



wwPDB EM Validation Summary Report ⓘ

May 27, 2024 – 06:16 PM EDT

PDB ID : 5IA9
EMDB ID : EMD-8084
Title : The structure of microsomal glutathione transferase 1 in complex with Meisenheimer complex
Authors : Kuang, Q.; Purhonen, P.; Jegerschold, C.; Morgenstern, R.; Hebert, H.
Deposited on : 2016-02-21
Resolution : 3.50 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 ⓘ 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.dev92
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) : 2.36.2

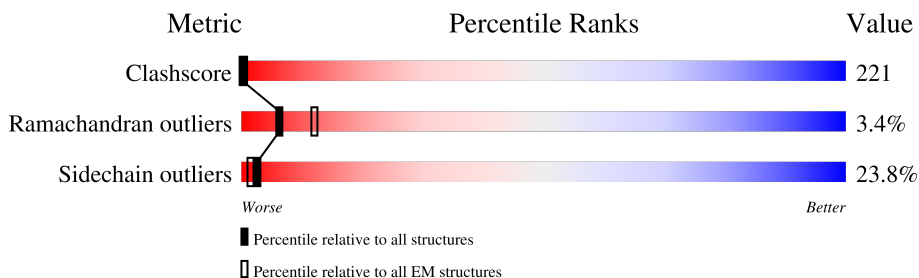
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.50 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	

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
3	PC1	A	202	X	-	X	-
3	PC1	A	203	X	-	-	-
4	PLM	A	204	-	-	X	-
4	PLM	A	205	-	-	X	-

2 Entry composition [i](#)

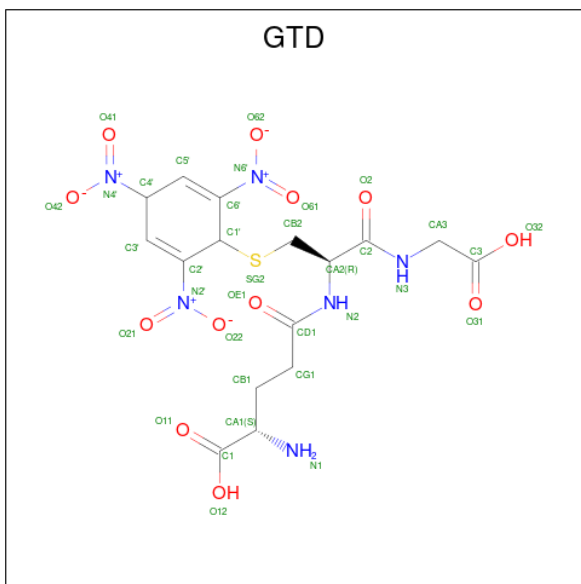
There are 4 unique types of molecules in this entry. The entry contains 1147 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Microsomal glutathione S-transferase 1.

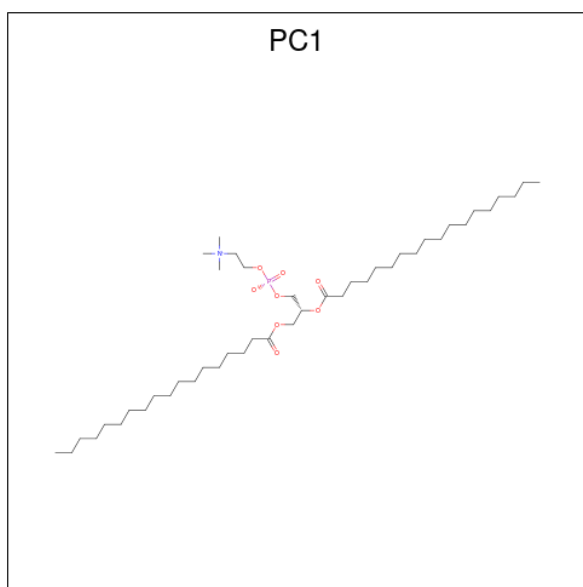
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	123	984	644	169	167	4	0	0

- Molecule 2 is 1-(S-GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE (three-letter code: GTD) (formula: C₁₆H₂₀N₆O₁₂S).



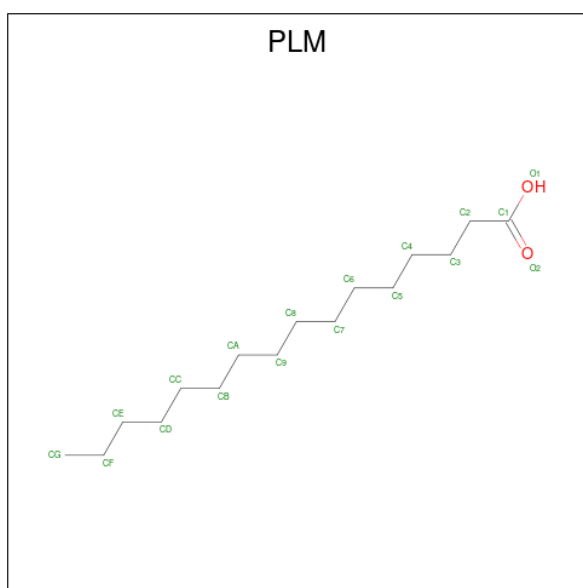
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	35	16	6	12	1	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	54	44	1	8	1	0
3	A	1	54	44	1	8	1	0

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

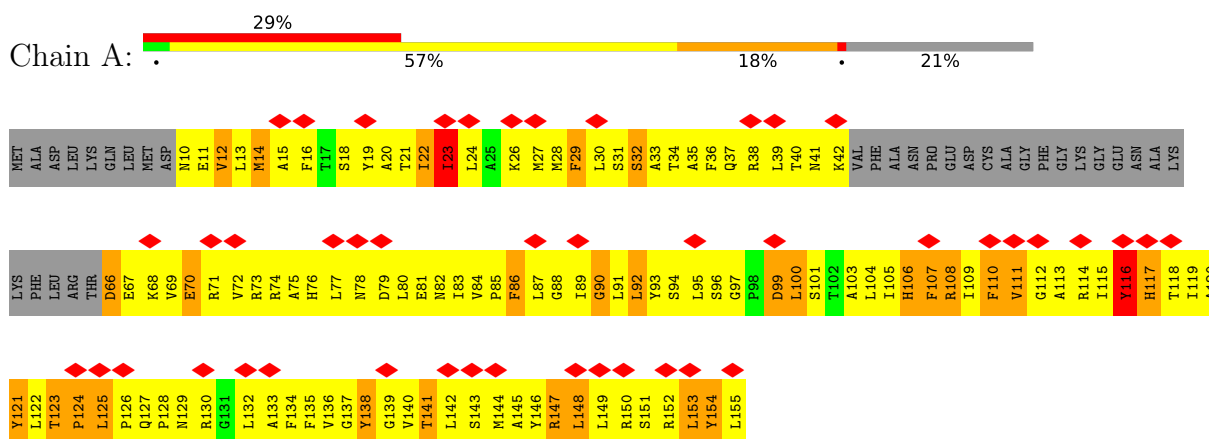


Mol	Chain	Residues	Atoms		AltConf
			Total	C	
4	A	1	10	10	0
4	A	1	10	10	0

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: Microsomal glutathione S-transferase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, $a=81.8 \text{ \AA}$, $b=81.8 \text{ \AA}$, $c=100.0 \text{ \AA}$, $\gamma=120.0^\circ$, space group=P 6	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL 2100F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.809	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.278	Depositor
Map size (\AA)	81.7992, 81.7992, 100.002	wwPDB
Map dimensions	73, 73, 84	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 120.0	wwPDB
Pixel spacing (\AA)	1.1361, 1.1361, 1.1905	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: GTD, PC1, PLM

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	1.16	2/1005 (0.2%)	1.32	4/1360 (0.3%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	TYR	CD2-CE2	5.49	1.47	1.39
1	A	116	TYR	CD1-CE1	5.37	1.47	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	VAL	CB-CA-C	-6.68	98.72	111.40
1	A	107	PHE	N-CA-C	-5.85	95.21	111.00
1	A	90	GLY	N-CA-C	-5.26	99.95	113.10
1	A	125	LEU	CB-CG-CD1	-5.03	102.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	TYR	Peptide

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	984	0	1019	526	5
2	A	35	0	17	1	0
3	A	108	0	176	33	2
4	A	20	0	32	47	0
All	All	1147	0	1244	528	5

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 221.

The worst 5 of 528 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:16:PHE:CZ	1:A:94:SER:HA	1.37	1.55
1:A:122:LEU:CA	4:A:204:PLM:H21	1.51	1.40
1:A:34:THR:HB	1:A:72:VAL:CG1	1.53	1.37
1:A:27:MET:CE	1:A:83:ILE:HG21	1.58	1.32
1:A:91:LEU:O	1:A:94:SER:HB3	1.32	1.30

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:SER:N	1:A:138:TYR:OH[3_665]	1.97	0.23
1:A:36:PHE:CZ	3:A:203:PC1:C36[4_665]	1.97	0.23
1:A:31:SER:OG	1:A:138:TYR:OH[3_665]	2.03	0.17
1:A:36:PHE:CE2	3:A:203:PC1:C36[4_665]	2.10	0.10
1:A:32:SER:CA	1:A:138:TYR:OH[3_665]	2.19	0.01

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	119/155 (77%)	80 (67%)	35 (29%)	4 (3%)	3 28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	THR
1	A	22	ILE
1	A	124	PRO
1	A	23	ILE

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	105/130 (81%)	80 (76%)	25 (24%)	0 4

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	116	TYR
1	A	154	TYR
1	A	111	VAL
1	A	117	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	78	ASN
1	A	117	HIS
1	A	129	ASN

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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLM	A	204	-	9,9,17	0.31	0	8,8,17	0.84	0
3	PC1	A	202	-	53,53,53	1.22	2 (3%)	59,61,61	1.08	4 (6%)
2	GTD	A	201	-	26,35,35	2.18	6 (23%)	25,48,48	1.66	2 (8%)
3	PC1	A	203	-	53,53,53	1.24	3 (5%)	59,61,61	1.55	12 (20%)
4	PLM	A	205	-	9,9,17	0.77	0	8,8,17	0.59	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
4	PLM	A	204	-	-	2/7/7/15	-
2	GTD	A	201	-	-	2/31/55/55	0/1/1/1
3	PC1	A	202	-	1/1/5/5	34/57/57/57	-
3	PC1	A	203	-	1/1/5/5	24/57/57/57	-
4	PLM	A	205	-	-	3/7/7/15	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	PC1	O31-C31	5.78	1.50	1.33
2	A	201	GTD	O2-C2	5.59	1.34	1.23
2	A	201	GTD	OE1-CD1	5.52	1.34	1.23
3	A	203	PC1	O31-C31	5.40	1.49	1.33
3	A	203	PC1	O21-C21	4.58	1.47	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	GTD	C5'-C6'-N6'	5.51	124.90	118.42
3	A	203	PC1	O21-C21-C22	4.66	121.55	111.50
2	A	201	GTD	C3'-C2'-N2'	-4.53	113.09	118.42
3	A	203	PC1	C3F-C3E-C3D	-4.10	93.61	114.42
3	A	202	PC1	O21-C21-C22	3.76	119.61	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	202	PC1	C2
3	A	203	PC1	C2

5 of 65 torsion outliers are listed below:

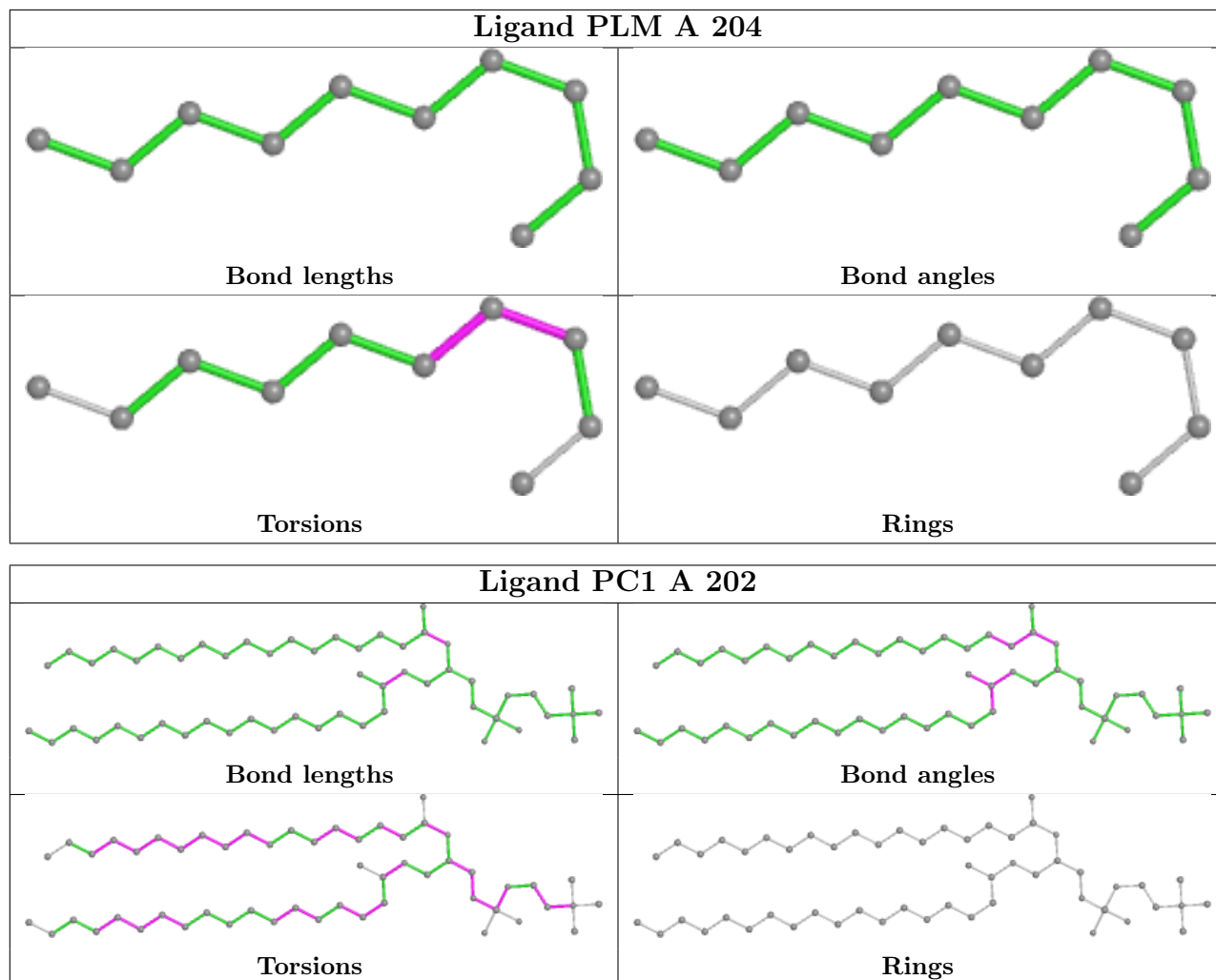
Mol	Chain	Res	Type	Atoms
3	A	202	PC1	C1-O11-P-O14
3	A	202	PC1	O13-C11-C12-N
3	A	203	PC1	C1-O11-P-O12
3	A	203	PC1	O32-C31-O31-C3
3	A	203	PC1	C32-C31-O31-C3

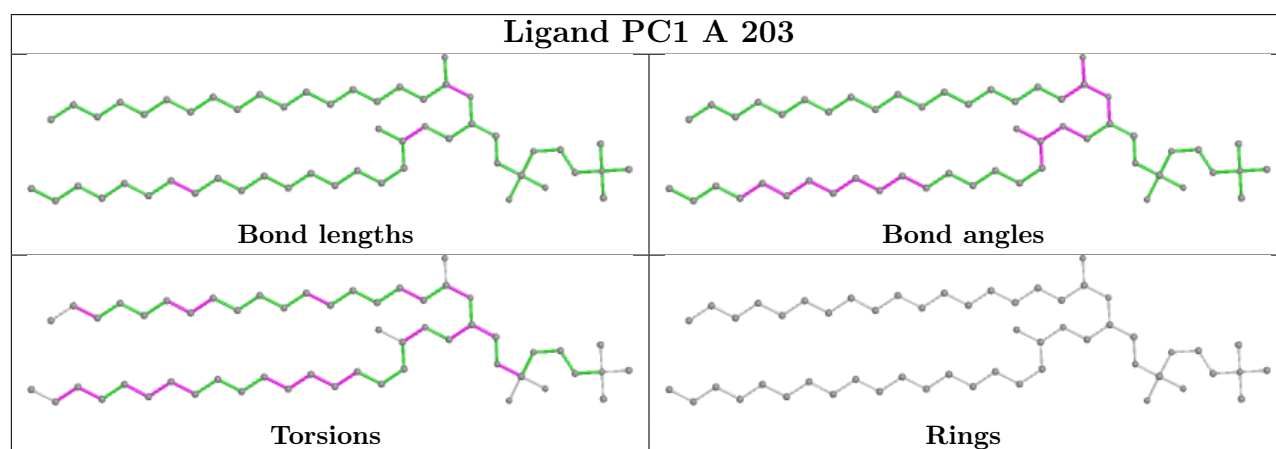
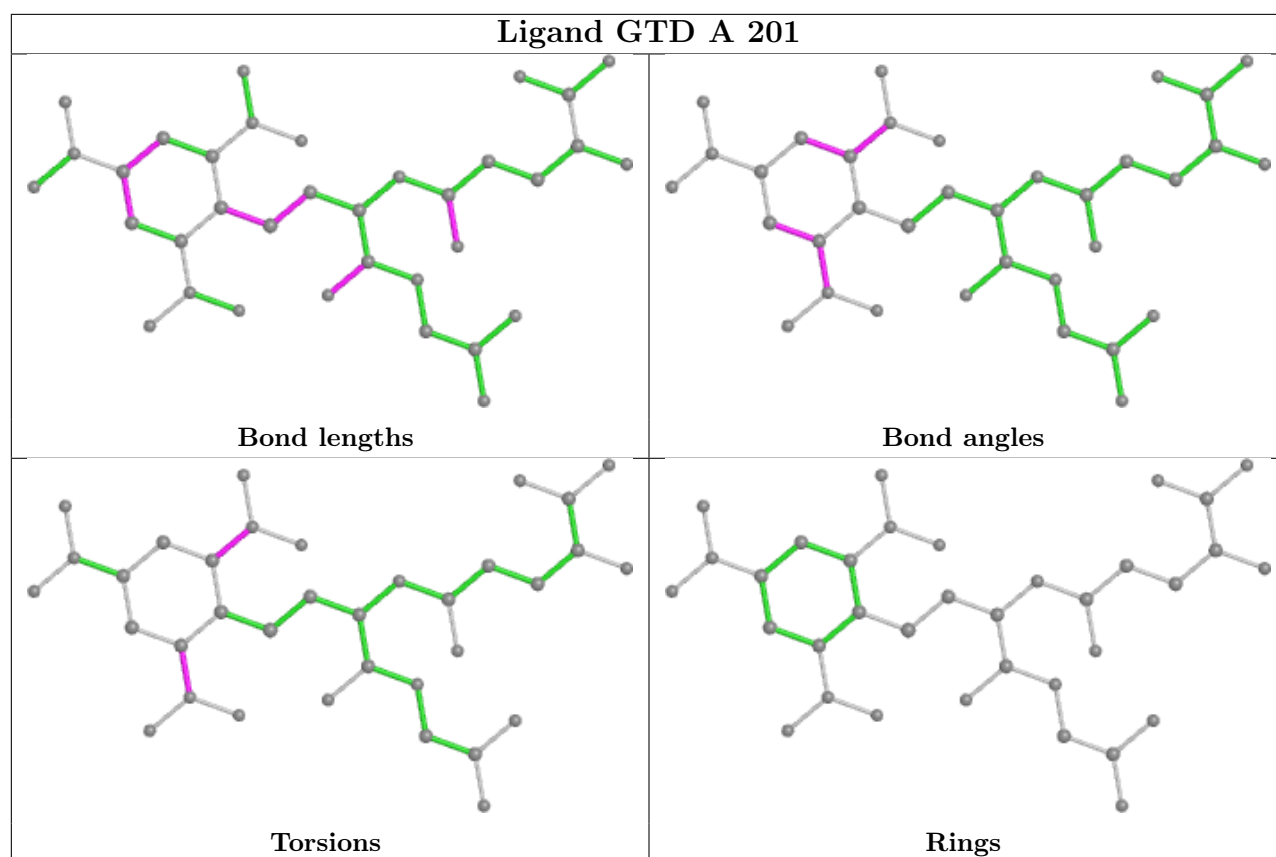
There are no ring outliers.

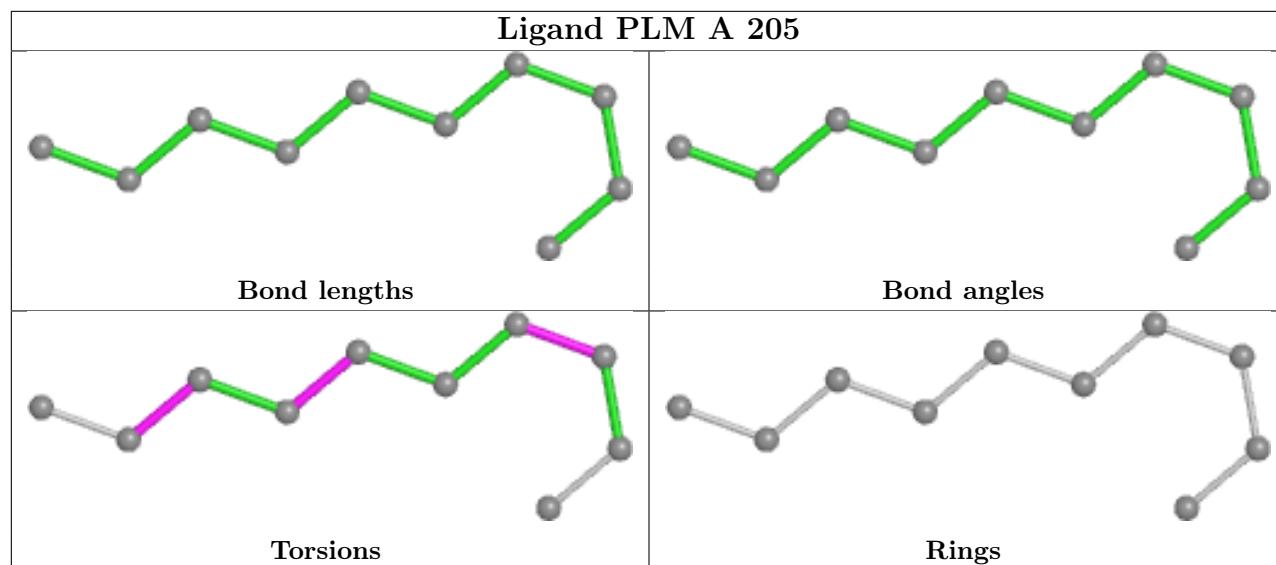
5 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	204	PLM	36	0
3	A	202	PC1	26	0
2	A	201	GTD	1	0
3	A	203	PC1	7	2
4	A	205	PLM	11	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8084. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

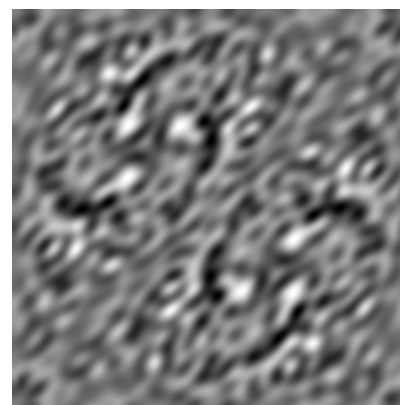
6.1.1 Primary map



X



Y

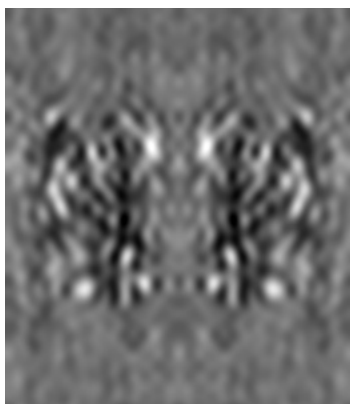


Z

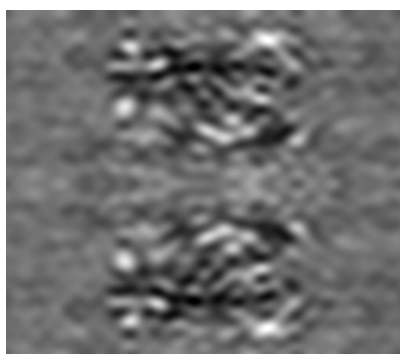
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

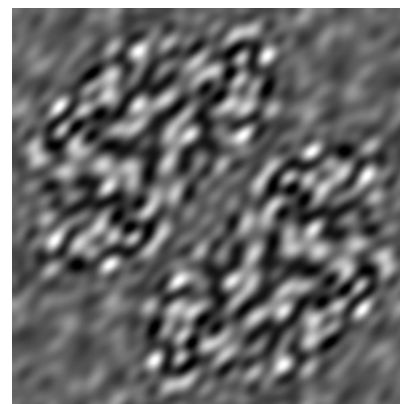
6.2.1 Primary map



X Index: 36



Y Index: 36

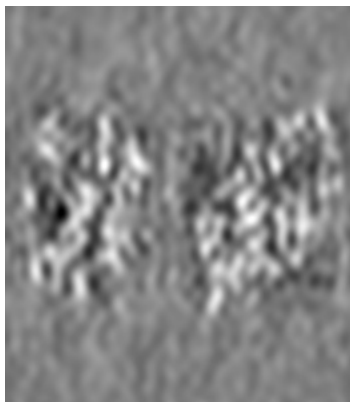


Z Index: 42

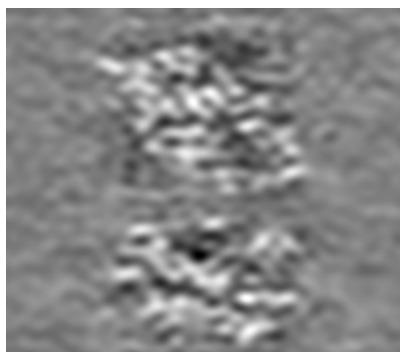
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

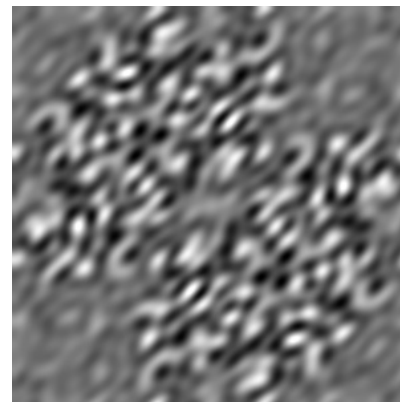
6.3.1 Primary map



X Index: 32



Y Index: 32

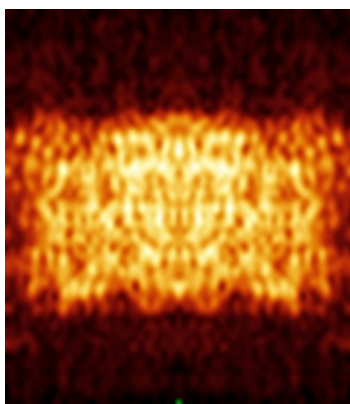


Z Index: 50

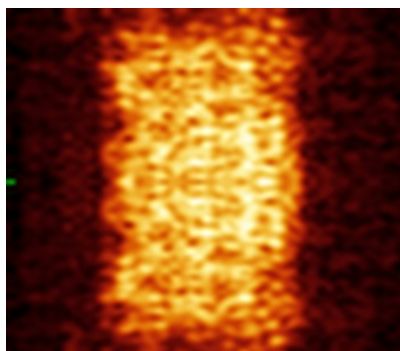
The images above show the largest variance slices of the map in three orthogonal directions.

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

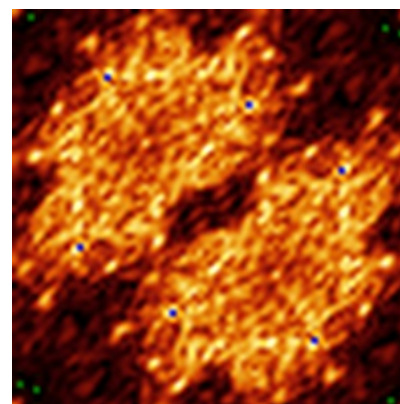
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.278. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

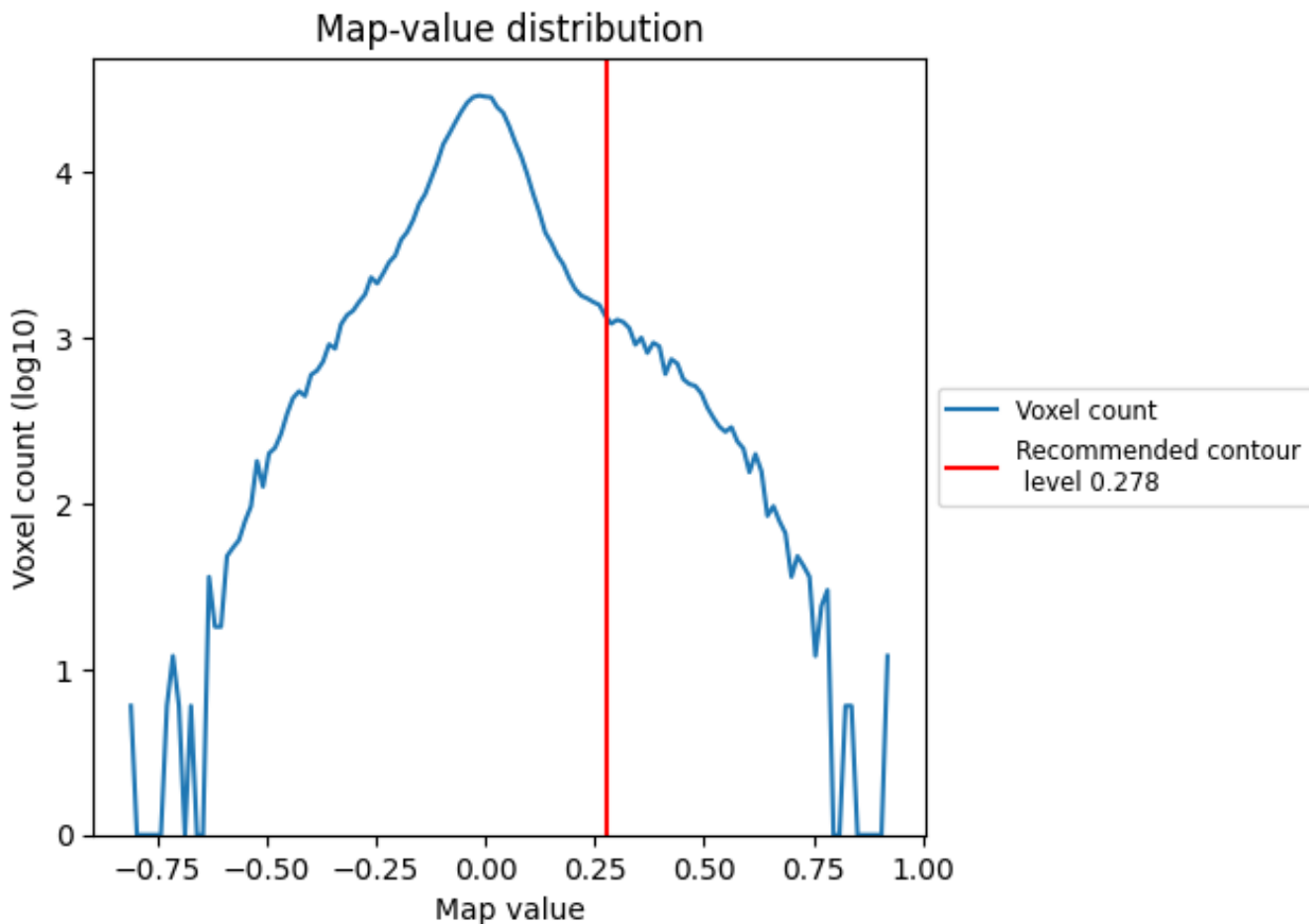
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

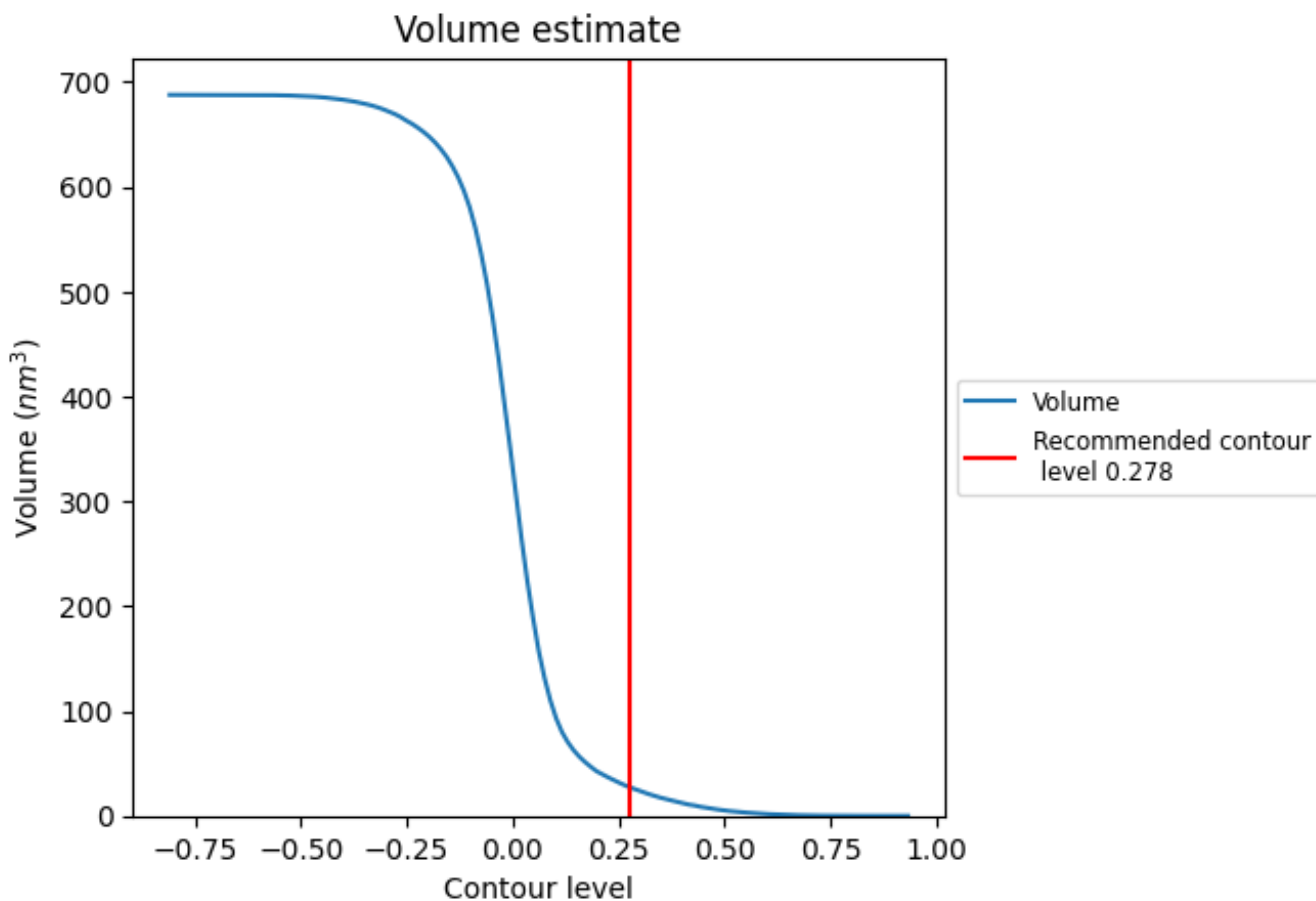
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 27 nm³; this corresponds to an approximate mass of 24 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.

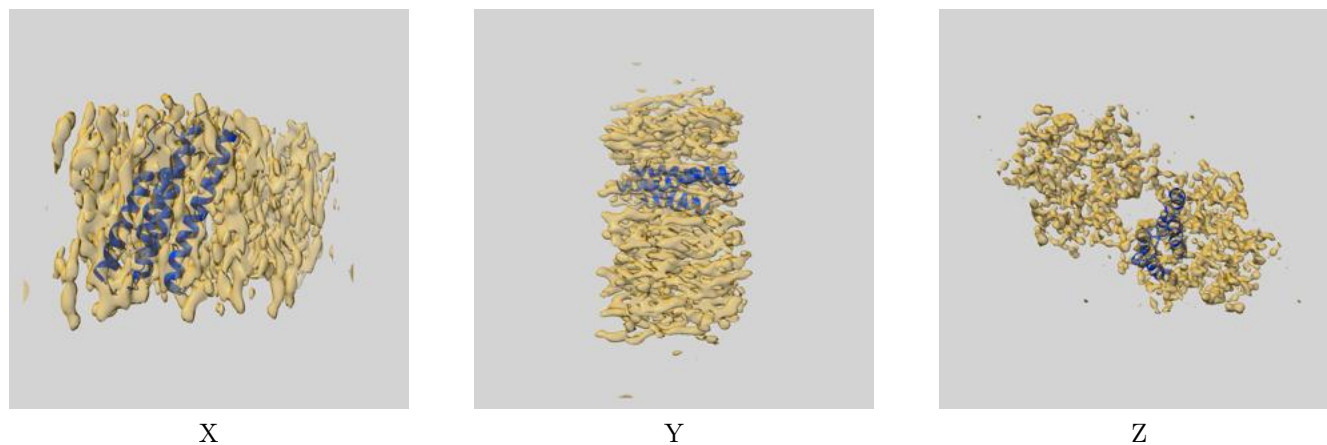
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

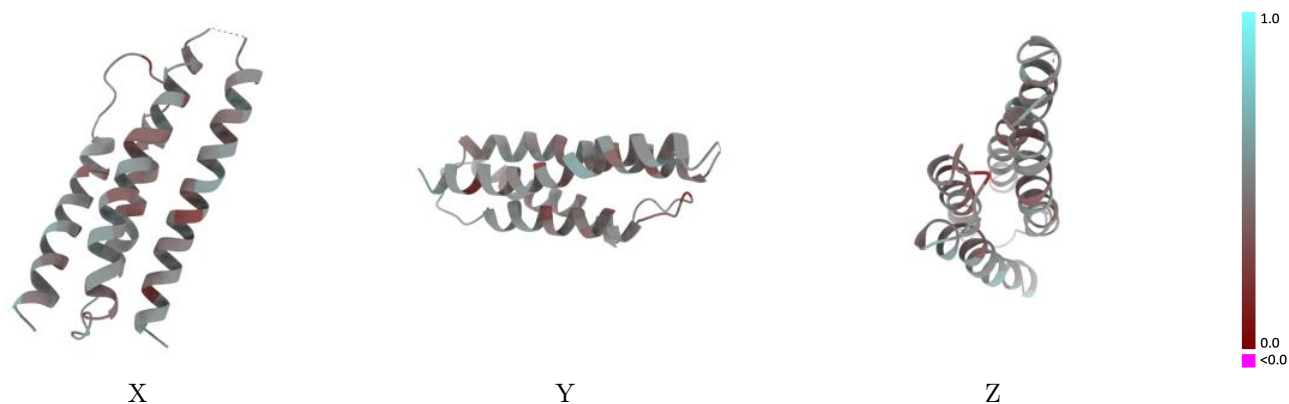
This section contains information regarding the fit between EMDB map EMD-8084 and PDB model 5IA9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



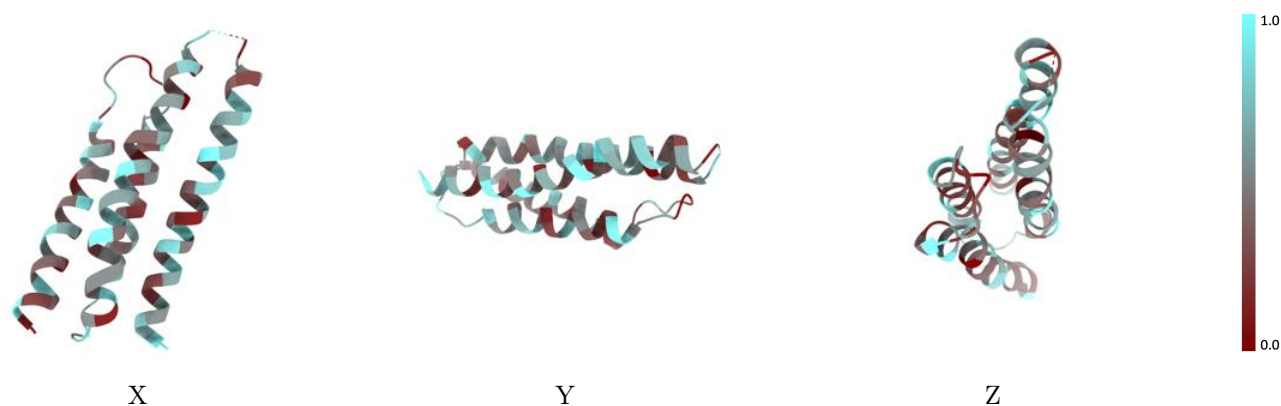
The images above show the 3D surface view of the map at the recommended contour level 0.278 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



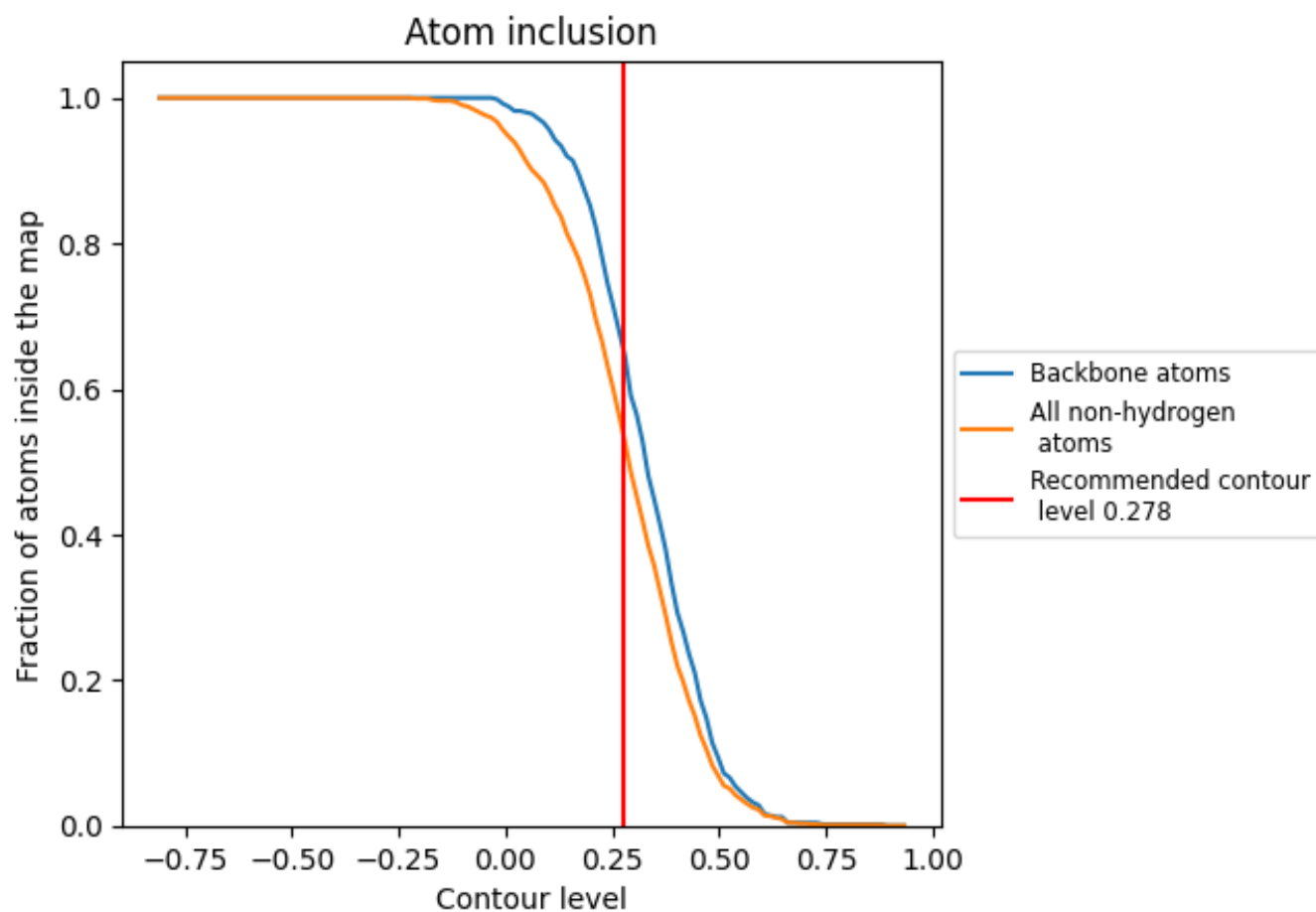
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.278).





9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.278) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5310	 0.4690
A	 0.5310	 0.4690

