Full wwPDB EM Validation Report

Oct 19, 2026 – 04:38 PM JST

PDB ID	:	9UHX / pdb_00009uhx
EMDB ID	:	EMD-64179
Title	:	Cryo-EM structure of the human adenosine A2A receptor bound to the antagonist ZM-241385 resolved via the fusion/crosslinking strategy
Authors	:	Han, S.C.; Li, M.H.
Deposited on	:	2025-04-14
Resolution	:	3.03 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:

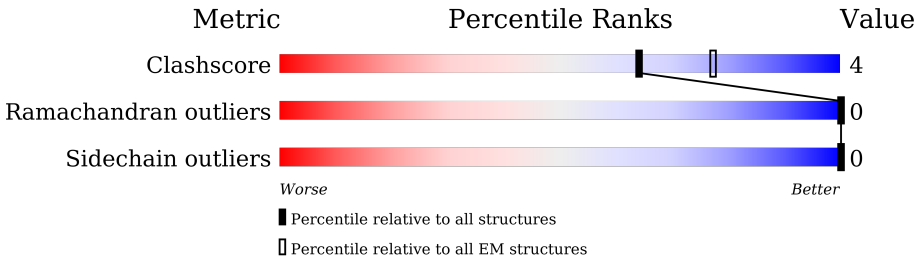
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

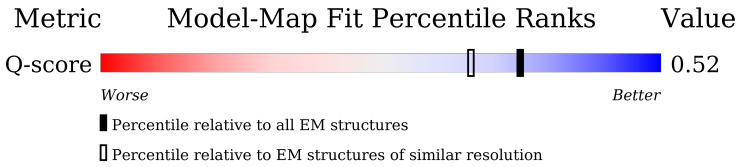
1 Overall quality at a glance

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

The reported resolution of this entry is 3.03 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	13929 (2.53 - 3.53)

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	331	83% 8% 8%
2	B	196	89% 10% ••
3	C	294	84% 14% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6128 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 Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	0	0
			2371	1569	391	391	20		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	GLY	-	linker	UNP P29274
A	1002	HIS	-	linker	UNP P29274
A	1003	TYR	-	linker	UNP P29274
A	1004	LEU	-	linker	UNP P29274
A	1005	SER	-	linker	UNP P29274
A	1006	THR	-	linker	UNP P29274
A	1007	GLN	-	linker	UNP P29274
A	1008	THR	-	linker	UNP P29274
A	1009	SER	-	linker	UNP P29274
A	1010	LEU	-	linker	UNP P29274
A	1011	SER	-	linker	UNP P29274
A	1012	LYS	-	linker	UNP P29274
A	1013	ASP	-	linker	UNP P29274
A	1014	LEU	-	linker	UNP P29274
A	1015	ASN	-	linker	UNP P29274
A	1016	GLU	-	linker	UNP P29274
A	1017	LYS	-	linker	UNP P29274
A	1018	ARG	-	linker	UNP P29274
A	1019	ASP	-	linker	UNP P29274
A	1020	HIS	-	linker	UNP P29274
A	1021	MET	-	linker	UNP P29274
A	1022	VAL	-	linker	UNP P29274
A	1023	LEU	-	linker	UNP P29274
A	1024	LEU	-	linker	UNP P29274
A	1025	GLU	-	linker	UNP P29274
A	1026	PHE	-	linker	UNP P29274
A	1027	VAL	-	linker	UNP P29274
A	1028	THR	-	linker	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1029	ALA	-	linker	UNP P29274
A	1030	ALA	-	linker	UNP P29274
A	1031	GLY	-	linker	UNP P29274

- Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total	C	N	O	S	0	0
			1569	999	269	296	5		

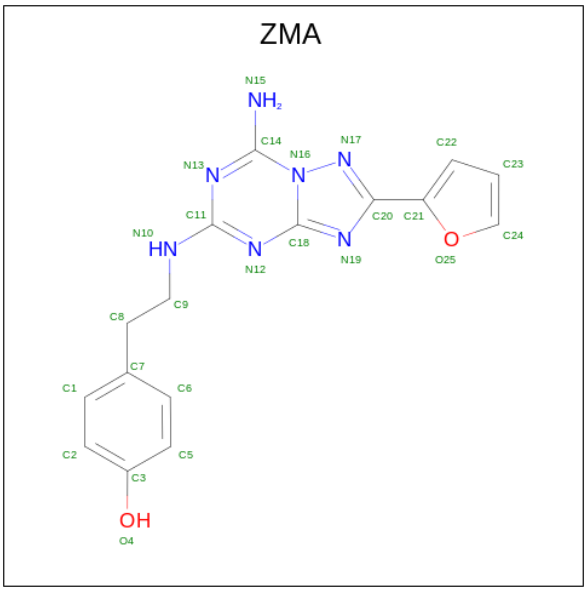
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A0A059PIQ0
B	2	GLY	-	expression tag	UNP A0A059PIQ0
B	3	THR	-	expression tag	UNP A0A059PIQ0
B	18	ILE	VAL	conflict	UNP A0A059PIQ0
B	32	ARG	SER	conflict	UNP A0A059PIQ0
B	41	TYR	ASN	conflict	UNP A0A059PIQ0
B	68	CRO	THR	conflict	UNP A0A059PIQ0
B	?	-	TYR	deletion	UNP A0A059PIQ0
B	?	-	GLY	deletion	UNP A0A059PIQ0
B	74	SER	ALA	conflict	UNP A0A059PIQ0
B	82	ARG	GLN	conflict	UNP A0A059PIQ0
B	101	TYR	SER	conflict	UNP A0A059PIQ0
B	155	MET	THR	conflict	UNP A0A059PIQ0
B	160	ASN	LYS	conflict	UNP A0A059PIQ0

- Molecule 3 is a protein called GFP-clamp.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	287	Total	C	N	O	S	0	0
			2163	1369	370	423	1		

- Molecule 4 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino] ethyl}phenol (CCD ID: ZMA) (formula: $C_{16}H_{15}N_7O_2$) (labeled as "Ligand of Interest" by depositor).



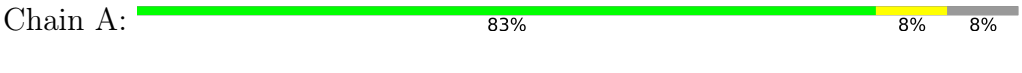
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	25	16	7	2	0

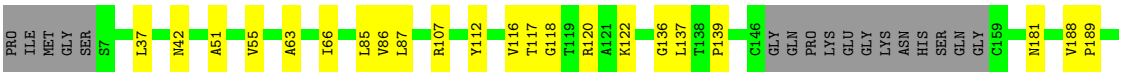
3 Residue-property plots (i)

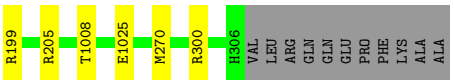
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Adenosine receptor A2a

Chain A:

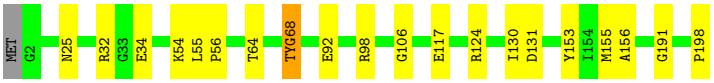






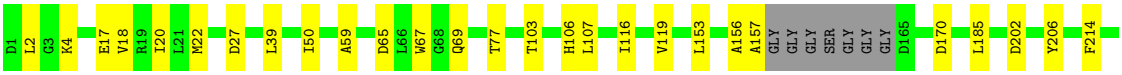
• Molecule 2: Green fluorescent protein

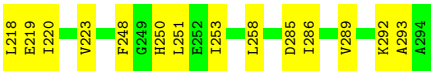
Chain B:



• Molecule 3: GFP-clamp

Chain C:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229906	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.503	Depositor
Minimum map value	-4.830	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRO, ZMA

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	0.15	0/2429	0.31	0/3313
2	B	0.46	2/1582 (0.1%)	0.51	3/2135 (0.1%)
3	C	0.33	0/2202	0.40	1/3000 (0.0%)
All	All	0.32	2/6213 (0.0%)	0.40	4/8448 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	LEU	CA-C	-7.61	1.44	1.52
2	B	54	LYS	CA-C	-6.90	1.43	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	153	LEU	N-CA-C	6.78	118.75	111.36
2	B	55	LEU	N-CA-C	-6.68	101.24	109.65
2	B	56	PRO	CA-C-N	5.73	129.77	121.68
2	B	56	PRO	C-N-CA	5.73	129.77	121.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2371	0	2441	17	0
2	B	1569	0	1528	10	0
3	C	2163	0	2115	25	0
4	A	25	0	15	1	0
All	All	6128	0	6099	50	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 (50) 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)
2:B:68:CRO:HB2	2:B:98:ARG:HH22	1.62	0.63
2:B:32:ARG:NH1	2:B:34:GLU:OE2	2.34	0.60
3:C:250:HIS:HB3	3:C:253:ILE:HD13	1.84	0.59
1:A:270:MET:HE2	4:A:1101:ZMA:H6	1.86	0.57
3:C:156:ALA:O	3:C:157:ALA:C	2.47	0.56
2:B:156:ALA:HB2	2:B:198:PRO:HG2	1.87	0.54
1:A:37:LEU:O	1:A:42:ASN:ND2	2.42	0.53
1:A:117:THR:HG22	1:A:120:ARG:HG3	1.90	0.52
3:C:39:LEU:HD11	3:C:59:ALA:HB1	1.92	0.52
3:C:202:ASP:OD1	3:C:206:TYR:N	2.43	0.52
2:B:64:THR:O	2:B:98:ARG:NH1	2.44	0.51
3:C:2:LEU:HD11	3:C:27:ASP:H	1.75	0.51
1:A:55:VAL:HG22	1:A:87:LEU:HD13	1.95	0.48
3:C:77:THR:OG1	3:C:107:LEU:HD23	2.13	0.48
3:C:285:ASP:N	3:C:285:ASP:OD1	2.47	0.48
2:B:25:ASN:H	2:B:130:ILE:HG22	1.79	0.48
3:C:18:VAL:O	3:C:22:MET:HG2	2.14	0.47
3:C:116:ILE:HA	3:C:119:VAL:HG12	1.96	0.47
3:C:220:ILE:HA	3:C:223:VAL:HG12	1.96	0.47
2:B:92:GLU:HG2	2:B:191:GLY:HA3	1.97	0.47
3:C:103:THR:OG1	3:C:106:HIS:ND1	2.40	0.47
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.80	0.46
3:C:4:LYS:H	3:C:4:LYS:HD2	1.81	0.46
1:A:118:GLY:O	1:A:122:LYS:HG2	2.16	0.45
3:C:185:LEU:HD22	3:C:219:GLU:HG3	1.99	0.45
3:C:170:ASP:OD1	3:C:170:ASP:N	2.47	0.45
1:A:1008:THR:HG22	1:A:1025:GLU:HG3	1.98	0.44
2:B:106:GLY:HA2	2:B:131:ASP:HB3	1.99	0.44
3:C:17:GLU:HA	3:C:20:ILE:HG12	1.99	0.44
1:A:300:ARG:HH11	1:A:300:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HA	1:A:107:ARG:HD2	1.86	0.43
2:B:153:TYR:HB3	3:C:214:PHE:CZ	2.53	0.43
1:A:205:ARG:HG3	1:A:205:ARG:O	2.19	0.43
3:C:65:ASP:C	3:C:67:TRP:H	2.25	0.43
1:A:85:LEU:HD22	1:A:181:ASN:HD21	1.83	0.43
1:A:112:TYR:O	1:A:116:VAL:HG22	2.19	0.43
1:A:51:ALA:O	1:A:55:VAL:HG23	2.19	0.43
3:C:258:LEU:HD21	3:C:293:ALA:HB2	2.01	0.43
2:B:117:GLU:OE2	2:B:124:ARG:NH2	2.52	0.42
2:B:155:MET:HE3	3:C:248:PHE:HB3	2.00	0.42
3:C:285:ASP:O	3:C:289:VAL:HG23	2.19	0.42
3:C:292:LYS:HA	3:C:292:LYS:HD2	1.92	0.41
1:A:86:VAL:HG22	1:A:136:GLY:HA3	2.01	0.41
3:C:218:LEU:HD12	3:C:253:ILE:HG13	2.01	0.41
1:A:63:ALA:HA	1:A:66:ILE:HG22	2.03	0.41
3:C:69:GLN:H	3:C:69:GLN:HG2	1.73	0.41
1:A:137:LEU:C	1:A:139:PRO:HD2	2.46	0.40
3:C:18:VAL:HG21	3:C:50:ILE:HD12	2.03	0.40
1:A:188:VAL:HB	1:A:189:PRO:HD3	2.03	0.40
3:C:251:LEU:HD13	3:C:286:ILE:HG12	2.02	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	299/331 (90%)	291 (97%)	8 (3%)	0	100	100
2	B	190/196 (97%)	182 (96%)	8 (4%)	0	100	100
3	C	283/294 (96%)	273 (96%)	10 (4%)	0	100	100
All	All	772/821 (94%)	746 (97%)	26 (3%)	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	256/278 (92%)	256 (100%)	0	100	100
2	B	168/169 (99%)	168 (100%)	0	100	100
3	C	217/218 (100%)	217 (100%)	0	100	100
All	All	641/665 (96%)	641 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	226	GLN
1	A	230	HIS
1	A	250	HIS
3	C	47	HIS
3	C	62	ASN
3	C	90	ASN
3	C	113	HIS
3	C	146	ASN
3	C	250	HIS
3	C	281	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CRO	B	68	2	23,23,24	2.68	8 (34%)	30,32,34	2.82	7 (23%)

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	CRO	B	68	2	-	1/12/31/32	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	CRO	C1-N2	7.13	1.42	1.32
2	B	68	CRO	CA2-C2	5.83	1.54	1.48
2	B	68	CRO	C1-N3	5.29	1.46	1.37
2	B	68	CRO	C2-N3	3.69	1.48	1.39
2	B	68	CRO	CG2-CB2	3.57	1.53	1.46
2	B	68	CRO	CB2-CA2	-2.84	1.32	1.35
2	B	68	CRO	CA2-N2	2.23	1.43	1.38
2	B	68	CRO	O2-C2	-2.08	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	68	CRO	CA2-C2-N3	8.61	107.44	103.37
2	B	68	CRO	O2-C2-CA2	-8.38	126.26	130.96
2	B	68	CRO	C2-N3-C1	-5.41	105.23	107.97
2	B	68	CRO	CA2-N2-C1	4.79	109.30	105.77
2	B	68	CRO	C2-CA2-N2	-3.80	106.27	108.93
2	B	68	CRO	CG2-CB2-CA2	-3.07	126.18	129.94
2	B	68	CRO	O3-C3-CA3	-2.27	119.53	126.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	68	CRO	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	68	CRO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	ZMA	A	1101	-	25,28,28	4.44	12 (48%)	29,39,39	2.32	6 (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	ZMA	A	1101	-	-	5/10/10/10	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ZMA	C18-N12	8.40	1.50	1.34
4	A	1101	ZMA	C2-C1	7.85	1.53	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	ZMA	C6-C5	7.72	1.52	1.38
4	A	1101	ZMA	C5-C3	7.38	1.53	1.38
4	A	1101	ZMA	C2-C3	7.34	1.52	1.38
4	A	1101	ZMA	C1-C7	6.55	1.53	1.38
4	A	1101	ZMA	C6-C7	6.54	1.52	1.38
4	A	1101	ZMA	C14-N15	6.19	1.45	1.34
4	A	1101	ZMA	C14-N13	4.89	1.43	1.34
4	A	1101	ZMA	C18-N16	-3.64	1.33	1.38
4	A	1101	ZMA	C11-N12	3.07	1.43	1.34
4	A	1101	ZMA	C11-N13	3.04	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1101	ZMA	C18-N19-C20	7.12	108.00	102.92
4	A	1101	ZMA	N17-C20-N19	-6.74	108.08	115.21
4	A	1101	ZMA	N13-C11-N12	-3.31	120.16	126.64
4	A	1101	ZMA	C18-N16-N17	-2.93	108.03	110.39
4	A	1101	ZMA	N16-C18-N12	-2.80	119.99	122.64
4	A	1101	ZMA	N12-C18-N19	2.55	132.03	127.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	ZMA	N17-C20-C21-O25
4	A	1101	ZMA	N19-C20-C21-C22
4	A	1101	ZMA	N19-C20-C21-O25
4	A	1101	ZMA	N17-C20-C21-C22
4	A	1101	ZMA	C8-C9-N10-C11

There are no ring outliers.

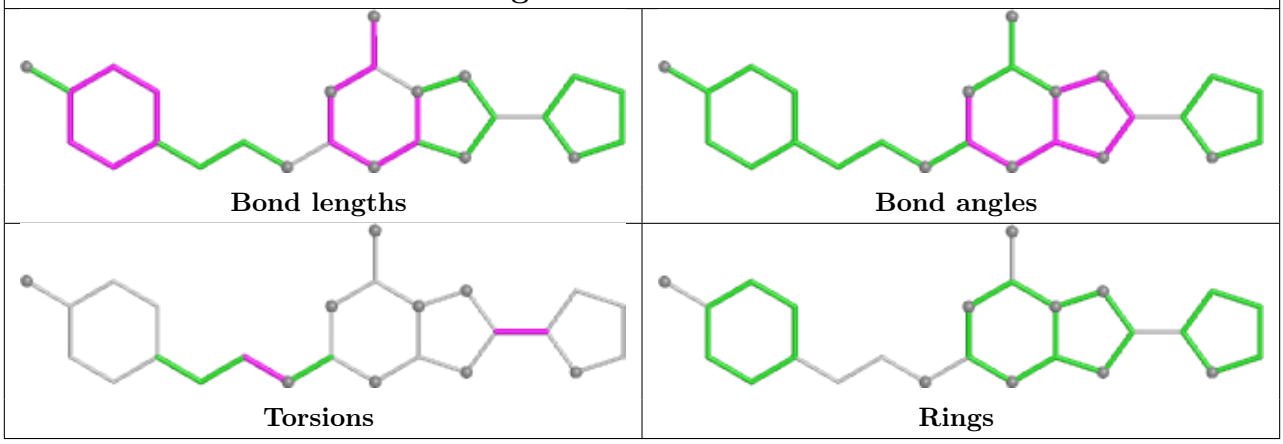
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	ZMA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

Ligand ZMA A 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

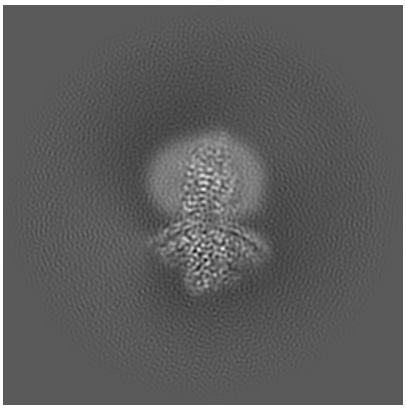
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64179. These allow visual inspection of the internal detail of the map and identification of artifacts.

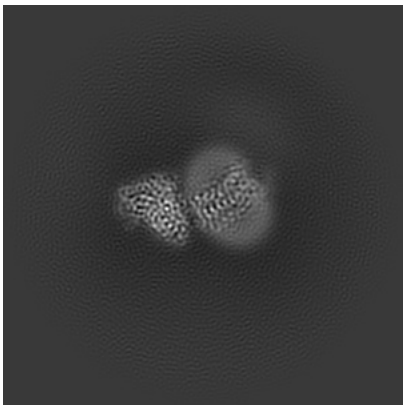
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

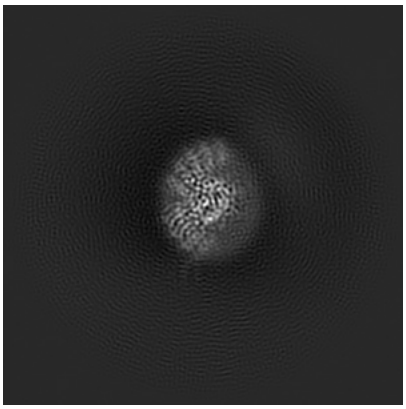
6.1.1 Primary map



X

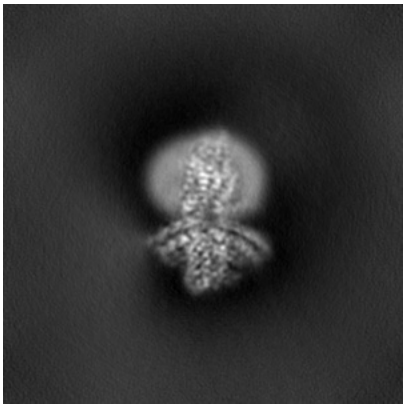


Y

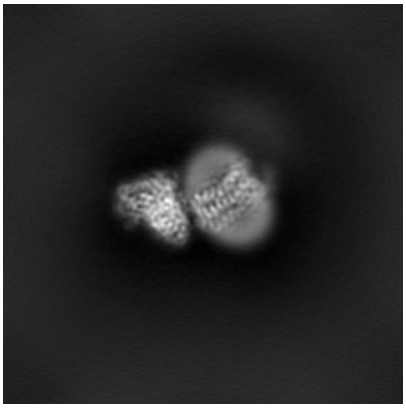


Z

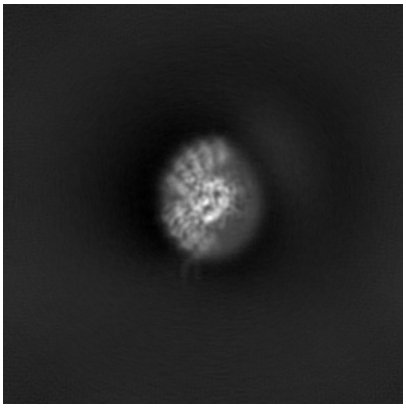
6.1.2 Raw map



X



Y

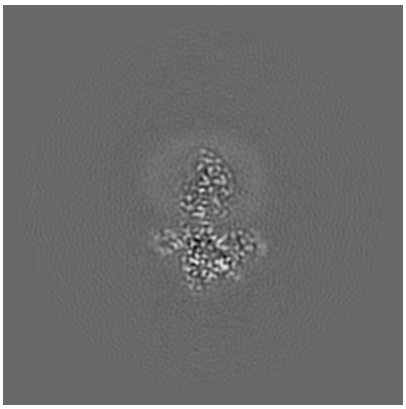


Z

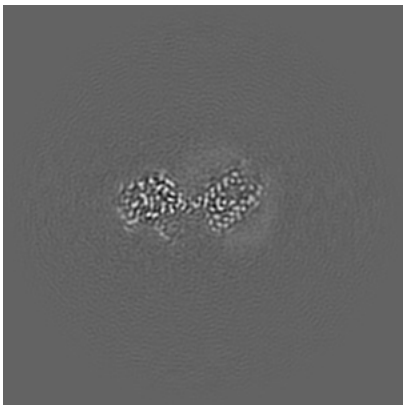
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

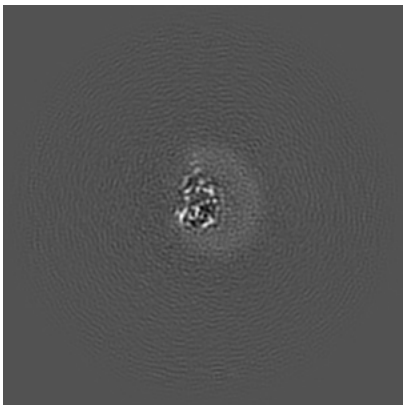
6.2.1 Primary map



X Index: 128

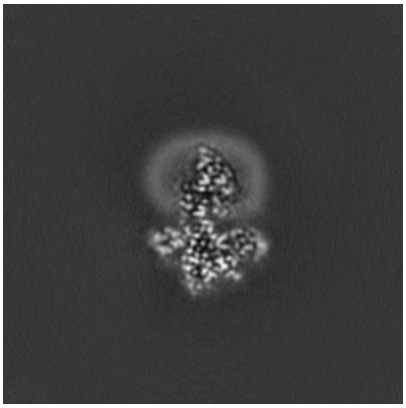


Y Index: 128

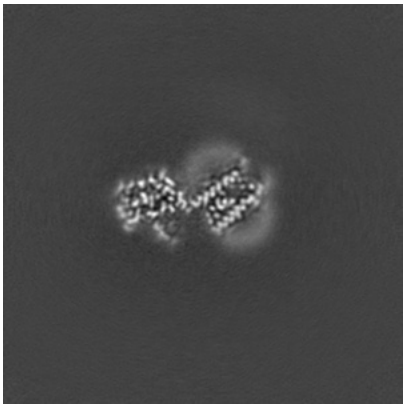


Z Index: 128

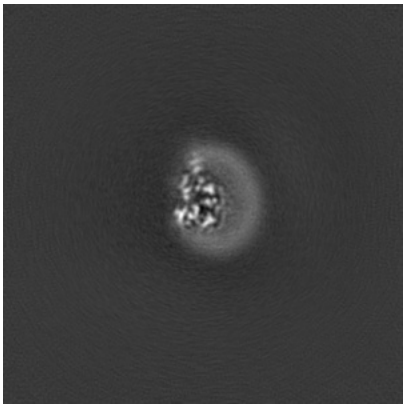
6.2.2 Raw map



X Index: 128



Y Index: 128

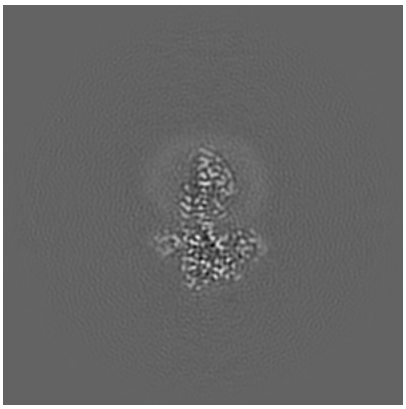


Z Index: 128

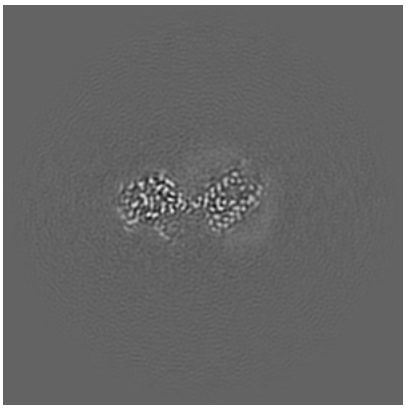
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

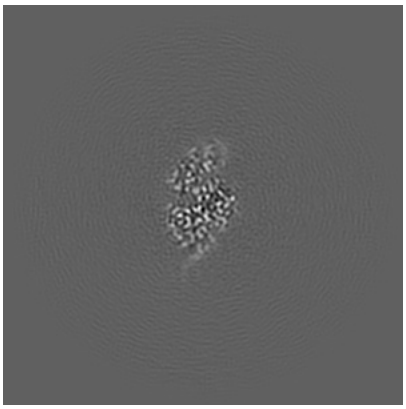
6.3.1 Primary map



X Index: 129

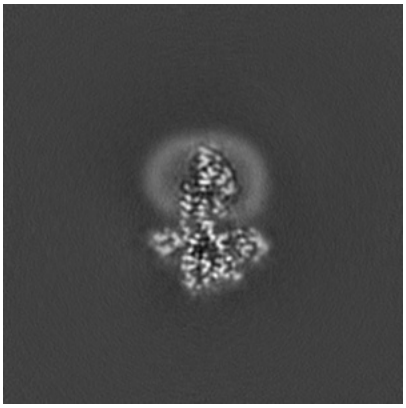


Y Index: 128

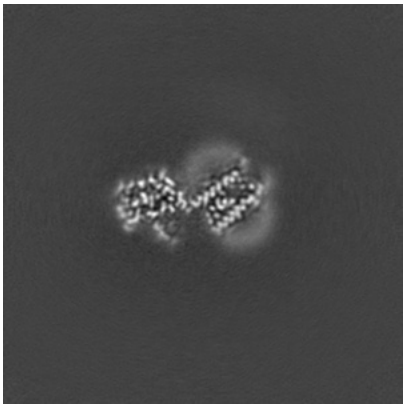


Z Index: 104

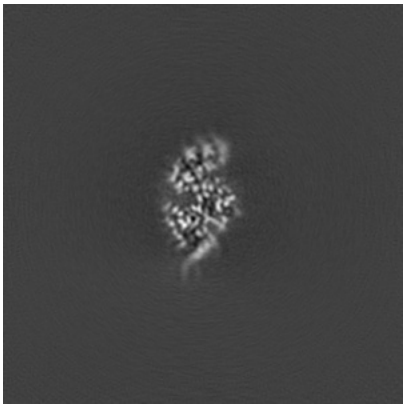
6.3.2 Raw map



X Index: 129



Y Index: 128

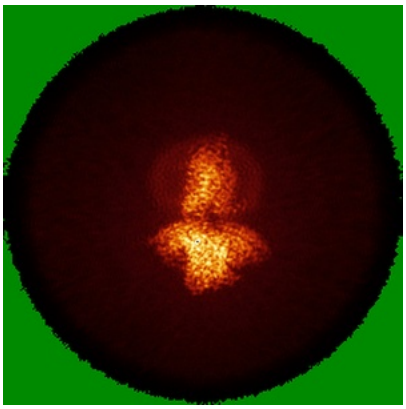


Z Index: 105

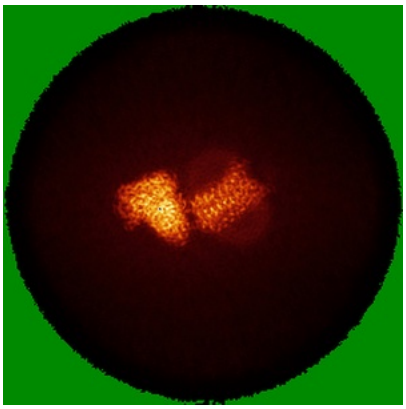
The images above show the largest variance slices of the map in three orthogonal directions.

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

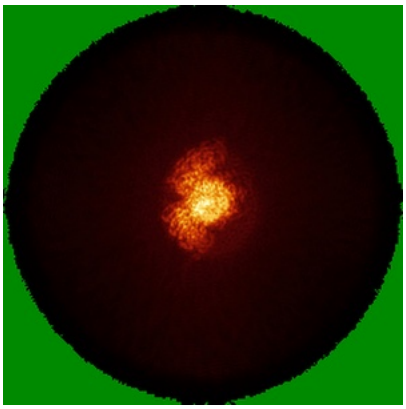
6.4.1 Primary map



X

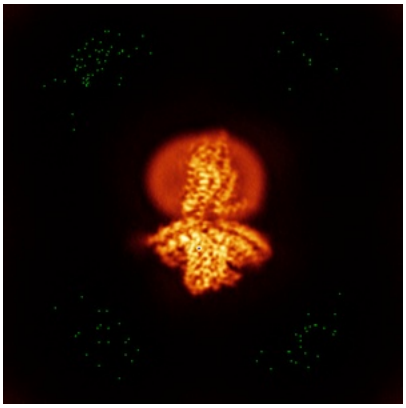


Y

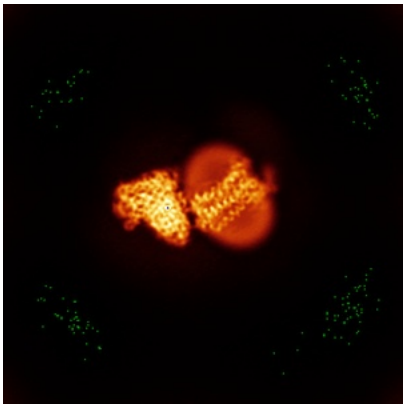


Z

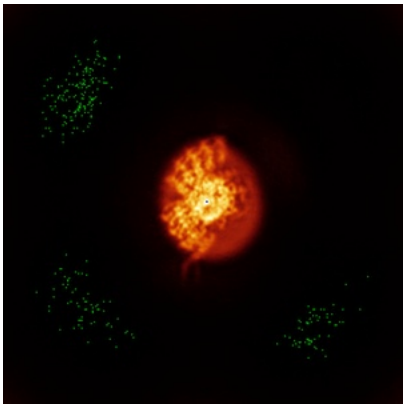
6.4.2 Raw map



X



Y

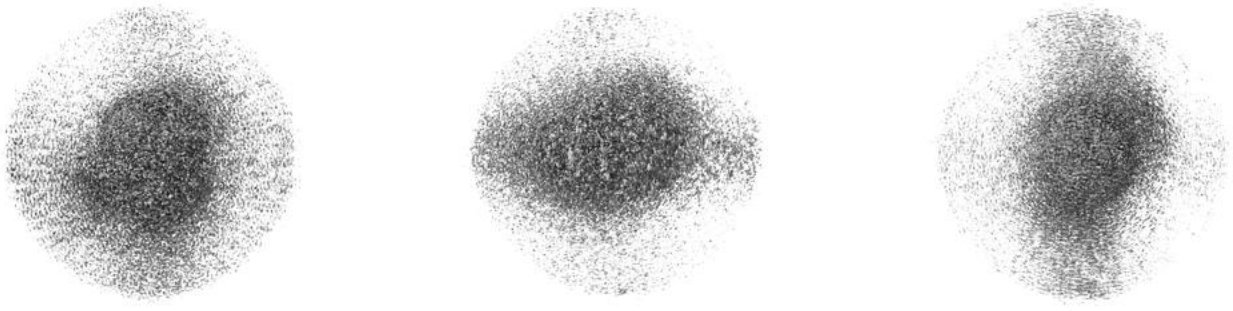


Z

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 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

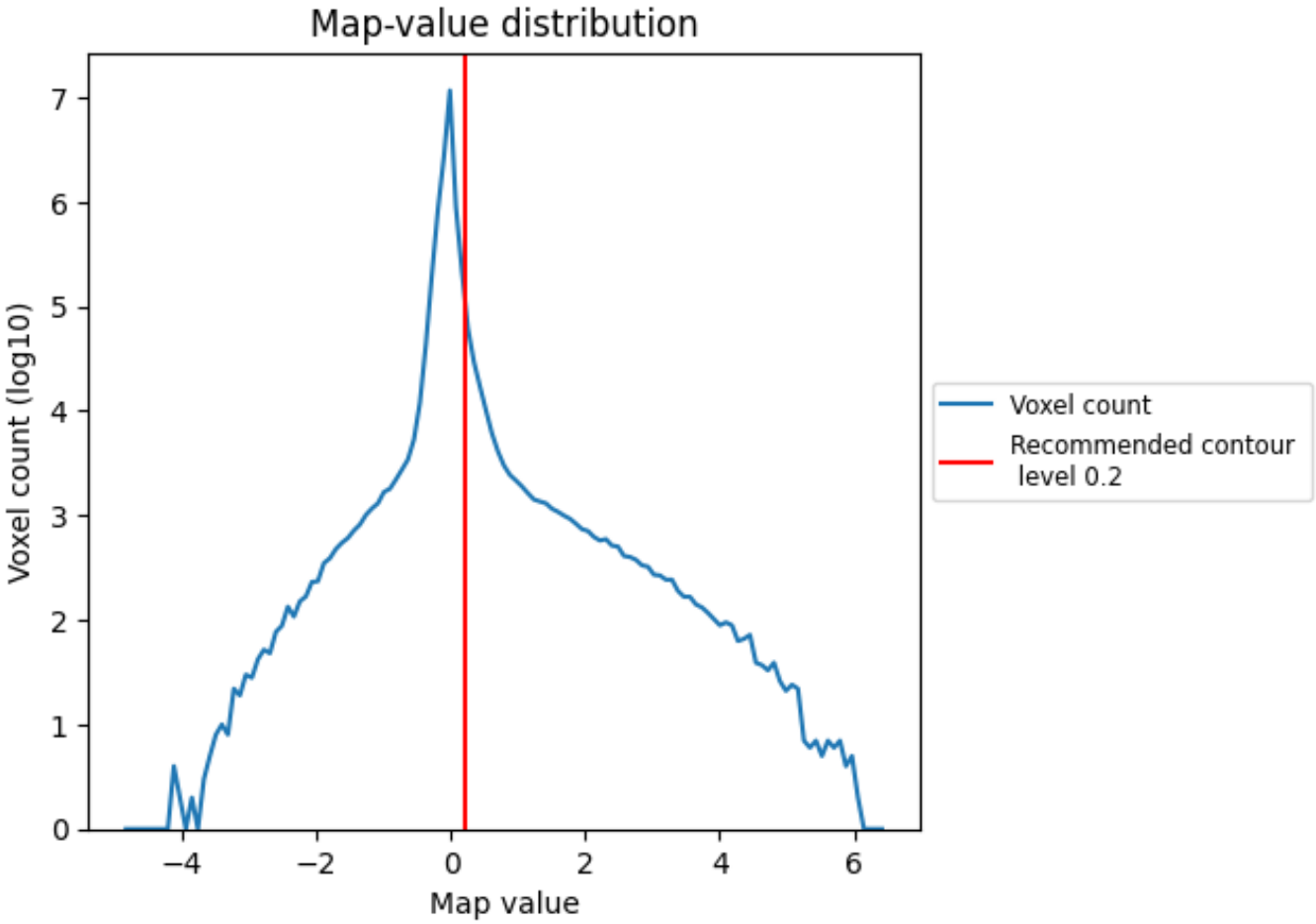
6.6 Mask visualisation (i)

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

7 Map analysis

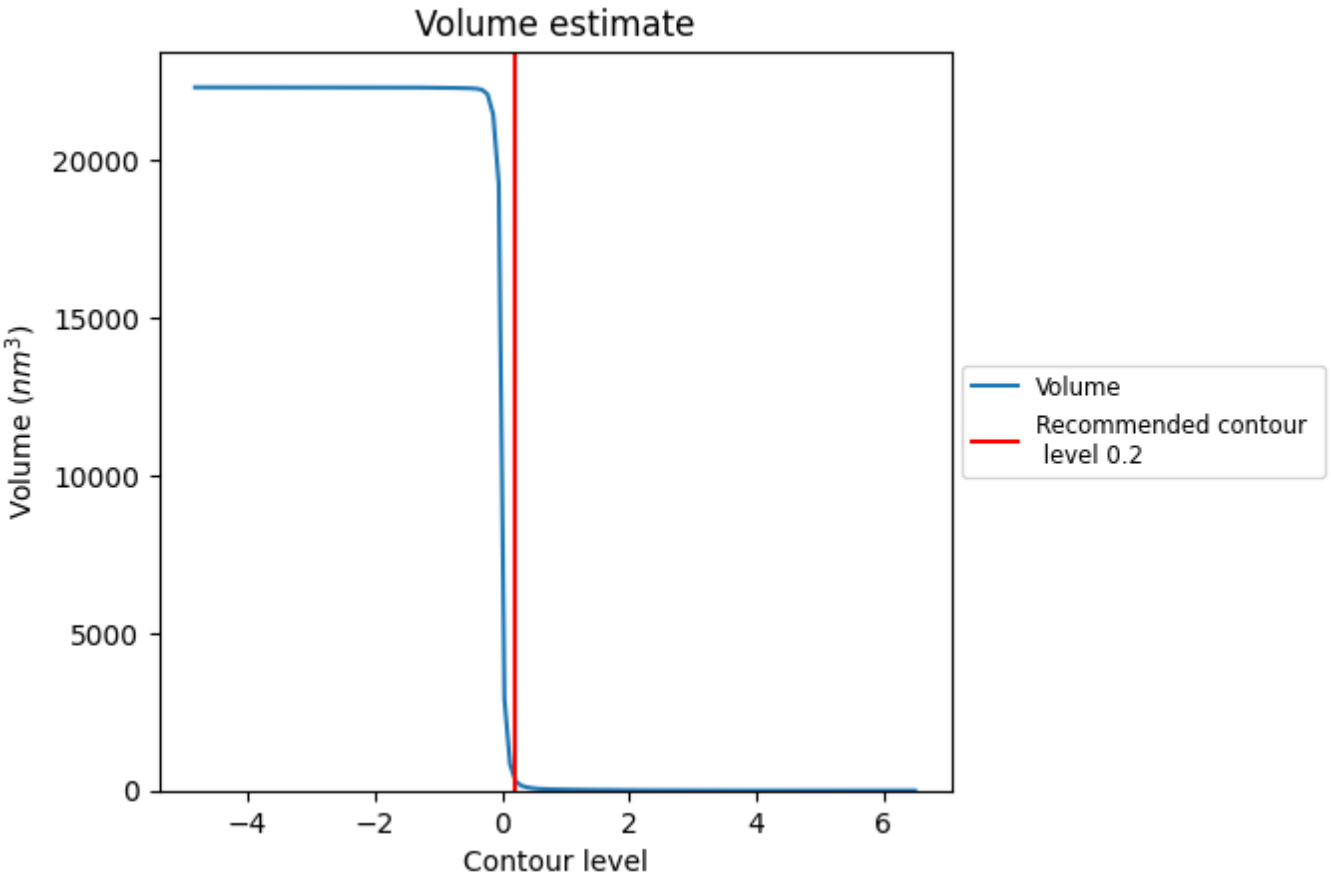
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

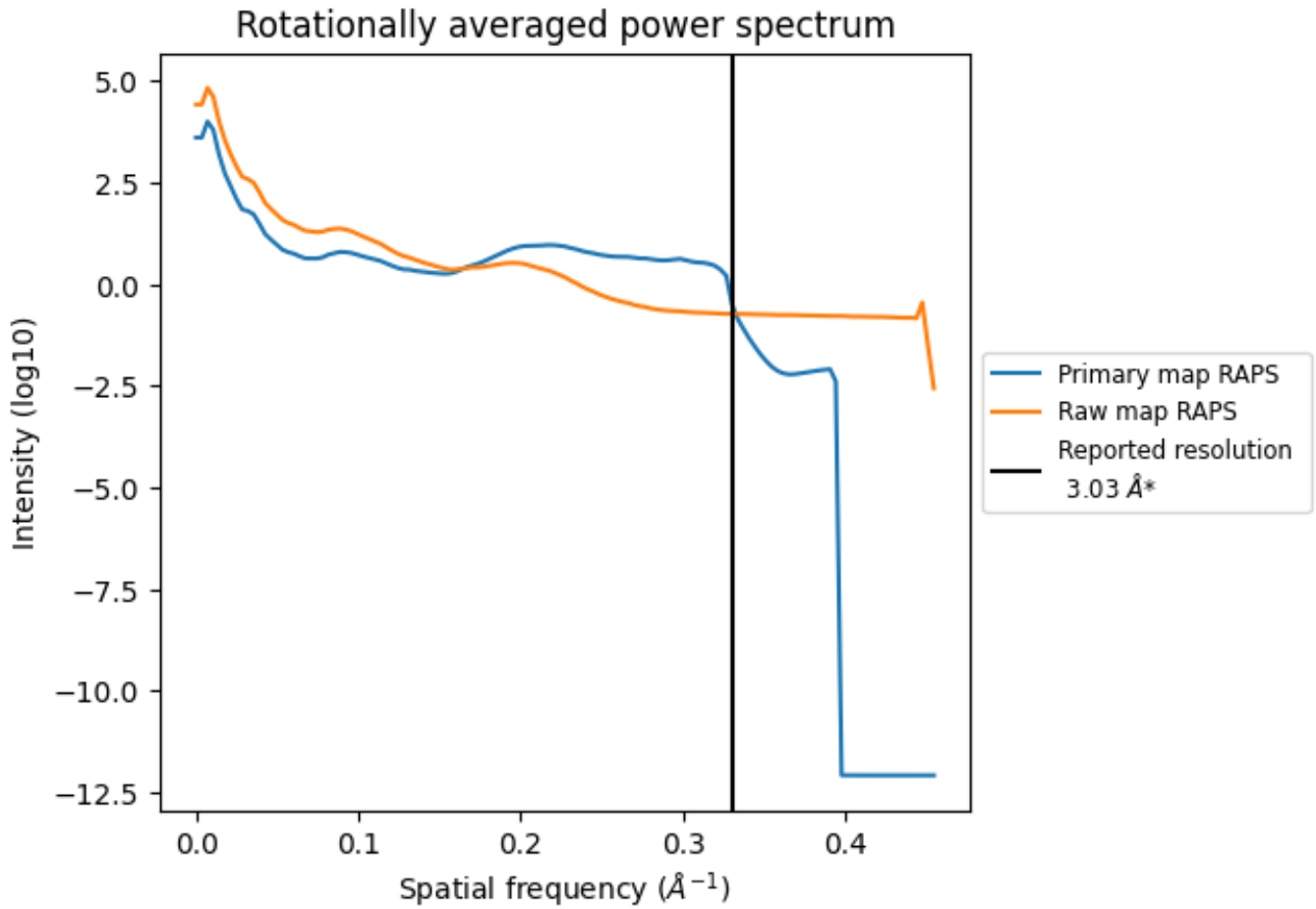
7.2 Volume estimate



The volume at the recommended contour level is 396 nm^3; this corresponds to an approximate mass of 358 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)

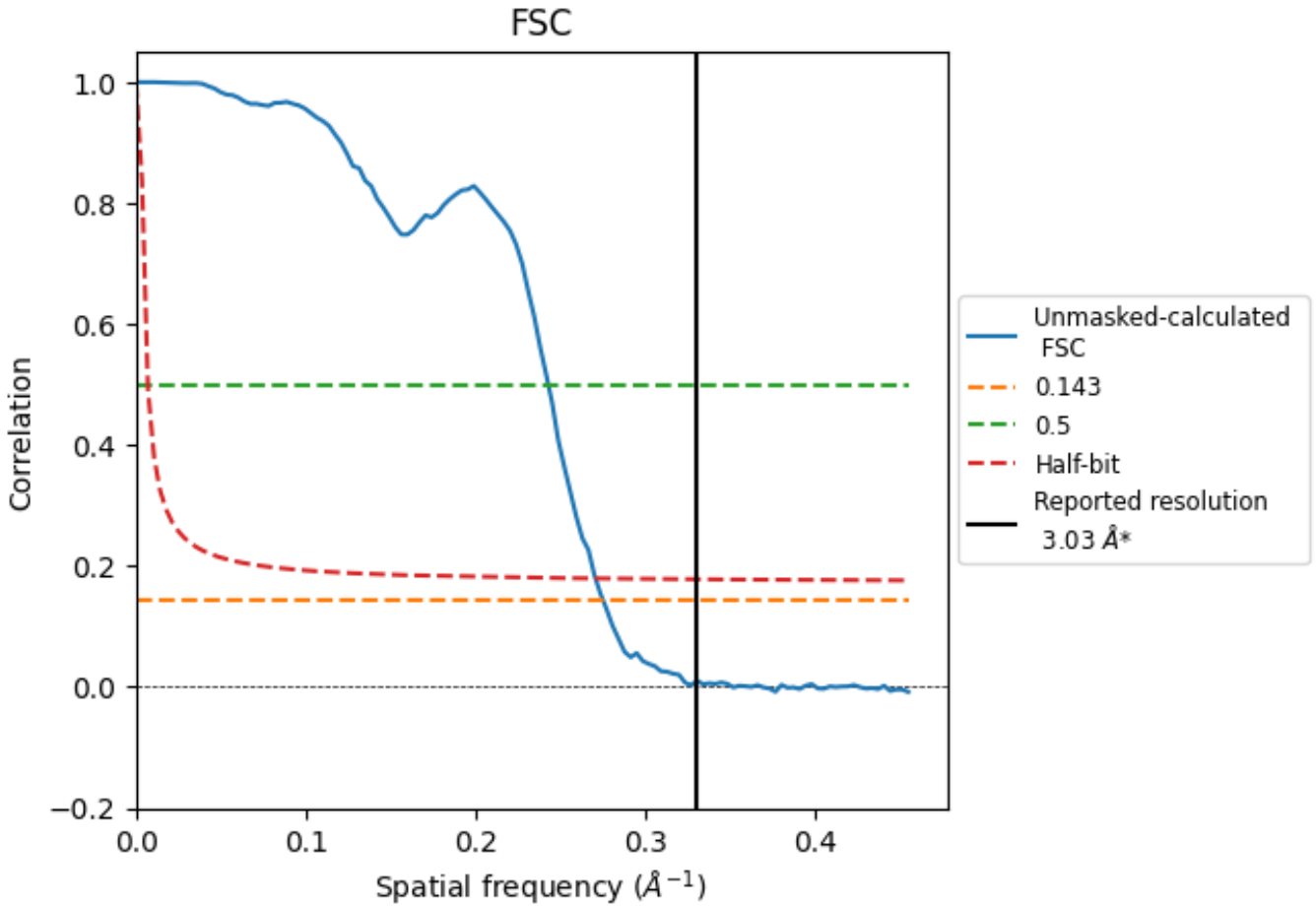


*Reported resolution corresponds to spatial frequency of 0.330 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.12	3.70

*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 3.64 differs from the reported value 3.03 by more than 10 %

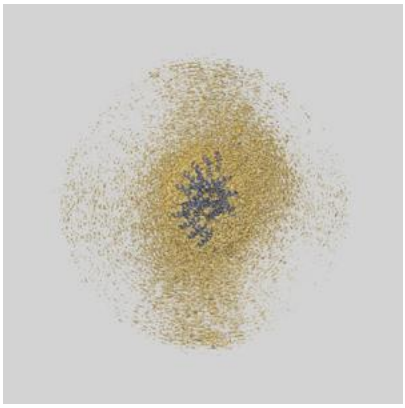
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64179 and PDB model 9UHX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay

X

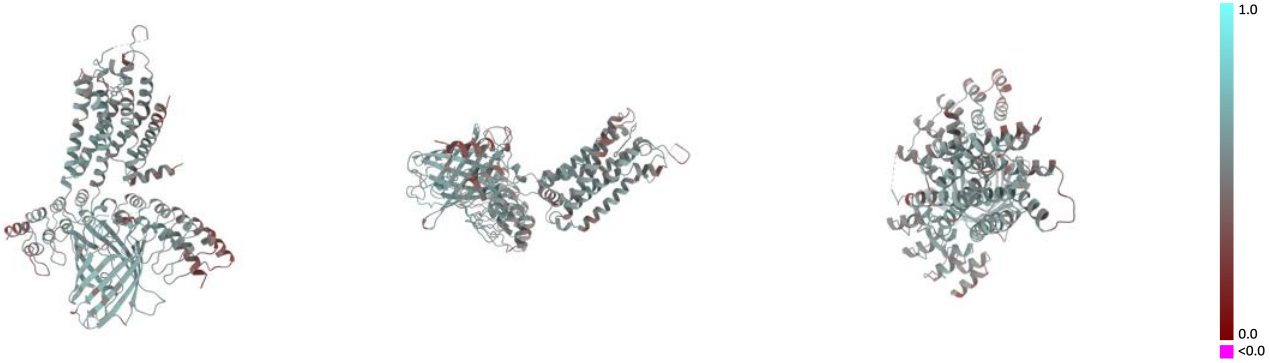
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

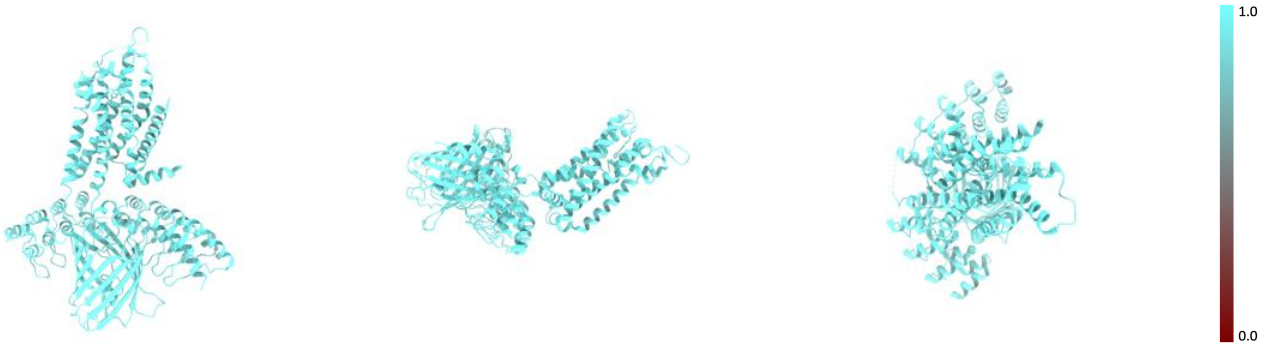
9.2 Q-score mapped to coordinate model (i)



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.

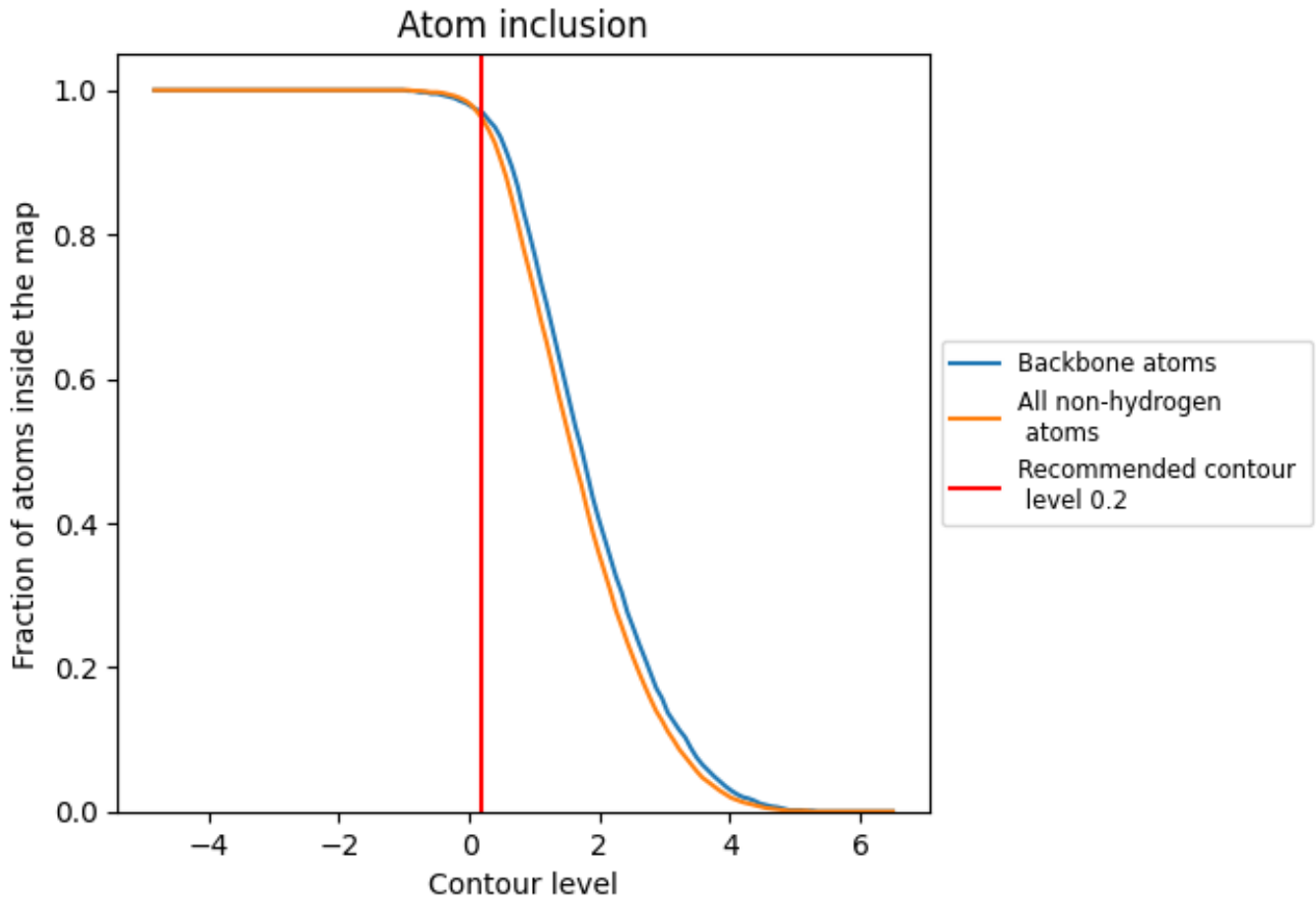
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.5200
A	0.9590	0.5210
B	0.9690	0.5590
C	0.9580	0.4920