



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 10:30 AM EST

PDB ID : 8DK3
EMDB ID : EMD-27482
Title : CryoEM structure of Pseudomonas aeruginosa PA14 JetC ATPase domain bound to DNA and cWHD domain of JetA
Authors : Deep, A.; Gu, Y.; Gao, Y.; Ego, K.; Herzik, M.; Zhou, H.; Corbett, K.
Deposited on : 2022-07-01
Resolution : 3.28 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

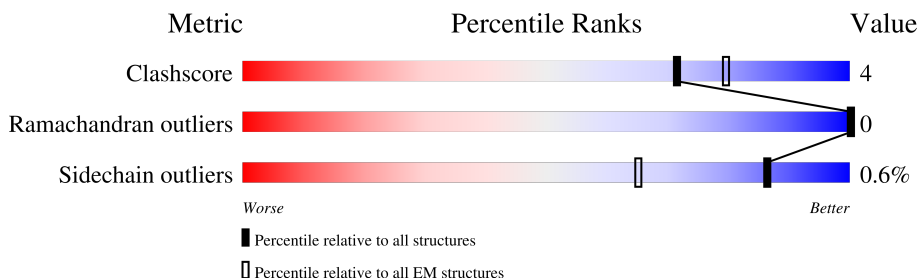
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1119	
1	B	1119	
2	C	517	
3	P	26	
4	Q	26	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8905 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 JetC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	455	Total	C	N	O	S	0	0
			3530	2208	643	669	10		
1	B	450	Total	C	N	O	S	0	0
			3494	2185	639	660	10		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A8G4Z850
A	-16	LYS	-	expression tag	UNP A0A8G4Z850
A	-15	SER	-	expression tag	UNP A0A8G4Z850
A	-14	SER	-	expression tag	UNP A0A8G4Z850
A	-13	HIS	-	expression tag	UNP A0A8G4Z850
A	-12	HIS	-	expression tag	UNP A0A8G4Z850
A	-11	HIS	-	expression tag	UNP A0A8G4Z850
A	-10	HIS	-	expression tag	UNP A0A8G4Z850
A	-9	HIS	-	expression tag	UNP A0A8G4Z850
A	-8	HIS	-	expression tag	UNP A0A8G4Z850
A	-7	GLU	-	expression tag	UNP A0A8G4Z850
A	-6	ASN	-	expression tag	UNP A0A8G4Z850
A	-5	LEU	-	expression tag	UNP A0A8G4Z850
A	-4	TYR	-	expression tag	UNP A0A8G4Z850
A	-3	PHE	-	expression tag	UNP A0A8G4Z850
A	-2	GLN	-	expression tag	UNP A0A8G4Z850
A	-1	SER	-	expression tag	UNP A0A8G4Z850
A	0	ASN	-	expression tag	UNP A0A8G4Z850
A	1	ALA	-	expression tag	UNP A0A8G4Z850
A	1022	GLN	GLU	conflict	UNP A0A8G4Z850
B	-17	MET	-	initiating methionine	UNP A0A8G4Z850
B	-16	LYS	-	expression tag	UNP A0A8G4Z850
B	-15	SER	-	expression tag	UNP A0A8G4Z850
B	-14	SER	-	expression tag	UNP A0A8G4Z850
B	-13	HIS	-	expression tag	UNP A0A8G4Z850
B	-12	HIS	-	expression tag	UNP A0A8G4Z850

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A8G4Z850
B	-10	HIS	-	expression tag	UNP A0A8G4Z850
B	-9	HIS	-	expression tag	UNP A0A8G4Z850
B	-8	HIS	-	expression tag	UNP A0A8G4Z850
B	-7	GLU	-	expression tag	UNP A0A8G4Z850
B	-6	ASN	-	expression tag	UNP A0A8G4Z850
B	-5	LEU	-	expression tag	UNP A0A8G4Z850
B	-4	TYR	-	expression tag	UNP A0A8G4Z850
B	-3	PHE	-	expression tag	UNP A0A8G4Z850
B	-2	GLN	-	expression tag	UNP A0A8G4Z850
B	-1	SER	-	expression tag	UNP A0A8G4Z850
B	0	ASN	-	expression tag	UNP A0A8G4Z850
B	1	ALA	-	expression tag	UNP A0A8G4Z850
B	1022	GLN	GLU	conflict	UNP A0A8G4Z850

- Molecule 2 is a protein called JetA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	94	751	481	123	146	1	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	initiating methionine	UNP A0A0H2ZJP9
C	-16	LYS	-	expression tag	UNP A0A0H2ZJP9
C	-15	SER	-	expression tag	UNP A0A0H2ZJP9
C	-14	SER	-	expression tag	UNP A0A0H2ZJP9
C	-13	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-12	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-11	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-10	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-9	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-8	HIS	-	expression tag	UNP A0A0H2ZJP9
C	-7	GLU	-	expression tag	UNP A0A0H2ZJP9
C	-6	ASN	-	expression tag	UNP A0A0H2ZJP9
C	-4	TYR	TRP	conflict	UNP A0A0H2ZJP9
C	-3	PHE	LYS	conflict	UNP A0A0H2ZJP9
C	-2	GLN	VAL	conflict	UNP A0A0H2ZJP9
C	-1	SER	ALA	conflict	UNP A0A0H2ZJP9
C	0	ASN	ALA	conflict	UNP A0A0H2ZJP9
C	1	ALA	MET	conflict	UNP A0A0H2ZJP9

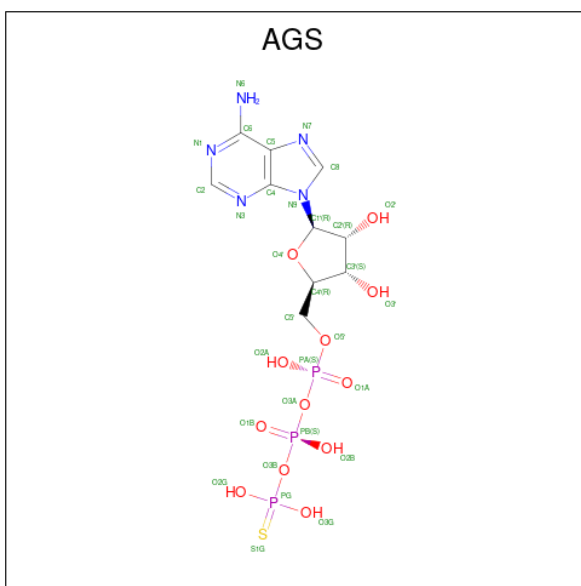
- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	26	520	260	52	182	26	0	0

- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	Q	26	546	260	130	130	26	0	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
5	A	1	31	10	5	12	3	1	0
5	B	1	31	10	5	12	3	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

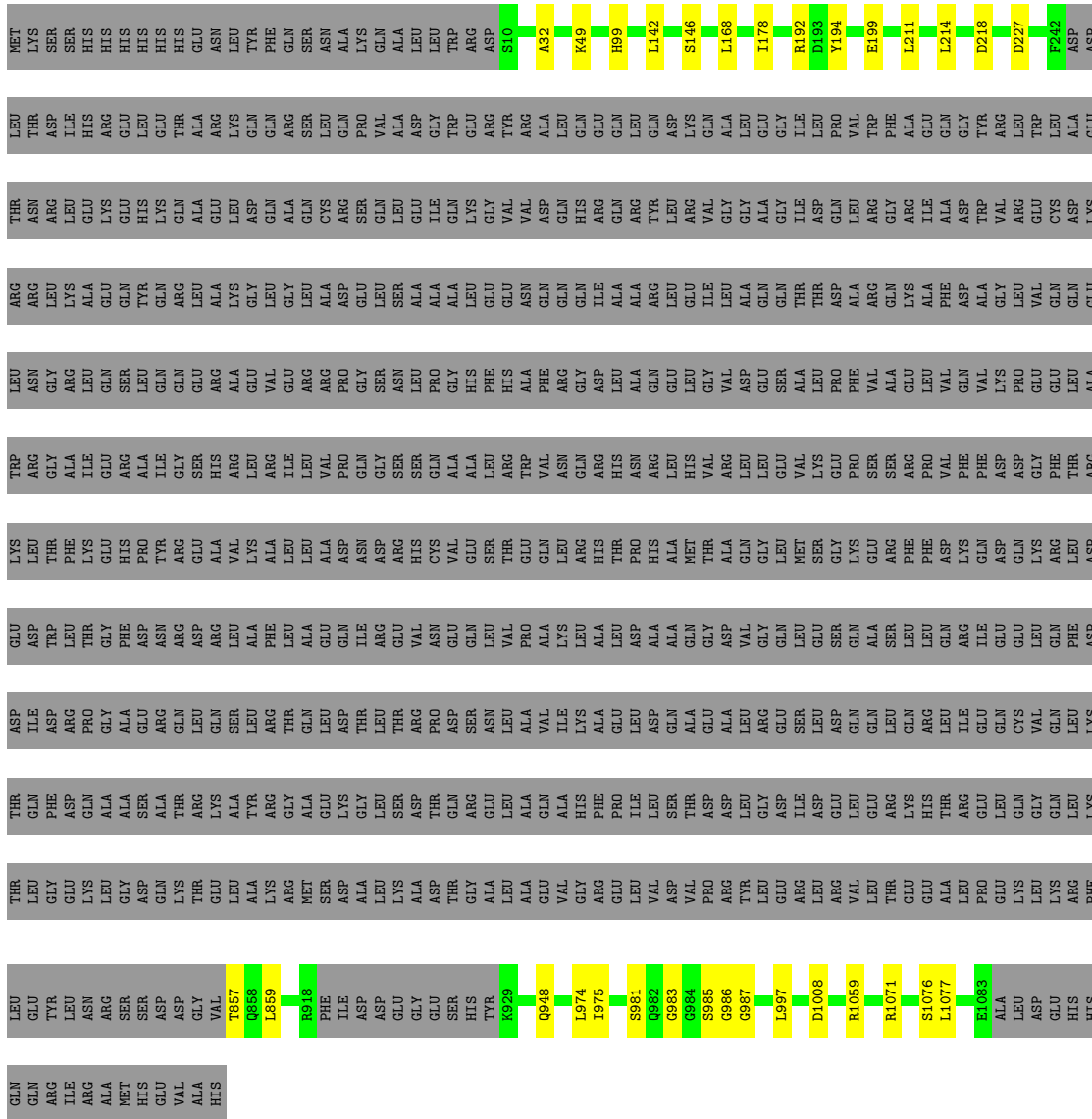
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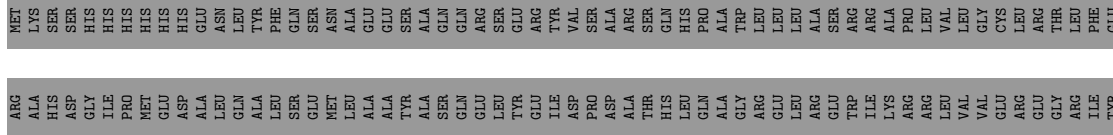
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	B	1	1	1	0



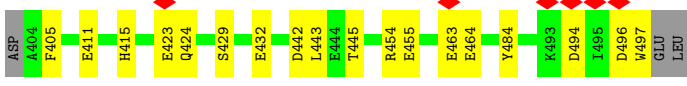
• Molecule 1: JetC



• Molecule 2: JetA



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

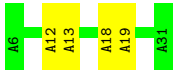
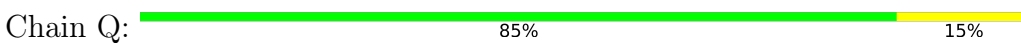


• Molecule 3: DNA (26-MER)



There are no outlier residues recorded for this chain.

• Molecule 4: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	323026	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.778	Depositor
Minimum map value	-0.334	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: MG, AGS

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	0.33	0/3593	0.52	0/4854
1	B	0.34	0/3556	0.53	0/4802
2	C	0.26	0/768	0.44	0/1047
3	P	0.58	0/571	1.29	0/880
4	Q	0.64	0/623	0.68	0/958
All	All	0.38	0/9111	0.62	0/12541

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	3530	0	3503	27	0
1	B	3494	0	3474	20	0
2	C	751	0	719	15	0
3	P	520	0	313	0	0
4	Q	546	0	287	2	0
5	A	31	0	12	3	0
5	B	31	0	12	2	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
All	All	8905	0	8320	61	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 4.

All (61) 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:214:LEU:HD11	1:A:996:VAL:HG21	1.71	0.73
1:B:192:ARG:NH2	1:B:199:GLU:OE2	2.24	0.67
5:B:1201:AGS:S1G	5:B:1201:AGS:O2B	2.53	0.66
1:B:857:THR:HG22	1:B:859:LEU:H	1.62	0.65
5:A:1201:AGS:O2G	5:A:1201:AGS:O2B	2.16	0.64
1:B:1059:ARG:NH1	2:C:442:ASP:OD2	2.31	0.63
1:A:1006:CYS:HB3	1:A:1013:PRO:HA	1.80	0.62
1:B:1076:SER:OG	2:C:454:ARG:NH1	2.33	0.61
2:C:429:SER:OG	2:C:432:GLU:OE1	2.16	0.61
1:A:77:ASP:OD2	1:B:983:GLY:N	2.34	0.59
1:A:874:LEU:HD11	1:A:894:LEU:HD23	1.88	0.56
1:B:214:LEU:O	1:B:981:SER:OG	2.24	0.56
1:A:227:ASP:O	1:A:957:ARG:NH1	2.40	0.55
1:A:875:ASP:HA	1:A:878:ASN:HD21	1.71	0.55
1:A:1054:GLU:OE2	1:A:1057:LEU:N	2.32	0.54
1:A:901:HIS:CD2	1:A:902:GLU:HG2	2.42	0.54
1:A:874:LEU:O	1:A:878:ASN:ND2	2.41	0.54
2:C:464:GLU:N	2:C:464:GLU:OE1	2.41	0.52
1:A:1074:GLU:OE1	1:A:1074:GLU:N	2.44	0.51
1:B:1008:ASP:OD1	1:B:1008:ASP:N	2.44	0.51
1:B:32:ALA:HB2	1:B:1077:LEU:HD23	1.93	0.50
1:A:973:ASN:N	1:A:973:ASN:OD1	2.45	0.50
1:A:48:GLY:N	5:A:1201:AGS:O1A	2.45	0.49
5:A:1201:AGS:S1G	1:B:987:GLY:N	2.86	0.48
2:C:496:ASP:OD1	2:C:497:TRP:N	2.46	0.48
1:B:211:LEU:HD23	1:B:997:LEU:HD11	1.96	0.47
1:B:227:ASP:OD1	1:B:227:ASP:N	2.37	0.47
1:B:49:LYS:NZ	5:B:1201:AGS:O2G	2.44	0.47
4:Q:12:DA:H2'	4:Q:13:DA:C8	2.51	0.46
1:B:1071:ARG:NH1	2:C:455:GLU:O	2.49	0.46
2:C:423:GLU:OE1	2:C:424:GLN:NE2	2.48	0.45
1:A:116:ARG:HG2	1:A:117:ASP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:ASP:N	2:C:442:ASP:OD1	2.50	0.45
2:C:411:GLU:O	2:C:415:HIS:ND1	2.46	0.44
1:A:218:ASP:OD1	1:A:219:GLU:N	2.50	0.44
1:B:142:LEU:HD23	1:B:168:LEU:HD13	2.00	0.43
2:C:463:GLU:OE1	2:C:463:GLU:N	2.47	0.43
1:A:33:GLU:N	1:A:33:GLU:OE1	2.52	0.43
2:C:443:LEU:HD12	2:C:443:LEU:HA	1.80	0.43
1:A:994:SER:O	1:A:998:THR:HG22	2.18	0.43
1:A:1006:CYS:N	1:A:1007:PRO:HD2	2.34	0.43
1:A:142:LEU:HD23	1:A:168:LEU:HD13	2.00	0.42
1:A:49:LYS:HE3	1:A:49:LYS:HB2	1.87	0.42
1:B:146:SER:HB3	1:B:178:ILE:HG13	2.01	0.42
1:B:974:LEU:HD23	1:B:975:ILE:N	2.35	0.42
1:A:985:SER:OG	1:A:986:GLY:N	2.52	0.42
1:B:948:GLN:H	1:B:948:GLN:CD	2.23	0.41
2:C:443:LEU:C	2:C:445:THR:H	2.23	0.41
1:B:985:SER:OG	1:B:986:GLY:N	2.54	0.41
2:C:463:GLU:H	2:C:463:GLU:CD	2.24	0.41
1:A:899:VAL:HG22	1:A:901:HIS:ND1	2.36	0.41
1:A:39:THR:HG22	1:A:1064:SER:HB3	2.02	0.41
1:B:218:ASP:N	1:B:218:ASP:OD1	2.51	0.41
1:A:875:ASP:HA	1:A:878:ASN:ND2	2.36	0.40
1:A:1012:ARG:HA	1:A:1012:ARG:NE	2.36	0.40
1:B:997:LEU:HD23	1:B:997:LEU:HA	1.92	0.40
4:Q:18:DA:H2"	4:Q:19:DA:C8	2.56	0.40
1:A:230:SER:OG	1:A:231:ALA:N	2.55	0.40
1:A:150:GLU:OE1	1:A:150:GLU:N	2.42	0.40
2:C:494:ASP:N	2:C:494:ASP:OD1	2.55	0.40
1:A:1055:MET:HE2	2:C:405:PHE:HE1	1.86	0.40

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	449/1119 (40%)	420 (94%)	29 (6%)	0	100	100
1	B	444/1119 (40%)	412 (93%)	32 (7%)	0	100	100
2	C	92/517 (18%)	86 (94%)	6 (6%)	0	100	100
All	All	985/2755 (36%)	918 (93%)	67 (7%)	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	374/936 (40%)	372 (100%)	2 (0%)	88	93
1	B	370/936 (40%)	368 (100%)	2 (0%)	88	93
2	C	78/440 (18%)	77 (99%)	1 (1%)	69	82
All	All	822/2312 (36%)	817 (99%)	5 (1%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	113	THR
1	B	99	HIS
1	B	194	TYR
2	C	484	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	878	ASN
1	A	1022	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	AGS	A	1201	6	26,33,33	0.73	0	26,52,52	1.14	2 (7%)
5	AGS	B	1201	6	26,33,33	0.71	0	26,52,52	1.05	2 (7%)

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
5	AGS	A	1201	6	-	2/17/38/38	0/3/3/3
5	AGS	B	1201	6	-	3/17/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1201	AGS	PA-O3A-PB	-4.17	118.53	132.83
5	B	1201	AGS	PA-O3A-PB	-3.58	120.55	132.83
5	B	1201	AGS	C5-C6-N6	2.25	123.77	120.35
5	A	1201	AGS	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

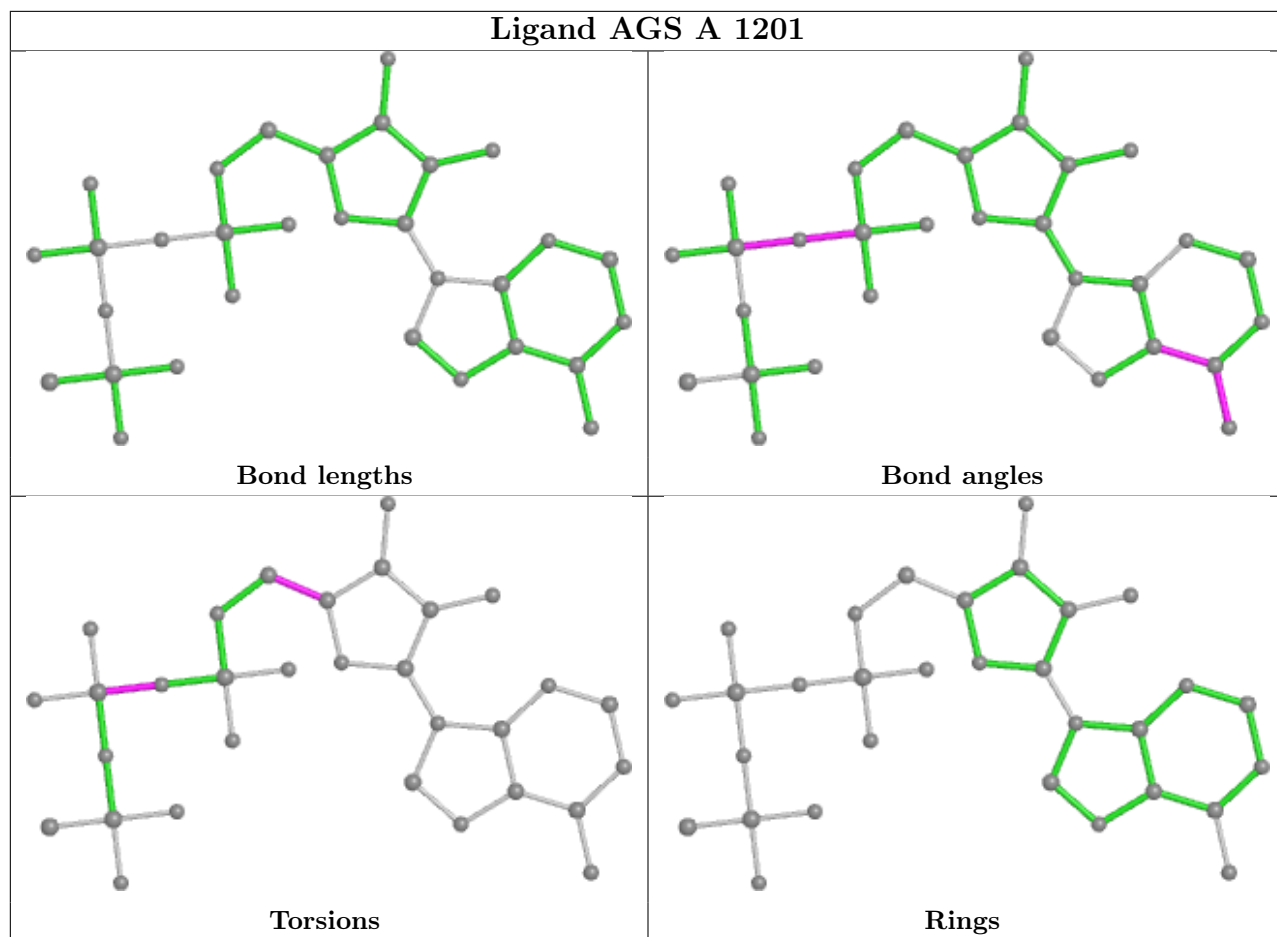
Mol	Chain	Res	Type	Atoms
5	B	1201	AGS	O4'-C4'-C5'-O5'
5	B	1201	AGS	C3'-C4'-C5'-O5'
5	B	1201	AGS	PG-O3B-PB-O2B
5	A	1201	AGS	C3'-C4'-C5'-O5'
5	A	1201	AGS	PA-O3A-PB-O1B

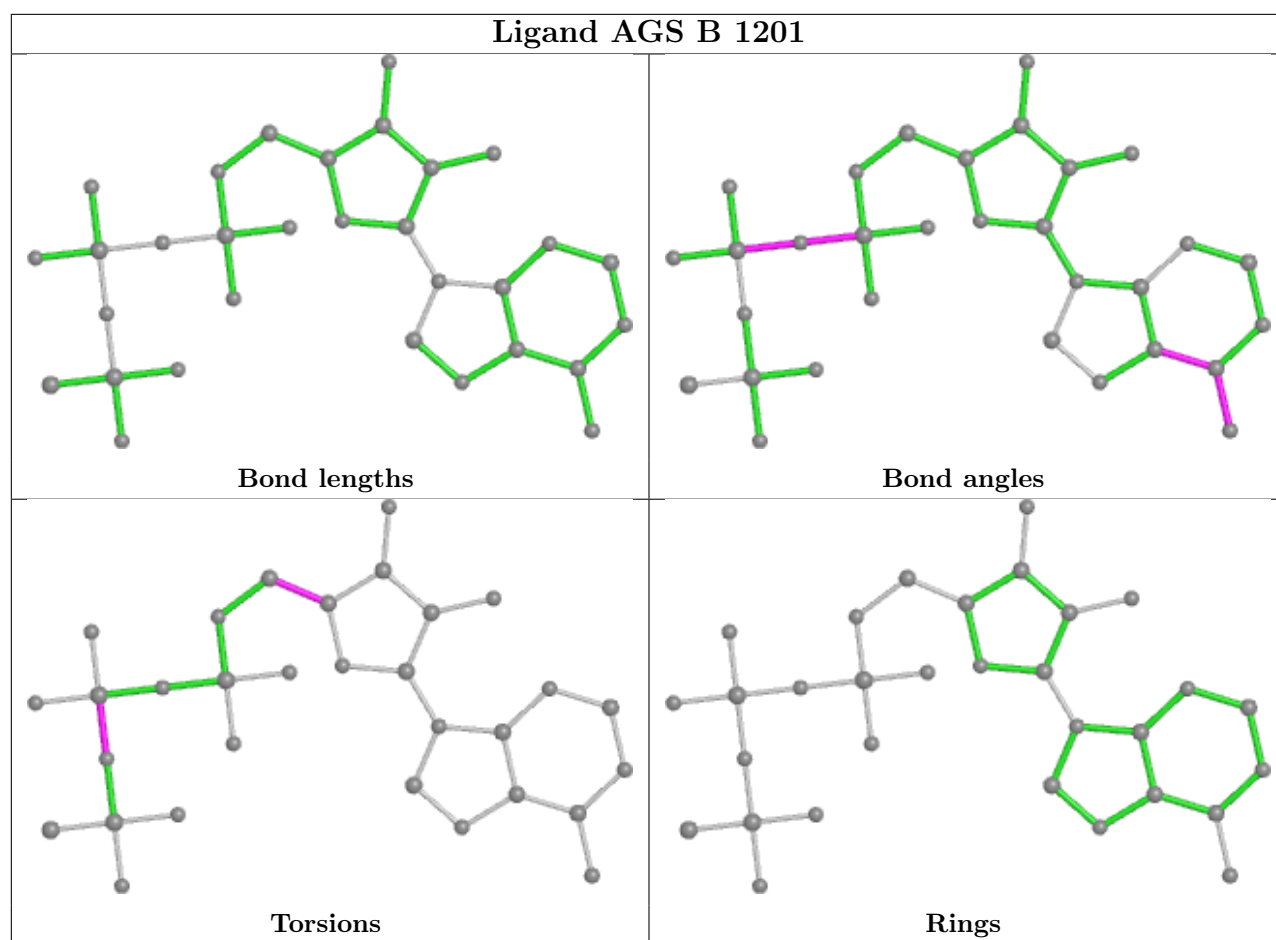
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	AGS	3	0
5	B	1201	AGS	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

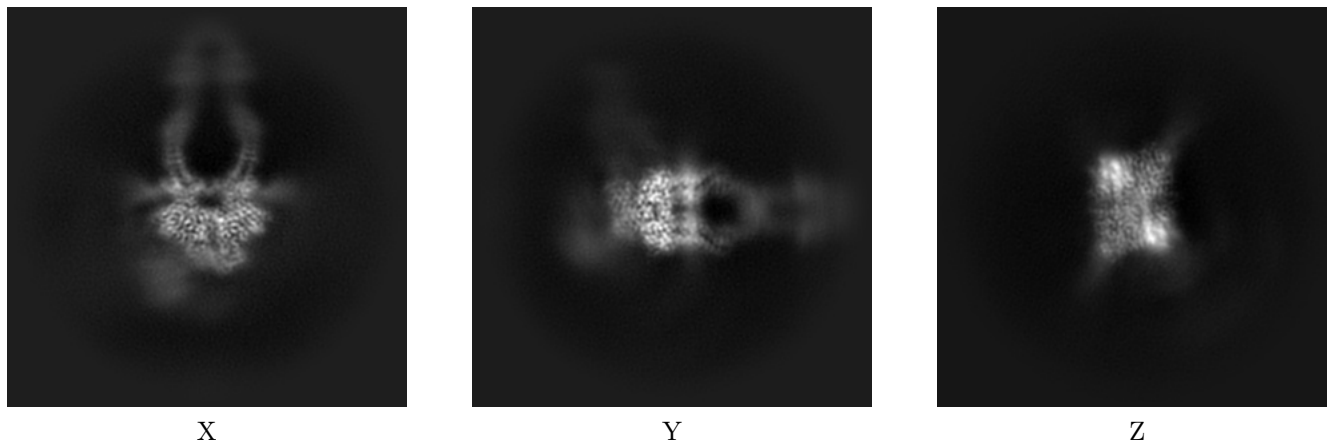
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27482. These allow visual inspection of the internal detail of the map and identification of artifacts.

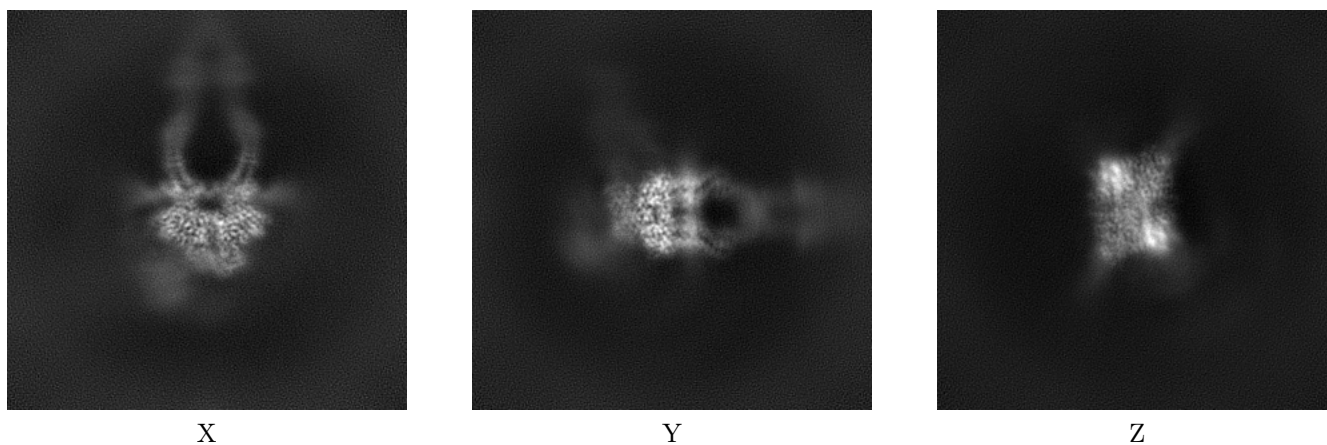
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



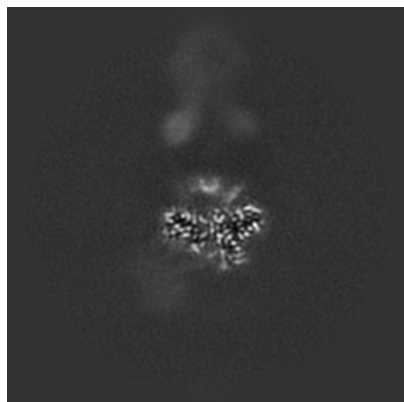
6.1.2 Raw map



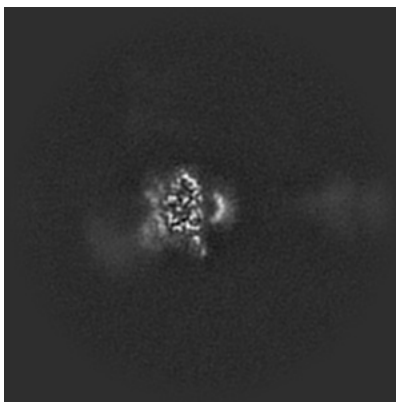
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

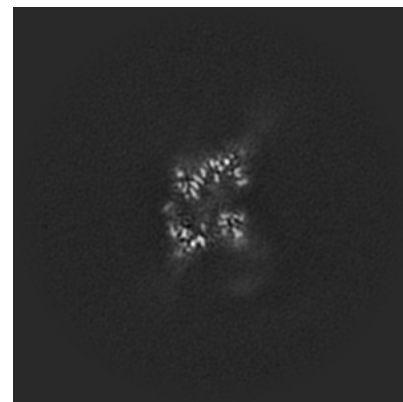
6.2.1 Primary map



X Index: 150

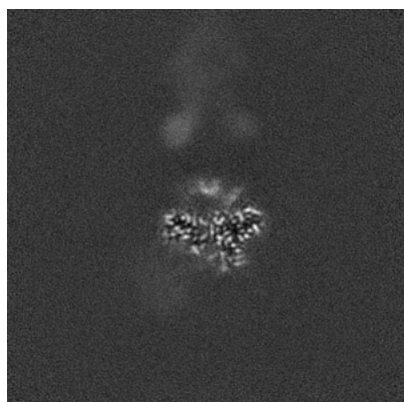


Y Index: 150

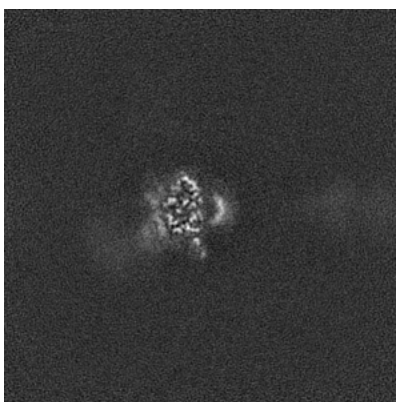


Z Index: 150

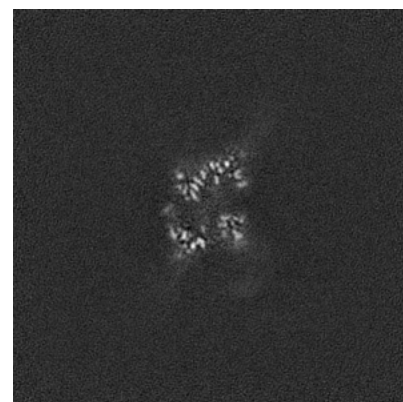
6.2.2 Raw map



X Index: 150



Y Index: 150

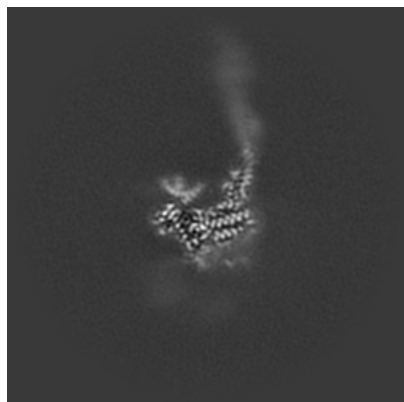


Z Index: 150

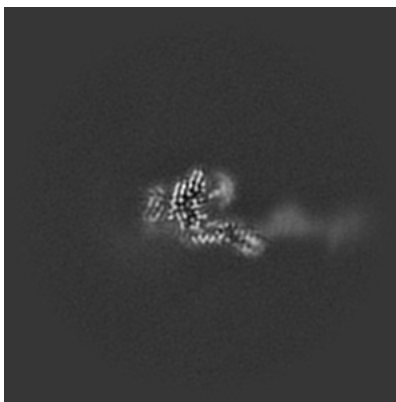
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

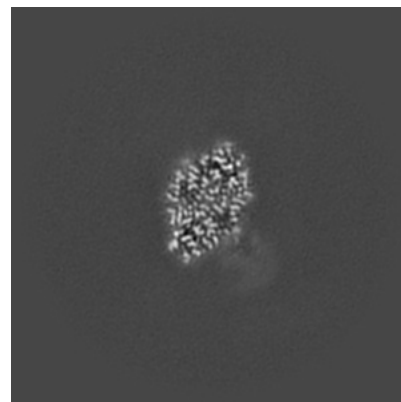
6.3.1 Primary map



X Index: 135

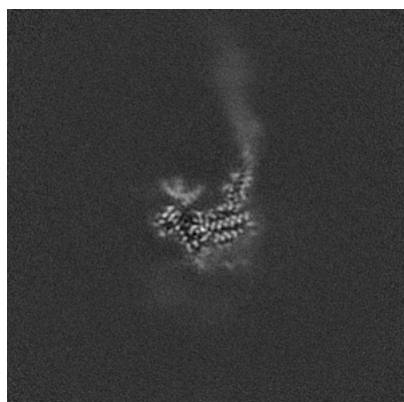


Y Index: 175

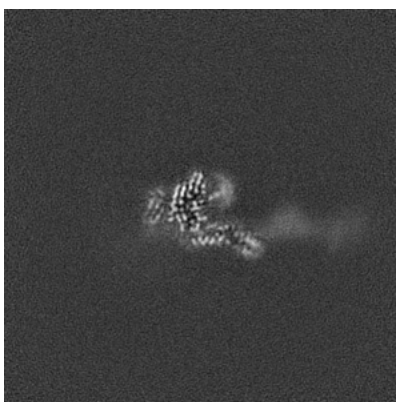


Z Index: 142

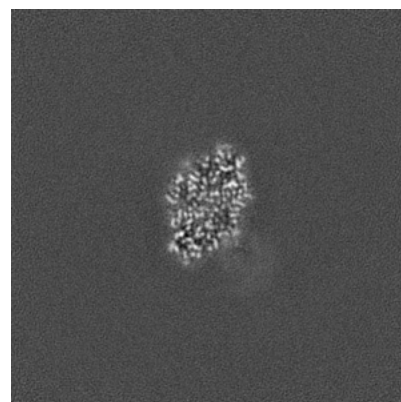
6.3.2 Raw map



X Index: 135



Y Index: 175

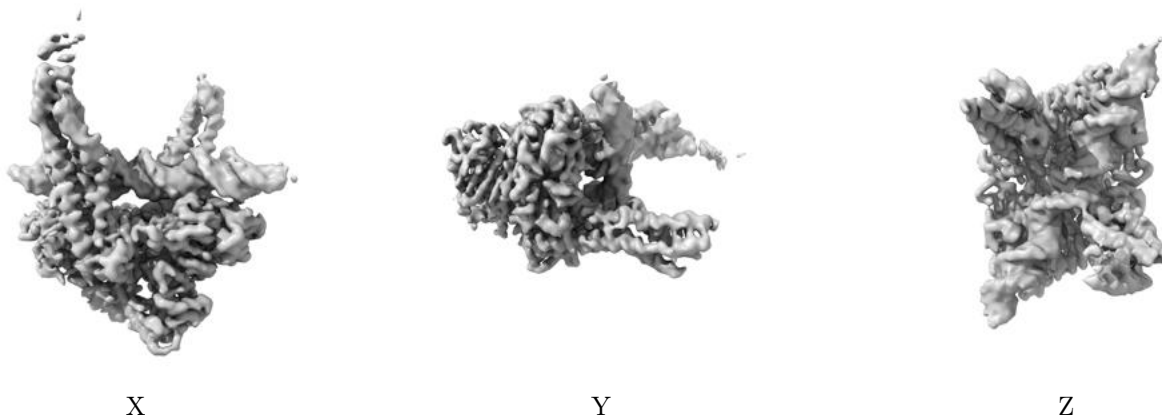


Z Index: 141

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

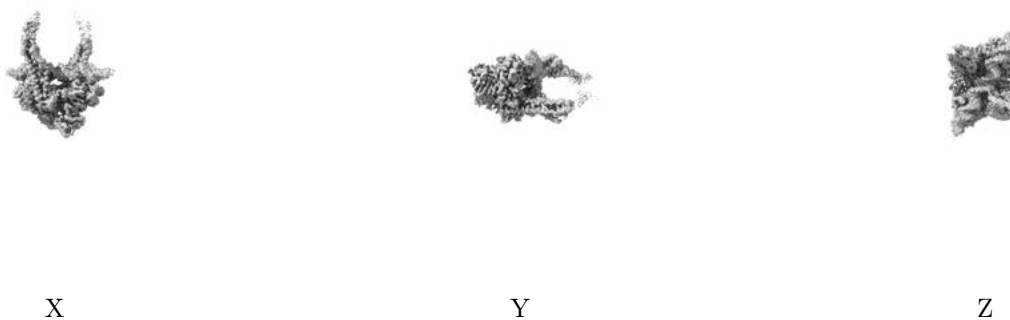
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

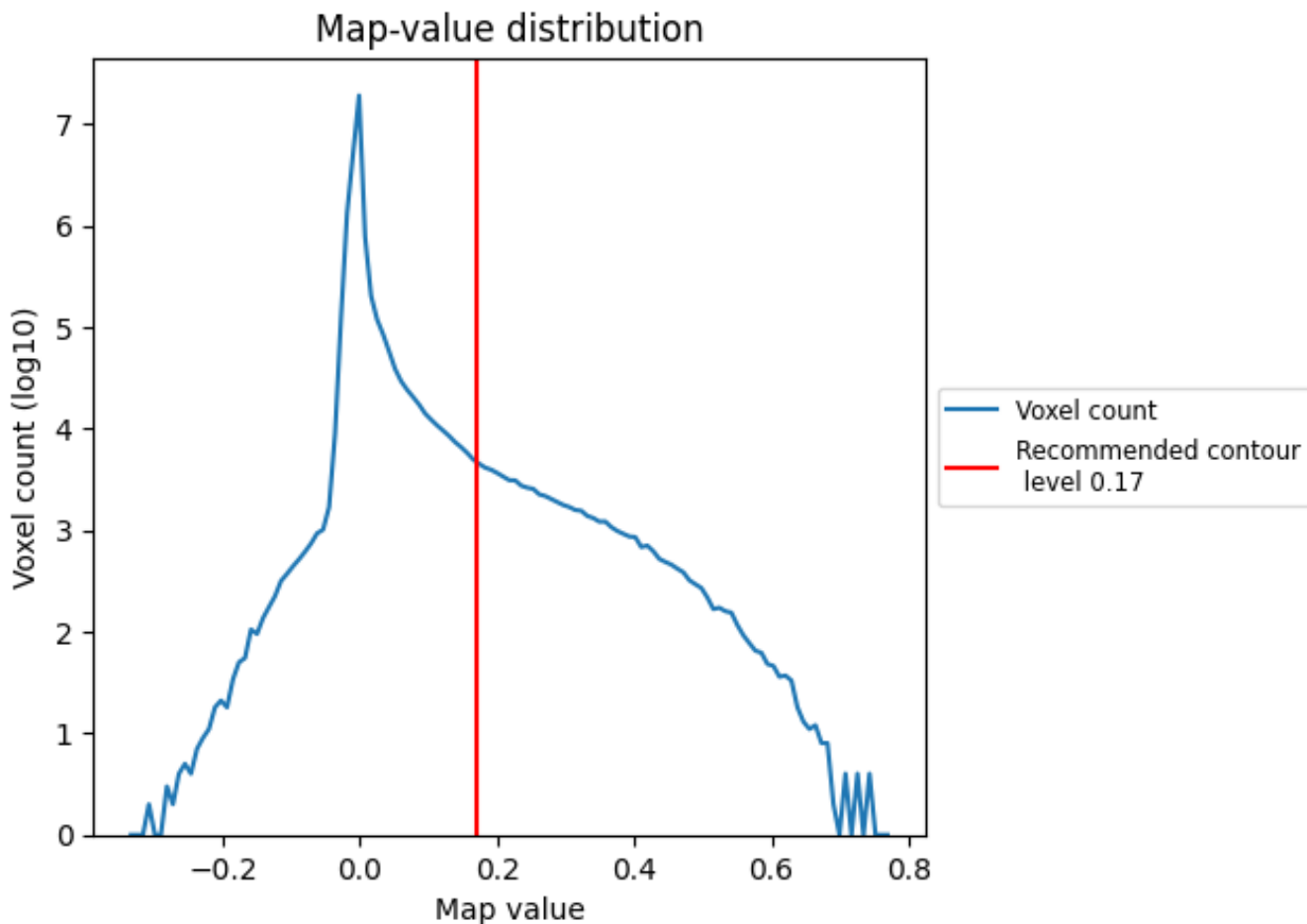
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

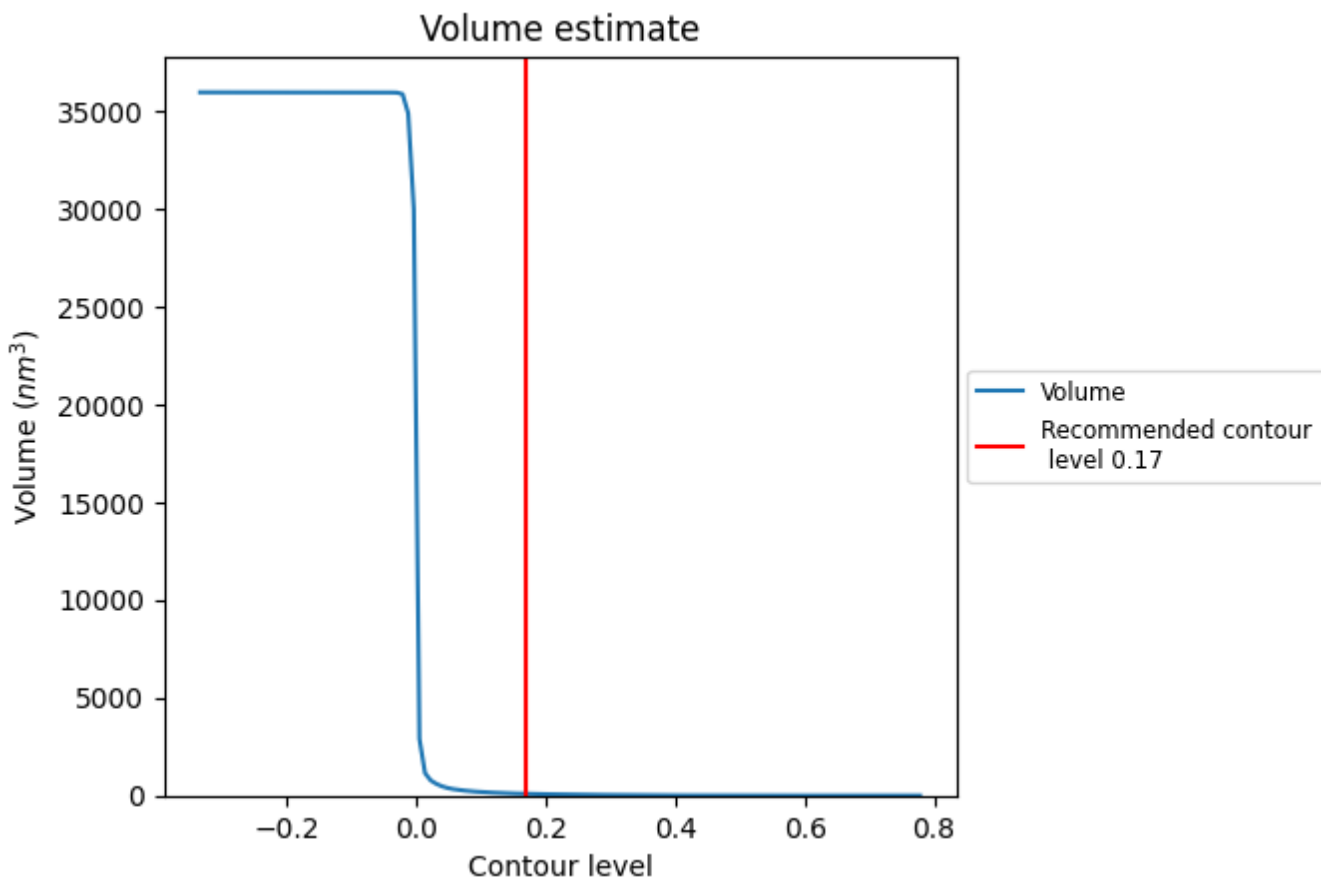
This section contains the results of statistical analysis of the map.

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.

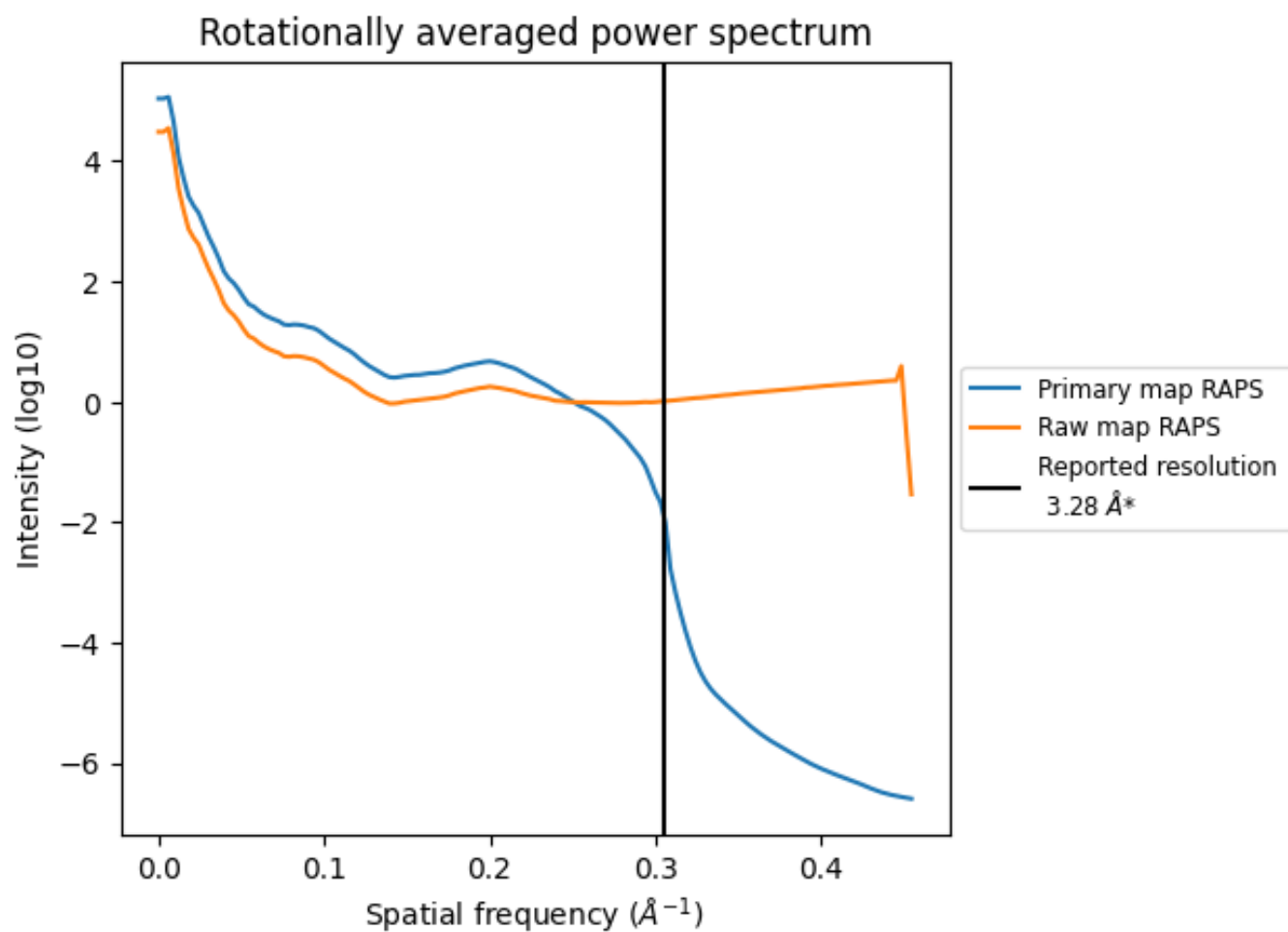
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 81 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

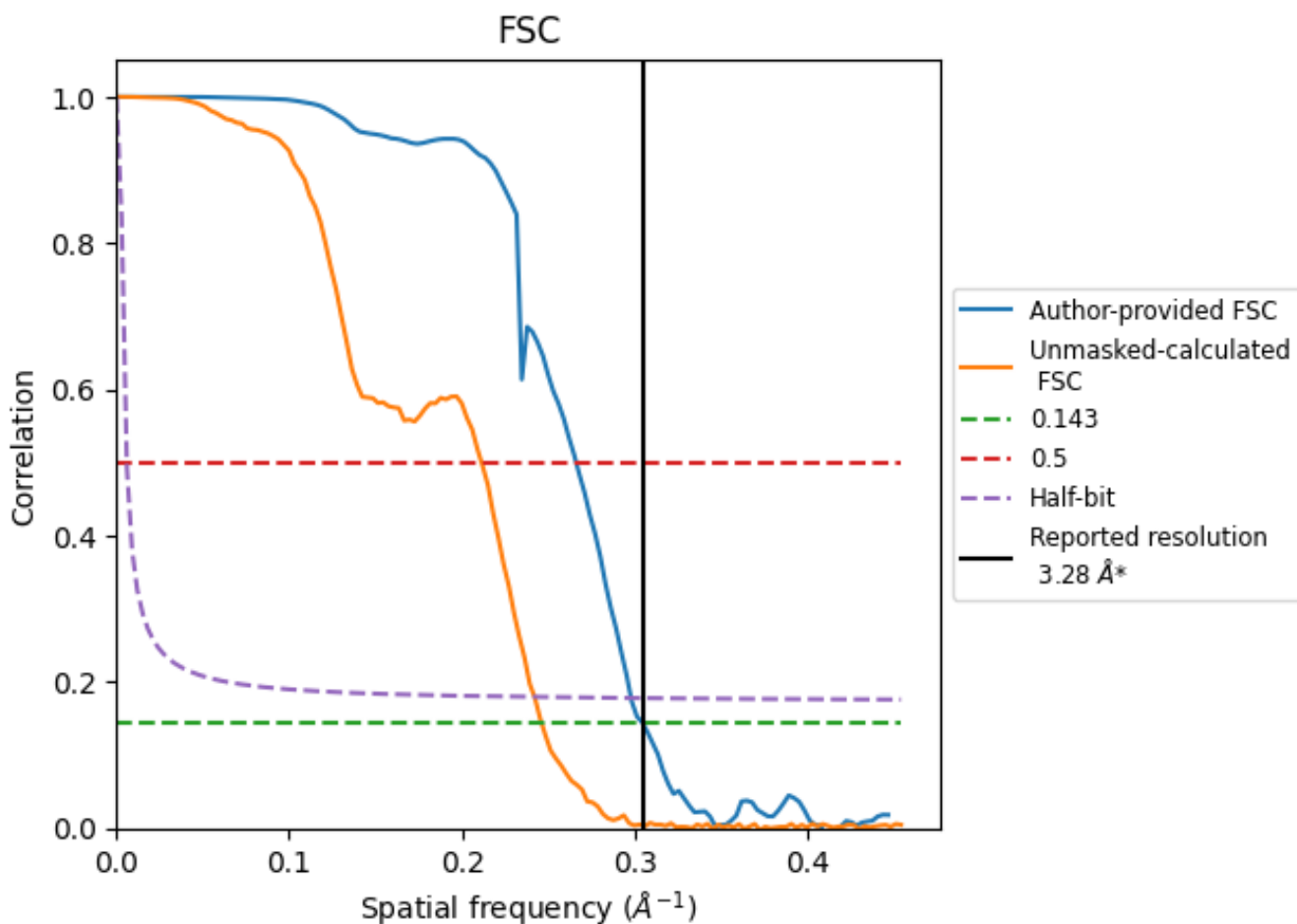


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 Å⁻¹

8.2 Resolution estimates

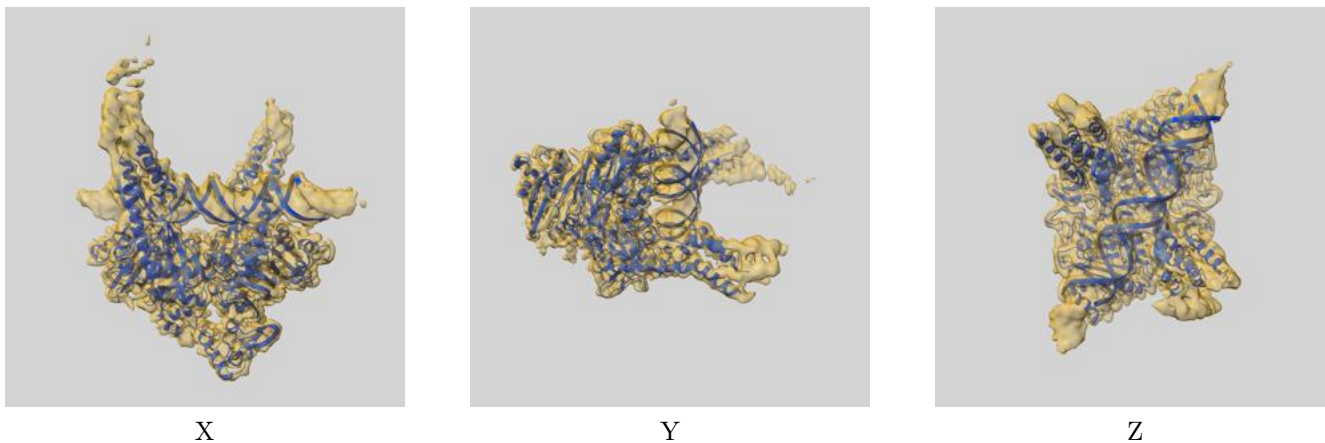
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.76	3.35
Unmasked-calculated*	4.06	4.73	4.13

*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 4.06 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

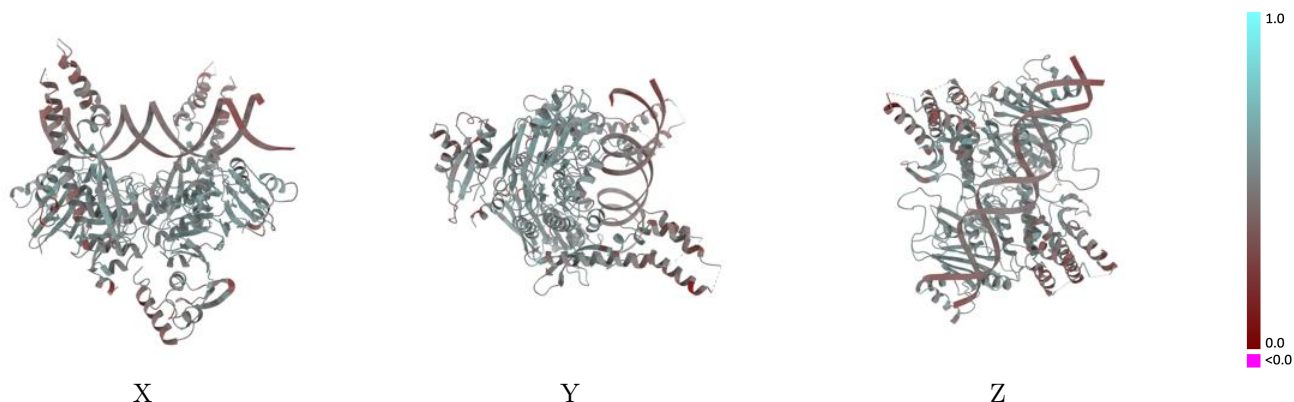
This section contains information regarding the fit between EMDB map EMD-27482 and PDB model 8DK3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



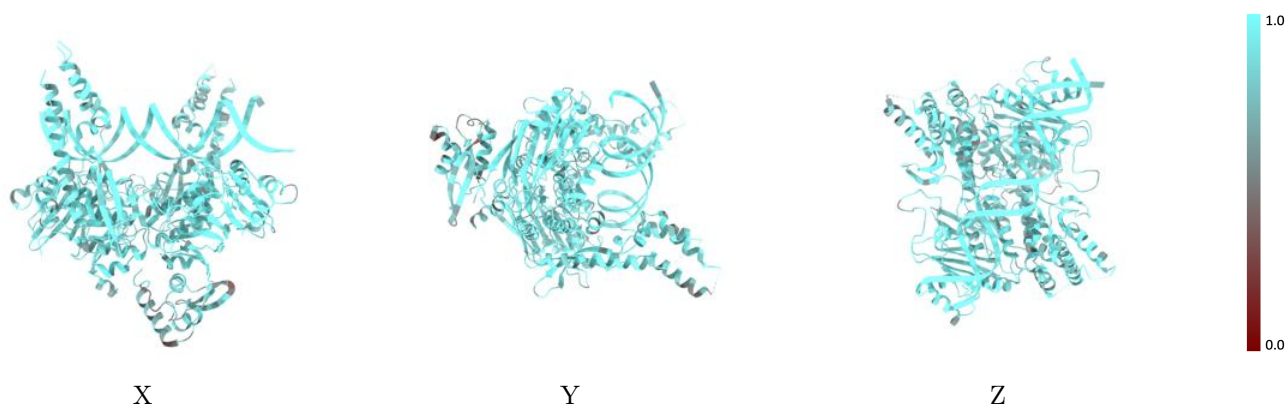
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



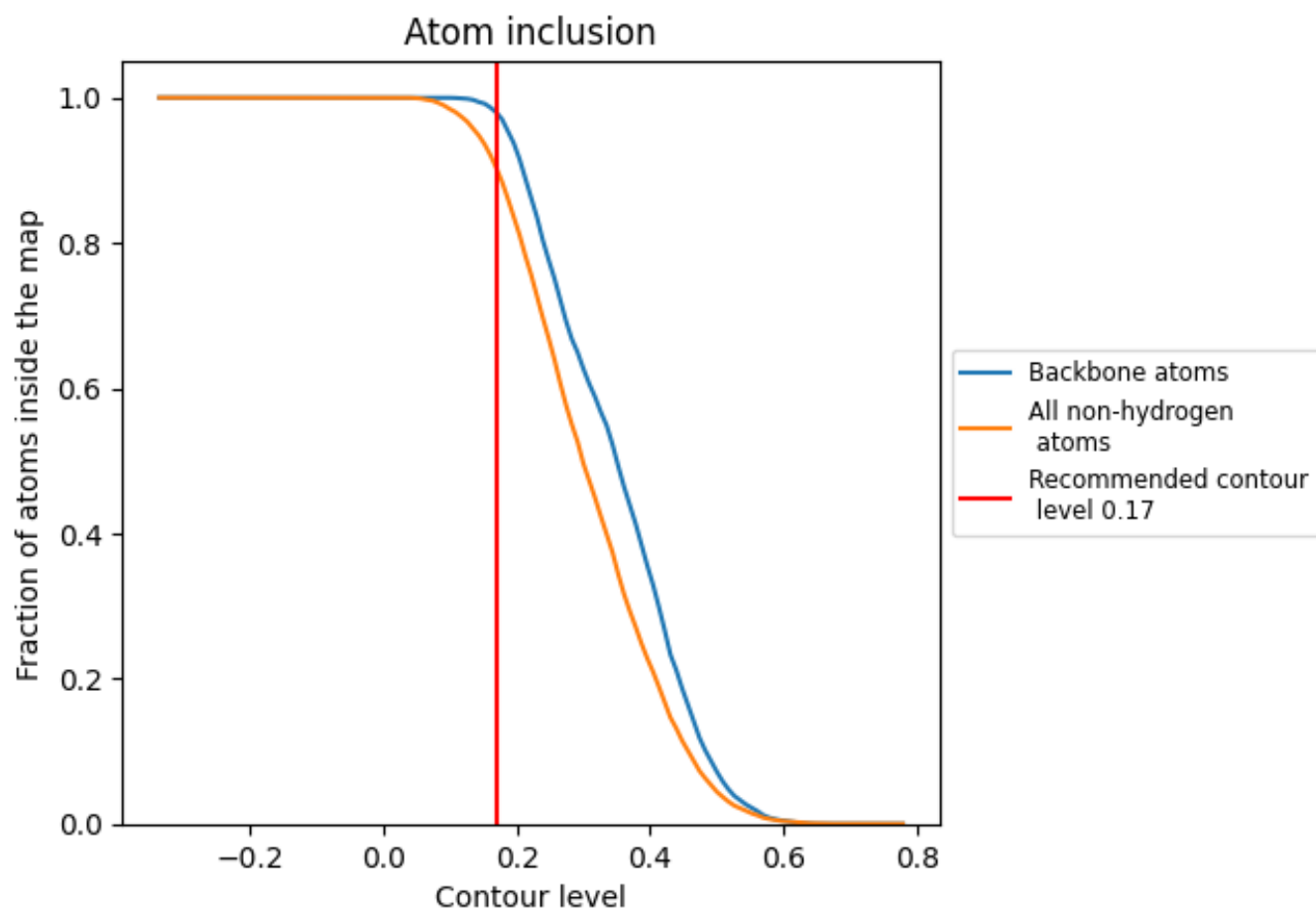
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).













9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9026	 0.4950
A	 0.9091	 0.5110
B	 0.9174	 0.5180
C	 0.7422	 0.4550
P	 0.9654	 0.3850
Q	 0.9249	 0.4040

