



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 11:05 PM EDT

PDB ID : 9CLO / pdb_00009clo
EMDB ID : EMD-45727
Title : DosP R97A with c-di-GMP
Authors : Kumar, P.; Kober, D.L.
Deposited on : 2024-07-11
Resolution : 3.10 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
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

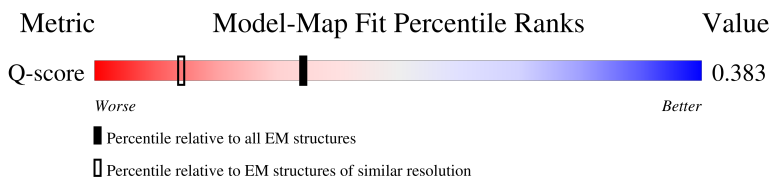
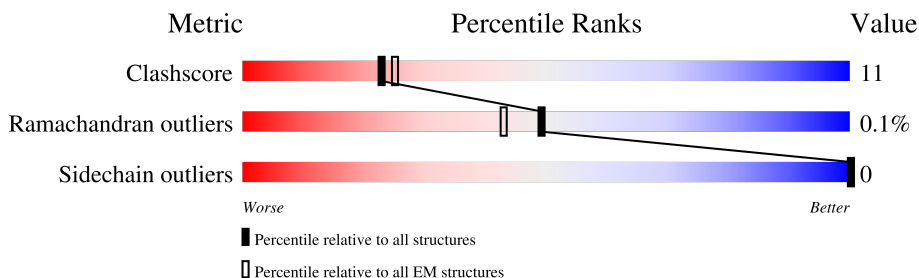
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	787	 71% 29%
1	B	787	 74% 26%

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.

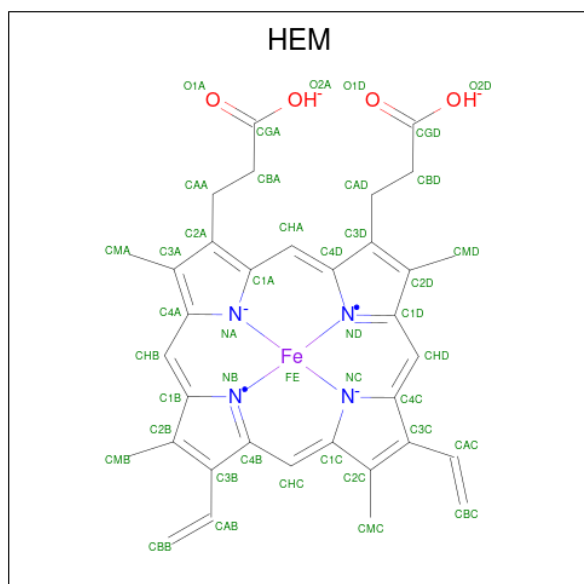
- Molecule 1 is a protein called Oxygen sensor protein DosP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	787	Total 6251	C 3958	N 1092	O 1168	S 33	0	0
1	B	787	Total 6247	C 3956	N 1092	O 1166	S 33	0	0

There are 4 discrepancies between the modelled and reference sequences:

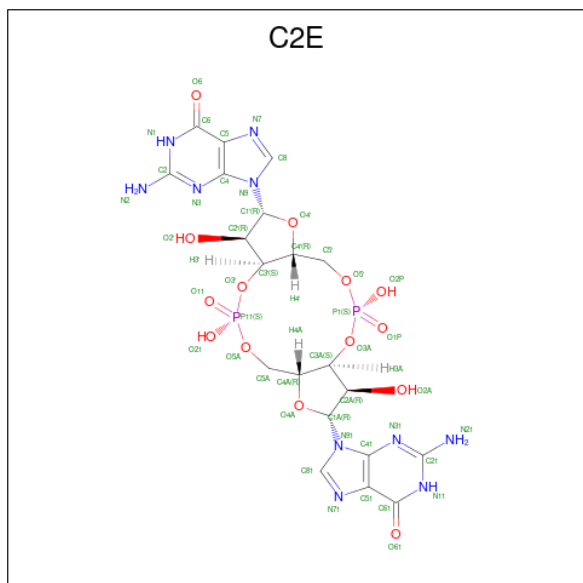
Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ALA	ARG	engineered mutation	UNP P76129
A	195	THR	ILE	conflict	UNP P76129
B	97	ALA	ARG	engineered mutation	UNP P76129
B	195	THR	ILE	conflict	UNP P76129

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			46	20	10	14	2	
3	B	1	Total	C	N	O	P	0
			46	20	10	14	2	

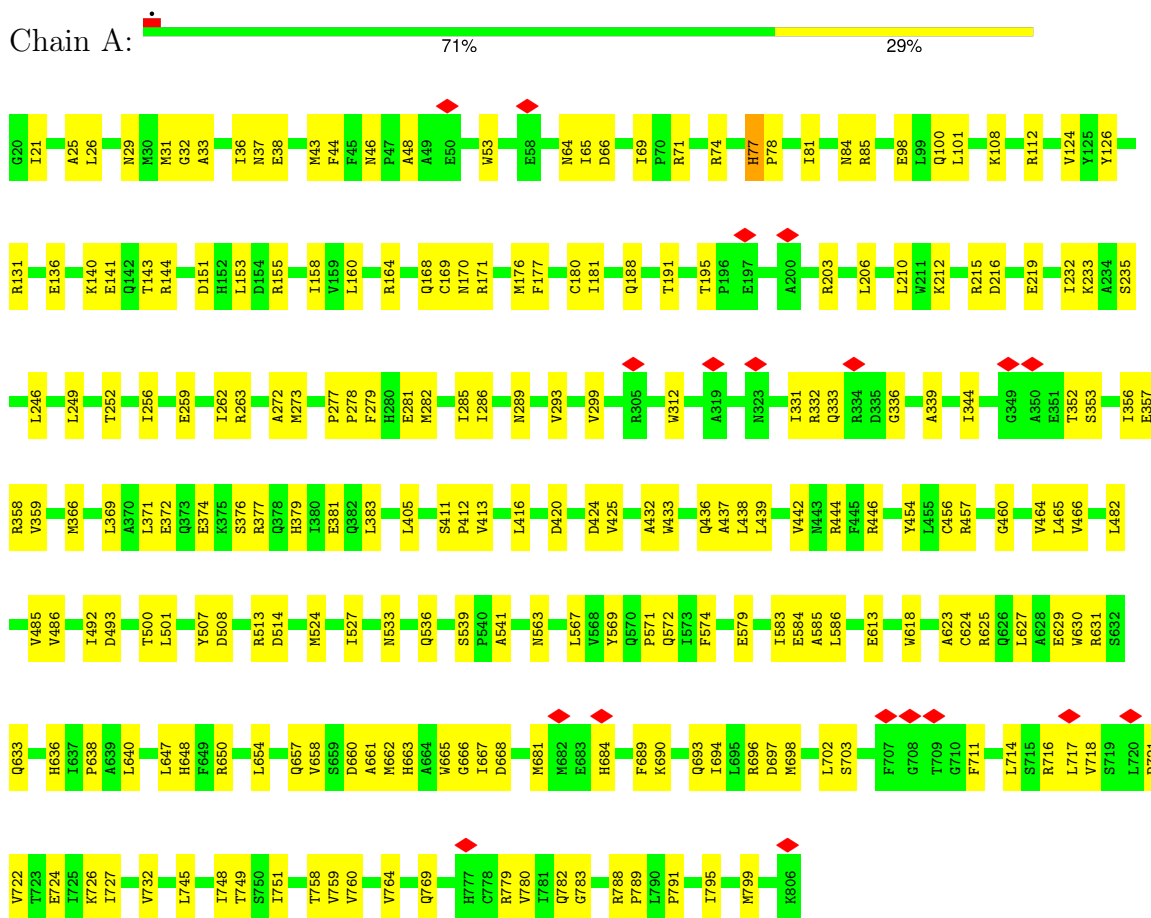
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

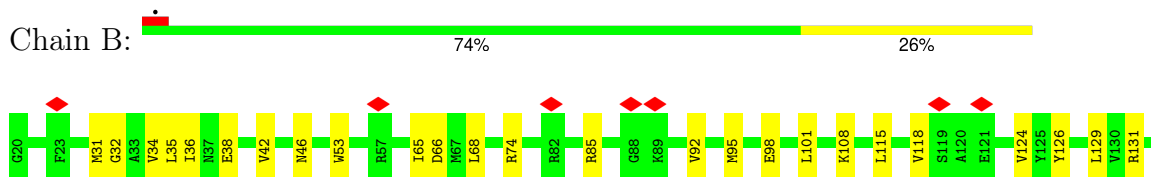
3 Residue-property plots

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: Oxygen sensor protein DosP



• Molecule 1: Oxygen sensor protein DosP



T749	V658	R513	L371	L249	M137
S750	S659	T519	S376	V250	L153
I751	D660	A520	S376	M251	D154
	M662	H521	I380	T252	P155
N755	H663	I527	L383	D255	P156
L757	G666	W535	I384	I256	V157
T758	I667	F538	Q385	T257	I158
V759	D668	F538	F386	E258	D161
V760		F538	D387	E259	
	T677	G553	P388	R260	H164
M772	F678	A554	L402	L265	H165
R779	S679	A555	D403		I166
V780	M680	E558	L416	I269	C169
I781	M681	W563	V419	L270	N170
Q782	M682	L567	D424	A271	R171
A792	E683	Y569	V425	A272	E175
	H684	Q570	D425	S275	H176
I795	F689	P571	L429	M282	F177
W798	Q693	Q572	W433		
M799	D697	I573	K450	I286	C180
		F574	Q453	C287	I181
	L702	E579	C456	R288	S182
	S703	I583	R457	N289	E183
	V704	E585	I458	I291	A184
	D705	P598	E459	S292	Q188
	D706	R601	V466	V293	P189
	F707	L605	D471		D190
	G708	W618	N474	M194	
	T709	A623	I475	T195	
	G710	L627	I478	P196	
	F711	W630	L482	E197	
		R631	V485	F198	
	L714	S632	I490	P199	
	S715	Q633	M491		
	R716	I637	D494	R203	
	L717	F649	L499	I204	
	V718	L654	T500	R205	
	S719	Q657	I503	L206	
	L720			Q207	
	P721			Q208	
	V722			L209	
	K726			L210	
	I727			W211	
	D728			K212	
	V732			R215	
	L736			L222	
	I741			L223	
	L744			T224	
	I748			S235	
				I236	
				S237	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186761	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.815	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	377.856, 377.856, 377.856	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98399997, 0.98399997, 0.98399997	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MG, C2E

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	0.12	0/6379	0.33	0/8643
1	B	0.12	0/6375	0.33	0/8638
All	All	0.12	0/12754	0.33	0/17281

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6251	0	6228	157	0
1	B	6247	0	6224	136	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	46	0	22	1	0
3	B	46	0	22	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	12680	0	12556	283	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 11.

The worst 5 of 283 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:732:VAL:HG12	1:A:769:GLN:HE21	1.44	0.81
1:B:101:LEU:O	1:B:108:LYS:HA	1.83	0.79
1:A:437:ALA:HB2	1:A:492:ILE:HD11	1.67	0.76
1:A:436:GLN:HG3	1:B:384:ILE:HG12	1.67	0.75
2:A:901:HEM:HHD	2:A:901:HEM:HBC2	1.70	0.73

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	785/787 (100%)	748 (95%)	36 (5%)	1 (0%)	48	78
1	B	785/787 (100%)	744 (95%)	41 (5%)	0	100	100
All	All	1570/1574 (100%)	1492 (95%)	77 (5%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	HIS

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	682/682 (100%)	682 (100%)	0	100	100
1	B	681/682 (100%)	681 (100%)	0	100	100
All	All	1363/1364 (100%)	1363 (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. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	373	GLN
1	B	436	GLN
1	B	399	HIS
1	B	474	ASN
1	A	633	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	C2E	A	902	4	52,52,52	0.42	0	78,82,82	0.44	0
3	C2E	B	901	4	52,52,52	0.40	0	78,82,82	0.52	0
2	HEM	A	901	-	50,50,50	1.47	8 (16%)	67,82,82	1.08	2 (2%)
2	HEM	B	902	-	50,50,50	1.44	8 (16%)	67,82,82	1.07	4 (5%)

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
3	C2E	A	902	4	-	8/30/62/62	0/6/7/7
3	C2E	B	901	4	-	8/30/62/62	0/6/7/7
2	HEM	A	901	-	-	4/14/54/54	-
2	HEM	B	902	-	-	2/14/54/54	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	FE-NB	3.58	2.05	1.94
2	A	901	HEM	FE-NA	3.57	2.06	1.95
2	B	902	HEM	FE-NB	3.56	2.05	1.94
2	A	901	HEM	FE-NC	3.45	2.06	1.95
2	B	902	HEM	FE-ND	3.24	2.04	1.94

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	HEM	C4D-ND-C1D	2.49	108.15	105.21
2	A	901	HEM	C4D-ND-C1D	2.38	108.02	105.21
2	B	902	HEM	C3D-C4D-ND	-2.26	107.69	110.17
2	B	902	HEM	C2A-C1A-NA	-2.12	107.80	110.15
2	B	902	HEM	C1B-NB-C4B	2.08	107.67	105.21

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	C2E	C5'-O5'-P1-O2P
3	A	902	C2E	C5'-O5'-P1-O1P

Continued on next page...

Continued from previous page...

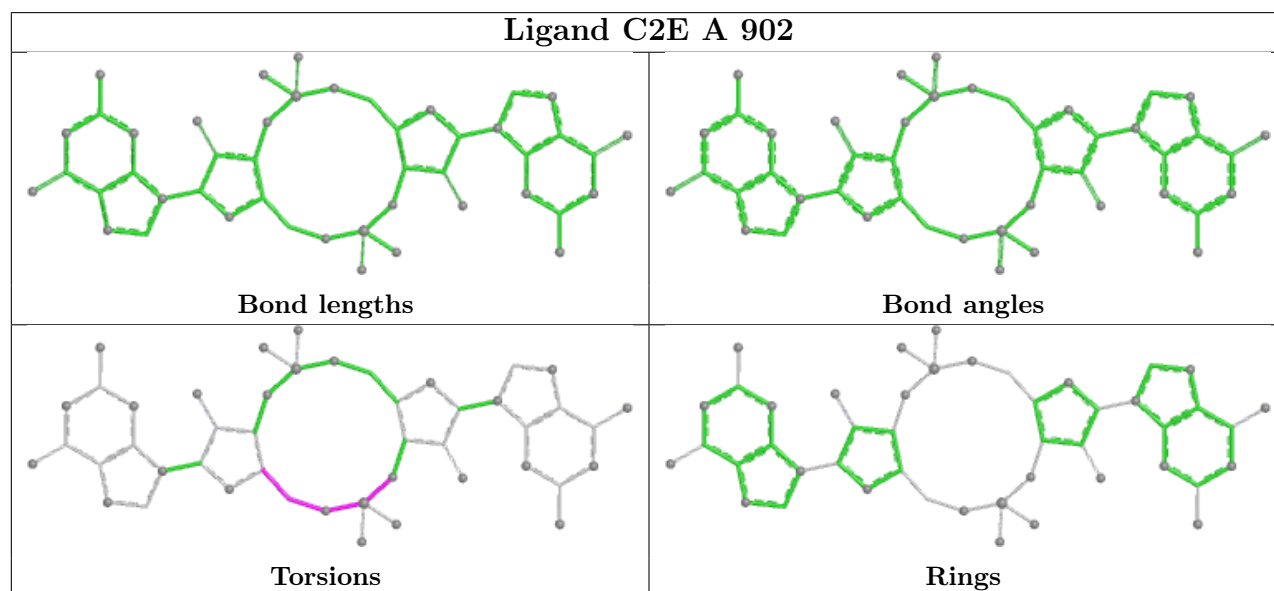
Mol	Chain	Res	Type	Atoms
3	A	902	C2E	C5'-O5'-P1-O3A
3	A	902	C2E	C3A-O3A-P1-O5'
3	B	901	C2E	C5'-O5'-P1-O2P

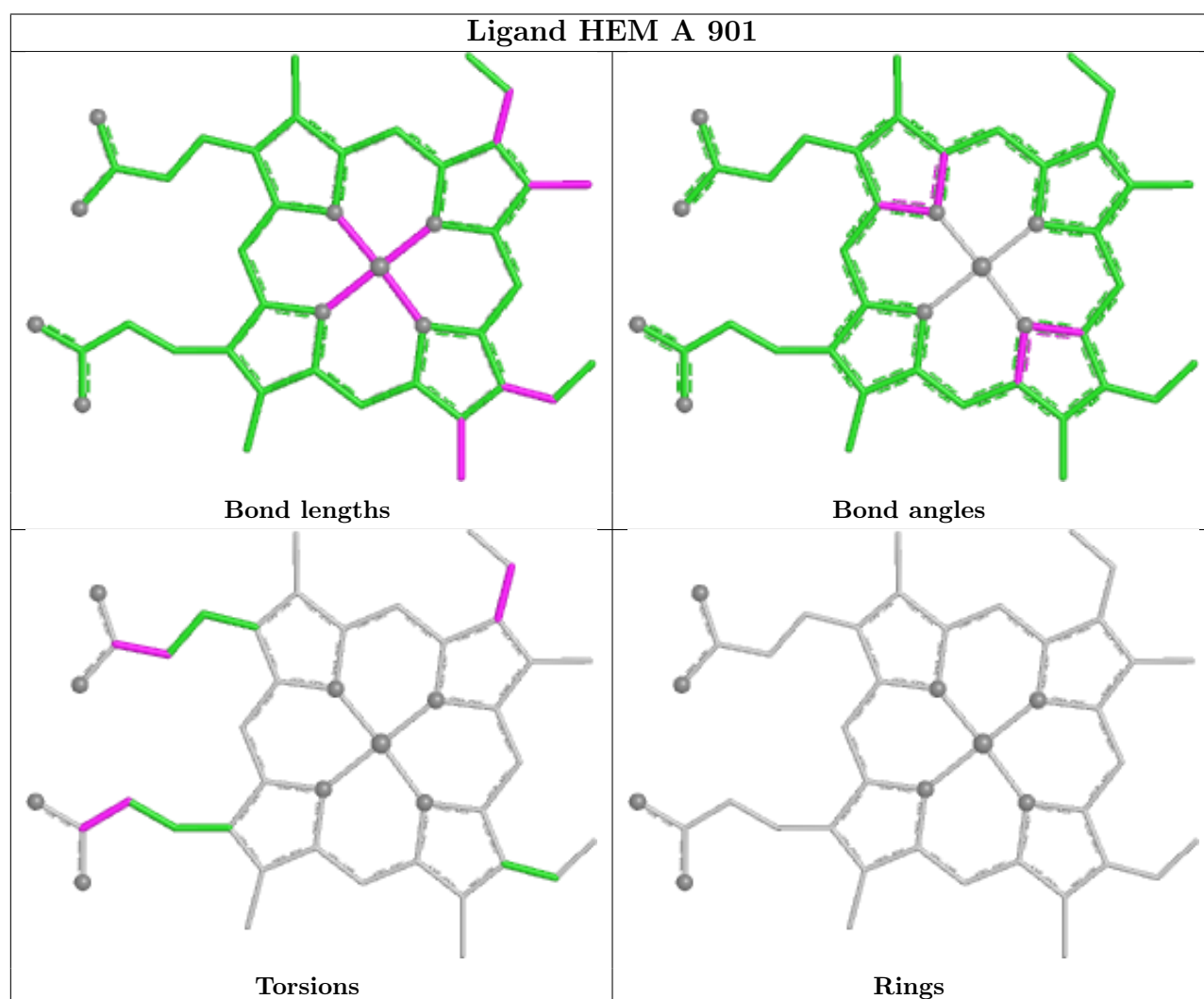
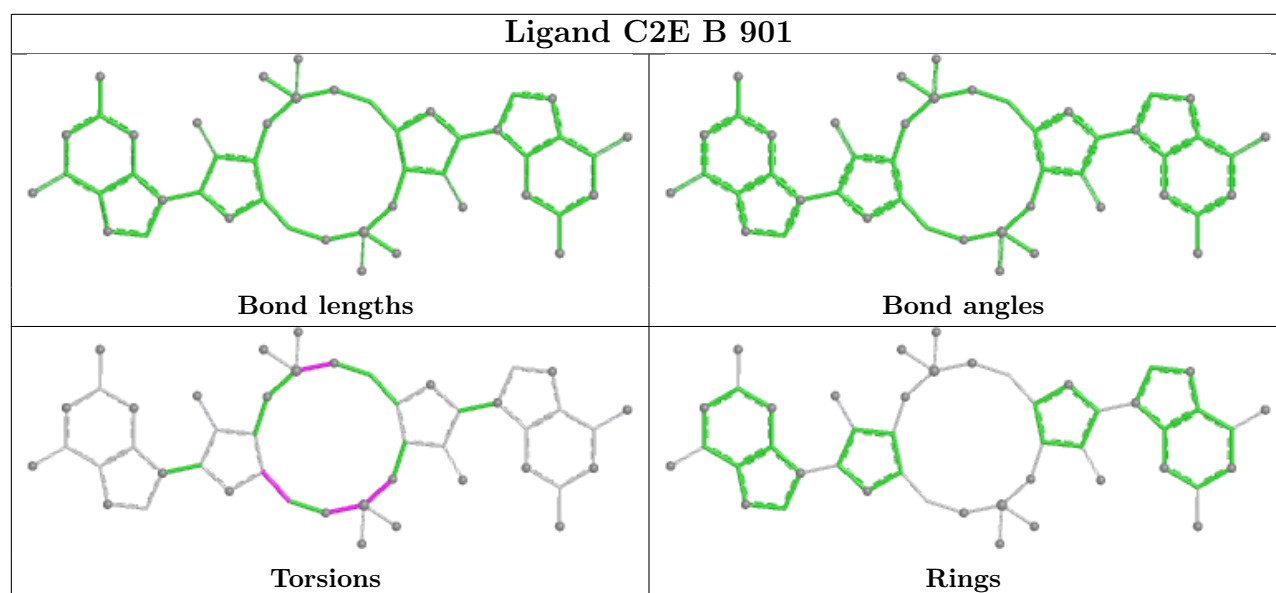
There are no ring outliers.

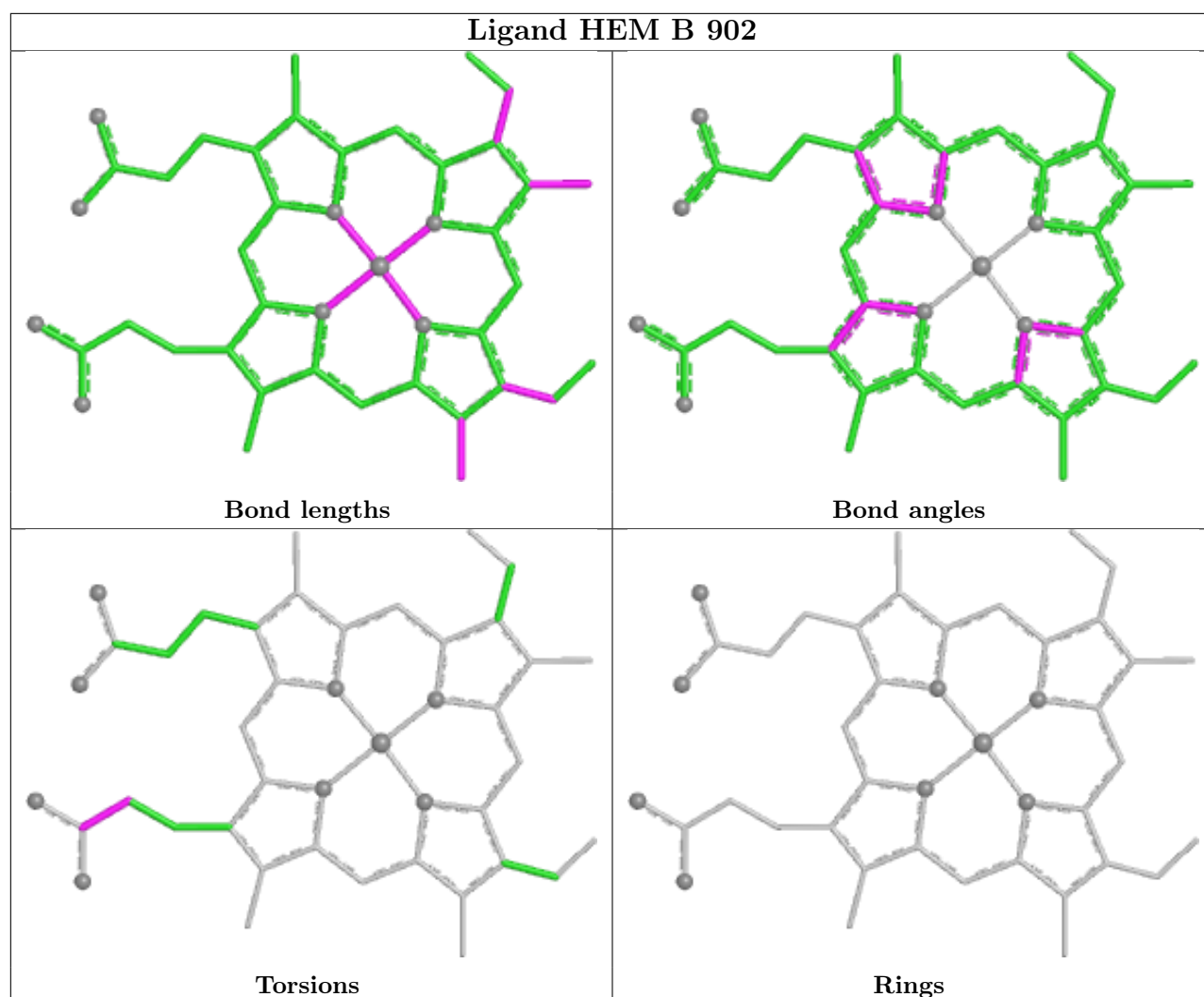
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	C2E	1	0
2	A	901	HEM	3	0
2	B	902	HEM	4	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.

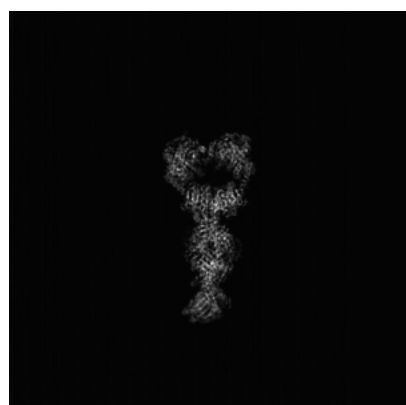
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45727. 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](#)

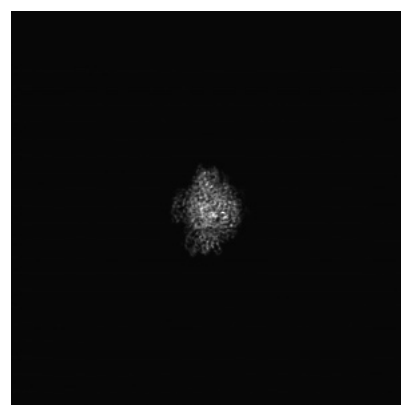
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

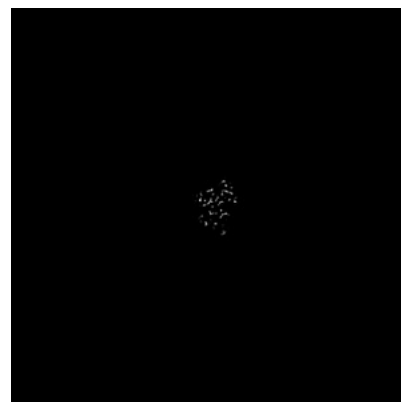
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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: 186



Y Index: 189

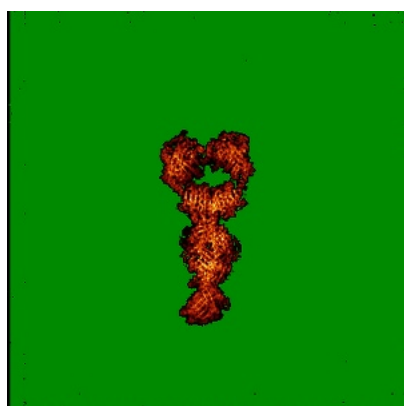


Z Index: 201

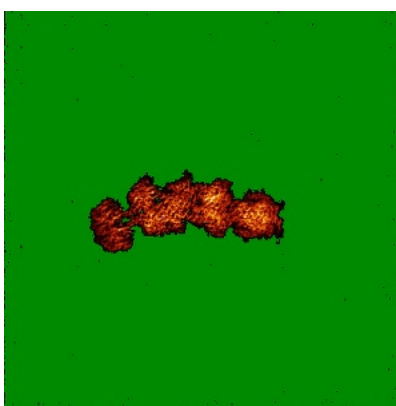
The images above show the largest variance slices of the map in three orthogonal directions.

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

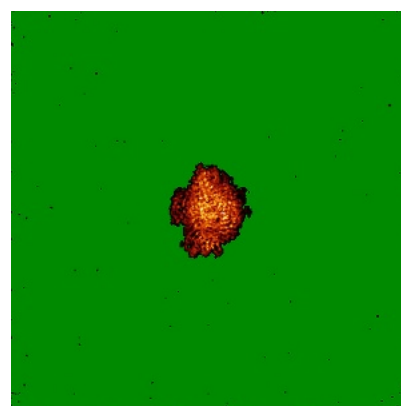
6.4.1 Primary map



X



Y

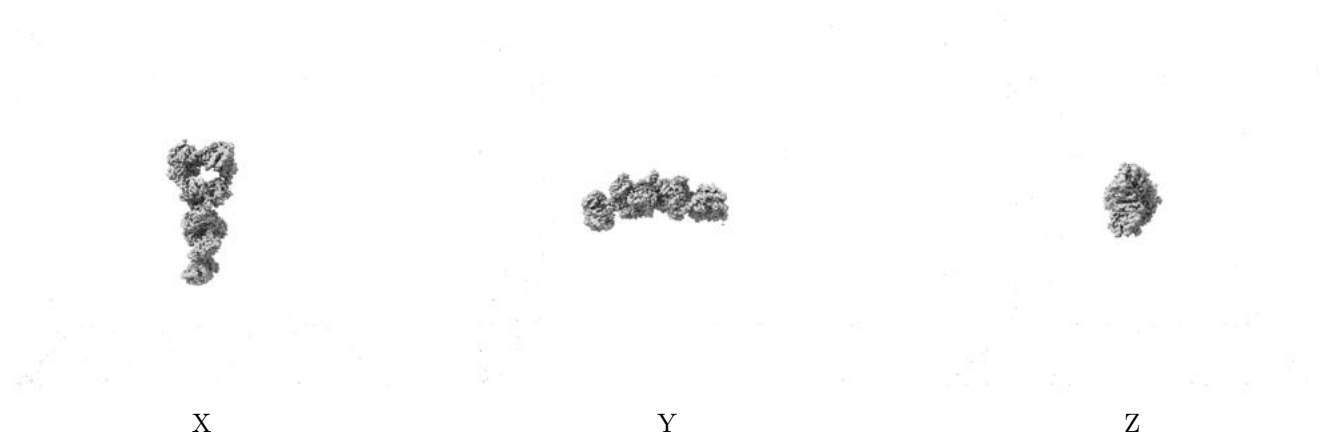


Z

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 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

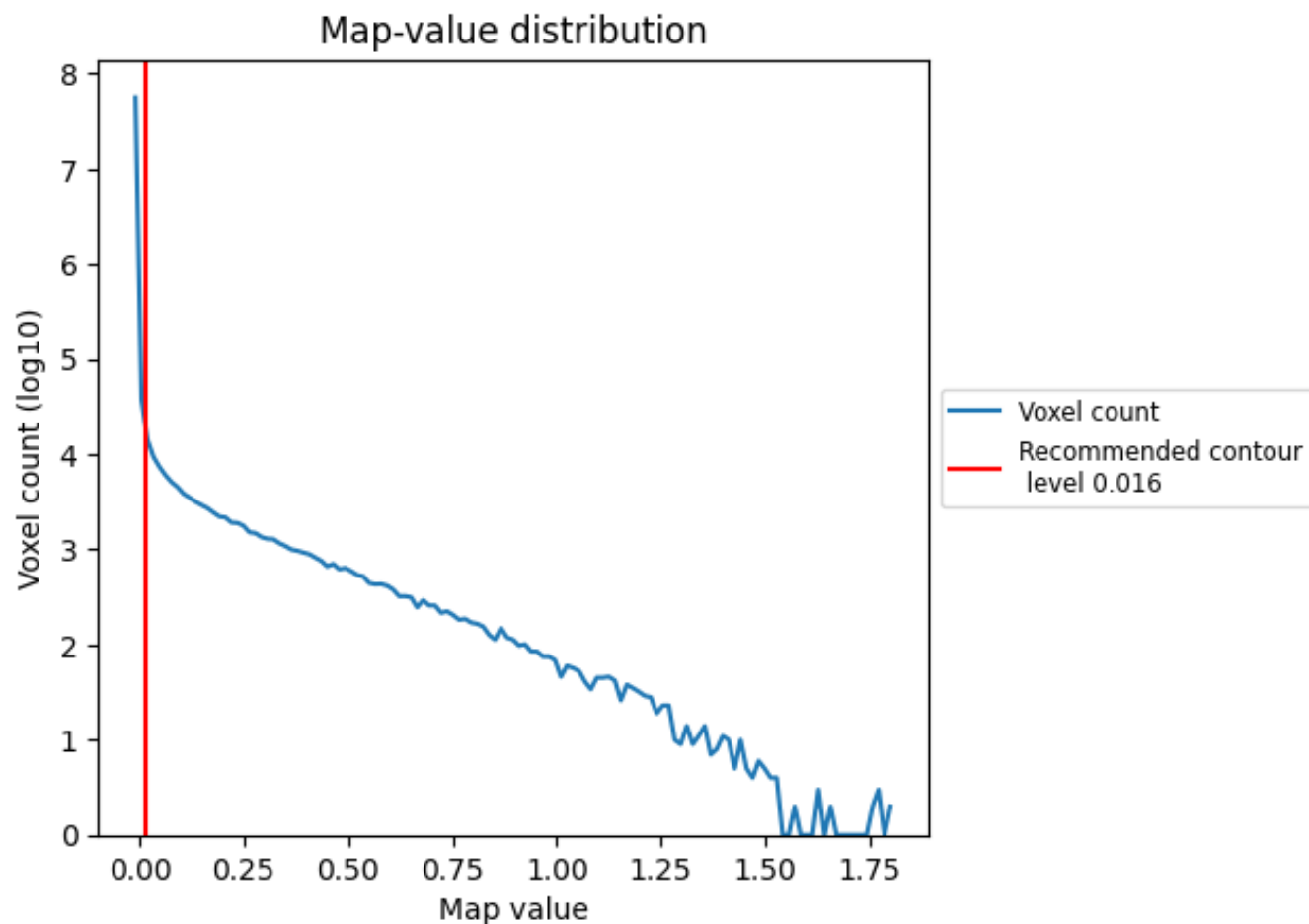
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

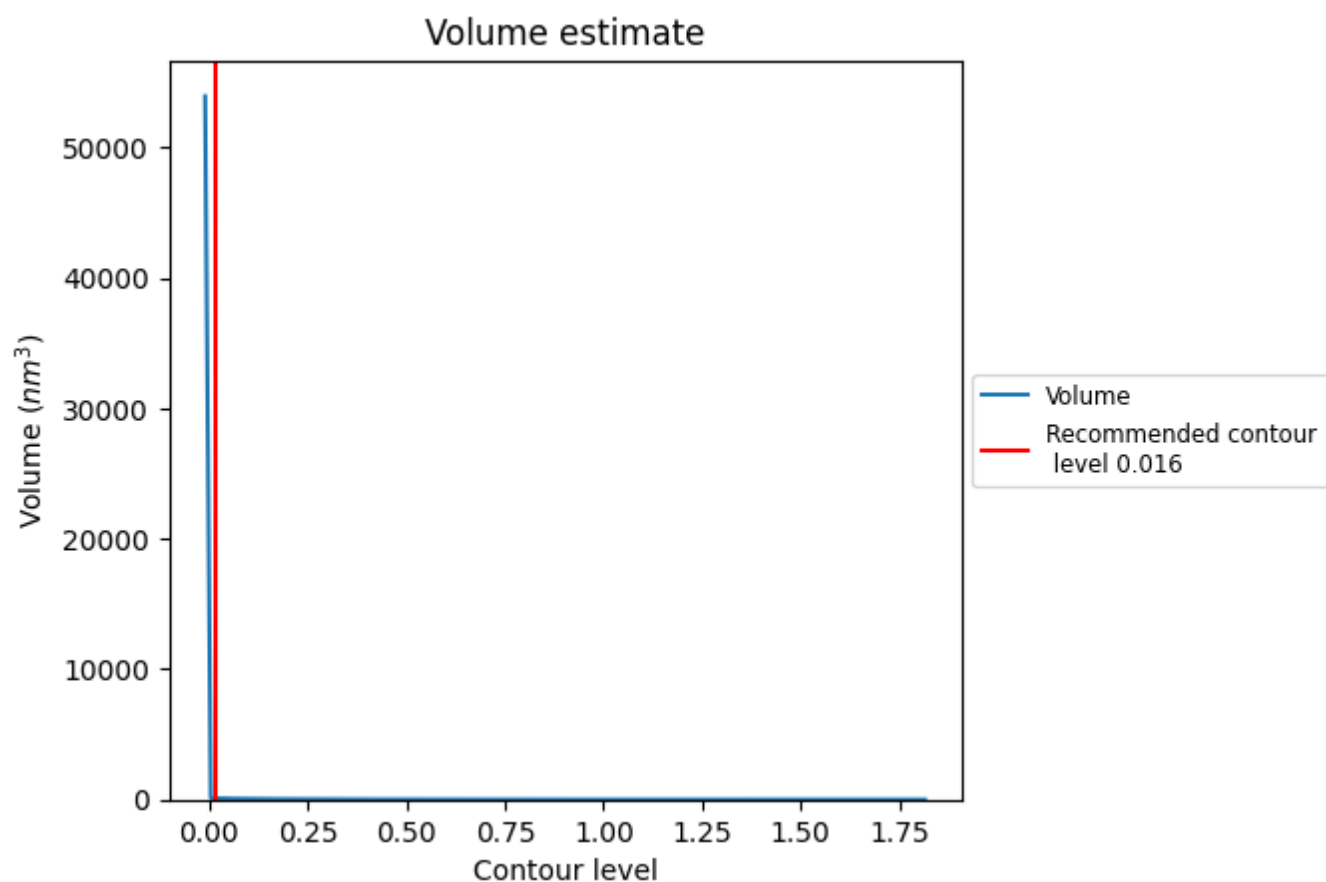
This section contains the results of statistical analysis of the map.

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.

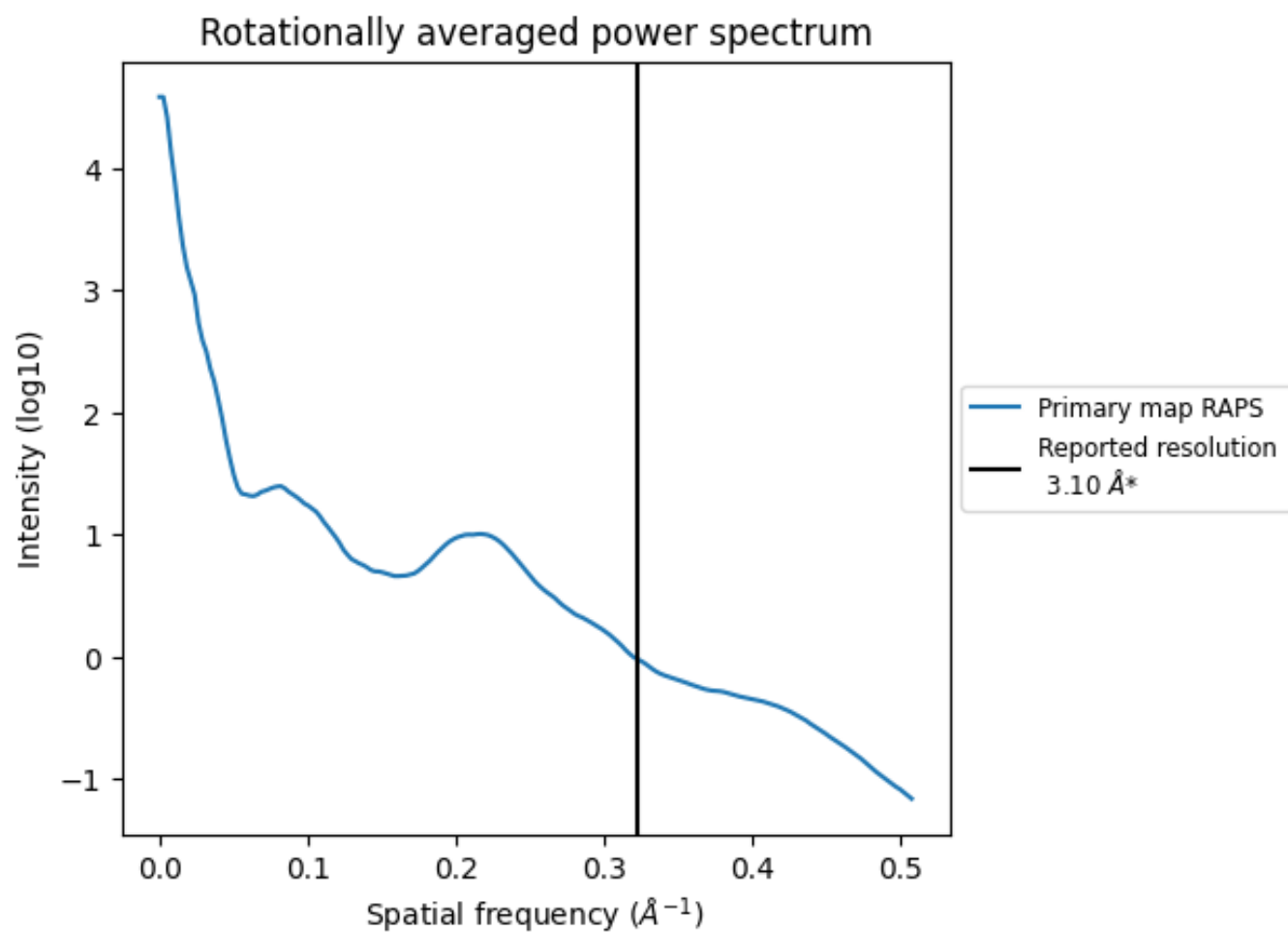
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

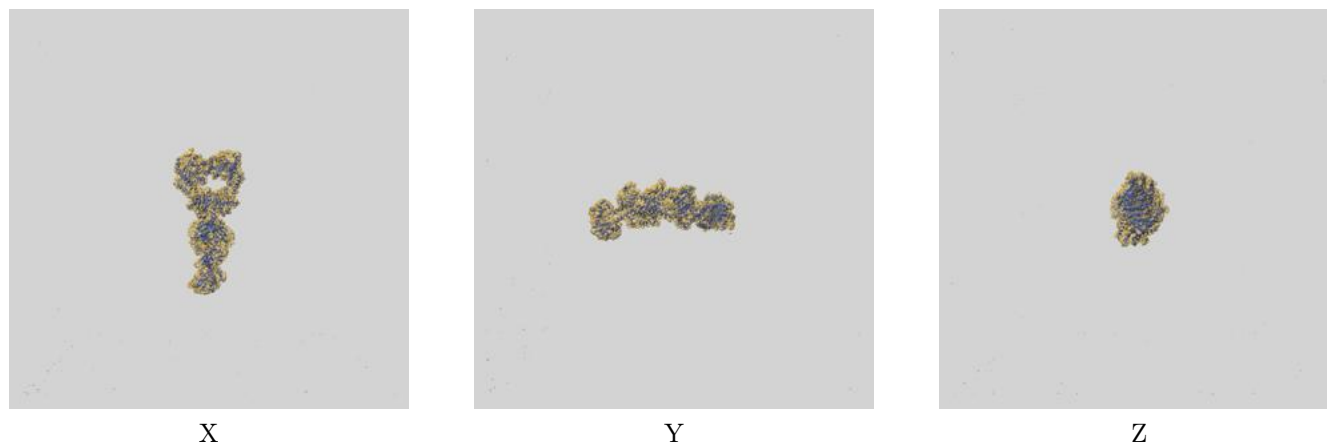
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

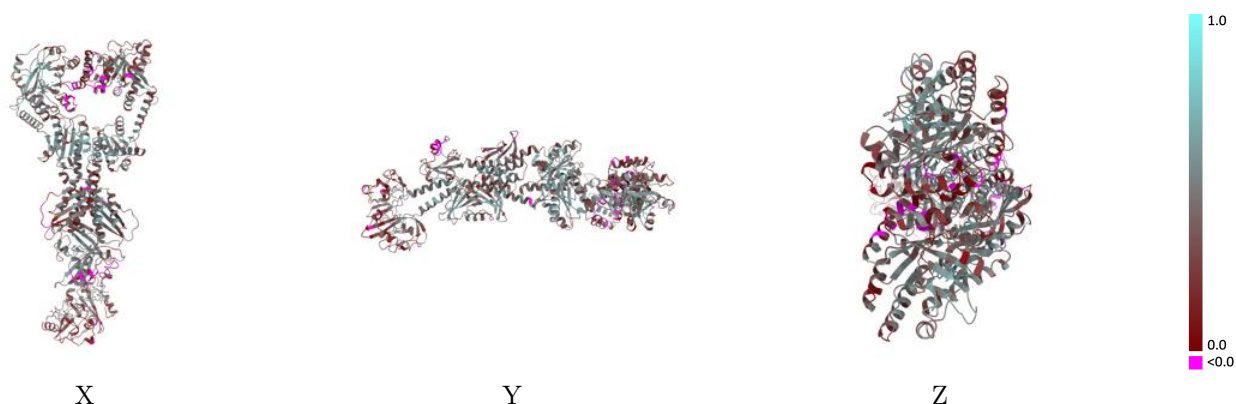
This section contains information regarding the fit between EMDB map EMD-45727 and PDB model 9CLO. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



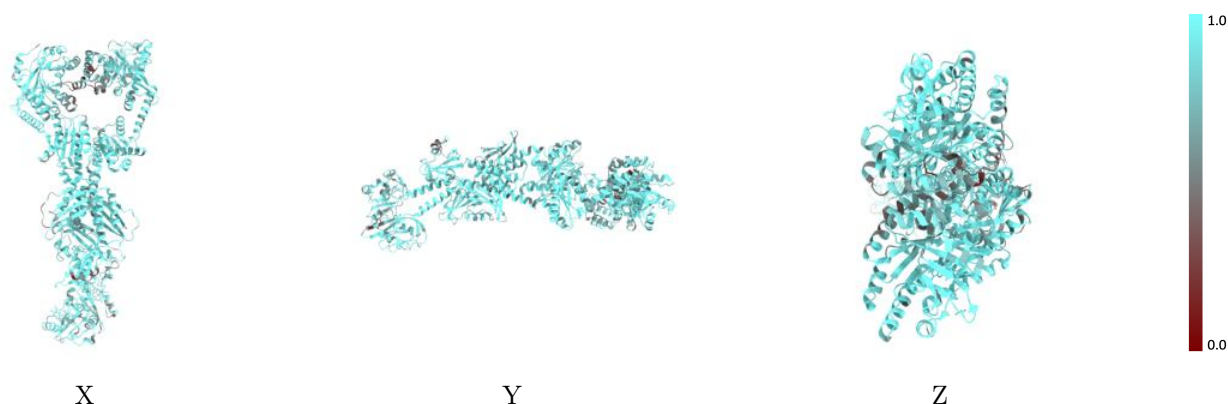
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



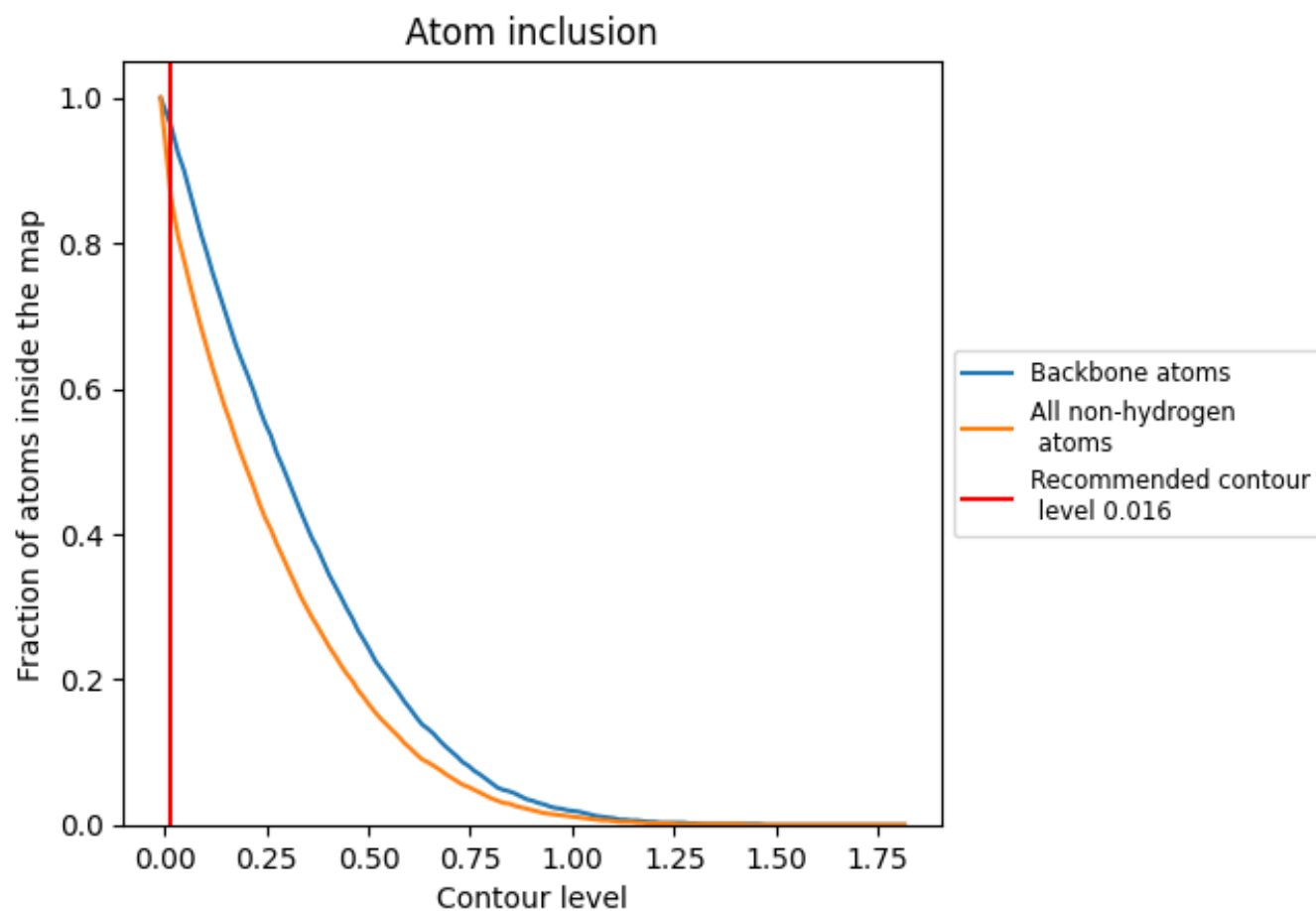
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.3830
A	0.8690	0.3860
B	0.8580	0.3800

