wwPDB EM Validation Summary Report (i)

Sep 23, 2026 – 06:20 PM EDT

PDB ID	:	9N8Z / pdb_00009n8z
EMDB ID	:	EMD-49154
Title	:	Cryo EM Structure of Full Length mGluR8 Bound to Agonist L-AP4 and PAM VU6005649, class 2
Authors	:	Marx, D.C.; Levitz, J.T.
Deposited on	:	2025-02-10
Resolution	:	2.97 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

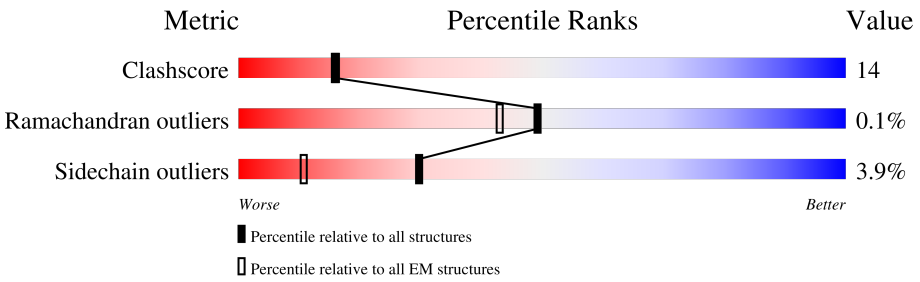
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

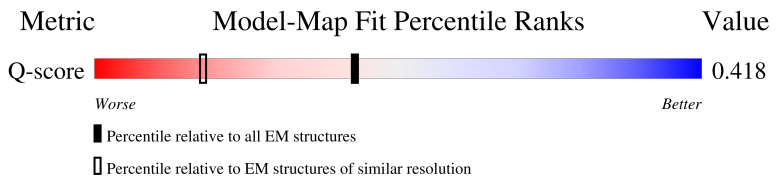
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	901	10% 59% 27% • 13%
1	B	901	5% 66% 19% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10501 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 Metabotropic glutamate receptor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	780	5243	3186	995	1035	27	0	0
1	B	772	5186	3160	976	1024	26	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP O00222
A	9	LYS	-	expression tag	UNP O00222
A	10	THR	-	expression tag	UNP O00222
A	11	ILE	-	expression tag	UNP O00222
A	12	ILE	-	expression tag	UNP O00222
A	13	ALA	-	expression tag	UNP O00222
A	14	LEU	-	expression tag	UNP O00222
A	15	SER	-	expression tag	UNP O00222
A	16	TYR	-	expression tag	UNP O00222
A	17	ILE	-	expression tag	UNP O00222
A	18	PHE	-	expression tag	UNP O00222
A	19	CYS	-	expression tag	UNP O00222
A	20	LEU	-	expression tag	UNP O00222
A	21	VAL	-	expression tag	UNP O00222
A	22	PHE	-	expression tag	UNP O00222
A	23	ALA	-	expression tag	UNP O00222
A	24	ASP	-	expression tag	UNP O00222
A	25	TYR	-	expression tag	UNP O00222
A	26	LYS	-	expression tag	UNP O00222
A	27	ASP	-	expression tag	UNP O00222
A	28	ASP	-	expression tag	UNP O00222
A	29	ASP	-	expression tag	UNP O00222
A	30	ASP	-	expression tag	UNP O00222
A	31	ALA	-	expression tag	UNP O00222
A	32	ALA	-	expression tag	UNP O00222
A	33	ALA	-	expression tag	UNP O00222

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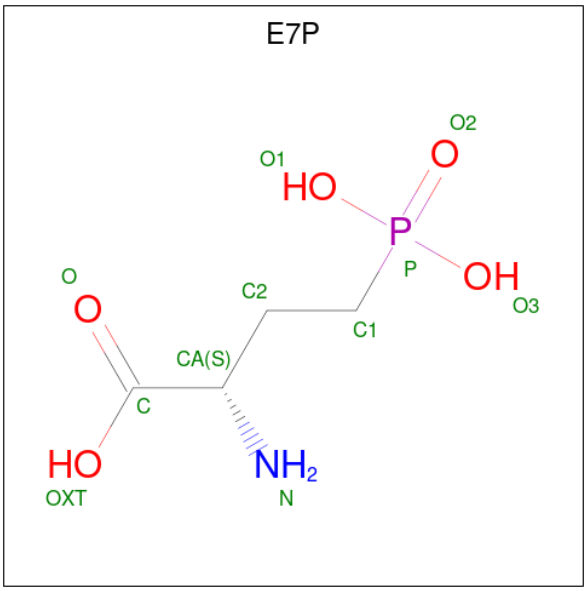
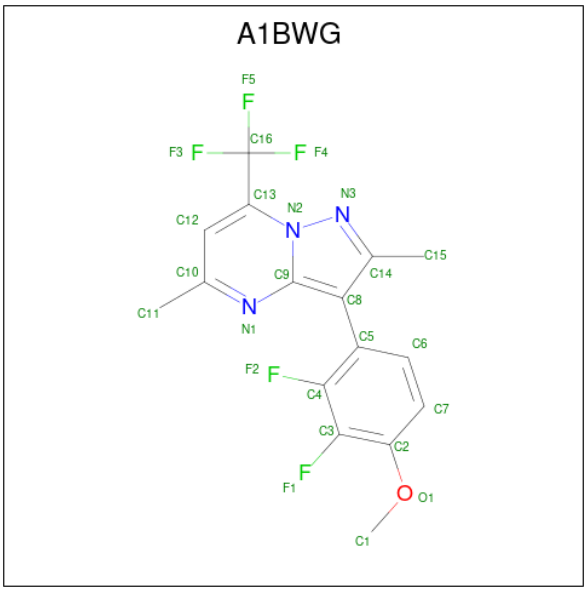
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	initiating methionine	UNP O00222
B	9	LYS	-	expression tag	UNP O00222
B	10	THR	-	expression tag	UNP O00222
B	11	ILE	-	expression tag	UNP O00222
B	12	ILE	-	expression tag	UNP O00222
B	13	ALA	-	expression tag	UNP O00222
B	14	LEU	-	expression tag	UNP O00222
B	15	SER	-	expression tag	UNP O00222
B	16	TYR	-	expression tag	UNP O00222
B	17	ILE	-	expression tag	UNP O00222
B	18	PHE	-	expression tag	UNP O00222
B	19	CYS	-	expression tag	UNP O00222
B	20	LEU	-	expression tag	UNP O00222
B	21	VAL	-	expression tag	UNP O00222
B	22	PHE	-	expression tag	UNP O00222
B	23	ALA	-	expression tag	UNP O00222
B	24	ASP	-	expression tag	UNP O00222
B	25	TYR	-	expression tag	UNP O00222
B	26	LYS	-	expression tag	UNP O00222
B	27	ASP	-	expression tag	UNP O00222
B	28	ASP	-	expression tag	UNP O00222
B	29	ASP	-	expression tag	UNP O00222
B	30	ASP	-	expression tag	UNP O00222
B	31	ALA	-	expression tag	UNP O00222
B	32	ALA	-	expression tag	UNP O00222
B	33	ALA	-	expression tag	UNP O00222

- Molecule 2 is (2S)-2-amino-4-phosphonobutanoic acid (CCD ID: E7P) (formula: $C_4H_{10}NO_5P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	11	4	1	5	1	0
			Total	C	N	O	P	
2	B	1	11	4	1	5	1	0

- Molecule 3 is (3P,8S)-3-(2,3-difluoro-4-methoxyphenyl)-2,5-dimethyl-7-(trifluoromethyl)pyrazolo[1,5-a]pyrimidine (CCD ID: A1BWG) (formula: $C_{16}H_{12}F_5N_3O$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
3	A	1	25	16	5	3	1	0

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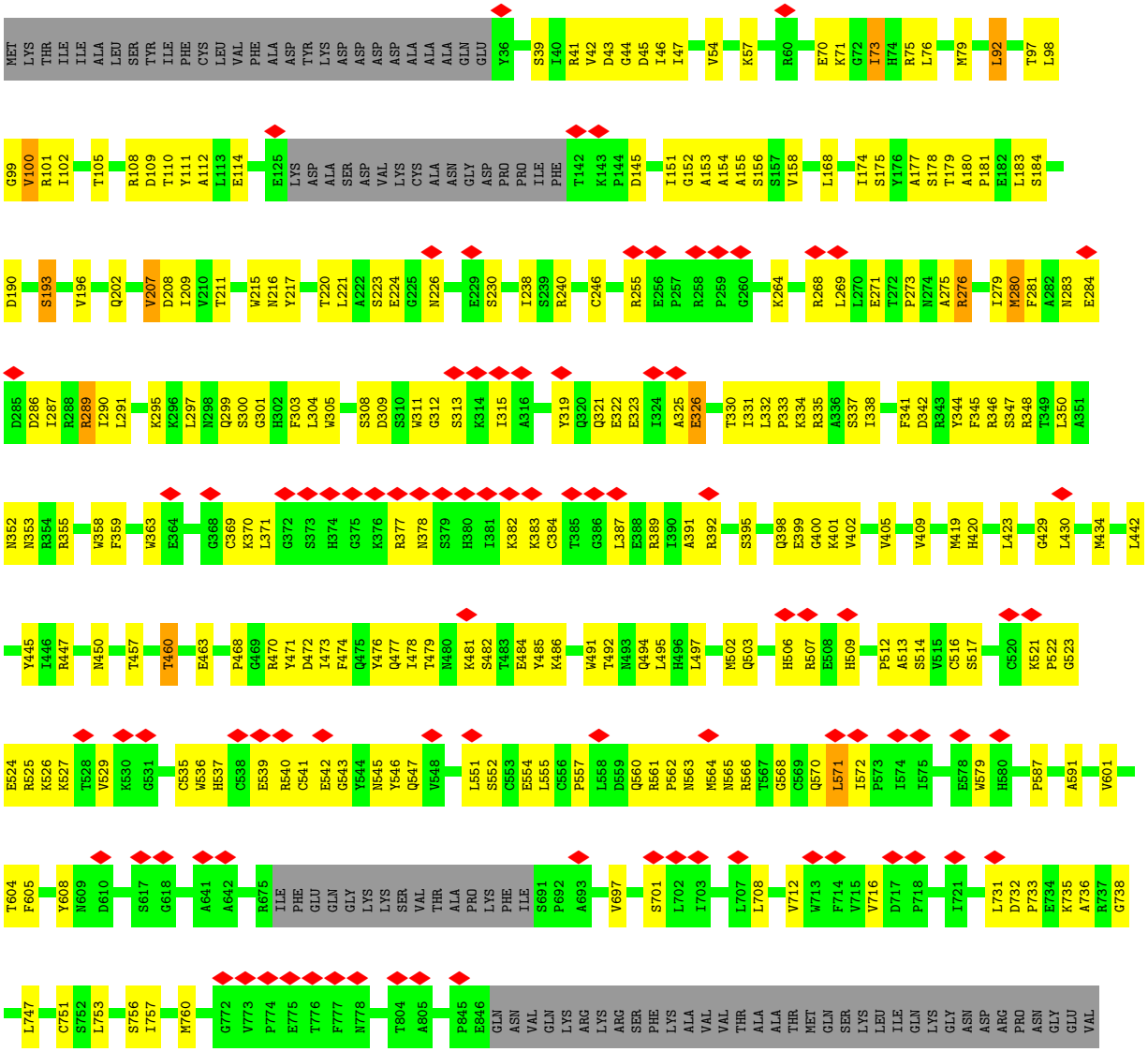
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
3	B	1	25	16	5	3	1	0

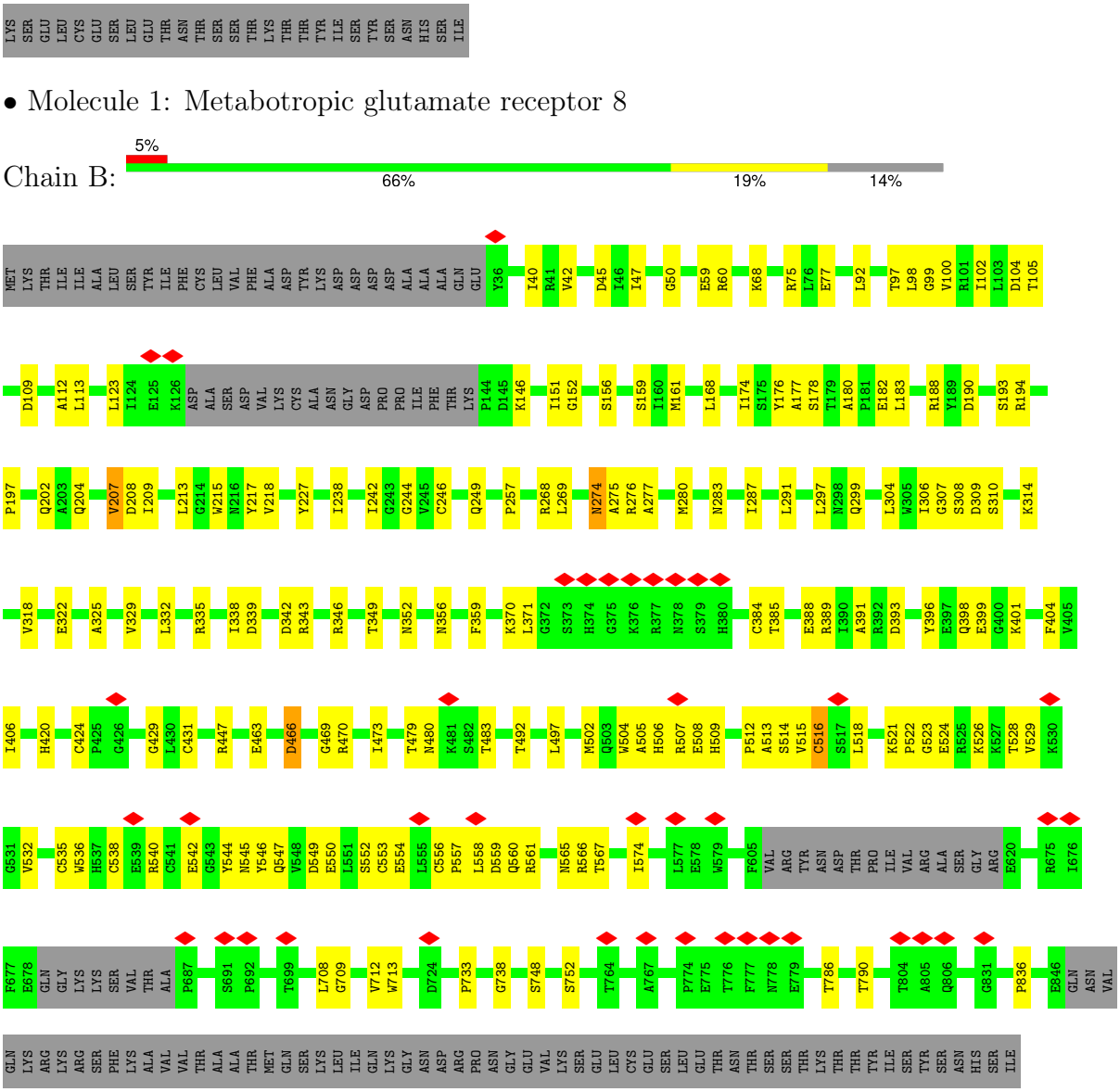
3 Residue-property plots (i)

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: Metabotropic glutamate receptor 8

Chain A:




LYS SER GLU LEU CYS GLU SER LEU GLU THR ASN THR SER SER THR LYS THR THR TYR ILE SER TYR SER ASN HIS SER ILE
• Molecule 1: Metabotropic glutamate receptor 8
Chain B:
5%
66%
19%
14%
MET LYS THR ILE ILE ALA LEU SER TYR ILE PHE CYS LEU VAL PHE ALA ASP TYR LYS ASP ASP ASP ALA ALA ALA GLN GLU Y36 I40 R41 V42 D45 I46 I47 G50 E59 R60 K68 R75 L76 E77 L92 T97 L98 G99 V100 R101 I102 L103 D104 T105
D109 A112 L113 L123 I124 E125 K126 ASP ALA SER ASP VAL LYS CYS ALA ASN GLY ASP PRO PRO ILE PHE THR LYS P144 D145 K146 I151 G152 S156 S159 I160 M161 L168 I174 S175 Y176 A177 S178 T179 A180 P181 E182 L183 R188 Y189 D190 S193 R194
P197 Q202 A203 Q204 V207 D208 I209 L213 G214 W215 N216 Y217 V218 Y227 I238 I242 G243 G244 V245 C246 Q249 P257 R268 L269 N274 A275 R276 A277 M280 N283 I287 L291 L297 N298 Q299 L304 W305 I306 G307 S308 D309 S310 K314
V318 E322 A325 V329 L332 R335 I338 D339 D342 R343 R346 T349 N352 N356 F359 K370 L371 G372 S373 H374 G375 K376 R377 N378 S379 H380 C384 T385 E388 R389 I390 A391 R392 D393 Y396 E397 Q398 E399 G400 K401 F404 V405
I406 H420 C424 P425 G426 G429 L430 C431 R447 E463 D466 G469 R470 I473 T479 N480 K481 S482 T483 T492 L497 M502 Q503 W504 A505 H506 R507 E508 H509 P512 A513 S514 V515 C516 S517 L518 K521 P522 G523 E524 R525 K526 K527 T528 V529 K530
G531 V532 C535 W536 H537 C538 E539 R540 C541 E542 G543 Y544 N545 Y546 Q547 V548 D549 E550 L551 S552 C553 E554 L555 C556 P557 L558 D559 Q560 R561 N565 R566 T567 I574 L577 E578 W579 F605 VAL ARG TYR ASN ASP THR PRO ILE ILE VAL ARG ALA SER GLY ARG E620 R675 I676
F677 E678 GLN GLY LYS LYS SER VAL THR ALA P687 S691 P692 T699 L708 G709 V712 W713 D724 P733 G738 S748 S752 T764 A767 P774 E775 T776 F777 W778 E779 T786 T790 T804 A805 Q806 G831 P836 E846 GLN ASN VAL
GLN LYS ARG LYS ARG SER PHE LYS ALA VAL VAL THR ALA ALA THR MET GLN SER LYS LEU ILE GLN LYS GLY ASN ASP ARG PRO ASN GLY GLU VAL LYS SER GLU LEU CYS GLU SER LEU GLU THR ASN THR SER SER THR LYS THR THR TYR ILE SER TYR SER ASN HIS SER ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298102	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 ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.396	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.265	Depositor
Map size (Å)	343.19998, 343.19998, 343.19998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8249999, 0.8249999, 0.8249999	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: E7P, A1BWG

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	0.16	0/5341	0.28	0/7132
1	B	0.21	0/5281	0.27	0/7063
All	All	0.19	0/10622	0.27	0/14195

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	5243	0	4452	167	0
1	B	5186	0	4391	115	0
2	A	11	0	0	2	0
2	B	11	0	0	3	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
All	All	10501	0	8843	279	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 14.

The worst 5 of 279 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:477:GLN:HE22	1:A:503:GLN:HB3	1.48	0.77
1:A:75:ARG:NH1	2:A:1001:E7P:O3	2.19	0.75
1:A:152:GLY:HA3	1:A:175:SER:HA	1.70	0.74
1:A:524:GLU:O	1:A:547:GLN:NE2	2.23	0.72
1:A:541:CYS:HB3	1:A:545:ASN:HB3	1.71	0.71

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	774/901 (86%)	720 (93%)	54 (7%)	0	100	100
1	B	764/901 (85%)	710 (93%)	53 (7%)	1 (0%)	48	78
All	All	1538/1802 (85%)	1430 (93%)	107 (7%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	836	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/779 (59%)	441 (95%)	22 (5%)	23	55
1	B	454/779 (58%)	440 (97%)	14 (3%)	35	66
All	All	917/1558 (59%)	881 (96%)	36 (4%)	30	60

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	VAL
1	B	516	CYS
1	B	385	THR
1	B	483	THR
1	A	290	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	B	226	ASN
1	B	366	ASN
1	A	274	ASN
1	A	249	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	$\#\|Z\| > 2$
2	E7P	B	1002	-	9,10,10	2.33	1 (11%)	10,14,14	2.18	1 (10%)
2	E7P	A	1001	-	9,10,10	2.51	1 (11%)	10,14,14	2.04	1 (10%)
3	A1BWG	B	1001	-	27,27,27	1.53	3 (11%)	39,42,42	2.09	13 (33%)
3	A1BWG	A	1002	-	27,27,27	1.55	4 (14%)	39,42,42	2.13	13 (33%)

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
2	E7P	B	1002	-	-	0/10/10/10	-
2	E7P	A	1001	-	-	3/10/10/10	-
3	A1BWG	B	1001	-	-	5/12/12/12	0/3/3/3
3	A1BWG	A	1002	-	-	2/12/12/12	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	E7P	P-C1	6.73	1.86	1.78
2	B	1002	E7P	P-C1	5.94	1.85	1.78
3	A	1002	A1BWG	C9-N2	-4.52	1.31	1.38
3	B	1001	A1BWG	C9-N2	-4.46	1.31	1.38
3	B	1001	A1BWG	C9-N1	2.39	1.39	1.34

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	E7P	P-C1-C2	-6.15	107.39	114.93
2	A	1001	E7P	P-C1-C2	-5.56	108.11	114.93
3	B	1001	A1BWG	O1-C2-C3	5.18	120.21	116.28
3	A	1002	A1BWG	C9-N1-C10	5.05	120.27	116.83
3	A	1002	A1BWG	O1-C2-C3	4.96	120.04	116.28

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	E7P	P-C1-C2-CA
2	A	1001	E7P	C1-C2-CA-C
2	A	1001	E7P	C1-C2-CA-N
3	A	1002	A1BWG	C3-C2-O1-C1
3	B	1001	A1BWG	C3-C2-O1-C1

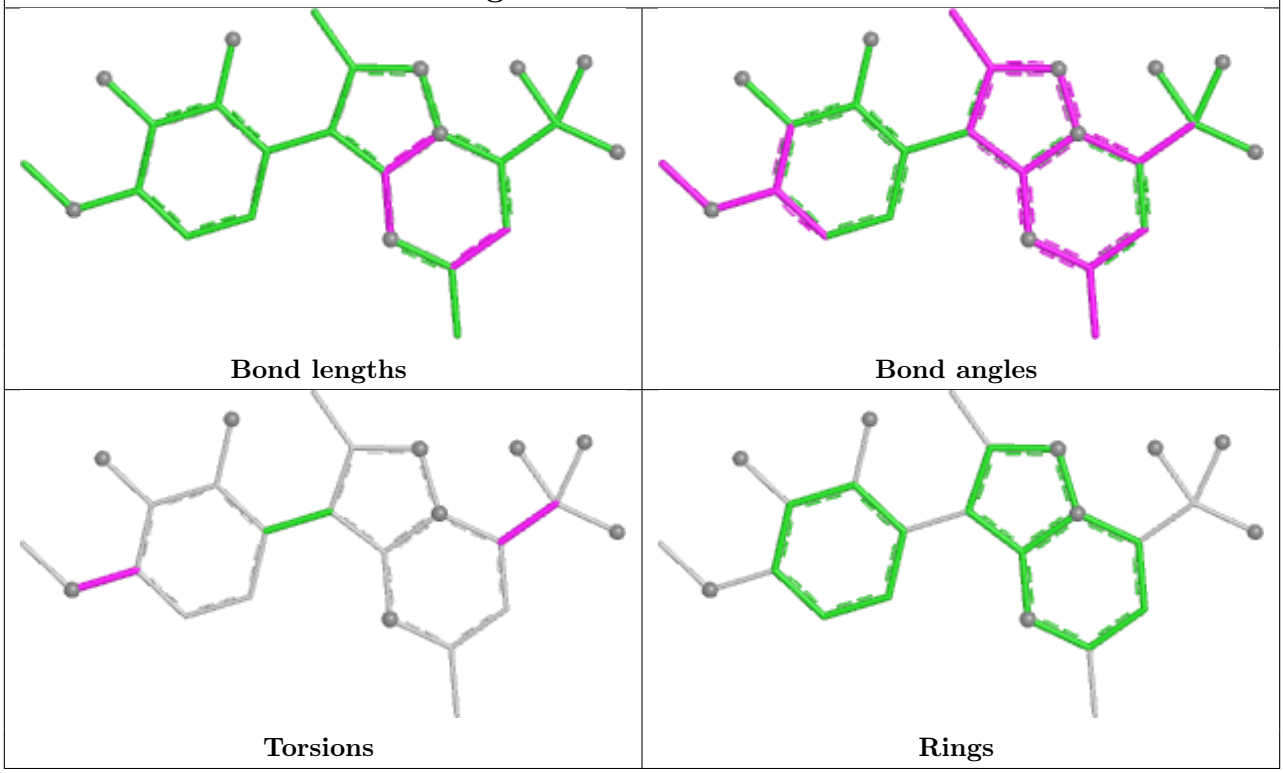
There are no ring outliers.

2 monomers are involved in 5 short contacts:

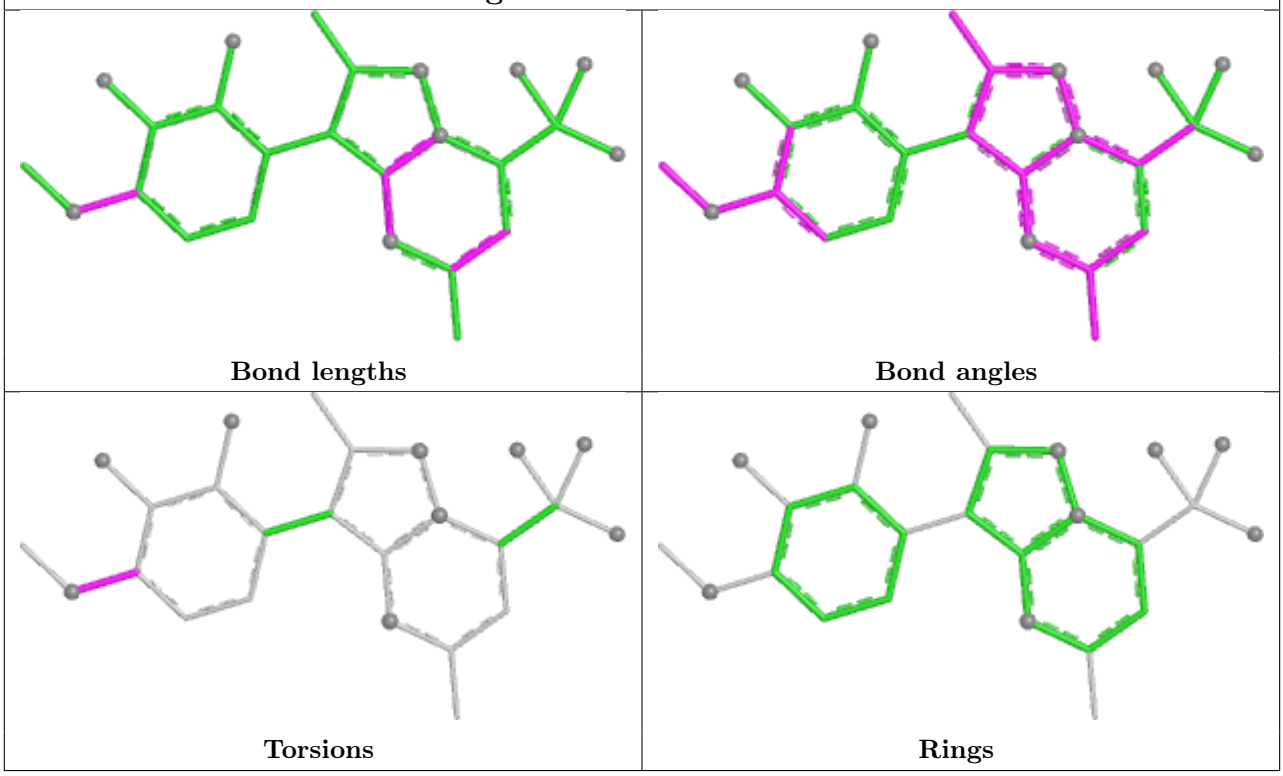
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	E7P	3	0
2	A	1001	E7P	2	0

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 A1BWG B 1001



Ligand A1BWG A 1002



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.

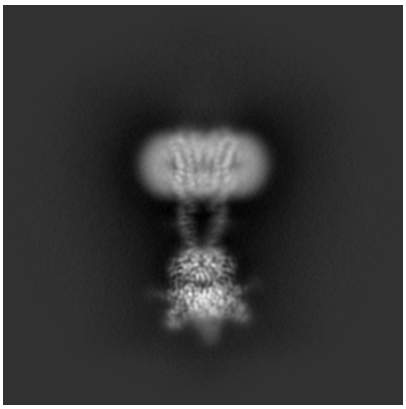
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-49154. These allow visual inspection of the internal detail of the map and identification of artifacts.

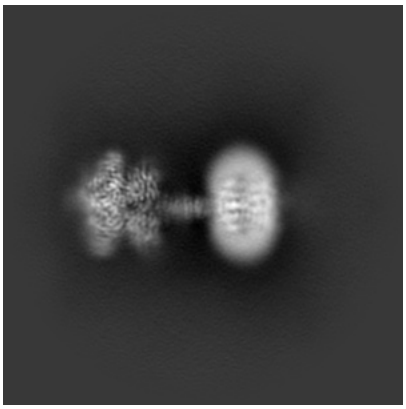
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

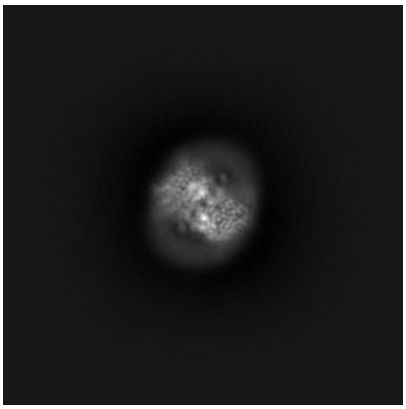
6.1.1 Primary map



X

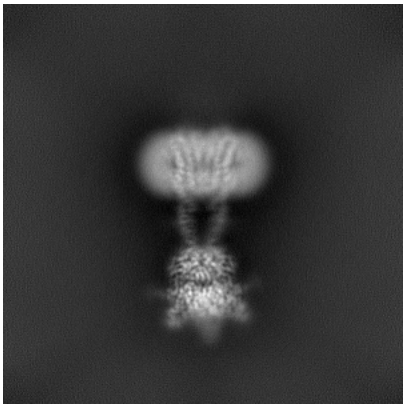


Y

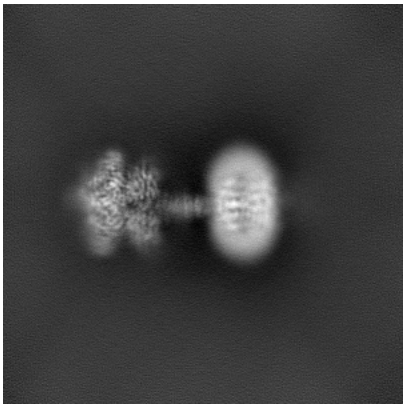


Z

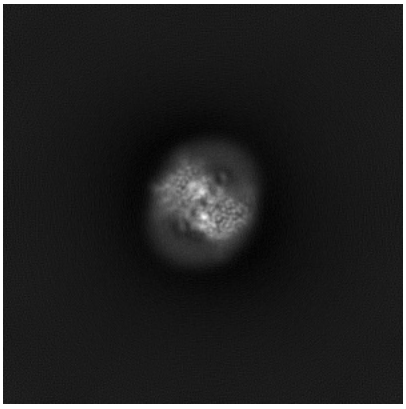
6.1.2 Raw map



X



Y

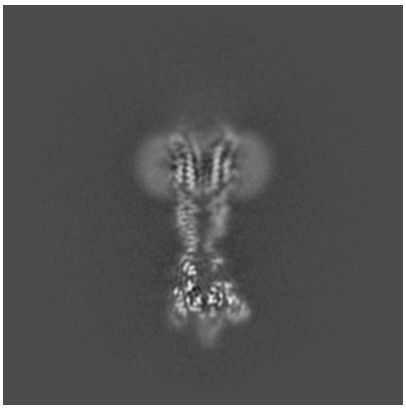


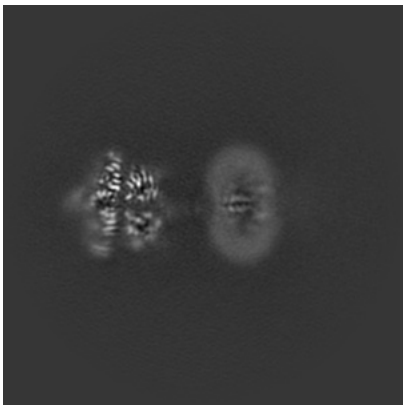
Z

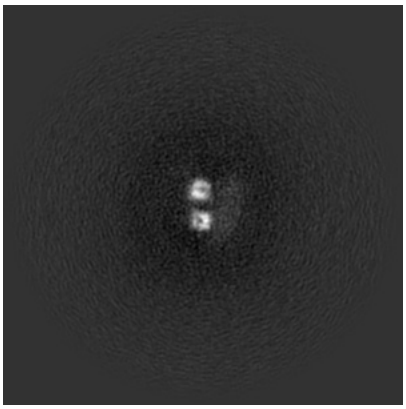
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

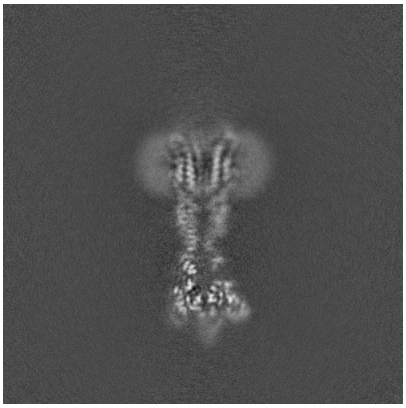
6.2.1 Primary map

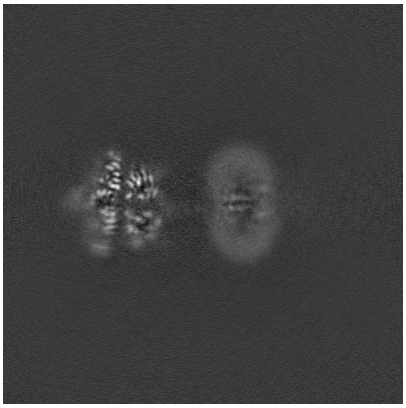

X Index: 208

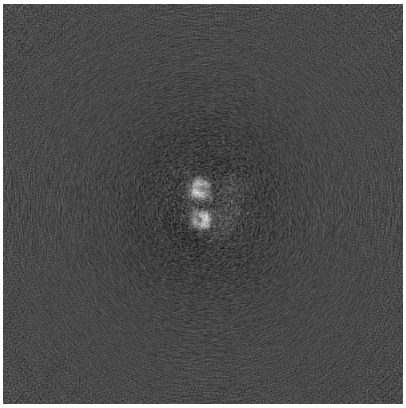

Y Index: 208


Z Index: 208

6.2.2 Raw map


X Index: 208

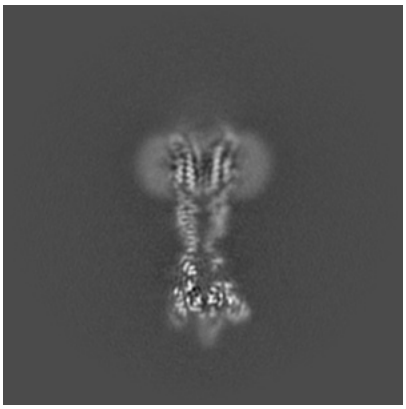

Y Index: 208

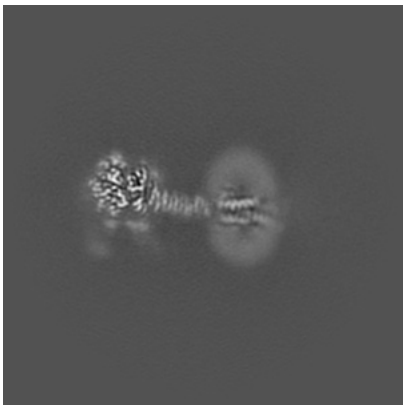

Z Index: 208

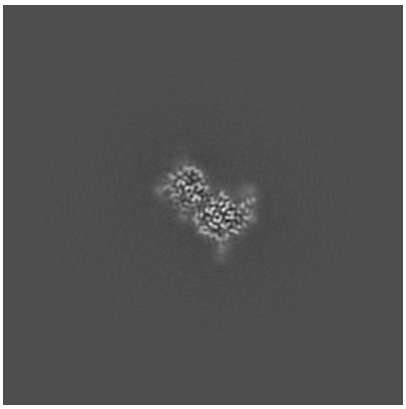
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

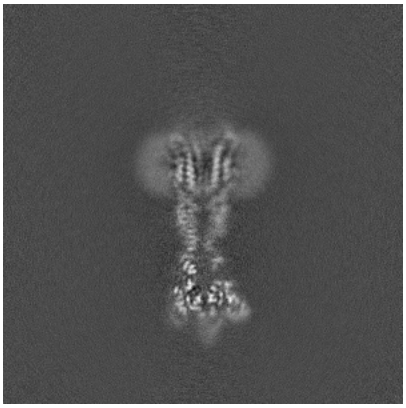
6.3.1 Primary map

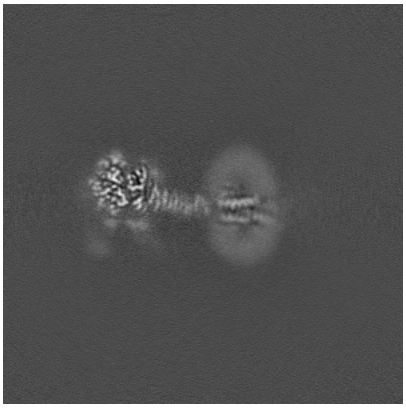

X Index: 208

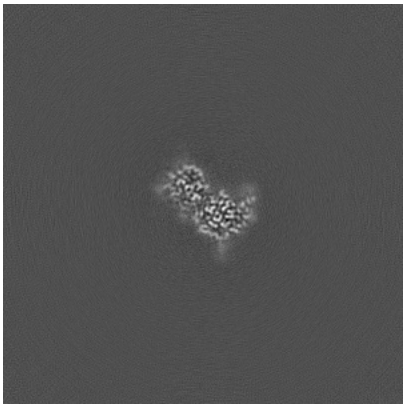

Y Index: 194


Z Index: 116

6.3.2 Raw map


X Index: 208

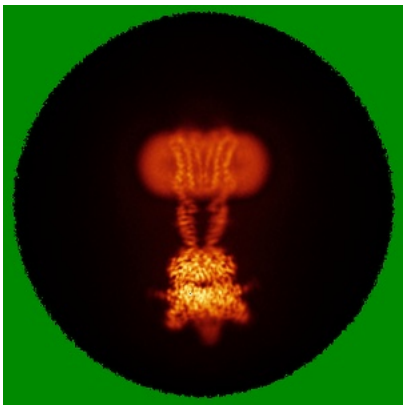

Y Index: 194

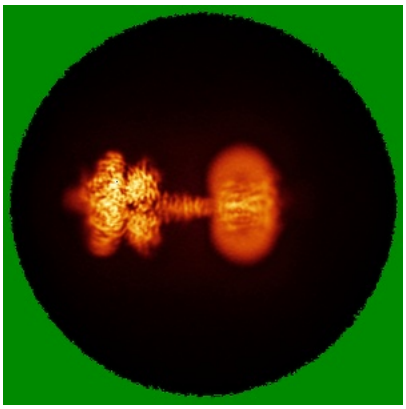

Z Index: 116

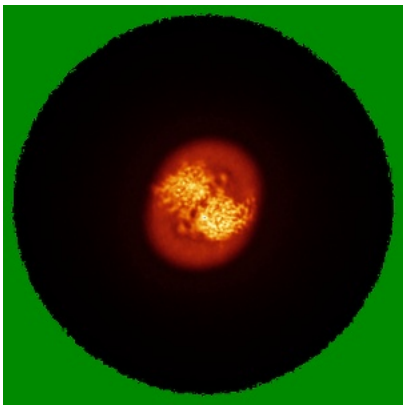
The images above show the largest variance slices of the map in three orthogonal directions.

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

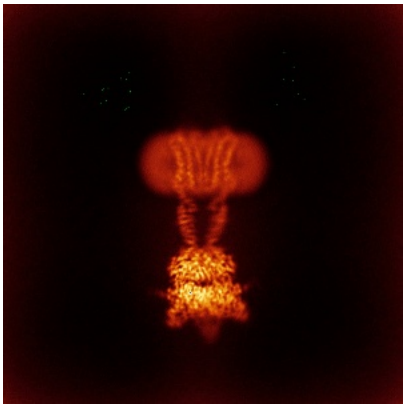
6.4.1 Primary map

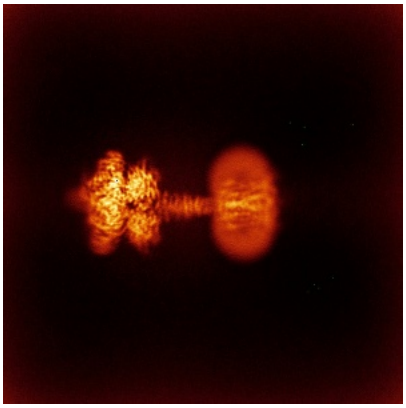

X

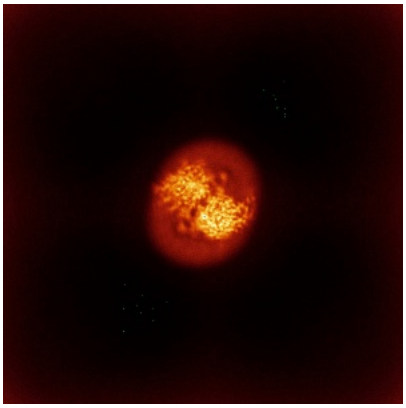

Y


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 0.265. 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.

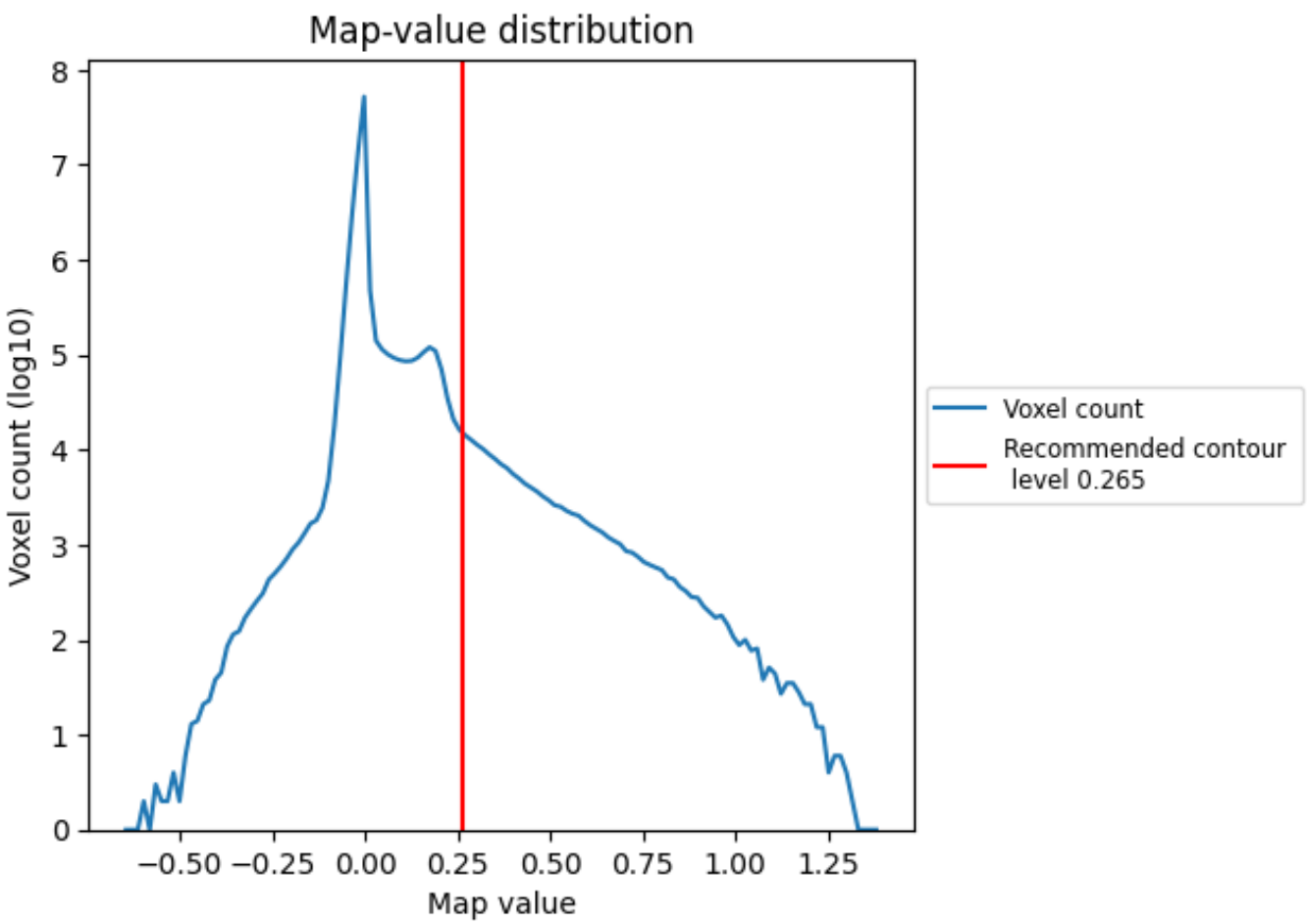
6.6 Mask visualisation (i)

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

7 Map analysis (i)

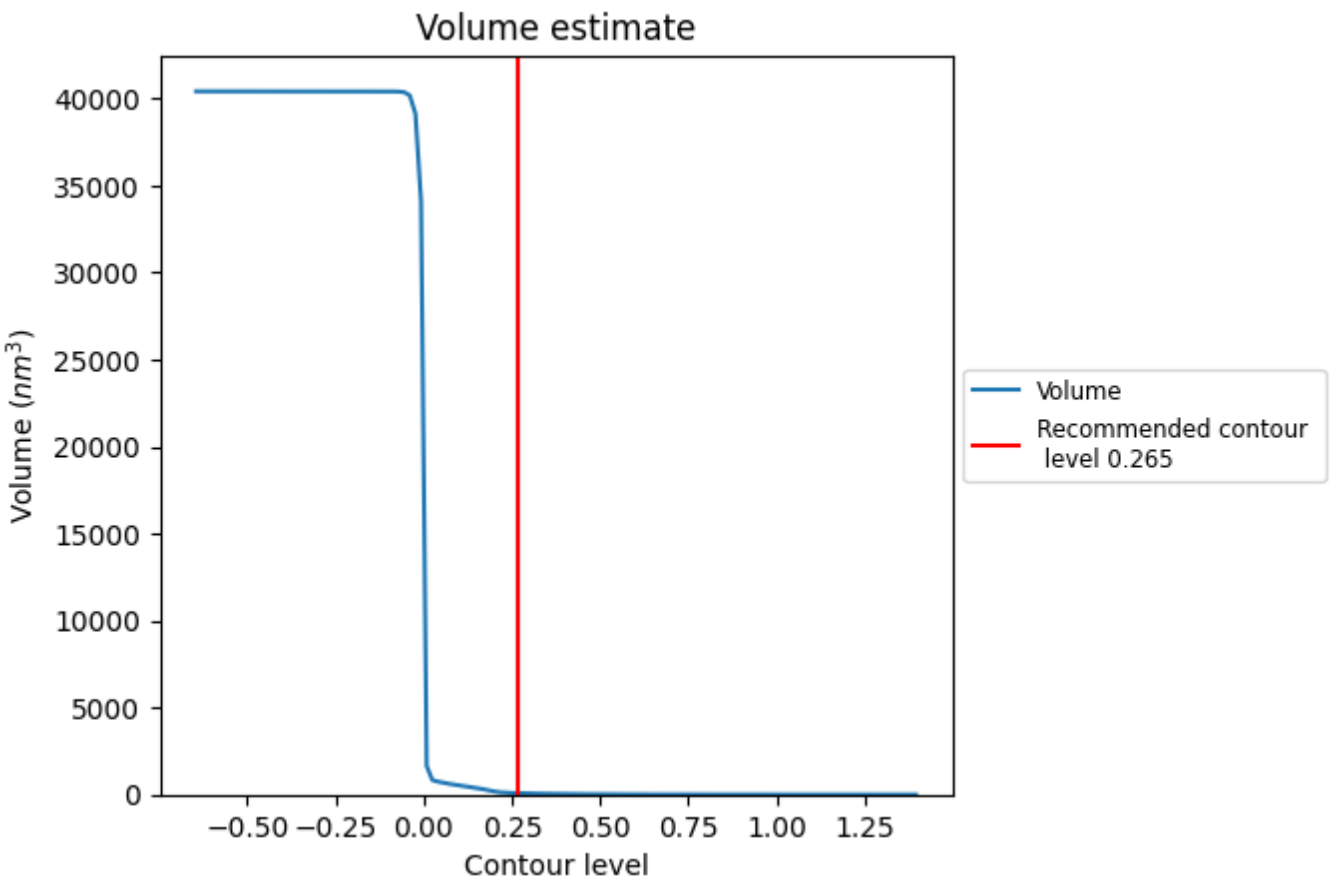
This section contains the results of statistical analysis of the map.

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.

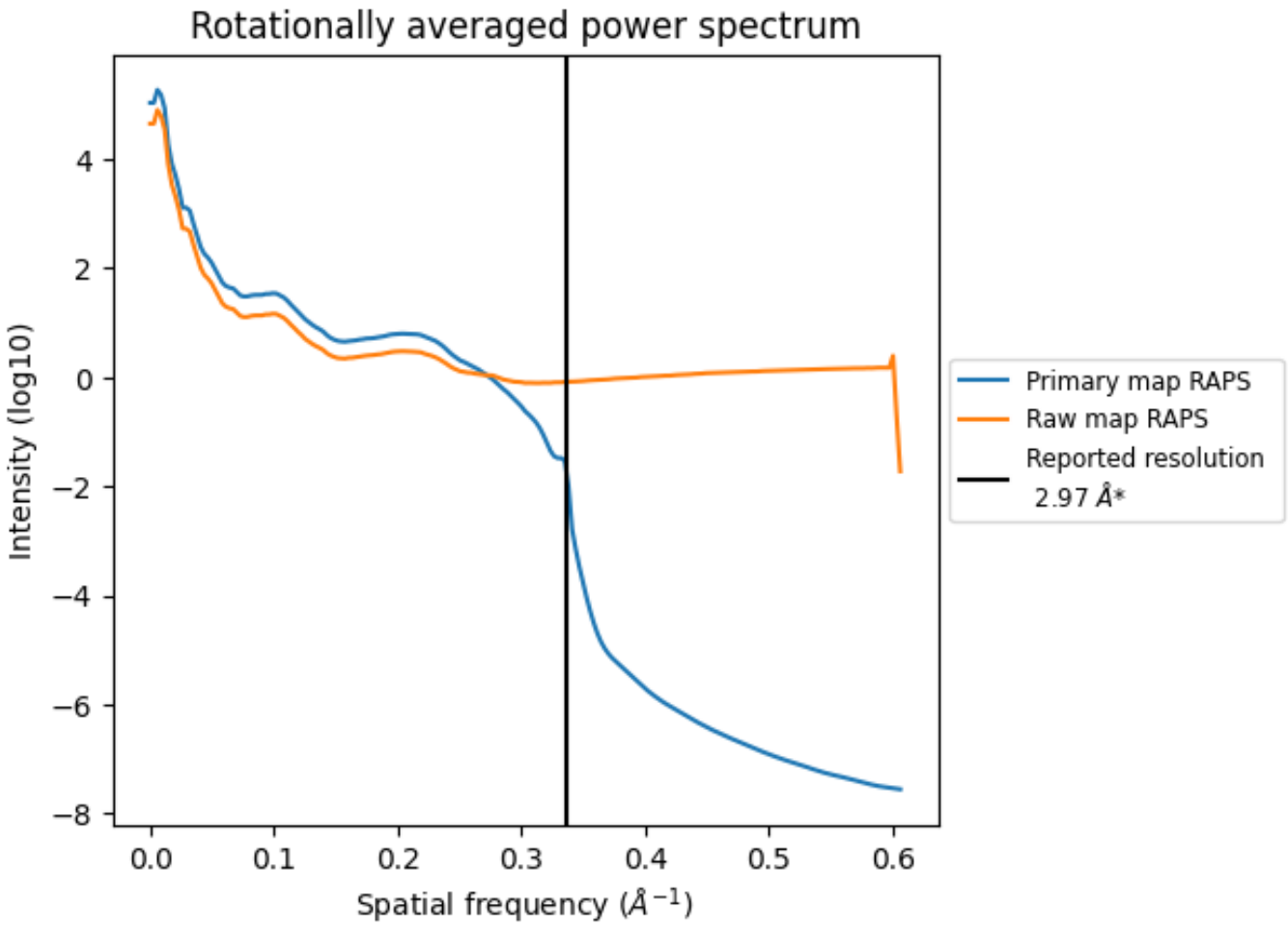
7.2 Volume estimate (i)



The volume at the recommended contour level is 80 nm^3; this corresponds to an approximate mass of 72 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)

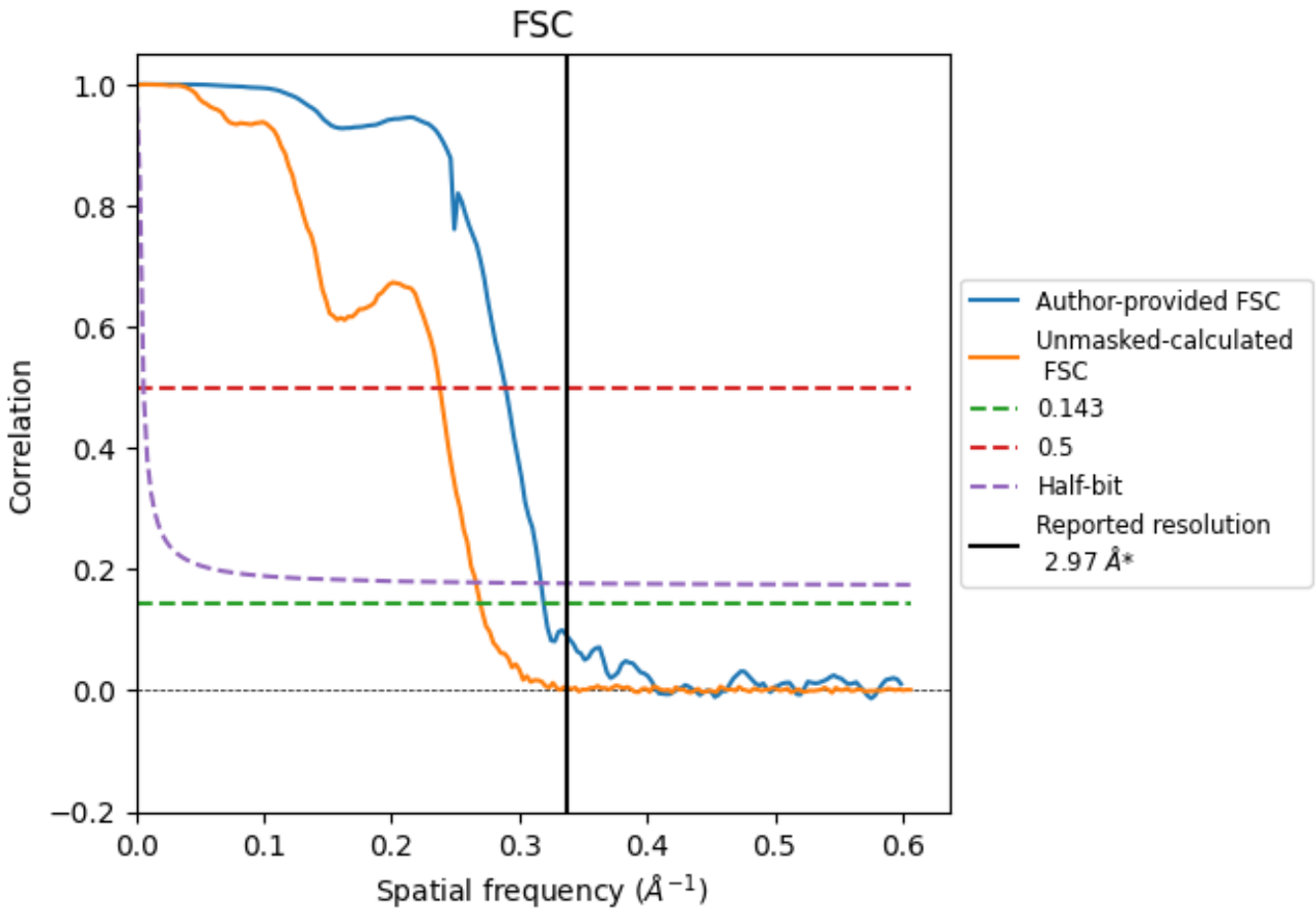


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

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 0.337 Å^{-1}

8.2 Resolution estimates (i)

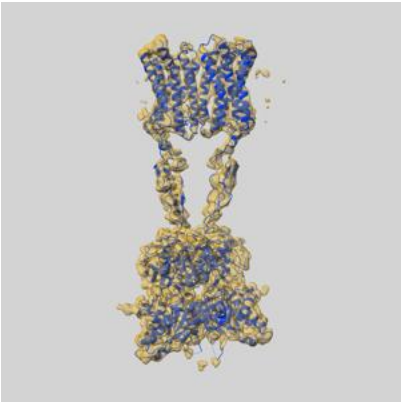
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	3.13	3.46	3.15
Unmasked-calculated*	3.71	4.21	3.76

*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 3.71 differs from the reported value 2.97 by more than 10 %

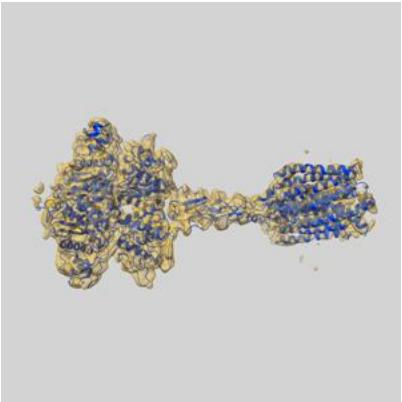
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-49154 and PDB model 9N8Z. Per-residue inclusion information can be found in section 3 on page 7.

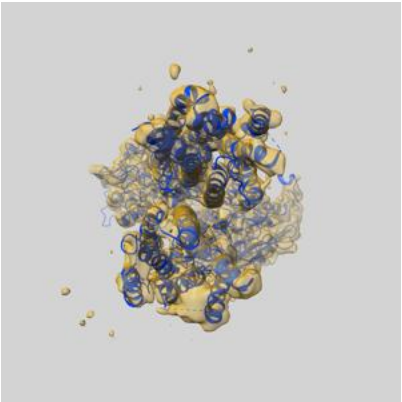
9.1 Map-model overlay (i)



X



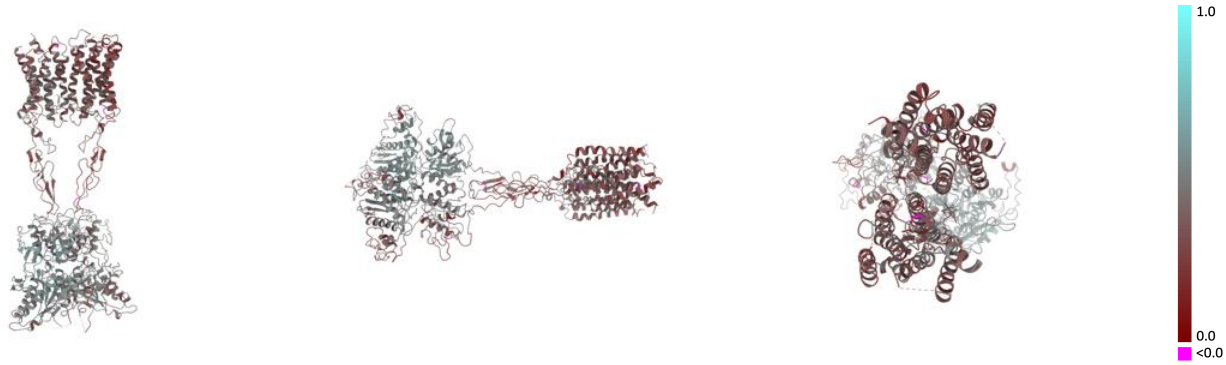
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.265 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.

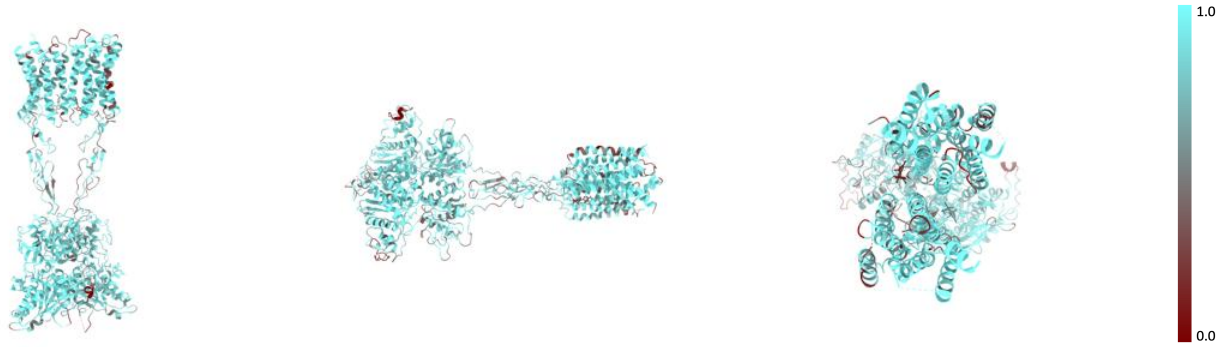
9.2 Q-score mapped to coordinate model (i)



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.

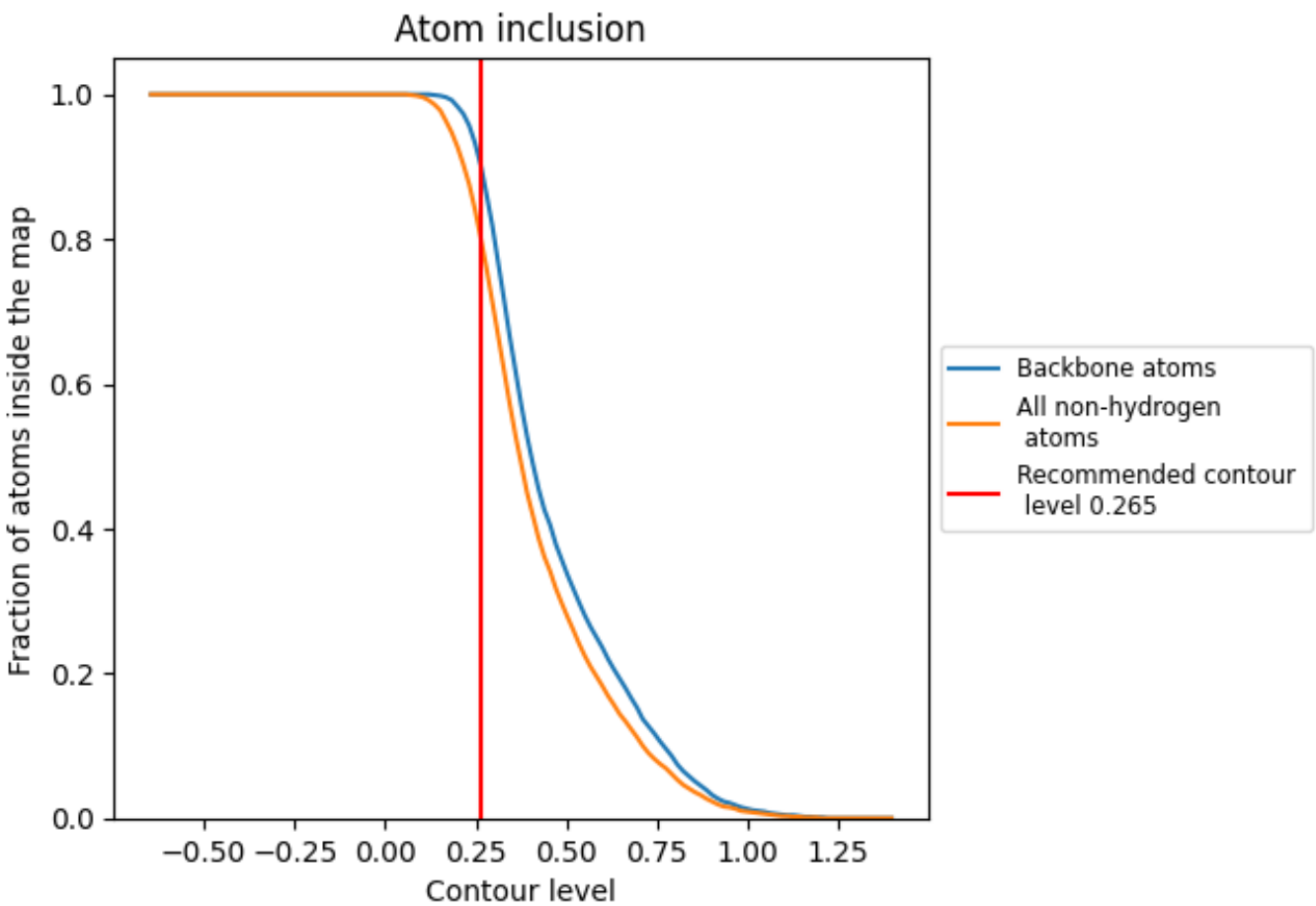
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.265).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.4180
A	0.7500	0.3750
B	0.8470	0.4600