



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:01 AM UTC

PDB ID : 6VEN / pdb_00006ven
EMDB ID : EMD-21157
Title : Yeast COMPASS in complex with a ubiquitinated nucleosome
Authors : Worden, E.J.; Wolberger, C.
Deposited on : 2020-01-02
Resolution : 3.37 Å(reported)
Based on initial models : 6BX3, 6CHG, 6NJ9

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:

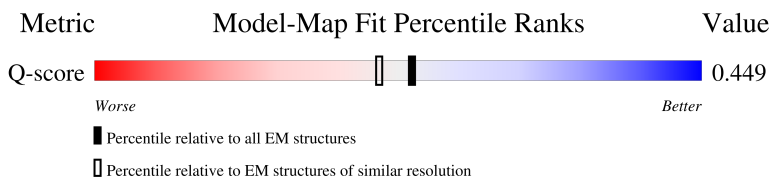
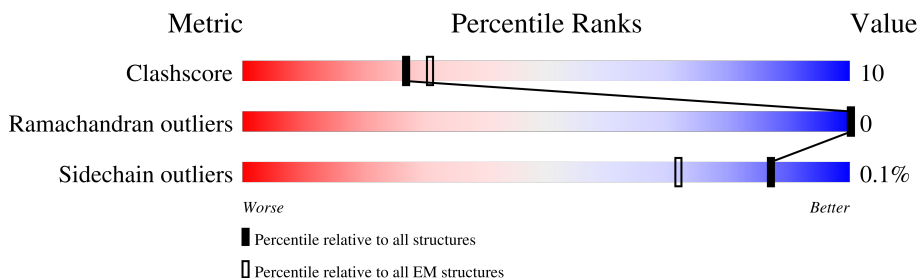
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.37 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.



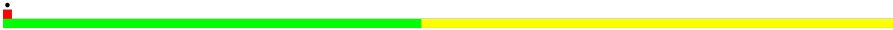
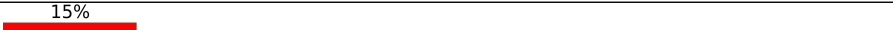
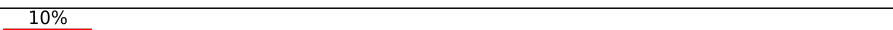
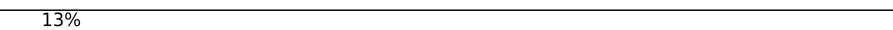
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14287 (2.87 - 3.87)

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	135	
1	E	135	
2	B	102	
2	F	102	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	129	 71%9%20%
3	G	129	 72%10%18%
4	D	122	 66%11%24%
4	H	122	 70%7%23%
5	I	146	 52%48%
6	J	146	 47%53%
7	K	80	 18%64%30%6%
8	L	315	 68%30%.
9	M	426	 65%28%7%
10	N	358	 8%49%12%39%
11	O	505	 15%43%19%38%
12	P	175	 17%21%.76%
12	Q	175	 10%10%7%83%
13	R	391	 13%25%8%67%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 24028 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			871	548	171	151	1		
1	E	97	Total	C	N	O	S	0	0
			802	508	155	138	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	NLE	LYS	engineered mutation	UNP P84233
A	90	NLE	MET	engineered mutation	UNP P84233
A	102	ALA	GLY	engineered mutation	UNP P84233
A	120	NLE	MET	engineered mutation	UNP P84233
E	4	NLE	LYS	engineered mutation	UNP P84233
E	90	NLE	MET	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233
E	120	NLE	MET	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
2	F	80	Total	C	N	O	S	0	0
			644	408	125	110	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	103	Total	C	N	O	0	0
			795	501	155	139		
3	G	106	Total	C	N	O	0	0
			818	516	160	142		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897
C	123	SER	ALA	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897
G	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			727	457	130	137	3		
4	H	94	Total	C	N	O	S	0	0
			732	460	131	138	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	THR	SER	engineered mutation	UNP P02281
D	120	CYS	LYS	engineered mutation	UNP P02281
H	32	THR	SER	engineered mutation	UNP P02281
H	120	CYS	LYS	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called 601 DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 6 is a DNA chain called 601 DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 7 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	75	Total	C	N	O	S	0	0
			597	376	104	116	1		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP P0CG48
K	-2	SER	-	expression tag	UNP P0CG48
K	-1	HIS	-	expression tag	UNP P0CG48
K	0	MET	-	expression tag	UNP P0CG48
K	76	CYS	GLY	engineered mutation	UNP P0CG48

- Molecule 8 is a protein called COMPASS component SWD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	308	Total	C	N	O	S	0	0
			2367	1500	394	454	19		

- Molecule 9 is a protein called COMPASS component SWD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	395	Total	C	N	O	S	0	0
			3183	2032	523	614	14		

- Molecule 10 is a protein called Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	218	Total	C	N	O	S	0	0
			1710	1072	315	314	9		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	723	MET	-	expression tag	UNP P38827
N	724	HIS	-	expression tag	UNP P38827
N	725	HIS	-	expression tag	UNP P38827
N	726	HIS	-	expression tag	UNP P38827
N	727	HIS	-	expression tag	UNP P38827
N	728	HIS	-	expression tag	UNP P38827
N	729	HIS	-	expression tag	UNP P38827
N	730	GLY	-	expression tag	UNP P38827
N	731	SER	-	expression tag	UNP P38827
N	732	SER	-	expression tag	UNP P38827
N	733	ASP	-	expression tag	UNP P38827
N	734	TYR	-	expression tag	UNP P38827
N	735	LYS	-	expression tag	UNP P38827
N	736	ASP	-	expression tag	UNP P38827
N	737	HIS	-	expression tag	UNP P38827
N	738	ASP	-	expression tag	UNP P38827

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	739	GLY	-	expression tag	UNP P38827
N	740	ASP	-	expression tag	UNP P38827
N	741	TYR	-	expression tag	UNP P38827
N	742	LYS	-	expression tag	UNP P38827
N	743	ASP	-	expression tag	UNP P38827
N	744	HIS	-	expression tag	UNP P38827
N	745	ASP	-	expression tag	UNP P38827
N	746	ILE	-	expression tag	UNP P38827
N	747	ASP	-	expression tag	UNP P38827
N	748	TYR	-	expression tag	UNP P38827
N	749	LYS	-	expression tag	UNP P38827
N	750	ASP	-	expression tag	UNP P38827
N	751	ASP	-	expression tag	UNP P38827
N	752	ASP	-	expression tag	UNP P38827
N	753	ASP	-	expression tag	UNP P38827
N	754	LYS	-	expression tag	UNP P38827
N	755	GLU	-	expression tag	UNP P38827
N	756	ASN	-	expression tag	UNP P38827
N	757	LEU	-	expression tag	UNP P38827
N	758	TYR	-	expression tag	UNP P38827
N	759	PHE	-	expression tag	UNP P38827
N	760	GLN	-	expression tag	UNP P38827
N	761	GLY	-	expression tag	UNP P38827

- Molecule 11 is a protein called COMPASS component BRE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	315	Total	C	N	O	S	0	0
			2595	1667	428	491	9		

- Molecule 12 is a protein called COMPASS component SDC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	42	Total	C	N	O	S	0	0
			336	212	60	63	1		
12	Q	29	Total	C	N	O	S	0	0
			225	142	40	42	1		

- Molecule 13 is a protein called COMPASS component SPP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	129	Total 966	C 605	N 164	O 189	S 8	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-37	MET	-	expression tag	UNP Q03012
R	-36	TRP	-	expression tag	UNP Q03012
R	-35	SER	-	expression tag	UNP Q03012
R	-34	HIS	-	expression tag	UNP Q03012
R	-33	PRO	-	expression tag	UNP Q03012
R	-32	GLN	-	expression tag	UNP Q03012
R	-31	PHE	-	expression tag	UNP Q03012
R	-30	GLU	-	expression tag	UNP Q03012
R	-29	LYS	-	expression tag	UNP Q03012
R	-28	GLY	-	expression tag	UNP Q03012
R	-27	GLY	-	expression tag	UNP Q03012
R	-26	GLY	-	expression tag	UNP Q03012
R	-25	SER	-	expression tag	UNP Q03012
R	-24	GLY	-	expression tag	UNP Q03012
R	-23	GLY	-	expression tag	UNP Q03012
R	-22	GLY	-	expression tag	UNP Q03012
R	-21	SER	-	expression tag	UNP Q03012
R	-20	GLY	-	expression tag	UNP Q03012
R	-19	GLY	-	expression tag	UNP Q03012
R	-18	SER	-	expression tag	UNP Q03012
R	-17	SER	-	expression tag	UNP Q03012
R	-16	ALA	-	expression tag	UNP Q03012
R	-15	TRP	-	expression tag	UNP Q03012
R	-14	SER	-	expression tag	UNP Q03012
R	-13	HIS	-	expression tag	UNP Q03012
R	-12	PRO	-	expression tag	UNP Q03012
R	-11	GLN	-	expression tag	UNP Q03012
R	-10	PHE	-	expression tag	UNP Q03012
R	-9	GLU	-	expression tag	UNP Q03012
R	-8	LYS	-	expression tag	UNP Q03012
R	-7	GLY	-	expression tag	UNP Q03012
R	-6	SER	-	expression tag	UNP Q03012
R	-5	GLU	-	expression tag	UNP Q03012
R	-4	ASN	-	expression tag	UNP Q03012
R	-3	LEU	-	expression tag	UNP Q03012
R	-2	TYR	-	expression tag	UNP Q03012
R	-1	PHE	-	expression tag	UNP Q03012

Continued on next page...

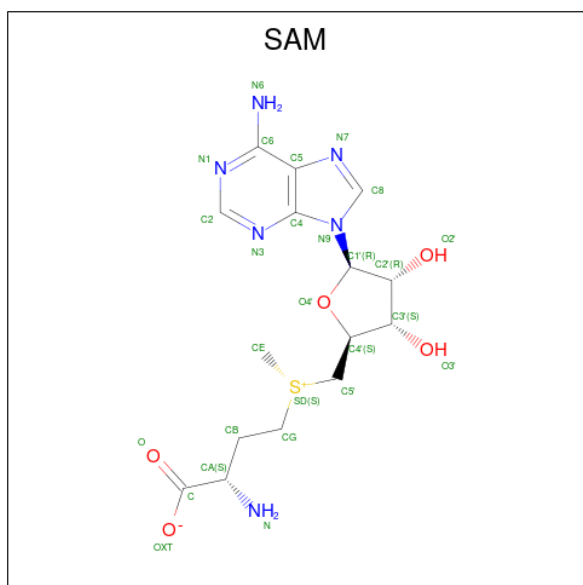
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	0	GLN	-	expression tag	UNP Q03012
R	1	GLY	-	expression tag	UNP Q03012

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	N	1	Total	Zn	0
			1	1	

- Molecule 15 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

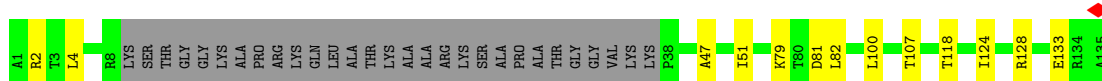


Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total	C	N	O	S	0
			27	15	6	5	1	

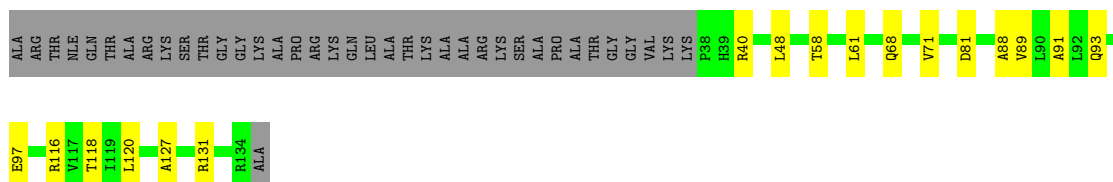
3 Residue-property plots

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: Histone H3.2



- Molecule 1: Histone H3.2



- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1



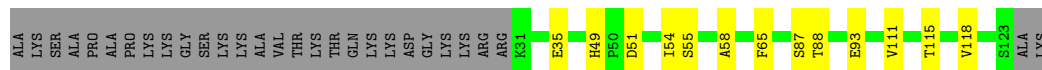
- Molecule 3: Histone H2A type 1

Chain G:  72% 10% 18%



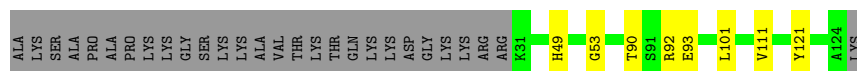
- Molecule 4: Histone H2B 1.1

Chain D:  66% 11% 24%



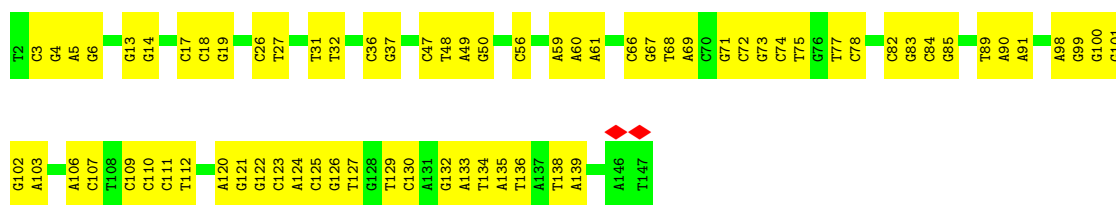
- Molecule 4: Histone H2B 1.1

Chain H:  70% 7% 23%

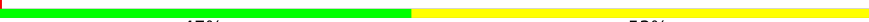


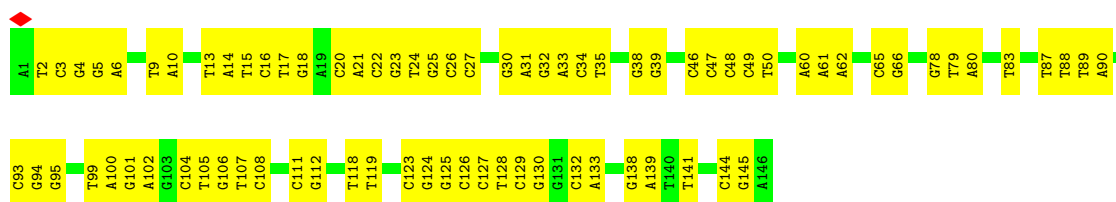
- Molecule 5: 601 DNA (146-MER)

Chain I:  52% 48%



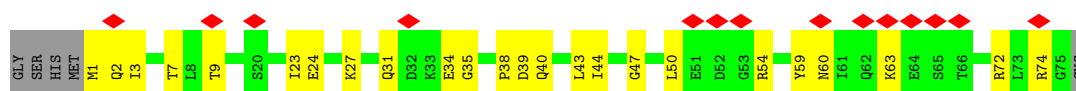
- Molecule 6: 601 DNA (146-MER)

Chain J:  47% 53%



- Molecule 7: Ubiquitin

Chain K:  18% 64% 30% 6%



Chain L:

Amino Acid	Percentage (%)
M1	68%
V8	68%
G9	68%
T10	68%
Q11	68%
L14	68%
K15	68%
S22	68%
F27	68%
L28	68%
Q32	68%
G33	68%
L34	68%
N35	68%
Y39	68%
D40	68%
I41	68%
ASN	2%
ARG	2%
R44	68%
S64	68%
D66	68%
P65	68%
T72	68%
A73	68%
S74	68%
D75	68%
D76	68%
F77	68%
S78	68%
V79	68%
E80	68%
I81	68%
I82	68%
S85	68%
L88	68%
L89	68%
H90	68%
T91	68%
F92	68%
H95	68%
T96	68%
A97	68%
P98	68%
L102	68%
T103	68%
F104	68%
L111	68%
F112	68%
T113	68%
S114	68%
S115	68%
M116	68%
K121	68%
I122	68%
W123	68%
D124	68%
T125	68%
L126	68%
M127	68%
G128	68%
K132	68%
E139	68%
A140	68%
V141	68%
V142	68%
V146	68%
S152	68%
T153	68%
L154	68%
Y159	68%
L162	68%
HIS	2%
I163	68%
E169	68%
T170	68%
G171	68%
H172	68%
D180	68%
P191	68%
V195	68%
R202	68%
L205	68%
V206	68%
W216	68%
D217	68%
C218	68%
T219	68%
G220	68%
G221	68%
R225	68%
T226	68%
F227	68%
Q230	68%
P231	68%
L232	68%
E233	68%
K234	68%
H239	68%
F245	68%
S252	68%
V256	68%
N262	68%
G263	68%
D264	68%
T265	68%
W268	68%
G269	68%
S270	68%
D271	68%
L279	68%
D280	68%
G281	68%
S282	68%
LEU	2%
TYR	2%
H296	68%
P289	68%
V290	68%
F296	68%
L299	68%
A304	68%
L305	68%
N306	68%
G307	68%
D308	68%
C309	68%
W312	68%
R313	68%
TRP	2%
VAL	2%

Chain M:

Amino Acid	Category
E313	Green
D317	Green
I318	Green
N319	Green
W320	Green
D321	Green
M325	Green
V328	Green
S329	Green
N330	Green
Y338	Green
V339	Green
W340	Green
P346	Green
D354	Green
F355	Green
E356	Green
E368	Green
D372	Green
E373	Green
V374	Green
ASP	Green
GLU	Green
ALA	Green
GLU	Green
GLN	Green
GLN	Green
GLY	Green
LEU	Green
GLU	Green
GLN	Green
E386	Green
E387	Green
E388	Green
L393	Green
V401	Green
K422	Green
MET	Green
GLN	Green
SER	Green
SER	Green
L220	Yellow
R228	Yellow
T231	Yellow
N232	Yellow
C233	Yellow
S234	Yellow
D235	Yellow
R236	Yellow
T237	Yellow
I238	Yellow
Y241	Yellow
E242	Yellow
D247	Yellow
E248	Yellow
N249	Yellow
V252	Yellow
L256	Yellow
E257	Yellow
H258	Yellow
K259	Yellow
N265	Yellow
K266	Yellow
L267	Yellow
Q268	Yellow
W269	Yellow
F274	Yellow
S275	Yellow
N276	Yellow
N277	Yellow
T278	Yellow
A279	Yellow
L282	Yellow
T286	Yellow
A291	Yellow
L294	Yellow
W297	Yellow
E298	Yellow
T299	Yellow
T300	Yellow
S301	Yellow
V305	Yellow
R306	Yellow
V307	Yellow
L308	Yellow
F135	Yellow
E136	Yellow
E137	Yellow
I3	Yellow
P8	Yellow
I143	Yellow
D144	Yellow
F145	Yellow
D148	Yellow
P149	Yellow
V150	Yellow
L153	Yellow
LEU	Yellow
SER	Yellow
LVS	Yellow
SER	Yellow
ASP	Yellow
GLU	Yellow
GLN	Yellow
LEU	Yellow
SER	Yellow
SER	Yellow
THR	Yellow
PRO	Yellow
ASP	Yellow
H168	Yellow
G169	Yellow
Y170	Yellow
V173	Yellow
I183	Yellow
I184	Yellow
I185	Yellow
S189	Yellow
W192	Yellow
L193	Yellow
D194	Yellow
F195	Yellow
Y196	Yellow
K197	Yellow
T204	Yellow
E205	Yellow
C206	Yellow
I207	Yellow
H208	Yellow
S209	Yellow
L210	Yellow
K211	Yellow
I212	Yellow
T213	Yellow
S214	Yellow
S215	Yellow
N216	Yellow
I217	Yellow
M1	Grey
N2	Grey
I3	Grey
P8	Grey
V11	Grey
L12	Grey
H15	Grey
L19	Grey
I23	Grey
R28	Grey
L32	Grey
Q33	Grey
F34	Grey
L43	Grey
G44	Grey
C45	Grey
A46	Grey
A49	Grey
L50	Grey
Y53	Grey
P60	Grey
R73	Grey
P74	Grey
I75	Grey
L88	Grey
S91	Grey
R92	Grey
L98	Grey
W99	Grey
D100	Grey
L108	Grey
W118	Grey
L123	Grey
D124	Grey
ALA	Grey
LVS	Grey
R127	Grey
R128	Grey
L129	Grey
C130	Grey
I134	Grey

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	650847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0128	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NLE, ZN, SAM

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	0.23	0/855	0.41	0/1140
1	E	0.24	0/796	0.42	0/1065
2	B	0.24	0/653	0.38	0/873
2	F	0.23	0/651	0.38	0/873
3	C	0.21	0/805	0.35	0/1088
3	G	0.22	0/828	0.38	0/1117
4	D	0.20	0/738	0.35	0/994
4	H	0.20	0/743	0.35	0/1001
5	I	0.21	0/3333	0.43	0/5137
6	J	0.22	0/3381	0.40	0/5221
7	K	0.20	0/603	0.50	0/811
8	L	0.15	0/2417	0.40	0/3281
9	M	0.21	0/3259	0.39	0/4438
10	N	0.14	0/1732	0.36	0/2317
11	O	0.18	0/2651	0.52	0/3575
12	P	0.18	0/341	0.53	0/463
12	Q	0.36	0/227	0.75	0/307
13	R	0.22	0/983	0.63	0/1335
All	All	0.20	0/24996	0.43	0/35036

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

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	871	0	918	9	0
1	E	802	0	843	13	0
2	B	646	0	687	8	0
2	F	644	0	690	12	0
3	C	795	0	846	11	0
3	G	818	0	877	10	0
4	D	727	0	747	11	0
4	H	732	0	752	9	0
5	I	2975	0	1639	47	0
6	J	3011	0	1639	55	0
7	K	597	0	626	17	0
8	L	2367	0	2330	64	0
9	M	3183	0	3085	87	0
10	N	1710	0	1723	33	0
11	O	2595	0	2506	69	0
12	P	336	0	345	6	0
12	Q	225	0	226	9	0
13	R	966	0	827	27	0
14	N	1	0	0	0	0
15	N	27	0	22	3	0
All	All	24028	0	21328	448	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 10.

The worst 5 of 448 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)
11:O:130:GLU:HA	11:O:241:LEU:HB2	1.67	0.76
8:L:9:GLY:HA3	8:L:309:CYS:HB3	1.72	0.71
11:O:66:TYR:HA	11:O:323:PHE:O	1.91	0.70
8:L:97:ALA:HB1	8:L:116:MET:HB2	1.73	0.69
8:L:290:VAL:HA	8:L:304:ALA:HA	1.73	0.69

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	99/135 (73%)	92 (93%)	7 (7%)	0	100	100
1	E	93/135 (69%)	86 (92%)	7 (8%)	0	100	100
2	B	79/102 (78%)	77 (98%)	2 (2%)	0	100	100
2	F	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	101/129 (78%)	99 (98%)	2 (2%)	0	100	100
3	G	104/129 (81%)	104 (100%)	0	0	100	100
4	D	91/122 (75%)	87 (96%)	4 (4%)	0	100	100
4	H	92/122 (75%)	89 (97%)	3 (3%)	0	100	100
7	K	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
8	L	302/315 (96%)	283 (94%)	19 (6%)	0	100	100
9	M	387/426 (91%)	356 (92%)	31 (8%)	0	100	100
10	N	210/358 (59%)	190 (90%)	20 (10%)	0	100	100
11	O	297/505 (59%)	281 (95%)	16 (5%)	0	100	100
12	P	40/175 (23%)	36 (90%)	4 (10%)	0	100	100
12	Q	25/175 (14%)	24 (96%)	1 (4%)	0	100	100
13	R	125/391 (32%)	111 (89%)	14 (11%)	0	100	100
All	All	2196/3401 (65%)	2062 (94%)	134 (6%)	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	88/107 (82%)	88 (100%)	0	100	100
1	E	83/107 (78%)	83 (100%)	0	100	100
2	B	66/78 (85%)	66 (100%)	0	100	100
2	F	67/78 (86%)	67 (100%)	0	100	100
3	C	82/101 (81%)	82 (100%)	0	100	100
3	G	84/101 (83%)	84 (100%)	0	100	100
4	D	80/102 (78%)	80 (100%)	0	100	100
4	H	80/102 (78%)	80 (100%)	0	100	100
7	K	68/72 (94%)	68 (100%)	0	100	100
8	L	272/279 (98%)	272 (100%)	0	100	100
9	M	359/388 (92%)	359 (100%)	0	100	100
10	N	179/318 (56%)	179 (100%)	0	100	100
11	O	282/449 (63%)	281 (100%)	1 (0%)	84	82
12	P	38/162 (24%)	38 (100%)	0	100	100
12	Q	25/162 (15%)	25 (100%)	0	100	100
13	R	91/355 (26%)	91 (100%)	0	100	100
All	All	1944/2961 (66%)	1943 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	O	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
10	N	987	ASN
13	R	304	HIS
11	O	116	GLN
11	O	306	ASN
8	L	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z > 2$
1	NLE	A	120	1	6,7,8	0.47	0	2,7,9	0.43	0
1	NLE	A	90	1	6,7,8	0.56	0	2,7,9	0.43	0
1	NLE	A	4	1	6,7,8	0.50	0	2,7,9	0.44	0
1	NLE	E	120	1	6,7,8	0.45	0	2,7,9	0.39	0
1	NLE	E	90	1	6,7,8	0.54	0	2,7,9	0.44	0

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
1	NLE	A	120	1	-	0/5/6/8	-
1	NLE	A	90	1	-	3/5/6/8	-
1	NLE	A	4	1	-	0/5/6/8	-
1	NLE	E	120	1	-	0/5/6/8	-
1	NLE	E	90	1	-	0/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	90	NLE	C-CA-CB-CG
1	A	90	NLE	CA-CB-CG-CD
1	A	90	NLE	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4	NLE	1	0
1	E	120	NLE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	SAM	N	1102	-	27,29,29	0.44	0	34,42,42	0.46	1 (2%)

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
15	SAM	N	1102	-	-	5/17/33/33	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	1102	SAM	CG-SD-C5'	-2.06	98.38	103.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

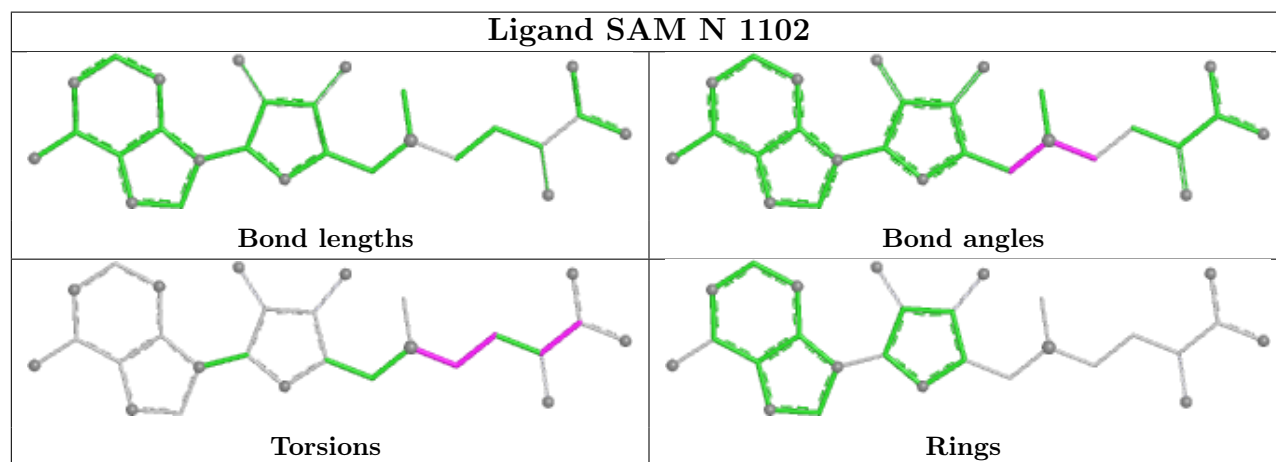
Mol	Chain	Res	Type	Atoms
15	N	1102	SAM	CA-CB-CG-SD
15	N	1102	SAM	CB-CG-SD-CE
15	N	1102	SAM	O-C-CA-CB
15	N	1102	SAM	OXT-C-CA-CB
15	N	1102	SAM	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	1102	SAM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

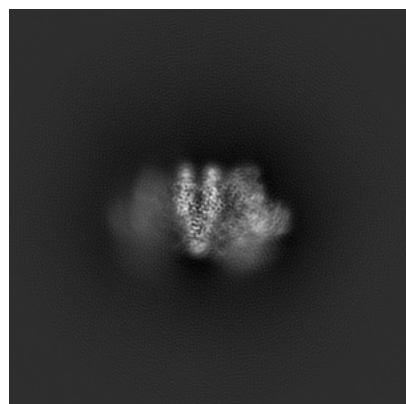
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21157. These allow visual inspection of the internal detail of the map and identification of artifacts.

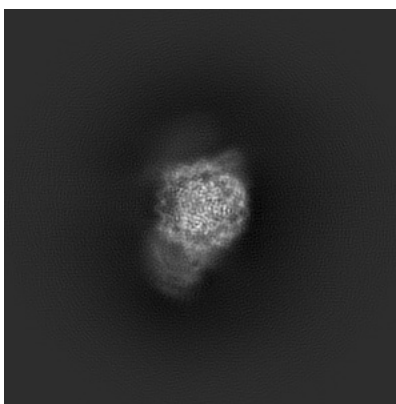
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

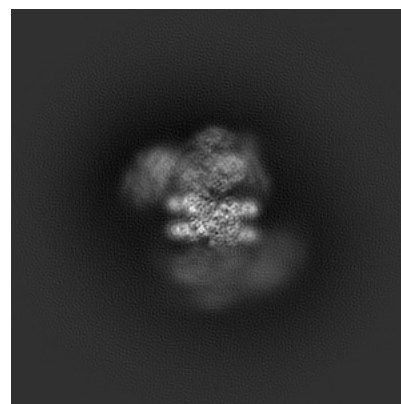
6.1.1 Primary map



X

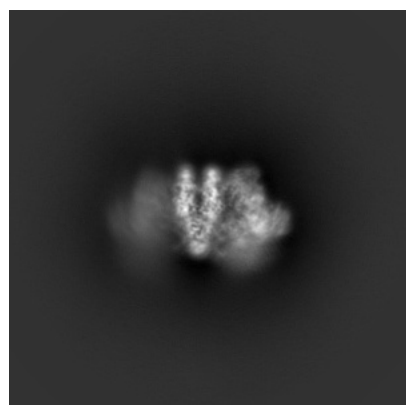


Y

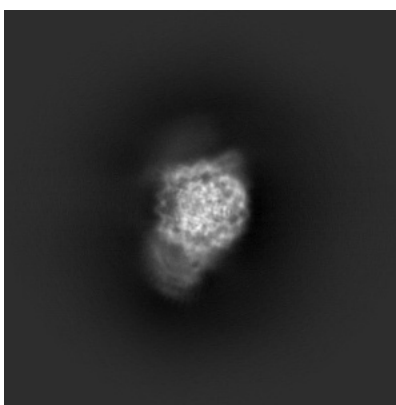


Z

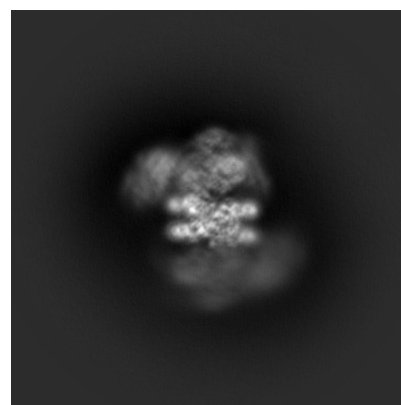
6.1.2 Raw map



X



Y

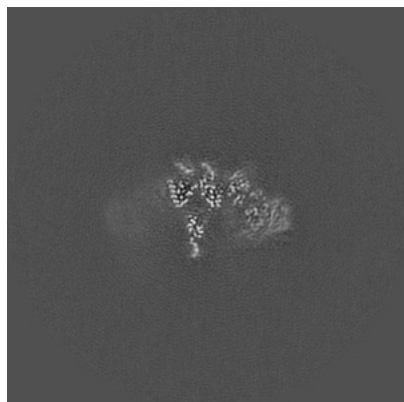


Z

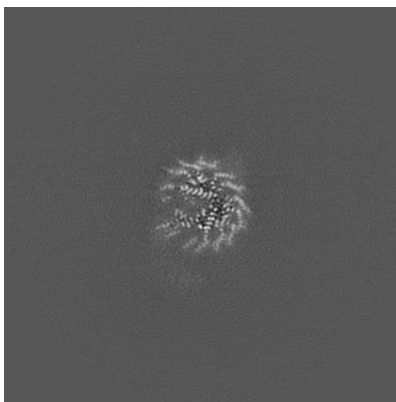
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

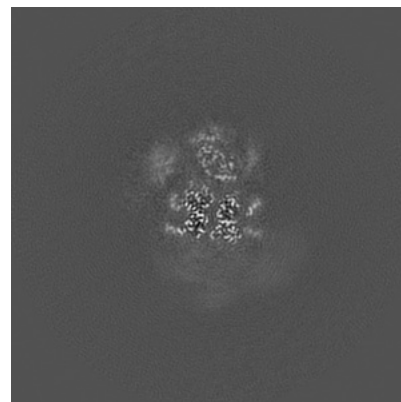
6.2.1 Primary map



X Index: 200

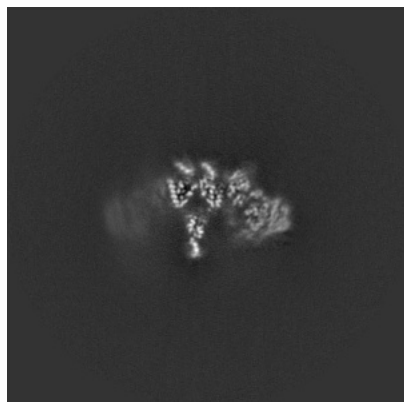


Y Index: 200

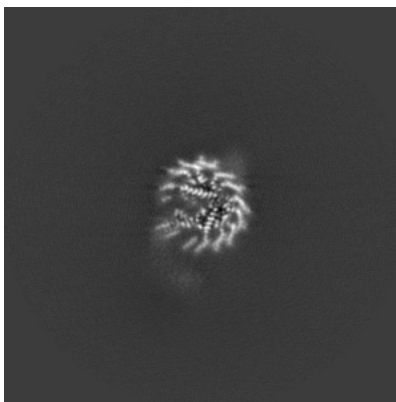


Z Index: 200

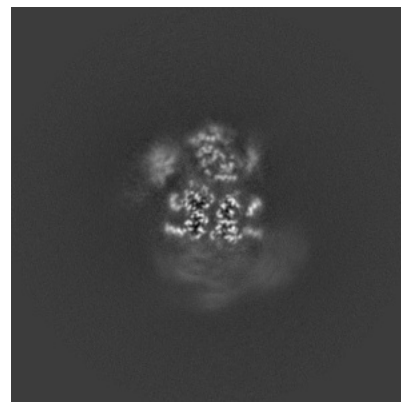
6.2.2 Raw map



X Index: 200



Y Index: 200

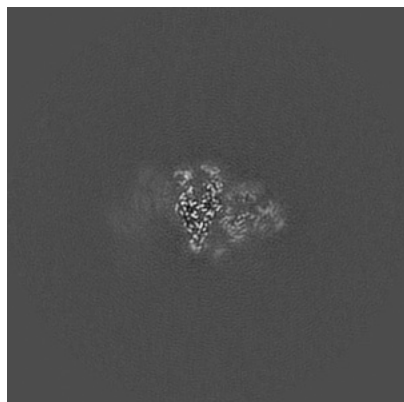


Z Index: 200

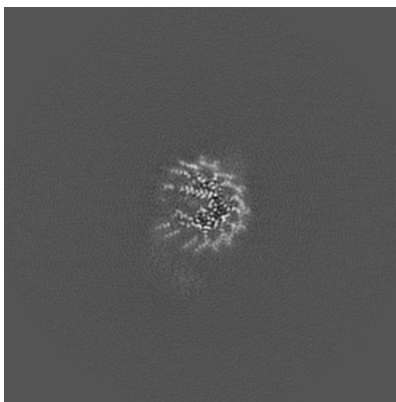
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

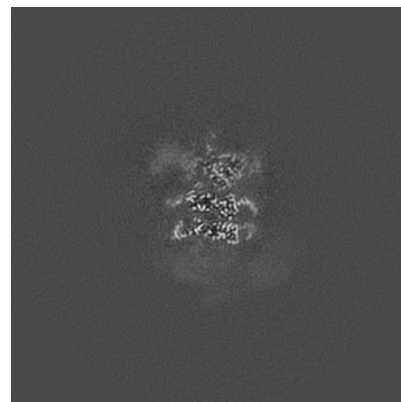
6.3.1 Primary map



X Index: 186

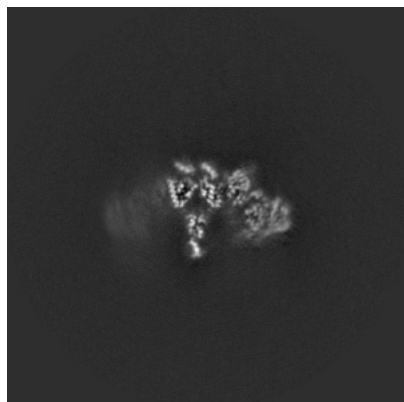


Y Index: 201

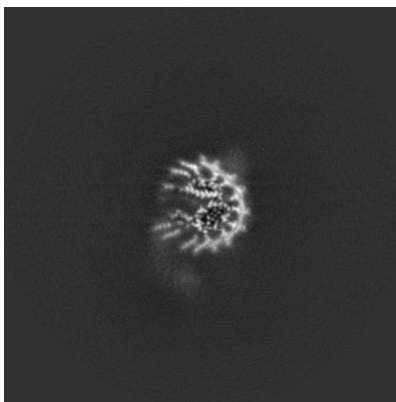


Z Index: 208

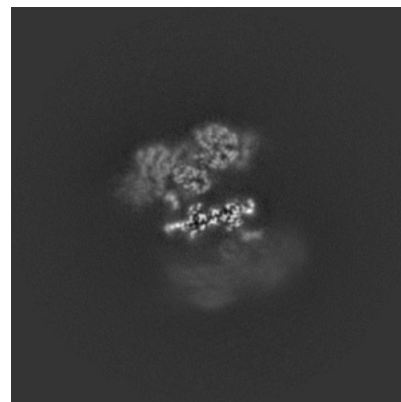
6.3.2 Raw map



X Index: 201



Y Index: 202

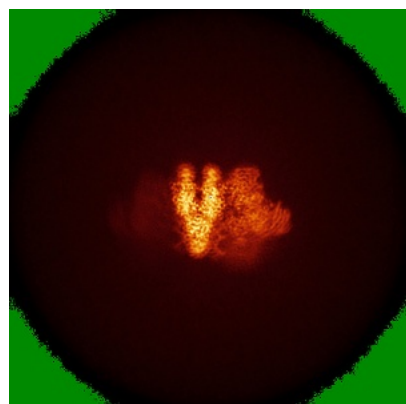


Z Index: 186

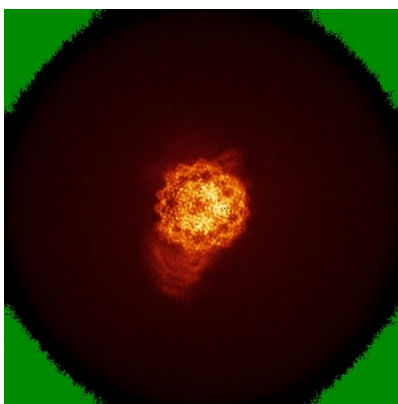
The images above show the largest variance slices of the map in three orthogonal directions.

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

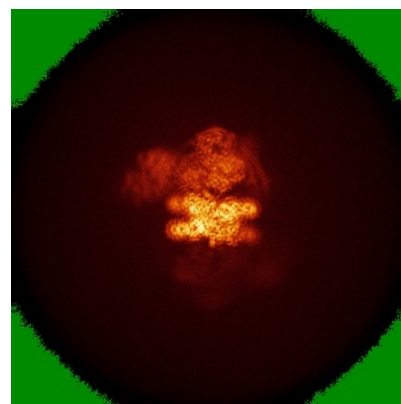
6.4.1 Primary map



X

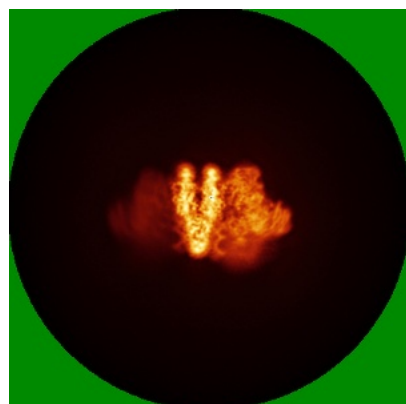


Y

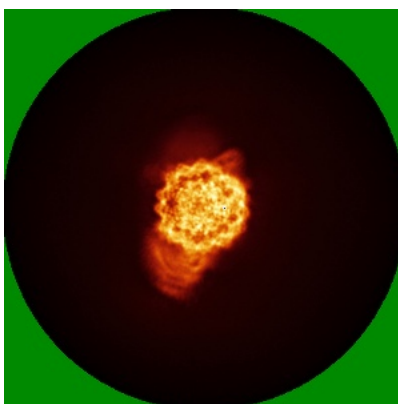


Z

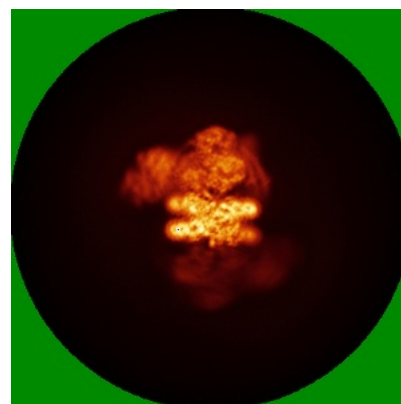
6.4.2 Raw map



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 0.0128. 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.

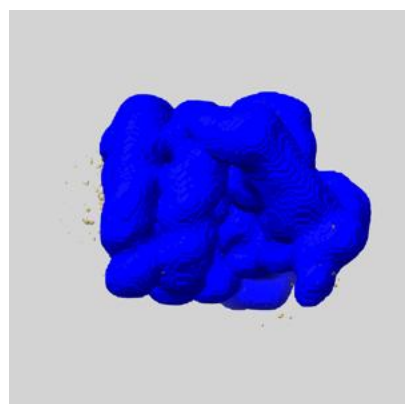
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

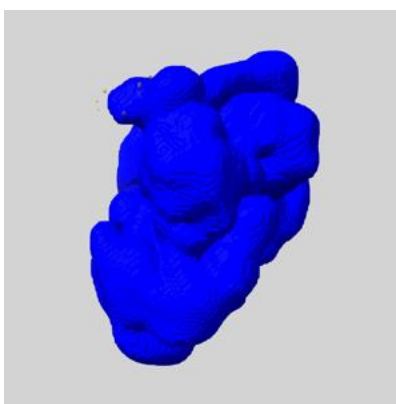
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

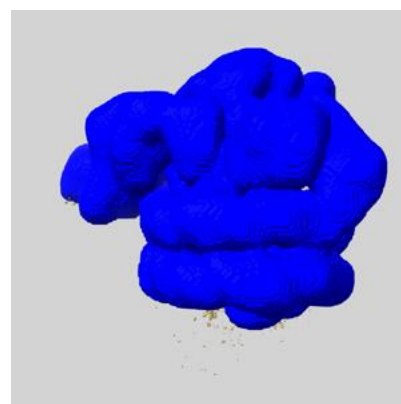
6.6.1 emd_21157_msk_1.map [i](#)



X



Y

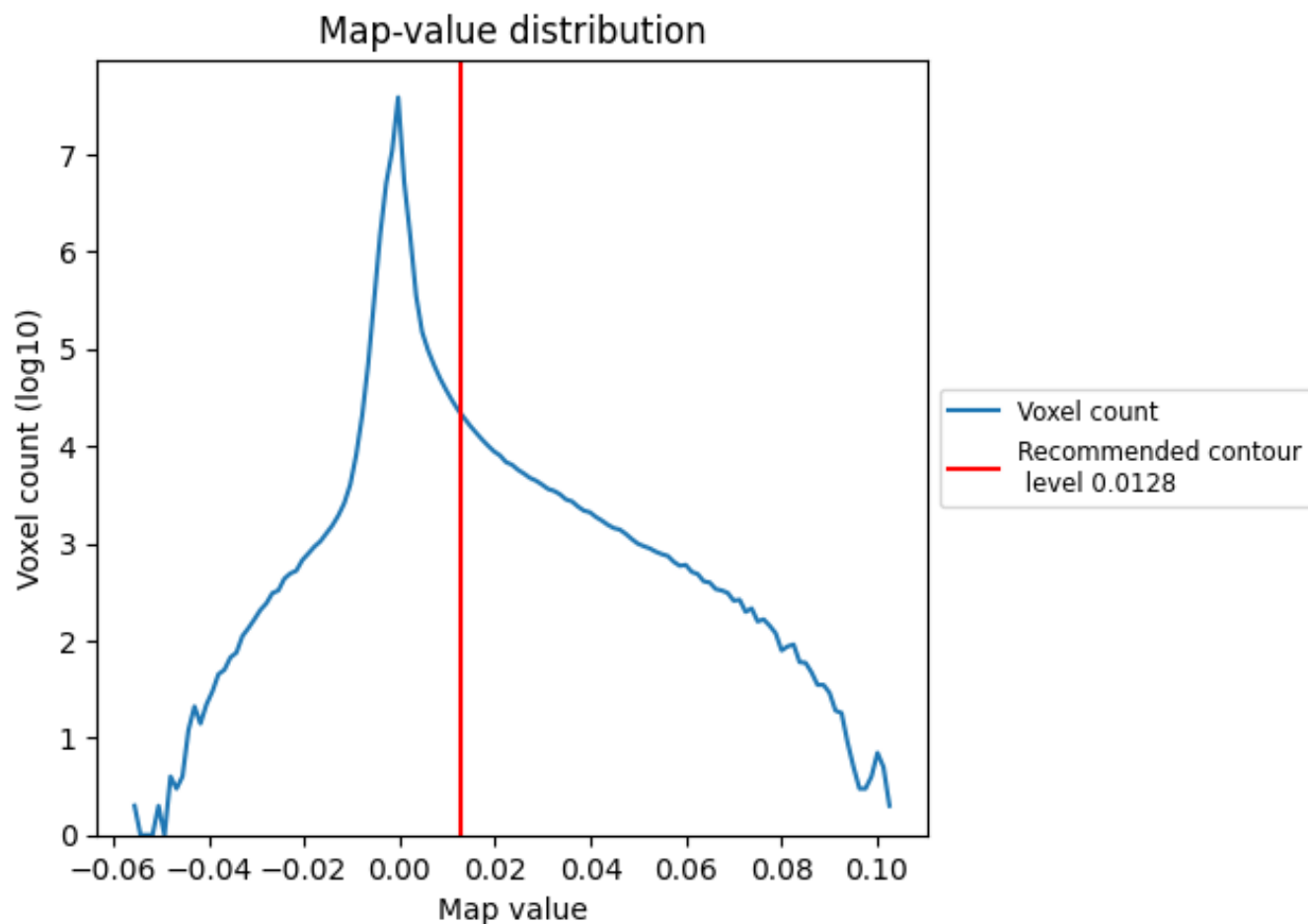


Z

7 Map analysis [i](#)

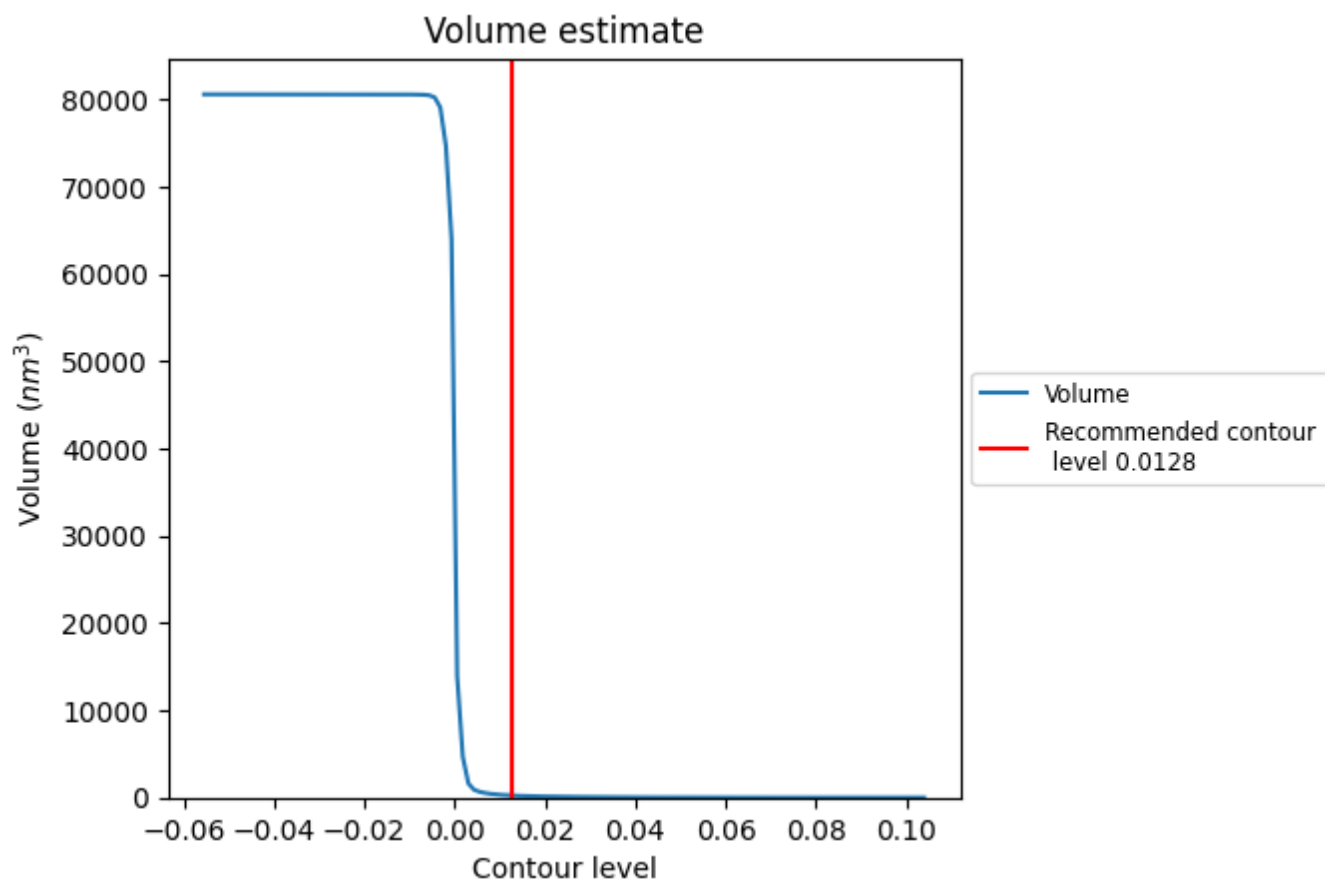
This section contains the results of statistical analysis of the map.

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.

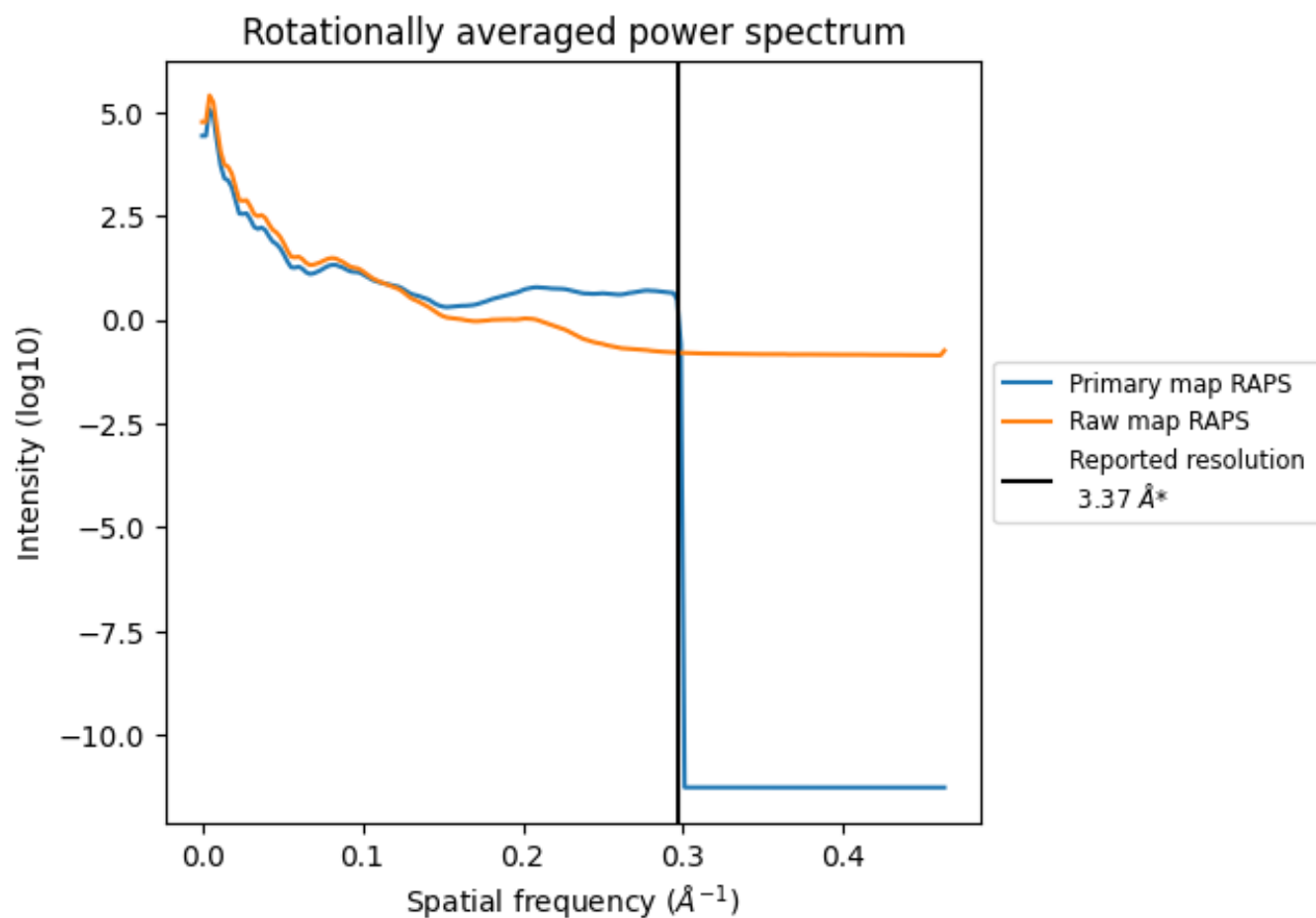
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm³; this corresponds to an approximate mass of 209 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 ⓘ

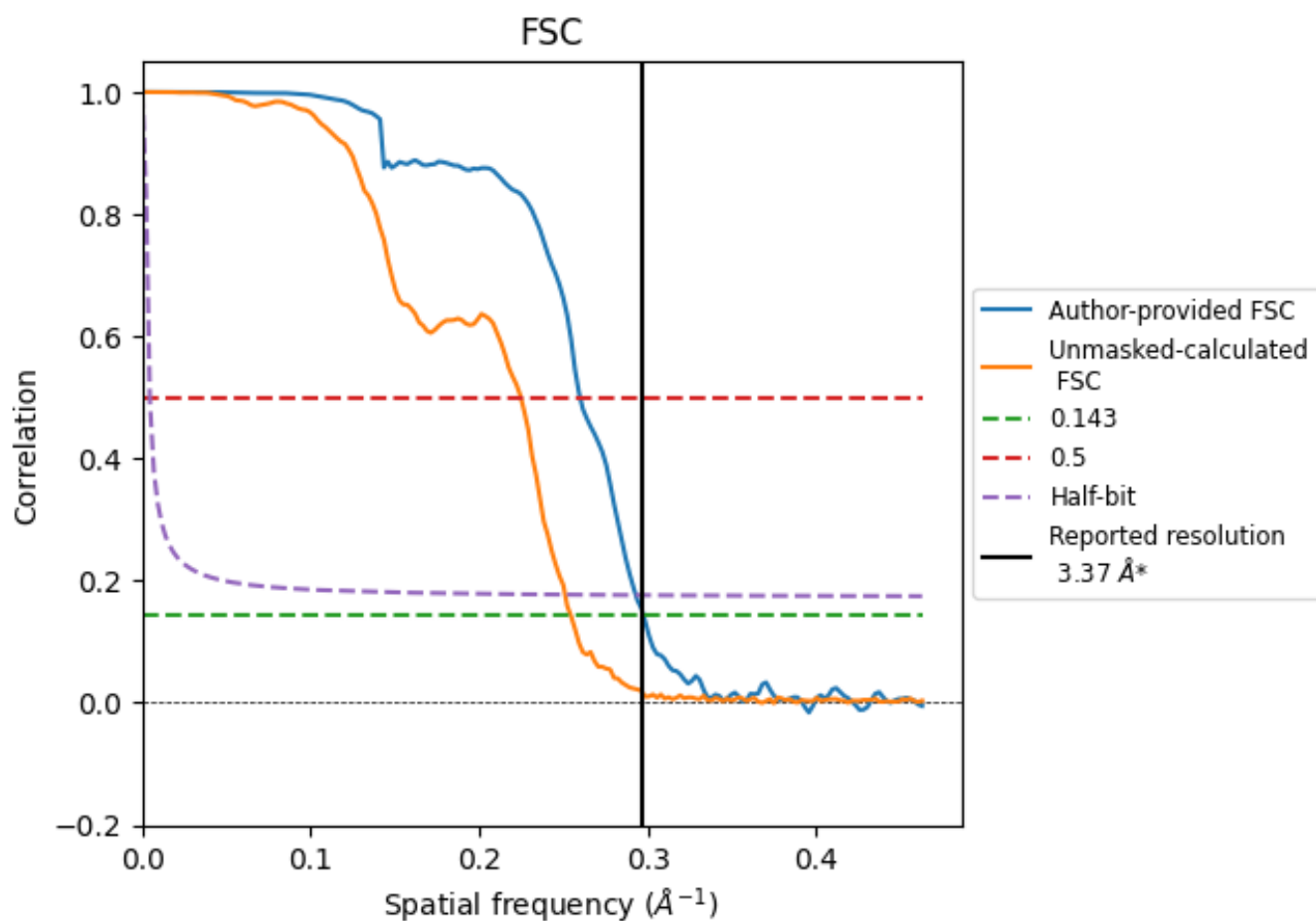


*Reported resolution corresponds to spatial frequency of 0.297 Å⁻¹

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 0.297 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

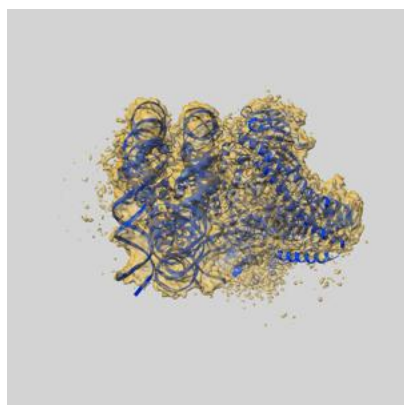
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	3.36	3.85	3.41
Unmasked-calculated*	3.93	4.45	3.98

*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 3.93 differs from the reported value 3.37 by more than 10 %

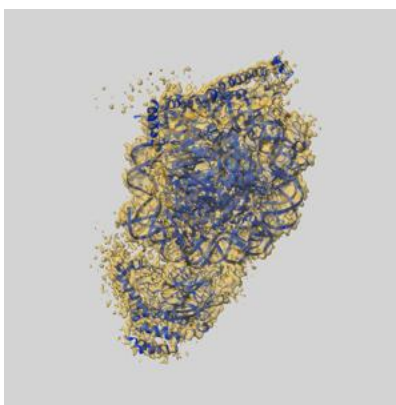
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21157 and PDB model 6VEN. Per-residue inclusion information can be found in section 3 on page 10.

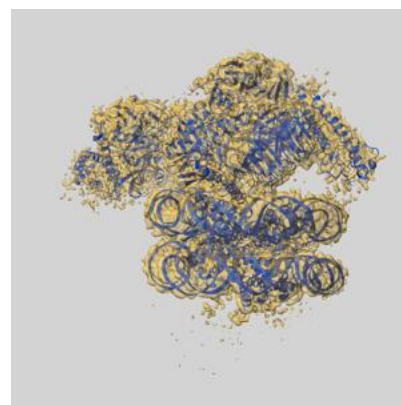
9.1 Map-model overlay [i](#)



X



Y



Z

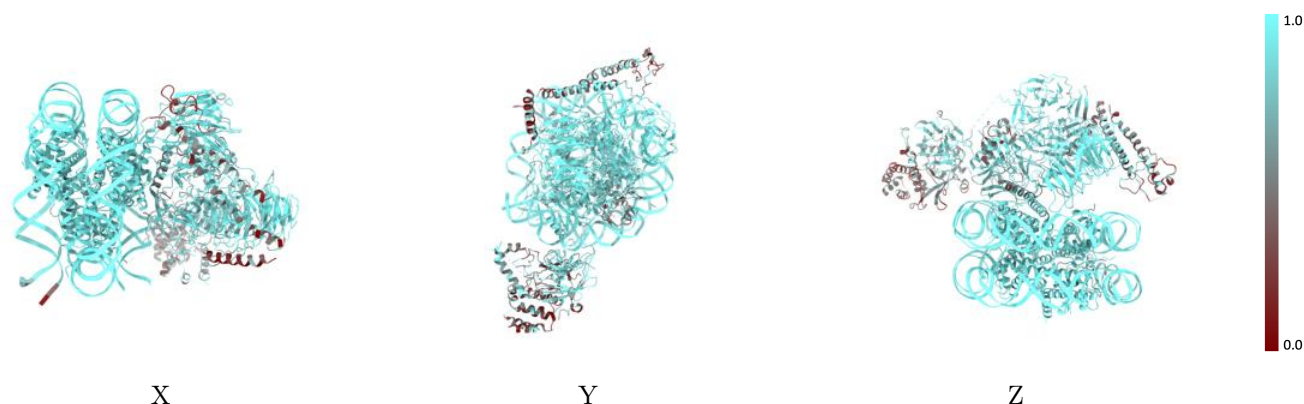
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



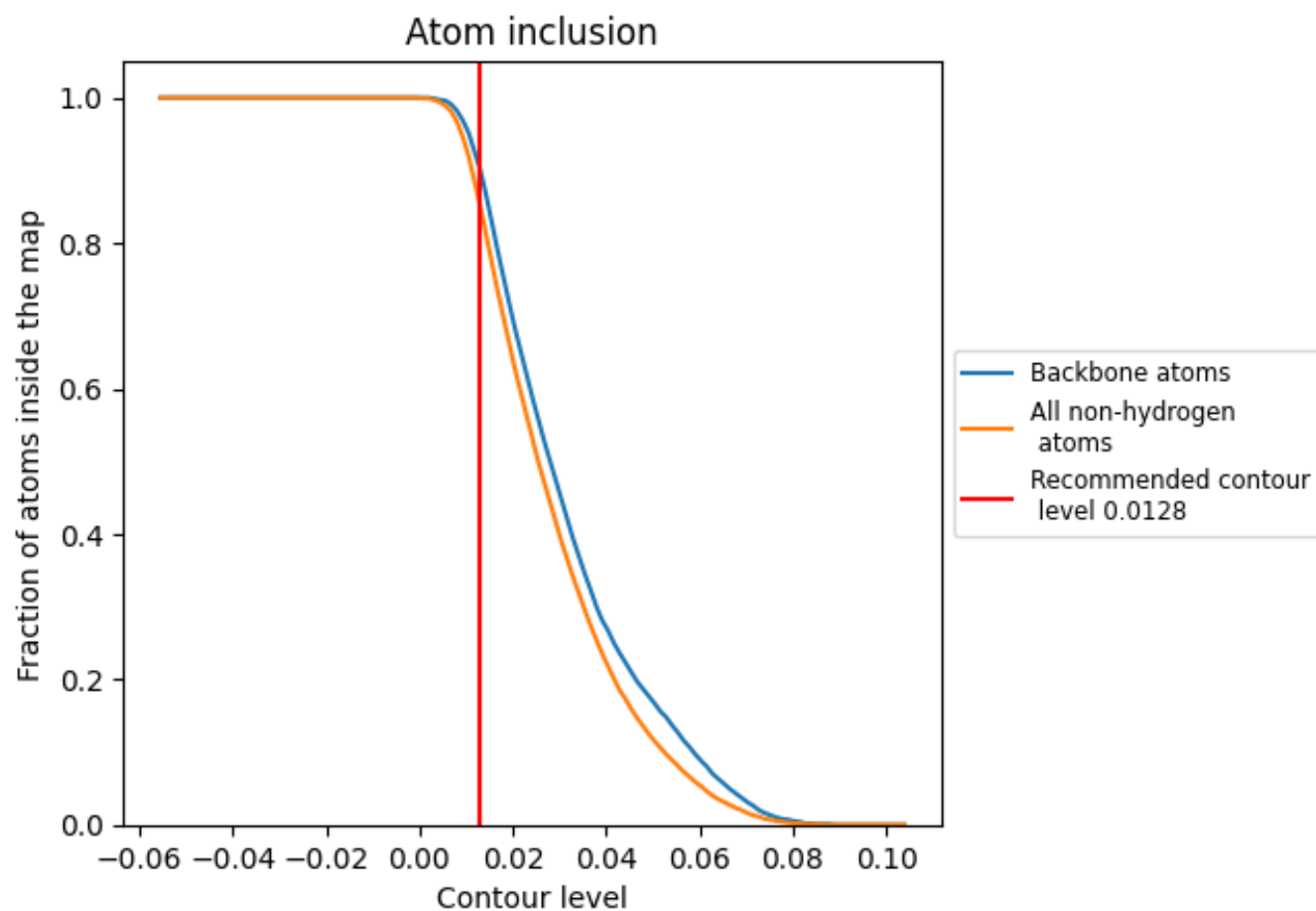
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0128).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.4490
A	 0.9580	 0.5560
B	 0.9630	 0.5530
C	 0.9560	 0.5530
D	 0.9540	 0.5430
E	 0.9560	 0.5500
F	 0.9580	 0.5540
G	 0.9470	 0.5550
H	 0.9500	 0.5490
I	 0.9670	 0.4590
J	 0.9730	 0.4620
K	 0.6070	 0.3220
L	 0.9050	 0.4550
M	 0.9140	 0.4920
N	 0.7640	 0.4600
O	 0.6050	 0.2620
P	 0.3350	 0.2150
Q	 0.3860	 0.2430
R	 0.5110	 0.2680

