



## wwPDB EM Validation Summary Report ⓘ

Apr 8, 2024 – 08:49 pm BST

PDB ID : 8S5M  
EMDB ID : EMD-19740  
Title : Full-length human cystathionine beta-synthase with C-terminal 6xHis-tag,  
SAM bound, activated state, helical reconstruction  
Authors : McCorvie, T.J.; Yue, W.W.  
Deposited on : 2024-02-23  
Resolution : 4.00 Å (reported)  
Based on initial models : 4UUU, ., 4PCU

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

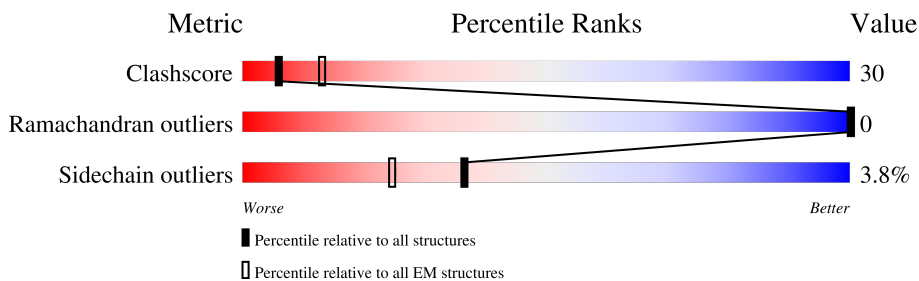
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	559	
1	B	559	
1	C	559	
1	D	559	
1	E	559	
1	F	559	
1	G	559	
1	H	559	

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Mol	Chain	Length	Quality of chain
1	I	559	 11% 15% 74%
1	J	559	 6% 14% 11% 74%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11620 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	144	1135	727	198	205	5	0	0
1	B	144	1135	727	198	205	5	0	0
1	C	144	1135	727	198	205	5	0	0
1	D	144	1135	727	198	205	5	0	0
1	E	144	1135	727	198	205	5	0	0
1	F	144	1135	727	198	205	5	0	0
1	G	144	1135	727	198	205	5	0	0
1	H	144	1135	727	198	205	5	0	0
1	I	144	1135	727	198	205	5	0	0
1	J	144	1135	727	198	205	5	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	-	expression tag	UNP P35520
A	146	ALA	-	expression tag	UNP P35520
A	147	HIS	-	expression tag	UNP P35520
A	148	HIS	-	expression tag	UNP P35520
A	149	HIS	-	expression tag	UNP P35520
A	150	HIS	-	expression tag	UNP P35520
A	151	HIS	-	expression tag	UNP P35520
A	152	HIS	-	expression tag	UNP P35520
B	145	ALA	-	expression tag	UNP P35520
B	146	ALA	-	expression tag	UNP P35520

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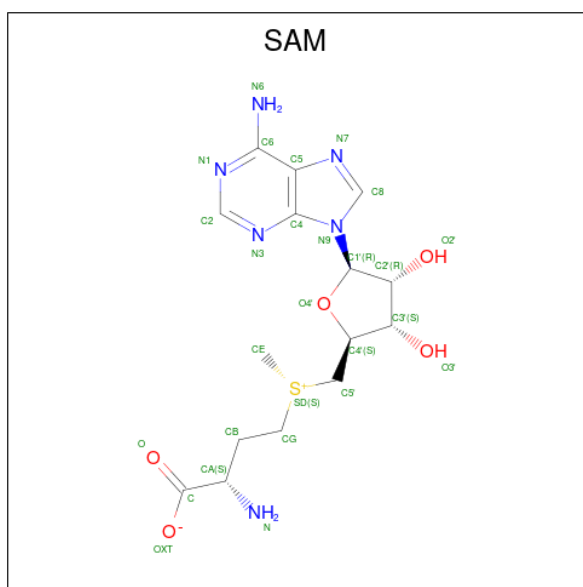
Chain	Residue	Modelled	Actual	Comment	Reference
B	147	HIS	-	expression tag	UNP P35520
B	148	HIS	-	expression tag	UNP P35520
B	149	HIS	-	expression tag	UNP P35520
B	150	HIS	-	expression tag	UNP P35520
B	151	HIS	-	expression tag	UNP P35520
B	152	HIS	-	expression tag	UNP P35520
C	145	ALA	-	expression tag	UNP P35520
C	146	ALA	-	expression tag	UNP P35520
C	147	HIS	-	expression tag	UNP P35520
C	148	HIS	-	expression tag	UNP P35520
C	149	HIS	-	expression tag	UNP P35520
C	150	HIS	-	expression tag	UNP P35520
C	151	HIS	-	expression tag	UNP P35520
C	152	HIS	-	expression tag	UNP P35520
D	145	ALA	-	expression tag	UNP P35520
D	146	ALA	-	expression tag	UNP P35520
D	147	HIS	-	expression tag	UNP P35520
D	148	HIS	-	expression tag	UNP P35520
D	149	HIS	-	expression tag	UNP P35520
D	150	HIS	-	expression tag	UNP P35520
D	151	HIS	-	expression tag	UNP P35520
D	152	HIS	-	expression tag	UNP P35520
E	145	ALA	-	expression tag	UNP P35520
E	146	ALA	-	expression tag	UNP P35520
E	147	HIS	-	expression tag	UNP P35520
E	148	HIS	-	expression tag	UNP P35520
E	149	HIS	-	expression tag	UNP P35520
E	150	HIS	-	expression tag	UNP P35520
E	151	HIS	-	expression tag	UNP P35520
E	152	HIS	-	expression tag	UNP P35520
F	145	ALA	-	expression tag	UNP P35520
F	146	ALA	-	expression tag	UNP P35520
F	147	HIS	-	expression tag	UNP P35520
F	148	HIS	-	expression tag	UNP P35520
F	149	HIS	-	expression tag	UNP P35520
F	150	HIS	-	expression tag	UNP P35520
F	151	HIS	-	expression tag	UNP P35520
F	152	HIS	-	expression tag	UNP P35520
G	145	ALA	-	expression tag	UNP P35520
G	146	ALA	-	expression tag	UNP P35520
G	147	HIS	-	expression tag	UNP P35520
G	148	HIS	-	expression tag	UNP P35520

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Chain	Residue	Modelled	Actual	Comment	Reference
G	149	HIS	-	expression tag	UNP P35520
G	150	HIS	-	expression tag	UNP P35520
G	151	HIS	-	expression tag	UNP P35520
G	152	HIS	-	expression tag	UNP P35520
H	145	ALA	-	expression tag	UNP P35520
H	146	ALA	-	expression tag	UNP P35520
H	147	HIS	-	expression tag	UNP P35520
H	148	HIS	-	expression tag	UNP P35520
H	149	HIS	-	expression tag	UNP P35520
H	150	HIS	-	expression tag	UNP P35520
H	151	HIS	-	expression tag	UNP P35520
H	152	HIS	-	expression tag	UNP P35520
I	145	ALA	-	expression tag	UNP P35520
I	146	ALA	-	expression tag	UNP P35520
I	147	HIS	-	expression tag	UNP P35520
I	148	HIS	-	expression tag	UNP P35520
I	149	HIS	-	expression tag	UNP P35520
I	150	HIS	-	expression tag	UNP P35520
I	151	HIS	-	expression tag	UNP P35520
I	152	HIS	-	expression tag	UNP P35520
J	145	ALA	-	expression tag	UNP P35520
J	146	ALA	-	expression tag	UNP P35520
J	147	HIS	-	expression tag	UNP P35520
J	148	HIS	-	expression tag	UNP P35520
J	149	HIS	-	expression tag	UNP P35520
J	150	HIS	-	expression tag	UNP P35520
J	151	HIS	-	expression tag	UNP P35520
J	152	HIS	-	expression tag	UNP P35520

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	B	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	C	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	D	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	E	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	F	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	G	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	H	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	I	1	Total	C	N	O	S	0
			27	15	6	5	1	
2	J	1	Total	C	N	O	S	0
			27	15	6	5	1	



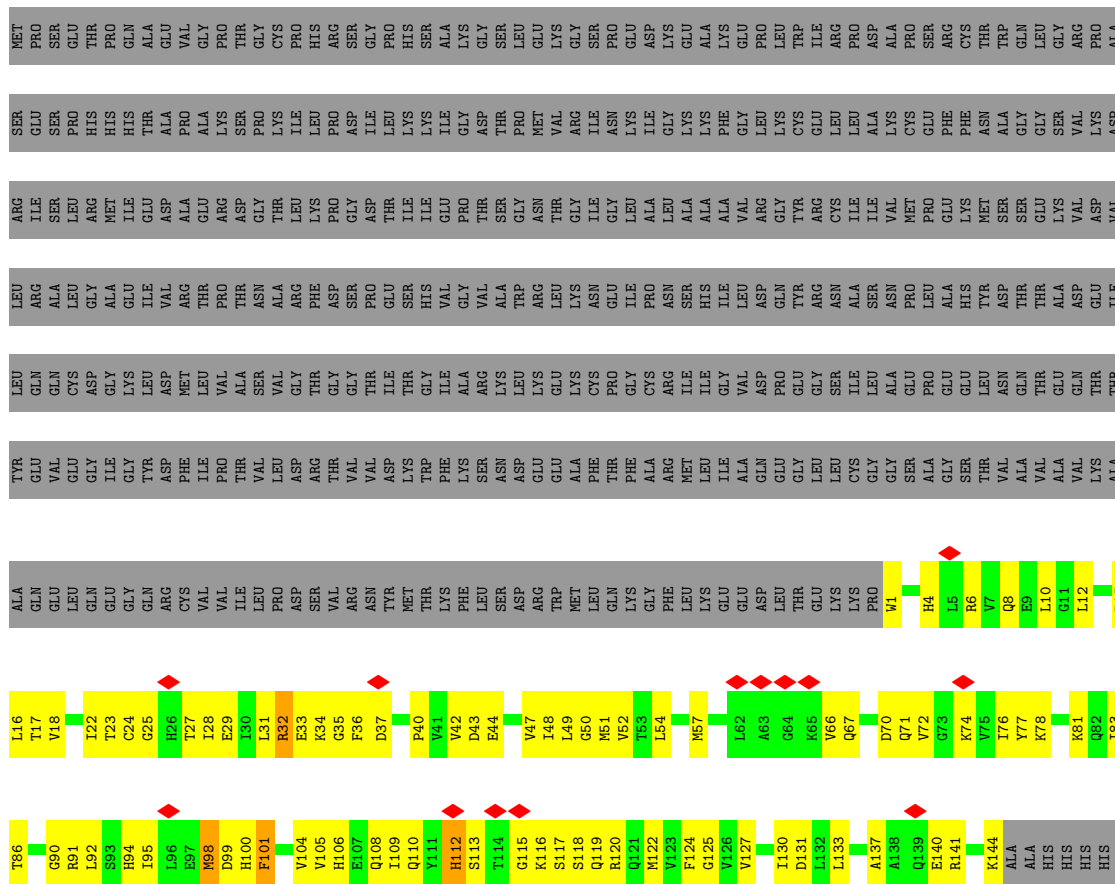






• Molecule 1: Cystathionine beta-synthase

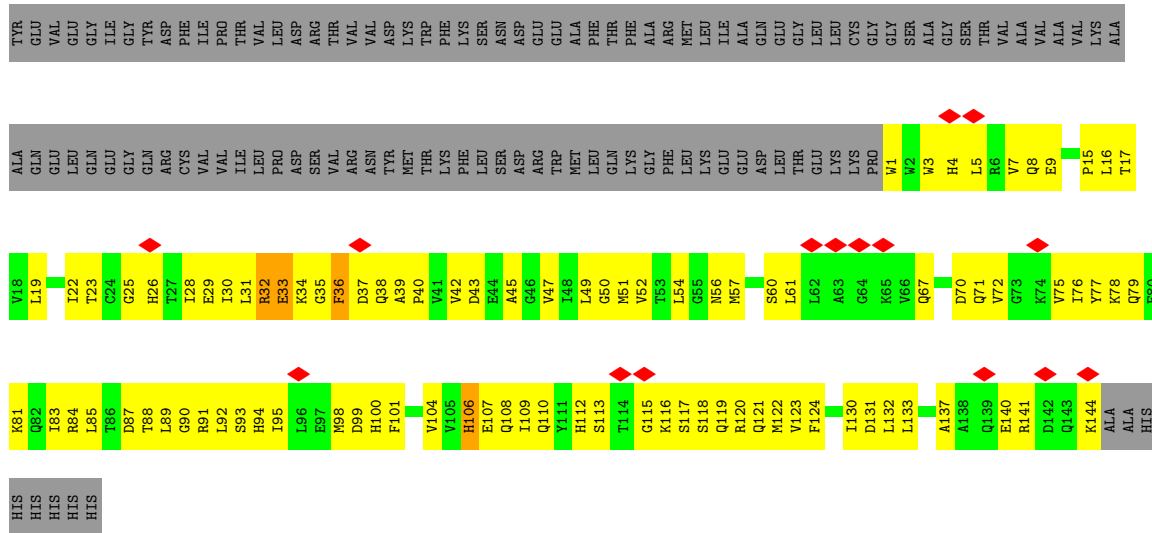
Chain D: 11% 14% . 74%



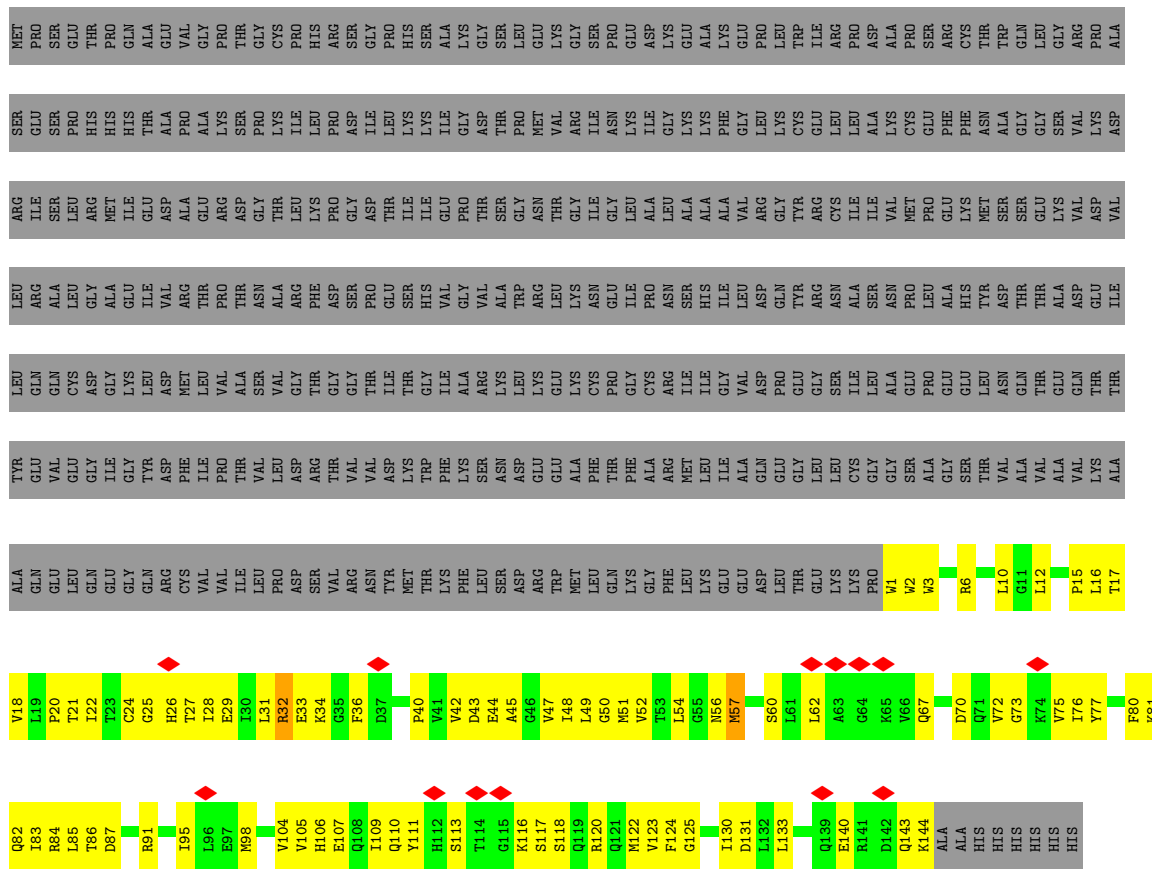
• Molecule 1: Cystathionine beta-synthase

Chain E: 9% 16% . 74%

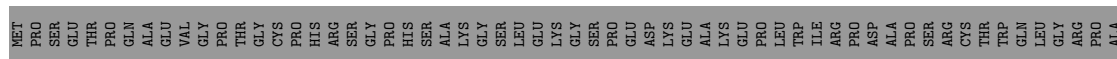


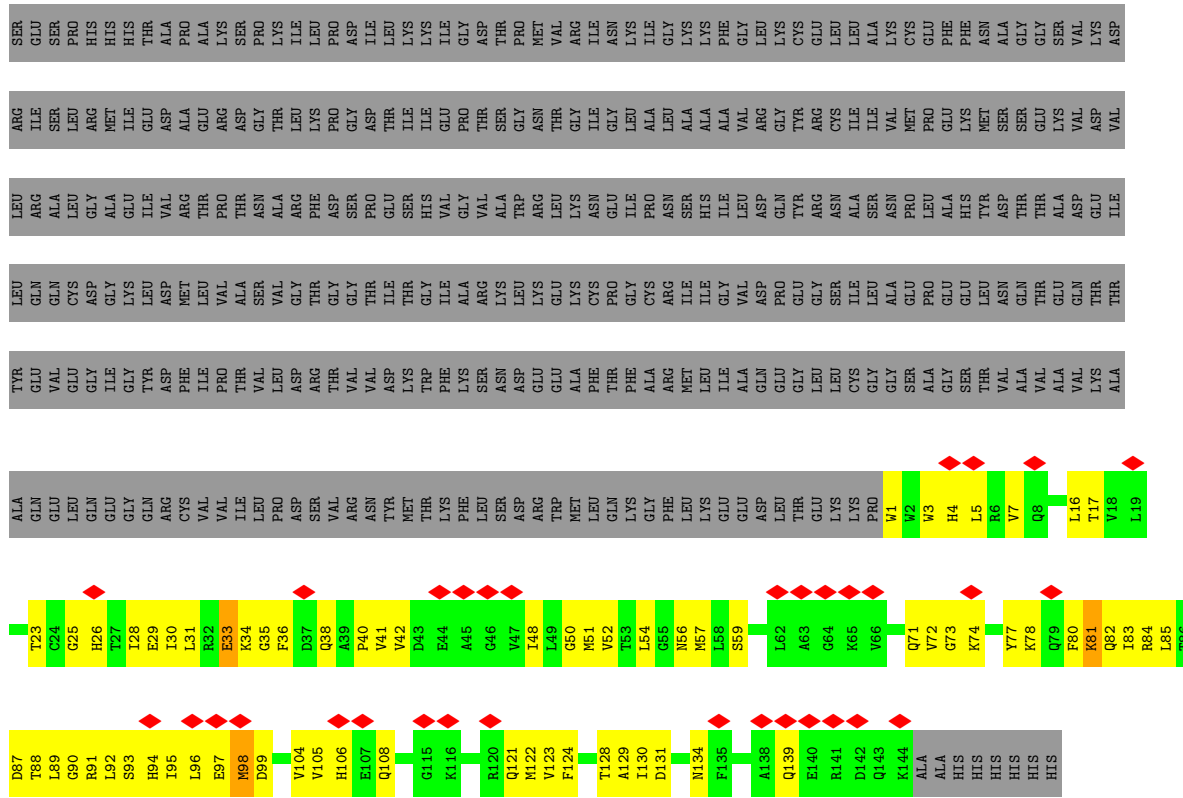


• Molecule 1: Cystathionine beta-synthase

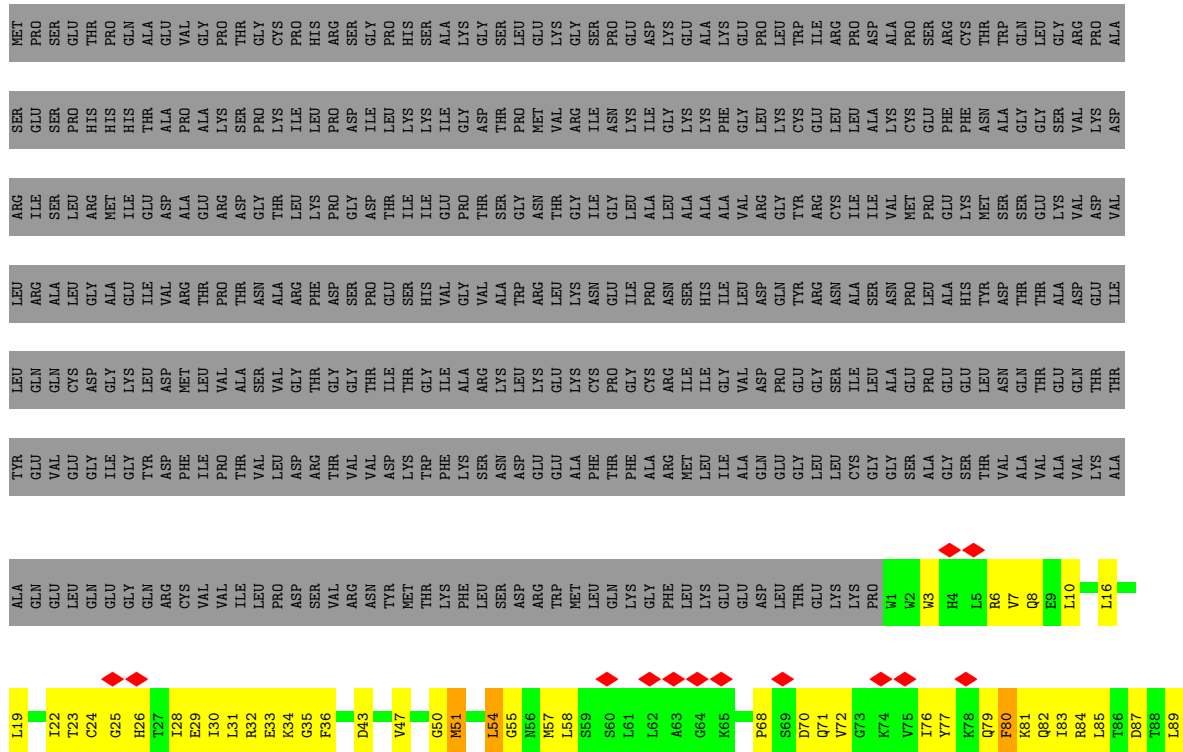


• Molecule 1: Cystathionine beta-synthase





● Molecule 1: Cystathionine beta-synthase





• Molecule 1: Cystathionine beta-synthase



MET	PRO	SER	GLU	THR	PRO	GLN	ALA	GLY	PRO	THR	GLY	CYS	HIS	ARG	SER	GLY	PRO	Q109	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
SER	GLU	SER	PRO	HIS	HIS	THR	ALA	ALA	LYS	PRO	THR	LYS	ILE	PRO	LEU	ASP	ILE	PRO	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
ARG	ILE	SER	LEU	ARG	MET	GLU	ASP	ALA	LYS	PRO	THR	LYS	ILE	PRO	LEU	ASP	ILE	PRO	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
LEU	ARG	ALA	GLY	ALA	GLY	ILE	VAL	THR	PRO	THR	ASN	ALA	GLY	THR	ASP	PRO	THR	GLU	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
LEU	GLN	CYS	GLY	GLY	LYS	LEU	ASP	VAL	THR	VAL	SER	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
TYR	GLU	VAL	GLY	ILE	GLY	TYR	ASP	ILE	THR	THR	VAL	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
ALA	GLN	LEU	GLN	GLY	GLY	ARG	CYS	VAL	VAL	ILE	LEU	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
L16	T17	V18	L19	P20	T21	T22	T23	C24	G25	H26	T27	I28	E29	L30	L31	R32	E33	K34	G35	F36	D37	Q38	A39	P40	V41	V42	D43	E44	A45	C46	V47	L48	L49	G50	M51	L54	L61	L62	A63	G64	R65	S69	D70	Q71	V72	G73	K74	V75	I76	V77	K78	K81	R84	L85
T86	D87	L89	L92	S93	H94	L96	F97	H98	D99	H100	V104	V105	H106	Q108	I109	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	A129	I130	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	D142	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

• Molecule 1: Cystathionine beta-synthase



MET	PRO	SER	THR	GLN	ALA	VAL	VAL	PRO	THR	THR	GLY	CYS	HIS	ARG	SER	GLY	PRO	Q109	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
SER	GLU	SER	PRO	HIS	HIS	THR	ALA	ALA	LYS	PRO	THR	LYS	ILE	PRO	LEU	ASP	ILE	PRO	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
ARG	ILE	SER	LEU	ARG	MET	GLU	ASP	ALA	LYS	PRO	THR	LYS	ILE	PRO	LEU	ASP	ILE	PRO	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
LEU	ARG	ALA	GLY	ALA	GLY	ILE	VAL	THR	PRO	THR	ASN	ALA	GLY	THR	ASP	PRO	THR	GLU	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
LEU	GLN	CYS	GLY	GLY	LYS	LEU	ASP	VAL	THR	VAL	SER	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
TYR	GLU	VAL	GLY	ILE	GLY	TYR	ASP	ILE	THR	THR	VAL	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
ALA	GLN	LEU	GLN	GLY	GLY	ARG	CYS	VAL	VAL	ILE	LEU	VAL	VAL	THR	ASP	THR	THR	ILE	Q110	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	V127	T128	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	
L16	T17	V18	L19	P20	T21	T22	T23	C24	G25	H26	T27	I28	E29	L30	L31	R32	E33	K34	G35	F36	D37	Q38	A39	P40	V41	V42	D43	E44	A45	C46	V47	L48	L49	G50	M51	L54	L61	L62	A63	G64	R65	S69	D70	Q71	V72	G73	K74	V75	I76	V77	K78	K81	R84	L85
T86	D87	L89	L92	S93	H94	L96	F97	H98	D99	H100	V104	V105	H106	Q108	I109	Y111	H112	S113	T114	G115	K116	Q119	R120	Q121	M122	V123	F124	A129	I130	D131	L132	L133	M134	F135	V136	A137	A138	Q139	E140	R141	D142	K144	ALA	ALA	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-178.6°, rise=46.7 Å, axial sym=D2	Depositor
Number of segments used	425260	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 ( $e^-/\text{Å}^2$ )	39.96	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.074	Depositor
Minimum map value	-1.990	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 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	0.29	0/1157	0.55	0/1568
1	B	0.29	0/1157	0.57	0/1568
1	C	0.29	0/1157	0.57	0/1568
1	D	0.29	0/1157	0.56	0/1568
1	E	0.28	0/1157	0.55	0/1568
1	F	0.29	0/1157	0.54	0/1568
1	G	0.27	0/1157	0.54	0/1568
1	H	0.28	0/1157	0.58	0/1568
1	I	0.28	0/1157	0.52	0/1568
1	J	0.28	0/1157	0.56	0/1568
All	All	0.28	0/11570	0.55	0/15680

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	1135	0	1161	73	0
1	B	1135	0	1161	80	0
1	C	1135	0	1161	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1135	0	1161	82	0
1	E	1135	0	1161	88	0
1	F	1135	0	1161	81	0
1	G	1135	0	1161	60	0
1	H	1135	0	1161	77	0
1	I	1135	0	1161	81	0
1	J	1135	0	1161	52	0
2	A	27	0	22	1	0
2	B	27	0	22	3	0
2	C	27	0	22	6	0
2	D	27	0	22	8	0
2	E	27	0	22	3	0
2	F	27	0	22	7	0
2	G	27	0	22	5	0
2	H	27	0	22	6	0
2	I	27	0	22	3	0
2	J	27	0	22	1	0
All	All	11620	0	11830	693	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 30.

The worst 5 of 693 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:J:12:LEU:HD21	1:J:125:GLY:HA3	1.56	0.88
1:B:122:MET:HG2	1:E:122:MET:HG2	1.55	0.88
1:F:84:ARG:HH22	1:F:107:GLU:HB3	1.37	0.87
1:H:81:LYS:NZ	1:H:95:ILE:O	2.09	0.85
1:C:84:ARG:HH22	1:C:107:GLU:HB3	1.41	0.85

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	142/559 (25%)	135 (95%)	7 (5%)	0	100	100
1	B	142/559 (25%)	134 (94%)	8 (6%)	0	100	100
1	C	142/559 (25%)	135 (95%)	7 (5%)	0	100	100
1	D	142/559 (25%)	136 (96%)	6 (4%)	0	100	100
1	E	142/559 (25%)	134 (94%)	8 (6%)	0	100	100
1	F	142/559 (25%)	133 (94%)	9 (6%)	0	100	100
1	G	142/559 (25%)	130 (92%)	12 (8%)	0	100	100
1	H	142/559 (25%)	131 (92%)	11 (8%)	0	100	100
1	I	142/559 (25%)	130 (92%)	12 (8%)	0	100	100
1	J	142/559 (25%)	134 (94%)	8 (6%)	0	100	100
All	All	1420/5590 (25%)	1332 (94%)	88 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/471 (26%)	119 (95%)	6 (5%)	25	53
1	B	125/471 (26%)	117 (94%)	8 (6%)	17	45
1	C	125/471 (26%)	123 (98%)	2 (2%)	62	79
1	D	125/471 (26%)	121 (97%)	4 (3%)	39	62
1	E	125/471 (26%)	119 (95%)	6 (5%)	25	53
1	F	125/471 (26%)	122 (98%)	3 (2%)	49	69
1	G	125/471 (26%)	120 (96%)	5 (4%)	31	57
1	H	125/471 (26%)	120 (96%)	5 (4%)	31	57
1	I	125/471 (26%)	121 (97%)	4 (3%)	39	62

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	125/471 (26%)	121 (97%)	4 (3%)	39 62
All	All	1250/4710 (26%)	1203 (96%)	47 (4%)	36 59

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	57	MET
1	H	54	LEU
1	G	3	TRP
1	G	98	MET
1	H	134	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	94	HIS
1	I	108	GLN
1	J	106	HIS
1	D	26	HIS
1	C	110	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands 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
2	SAM	C	201	-	24,29,29	1.25	3 (12%)	23,42,42	1.61	4 (17%)
2	SAM	F	201	-	24,29,29	1.23	3 (12%)	23,42,42	1.57	3 (13%)
2	SAM	G	201	-	24,29,29	1.22	3 (12%)	23,42,42	1.60	4 (17%)
2	SAM	A	201	-	24,29,29	1.23	3 (12%)	23,42,42	1.63	4 (17%)
2	SAM	E	201	-	24,29,29	1.24	3 (12%)	23,42,42	1.59	4 (17%)
2	SAM	D	201	-	24,29,29	1.22	2 (8%)	23,42,42	1.61	5 (21%)
2	SAM	I	201	-	24,29,29	1.21	3 (12%)	23,42,42	1.66	5 (21%)
2	SAM	B	201	-	24,29,29	1.22	3 (12%)	23,42,42	1.64	4 (17%)
2	SAM	H	201	-	24,29,29	1.23	3 (12%)	23,42,42	1.67	4 (17%)
2	SAM	J	201	-	24,29,29	1.24	3 (12%)	23,42,42	1.65	4 (17%)

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	SAM	C	201	-	-	8/12/33/33	0/3/3/3
2	SAM	F	201	-	-	5/12/33/33	0/3/3/3
2	SAM	G	201	-	-	5/12/33/33	0/3/3/3
2	SAM	A	201	-	-	3/12/33/33	0/3/3/3
2	SAM	E	201	-	-	7/12/33/33	0/3/3/3
2	SAM	D	201	-	-	6/12/33/33	0/3/3/3
2	SAM	I	201	-	-	4/12/33/33	0/3/3/3
2	SAM	B	201	-	-	9/12/33/33	0/3/3/3
2	SAM	H	201	-	-	3/12/33/33	0/3/3/3
2	SAM	J	201	-	-	4/12/33/33	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	SAM	C2-N3	3.90	1.38	1.32

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	SAM	C2-N3	3.90	1.38	1.32
2	H	201	SAM	C2-N3	3.87	1.38	1.32
2	G	201	SAM	C2-N3	3.84	1.38	1.32
2	D	201	SAM	C2-N3	3.80	1.38	1.32

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	SAM	N3-C2-N1	-5.55	120.00	128.68
2	B	201	SAM	N3-C2-N1	-5.49	120.09	128.68
2	H	201	SAM	N3-C2-N1	-5.47	120.12	128.68
2	E	201	SAM	N3-C2-N1	-5.46	120.15	128.68
2	J	201	SAM	N3-C2-N1	-5.43	120.19	128.68

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	SAM	CA-CB-CG-SD
2	A	201	SAM	CB-CG-SD-C5'
2	B	201	SAM	O-C-CA-N
2	B	201	SAM	N-CA-CB-CG
2	B	201	SAM	C-CA-CB-CG

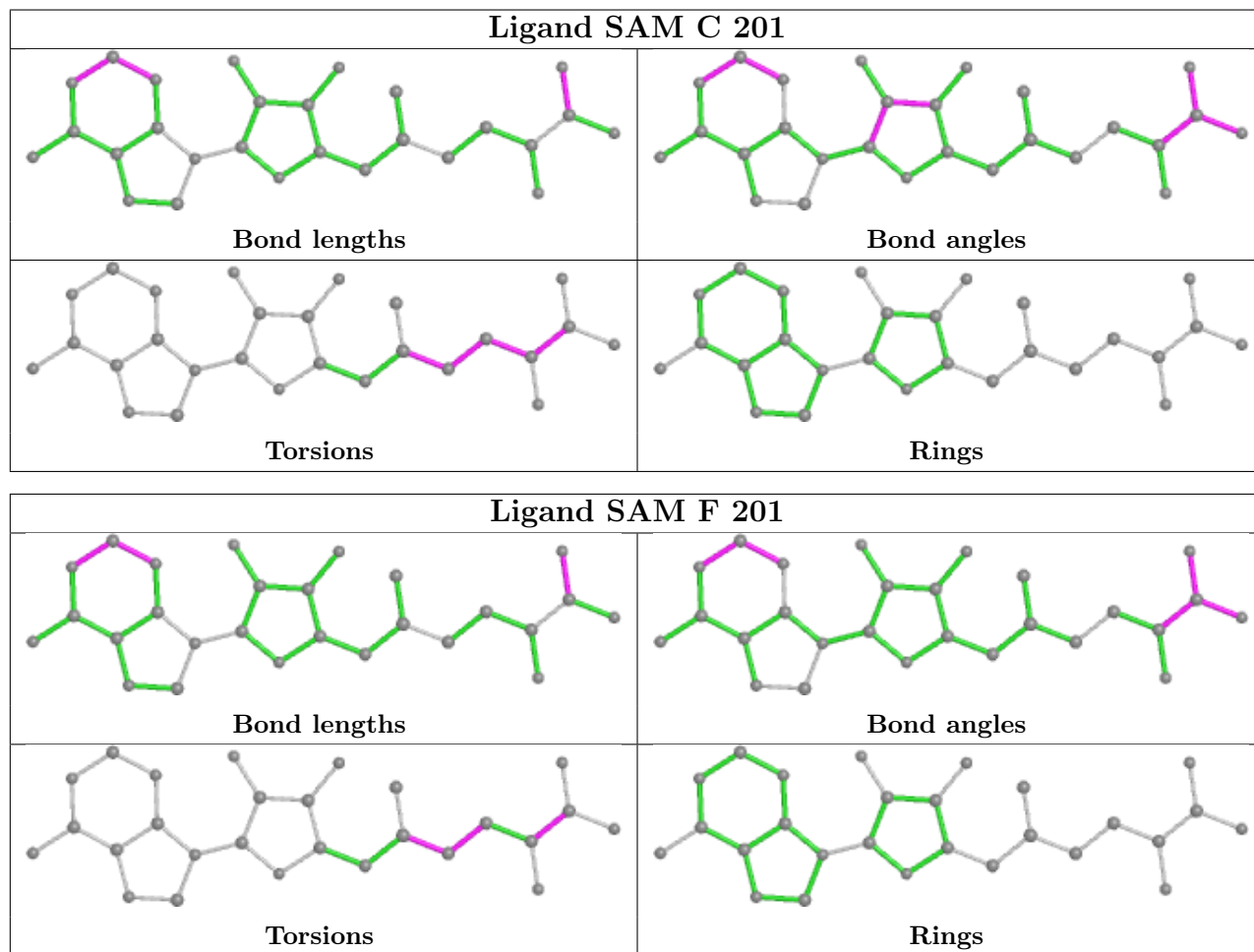
There are no ring outliers.

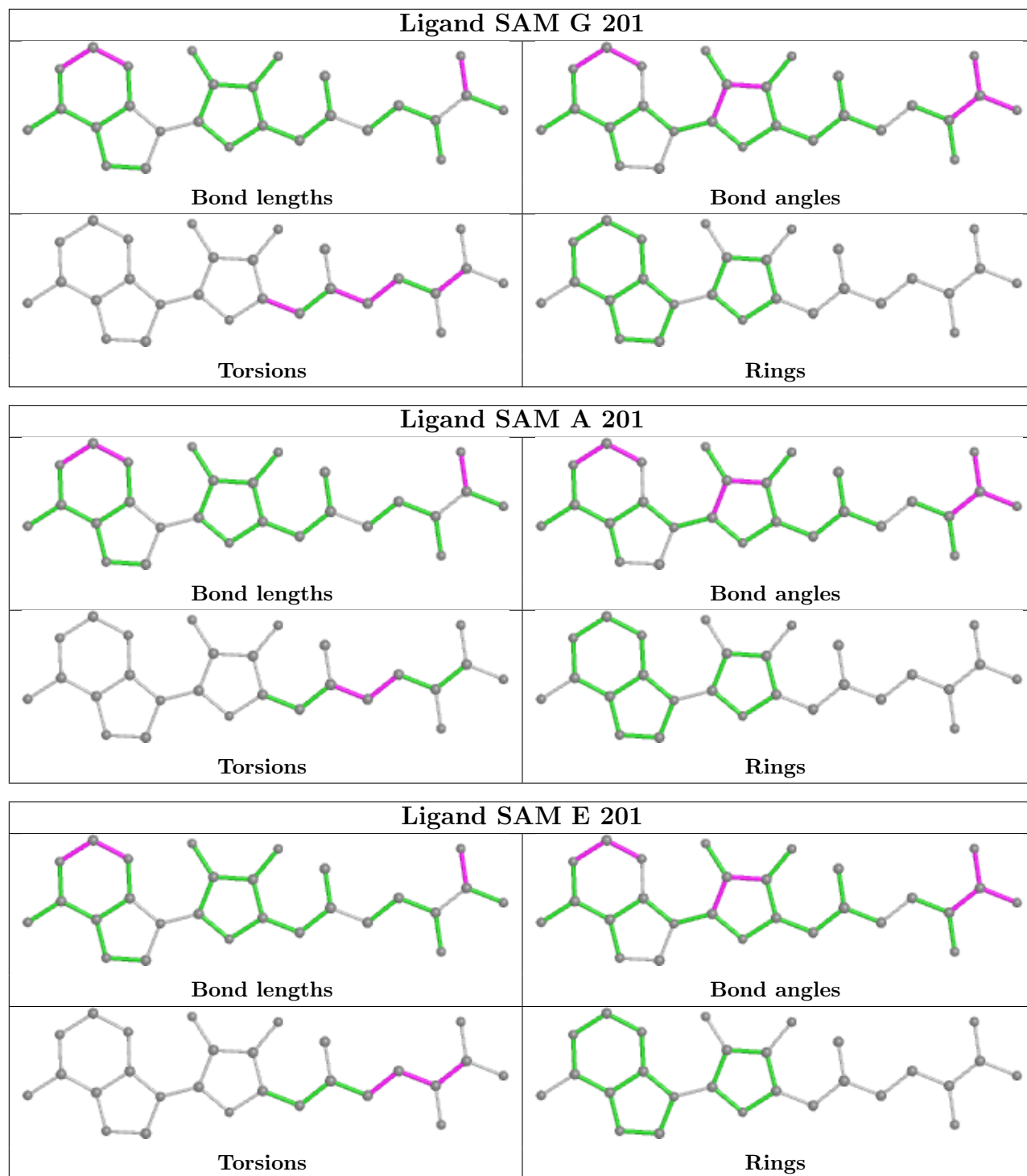
10 monomers are involved in 43 short contacts:

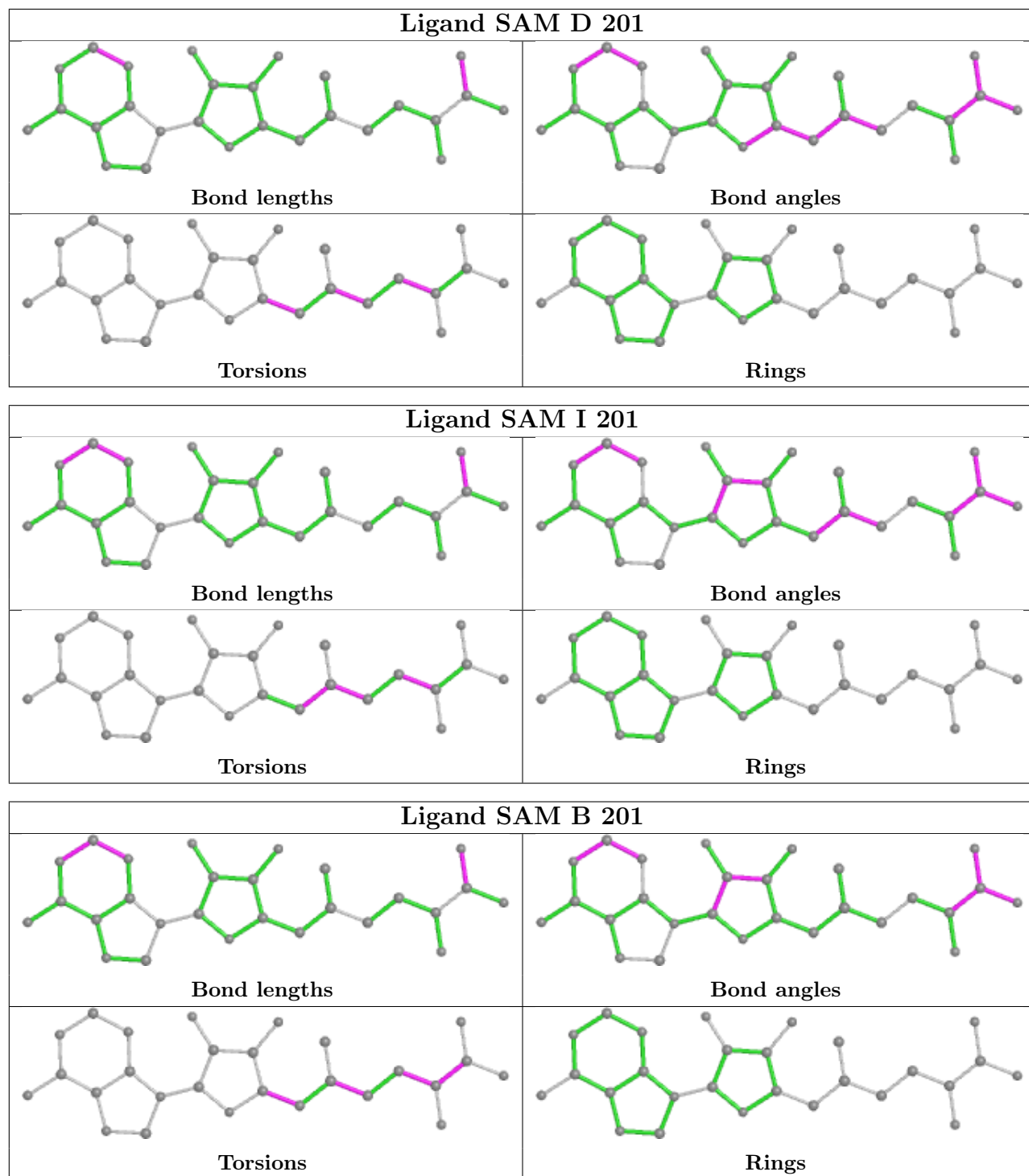
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	SAM	6	0
2	F	201	SAM	7	0
2	G	201	SAM	5	0
2	A	201	SAM	1	0
2	E	201	SAM	3	0
2	D	201	SAM	8	0
2	I	201	SAM	3	0
2	B	201	SAM	3	0
2	H	201	SAM	6	0
2	J	201	SAM	1	0

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

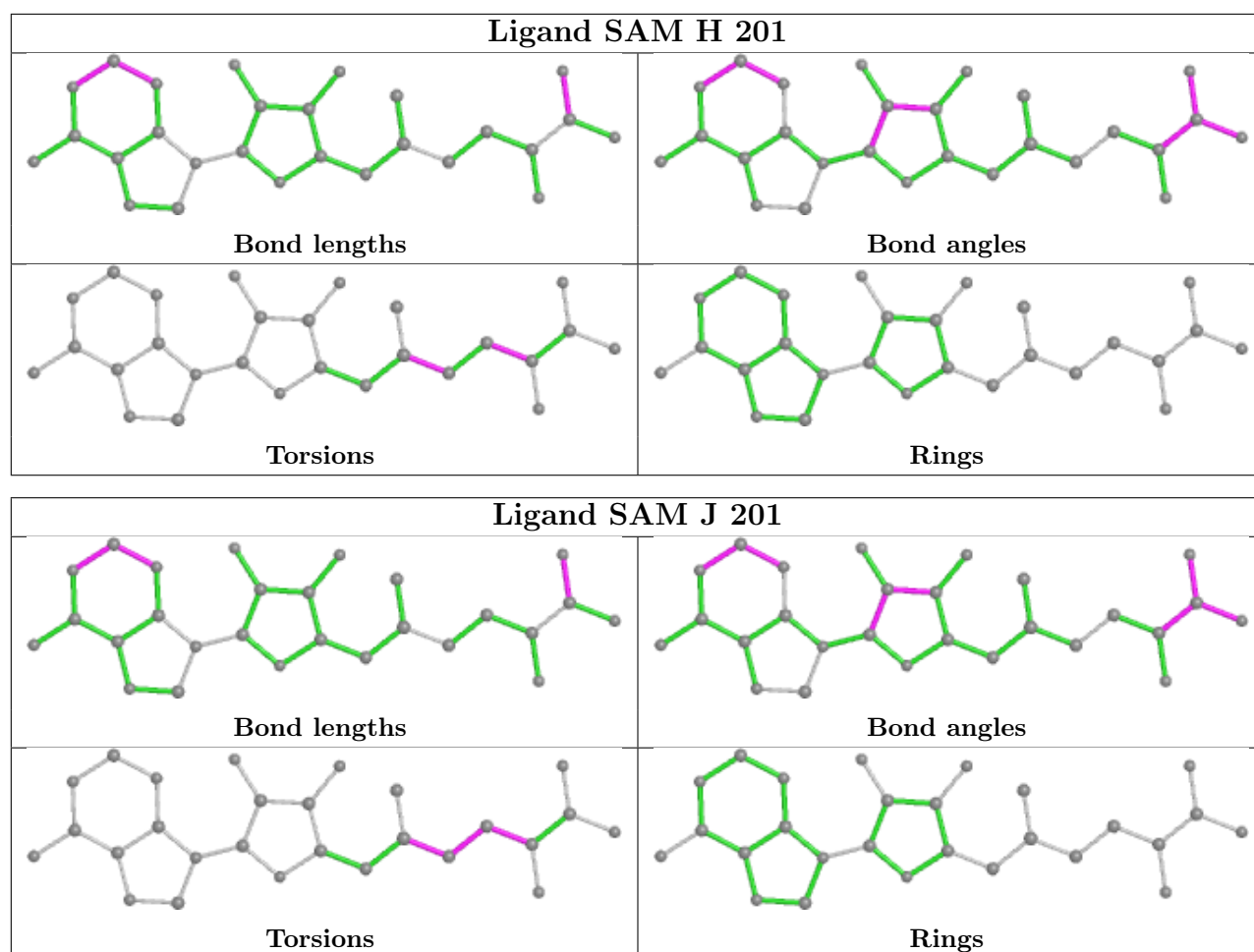
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

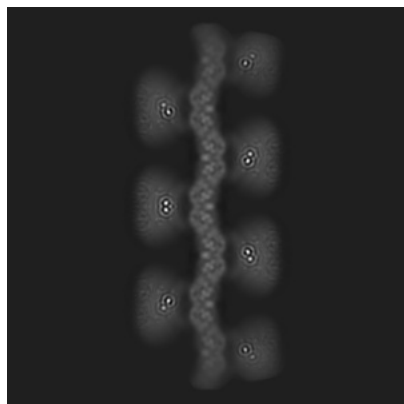
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19740. These allow visual inspection of the internal detail of the map and identification of artifacts.

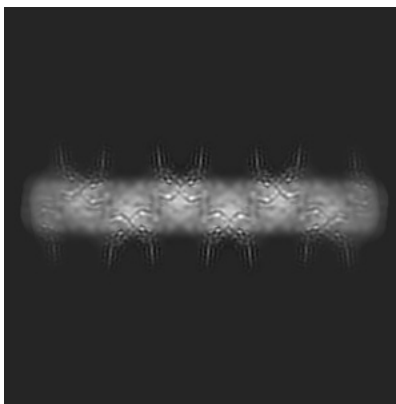
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

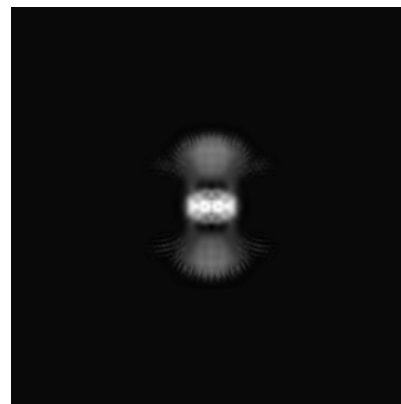
#### 6.1.1 Primary map



X

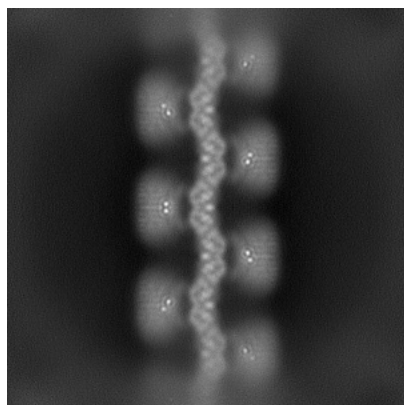


Y

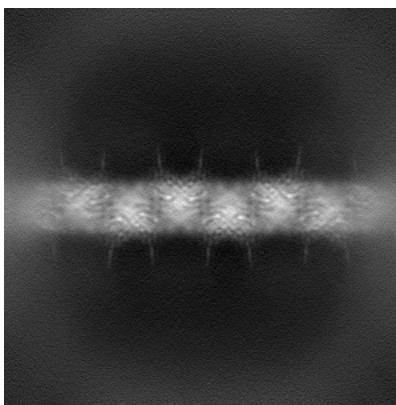


Z

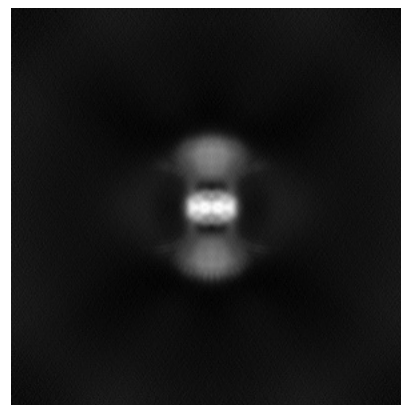
#### 6.1.2 Raw map



X



Y

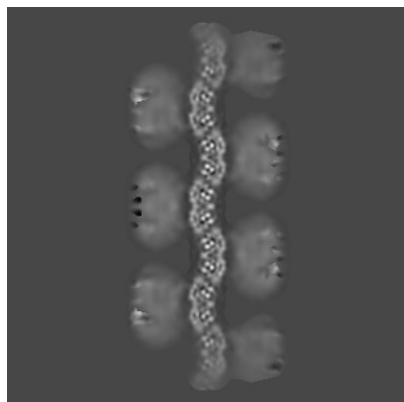


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 180

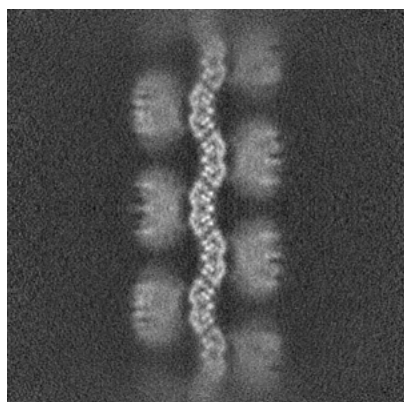


Y Index: 180

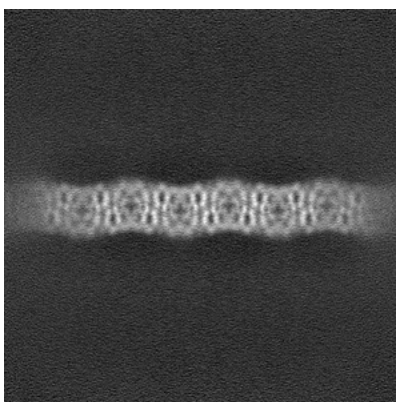


Z Index: 180

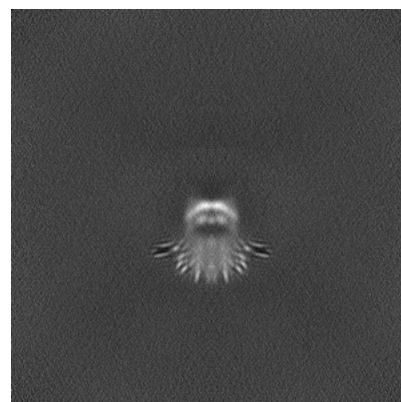
### 6.2.2 Raw map



X Index: 180



Y Index: 180

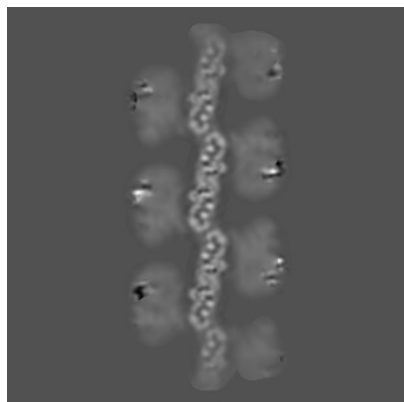


Z Index: 180

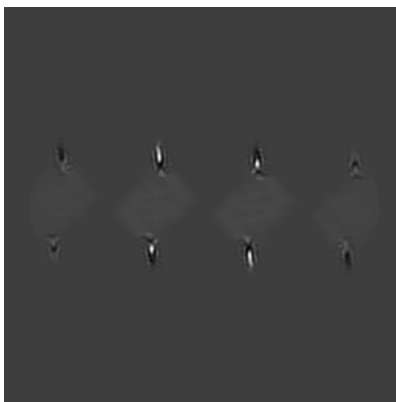
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 172

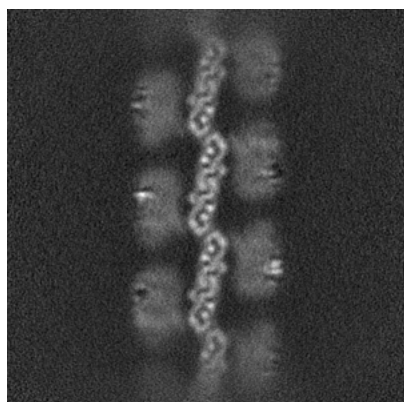


Y Index: 217

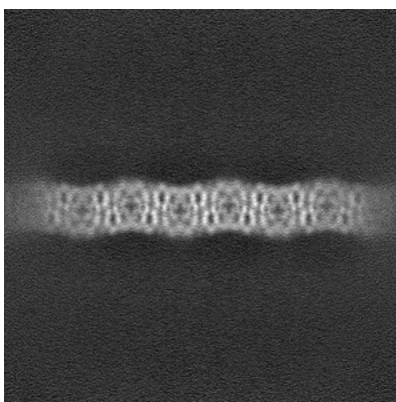


Z Index: 177

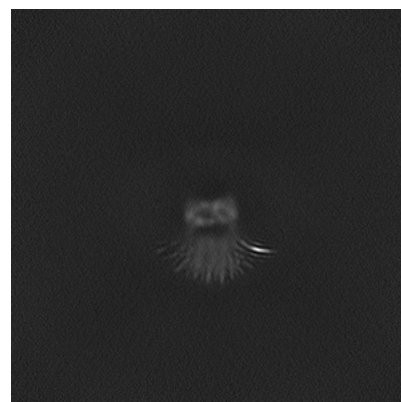
### 6.3.2 Raw map



X Index: 173



Y Index: 180

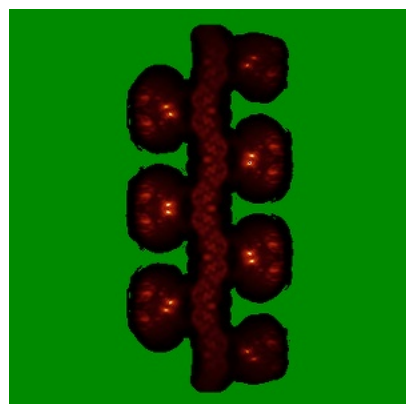


Z Index: 177

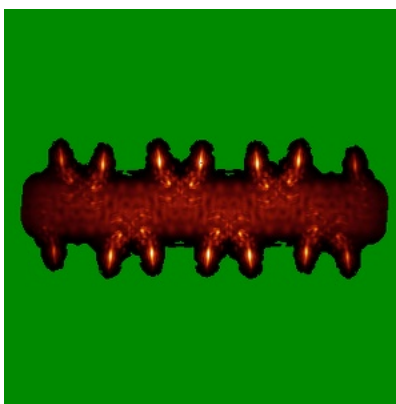
The images above show the largest variance slices of the map in three orthogonal directions.

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

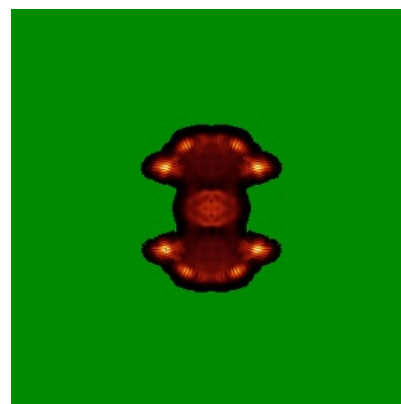
### 6.4.1 Primary map



X

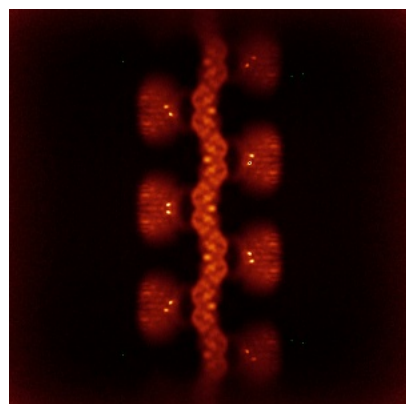


Y

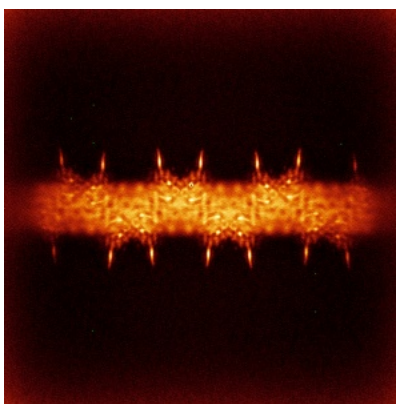


Z

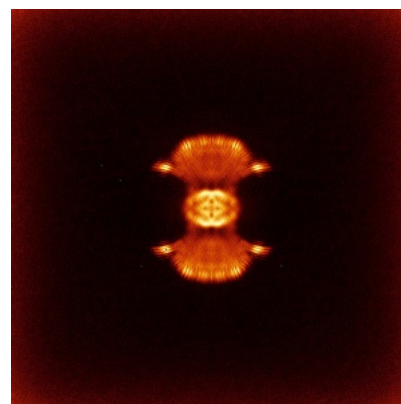
### 6.4.2 Raw map



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](#)

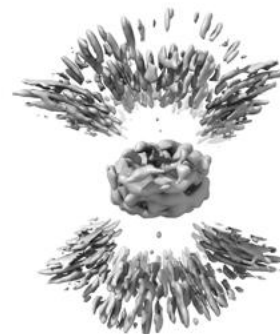
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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.

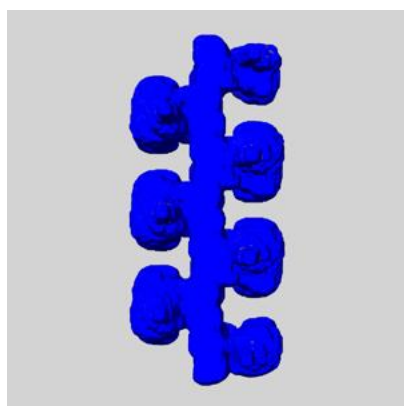
## 6.6 Mask visualisation [i](#)

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

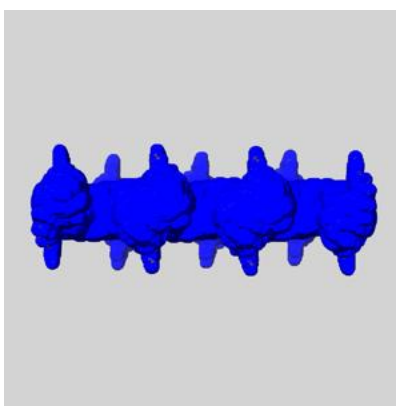
A mask typically either:

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

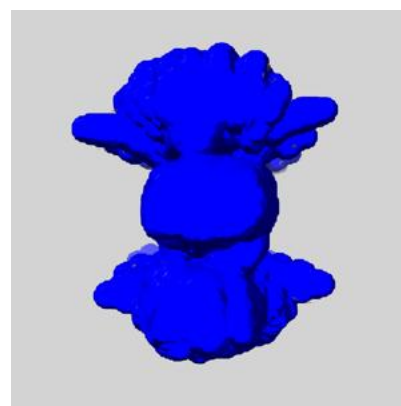
### 6.6.1 emd\_19740\_msk\_1.map [i](#)



X



Y



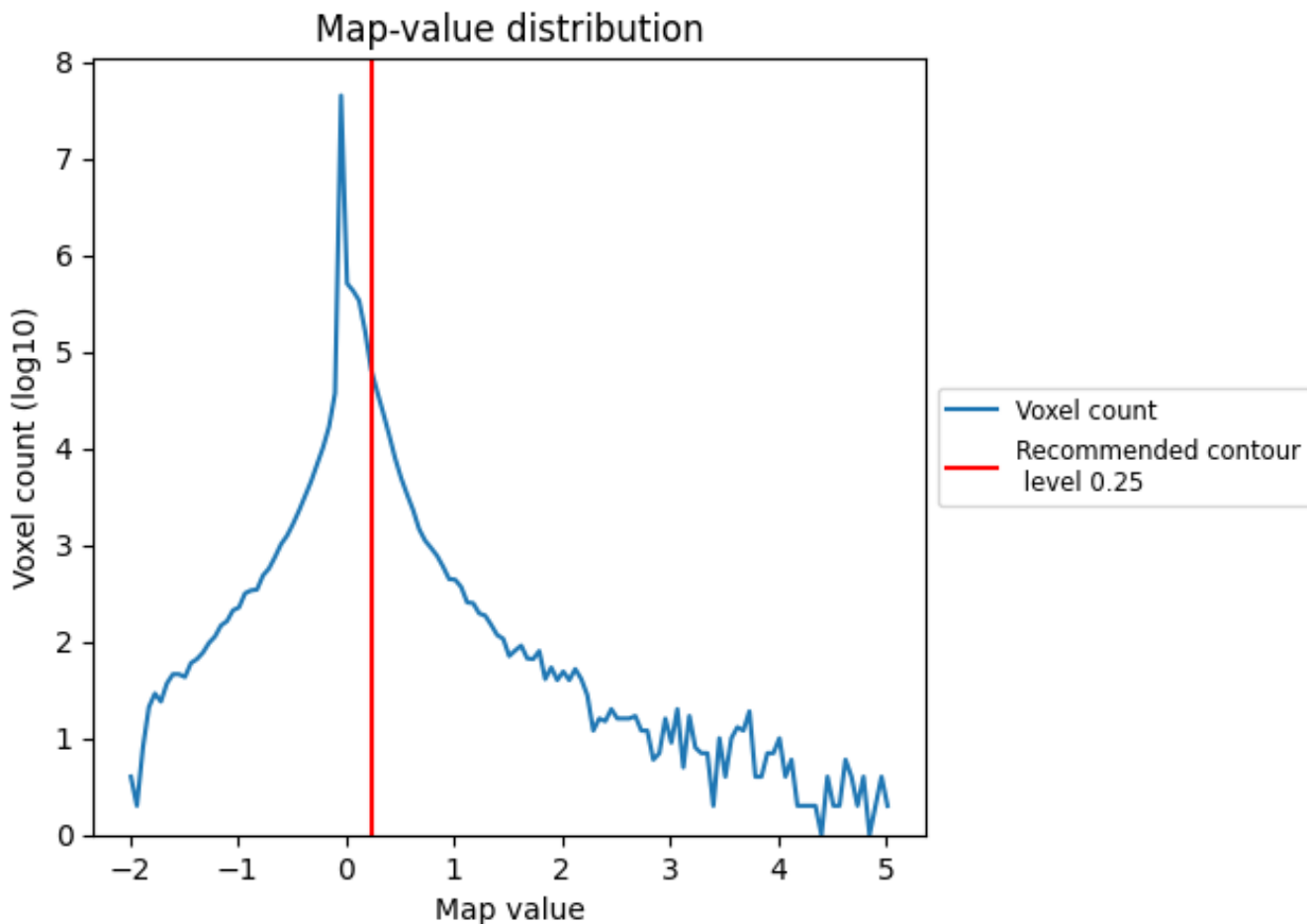
Z



## 7 Map analysis [i](#)

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

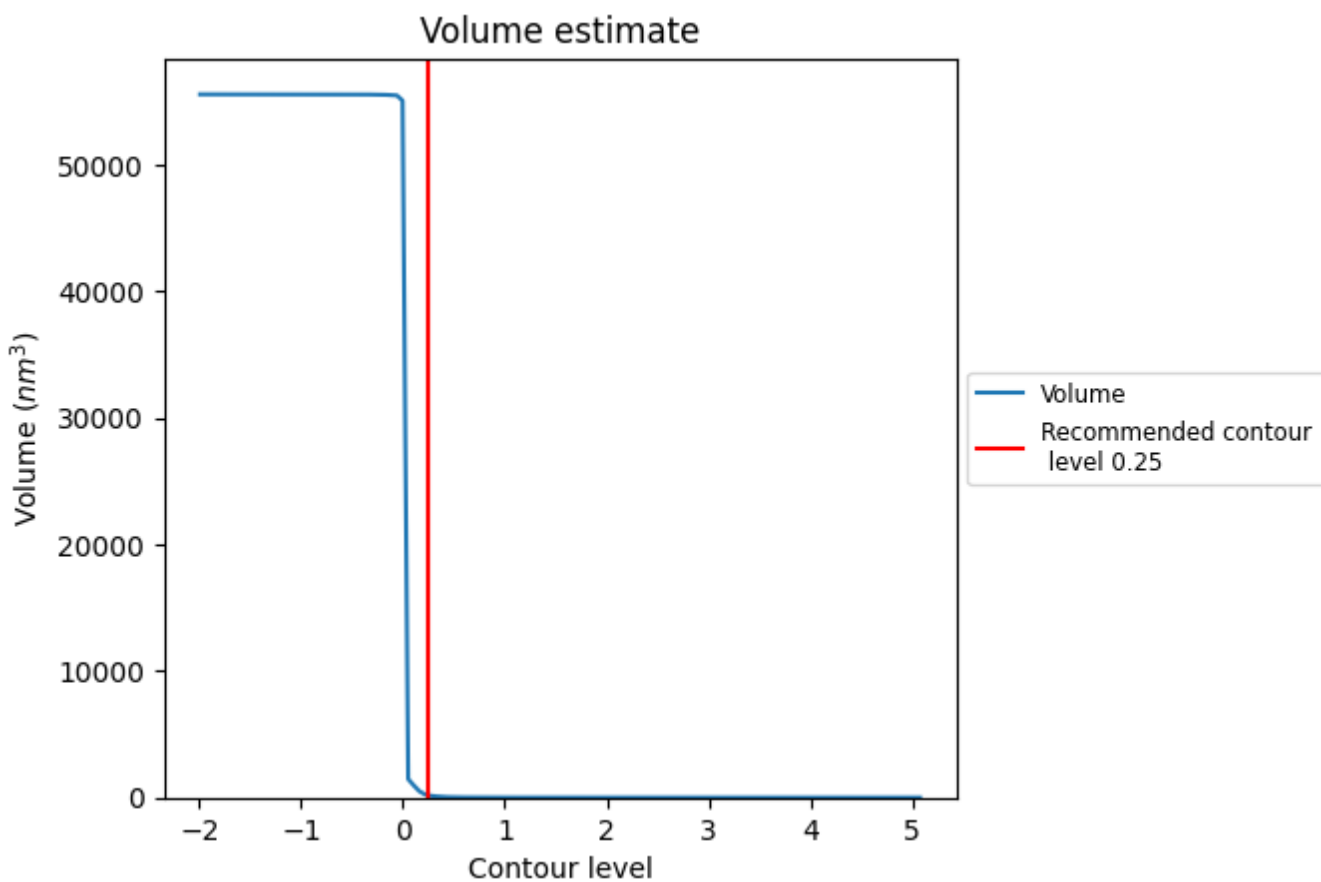
### 7.1 Map-value distribution [i](#)



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.



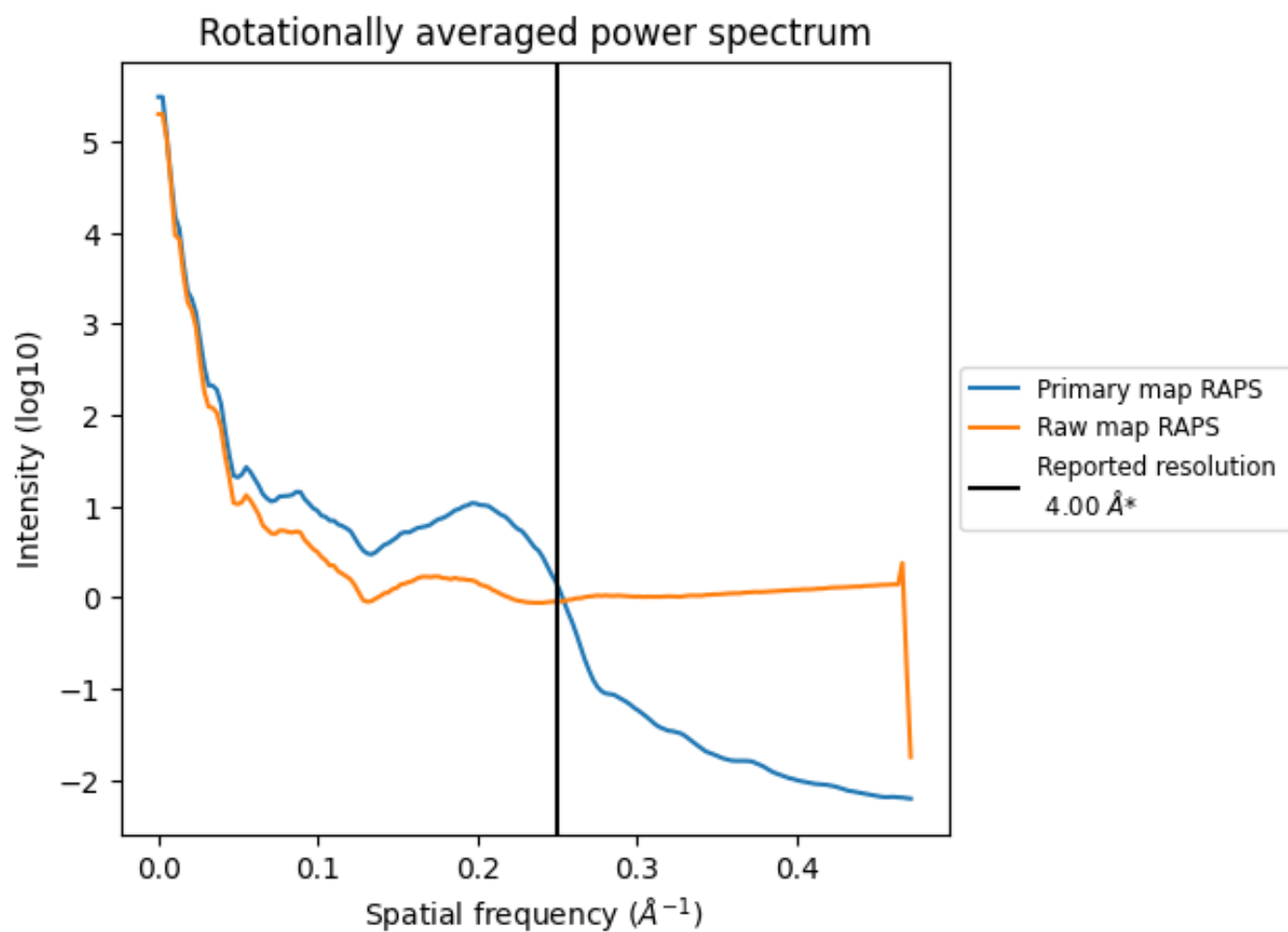
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm<sup>3</sup>; this corresponds to an approximate mass of 166 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](#)

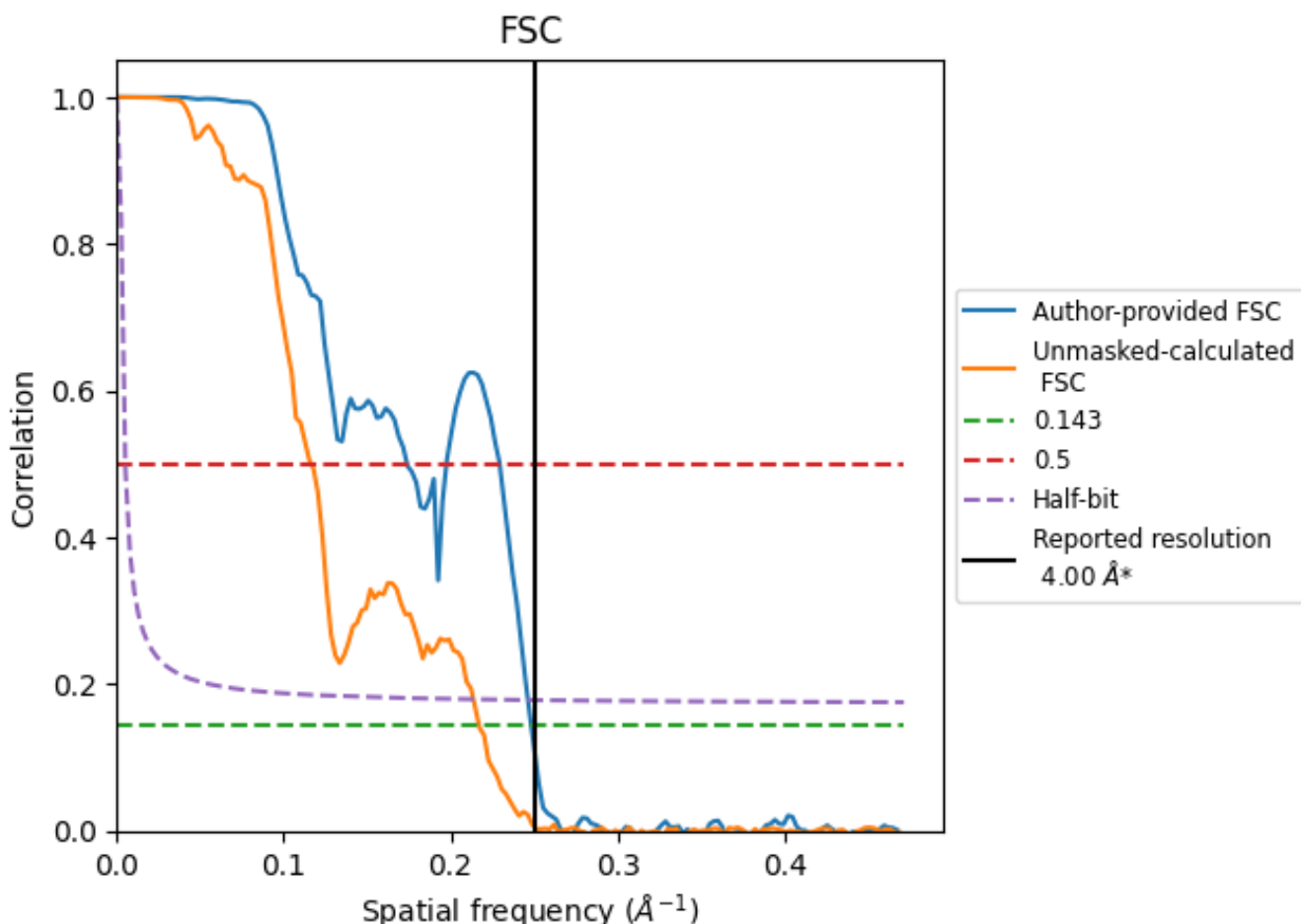


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates

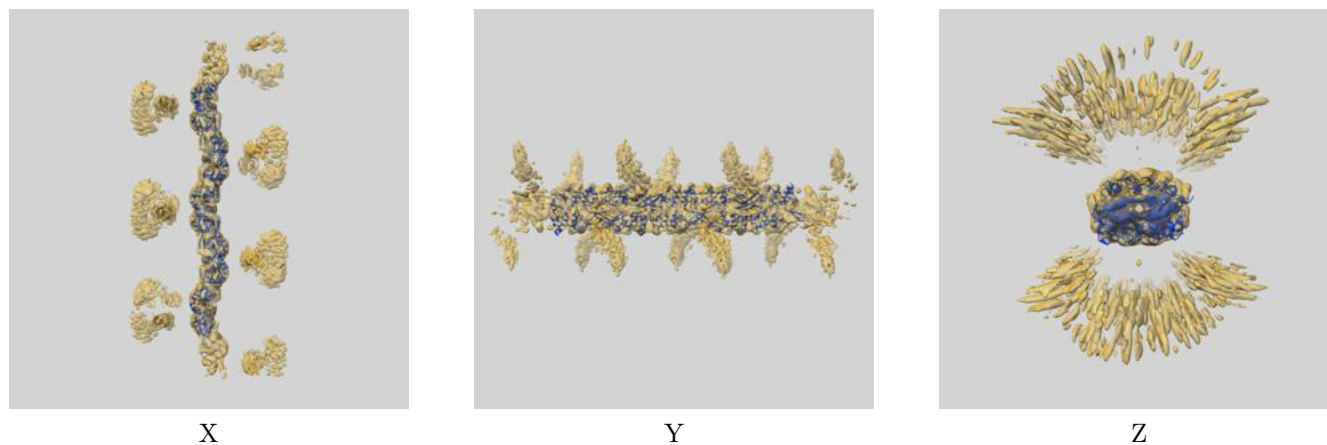
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.03	5.75	4.06
Unmasked-calculated*	4.61	8.58	4.68

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.61 differs from the reported value 4.0 by more than 10 %

## 9 Map-model fit [i](#)

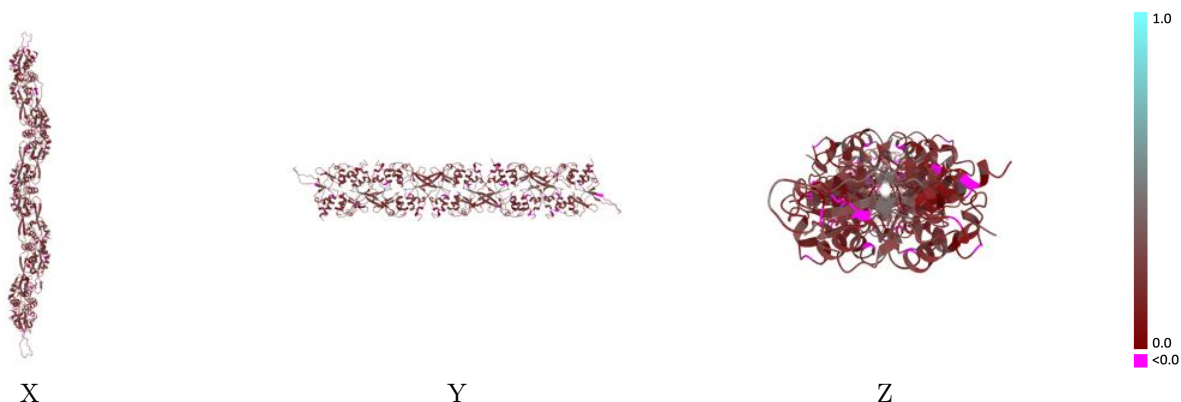
This section contains information regarding the fit between EMDB map EMD-19740 and PDB model 8S5M. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



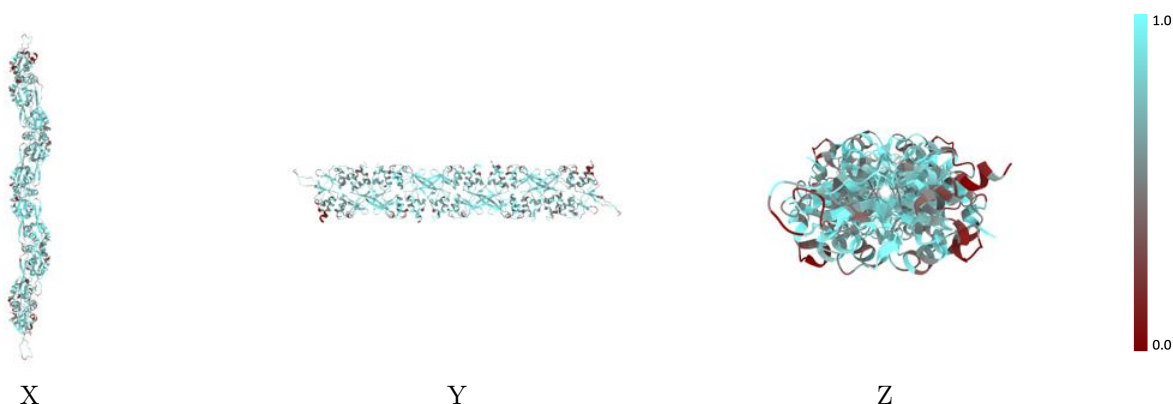
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



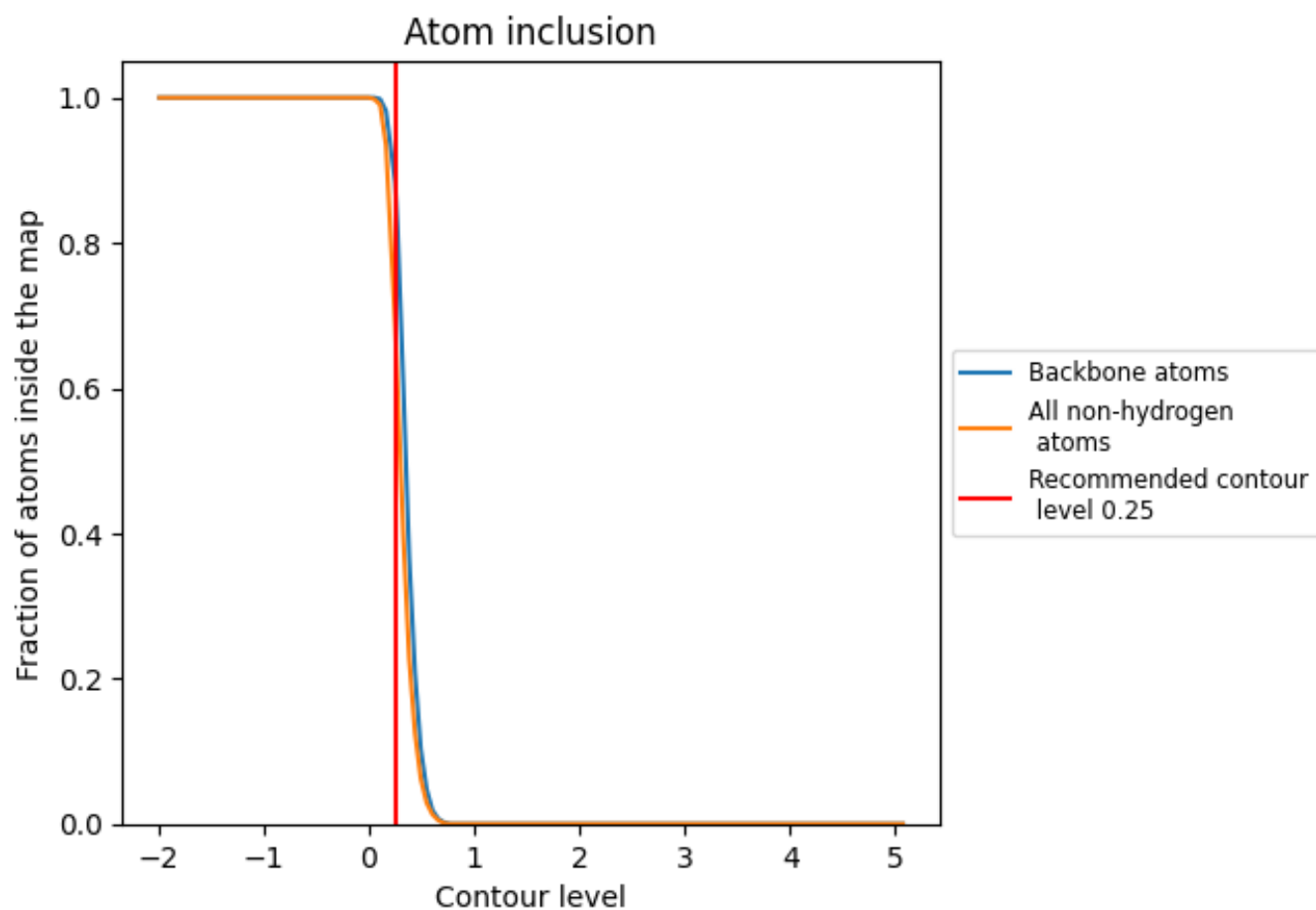
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.2220
A	 0.7280	 0.2270
B	 0.7280	 0.2180
C	 0.7080	 0.2230
D	 0.7070	 0.2220
E	 0.7350	 0.2250
F	 0.7070	 0.2230
G	 0.5980	 0.2150
H	 0.6780	 0.2220
I	 0.6750	 0.2230
J	 0.6010	 0.2200

