wwPDB EM Validation Summary Report (i)

Oct 5, 2026 – 01:12 am BST

PDB ID	:	9SV7 / pdb_00009sv7
EMDB ID	:	EMD-55242
Title	:	Cryo-EM structure of CARM1 in complex with ALIX
Authors	:	Marechal, N.; Cavarelli, J.
Deposited on	:	2025-10-02
Resolution	:	3.10 Å(reported)
Based on initial model	:	5IH3

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:

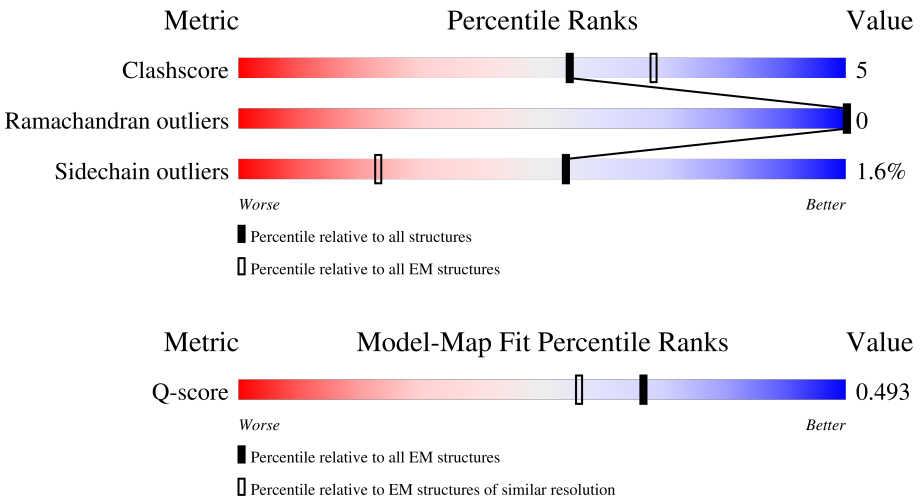
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 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 <=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	608	53% 7% 40%
1	B	608	49% 7% • 43%
1	C	608	51% 8% 40%
1	D	608	51% 5% 43%

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Mol	Chain	Length	Quality of chain
2	E	868	96%
2	F	868	96%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23624 atoms, of which 11638 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.

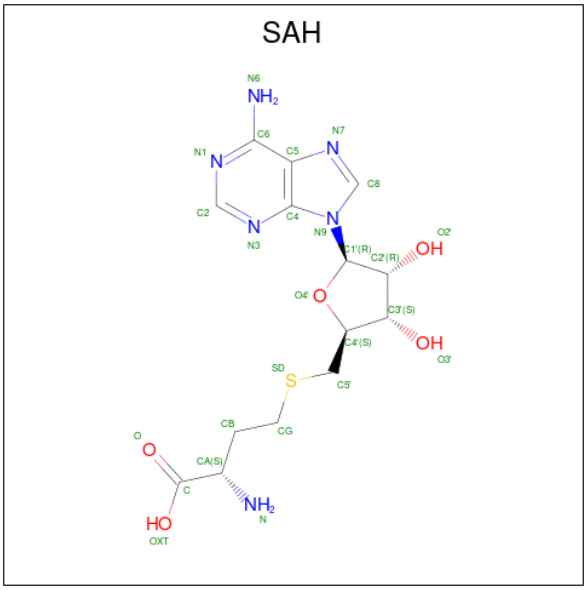
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	364	5742	1873	2834	480	540	15	0	0
1	B	344	5457	1778	2702	455	508	14	0	0
1	C	364	5742	1873	2834	480	540	15	0	0
1	D	344	5457	1778	2702	455	508	14	0	0

- Molecule 2 is a protein called Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	F	34	523	187	245	38	48	5	0	0
2	E	34	523	187	245	38	48	5	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



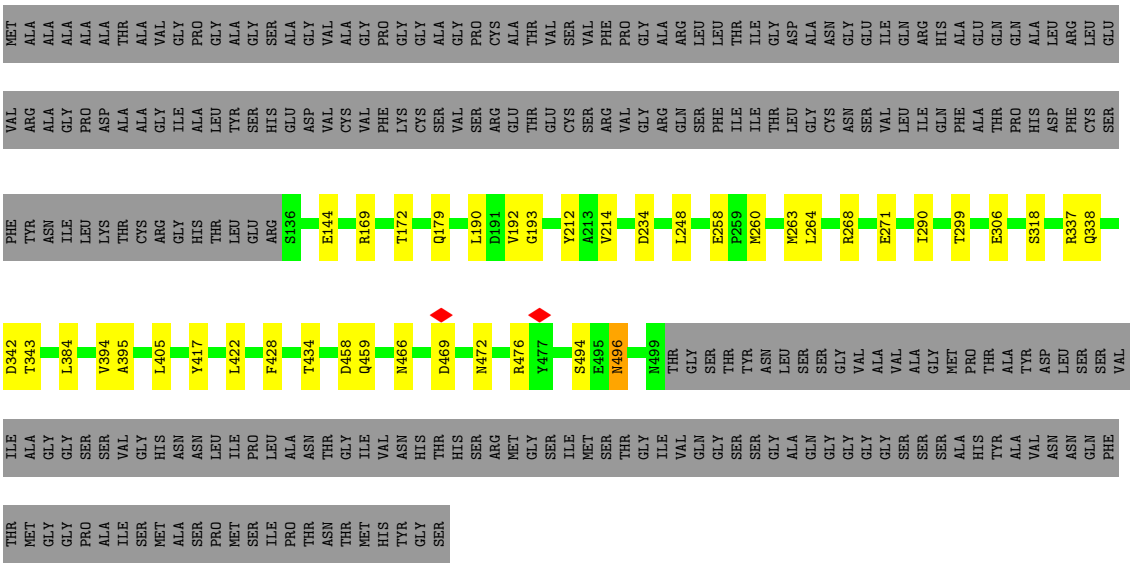
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
3	A	1	45	14	19	6	5	1	0
			Total	C	H	N	O	S	
3	B	1	45	14	19	6	5	1	0
			Total	C	H	N	O	S	
3	C	1	45	14	19	6	5	1	0
			Total	C	H	N	O	S	
3	D	1	45	14	19	6	5	1	0

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.

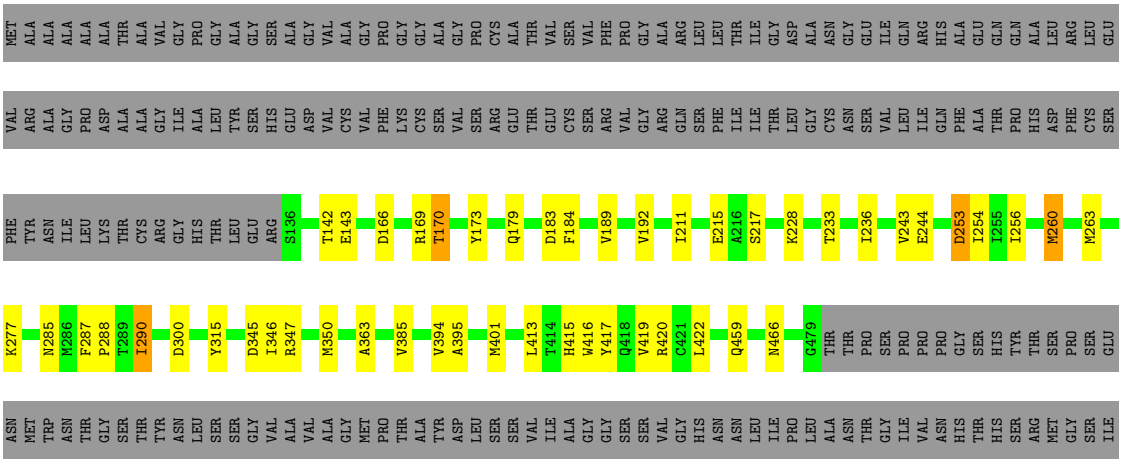
• Molecule 1: Histone-arginine methyltransferase CARM1

Chain A: 53% 7% 40%



• Molecule 1: Histone-arginine methyltransferase CARM1

Chain B: 49% 7% • 43%



MET SER THR GLY ILE VAL GLN GLY SER SER GLY ALA GLN GLY GLY GLY GLY SER SER SER ALA HIS TYR ALA VAL ASN ASN GLN PHE THR MET GLY GLY PRO ALA ILE SER MET ALA SER PRO MET SER ILE PRO THR ASN THR MET HIS TYR GLY SER

- Molecule 1: Histone-arginine methyltransferase CARM1

Chain C: 51% 8% 40%

MET ALA ALA ALA ALA ALA THR ALA VAL GLY PRO GLY ALA GLY SER ALA GLY VAL ALA GLY PRO GLY GLY ALA GLY PRO CYS ALA THR VAL SER VAL PHE PRO GLY ALA ARG LEU LEU THR ILE ILE GLY ASP ALA ASN GLY GLU ILE GLN ARG HIS ALA GLU GLN GLN ALA LEU ARG LEU GLU

VAL ARG ALA GLY PRO ASP ALA ALA GLY ILE ALA LEU TYR SER HIS GLU ASP VAL CYS VAL PHE LYS CYS SER VAL SER ARG GLU THR GLU CYS SER ARG VAL GLY ARG GLN SER PHE ILE ILE THR LEU GLY CYS ASN SER VAL LEU ILE GLN PHE ALA THR PRO HIS ASP PHE CYS SER

PHE TYR ASN ILE LEU LYS THR CYS ARG GLY HIS THR LEU GLU ARG S136 T142 E143 T172 V189 L190 G193 A204 I211 V214 E215 D234 R235 E244 E245 L248 I254 E258 P259 M260 M263 L264 L270 N285 I290 T299 D345

K355 Y356 T357 F360 L384 L388 A395 L405 S406 T407 T414 Y417 L422 L427 F428 S436 C439 L440 L441 Q447 S448 I453 D458 Q459 S464 S465 N466 F475 T480 Y490 N499 THR GLY SER THR TYR ASN LEU SER SER

GLY VAL ALA VAL ALA GLY MET PRO THR ALA TYR ASP LEU SER SER VAL ILE ALA GLY GLY SER SER VAL VAL GLY HIS ASN ASN LEU ILE PRO LEU ALA ASN THR GLY ILE VAL ASN HIS THR HIS SER ARG MET GLY SER ILE MET SER THR GLY ILE VAL GLN GLY SER SER GLY ALA GLN

GLY GLY GLY GLY SER SER SER ALA HIS TYR ALA VAL ASN ASN GLN PHE THR MET GLY GLY GLY PRO ALA ILE SER MET ALA SER PRO MET SER ILE PRO THR ASN THR MET HIS TYR GLY SER

- Molecule 1: Histone-arginine methyltransferase CARM1

Chain D: 51% 5% 43%

MET ALA ALA ALA ALA ALA THR ALA VAL GLY PRO GLY ALA GLY SER ALA GLY VAL ALA GLY PRO GLY GLY ALA GLY PRO CYS ALA THR VAL SER VAL PHE PRO GLY ALA ARG LEU LEU THR ILE ILE GLY ASP ALA ASN GLY GLU ILE GLN ARG HIS ALA GLU GLN GLN ALA LEU ARG LEU GLU

VAL ARG ALA GLY PRO ASP ALA ALA GLY ILE ALA LEU TYR SER HIS GLU ASP VAL CYS VAL PHE LYS CYS SER VAL SER ARG GLU THR GLU CYS SER ARG VAL GLY ARG GLN SER PHE ILE ILE THR LEU GLY CYS ASN SER VAL LEU ILE GLN PHE ALA THR PRO HIS ASP PHE CYS SER

PHE TYR ASN ILE LEU LYS THR CYS ARG GLY HIS THR LEU GLU ARG S136 Q160 R169 F184 L190 Y212 E215 A216 S217 T218 M219 L248 I254 L264 L270 F287 I290 Y315 V322 V341 D342 T343 I346 D393 V394 A395 H415

L422 L427 D433 L440 L441 I442 I453 S464 S465 N466 C479 THR THR PRO SER PRO PRO PRO PRO GLY SER HIS TYR THR SER PRO SER GLU ASN MET TRP ASN THR GLY SER THR TYR ASN LEU SER SER GLY VAL ALA VAL ALA GLY MET PRO THR ALA TYR ASP LEU

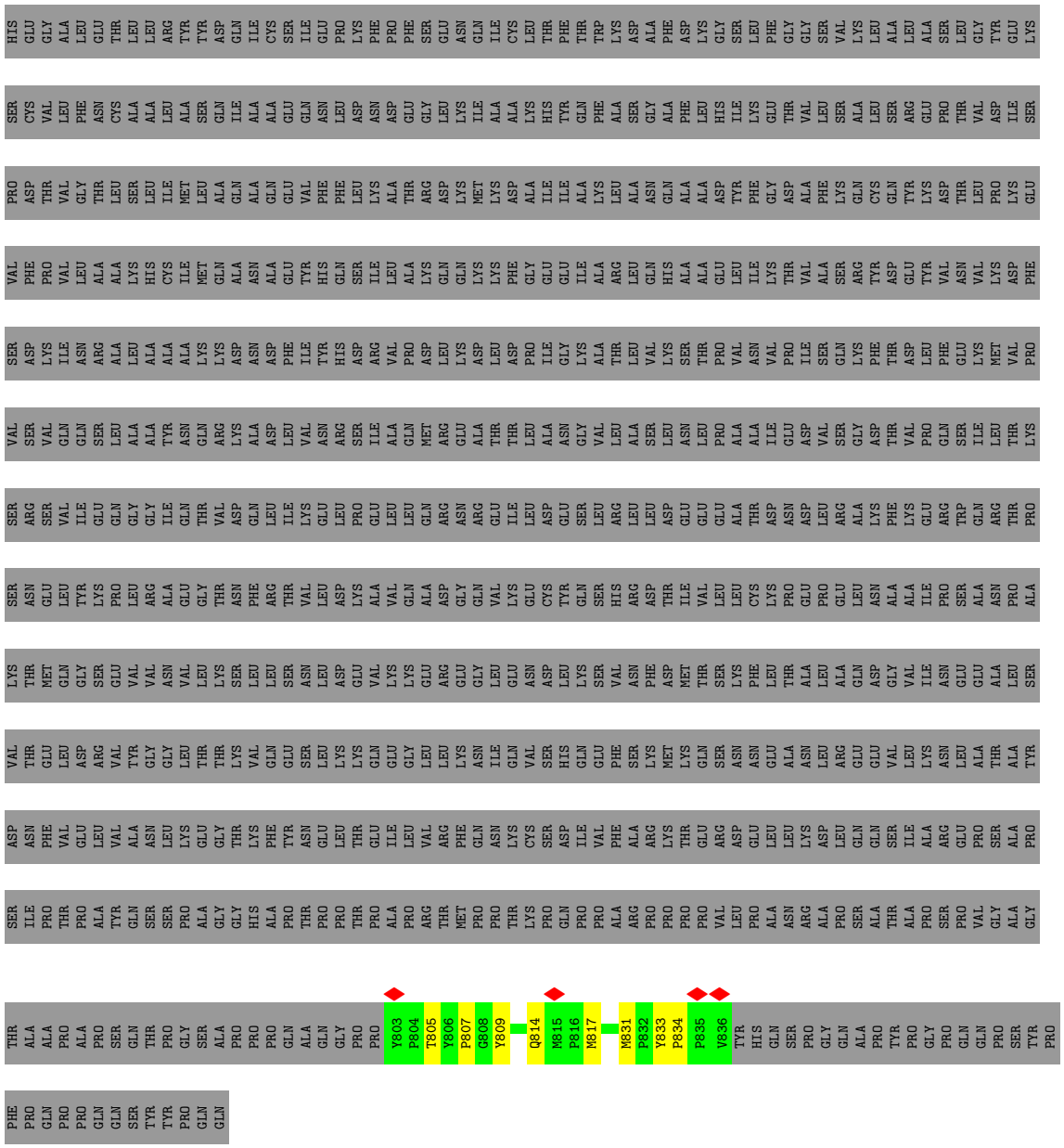
SER SER VAL ILE ALA GLY GLY SER VAL GLY HIS ASN ASN LEU ILE PRO LEU ALA ASN THR GLY ILE VAL ASN HIS THR HIS SER ARG MET GLY SER ILE MET SER THR GLY ILE VAL GLN GLY SER SER GLY ALA GLN GLY GLY GLY GLY SER SER SER ALA HIS TYR ALA VAL ASN

ASN GLN PHE THR MET GLY GLY PRO ALA ILE SER MET ALA SER PRO MET SER ILE PRO THR ASN THR MET HIS TYR GLY SER

- Molecule 2: Programmed cell death 6-interacting protein

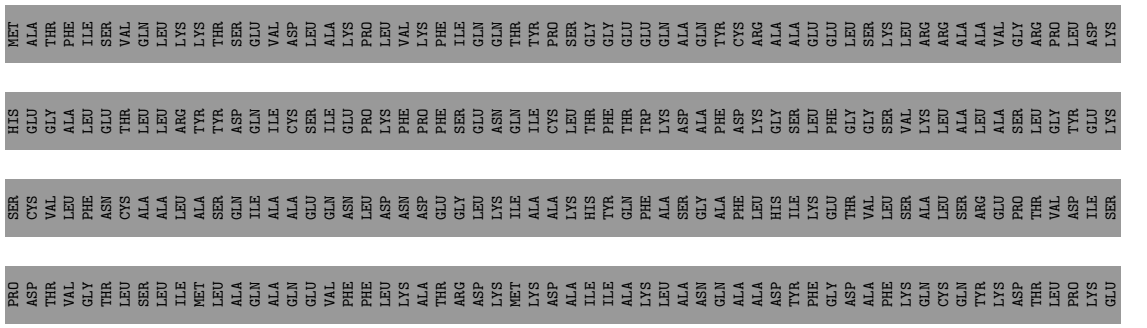
Chain F: 96%

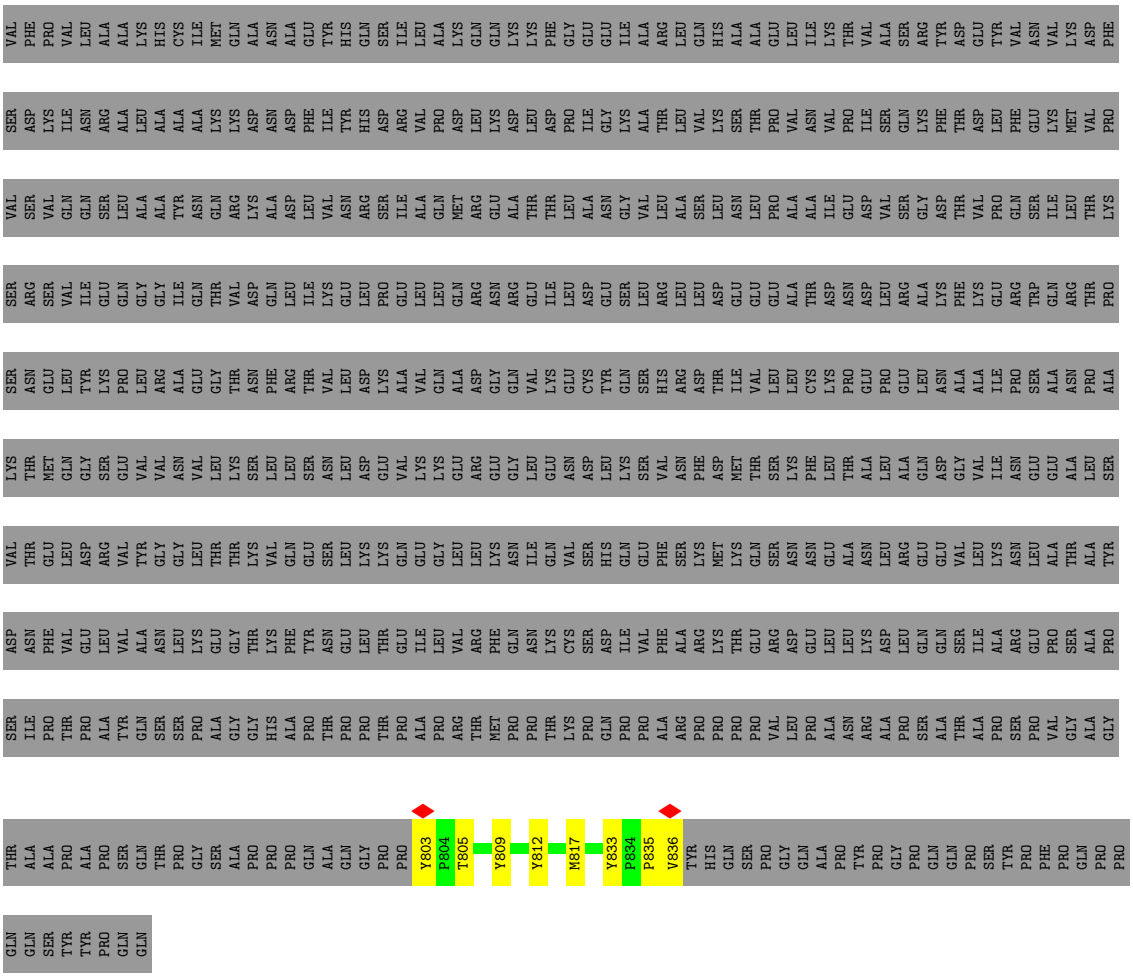
MET ALA THR PHE ILE SER VAL GLN LEU LYS LYS THR SER GLU VAL ASP LEU ALA LYS PRO LEU VAL LYS PHE ILE GLN GLN THR TYR PRO SER GLY GLY GLU GLU GLN ALA GLN TYR CYS ARG ALA ALA GLU GLU LEU SER LYS LEU ARG ARG ALA ALA VAL GLY ARG PRO LEU ASP LYS



- Molecule 2: Programmed cell death 6-interacting protein

Chain E: 96%




Y803
P804
T805
Y809
Y812
M817
Y833
P834
P835
V836

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.622	Depositor
Minimum map value	-0.737	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	297.33002, 297.33002, 297.33002	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.901, 0.901, 0.901	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: SAH

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	0.27	0/2987	0.31	0/4055
1	B	0.26	0/2825	0.31	0/3828
1	C	0.26	0/2987	0.32	0/4055
1	D	0.26	0/2825	0.31	0/3828
2	E	0.31	0/295	0.43	0/408
2	F	0.29	0/295	0.41	0/408
All	All	0.26	0/12214	0.32	0/16582

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 (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	A	2908	2834	2834	25	0
1	B	2755	2702	2702	32	0
1	C	2908	2834	2834	35	0
1	D	2755	2702	2702	24	0
2	E	278	245	245	5	0
2	F	278	245	245	11	0
3	A	26	19	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	19	19	2	0
3	C	26	19	19	1	0
3	D	26	19	19	1	0
All	All	11986	11638	11638	121	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 5.

The worst 5 of 121 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:C:215:GLU:OE1	3:C:701:SAH:O2'	1.87	0.91
1:A:422:LEU:O	1:A:466:ASN:ND2	2.18	0.77
2:F:814:GLN:HB2	2:F:817:MET:HE3	1.66	0.77
1:A:417:TYR:OH	2:E:805:THR:O	2.03	0.76
1:B:422:LEU:O	1:B:466:ASN:ND2	2.20	0.74

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	362/608 (60%)	350 (97%)	12 (3%)	0	100	100
1	B	342/608 (56%)	331 (97%)	11 (3%)	0	100	100
1	C	362/608 (60%)	349 (96%)	13 (4%)	0	100	100
1	D	342/608 (56%)	337 (98%)	5 (2%)	0	100	100
2	E	32/868 (4%)	25 (78%)	7 (22%)	0	100	100
2	F	32/868 (4%)	25 (78%)	7 (22%)	0	100	100
All	All	1472/4168 (35%)	1417 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/498 (64%)	315 (99%)	3 (1%)	70	80
1	B	299/498 (60%)	290 (97%)	9 (3%)	36	65
1	C	318/498 (64%)	314 (99%)	4 (1%)	61	77
1	D	299/498 (60%)	295 (99%)	4 (1%)	61	77
2	E	29/740 (4%)	28 (97%)	1 (3%)	32	63
2	F	29/740 (4%)	29 (100%)	0	100	100
All	All	1292/3472 (37%)	1271 (98%)	21 (2%)	54	75

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	299	THR
1	D	322	VAL
2	E	803	TYR
1	D	393	ASP
1	D	315	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	222	HIS
1	D	149	GLN
2	E	814	GLN
1	A	415	HIS
1	B	179	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)

4 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	$\#\|Z\| > 2$
3	SAH	C	701	-	27,28,28	1.06	4 (14%)	38,40,40	1.97	9 (23%)
3	SAH	A	701	-	27,28,28	1.06	4 (14%)	38,40,40	1.99	11 (28%)
3	SAH	B	701	-	27,28,28	1.06	5 (18%)	38,40,40	2.01	10 (26%)
3	SAH	D	701	-	27,28,28	1.03	3 (11%)	38,40,40	1.98	11 (28%)

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	SAH	C	701	-	-	3/15/31/31	0/3/3/3
3	SAH	A	701	-	-	1/15/31/31	0/3/3/3
3	SAH	B	701	-	-	1/15/31/31	0/3/3/3
3	SAH	D	701	-	-	1/15/31/31	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	SAH	C2-N1	2.26	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	SAH	C2-N1	2.26	1.38	1.33
3	C	701	SAH	C2-N1	2.25	1.38	1.33
3	D	701	SAH	C2-N1	2.21	1.38	1.33
3	B	701	SAH	C2-N3	2.16	1.37	1.33

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	SAH	N3-C2-N1	-5.48	120.03	128.60
3	B	701	SAH	N3-C2-N1	-5.45	120.07	128.60
3	D	701	SAH	N3-C2-N1	-5.44	120.10	128.60
3	C	701	SAH	N3-C2-N1	-5.43	120.11	128.60
3	C	701	SAH	C5-C4-N3	-4.74	120.56	126.75

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	SAH	C-CA-CB-CG
3	C	701	SAH	N-CA-CB-CG
3	D	701	SAH	CB-CG-SD-C5'
3	B	701	SAH	CB-CG-SD-C5'
3	C	701	SAH	C4'-C5'-SD-CG

There are no ring outliers.

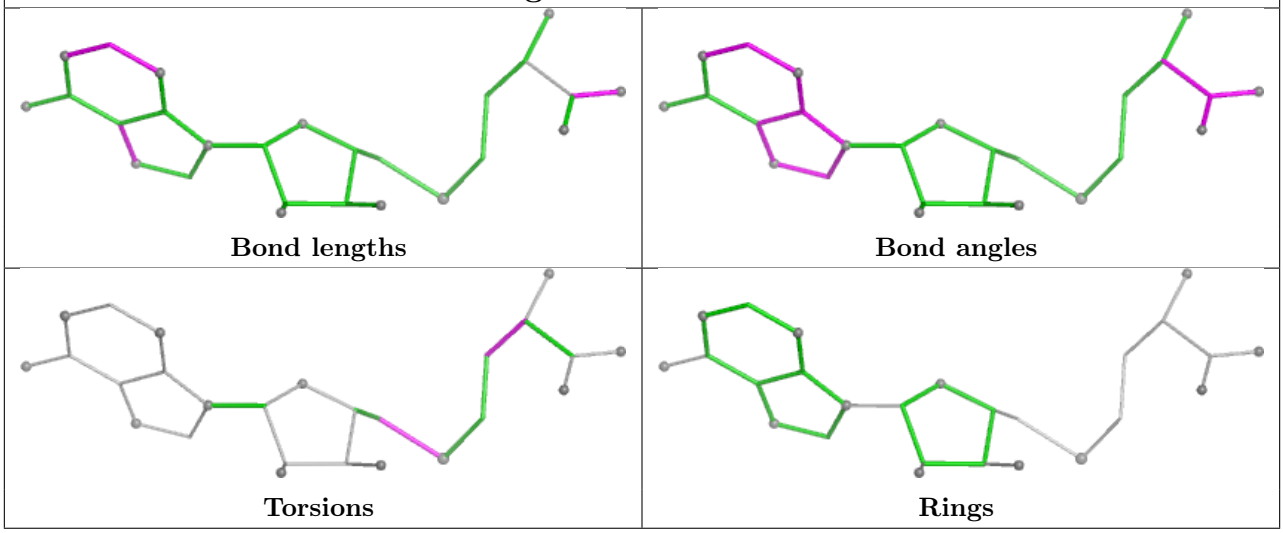
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	SAH	1	0
3	A	701	SAH	1	0
3	B	701	SAH	2	0
3	D	701	SAH	1	0

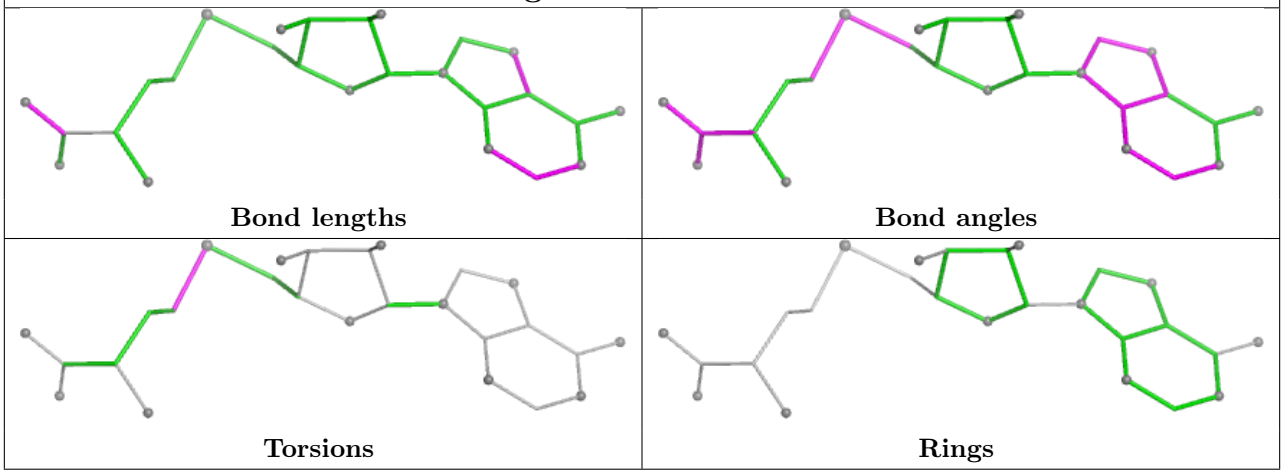
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

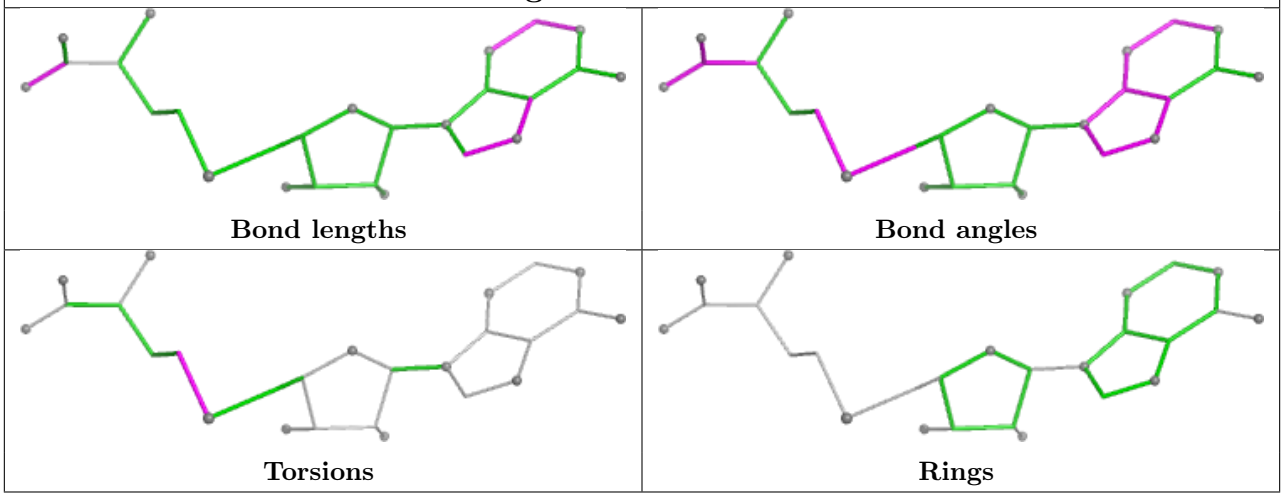
Ligand SAH C 701

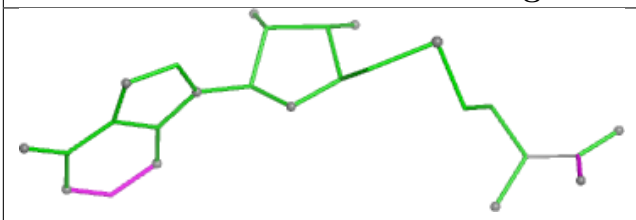
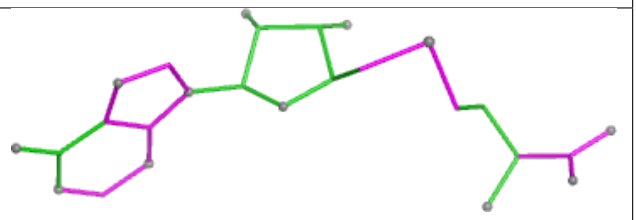
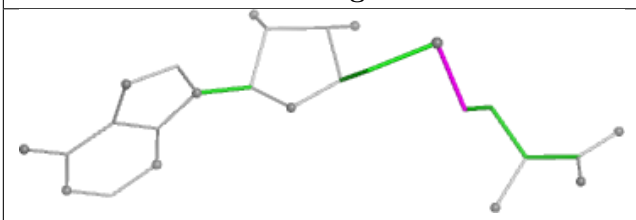
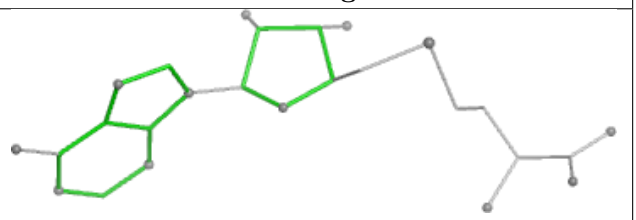


Ligand SAH A 701



Ligand SAH B 701



Ligand SAH D 701	
 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.

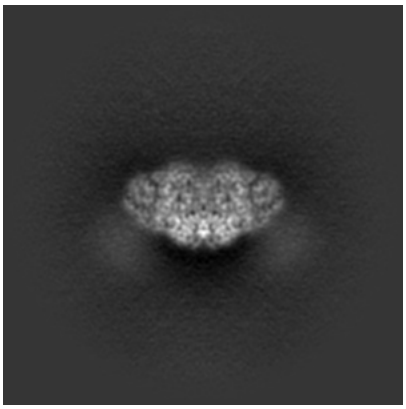
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55242. These allow visual inspection of the internal detail of the map and identification of artifacts.

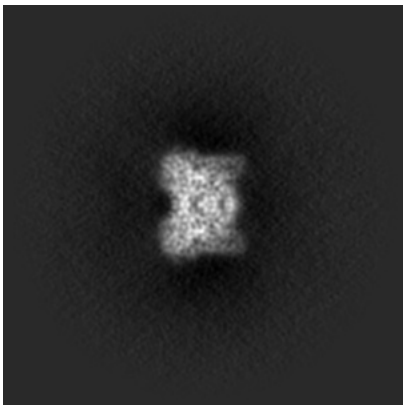
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

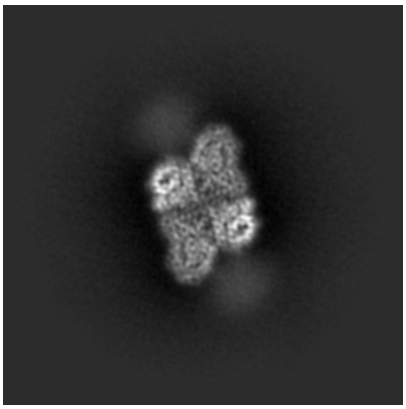
6.1.1 Primary map



X

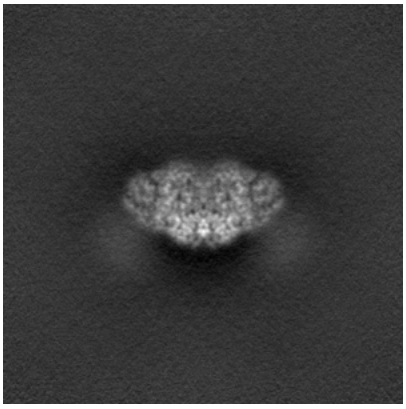


Y

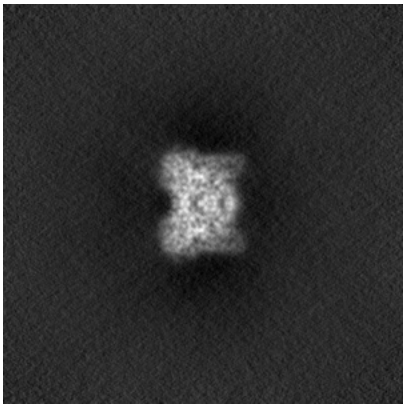


Z

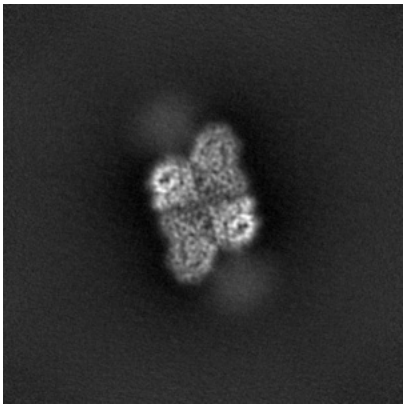
6.1.2 Raw map



X



Y

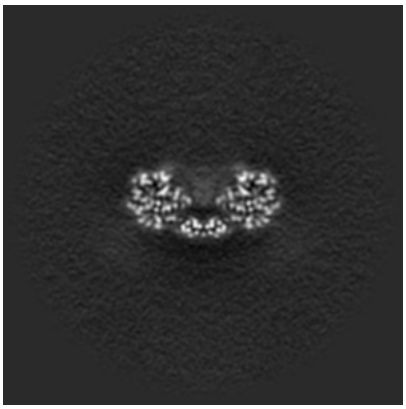


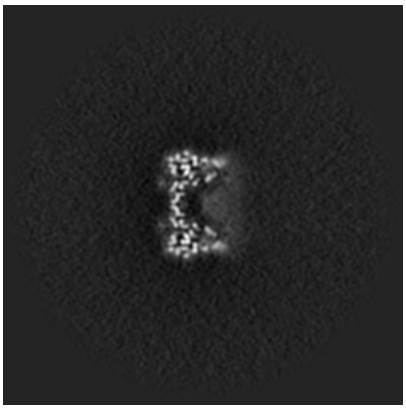
Z

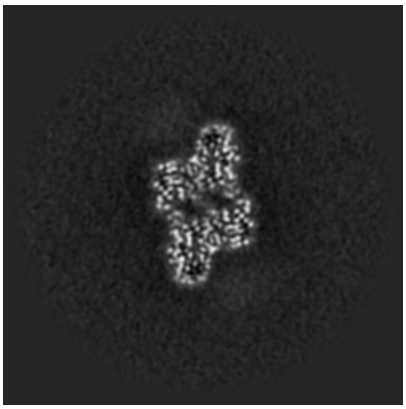
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

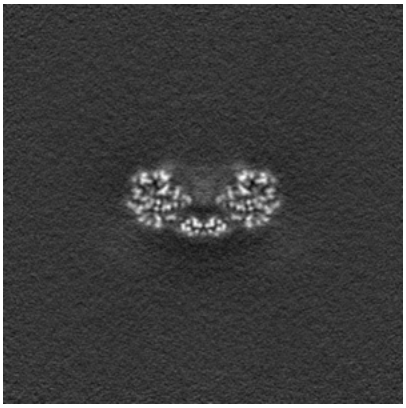
6.2.1 Primary map

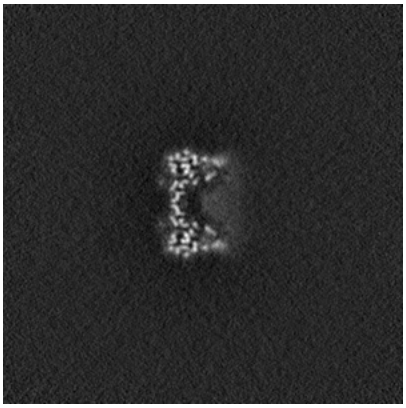

X Index: 165

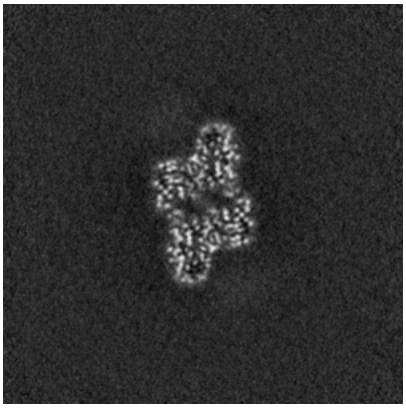

Y Index: 165


Z Index: 165

6.2.2 Raw map


X Index: 165

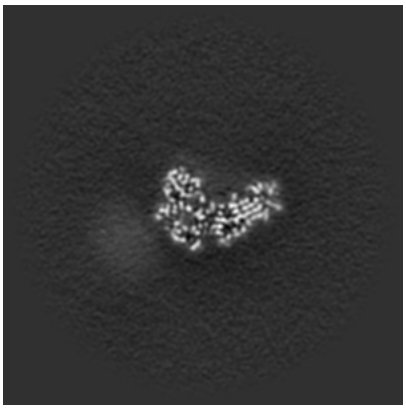

Y Index: 165

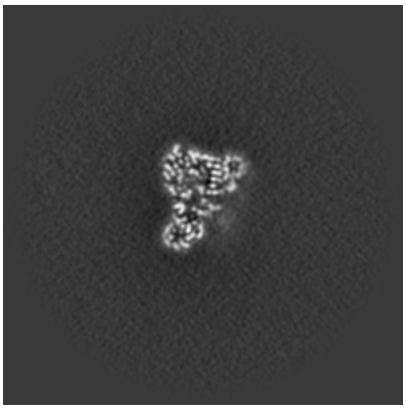

Z Index: 165

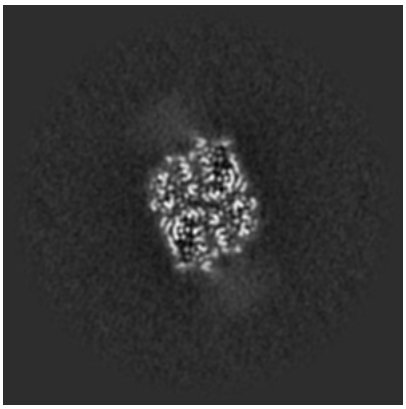
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

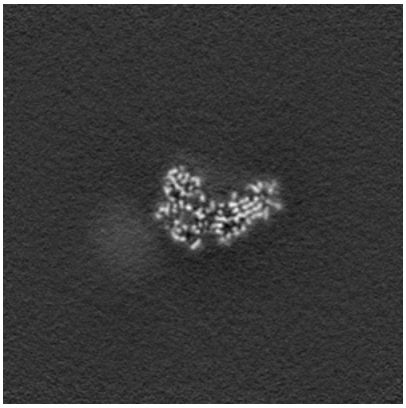
6.3.1 Primary map

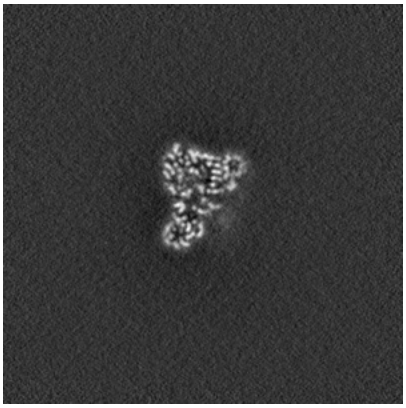

X Index: 187

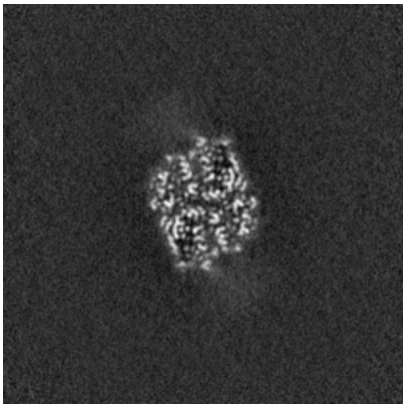

Y Index: 149


Z Index: 152

6.3.2 Raw map


X Index: 187

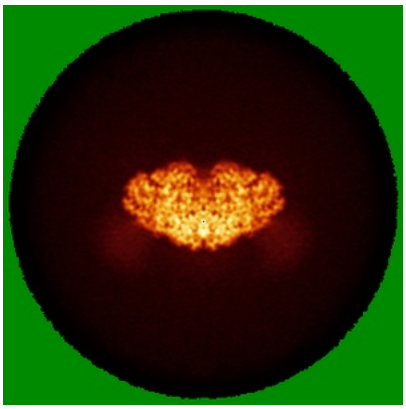

Y Index: 149


Z Index: 152

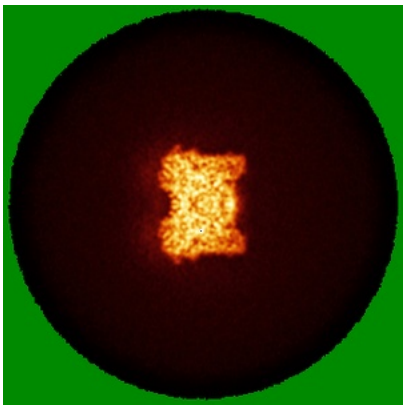
The images above show the largest variance slices of the map in three orthogonal directions.

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

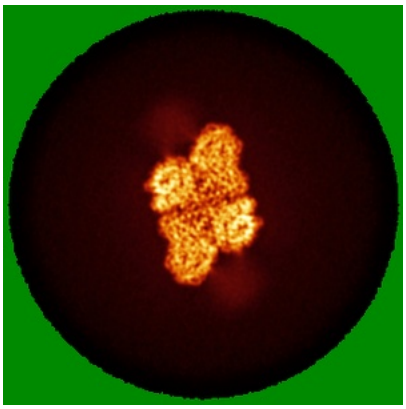
6.4.1 Primary map



X

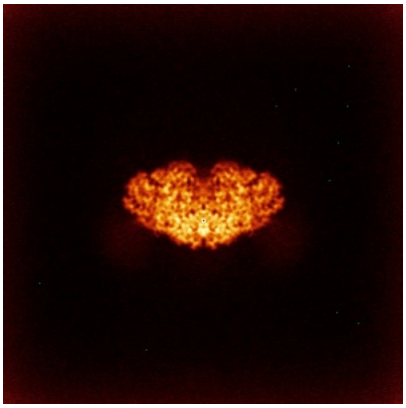


Y

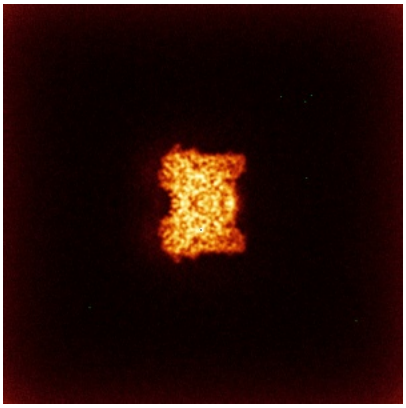


Z

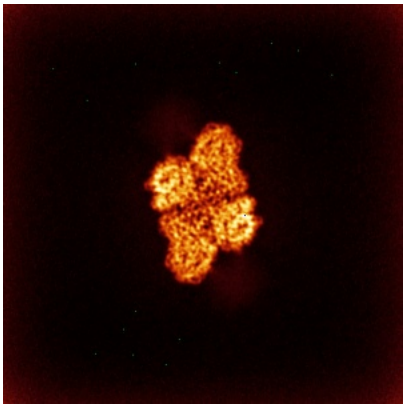
6.4.2 Raw map



X



Y

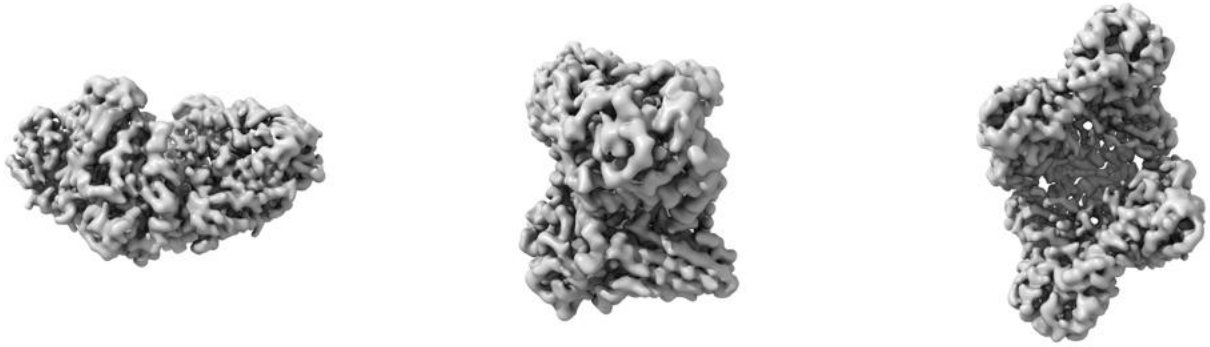


Z

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)

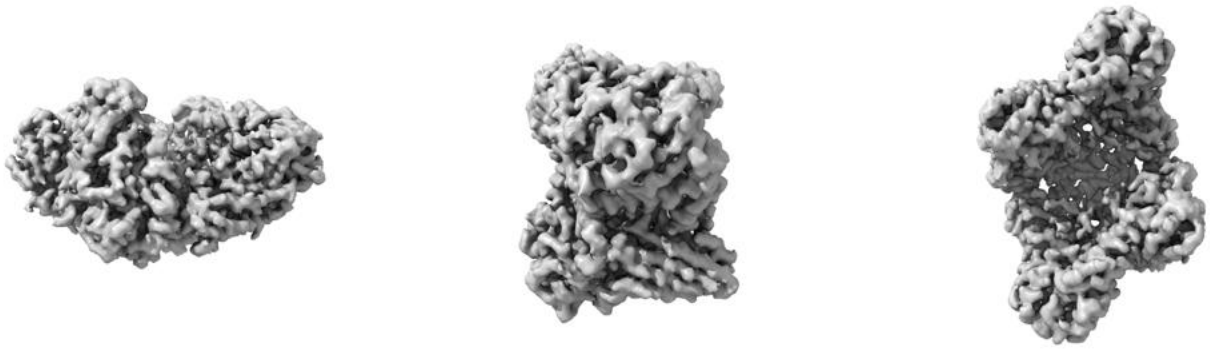
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

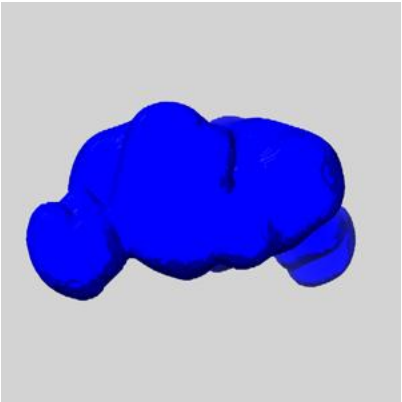
6.6 Mask visualisation (i)

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

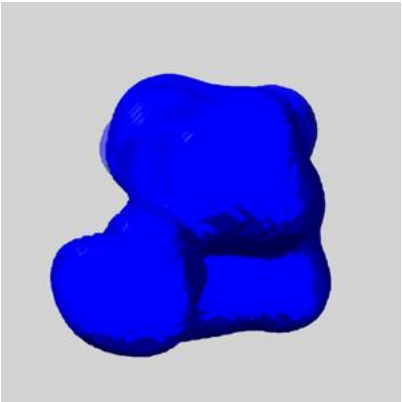
A mask typically either:

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

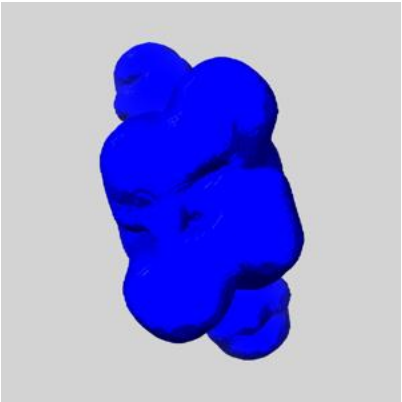
6.6.1 emd_55242_msk_1.map (i)



X



Y

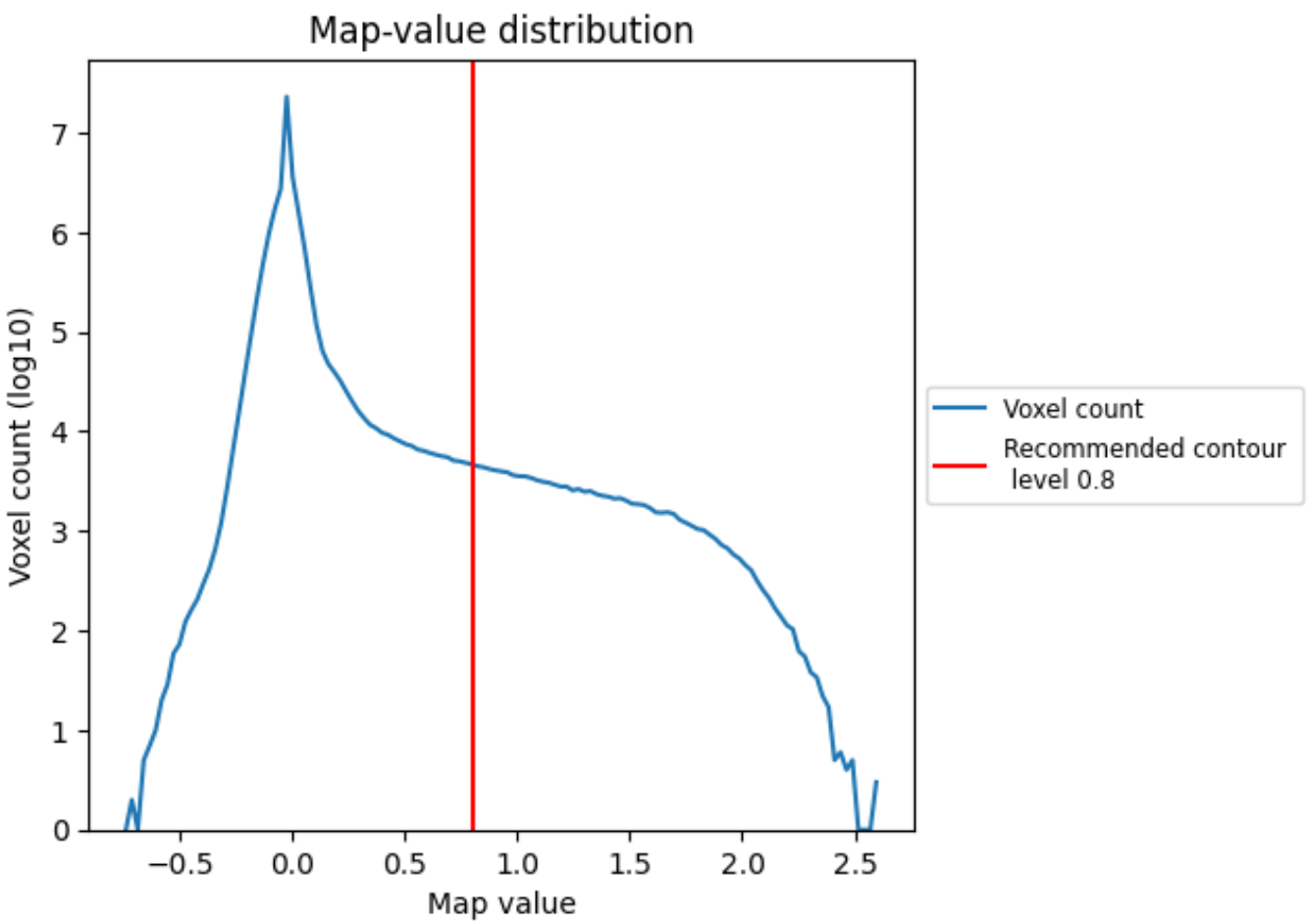


Z

7 Map analysis (i)

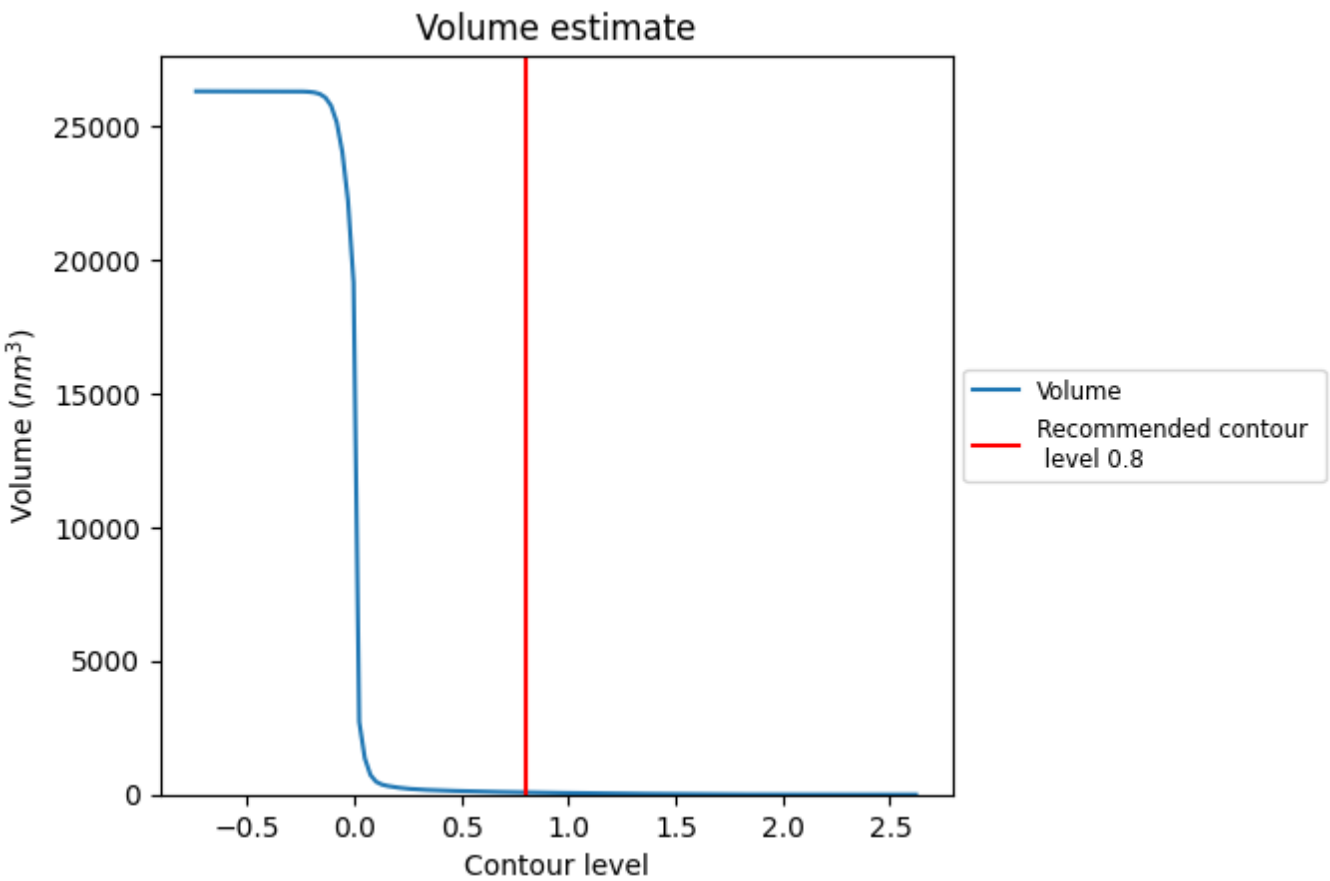
This section contains the results of statistical analysis of the map.

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.

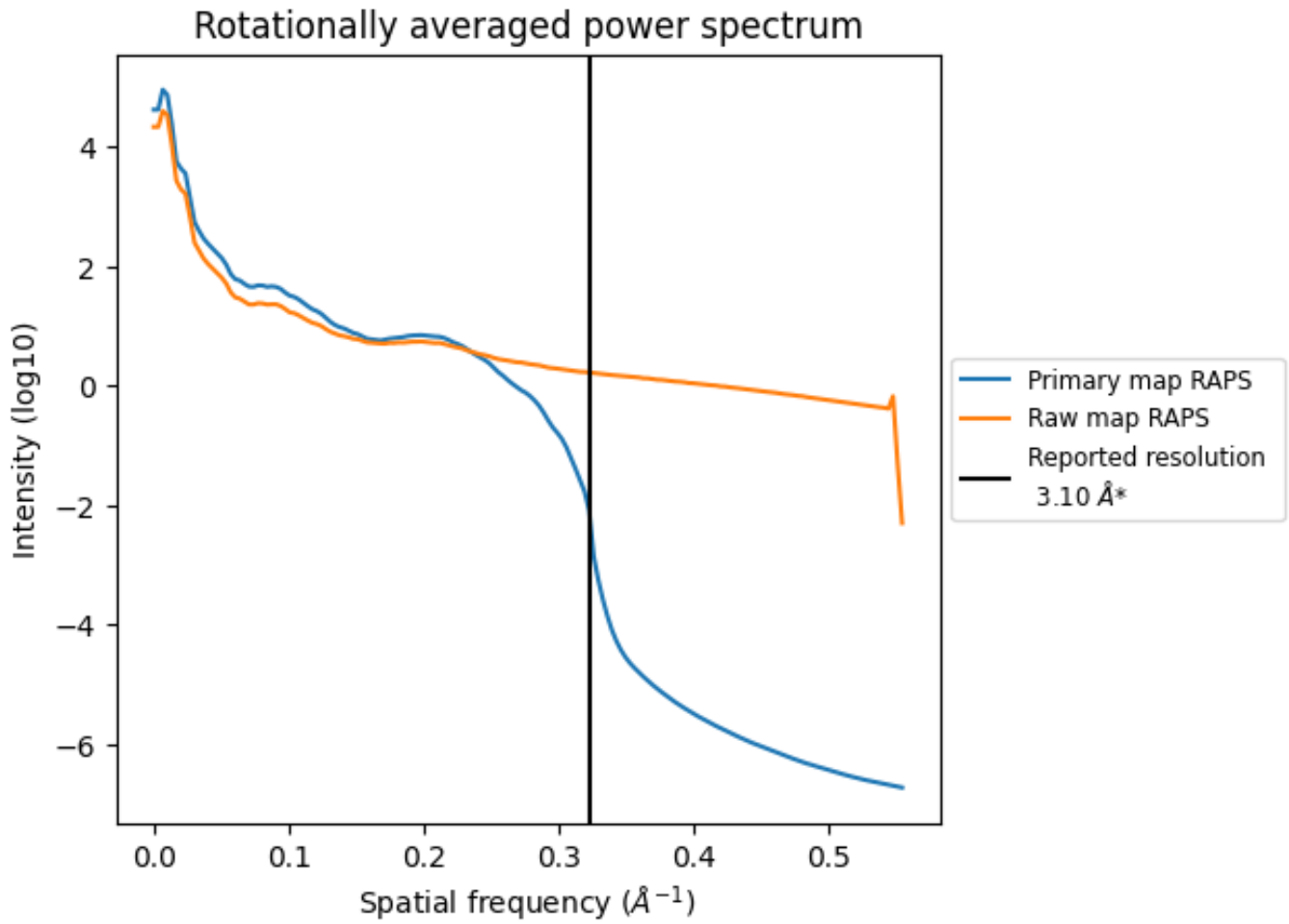
7.2 Volume estimate (i)



The volume at the recommended contour level is 81 nm^3; this corresponds to an approximate mass of 73 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)

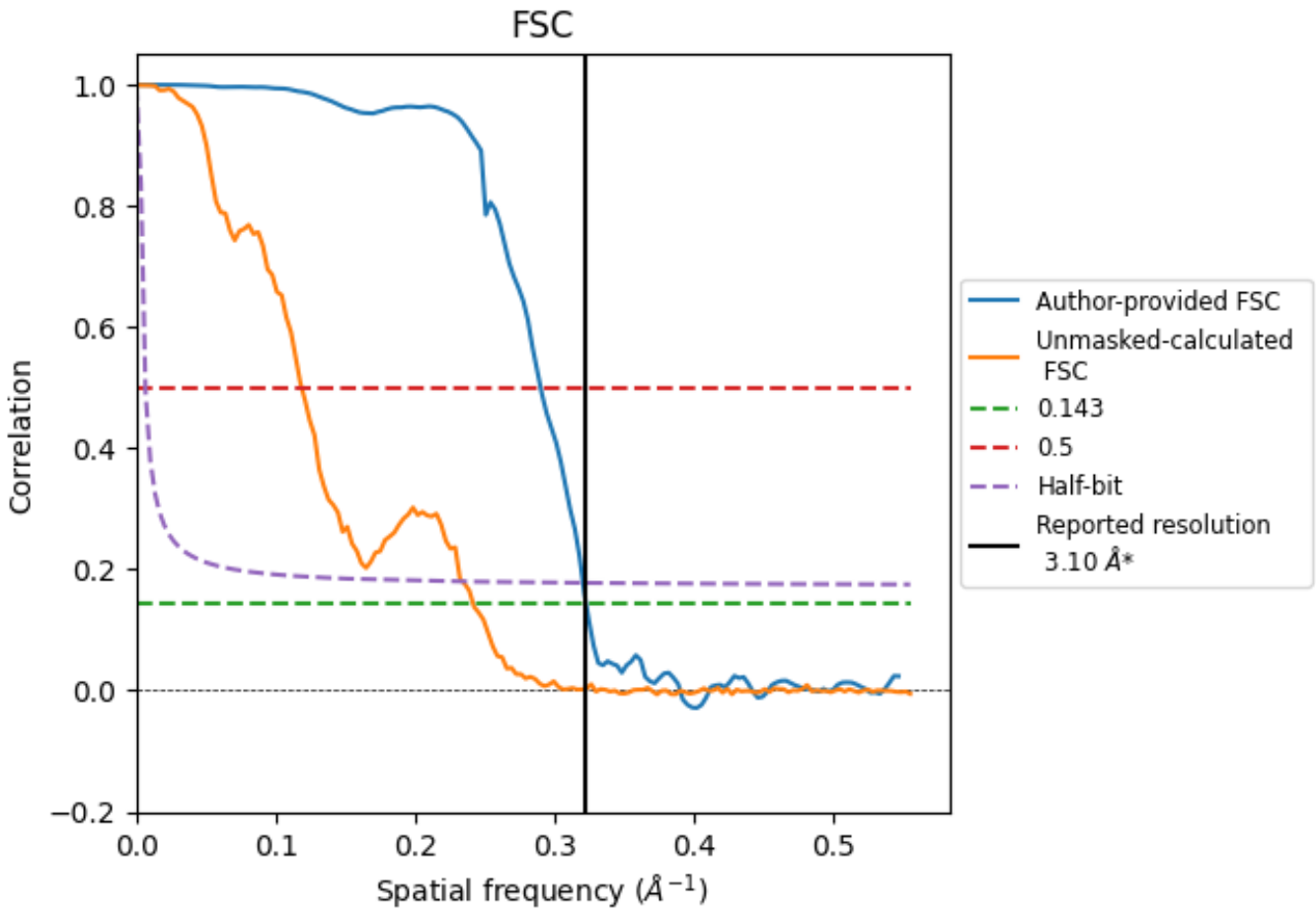


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

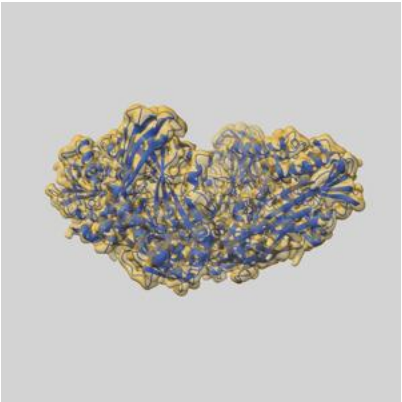
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.45	3.12
Unmasked-calculated*	4.14	8.43	4.28

*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 4.14 differs from the reported value 3.1 by more than 10 %

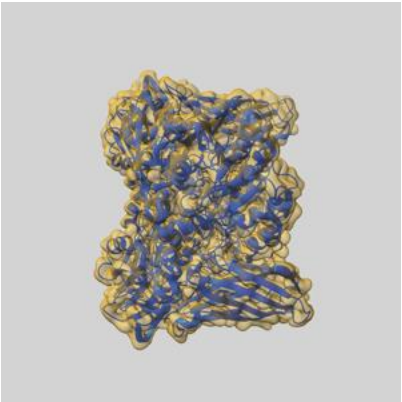
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55242 and PDB model 9SV7. Per-residue inclusion information can be found in section 3 on page 6.

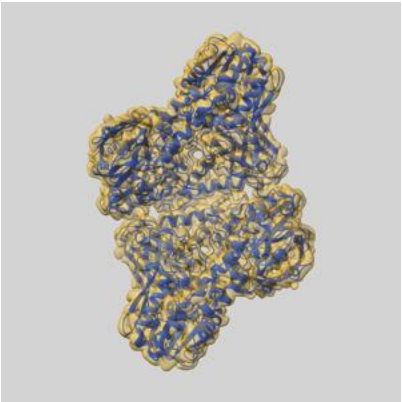
9.1 Map-model overlay (i)



X



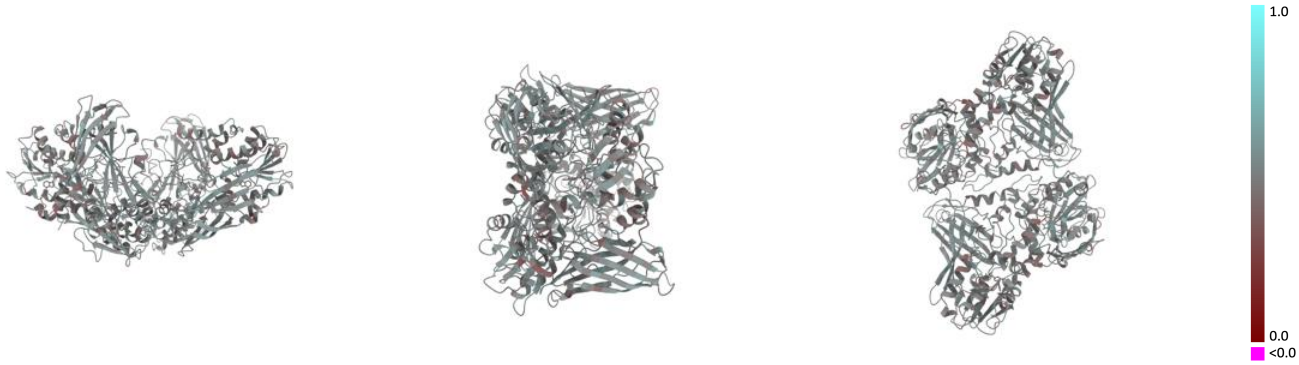
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

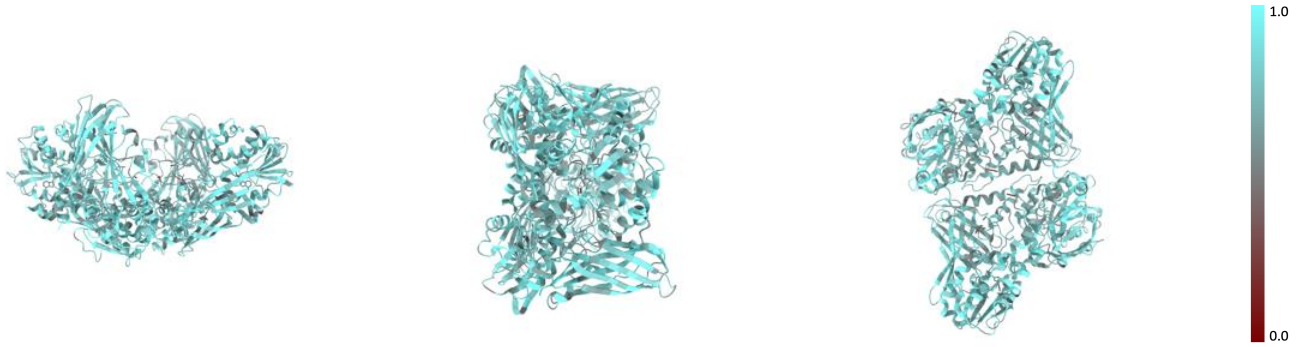
9.2 Q-score mapped to coordinate model (i)



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.

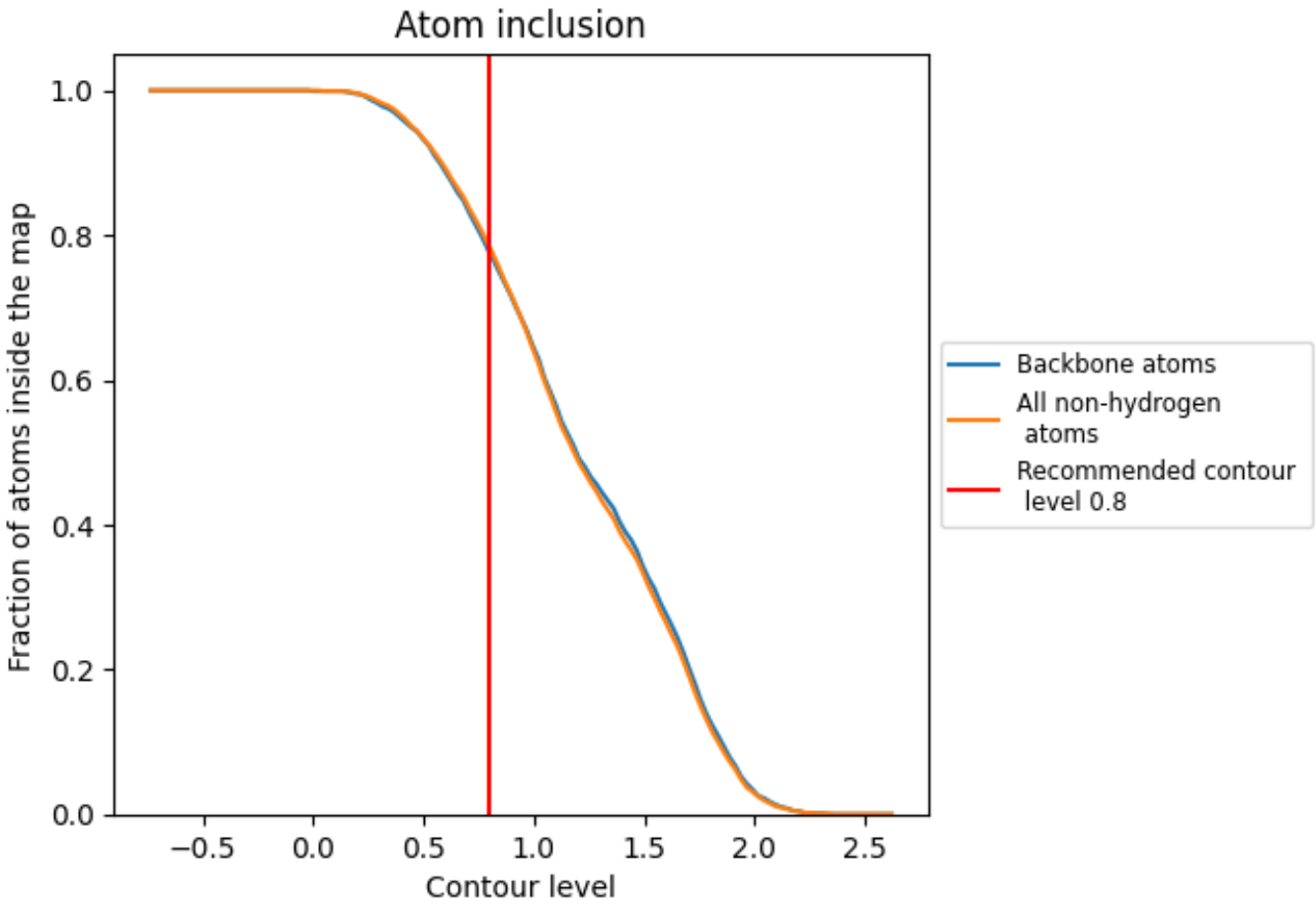
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.4930
A	0.8000	0.4950
B	0.8010	0.4940
C	0.7900	0.4950
D	0.7880	0.4900
E	0.7620	0.4910
F	0.6390	0.4790