



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:32 AM UTC

PDB ID : 7YE2 / pdb_00007ye2
EMDB ID : EMD-33762
Title : The cryo-EM structure of C. crescentus GcrA-TACdown
Authors : Wu, X.X.; Zhang, Y.
Deposited on : 2022-07-05
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

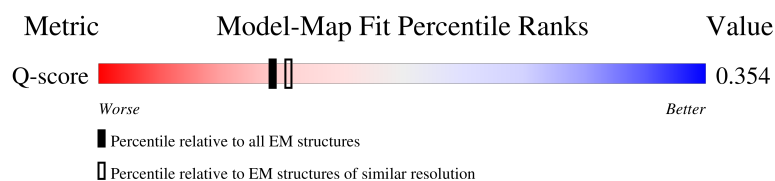
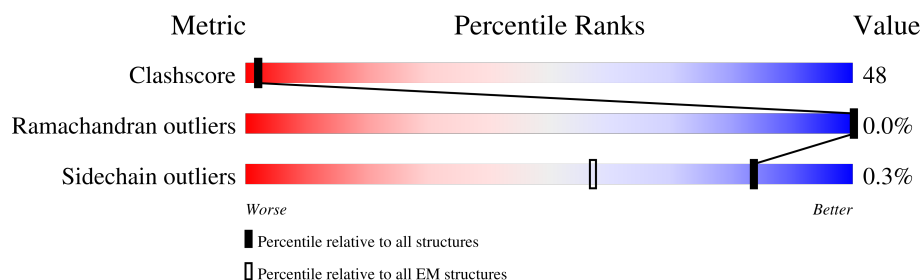
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.80 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.



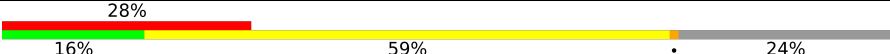
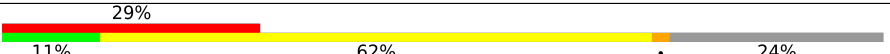
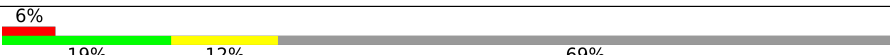
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	338	
1	B	338	
2	C	1356	
3	D	1396	

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Mol	Chain	Length	Quality of chain
4	E	119	
5	F	652	
6	H	90	
7	I	90	
8	G	173	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28925 atoms, of which 12 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2054	1300	353	397	4		
1	B	220	Total	C	N	O	S	0	0
			1633	1044	274	311	4		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1303	Total	C	H	N	O	S	0	0
			9603	6112	12	1598	1841	40		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1140	Total	C	N	O	S	0	0
			8691	5586	1432	1630	43		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	69	Total	C	N	O	S	0	0
			510	323	85	101	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	497	Total	C	N	O	S	0	0
			3266	2049	576	631	10		

- Molecule 6 is a DNA chain called DNA (90-MER)-non template.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	68	Total	C	N	O	P	0	0
			1396	663	257	408	68		

- Molecule 7 is a DNA chain called DNA (90-MER)-template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	68	Total	C	N	O	P	0	0
			1396	663	257	408	68		

- Molecule 8 is a protein called Cell cycle regulatory protein GcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	53	Total	C	N	O	S	0	0
			372	237	61	70	4		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	
9	G	1	Total	Zn	0
			1	1	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

K199	ASP	VAL
L200	GLU	PRO
I201	LEU	ASN
L202	GLU	TRP
E203	LEU	PRO
V204	SER	PRO
E205	VAL	GLU
T206	ARG	ASN
N207	SER	ILE
A208	ALA	GLU
A209	ASN	ASP
V210	CYS	LEU
T211	ALA	ALA
P212	LYS	LYS
V213	ASN	LYS
D214	ASP	PHE
A215	ASN	GLU
V216	ILE	ASP
A217	VAL	GLN
Y218	TYR	ILE
A219	ILE	GLY
A220	ASP	LEU
I222	ASP	ILE
L223	ILE	L27
Q224	GLN	L28
D225	LYS	E29
Q226	THR	E32
L227	GLU	R32
Q228	ALA	Y35
I229	GLU	E36
F230	MET	Q37
I231	LEU	F38
T232	ARG	L39
F233	THR	T43
E234	PRO	R44
GLU	ASN	P45
PRO	PHE	G46
LYS	GLY	L47
ALA	ARG	R48
LYS	LYS	E54
SER	SER	F57
ALA	LEU	K58
ASP	ASN	S59
GLU	ASP	V60
SER	ILE	Y61
LYS	LYS	P62
PRO	GLU	L63
PRO	VAL	K64
LEU	VAL	D65
PHE	LEU	F66
ASN	MET	A70
PRO	GLY	V71
ALA	LEU	L72
LEU	HIS	E73
LYS	LEU	
LYS	GLY	
VAL	MET	
ASP	ASP	

• Molecule 2: DNA-directed RNA polymerase subunit beta

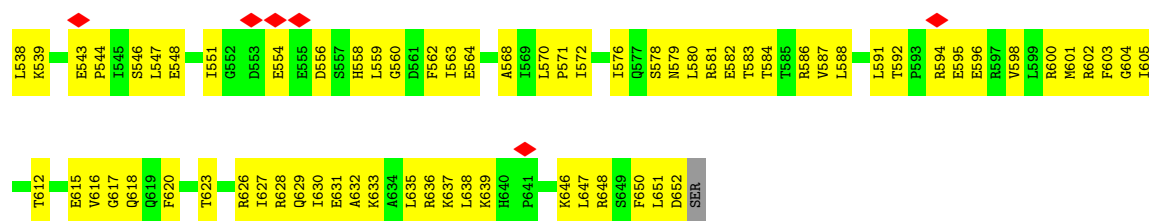


A716	R717	D718	S719	G720	A721	V722	S663	P664	R665	Q666	V667	P668	S669	V670	A671	A672	A673	L674	L675	P676	F677	L678	E679	N680	D681	D682	A683	N684	R685	A686	L687	M688	D689	S690	N691	M692	Q693	R694	Q695	A696	V697	P698	L699	V700	S702	D703	G704	P705	L706	T707	T708	C770	I771	N772	Q773	R774	P775	L776	V777	K778																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
F522	M523	D524	Q525	T526	N527	P528	L529	S530	E531	I532	T533	H534	K535	R536	R537	L538	S539	A540	L541	G542	P543	L546	T547	R548	E549	R550	A551	G552	F553	E554	V555	R556	D557	V558	H559	P560	T561	H562	Y563	G564	R565	I566	C567	P568	I569	K570	T571	P572	E573	G574	P575	N576	I577	G578	L579	I580	N581	S582																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L371	F372	D373	I374	V377	M378	G381	A389	E390	K394	S395	L396	F397	F398	D399	Y403	D404	L405	S406	S407	V408	G409	R410	V411	K412	M413	M414	M415	R416	L417	S422	V425	R426	I427	L428	R429	K430	E431	D432	V433	L434	A435	V436	L437	K438	V439	L440	V441	G442	L443	R444	D445	G446																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
R447	D451	D452	M455	L456	G457	M458	R459	R460	V461	R462	S463	V464	L467	L468	K469	A470	Q471	Y472	R473	L477	R478	M479	E480	I483	K484	E485	R486	M487	D491	I492	D493	P497	Y498	H499	D499	L500	I501	N502	A503	K504	P505	A506	V510	F513	F514	S517	Q518	L519	S520	Q521																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
ALA	PRO	GLU	ALA	L300	A309	VAL	ASN	MET	ALA	THR	GLY	E316	A321	G322	D323	E324	L325	D326	V327	T328	S329	D335	GLN	GLY	PHE	SER	THR	ILE	ASP	VAL	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP

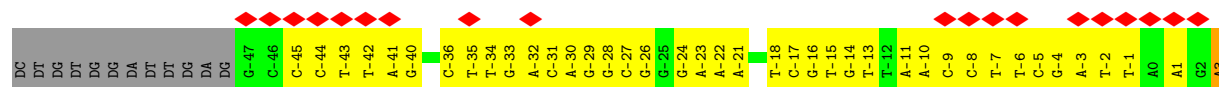
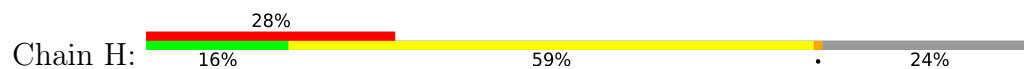


E205	E206	G209	S212	K215	Q216	F219	R222	K224	L225	L226	E227	A228	F229	N234	R235	P236	E237	W238	M239	V240	L241	T242	V243	V244	P245	V246	I247	P248	P249	E250	L251	R252	P253	L254	V255	P256	L257	D258	G259	G260	R261	A263	T264	S265	D266	L267	L270	Y271	T272										
K134	D135	I136	E137	R138	V139	L140	Y141	F142	E143	Y144	Y145	I146	V147	G151	LEU	THR	F154	L155	K156	Q157	H158	Q159	L160	L161	S162	Y166	Q170	E171	E172	I173	G174	D175	D176	S177	F178	E181	I182	G183	A184	E185	A186	I187	Q188	M189	L190	L191	I194	D195	L196	E199									
F63	G64	P65	T66	K67	D68	Y69	E70	C71	L72		K77		Y81	K82	G83	I84	I85	C86		V91	E92	I93	V93	T94	L95		V98	R99		R102	M103	G104	H105	I106	E107	L108	A109		V112	A113	H114	I115	M116	F117	L118	K119	S120	L121	P122	S123	R124	I125	A126	M127	M128	L129	D130	M131	P132
ASN	GLN	GLU	VAL	LEU	ASN	LEU	ASN	ILE	PRO	ASN	VAL	GLN	ALA	ALA	PRO	T17	F18	D19	Q20	I21	R22	I23	S24	L25	A26	S27		K30	I31		W34	S35	F36	G37	E38	I39	K40	K41	E43	T44	N46	Y47	R48	T49	F50	K51	P52	E53	R54	D55	G56	F57	L58	C59	A60	R61	L62		

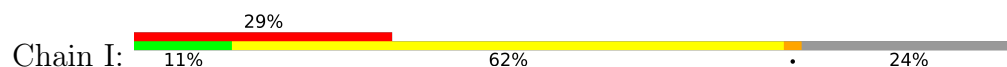




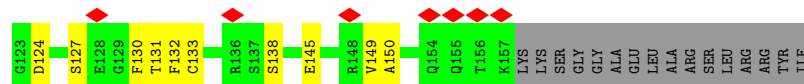
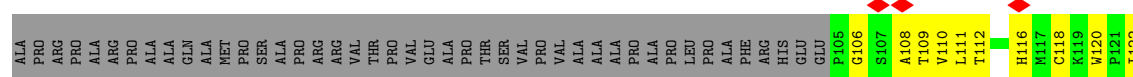
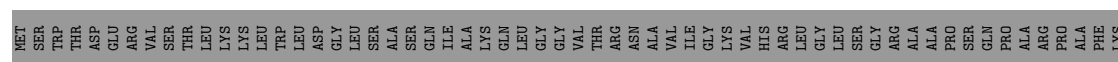
• Molecule 6: DNA (90-MER)-non template



• Molecule 7: DNA (90-MER)-template



• Molecule 8: Cell cycle regulatory protein GcrA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	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: 6MA, MG, ZN

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	0.08	0/2078	0.23	0/2838
1	B	0.08	0/1657	0.24	0/2249
2	C	0.08	0/9735	0.23	0/13133
3	D	0.08	0/8829	0.21	0/11870
4	E	0.08	0/514	0.19	0/695
5	F	0.09	0/3294	0.25	0/4467
6	H	0.17	0/1513	0.45	0/2328
7	I	0.17	0/1513	0.36	0/2328
8	G	0.07	0/384	0.19	0/522
All	All	0.09	0/29517	0.25	0/40430

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	2054	0	1816	221	0
1	B	1633	0	1618	203	0
2	C	9591	12	9110	1052	0
3	D	8691	0	8727	1040	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	510	0	505	59	0
5	F	3266	0	2751	255	0
6	H	1396	0	768	83	0
7	I	1396	0	768	88	0
8	G	372	0	325	14	0
9	D	2	0	0	0	0
9	G	1	0	0	0	0
10	D	1	0	0	0	0
All	All	28913	12	26388	2655	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 48.

The worst 5 of 2655 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:45:ALA:O	1:A:49:VAL:HG12	1.48	1.11
1:A:50:LEU:HB2	1:A:220:ALA:CB	1.84	1.07
5:F:123:MET:HE2	5:F:123:MET:HA	1.33	1.06
1:A:51:LEU:HD21	2:C:1100:ILE:HG13	1.40	1.04
3:D:504:PRO:HB3	3:D:508:ILE:HB	1.39	1.04

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	300/338 (89%)	280 (93%)	19 (6%)	1 (0%)	36	67
1	B	214/338 (63%)	202 (94%)	12 (6%)	0	100	100
2	C	1291/1356 (95%)	1207 (94%)	84 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1128/1396 (81%)	1072 (95%)	56 (5%)	0	100	100
4	E	67/119 (56%)	64 (96%)	3 (4%)	0	100	100
5	F	493/652 (76%)	477 (97%)	16 (3%)	0	100	100
8	G	51/173 (30%)	49 (96%)	2 (4%)	0	100	100
All	All	3544/4372 (81%)	3351 (95%)	192 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LEU

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	176/285 (62%)	175 (99%)	1 (1%)	78	79
1	B	173/285 (61%)	173 (100%)	0	100	100
2	C	975/1137 (86%)	971 (100%)	4 (0%)	84	83
3	D	941/1157 (81%)	940 (100%)	1 (0%)	88	89
4	E	56/100 (56%)	56 (100%)	0	100	100
5	F	247/542 (46%)	244 (99%)	3 (1%)	63	72
8	G	37/134 (28%)	37 (100%)	0	100	100
All	All	2605/3640 (72%)	2596 (100%)	9 (0%)	84	84

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	426	LEU
5	F	581	ARG
2	C	231	TYR
2	C	550	ARG
3	D	776	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	46	ASN
3	D	491	ASN
5	F	629	GLN
3	D	1374	GLN
3	D	114	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
6	6MA	H	3	6	21,24,25	3.13	10 (47%)	27,34,37	3.05	16 (59%)
7	6MA	I	-13	6,7	21,24,25	3.16	11 (52%)	27,34,37	2.96	13 (48%)
7	6MA	I	-5	7	21,24,25	3.17	11 (52%)	27,34,37	3.04	14 (51%)
6	6MA	H	11	6,7	21,24,25	3.15	10 (47%)	27,34,37	2.98	13 (48%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	6MA	H	3	6	-	3/9/23/24	0/3/3/3
7	6MA	I	-13	6,7	-	4/9/23/24	0/3/3/3
7	6MA	I	-5	7	-	7/9/23/24	0/3/3/3
6	6MA	H	11	6,7	-	5/9/23/24	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	-13	6MA	C3'-C4'	-8.24	1.31	1.53
6	H	11	6MA	C3'-C4'	-8.17	1.31	1.53
7	I	-5	6MA	C3'-C4'	-8.09	1.31	1.53
7	I	-5	6MA	O4'-C4'	8.08	1.63	1.45
6	H	3	6MA	C3'-C4'	-7.98	1.32	1.53

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	-13	6MA	C1'-N9-C8	-7.12	102.04	126.95
7	I	-5	6MA	C1'-N9-C8	-7.12	102.05	126.95
6	H	11	6MA	C1'-N9-C8	-7.08	102.18	126.95
6	H	3	6MA	C1'-N9-C8	-7.02	102.39	126.95
7	I	-13	6MA	N3-C2-N1	-5.74	119.89	128.58

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	3	6MA	C5-C6-N6-C1
6	H	3	6MA	N1-C6-N6-C1
6	H	11	6MA	C5-C6-N6-C1
6	H	11	6MA	N1-C6-N6-C1
7	I	-13	6MA	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	6MA	2	0
7	I	-13	6MA	3	0
7	I	-5	6MA	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

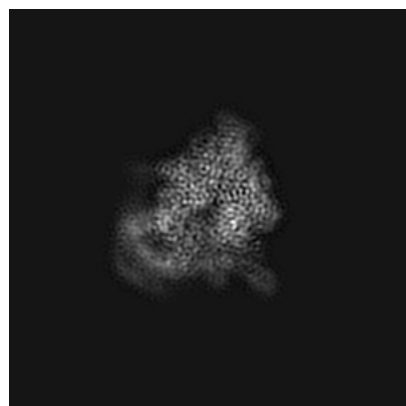
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33762. These allow visual inspection of the internal detail of the map and identification of artifacts.

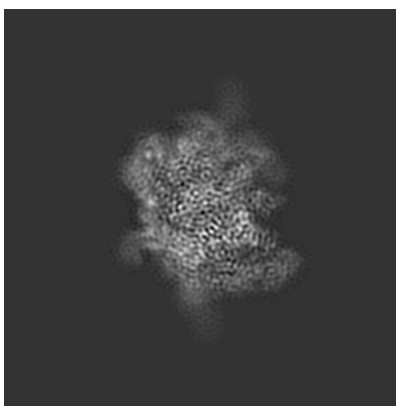
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

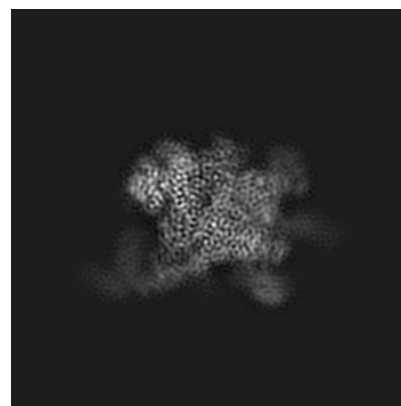
6.1.1 Primary map



X

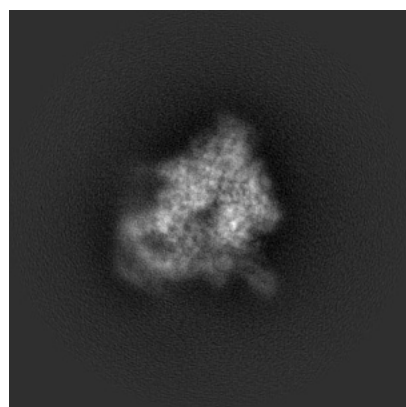


Y

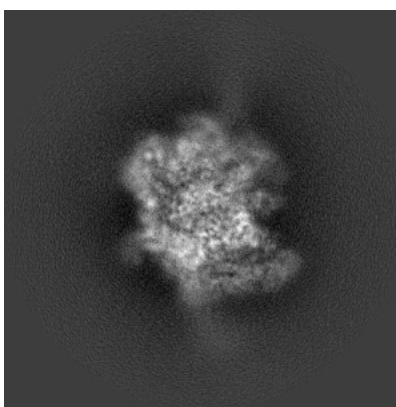


Z

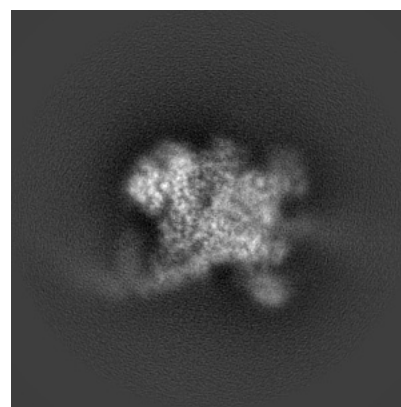
6.1.2 Raw map



X



Y

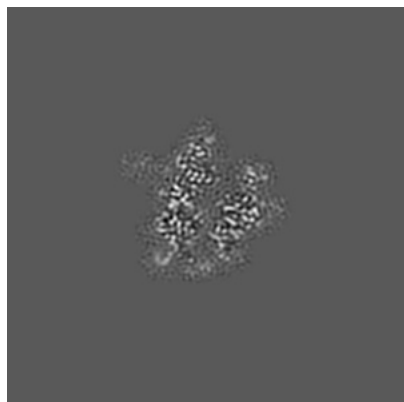


Z

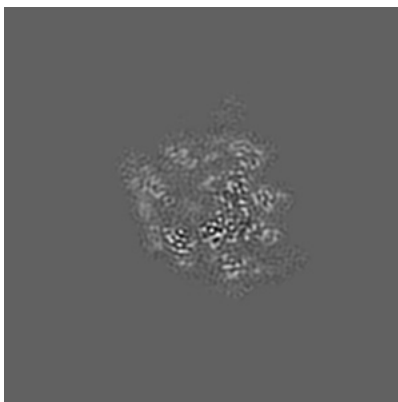
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

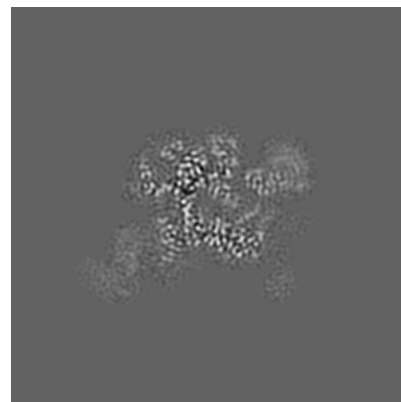
6.2.1 Primary map



X Index: 150

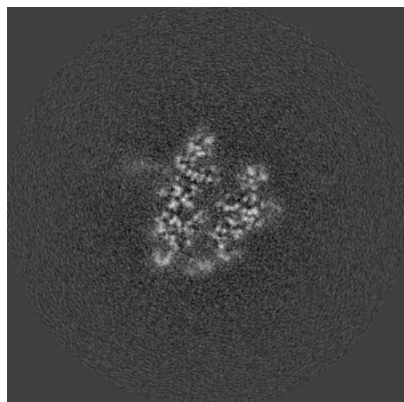


Y Index: 150

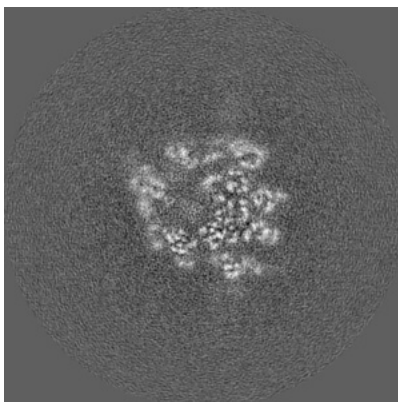


Z Index: 150

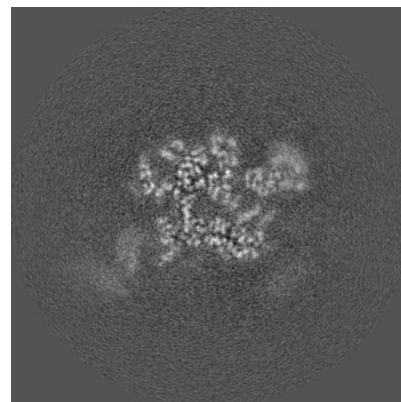
6.2.2 Raw map



X Index: 150



Y Index: 150

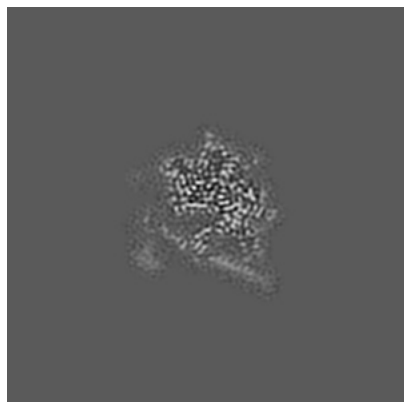


Z Index: 150

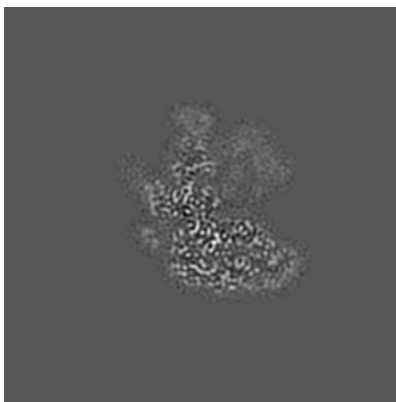
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

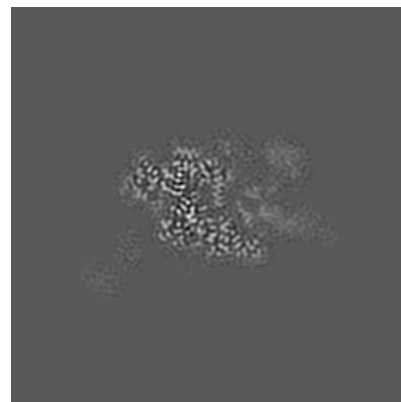
6.3.1 Primary map



X Index: 131

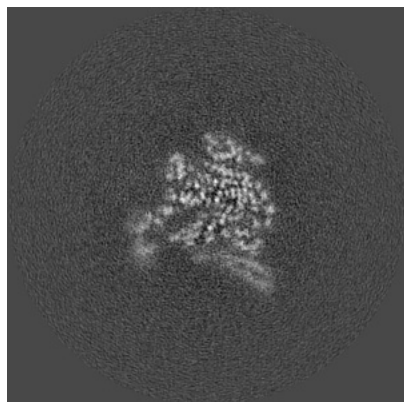


Y Index: 165

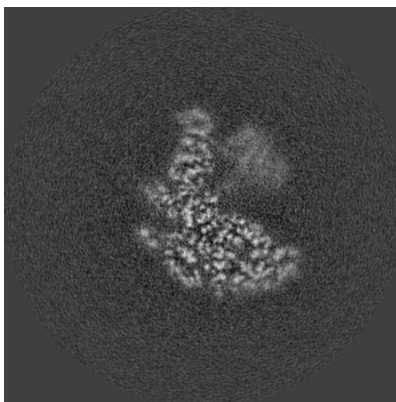


Z Index: 159

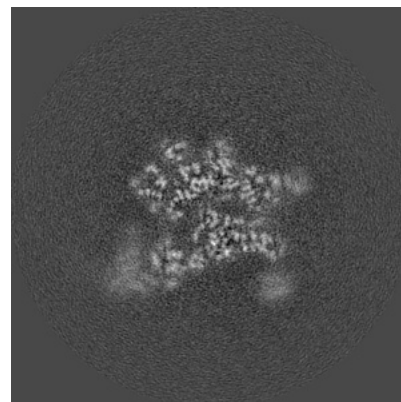
6.3.2 Raw map



X Index: 125



Y Index: 168

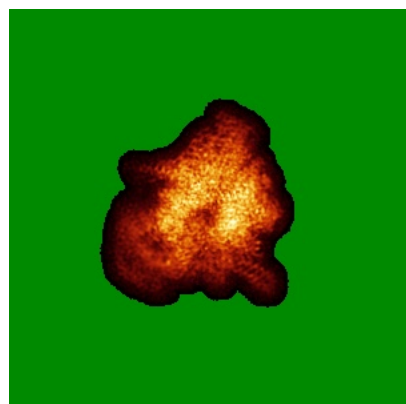


Z Index: 138

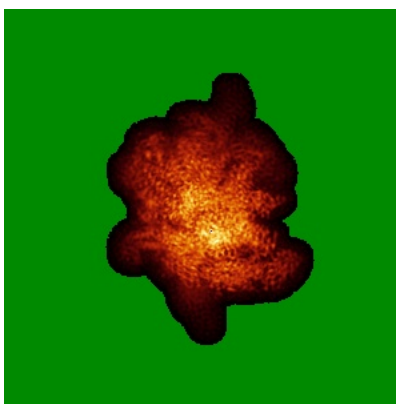
The images above show the largest variance slices of the map in three orthogonal directions.

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

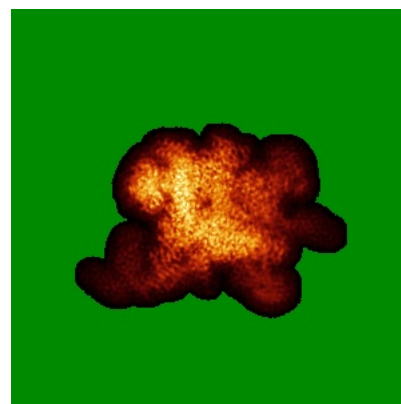
6.4.1 Primary map



X

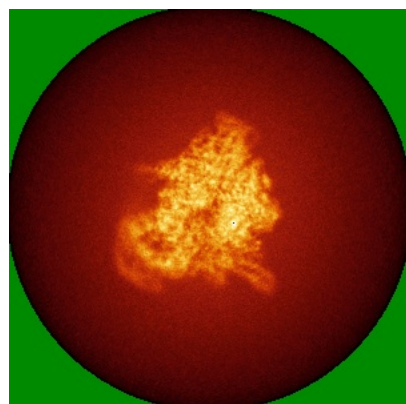


Y

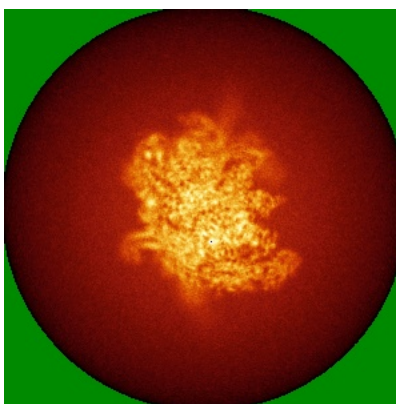


Z

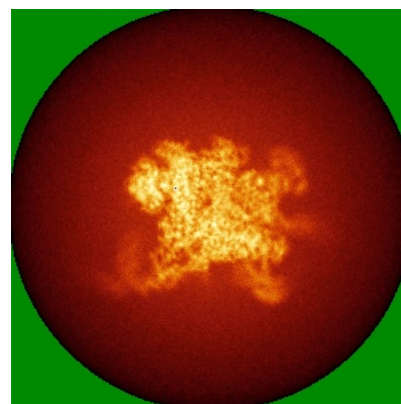
6.4.2 Raw map



X



Y

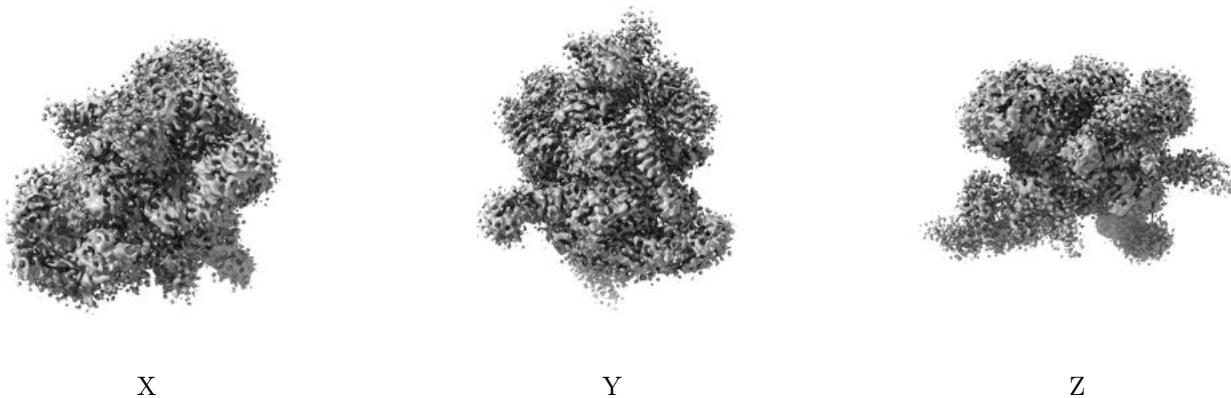


Z

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.

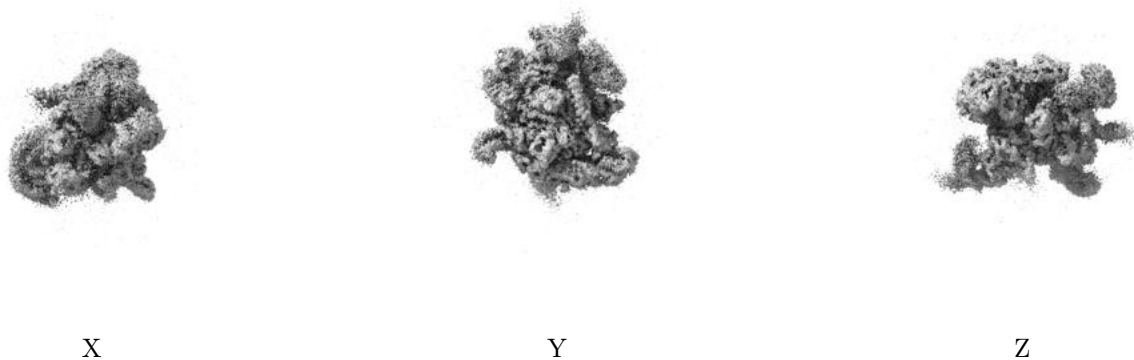
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

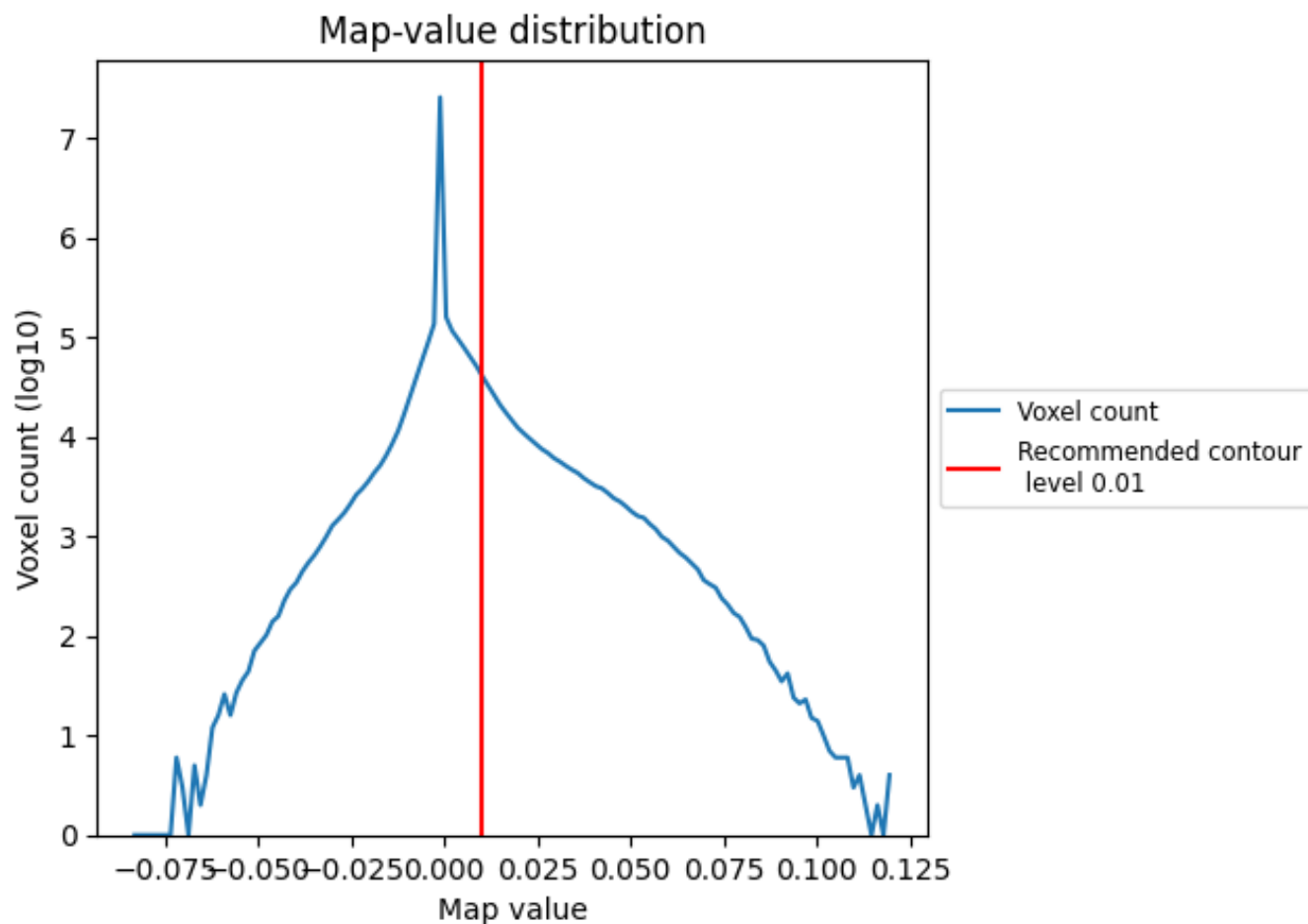
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

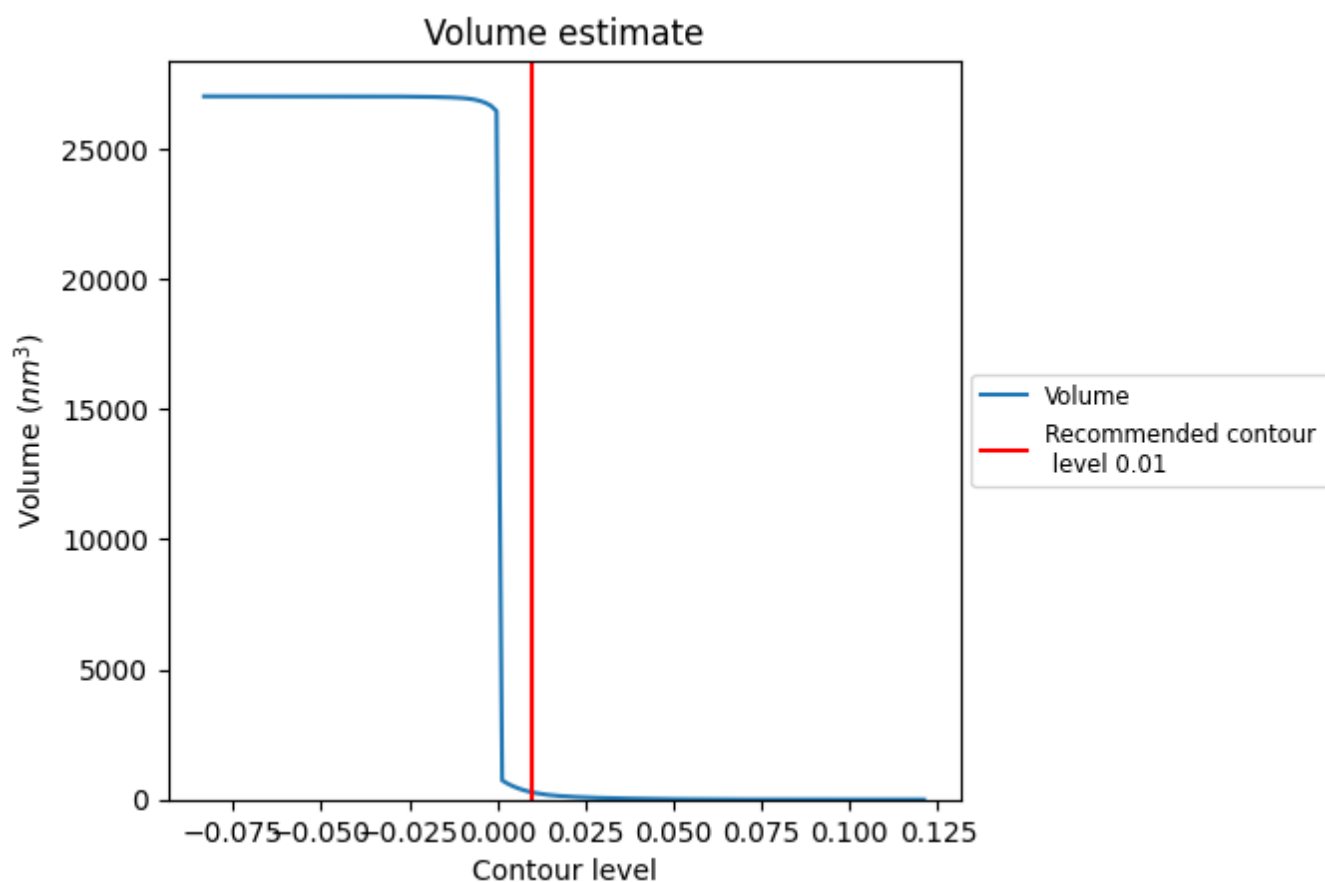
This section contains the results of statistical analysis of the map.

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.

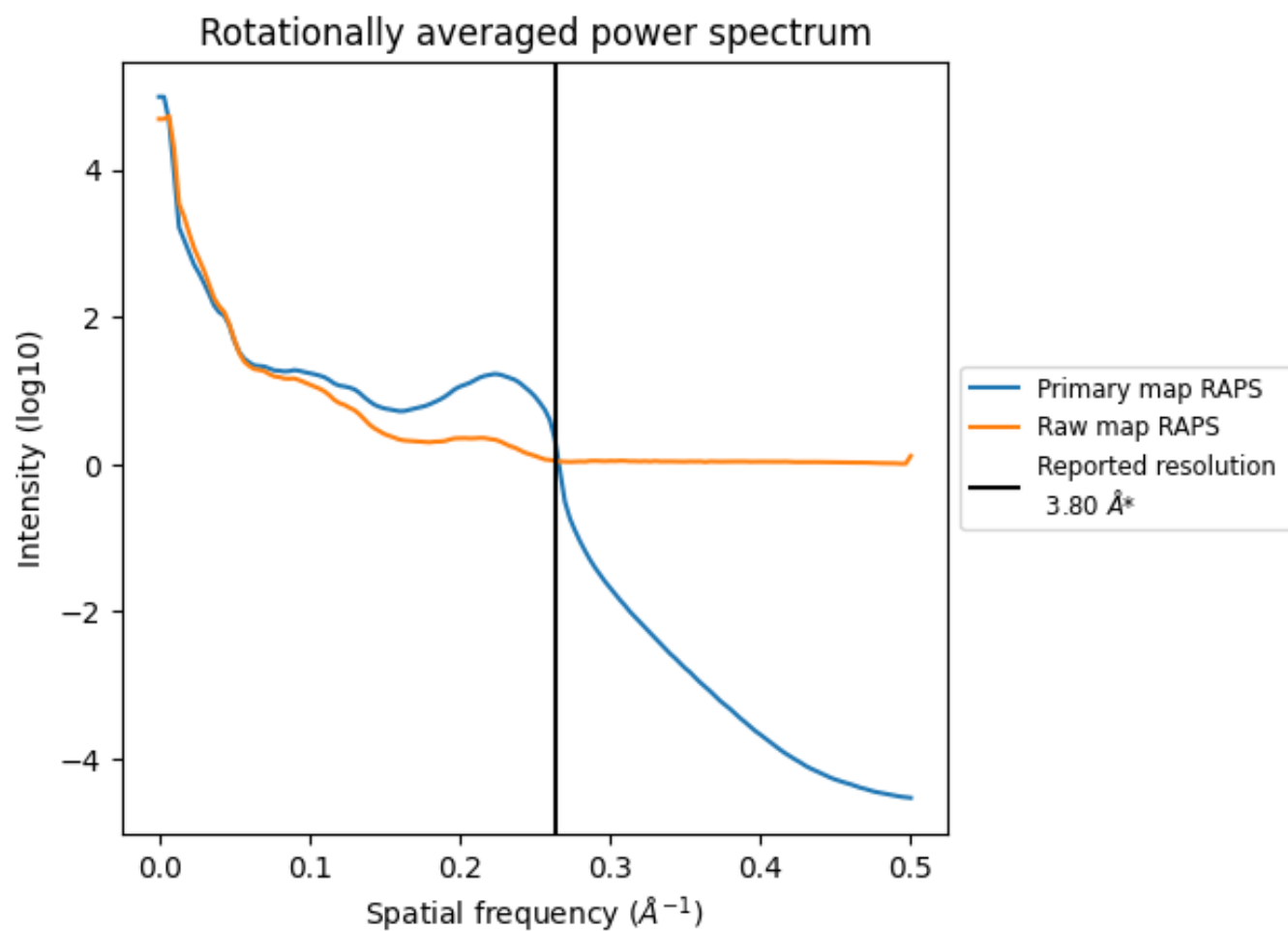
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 250 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 ⓘ

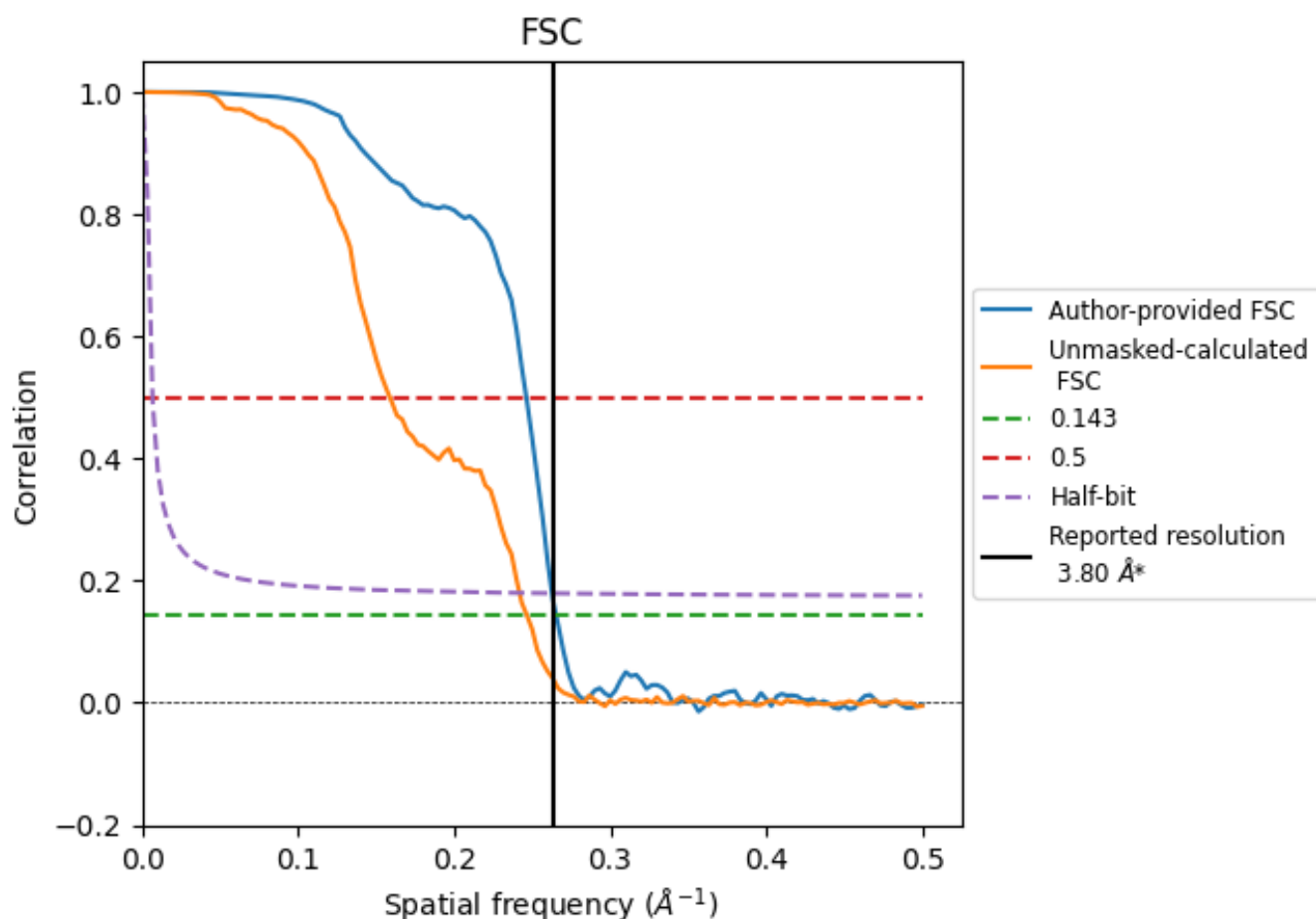


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

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 $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

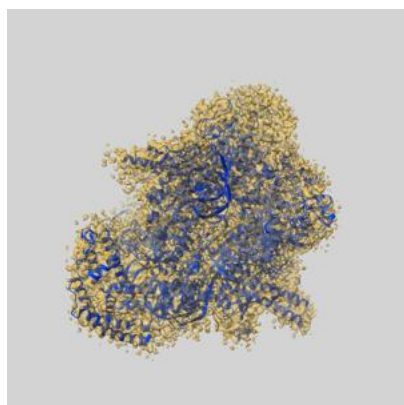
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.06	3.81
Unmasked-calculated*	4.06	6.30	4.13

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

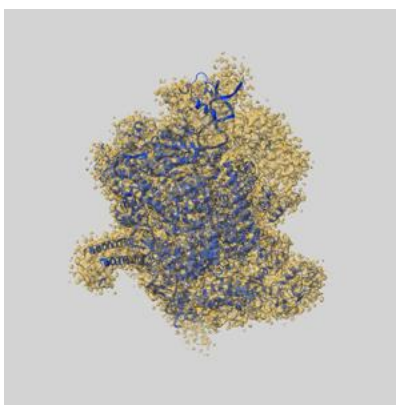
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33762 and PDB model 7YE2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

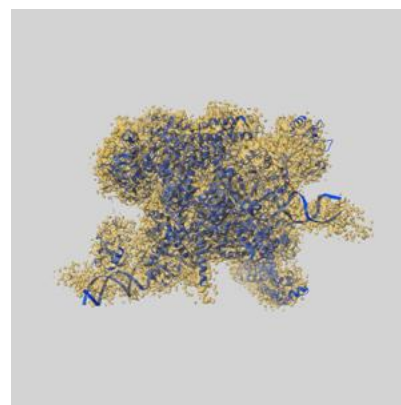
9.1 Map-model overlay [i](#)



X



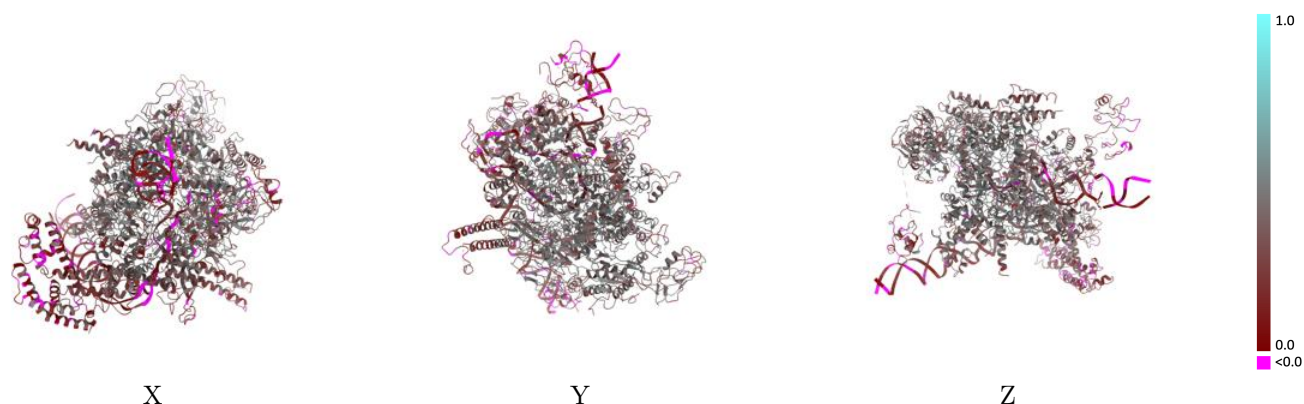
Y



Z

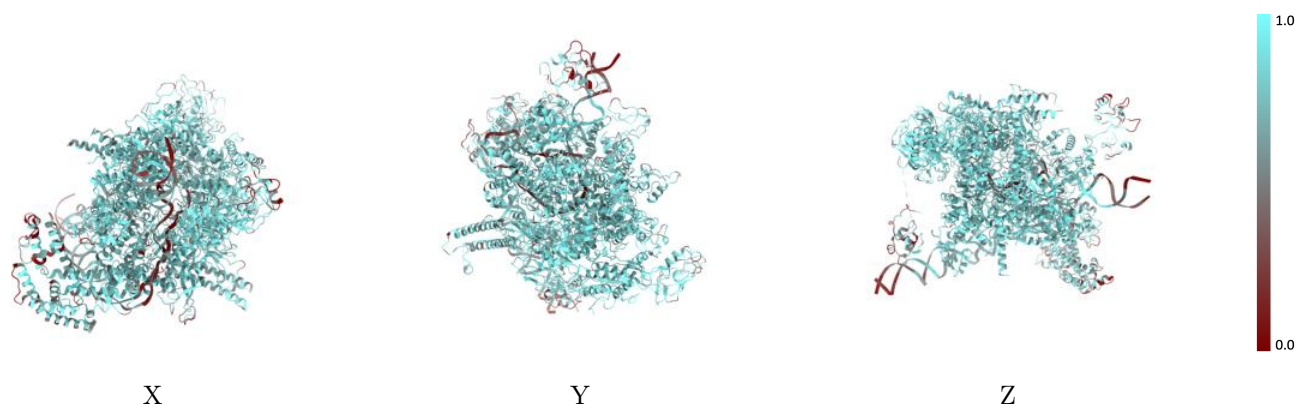
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



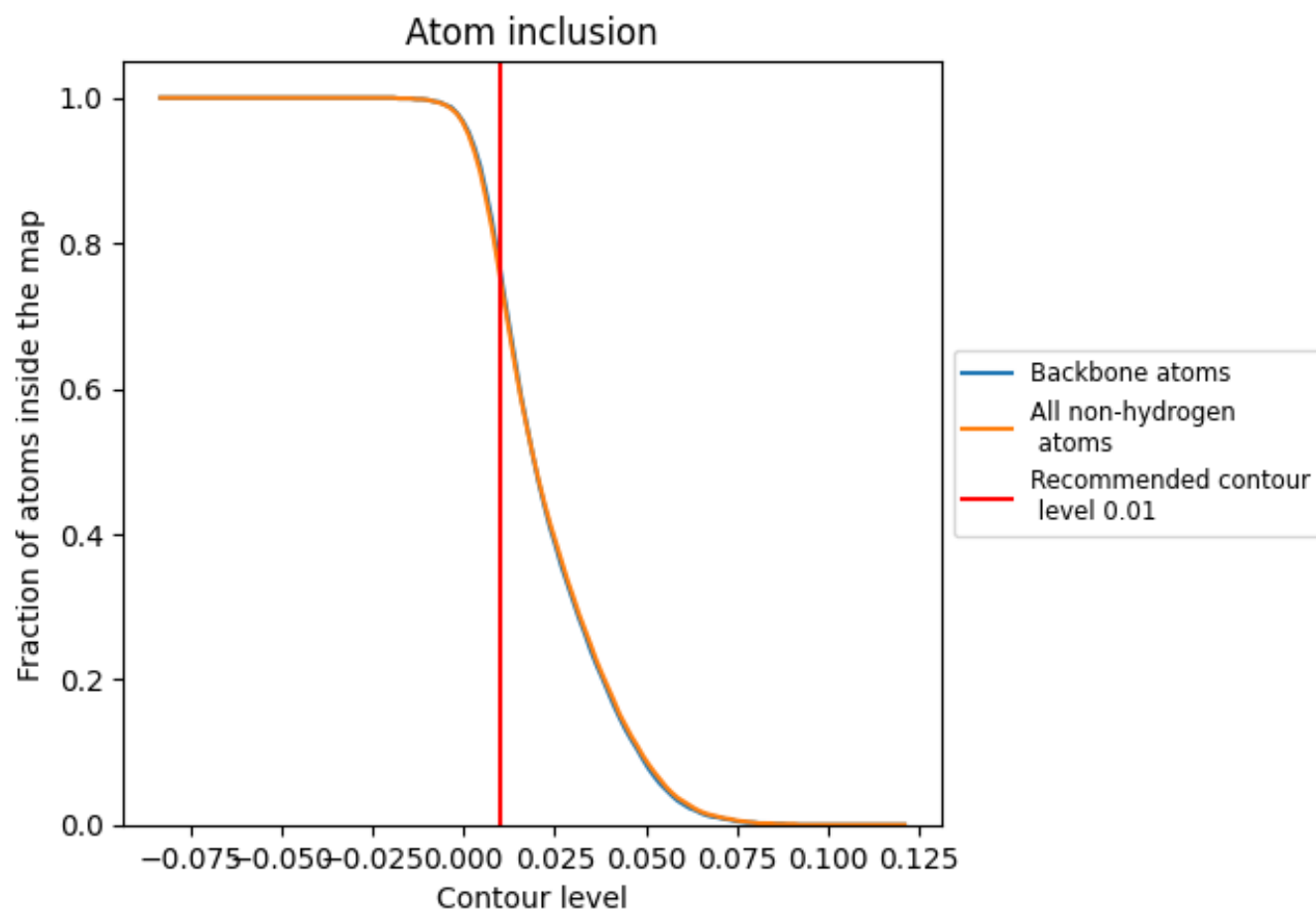
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.3540
A	0.7690	0.3850
B	0.8060	0.3890
C	0.7850	0.3840
D	0.8030	0.4060
E	0.8140	0.4120
F	0.7330	0.3080
G	0.6820	0.2680
H	0.4960	0.0990
I	0.4880	0.0920

1.0

0.0

<0.0