



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:01 PM UTC

PDB ID : 8I0N / pdb_00008i0n
EMDB ID : EMD-35104
Title : Structure of beta-arrestin1 in complex with a phosphopeptide corresponding to the human C5a anaphylatoxin chemotactic receptor 1, C5aR1 (Local refine)
Authors : Maharana, J.; Sarma, P.; Yadav, M.K.; Banerjee, R.; Shukla, A.K.
Deposited on : 2023-01-11
Resolution : 3.26 Å(reported)
Based on initial model : 8GO8

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

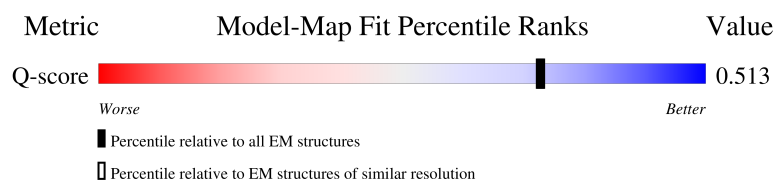
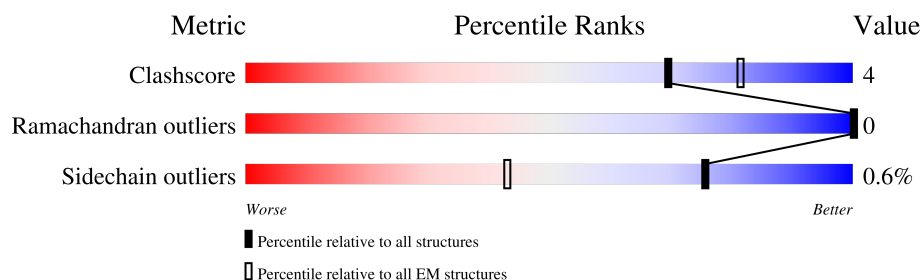
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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.



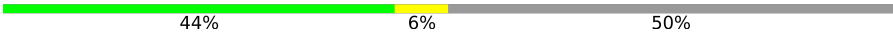
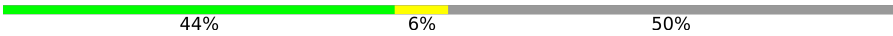
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	418	
1	B	418	
2	H	237	
2	I	237	

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Mol	Chain	Length	Quality of chain
3	L	215	 44% 6% 50%
3	M	215	 44% 6% 50%
4	U	20	 25% 20% 55%
4	V	20	 25% 20% 55%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9141 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-arrestin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	362	Total	C	N	O	S	0	0
			2775	1775	477	513	10		
1	B	362	Total	C	N	O	S	0	0
			2767	1769	476	512	10		

- Molecule 2 is a protein called Fab30 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			908	578	153	174	3		
2	I	117	Total	C	N	O	S	0	0
			908	578	153	174	3		

- Molecule 3 is a protein called Fab30 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			804	508	132	161	3		
3	M	107	Total	C	N	O	S	0	0
			799	506	131	159	3		

- Molecule 4 is a protein called C5a anaphylatoxin chemotactic receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	9	Total	C	N	O	P	0	0
			90	42	12	31	5		
4	V	9	Total	C	N	O	P	0	0
			90	42	12	31	5		

There are 22 discrepancies between the modelled and reference sequences:

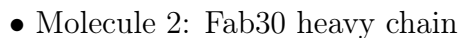
Chain	Residue	Modelled	Actual	Comment	Reference
U	331	GLU	-	expression tag	UNP P21730

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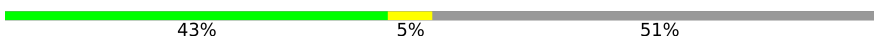
Chain	Residue	Modelled	Actual	Comment	Reference
U	332	SEP	-	expression tag	UNP P21730
U	333	LYS	-	expression tag	UNP P21730
U	343	MET	-	expression tag	UNP P21730
U	344	ALA	-	expression tag	UNP P21730
U	345	GLN	-	expression tag	UNP P21730
U	346	LYS	-	expression tag	UNP P21730
U	347	THR	-	expression tag	UNP P21730
U	348	GLN	-	expression tag	UNP P21730
U	349	ALA	-	expression tag	UNP P21730
U	350	VAL	-	expression tag	UNP P21730
V	331	GLU	-	expression tag	UNP P21730
V	332	SEP	-	expression tag	UNP P21730
V	333	LYS	-	expression tag	UNP P21730
V	343	MET	-	expression tag	UNP P21730
V	344	ALA	-	expression tag	UNP P21730
V	345	GLN	-	expression tag	UNP P21730
V	346	LYS	-	expression tag	UNP P21730
V	347	THR	-	expression tag	UNP P21730
V	348	GLN	-	expression tag	UNP P21730
V	349	ALA	-	expression tag	UNP P21730
V	350	VAL	-	expression tag	UNP P21730

- Molecule 1: Beta-arrestin-1



SER
GLU
ASN
THR
LYS
VAL
ASP
LYS
LYS
VAL
GLU
PRO
LYS
SER
CYS
ASP
LYS
THR
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 2: Fab30 heavy chain

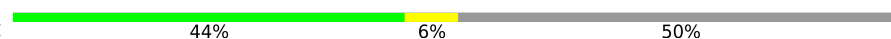
Chain I:  43% 5% 51%

GLU
ILE
SER
GLU
V5
L14
S20
L21
M31
N80
M86
R90
C99
D111
G114
Q115
V119
T120
V121
SER
SER
ALA
SER
THR
LYS
GLY
PRO
SER
VAL
PHE
PRO
LEU
PRO
ALA
PRO
SER
SER
LYS
SER
LYS
THR
GLY
THR
ALA
ALA
GLY
CYS
LEU
VAL

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

SER
ASN
THR
LYS
VAL
ASP
LYS
LYS
VAL
GLU
PRO
LYS
SER
CYS
ASP
LYS
THR
HIS
HIS
HIS
HIS
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HIS
HIS

• Molecule 3: Fab30 light chain

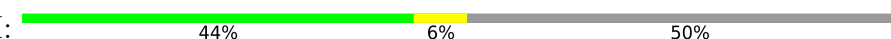
Chain L:  44% 6% 50%

S1
M5
D18
R19
R25
Q80
P81
E82
D83
F84
C89
Q90
Q91
V97
G100
T107
LYS
ARG
THR
VAL
ALA
ALA
PRO
SER
SER
VAL
PHE
SER
ILE
PHE
PRO
SER
ASP
SER
GLN
LEU
LYS
GLY
THR
ALA
VAL
CYS
LEU
ASN
ASN
PHE
TYR
PRO
ARG

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

SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

• Molecule 3: Fab30 light chain

Chain M:  44% 6% 50%

S1
Q7
D18
R19
R25
R62
P81
E82
D83
F84
C89
Q90
Q91
V97
G100
T103
T107
LYS
ARG
THR
VAL
ALA
PRO
SER
SER
VAL
SER
PHE
THR
THR
THR
THR
THR
THR
THR
SER
SER
ASP
SER
GLN
LEU
LYS
GLY
THR
ALA
VAL
CYS
LEU
ASN
ASN
PHE

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

GLY
LEU
SER
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

• Molecule 4: C5a anaphylatoxin chemotactic receptor 1

Chain U:  25% 20% 55%

GLU
SEP
LYS
S334
F335
T336
H337
S338
T339
T342
MET
ALA
GLN
LYS
THR
GLN
ALA
VAL

• Molecule 4: C5a anaphylatoxin chemotactic receptor 1

Chain V:  25% 20% 55%

GLU	SEP	LYS	S334	F336	T336	R337	S338	T339	T342	MET	ALA	GLN	LYS	THR	GLN	ALA	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	80437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.893	Depositor
Minimum map value	-1.482	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	393.60962, 393.60962, 393.60962	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3667, 1.3667, 1.3667	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: TPO, SEP

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	0/2836	0.32	0/3859
1	B	0.16	0/2828	0.33	1/3850 (0.0%)
2	H	0.14	0/932	0.28	0/1267
2	I	0.14	0/932	0.29	0/1267
3	L	0.14	0/822	0.31	0/1119
3	M	0.15	0/817	0.30	0/1113
4	U	0.10	0/35	0.26	0/42
4	V	0.09	0/35	0.19	0/42
All	All	0.15	0/9237	0.31	1/12559 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	PRO	N-CA-C	-6.01	103.37	110.70

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	2775	0	2779	17	0
1	B	2767	0	2765	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	908	0	860	9	0
2	I	908	0	860	9	0
3	L	804	0	776	8	0
3	M	799	0	767	7	0
4	U	90	0	59	0	0
4	V	90	0	59	0	0
All	All	9141	0	8925	65	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 (65) 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:B:76:ARG:NH1	1:B:78:ASP:OD1	2.27	0.68
3:L:82:GLU:N	3:L:82:GLU:OE2	2.28	0.66
2:I:86:MET:HE1	2:I:119:VAL:HG21	1.84	0.58
1:A:26:ASP:OD2	1:A:363:ARG:NH2	2.35	0.58
1:B:232:LYS:NZ	1:B:257:GLU:OE2	2.38	0.57
2:H:31:ASN:HA	2:H:80:ASN:ND2	2.20	0.56
2:H:86:MET:HE1	2:H:119:VAL:HG21	1.87	0.56
2:I:31:ASN:HA	2:I:80:ASN:ND2	2.20	0.56
1:A:232:LYS:NZ	1:A:257:GLU:OE2	2.40	0.55
2:I:14:LEU:HD12	2:I:120:THR:HB	1.88	0.55
3:L:81:PRO:HA	3:L:84:PHE:HE1	1.72	0.54
2:H:5:VAL:HG12	2:H:29:GLY:HA3	1.90	0.54
3:M:81:PRO:HA	3:M:84:PHE:HE1	1.73	0.53
2:H:99:CYS:O	2:H:114:GLY:N	2.41	0.53
1:A:257:GLU:N	1:A:257:GLU:OE1	2.42	0.51
1:B:257:GLU:N	1:B:257:GLU:OE1	2.43	0.51
2:I:90:ARG:O	2:I:121:VAL:HG21	2.11	0.51
1:B:175:PRO:HD2	1:B:207:ILE:HD11	1.93	0.50
1:B:33:LEU:HD12	1:B:34:VAL:N	2.27	0.49
1:B:39:GLY:O	1:B:101:GLN:NE2	2.45	0.49
1:B:357:LYS:HA	1:B:357:LYS:HE2	1.95	0.49
3:M:62:ARG:NH2	3:M:82:GLU:OE1	2.47	0.47
1:A:338:LEU:HD23	1:B:249:TYR:CE2	2.49	0.47
2:I:99:CYS:O	2:I:114:GLY:N	2.47	0.47
3:M:89:CYS:O	3:M:100:GLY:N	2.45	0.47
1:A:249:TYR:CE1	1:B:338:LEU:HD23	2.50	0.46
2:I:20:SER:O	2:I:21:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:ASP:N	2:I:111:ASP:OD1	2.48	0.46
1:B:277:PHE:CE2	1:B:279:ALA:HB3	2.50	0.46
1:B:26:ASP:OD2	1:B:363:ARG:NH2	2.46	0.46
1:A:277:PHE:CE2	1:A:279:ALA:HB3	2.51	0.45
1:B:296:GLU:OE1	1:B:363:ARG:HB3	2.16	0.44
1:A:39:GLY:O	1:A:101:GLN:NE2	2.50	0.44
1:B:211:GLY:O	2:I:31:ASN:ND2	2.51	0.44
1:A:227:THR:HG22	1:A:264:PRO:HD3	1.99	0.44
3:L:89:CYS:O	3:L:100:GLY:N	2.44	0.44
3:L:18:ASP:OD2	3:L:19:ARG:N	2.49	0.44
2:H:46:LYS:HB3	2:H:46:LYS:HE3	1.87	0.44
1:A:214:ILE:N	1:A:274:LEU:O	2.44	0.43
2:H:90:ARG:O	2:H:121:VAL:HG21	2.17	0.43
1:B:83:ASN:OD1	1:B:83:ASN:C	2.61	0.43
1:B:227:THR:HG22	1:B:264:PRO:HD3	2.00	0.43
1:B:239:ALA:HB3	1:B:249:TYR:CE1	2.53	0.43
1:B:303:SER:O	1:B:352:MET:HE3	2.18	0.43
3:L:5:MET:HE3	3:L:5:MET:HB3	1.91	0.43
1:A:62:ARG:NH1	1:A:138:LYS:HD2	2.34	0.42
2:I:115:GLN:HA	2:I:115:GLN:OE1	2.18	0.42
1:B:33:LEU:HD12	1:B:34:VAL:H	1.84	0.42
3:M:18:ASP:OD2	3:M:19:ARG:N	2.50	0.42
3:L:91:GLN:O	3:L:97:VAL:HG13	2.19	0.42
1:A:52:ARG:HB2	1:A:151:ALA:O	2.20	0.42
1:A:239:ALA:HB3	1:A:249:TYR:CE2	2.55	0.42
2:H:22:ARG:HH21	2:H:85:GLN:HB2	1.84	0.42
3:M:25:ARG:CZ	3:M:25:ARG:HB2	2.50	0.42
3:L:80:GLN:N	3:L:83:ASP:OD1	2.49	0.42
2:H:23:LEU:HG	2:H:86:MET:HE2	2.02	0.42
3:M:7:GLN:HE22	3:M:103:THR:HG22	1.84	0.41
1:B:245:ASN:OD1	1:B:245:ASN:N	2.52	0.41
3:M:91:GLN:O	3:M:97:VAL:HG13	2.20	0.41
1:A:296:GLU:OE1	1:A:363:ARG:HB3	2.21	0.41
1:A:303:SER:O	1:A:352:MET:HE3	2.21	0.41
1:A:365:VAL:HB	1:A:366:PRO:HD3	2.02	0.41
3:L:25:ARG:CZ	3:L:25:ARG:HB2	2.51	0.41
1:A:211:GLY:O	2:H:31:ASN:ND2	2.53	0.41
1:A:67:ASP:OD1	1:A:67:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	360/418 (86%)	340 (94%)	20 (6%)	0	100	100
1	B	360/418 (86%)	342 (95%)	18 (5%)	0	100	100
2	H	115/237 (48%)	111 (96%)	4 (4%)	0	100	100
2	I	115/237 (48%)	110 (96%)	5 (4%)	0	100	100
3	L	105/215 (49%)	102 (97%)	3 (3%)	0	100	100
3	M	105/215 (49%)	102 (97%)	3 (3%)	0	100	100
4	U	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
4	V	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
All	All	1168/1780 (66%)	1113 (95%)	55 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	301/372 (81%)	300 (100%)	1 (0%)	86	86
1	B	300/372 (81%)	297 (99%)	3 (1%)	68	75
2	H	94/200 (47%)	93 (99%)	1 (1%)	65	75
2	I	94/200 (47%)	93 (99%)	1 (1%)	65	75
3	L	89/190 (47%)	89 (100%)	0	100	100
3	M	87/190 (46%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	U	4/12 (33%)	4 (100%)	0	100	100
4	V	4/12 (33%)	4 (100%)	0	100	100
All	All	973/1548 (63%)	967 (99%)	6 (1%)	76	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	B	135	ASP
1	B	245	ASN
1	B	337	ASP
2	H	31	ASN
2	I	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	225	ASN
1	B	15	ASN
1	B	162	ASN
1	B	189	GLN
2	H	42	GLN
2	I	42	GLN
3	L	7	GLN
3	L	39	GLN
3	M	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	TPO	U	336	4	8,10,11	1.08	0	10,14,16	2.03	1 (10%)
4	TPO	V	342	4	8,10,11	1.69	1 (12%)	10,14,16	1.72	2 (20%)
4	SEP	V	338	4	8,9,10	1.59	1 (12%)	7,12,14	1.01	0
4	SEP	U	338	4	8,9,10	1.60	1 (12%)	7,12,14	0.96	0
4	TPO	V	336	4	8,10,11	1.09	0	10,14,16	2.05	1 (10%)
4	SEP	V	334	4	8,9,10	0.59	0	7,12,14	0.63	0
4	TPO	V	339	4	8,10,11	1.63	1 (12%)	10,14,16	2.14	1 (10%)
4	SEP	U	334	4	8,9,10	0.60	0	7,12,14	0.63	0
4	TPO	U	339	4	8,10,11	1.10	0	10,14,16	2.09	1 (10%)
4	TPO	U	342	4	8,10,11	1.71	1 (12%)	10,14,16	1.35	2 (20%)

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
4	TPO	U	336	4	-	0/9/11/13	-
4	TPO	V	342	4	-	2/9/11/13	-
4	SEP	V	338	4	-	0/6/8/10	-
4	SEP	U	338	4	-	0/6/8/10	-
4	TPO	V	336	4	-	0/9/11/13	-
4	SEP	V	334	4	-	6/6/8/10	-
4	TPO	V	339	4	-	2/9/11/13	-
4	SEP	U	334	4	-	5/6/8/10	-
4	TPO	U	339	4	-	2/9/11/13	-
4	TPO	U	342	4	-	4/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	342	TPO	P-O1P	3.58	1.61	1.50
4	U	342	TPO	P-O1P	3.55	1.61	1.50
4	V	339	TPO	P-O1P	3.53	1.61	1.50
4	U	338	SEP	P-O1P	3.53	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	338	SEP	P-O1P	3.50	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	339	TPO	P-OG1-CB	-6.11	106.72	123.33
4	U	339	TPO	P-OG1-CB	-5.96	107.13	123.33
4	V	336	TPO	P-OG1-CB	-5.87	107.38	123.33
4	U	336	TPO	P-OG1-CB	-5.80	107.56	123.33
4	V	342	TPO	P-OG1-CB	-4.33	111.56	123.33
4	U	342	TPO	P-OG1-CB	-2.62	116.21	123.33
4	V	342	TPO	CG2-CB-CA	-2.38	108.62	113.26
4	U	342	TPO	CG2-CB-CA	-2.23	108.91	113.26

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	334	SEP	N-CA-CB-OG
4	U	334	SEP	C-CA-CB-OG
4	U	334	SEP	CB-OG-P-O2P
4	U	339	TPO	N-CA-CB-OG1
4	U	342	TPO	CG2-CB-OG1-P
4	V	334	SEP	N-CA-CB-OG
4	V	334	SEP	C-CA-CB-OG
4	V	334	SEP	CB-OG-P-O1P
4	V	334	SEP	CB-OG-P-O2P
4	V	334	SEP	CB-OG-P-O3P
4	V	339	TPO	N-CA-CB-OG1
4	U	334	SEP	CB-OG-P-O3P
4	V	334	SEP	CA-CB-OG-P
4	U	342	TPO	C-CA-CB-CG2
4	U	334	SEP	CB-OG-P-O1P
4	U	342	TPO	CB-OG1-P-O3P
4	U	339	TPO	O-C-CA-CB
4	U	342	TPO	O-C-CA-CB
4	V	339	TPO	O-C-CA-CB
4	V	342	TPO	C-CA-CB-CG2
4	V	342	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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.

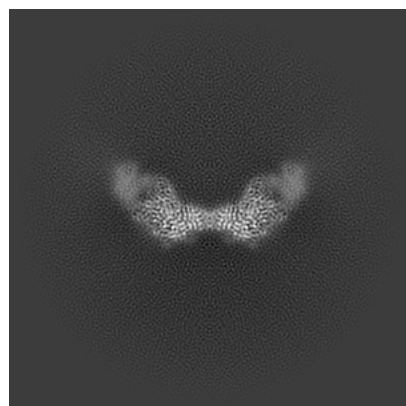
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35104. These allow visual inspection of the internal detail of the map and identification of artifacts.

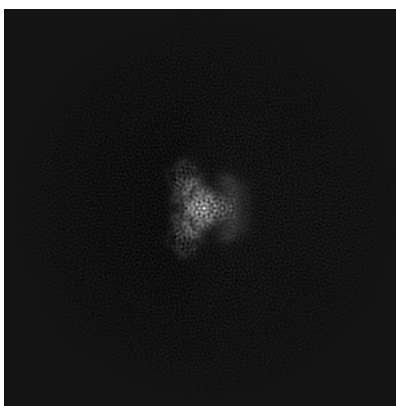
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

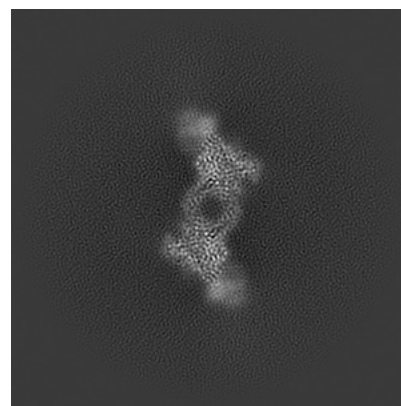
6.1.1 Primary map



X

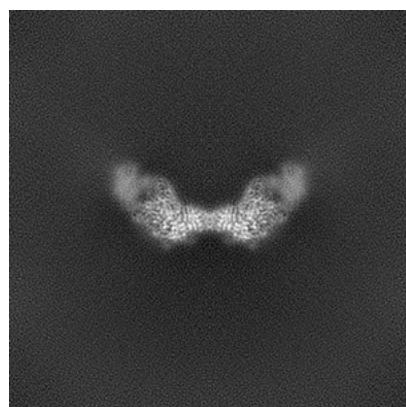


Y

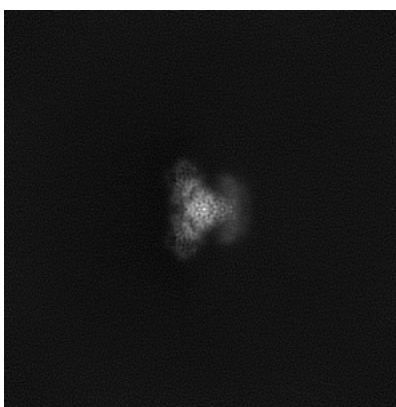


Z

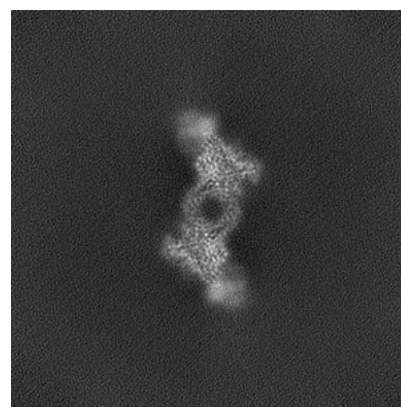
6.1.2 Raw map



X



Y

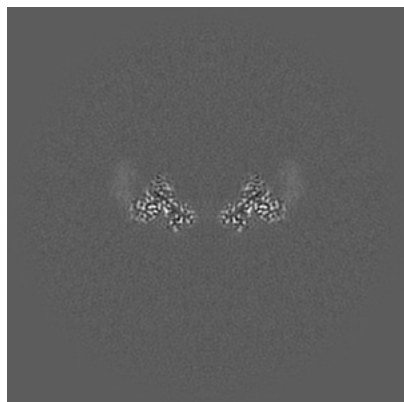


Z

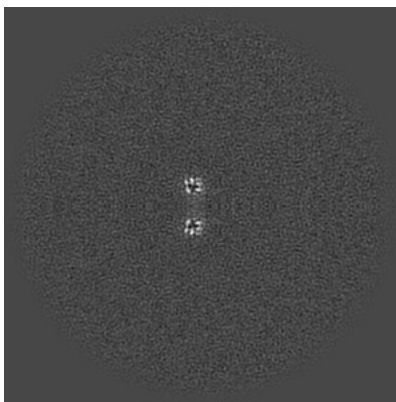
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

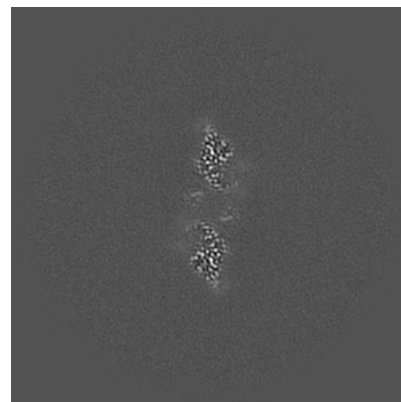
6.2.1 Primary map



X Index: 144

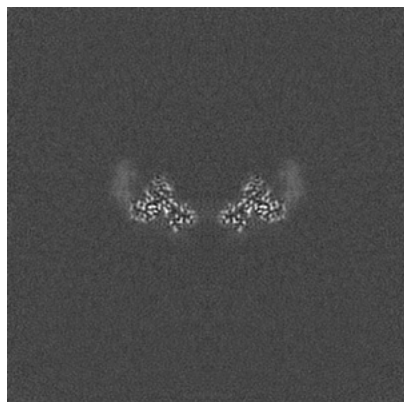


Y Index: 144

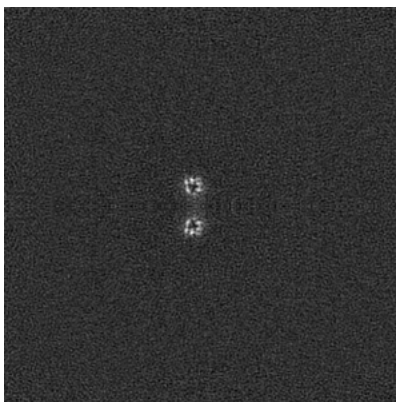


Z Index: 144

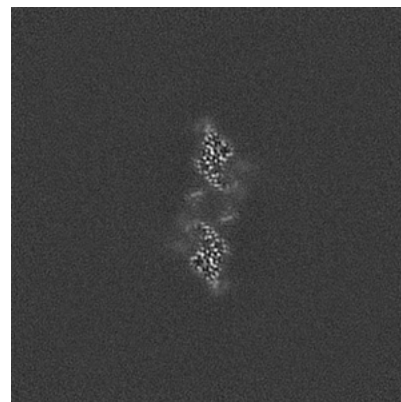
6.2.2 Raw map



X Index: 144



Y Index: 144

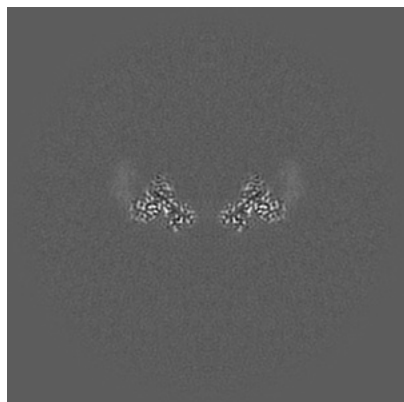


Z Index: 144

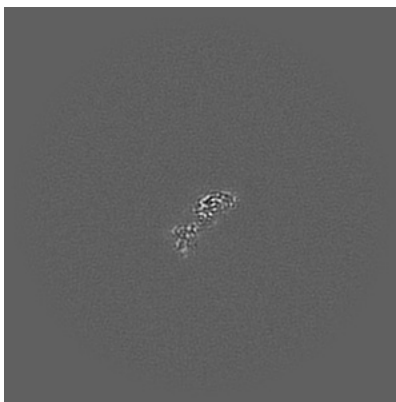
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

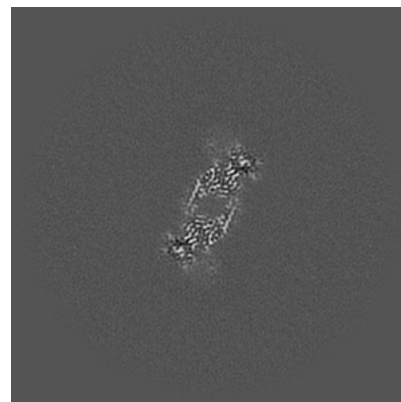
6.3.1 Primary map



X Index: 144

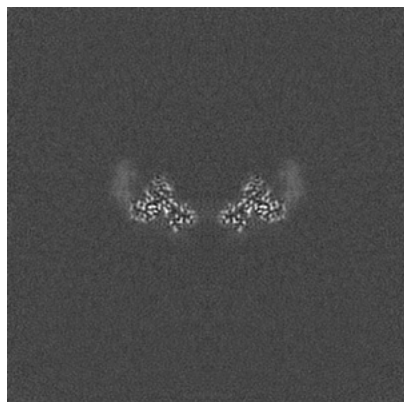


Y Index: 109

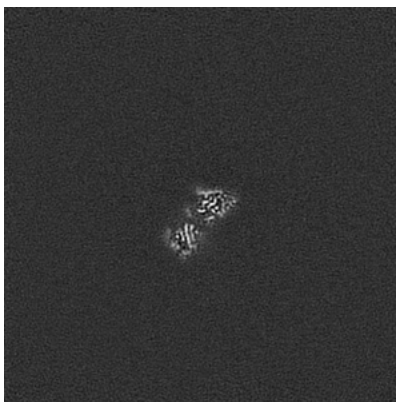


Z Index: 132

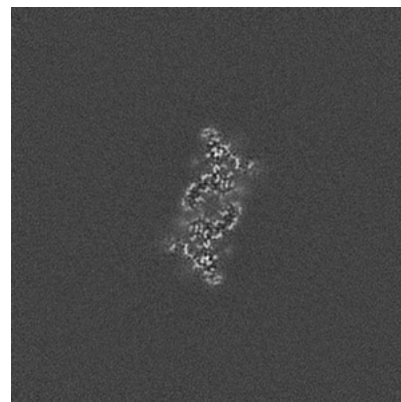
6.3.2 Raw map



X Index: 144



Y Index: 112

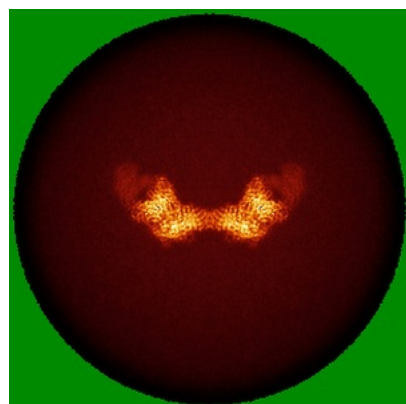


Z Index: 138

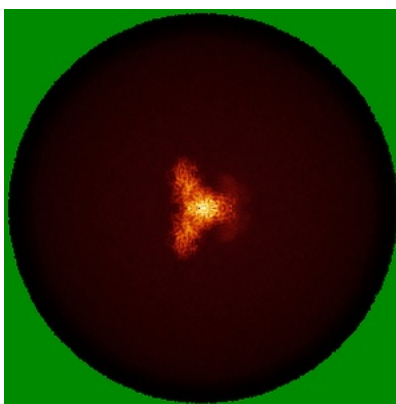
The images above show the largest variance slices of the map in three orthogonal directions.

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

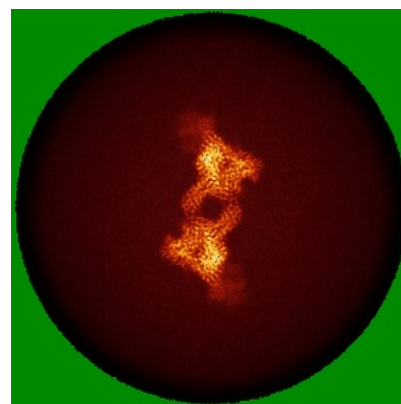
6.4.1 Primary map



X

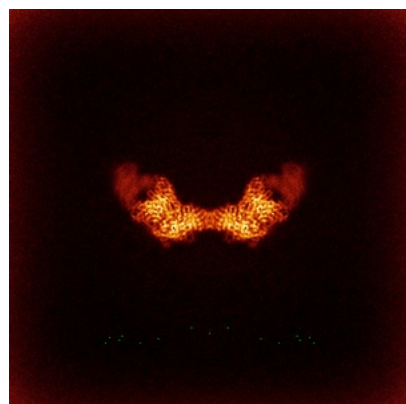


Y

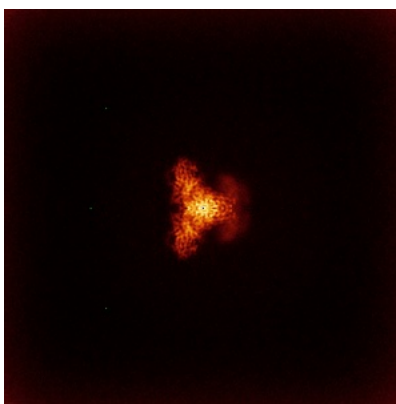


Z

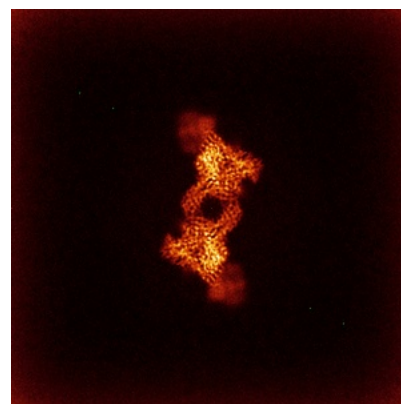
6.4.2 Raw map



X



Y

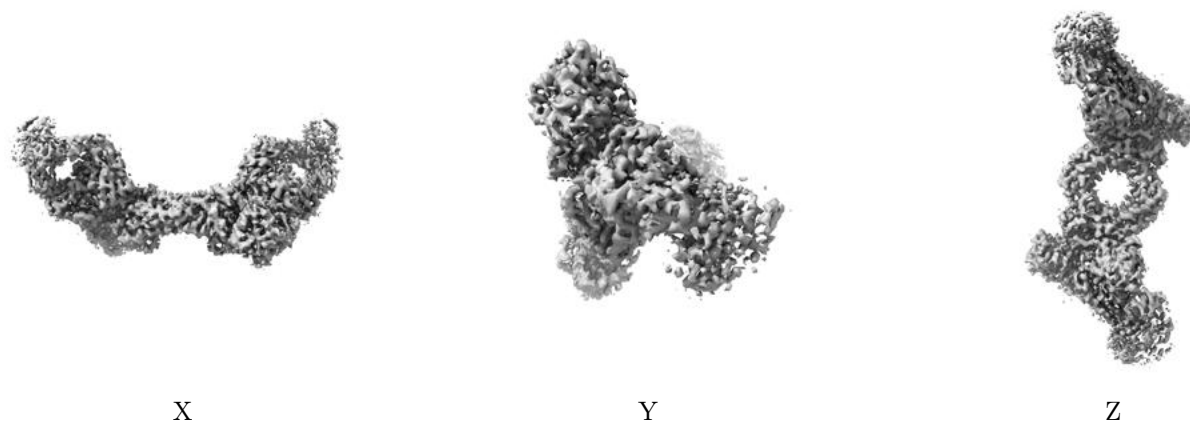


Z

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.

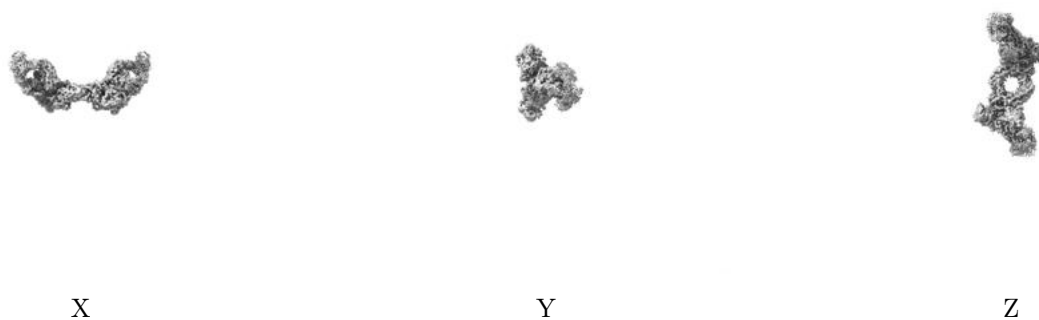
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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



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.

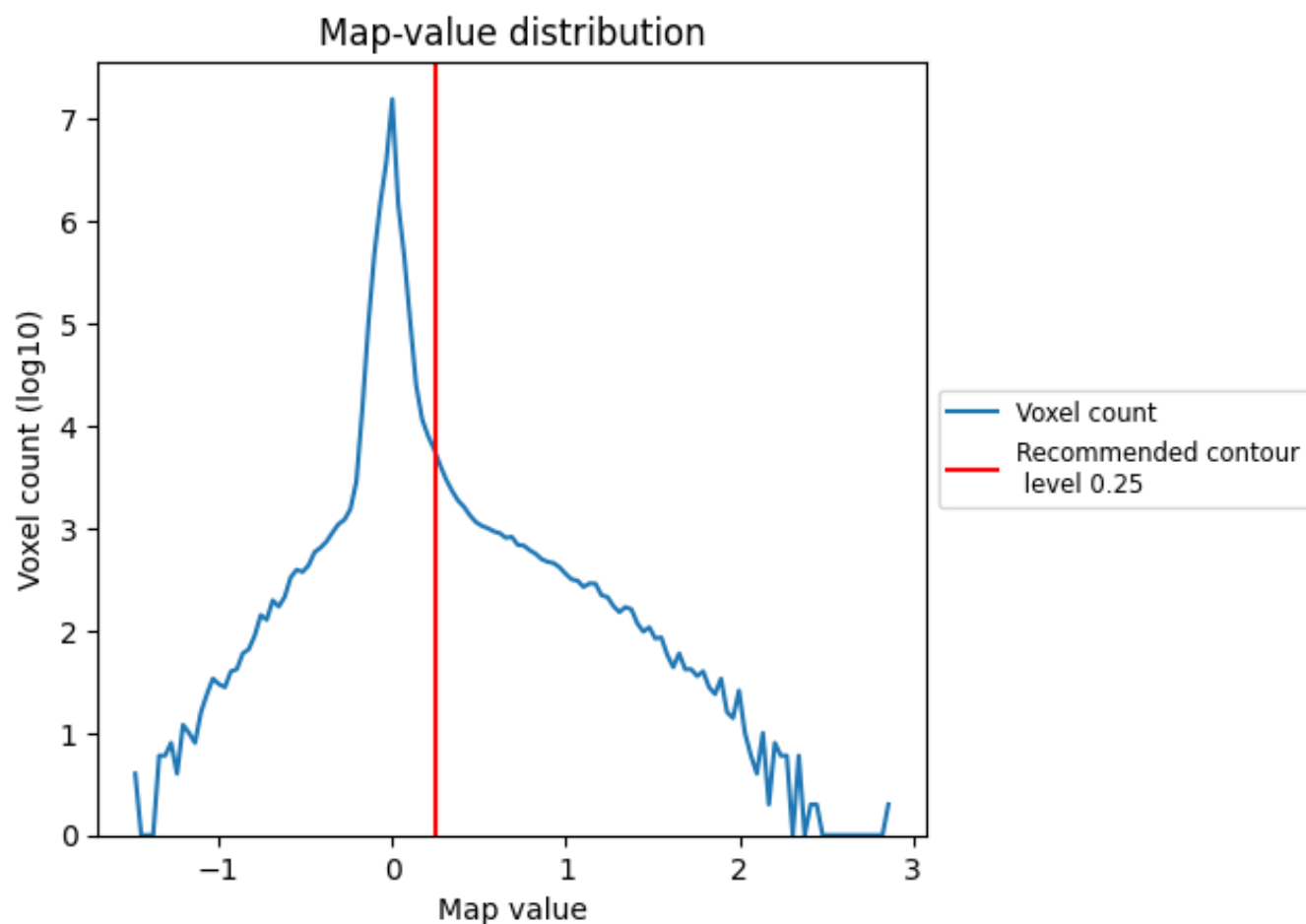
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

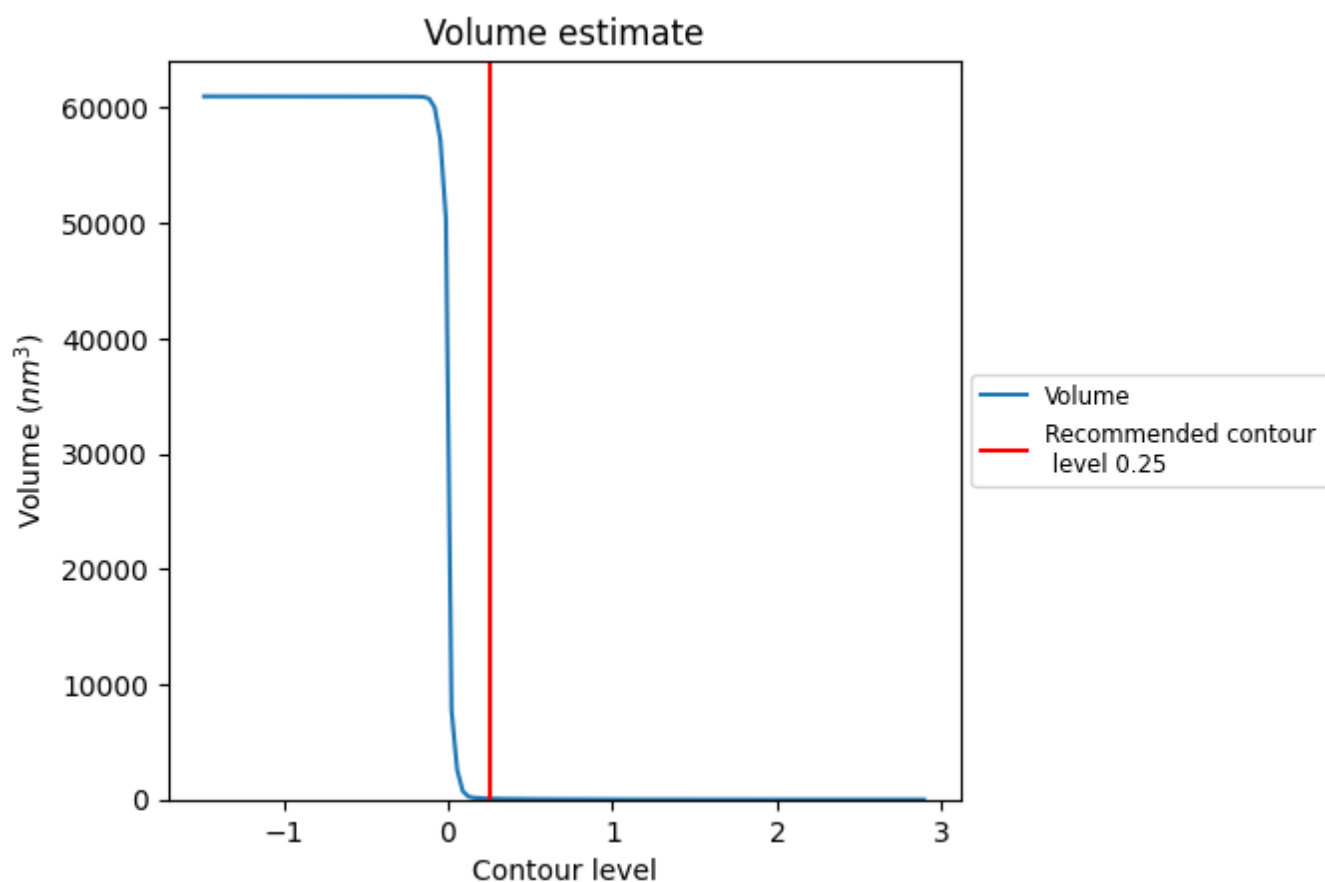
This section contains the results of statistical analysis of the map.

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.

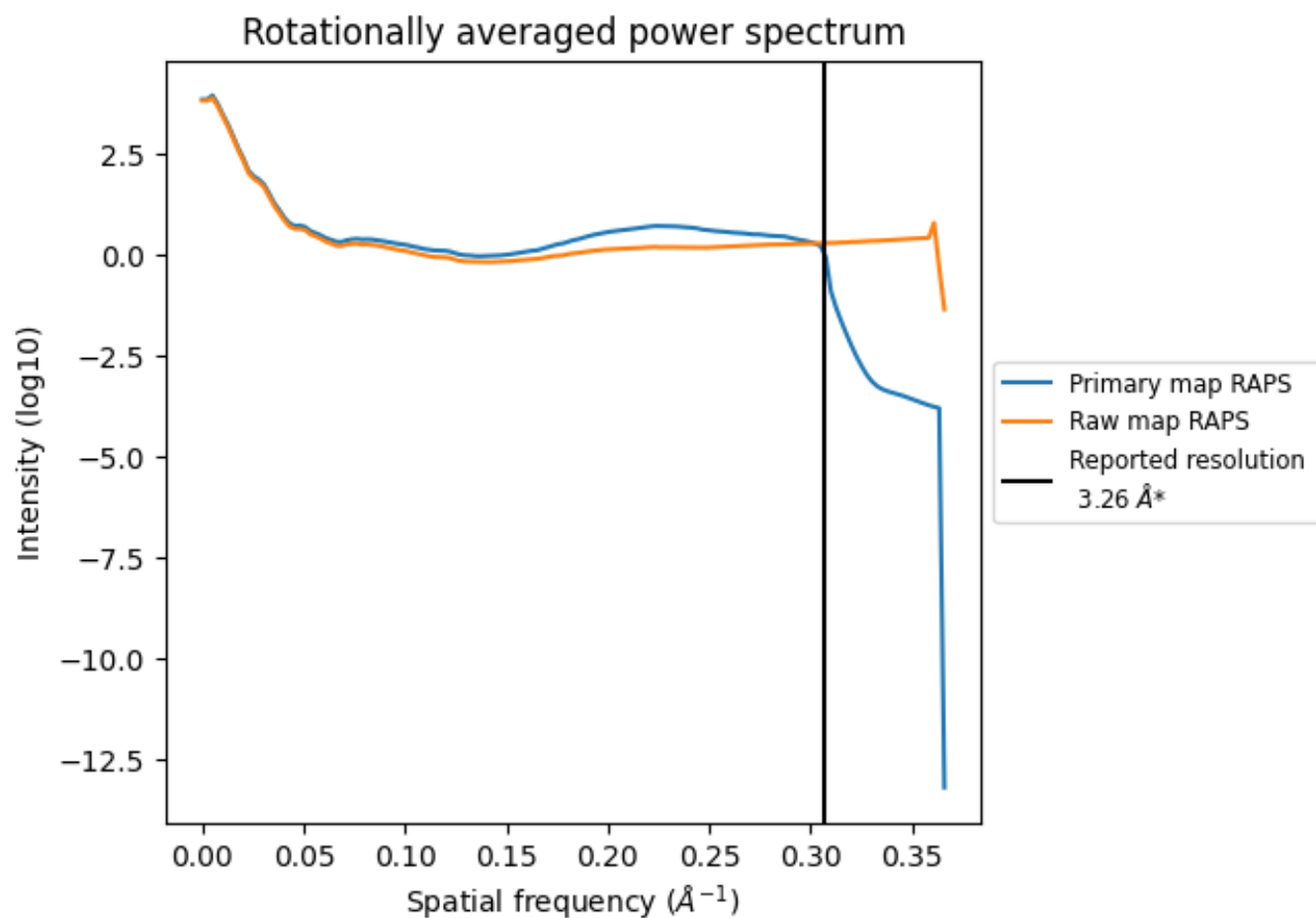
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 78 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

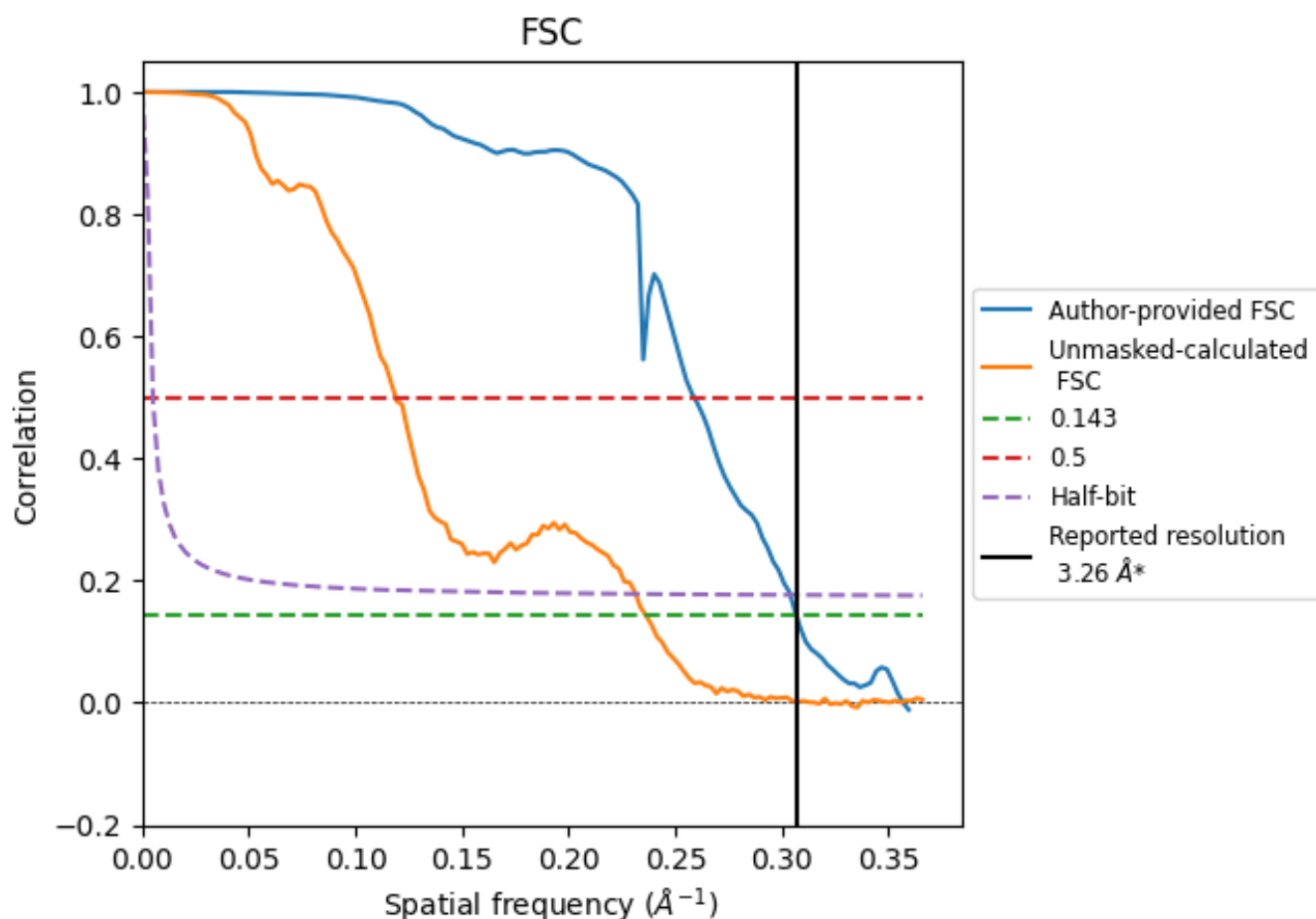


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 $0.307 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

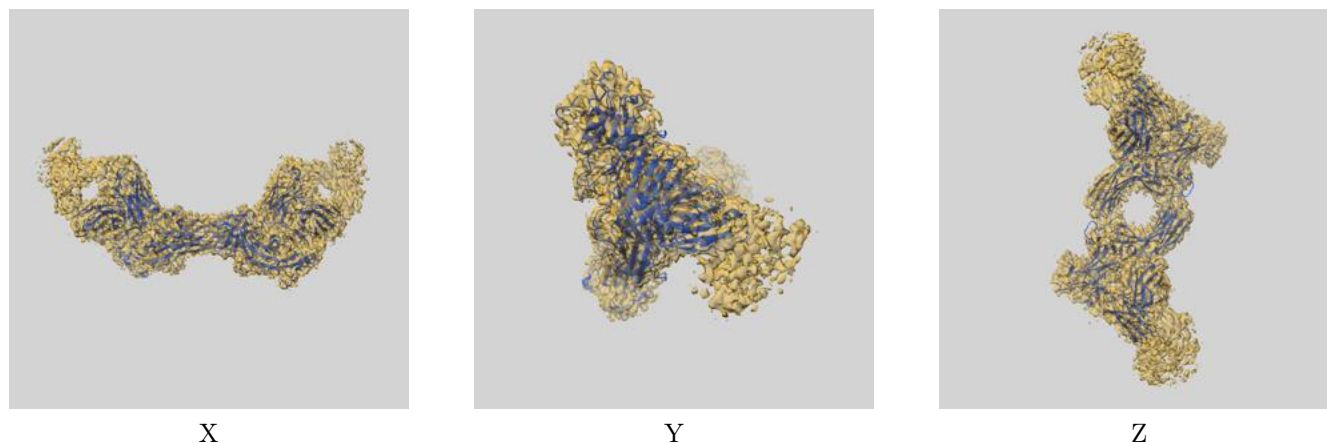
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.86	3.29
Unmasked-calculated*	4.23	8.42	4.32

*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 4.23 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

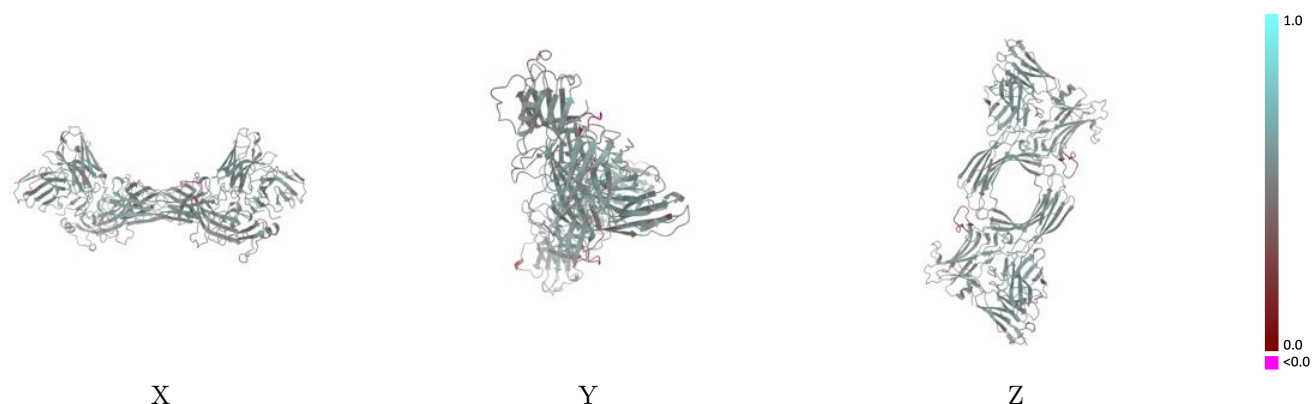
This section contains information regarding the fit between EMDB map EMD-35104 and PDB model 8I0N. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



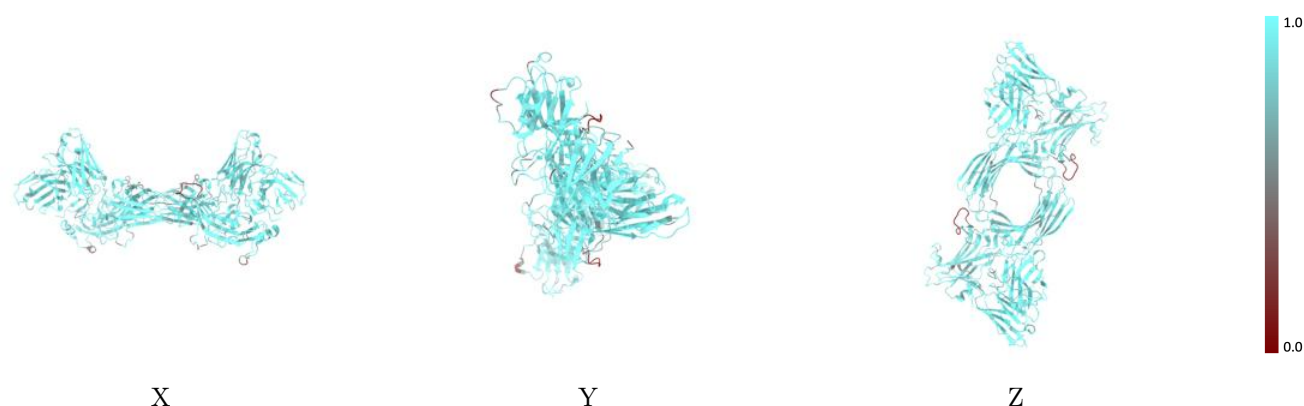
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



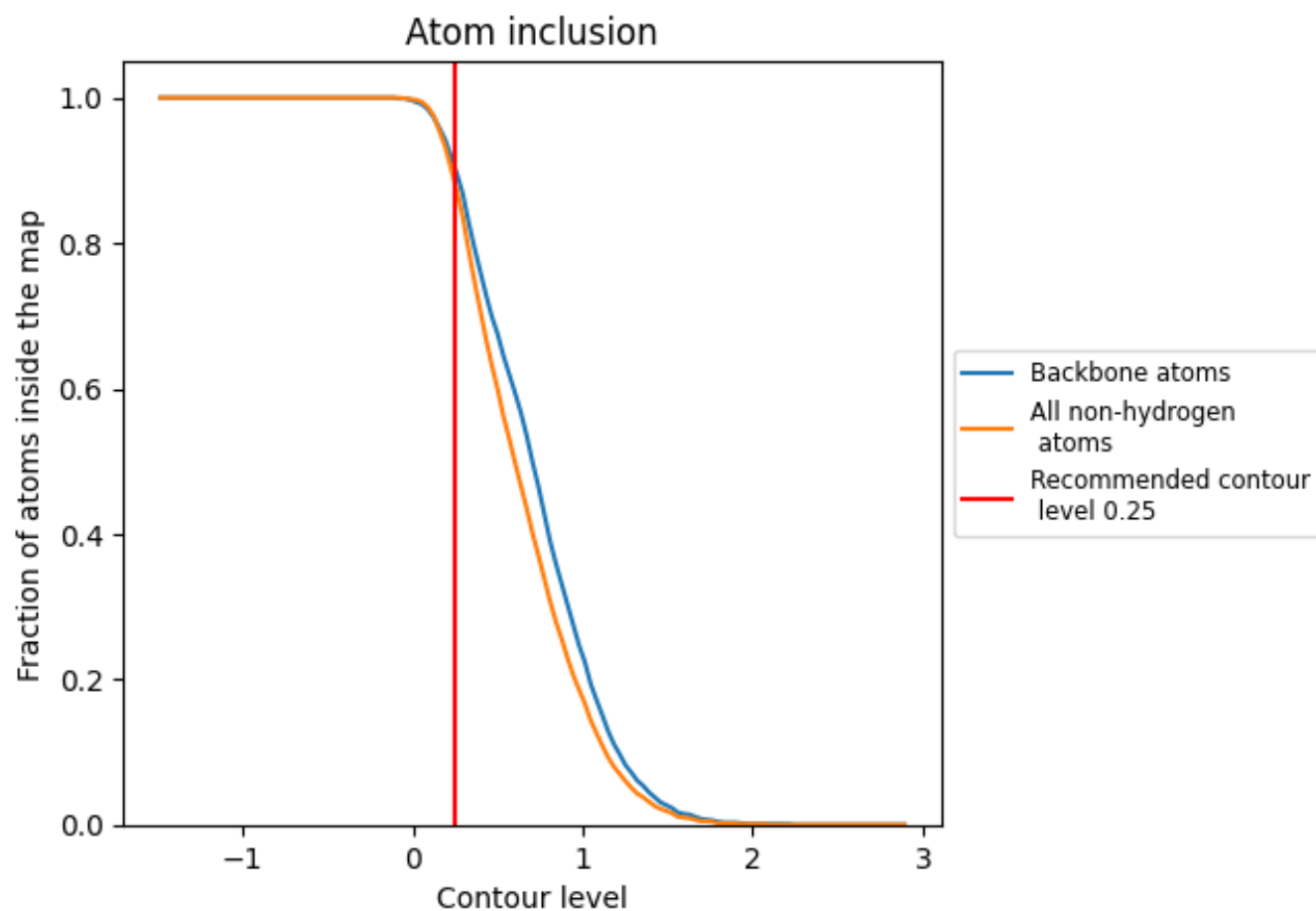
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.5130
A	0.8550	0.5020
B	0.8510	0.5020
H	0.9300	0.5360
I	0.9300	0.5350
L	0.9150	0.5260
M	0.9230	0.5270
U	0.9430	0.5020
V	0.9200	0.5000

1.0

0.0

<0.0