 100
4	D	97/109 (89%)	88 (91%)	9 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1199/1291 (93%)	1143 (95%)	55 (5%)	1 (0%)	54 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	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	A	544/547 (100%)	494 (91%)	50 (9%)	9 12
2	B	218/262 (83%)	202 (93%)	16 (7%)	14 20
3	C	153/166 (92%)	132 (86%)	21 (14%)	3 4
4	D	86/94 (92%)	71 (83%)	15 (17%)	2 2
All	All	1001/1069 (94%)	899 (90%)	102 (10%)	11 9

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	171	MET
3	C	65	GLU
4	D	77	ASN
2	B	192	ARG
2	B	258	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
9	3PE	A	1006	-	27,27,50	1.20	4 (14%)	29,29,55	1.43	4 (13%)
9	3PE	A	1005	-	46,46,50	0.89	4 (8%)	49,51,55	1.13	2 (4%)
9	3PE	A	1007	-	9,9,50	0.29	0	8,8,55	0.78	0
9	3PE	C	401	-	46,46,50	0.90	4 (8%)	49,51,55	1.08	2 (4%)
9	3PE	A	1009	-	23,25,50	1.16	3 (13%)	24,28,55	1.30	2 (8%)
9	3PE	B	401	-	13,13,50	1.01	2 (15%)	13,13,55	1.00	1 (7%)
5	HEM	A	1001	1	41,50,50	1.33	4 (9%)	45,82,82	1.89	10 (22%)
9	3PE	C	402	-	39,39,50	0.97	4 (10%)	42,44,55	1.07	2 (4%)
9	3PE	D	202	-	16,16,50	0.29	0	15,15,55	0.77	0
10	U9V	A	1008	-	33,33,36	0.82	2 (6%)	33,33,37	1.07	0
9	3PE	D	201	-	44,44,50	0.92	4 (9%)	47,49,55	1.16	2 (4%)
8	UQ8	A	1004	-	53,53,53	2.72	18 (33%)	64,67,67	2.18	20 (31%)
6	HEO	A	1002	1	63,66,66	3.92	13 (20%)	71,102,102	4.44	38 (53%)

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
9	3PE	A	1006	-	-	10/28/28/54	-
9	3PE	A	1005	-	-	28/50/50/54	-
9	3PE	A	1007	-	-	2/7/7/54	-
9	3PE	C	401	-	-	15/50/50/54	-
9	3PE	A	1009	-	-	12/25/27/54	-
9	3PE	B	401	-	-	4/12/12/54	-
5	HEM	A	1001	1	-	6/12/54/54	-
9	3PE	C	402	-	-	19/43/43/54	-
9	3PE	D	202	-	-	5/14/14/54	-
10	U9V	A	1008	-	-	13/29/29/36	-
9	3PE	D	201	-	-	24/48/48/54	-
8	UQ8	A	1004	-	-	20/51/75/75	0/1/1/1
6	HEO	A	1002	1	3/3/17/25	16/32/114/114	-

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	HEO	CHA-C1A	13.21	1.64	1.38
6	A	1002	HEO	CHC-C4B	11.67	1.64	1.35
6	A	1002	HEO	CHB-C4A	11.63	1.61	1.38
6	A	1002	HEO	CHB-C1B	10.80	1.63	1.39
6	A	1002	HEO	CHD-C1D	10.78	1.62	1.35

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	HEO	CHA-C4D-C3D	-12.26	106.82	124.84
6	A	1002	HEO	C1A-CHA-C4D	-10.29	103.86	126.06
6	A	1002	HEO	C3D-C4D-ND	9.61	119.67	110.36
6	A	1002	HEO	C4A-NA-C1A	-9.13	96.41	105.35
6	A	1002	HEO	C1D-ND-C4D	-9.10	95.67	105.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1002	HEO	NB
6	A	1002	HEO	ND
6	A	1002	HEO	NA

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEM	C2B-C3B-CAB-CBB
5	A	1001	HEM	C4B-C3B-CAB-CBB
6	A	1002	HEO	C2D-C3D-CAD-CBD
6	A	1002	HEO	C4D-C3D-CAD-CBD
6	A	1002	HEO	C3B-C11-C12-C13

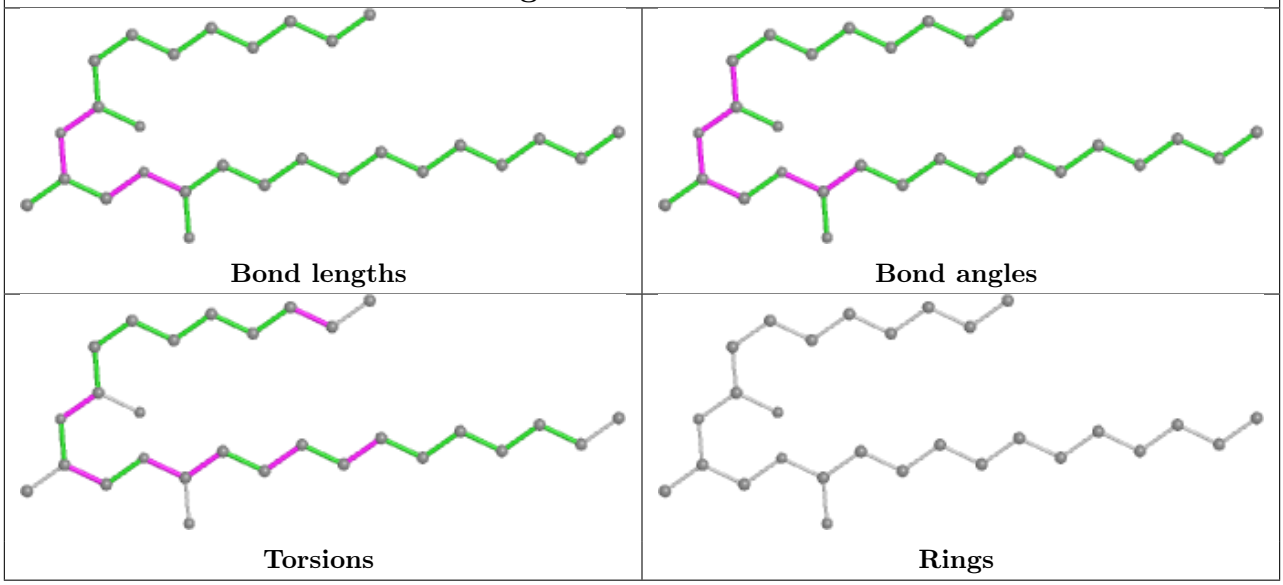
There are no ring outliers.

5 monomers are involved in 26 short contacts:

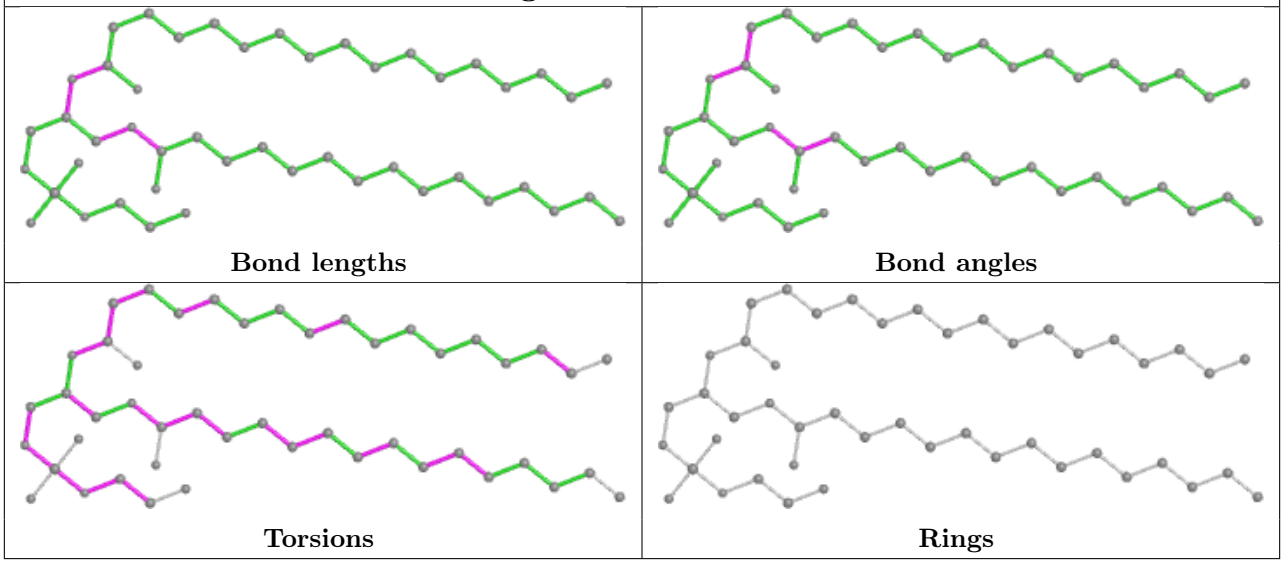
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	401	3PE	1	0
9	A	1009	3PE	1	0
5	A	1001	HEM	9	0
8	A	1004	UQ8	8	0
6	A	1002	HEO	7	0

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

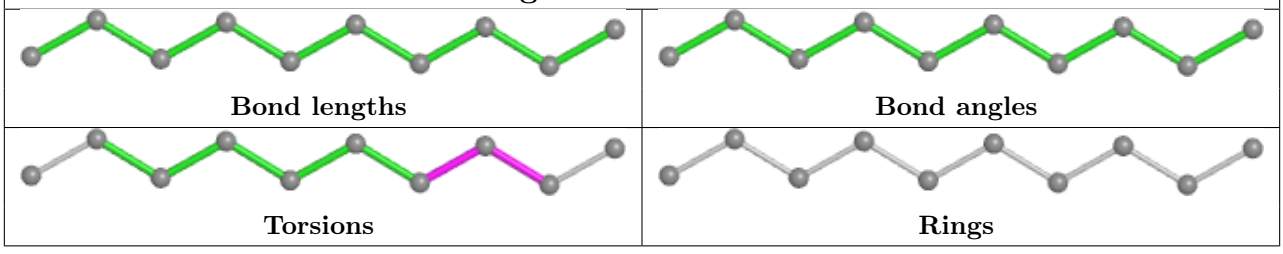
Ligand 3PE A 1006



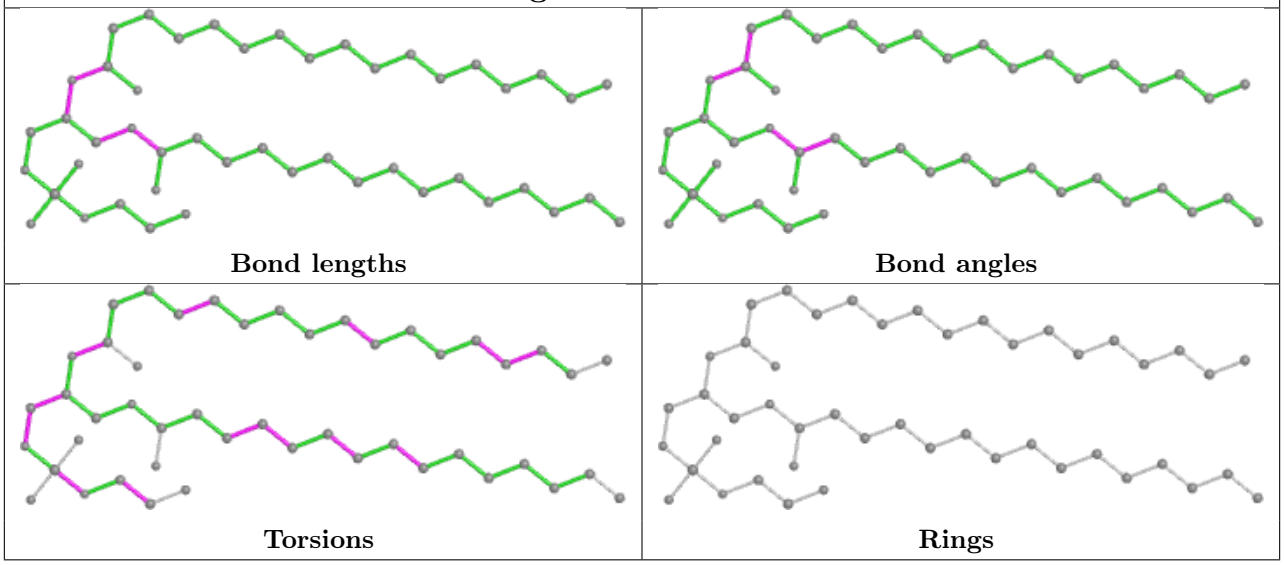
Ligand 3PE A 1005



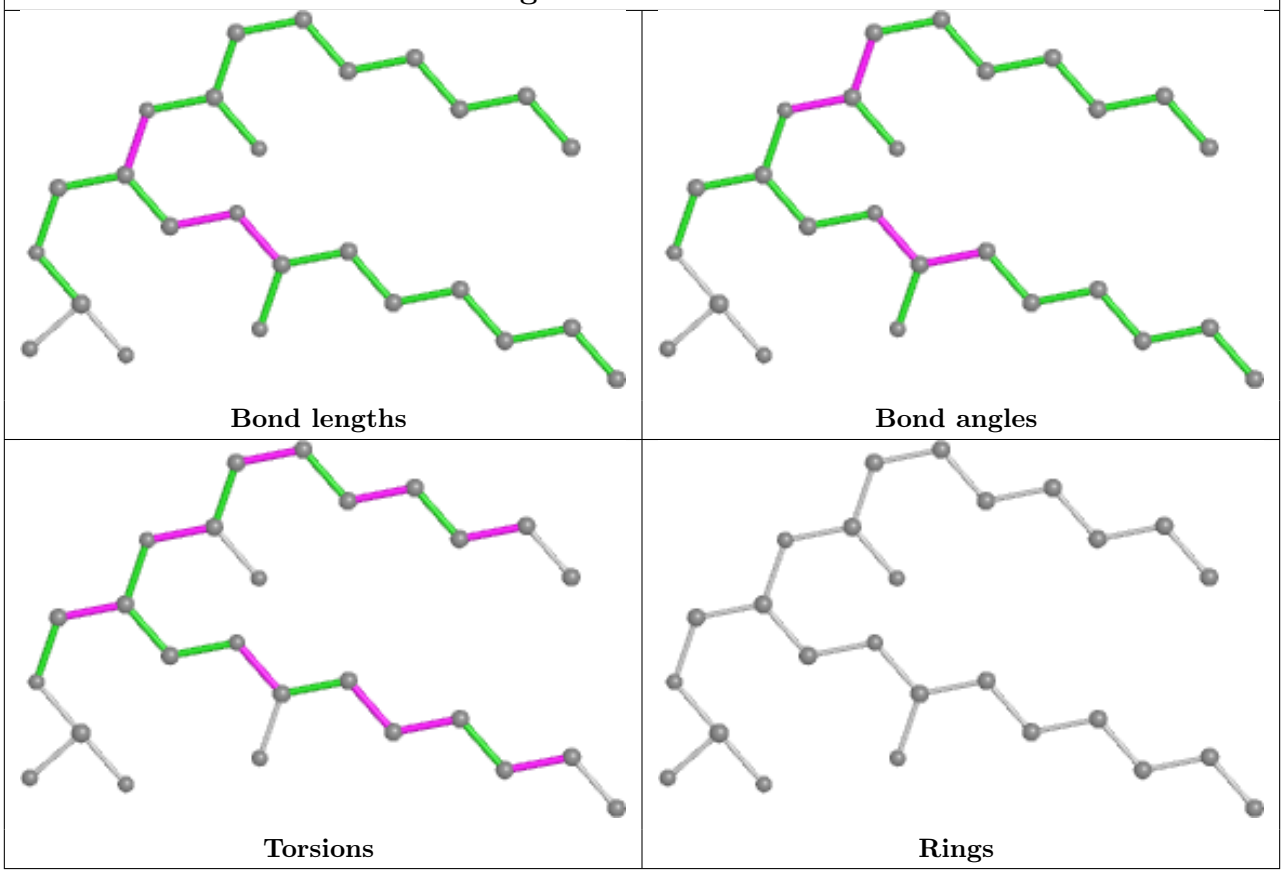
Ligand 3PE A 1007



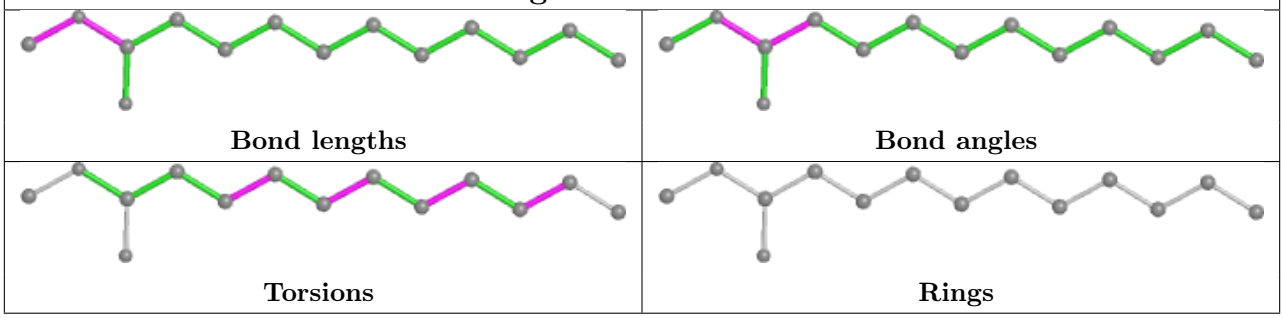
Ligand 3PE C 401



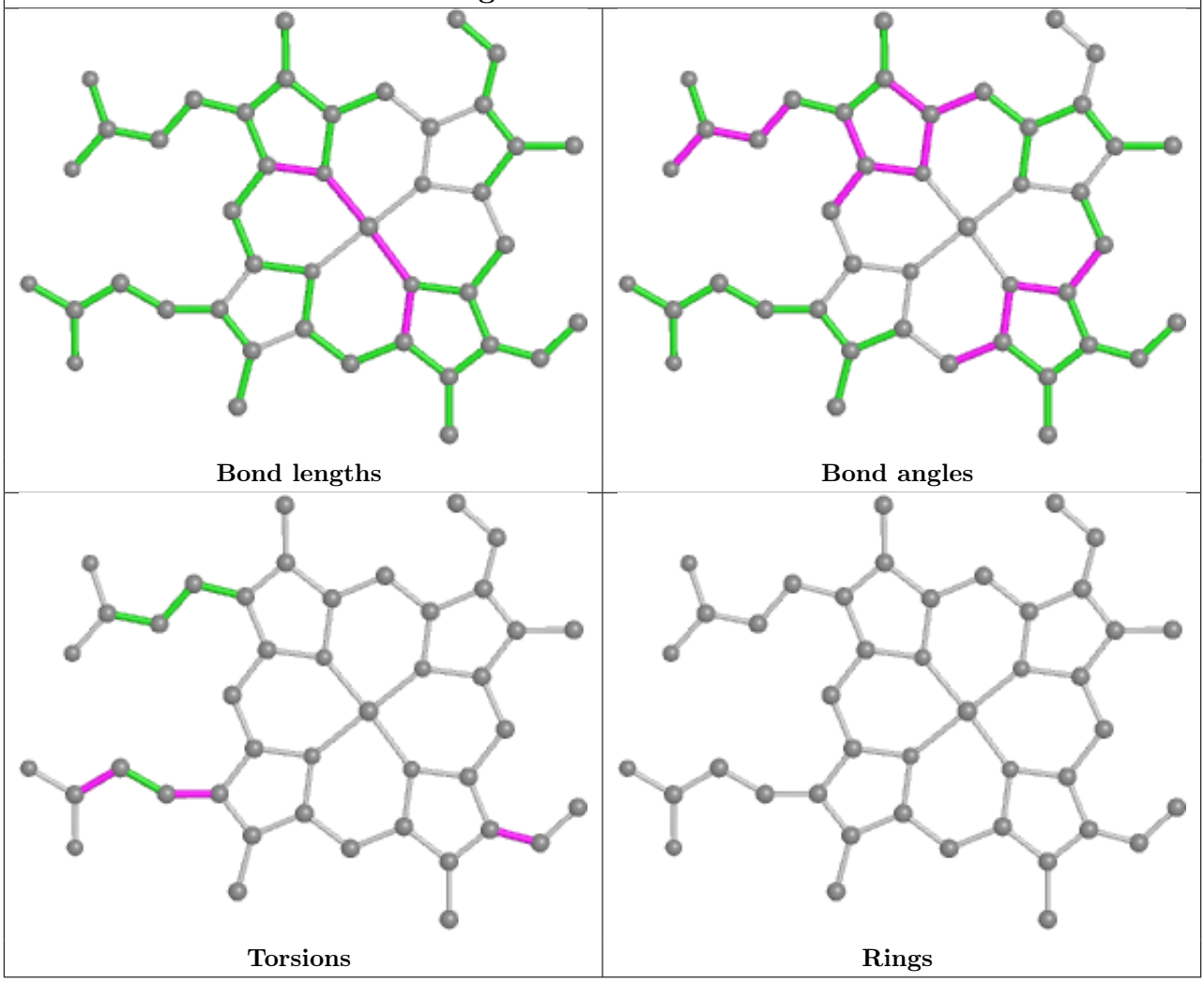
Ligand 3PE A 1009



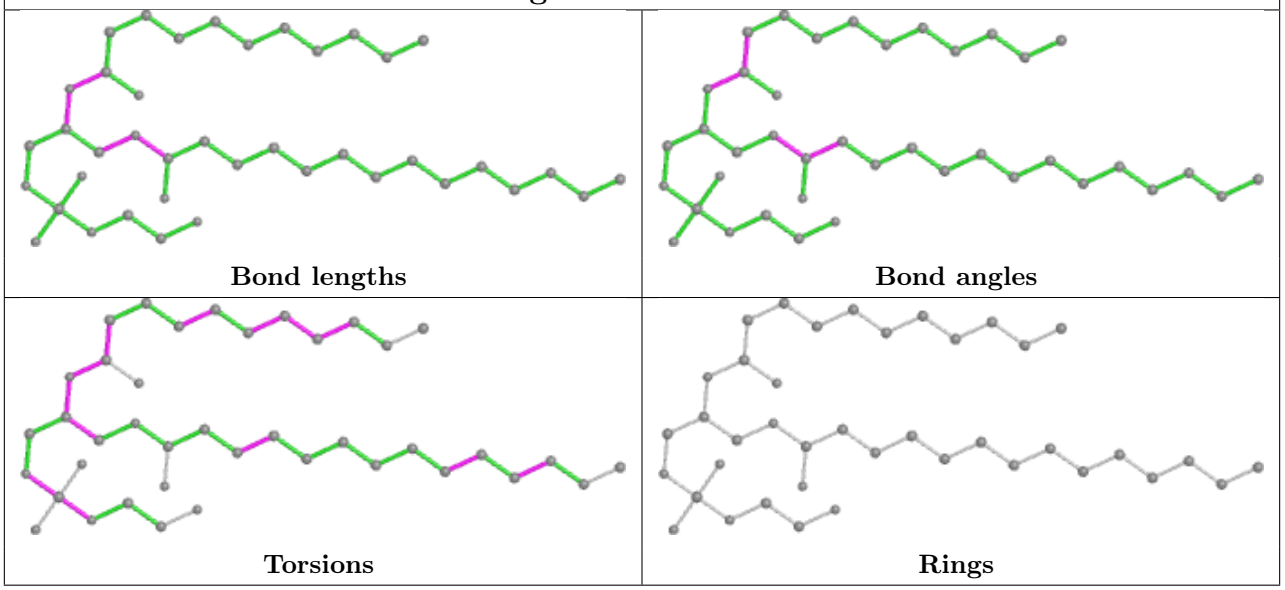
Ligand 3PE B 401



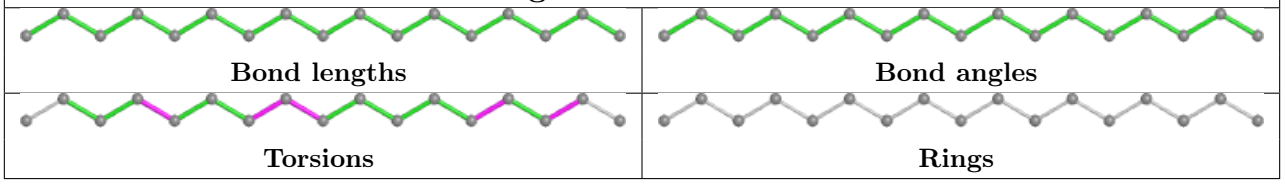
Ligand HEM A 1001



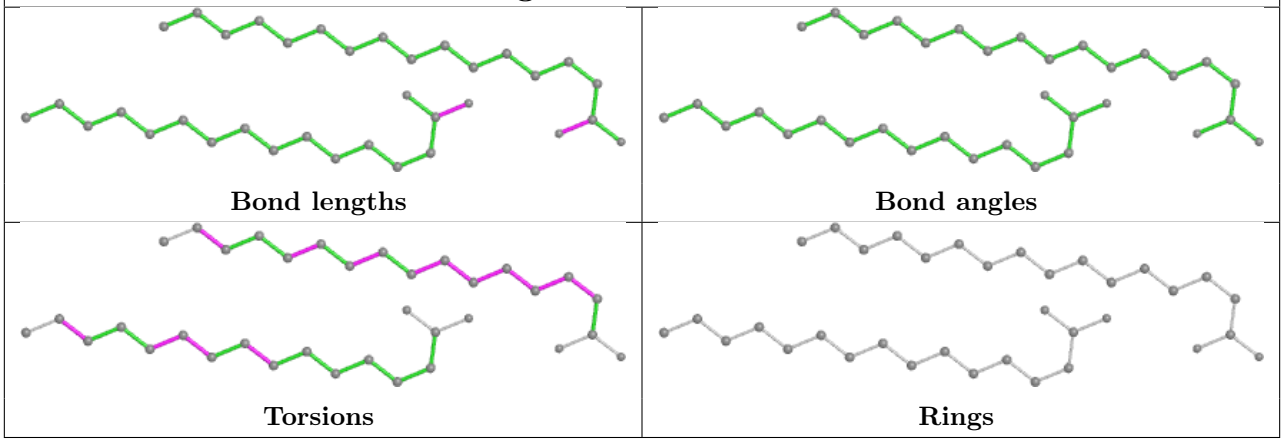
Ligand 3PE C 402



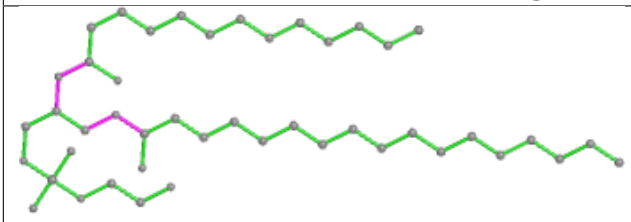
Ligand 3PE D 202



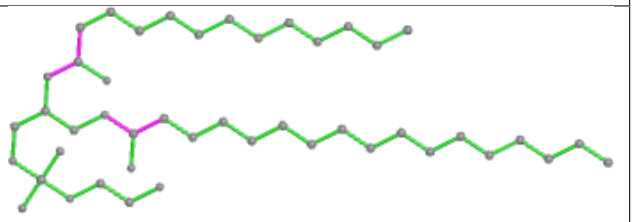
Ligand U9V A 1008



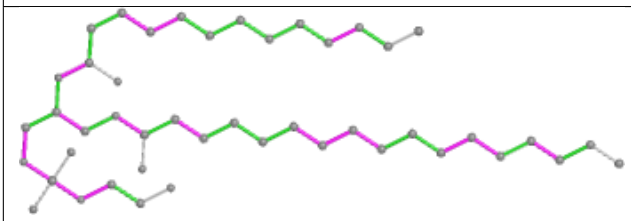
Ligand 3PE D 201



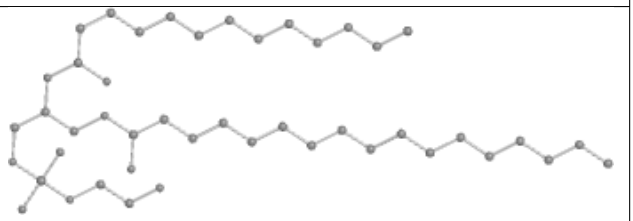
Bond lengths



Bond angles

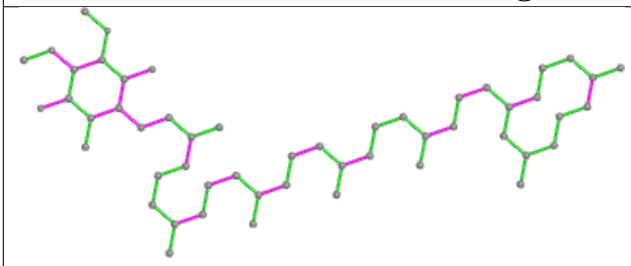


Torsions

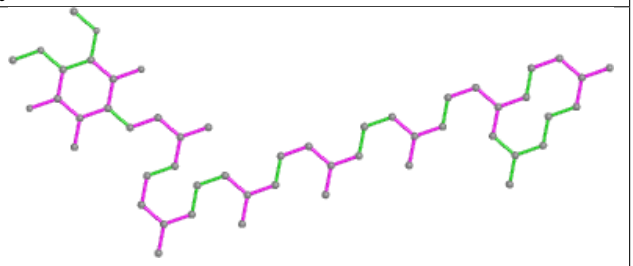


Rings

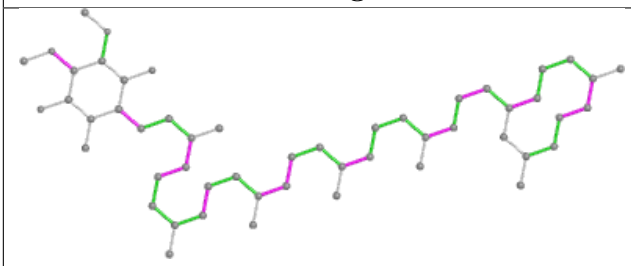
Ligand UQ8 A 1004



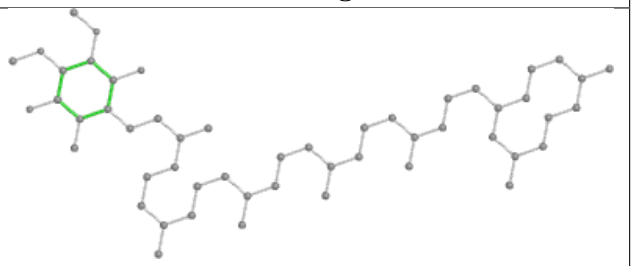
Bond lengths



Bond angles

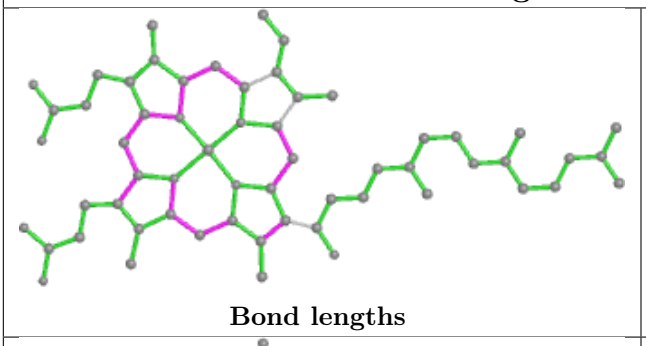


Torsions

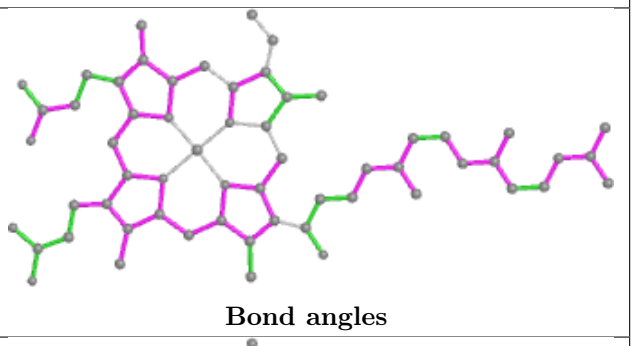


Rings

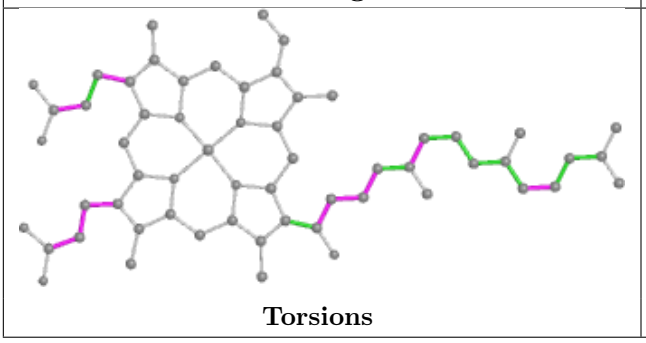
Ligand HEO A 1002



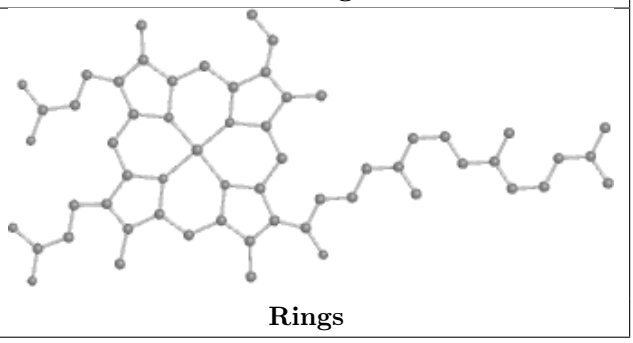
Bond lengths



Bond angles



Torsions



Rings

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.

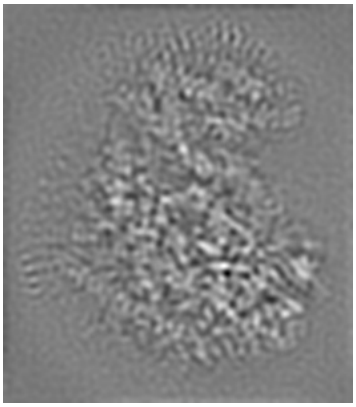
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21897. These allow visual inspection of the internal detail of the map and identification of artifacts.

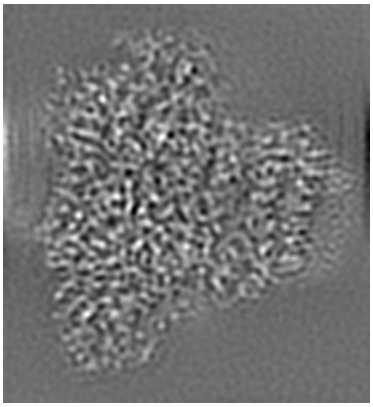
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

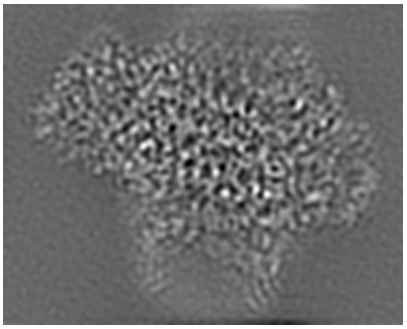
6.1.1 Primary map



X



Y

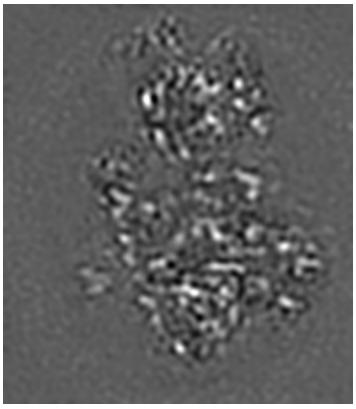


Z

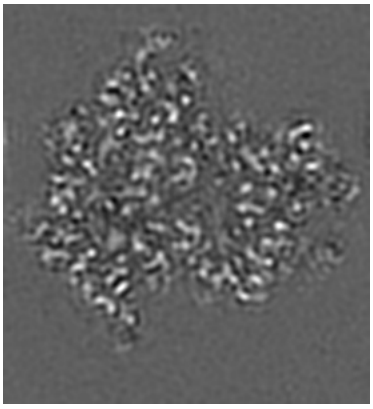
The images above show the map projected in three orthogonal directions.

6.2 Central slices

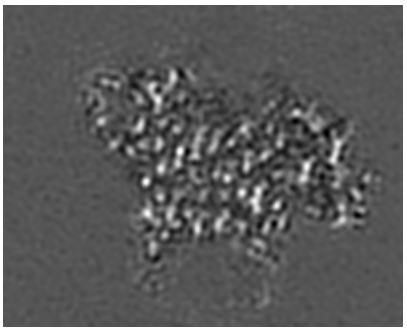
6.2.1 Primary map



X Index: 53



Y Index: 42

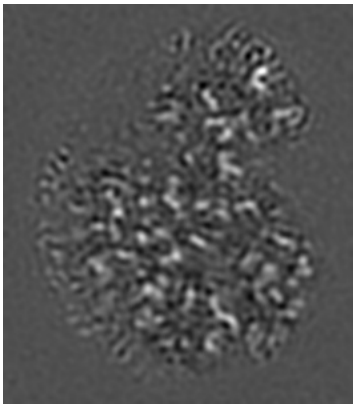


Z Index: 48

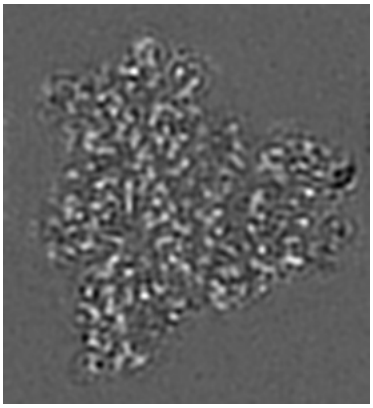
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

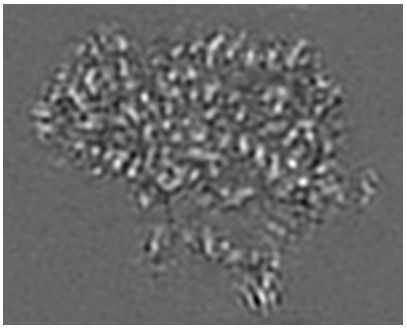
6.3.1 Primary map



X Index: 41



Y Index: 52

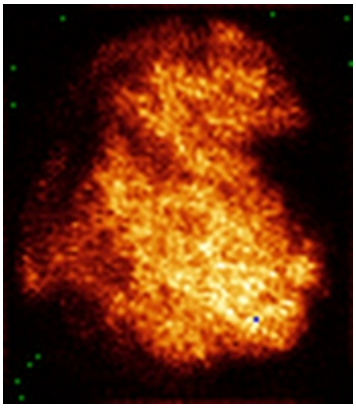


Z Index: 30

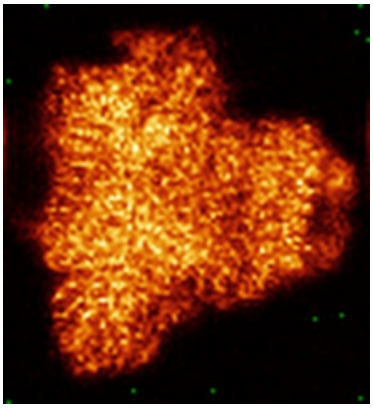
The images above show the largest variance slices of the map in three orthogonal directions.

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

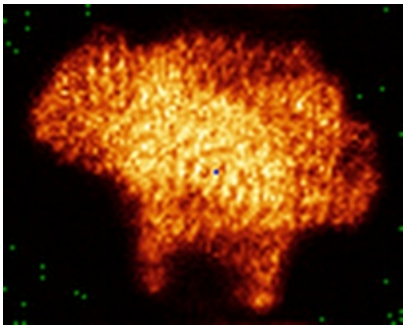
6.4.1 Primary map



X



Y

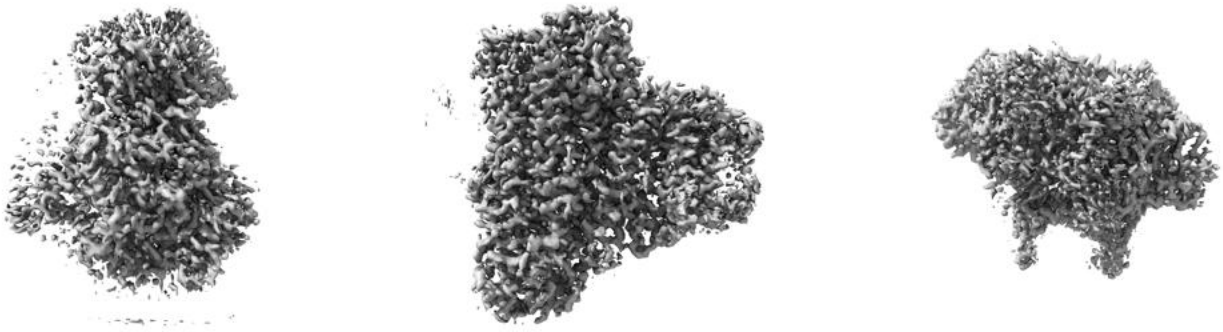


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

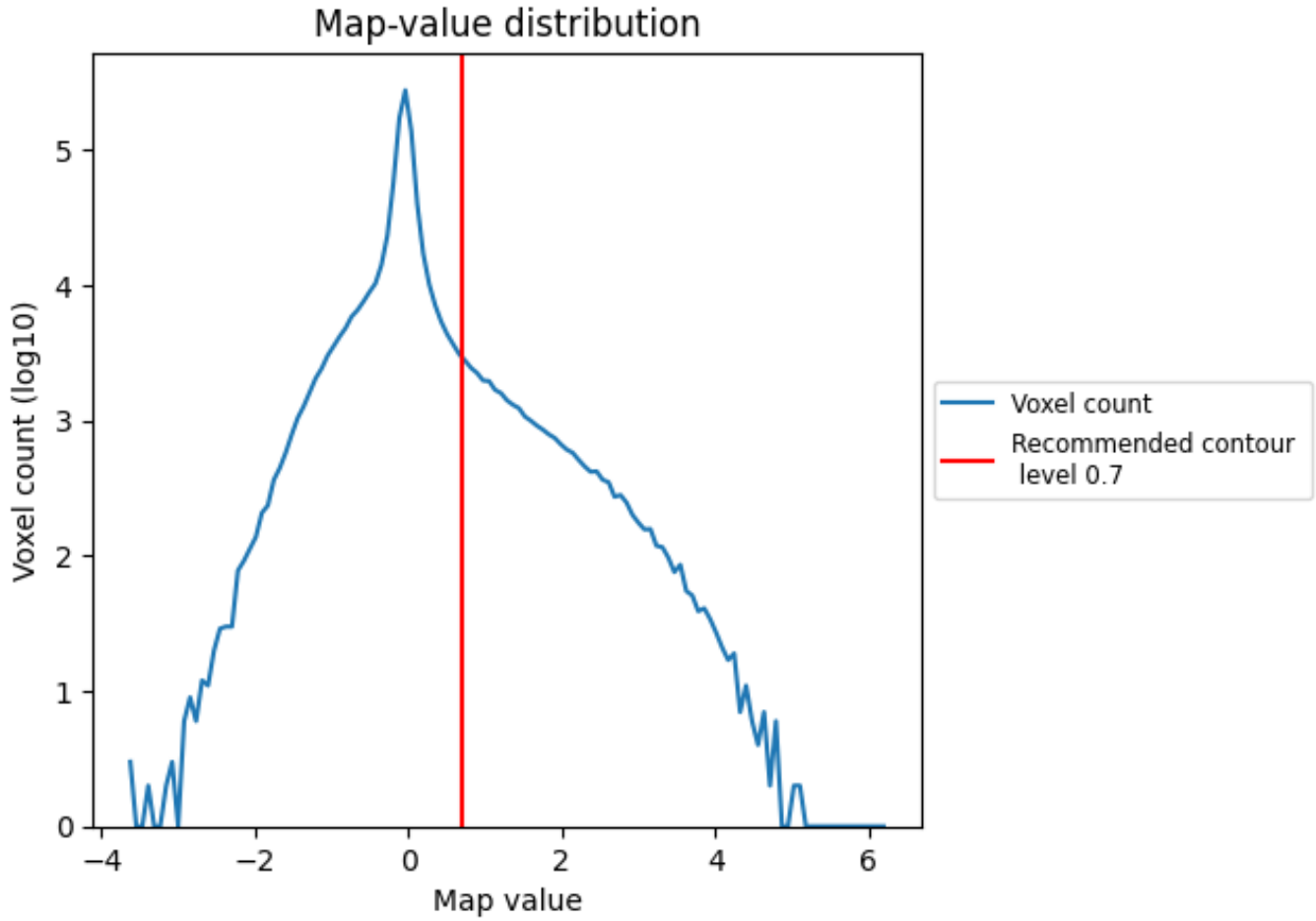
6.6 Mask visualisation (i)

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

7 Map analysis

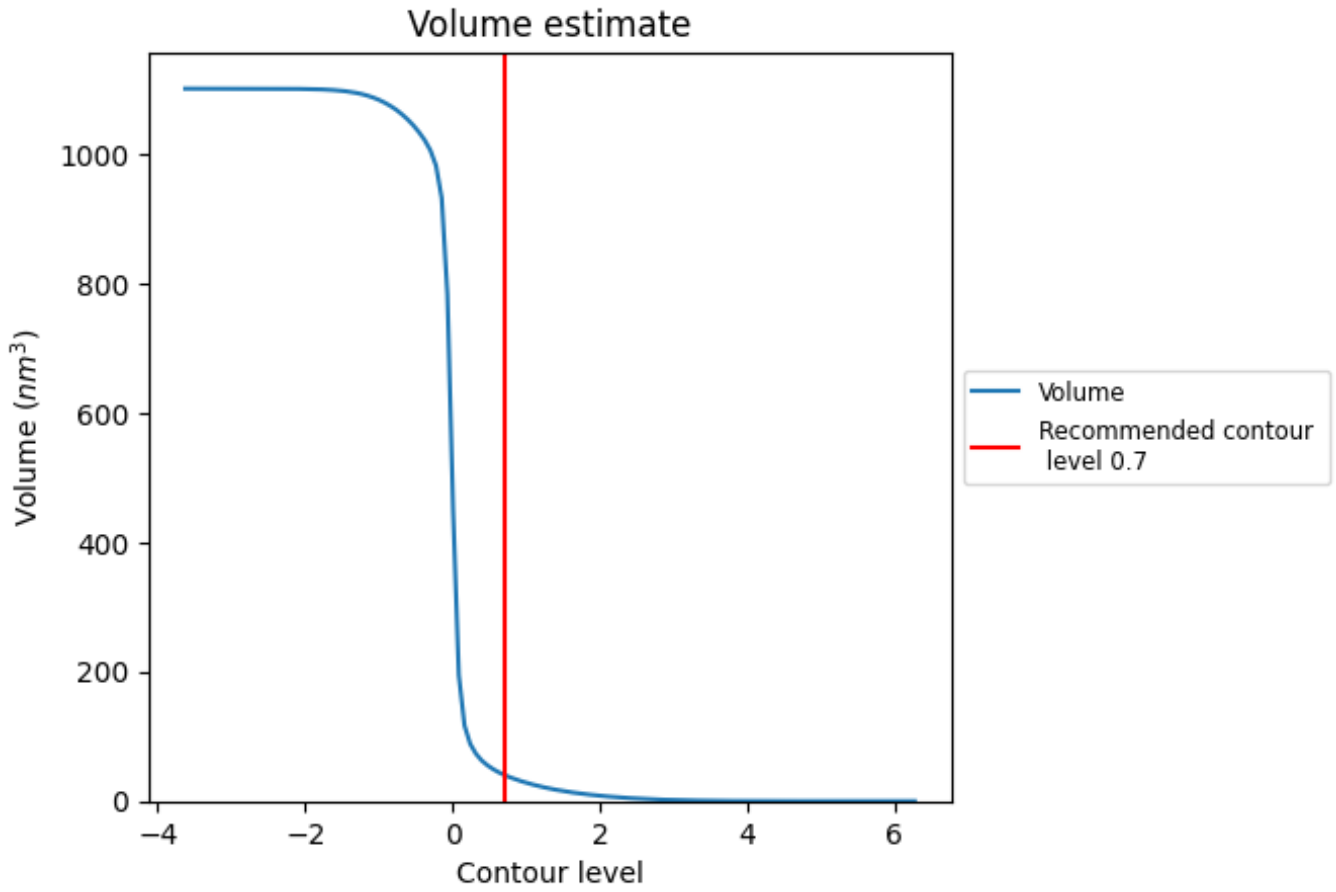
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 41 nm^3; this corresponds to an approximate mass of 37 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)

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

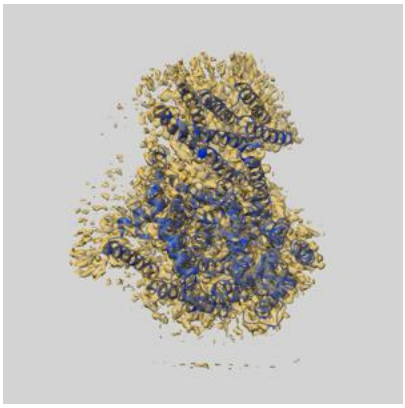
8 Fourier-Shell correlation (i)

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

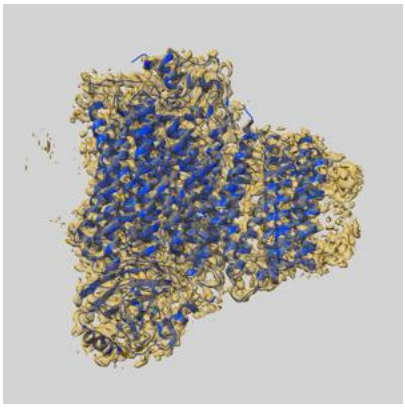
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21897 and PDB model 6WTI. Per-residue inclusion information can be found in section 3 on page 7.

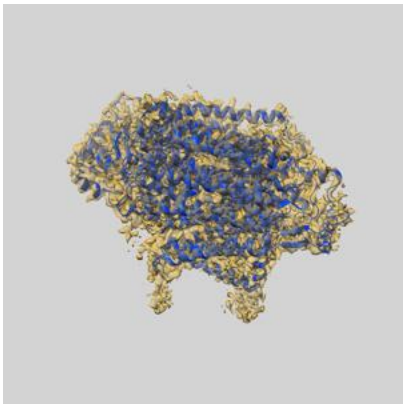
9.1 Map-model overlay



X



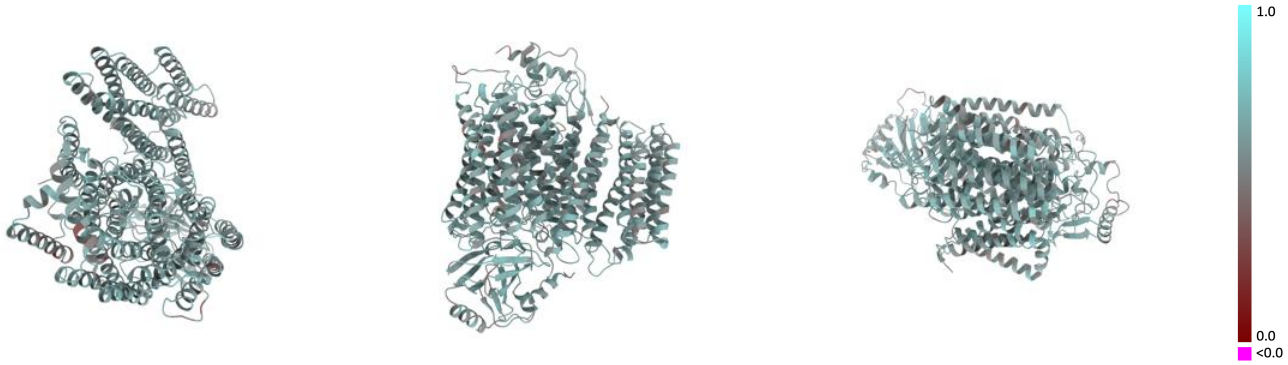
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

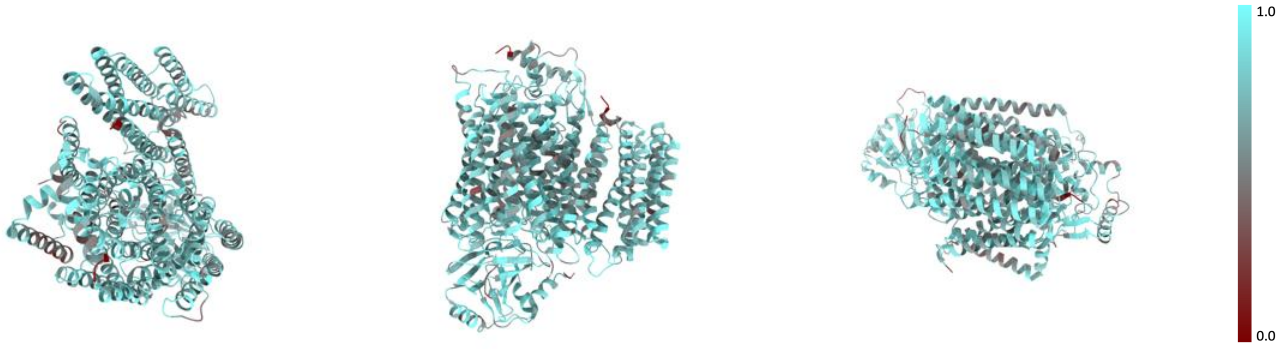
9.2 Q-score mapped to coordinate model



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.

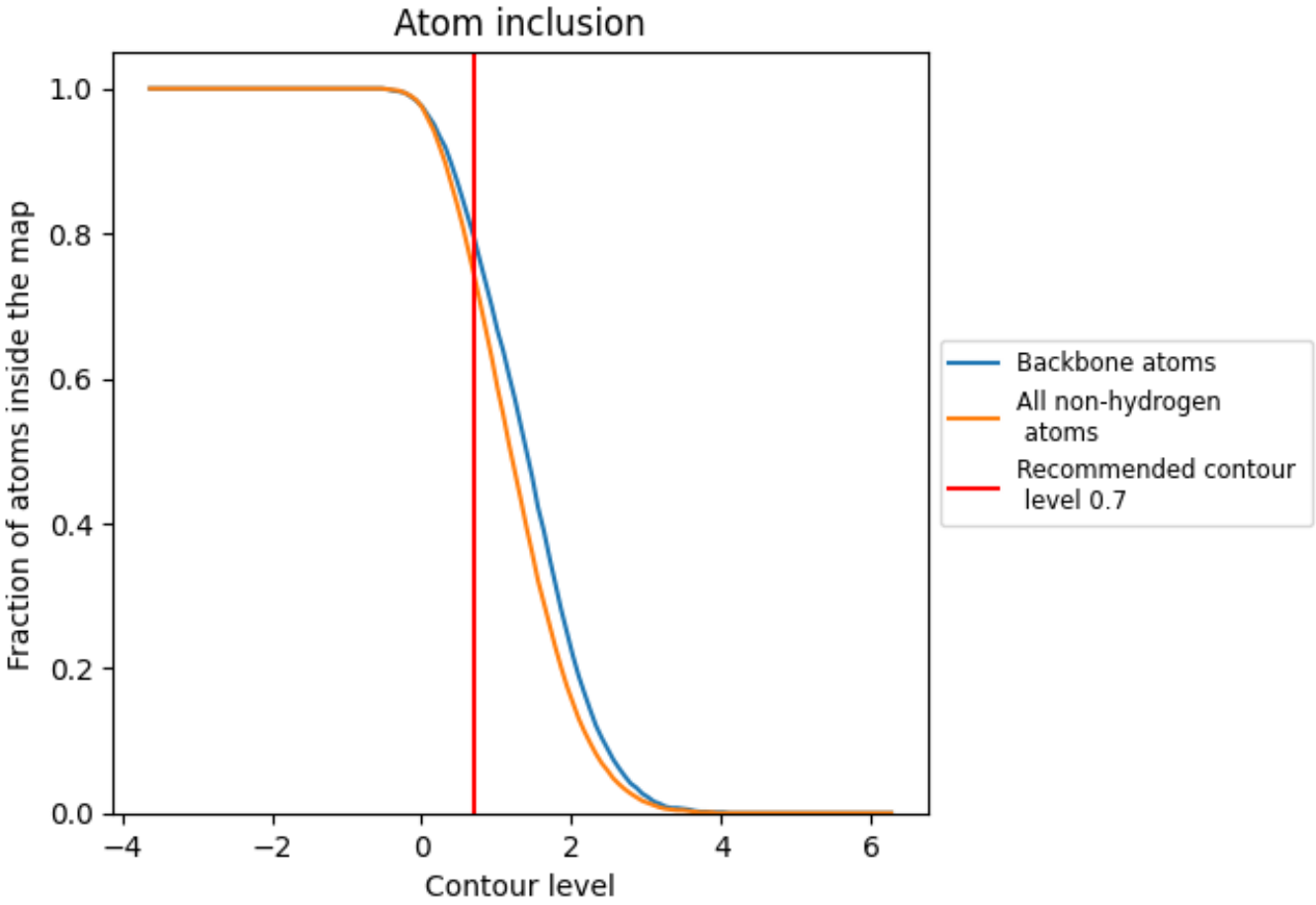
9.3 Atom inclusion mapped to coordinate model



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.5910
A	0.7460	0.5930
B	0.7580	0.5900
C	0.7470	0.5940
D	0.6910	0.5790