wwPDB EM Validation Summary Report

Sep 14, 2026 – 01:19 pm BST

PDB ID	:	9SQP / pdb_00009sqp
EMDB ID	:	EMD-55114
Title	:	Structure of a disulfide-bridged complex between HLA-A*02:01-K127N/Y84C and ERp57/tapasin-K16C - State 3
Authors	:	Mitlehner, A.; Loll, B.; Hilal, T.
Deposited on	:	2025-09-23
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:

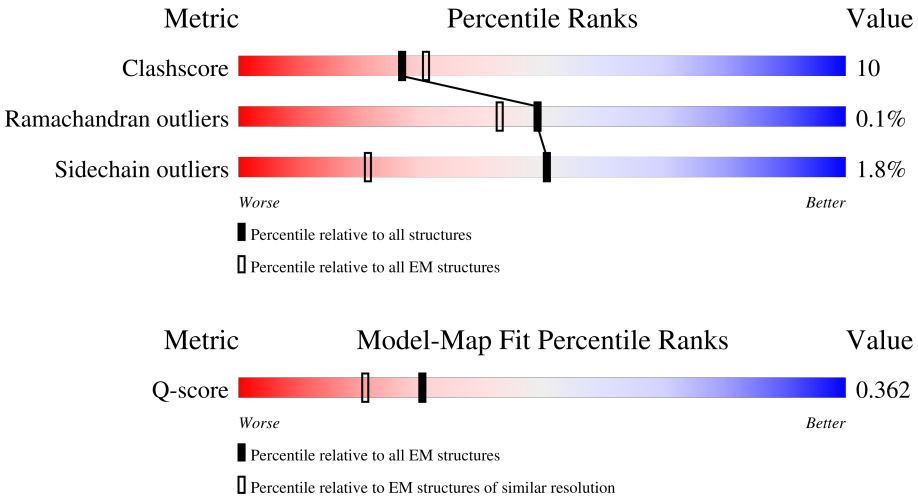
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal 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 (i)

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

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	B	99	65% 34%
2	D	398	76% 19%
3	E	481	75% 22%
4	A	301	63% 18% 19%

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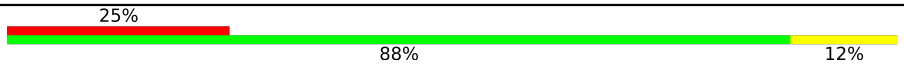
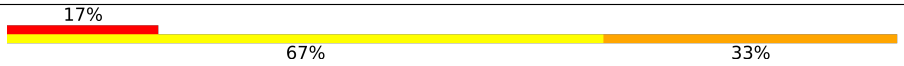
Mol	Chain	Length	Quality of chain
5	C	8	
6	F	6	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9548 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	99	Total	C	N	O	S	0	0
			828	527	140	157	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	CYS	THR	engineered mutation	UNP P61769

- Molecule 2 is a protein called Tapasin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	381	Total	C	N	O	S	0	0
			2882	1839	510	520	13		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	16	CYS	LYS	engineered mutation	UNP O15533
D	240	ARG	THR	variant	UNP O15533
D	304	CYS	GLY	engineered mutation	UNP O15533
D	393	HIS	-	expression tag	UNP O15533
D	394	HIS	-	expression tag	UNP O15533
D	395	HIS	-	expression tag	UNP O15533
D	396	HIS	-	expression tag	UNP O15533
D	397	HIS	-	expression tag	UNP O15533
D	398	HIS	-	expression tag	UNP O15533

- Molecule 3 is a protein called Protein disulfide-isomerase A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	469	Total	C	N	O	S	0	0
			3724	2362	625	724	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	85	ALA	CYS	engineered mutation	UNP P30101

- Molecule 4 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	244	Total	C	N	O	S	0	0
			1983	1242	359	373	9		

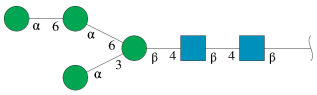
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	CYS	TYR	engineered mutation	UNP Q9TQB6
A	277	GLY	-	expression tag	UNP Q9TQB6
A	278	SER	-	expression tag	UNP Q9TQB6
A	279	GLY	-	expression tag	UNP Q9TQB6
A	280	GLY	-	expression tag	UNP Q9TQB6
A	281	SER	-	expression tag	UNP Q9TQB6
A	282	GLY	-	expression tag	UNP Q9TQB6
A	283	GLY	-	expression tag	UNP Q9TQB6
A	284	SER	-	expression tag	UNP Q9TQB6
A	285	ALA	-	expression tag	UNP Q9TQB6
A	286	GLY	-	expression tag	UNP Q9TQB6
A	287	GLY	-	expression tag	UNP Q9TQB6
A	288	GLY	-	expression tag	UNP Q9TQB6
A	289	LEU	-	expression tag	UNP Q9TQB6
A	290	ASN	-	expression tag	UNP Q9TQB6
A	291	ASP	-	expression tag	UNP Q9TQB6
A	292	ILE	-	expression tag	UNP Q9TQB6
A	293	PHE	-	expression tag	UNP Q9TQB6
A	294	GLU	-	expression tag	UNP Q9TQB6
A	295	ALA	-	expression tag	UNP Q9TQB6
A	296	GLN	-	expression tag	UNP Q9TQB6
A	297	LYS	-	expression tag	UNP Q9TQB6
A	298	ILE	-	expression tag	UNP Q9TQB6
A	299	GLU	-	expression tag	UNP Q9TQB6
A	300	TRP	-	expression tag	UNP Q9TQB6
A	301	HIS	-	expression tag	UNP Q9TQB6

- Molecule 5 is a protein called LYS-ILE-LEU-GLY-PHE-VAL-NFA; pKV9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	8	Total	C	N	O	0	1
			59	43	9	7		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



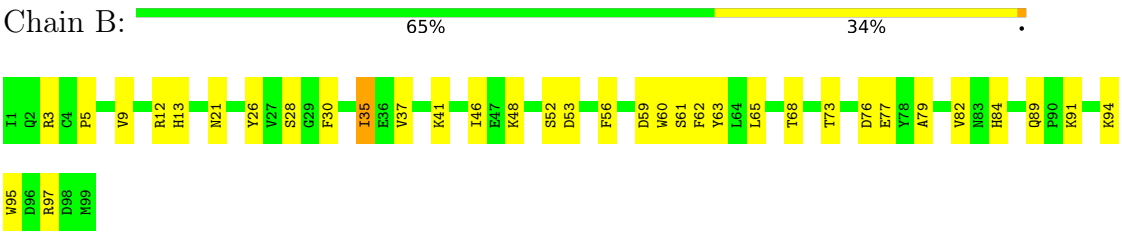
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	6	Total	C	N	O	0	0
			72	40	2	30		

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.

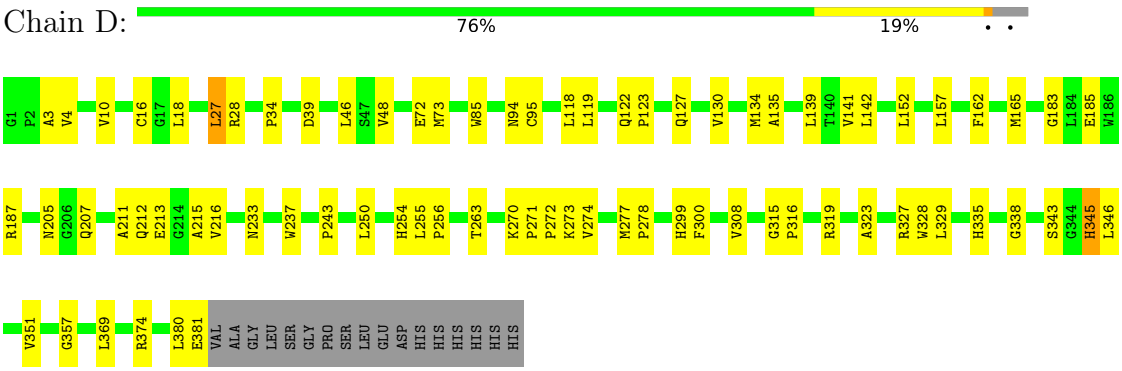
• Molecule 1: Beta-2-microglobulin

Chain B:



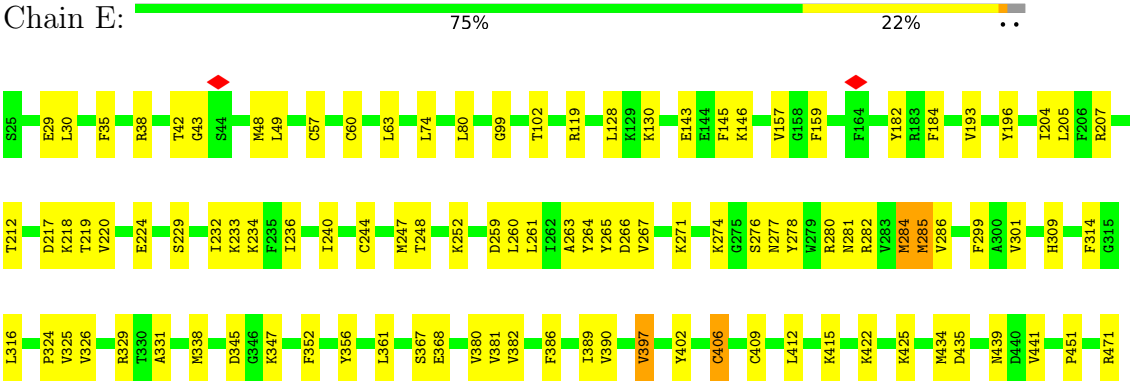
• Molecule 2: Tapasin

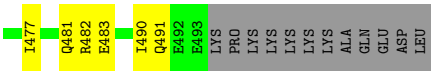
Chain D:



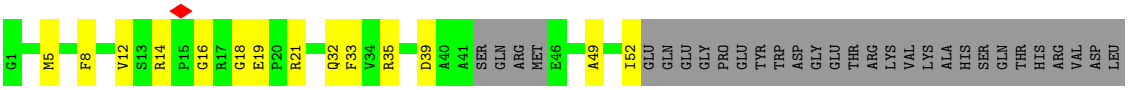
• Molecule 3: Protein disulfide-isomerase A3

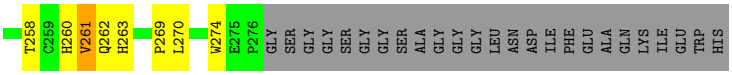
Chain E:



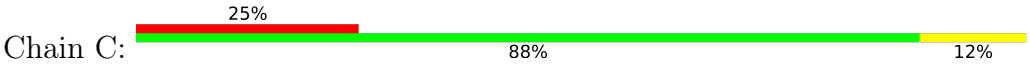


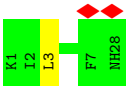
• Molecule 4: MHC class I antigen



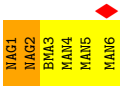


• Molecule 5: LYS-ILE-LEU-GLY-PHE-VAL-NFA; pKV9





• Molecule 6: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	235772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.521	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	235.87201, 235.87201, 235.87201	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.819, 0.819, 0.819	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, BMA, MAN, NAG

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	B	0.13	0/851	0.36	0/1150
2	D	0.11	0/2980	0.30	0/4090
3	E	0.10	0/3808	0.31	3/5142 (0.1%)
4	A	0.10	0/2040	0.33	1/2771 (0.0%)
5	C	0.16	0/59	0.40	0/77
All	All	0.11	0/9738	0.32	4/13230 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	84	CYS	CA-CB-SG	7.45	131.53	114.40
3	E	285	MET	CA-CB-CG	5.45	125.00	114.10
3	E	284	MET	CA-C-N	-5.05	112.30	121.14
3	E	284	MET	C-N-CA	-5.05	112.30	121.14

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	B	828	0	792	31	0
2	D	2882	0	2833	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3724	0	3622	73	0
4	A	1983	0	1845	40	0
5	C	59	0	67	1	0
6	F	72	0	61	3	0
All	All	9548	0	9220	186	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 10.

The worst 5 of 186 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)
3:E:278:TYR:HA	3:E:281:ASN:HD22	1.53	0.71
4:A:138:MET:SD	4:A:138:MET:N	2.62	0.71
2:D:16:CYS:HA	4:A:84:CYS:HB2	1.74	0.69
1:B:94:LYS:HZ1	2:D:328:TRP:CG	2.10	0.69
3:E:390:VAL:HG12	3:E:397:VAL:HG21	1.74	0.68

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	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	D	379/398 (95%)	354 (93%)	24 (6%)	1 (0%)	36	67
3	E	467/481 (97%)	459 (98%)	8 (2%)	0	100	100
4	A	238/301 (79%)	231 (97%)	7 (3%)	0	100	100
5	C	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1187/1287 (92%)	1144 (96%)	42 (4%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	28	ARG

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	B	94/94 (100%)	92 (98%)	2 (2%)	47	66
2	D	303/317 (96%)	294 (97%)	9 (3%)	36	60
3	E	402/413 (97%)	396 (98%)	6 (2%)	57	71
4	A	204/247 (83%)	203 (100%)	1 (0%)	81	80
5	C	6/6 (100%)	6 (100%)	0	100	100
All	All	1009/1077 (94%)	991 (98%)	18 (2%)	51	69

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	397	VAL
4	A	261	VAL
3	E	441	VAL
2	D	274	VAL
3	E	380	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	360	ASN
3	E	428	ASN
4	A	115	GLN
4	A	32	GLN
4	A	96	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)

6 monosaccharides 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	$\#\|Z\| > 2$
6	NAG	F	1	2,6	14,14,15	0.97	1 (7%)	17,19,21	1.59	3 (17%)
6	NAG	F	2	6	14,14,15	0.71	0	17,19,21	1.18	2 (11%)
6	BMA	F	3	6	11,11,12	0.82	0	15,15,17	2.29	6 (40%)
6	MAN	F	4	6	11,11,12	0.77	0	15,15,17	1.02	1 (6%)
6	MAN	F	5	6	11,11,12	0.72	0	15,15,17	1.17	1 (6%)
6	MAN	F	6	6	11,11,12	0.70	0	15,15,17	1.17	1 (6%)

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
6	NAG	F	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	2/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1	NAG	C1-C2	2.44	1.56	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	3	BMA	C1-O5-C5	6.31	120.74	112.19
6	F	1	NAG	O5-C1-C2	-3.94	105.06	111.29
6	F	5	MAN	C1-O5-C5	3.49	116.92	112.19
6	F	6	MAN	C1-O5-C5	3.36	116.74	112.19
6	F	3	BMA	C3-C4-C5	3.00	115.60	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
6	F	4	MAN	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	4	MAN	O5-C5-C6-O6

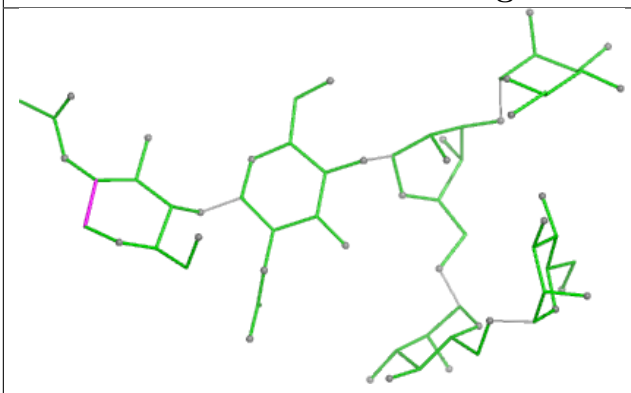
There are no ring outliers.

2 monomers are involved in 3 short contacts:

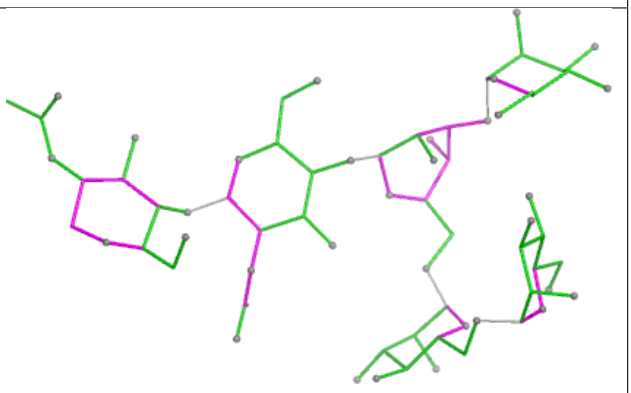
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	2	0
6	F	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

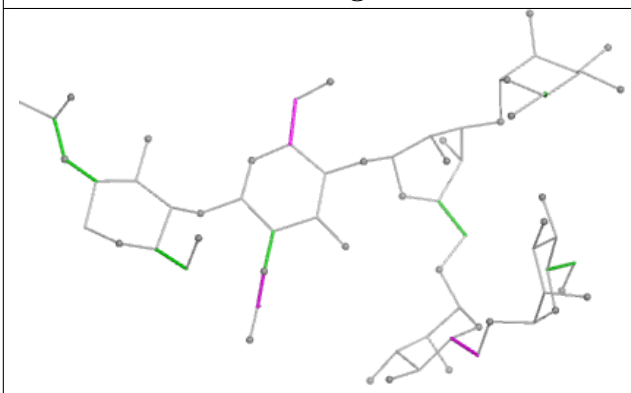
Oligosaccharide Chain F



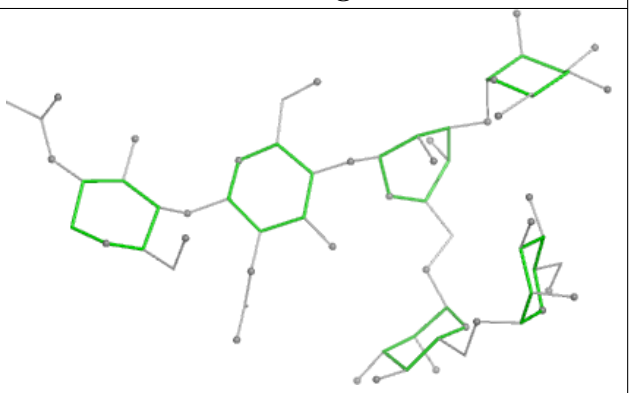
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

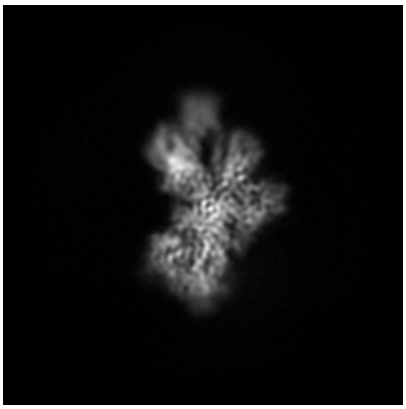
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55114. These allow visual inspection of the internal detail of the map and identification of artifacts.

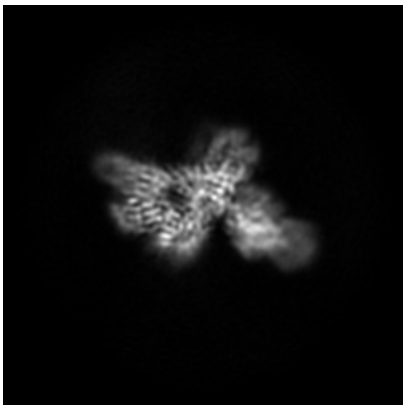
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

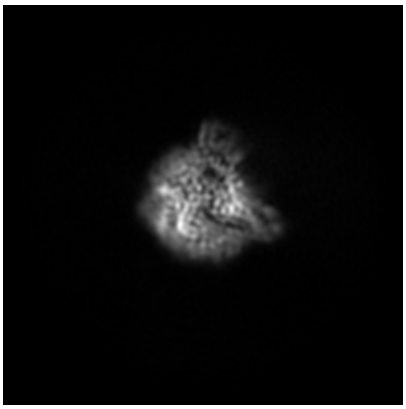
6.1.1 Primary map



X

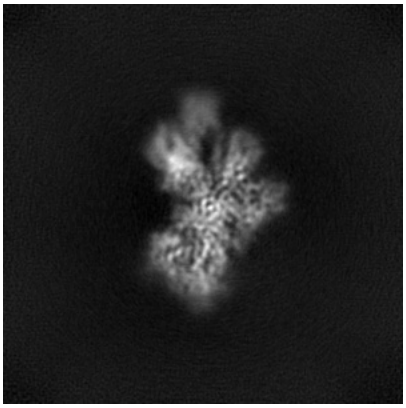


Y

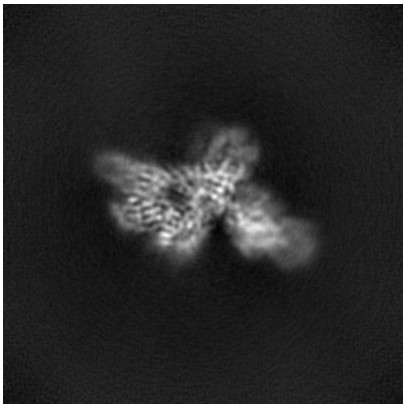


Z

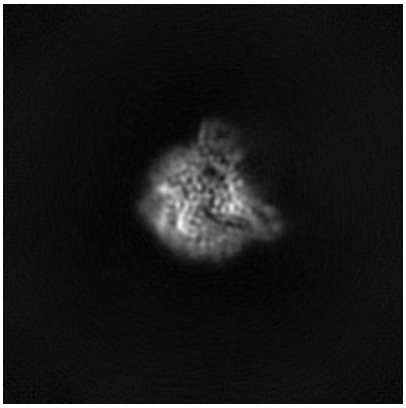
6.1.2 Raw map



X



Y

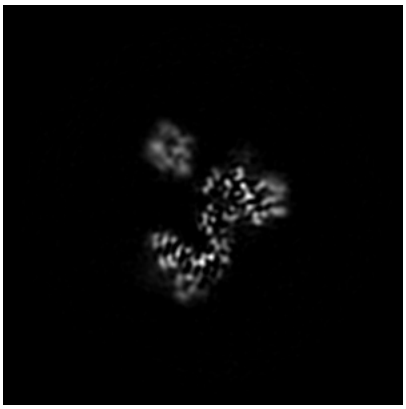


Z

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

6.2 Central slices (i)

6.2.1 Primary map

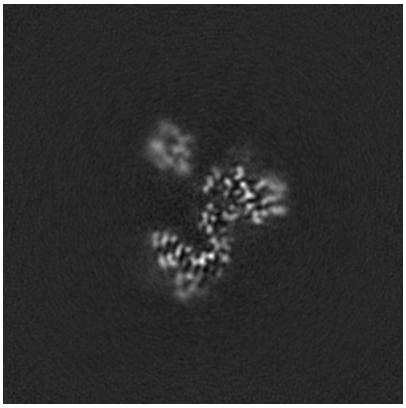


X Index: 144

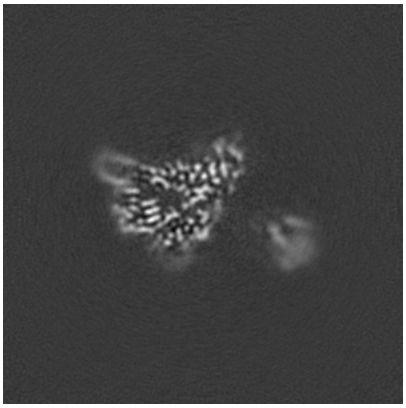
Y Index: 144

Z Index: 144

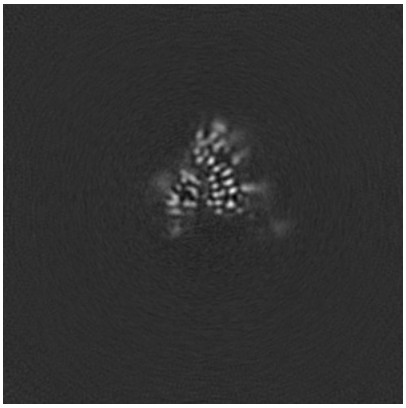
6.2.2 Raw map



X Index: 144



Y Index: 144

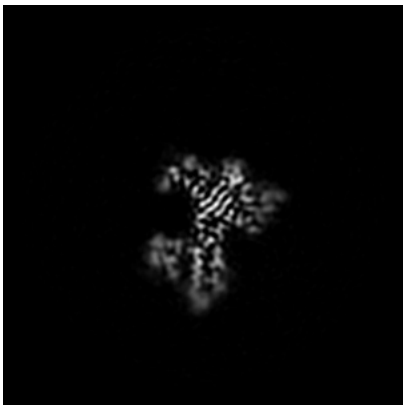


Z Index: 144

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

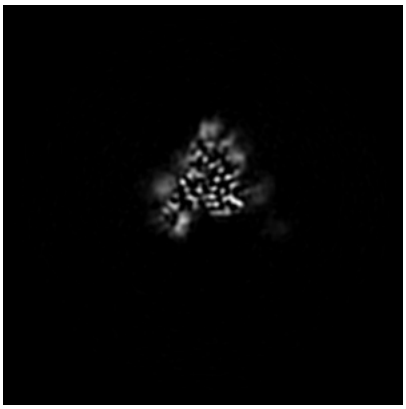
6.3 Largest variance slices (i)

6.3.1 Primary map



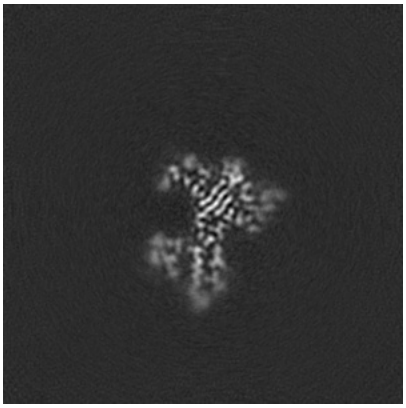
X Index: 164

Y Index: 144

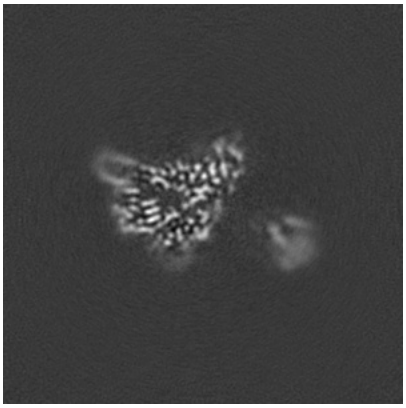


Z Index: 140

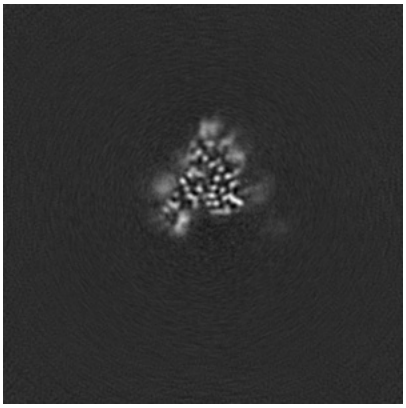
6.3.2 Raw map



X Index: 164



Y Index: 144

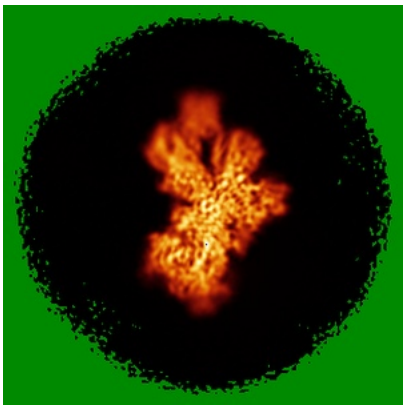


Z Index: 140

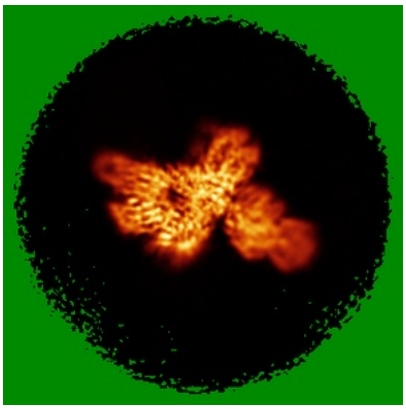
The images above show the largest variance slices of the map in three orthogonal directions.

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

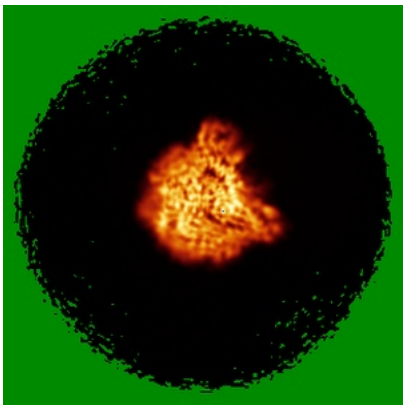
6.4.1 Primary map



X

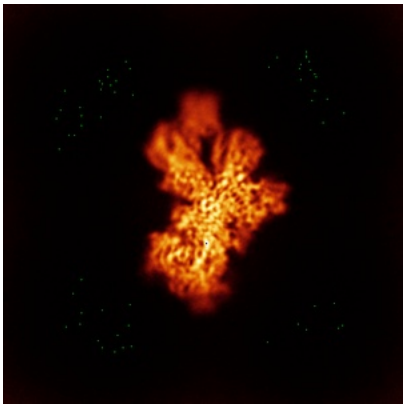


Y

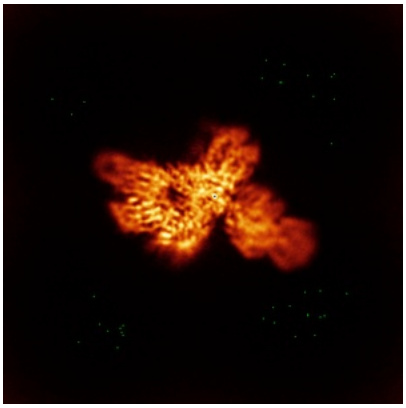


Z

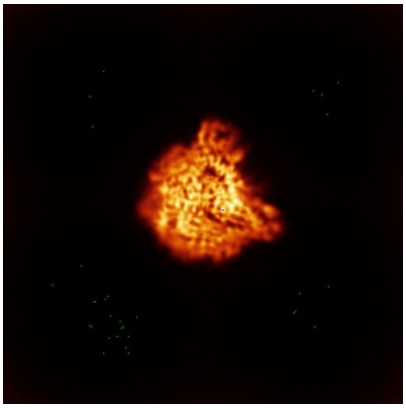
6.4.2 Raw map



X



Y

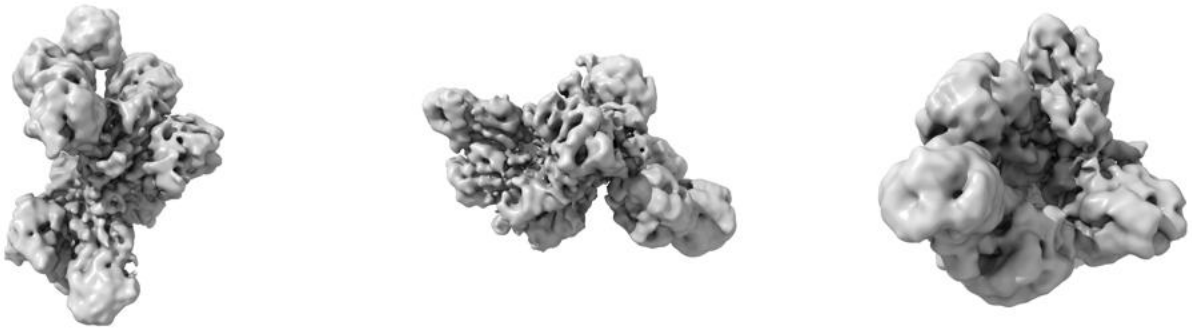


Z

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 0.18. 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.

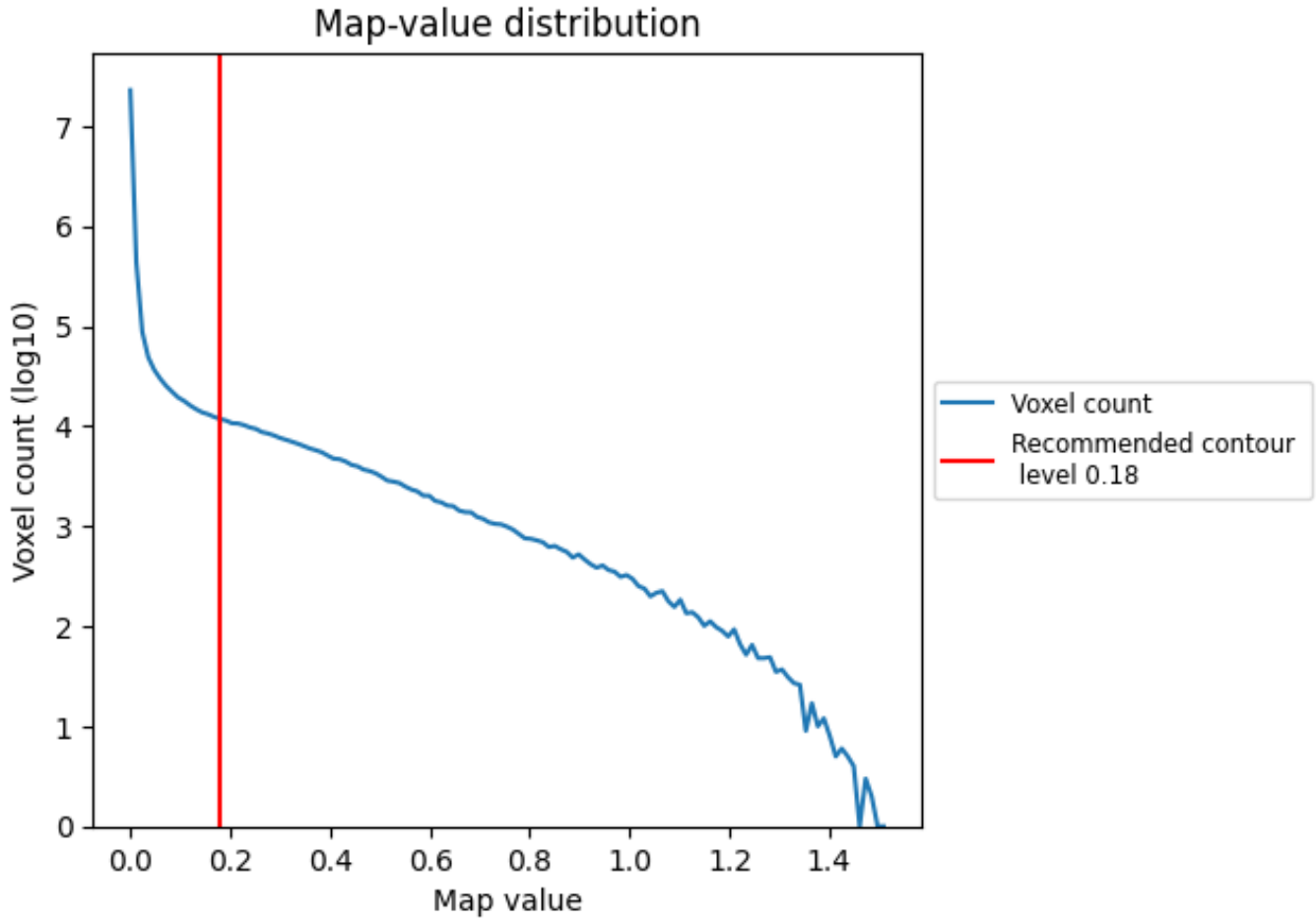
6.6 Mask visualisation (i)

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

7 Map analysis

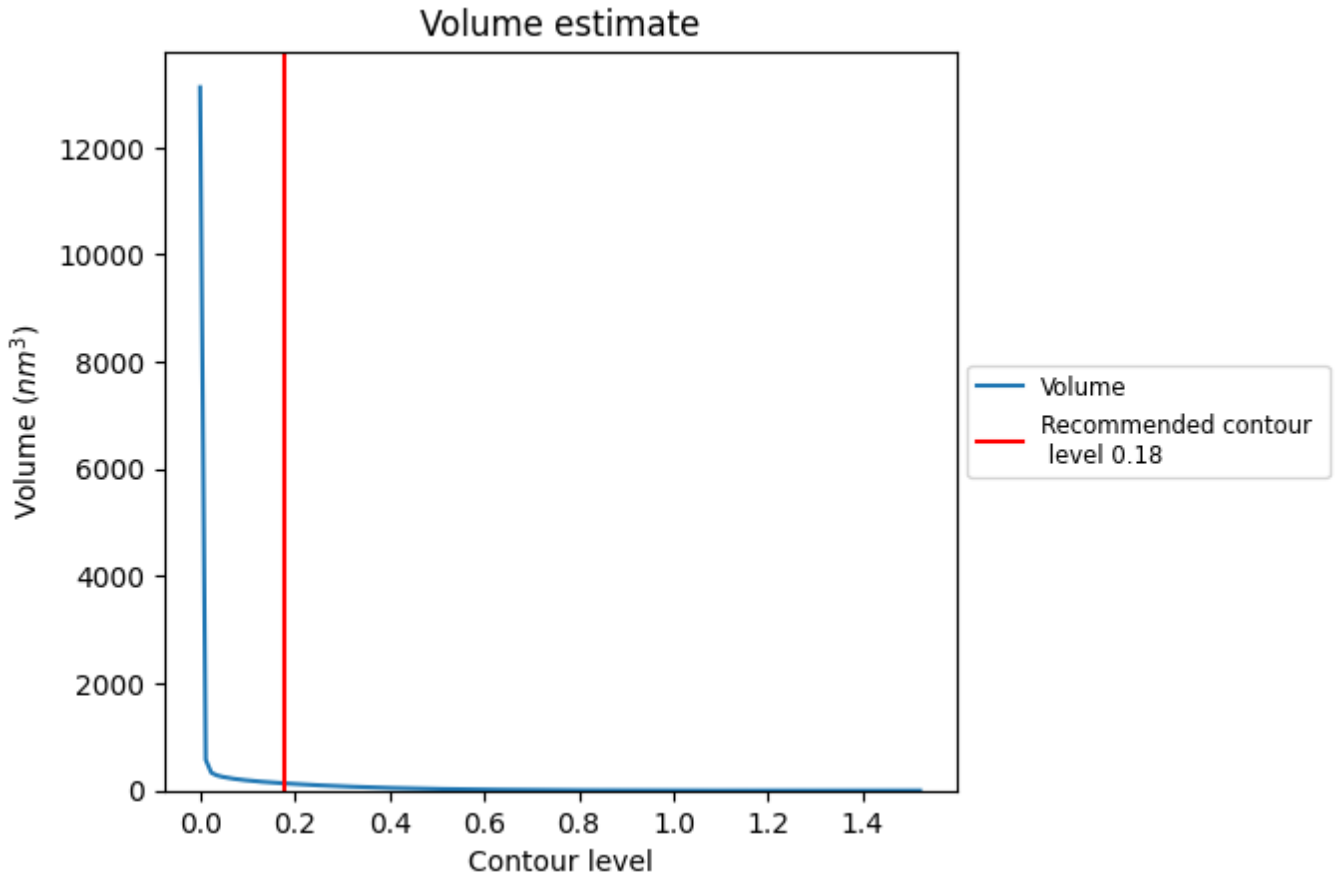
This section contains the results of statistical analysis of the map.

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.

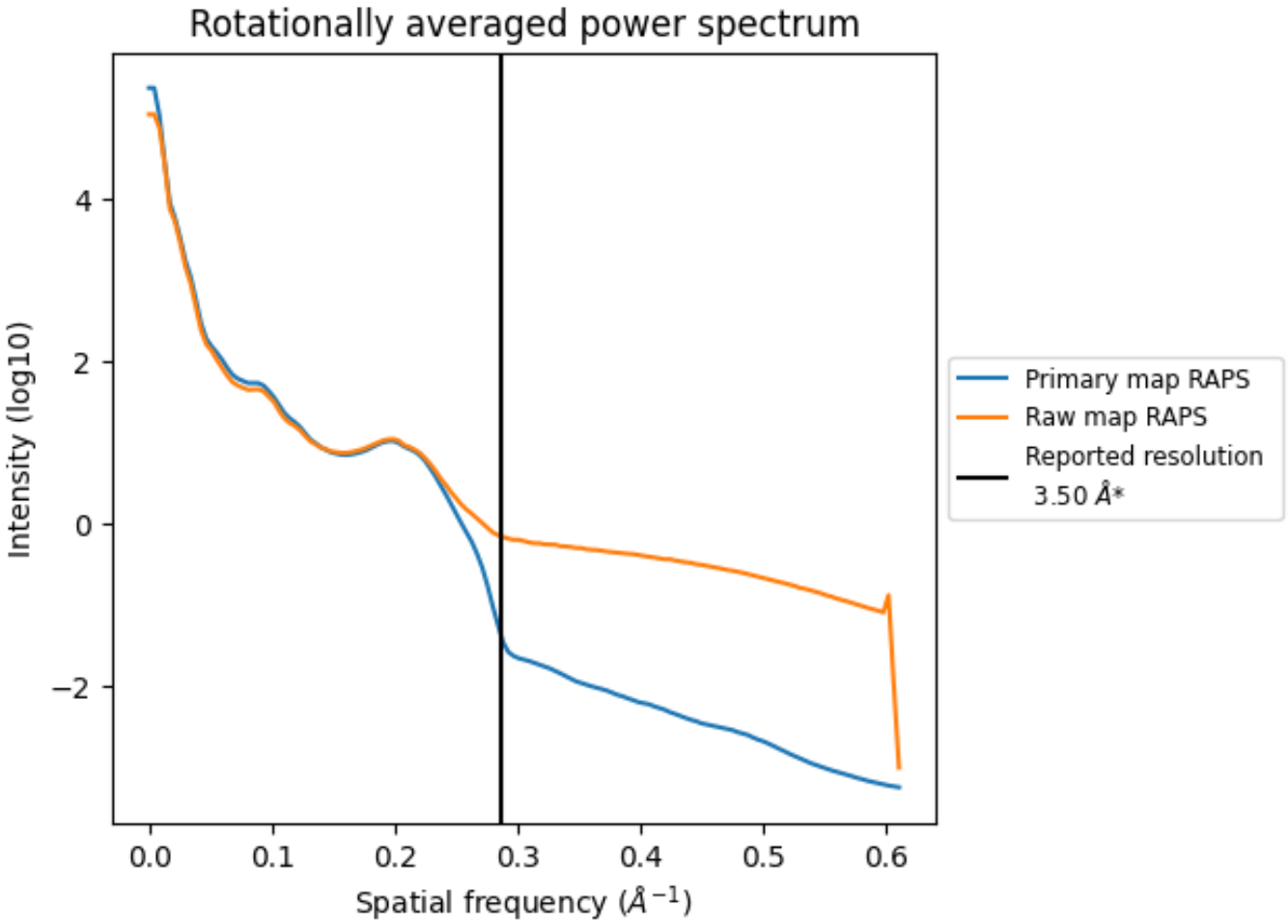
7.2 Volume estimate (i)



The volume at the recommended contour level is 134 nm^3; this corresponds to an approximate mass of 121 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)

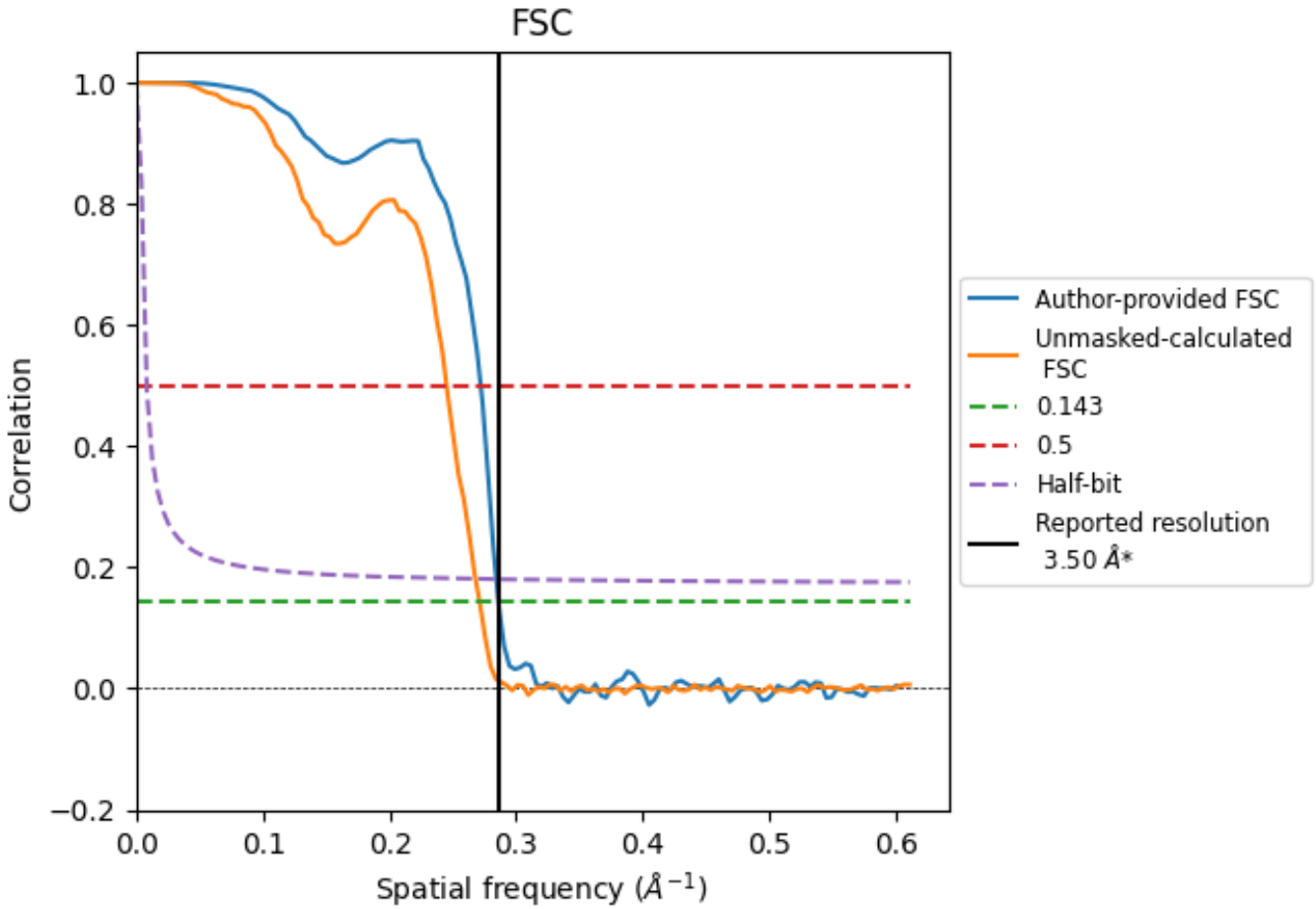


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

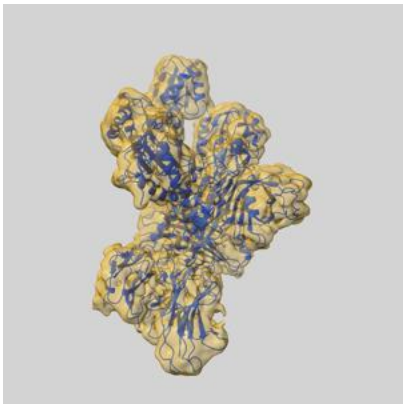
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	3.68	3.52
Unmasked-calculated*	3.69	4.08	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

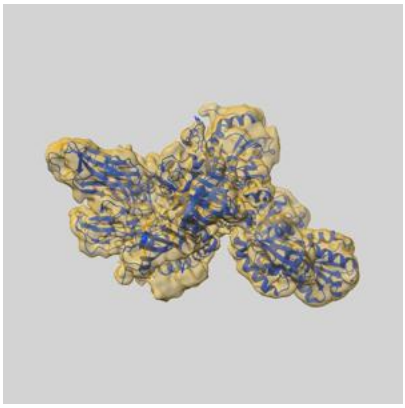
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55114 and PDB model 9SQP. Per-residue inclusion information can be found in section 3 on page 7.

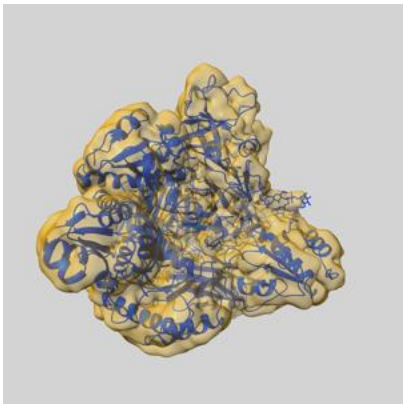
9.1 Map-model overlay



X



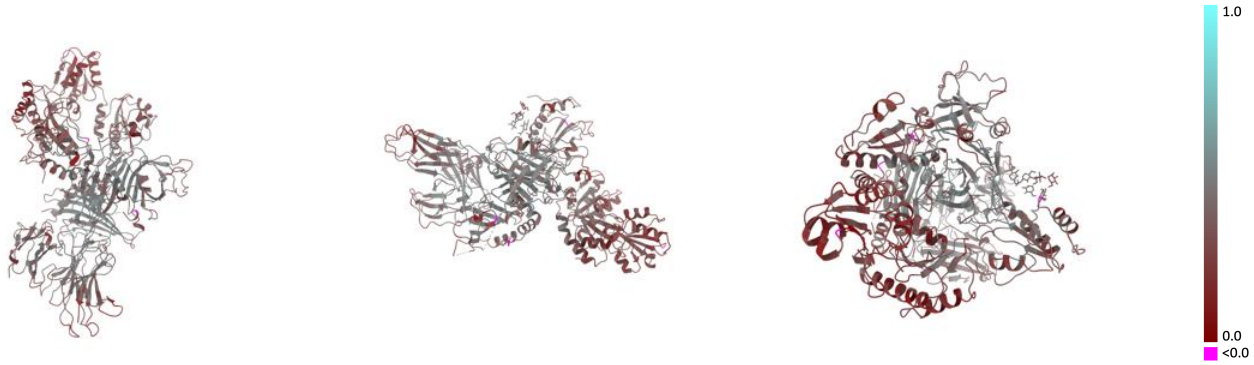
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

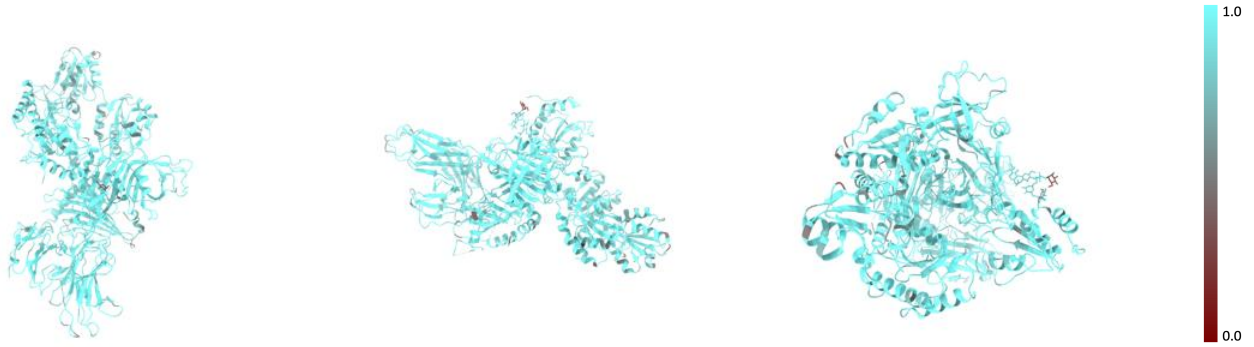
9.2 Q-score mapped to coordinate model (i)



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.

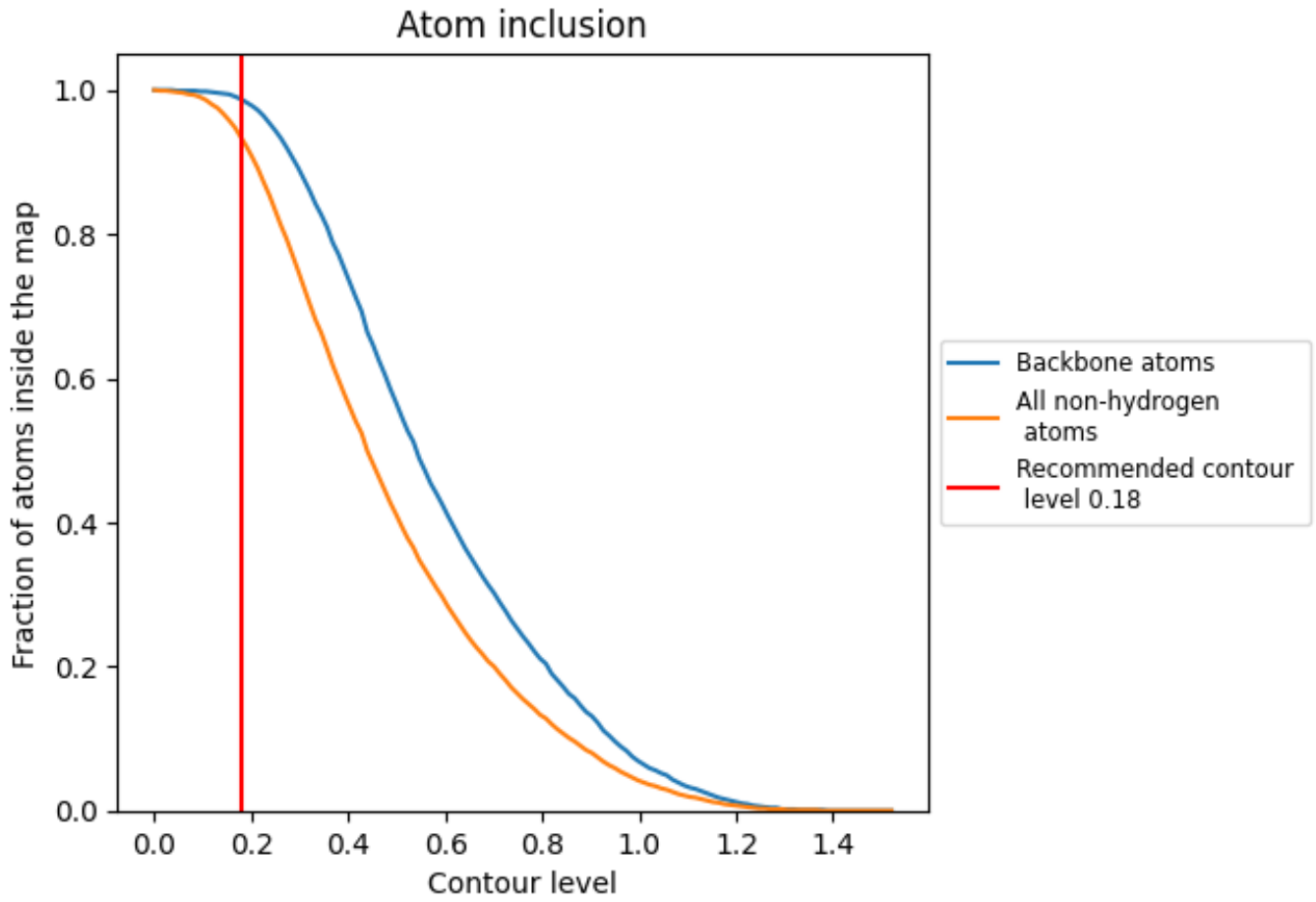
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.3620
A	0.9380	0.3970
B	0.9520	0.4210
C	0.7460	0.1120
D	0.9530	0.4170
E	0.9180	0.2920
F	0.7780	0.3880