



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:49 AM UTC

PDB ID : 8GF5 / pdb_00008gf5
EMDB ID : EMD-29978
Title : McrD binds asymmetrically to methyl-coenzyme M reductase improving active site accessibility during assembly
Authors : Joiner, A.M.N.; Chadwick, G.L.; Nayak, D.D.
Deposited on : 2023-03-07
Resolution : 3.00 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
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

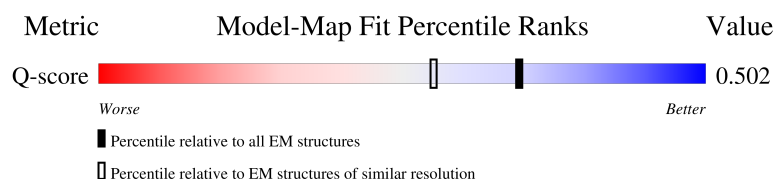
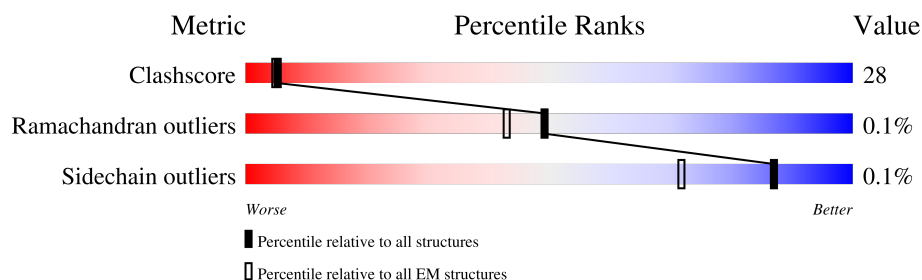
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	570	
1	B	570	
2	C	434	
2	D	434	

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Mol	Chain	Length	Quality of chain
3	E	248	 54% 46%
3	F	248	 51% 48%
4	X	193	 5% 23% 38% 39%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19178 atoms, of which 51 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 Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	560	Total	C	N	O	S	0	0
			4282	2695	731	828	28		
1	B	483	Total	C	N	O	S	0	0
			3682	2316	626	716	24		

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	429	Total	C	N	O	S	0	0
			3133	1963	540	612	18		
2	D	431	Total	C	N	O	S	0	0
			3143	1968	542	615	18		

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	247	Total	C	N	O	S	0	0
			1926	1192	352	369	13		
3	F	247	Total	C	N	O	S	0	0
			1926	1192	352	369	13		

- Molecule 4 is a protein called Methyl coenzyme M reductase, subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	118	Total	C	N	O	S	0	0
			945	600	170	172	3		

There are 23 discrepancies between the modelled and reference sequences:

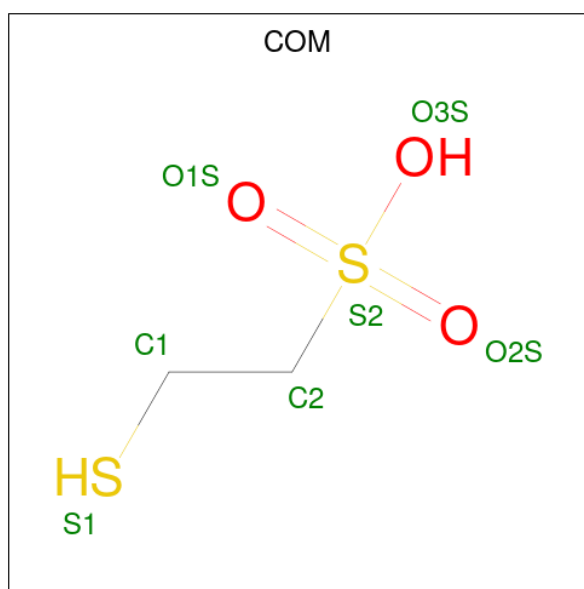
Chain	Residue	Modelled	Actual	Comment	Reference
X	-22	MET	-	expression tag	UNP Q8THG8
X	-21	ASP	-	expression tag	UNP Q8THG8
X	-20	TYR	-	expression tag	UNP Q8THG8

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-19	LYS	-	expression tag	UNP Q8THG8
X	-18	ASP	-	expression tag	UNP Q8THG8
X	-17	ASP	-	expression tag	UNP Q8THG8
X	-16	ASP	-	expression tag	UNP Q8THG8
X	-15	ASP	-	expression tag	UNP Q8THG8
X	-14	LYS	-	expression tag	UNP Q8THG8
X	-13	GLY	-	expression tag	UNP Q8THG8
X	-12	GLY	-	expression tag	UNP Q8THG8
X	-11	GLY	-	expression tag	UNP Q8THG8
X	-10	TRP	-	expression tag	UNP Q8THG8
X	-9	SER	-	expression tag	UNP Q8THG8
X	-8	HIS	-	expression tag	UNP Q8THG8
X	-7	PRO	-	expression tag	UNP Q8THG8
X	-6	GLN	-	expression tag	UNP Q8THG8
X	-5	PHE	-	expression tag	UNP Q8THG8
X	-4	GLU	-	expression tag	UNP Q8THG8
X	-3	LYS	-	expression tag	UNP Q8THG8
X	-2	GLY	-	expression tag	UNP Q8THG8
X	-1	GLY	-	expression tag	UNP Q8THG8
X	0	GLY	-	expression tag	UNP Q8THG8

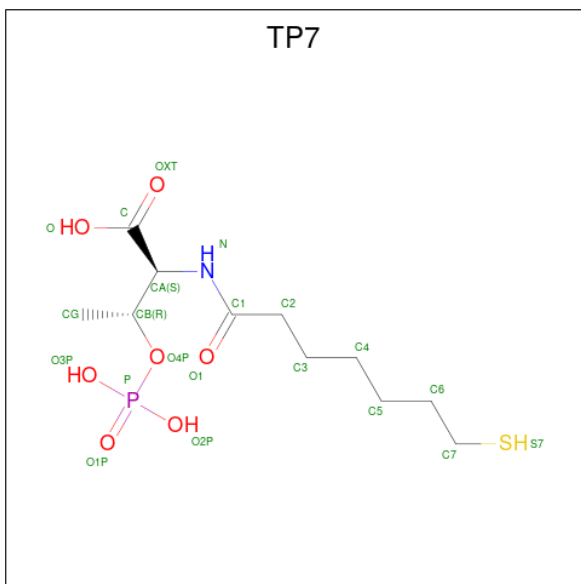
- Molecule 5 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	S	0
			7	2	3	2	

- ### F43

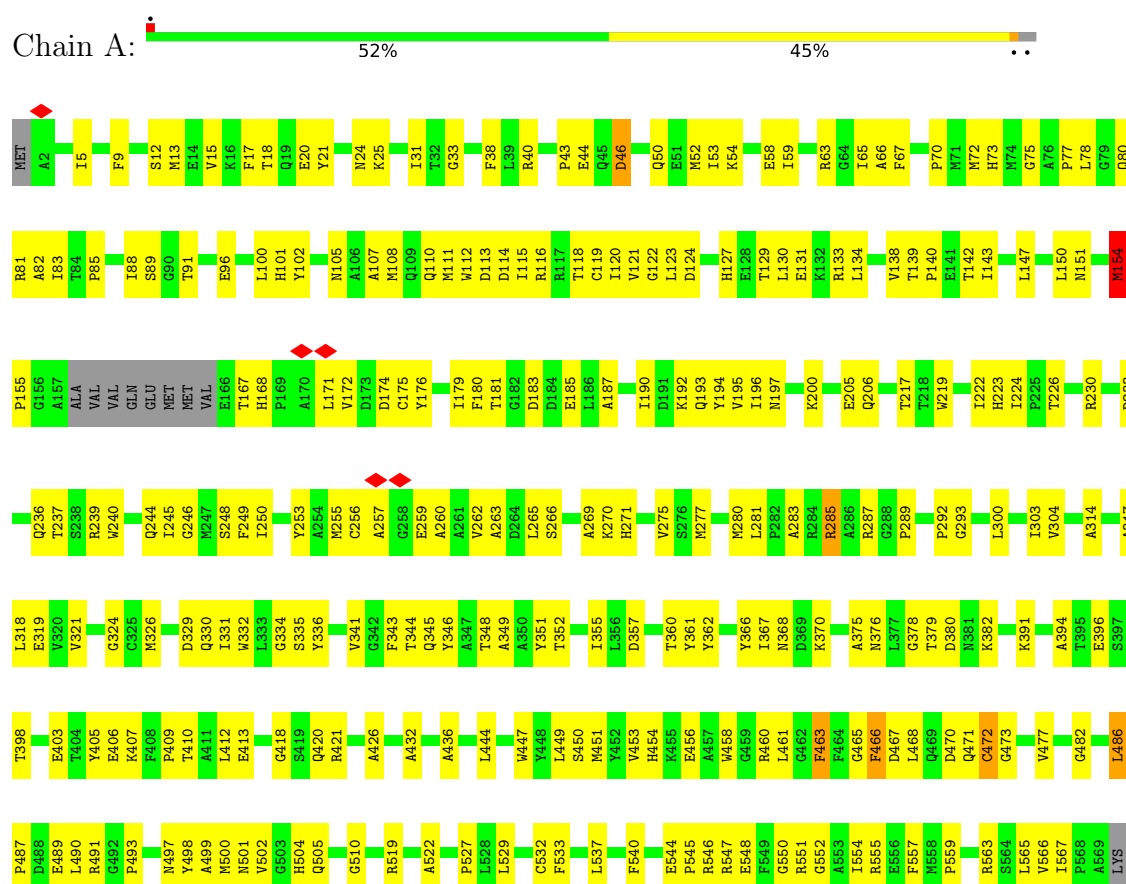
- Molecule 7 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$) (labeled as "Ligand of Interest" by depositor).



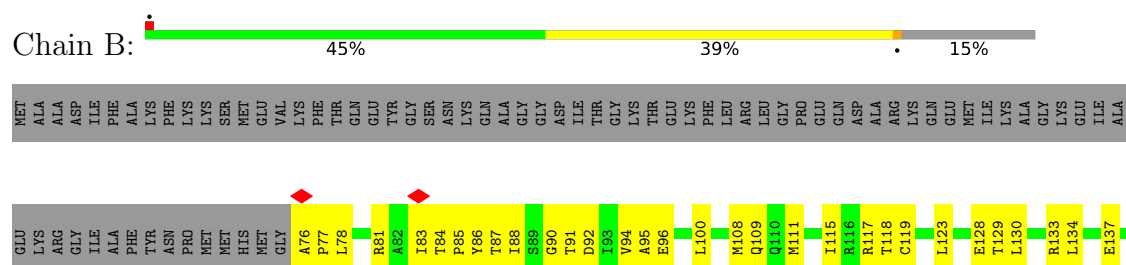
3 Residue-property plots

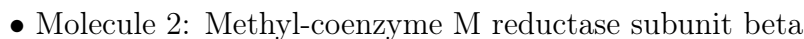
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



- Molecule 1: Methyl-coenzyme M reductase subunit alpha

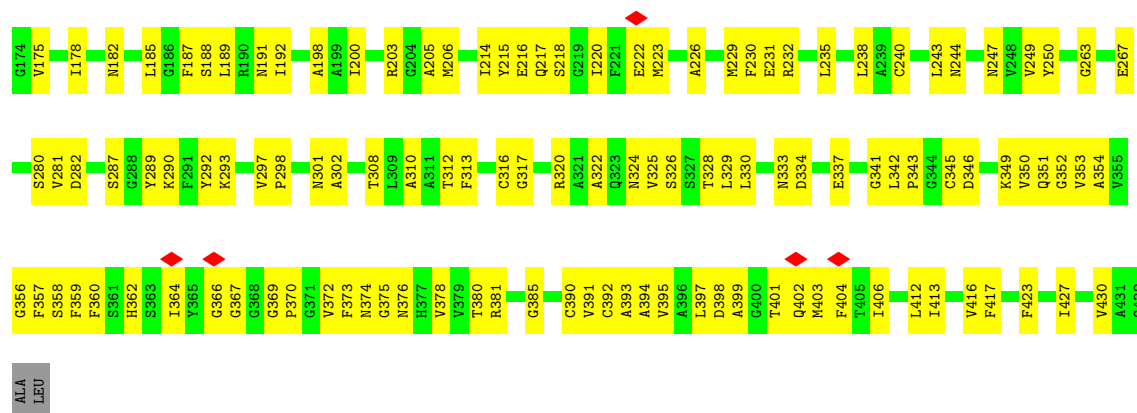




MET SER	L110	M193	A285	N374
	G121	A194	P286	N375
	A122		K290	H377
	D123	I200	F291	V378
	Y124		V292	V379
	M125	R203	K293	T380
	S126		A294	R381
	A132	A209		H382
	A133		V297	S383
	A134	I214	P298	R384
I21	V135	E216	M299	G385
	T136	Q217	Y303	
	Q137		A304	
	T138	I220	A305	
	I139			
	T140	M223	A310	
	D141		A311	
	M142	A226	T312	
	F143		F313	
	G144	M229	V314	
A48	D145	F230	G317	
	T146	E231	A318	M403
	M147	R232	G319	F404
	Y148	H233	R320	T405
	D149	Q234	V325	L406
	A150	L235		E407
	A153	G237	S326	S408
	F154	L238	S327	
	S155	A239	T328	V416
	K58	C240	L329	F417
G61	Y161		D334	G418
	P162	L243	I335	L420
	Q164	N244	T336	E421
	T164	A245	L336	E422
	M165	V246	E337	F423
	D166	N247	K338	A424
	L167	V248	L342	P426
	M168	V249	P343	
	D169	Y250	G344	V430
	V172	D251	C345	A431
D80	L176	I252	C346	GLY
	S177	V253	Y347	ALA
	A181	E255		LEU
	A83	T261	Q351	
	Q180		G352	
	P180	V265	V353	
	H161	I266	A354	
	M182		G355	
	L185	D276	V356	
	V100		F357	
K101	S188	I279	S358	
	L189	S280	I364	
	R190	V281	G371	
	M191	D282		
	I192			

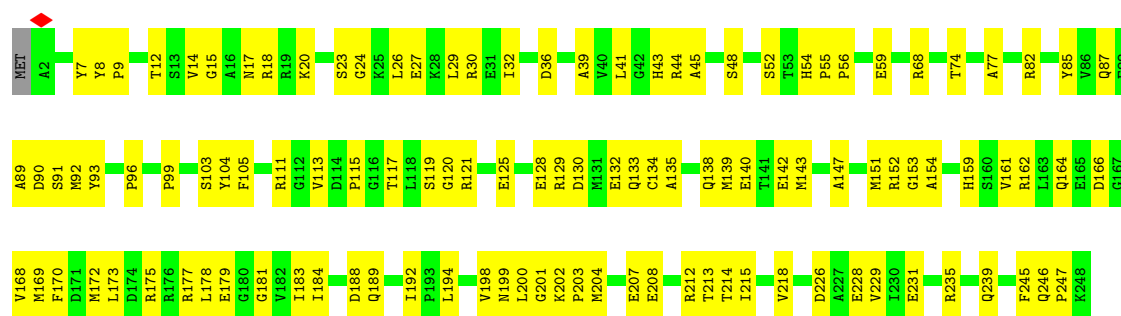
- Molecule 2: Methyl-coenzyme M reductase subunit beta

K87	Q81	V92	S99	V100	K101	V102	D10	R11	G105	G106	L109	L110	I111	Q112	H113	P114	S115	S116	R117	D28	I22	A123	Y124	M125	G131	V135	I140	D141	M142	F143	G144	T145	D149	P151	I152	A153	K154	S155	A156	S160	Y161	P162	Q163	T164	M168	N171	V172	Q173
NET	S2	D3	T4	V5	D6	T7	D9	D10	R11	G12	K13	L14	L15	V19	D20	I21	M22	S23	L24	A25	R28	I32	L36	L37	K40	R41	S42	V43	A44	V45	S46	L47	G51	G57	K58	M59	G60	G61	K62	G63	R64	Q65	L66	Y73	D74	L75	I82	



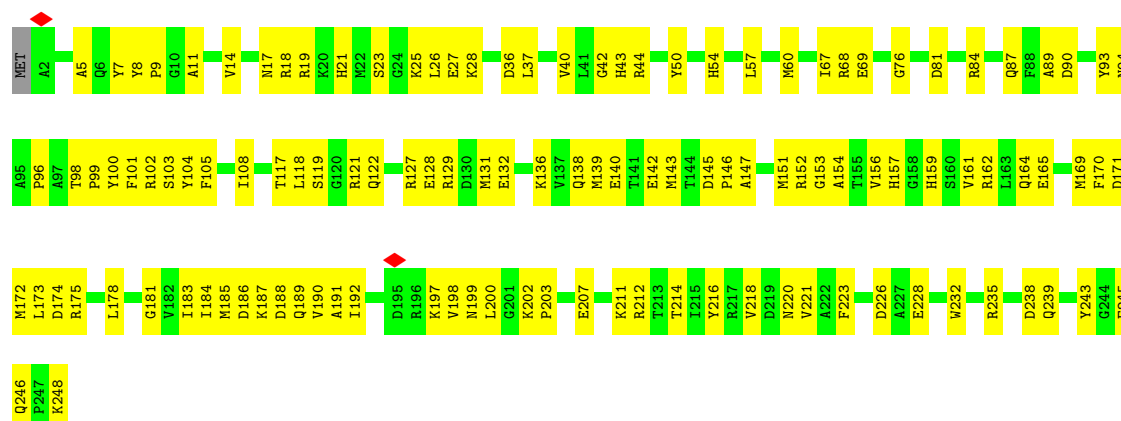
• Molecule 3: Methyl-coenzyme M reductase subunit gamma

Chain E: 54% 46%



• Molecule 3: Methyl-coenzyme M reductase subunit gamma

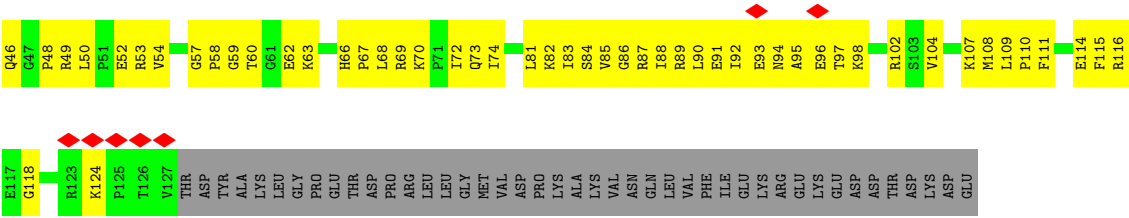
Chain F: 51% 48%



• Molecule 4: Methyl coenzyme M reductase, subunit D

Chain X: 5% 23% 38% 39%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.696	Depositor
Minimum map value	-0.782	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	249.76001, 249.76001, 249.76001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.115, 1.115, 1.115	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COM, AGM, TP7, SMC, F43, MHS

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	0.37	0/4339	0.56	8/5870 (0.1%)
1	B	0.34	0/3727	0.46	1/5060 (0.0%)
2	C	0.26	0/3180	0.38	0/4304
2	D	0.25	0/3190	0.40	0/4317
3	E	0.26	0/1965	0.43	2/2653 (0.1%)
3	F	0.27	0/1965	0.40	0/2653
4	X	0.20	0/961	0.41	0/1293
All	All	0.30	0/19327	0.45	11/26150 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	LEU	N-CA-C	-12.19	97.25	108.22
1	A	482	GLY	N-CA-C	7.38	121.06	112.50
1	A	466	PHE	N-CA-C	-7.25	104.58	113.50
1	A	283	ALA	N-CA-C	7.12	118.69	111.07
1	A	151	ASN	N-CA-C	6.78	119.51	111.71

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	4282	0	4142	271	0
1	B	3682	0	3547	243	0
2	C	3133	0	3116	163	0
2	D	3143	0	3124	213	0
3	E	1926	0	1871	109	0
3	F	1926	0	1871	152	0
4	X	945	0	987	94	0
5	A	7	0	6	1	0
6	A	62	51	43	5	0
7	B	21	0	19	1	0
All	All	19127	51	18726	1073	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 28.

The worst 5 of 1073 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD11	1:B:179:ILE:HD12	1.36	1.05
3:F:26:LEU:HD11	3:F:143:MET:HE3	1.38	1.04
1:A:500:MET:HE1	2:C:379:VAL:HA	1.44	1.00
1:A:468:LEU:HD12	2:C:356:GLY:HA3	1.41	0.99
4:X:28:GLN:HG2	4:X:72:ILE:HG23	1.41	0.99

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	553/570 (97%)	525 (95%)	27 (5%)	1 (0%)	43 76
1	B	476/570 (84%)	448 (94%)	27 (6%)	1 (0%)	43 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	427/434 (98%)	416 (97%)	11 (3%)	0	100	100
2	D	429/434 (99%)	409 (95%)	20 (5%)	0	100	100
3	E	245/248 (99%)	234 (96%)	11 (4%)	0	100	100
3	F	245/248 (99%)	227 (93%)	18 (7%)	0	100	100
4	X	116/193 (60%)	109 (94%)	7 (6%)	0	100	100
All	All	2491/2697 (92%)	2368 (95%)	121 (5%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	PHE
1	B	465	GLY

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	433/442 (98%)	432 (100%)	1 (0%)	87	92
1	B	374/442 (85%)	373 (100%)	1 (0%)	86	91
2	C	324/327 (99%)	324 (100%)	0	100	100
2	D	325/327 (99%)	325 (100%)	0	100	100
3	E	199/200 (100%)	199 (100%)	0	100	100
3	F	199/200 (100%)	199 (100%)	0	100	100
4	X	107/171 (63%)	107 (100%)	0	100	100
All	All	1961/2109 (93%)	1959 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	MET
1	B	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	402	GLN
2	D	333	ASN
4	X	28	GLN
2	D	182	ASN
1	B	415	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	AGM	B	285	1	10,11,12	1.27	1 (10%)	7,13,15	1.22	0
1	MHS	B	271	1	10,11,12	1.66	2 (20%)	5,14,16	1.17	1 (20%)
1	SMC	B	472	1	5,6,7	1.17	0	3,6,8	2.60	1 (33%)
1	MHS	A	271	1	10,11,12	1.75	1 (10%)	5,14,16	1.03	1 (20%)
1	SMC	A	472	1	5,6,7	1.14	0	3,6,8	1.96	1 (33%)
1	AGM	A	285	1	10,11,12	0.85	0	7,13,15	1.00	1 (14%)

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	AGM	B	285	1	-	7/10/11/13	-
1	MHS	B	271	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	B	472	1	-	1/3/5/7	-
1	MHS	A	271	1	-	4/5/6/8	0/1/1/1
1	SMC	A	472	1	-	1/3/5/7	-
1	AGM	A	285	1	-	2/10/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	MHS	CD2-CG	3.71	1.41	1.36
1	B	271	MHS	CD2-CG	3.36	1.41	1.36
1	B	285	AGM	CZ-NE1	2.95	1.38	1.33
1	B	271	MHS	CM-ND1	-2.07	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	472	SMC	CA-CB-SG	-4.42	106.89	114.04
1	A	472	SMC	CA-CB-SG	-2.78	109.54	114.04
1	A	285	AGM	CD-NE1-CZ	-2.51	118.93	123.59
1	B	271	MHS	ND1-CE1-NE2	-2.37	111.53	112.94
1	A	271	MHS	ND1-CE1-NE2	-2.08	111.70	112.94

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	271	MHS	N-CA-CB-CG
1	A	271	MHS	C-CA-CB-CG
1	A	271	MHS	CA-CB-CG-ND1
1	A	285	AGM	N-CA-CB-CG
1	A	472	SMC	CA-CB-SG-CS

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	285	AGM	3	0
1	B	472	SMC	1	0
1	A	472	SMC	3	0
1	A	285	AGM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
6	F43	A	602	-	63,71,71	1.74	5 (7%)	73,118,118	1.38	12 (16%)
5	COM	A	601	-	6,6,6	1.64	1 (16%)	8,8,8	2.39	4 (50%)
7	TP7	B	601	-	19,20,20	2.71	2 (10%)	24,26,26	2.45	4 (16%)

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	F43	A	602	-	-	10/28/185/185	-
5	COM	A	601	-	-	0/4/4/4	-
7	TP7	B	601	-	-	5/24/24/24	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TP7	O1-C1	10.18	1.43	1.23
6	A	602	F43	NI-NA	8.56	2.10	1.89
6	A	602	F43	NI-NB	7.79	2.08	1.89
6	A	602	F43	NI-ND	5.92	2.03	1.89
7	B	601	TP7	C1-N	5.25	1.45	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	601	TP7	O1-C1-N	-8.29	108.91	122.95
7	B	601	TP7	O1-C1-C2	-6.36	110.50	122.02
5	A	601	COM	O3S-S2-O1S	-4.10	101.14	111.40
6	A	602	F43	C9D-C3D-C4D	-3.54	105.32	114.63
6	A	602	F43	C2A-C3A-C4A	-3.50	97.06	102.36

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	TP7	O1-C1-N-CA
6	A	602	F43	C3A-CAA-CBA-CCA
7	B	601	TP7	O1-C1-C2-C3
6	A	602	F43	C2D-C3D-C9D-CAD
6	A	602	F43	C2C-C5C-C6C-O7C

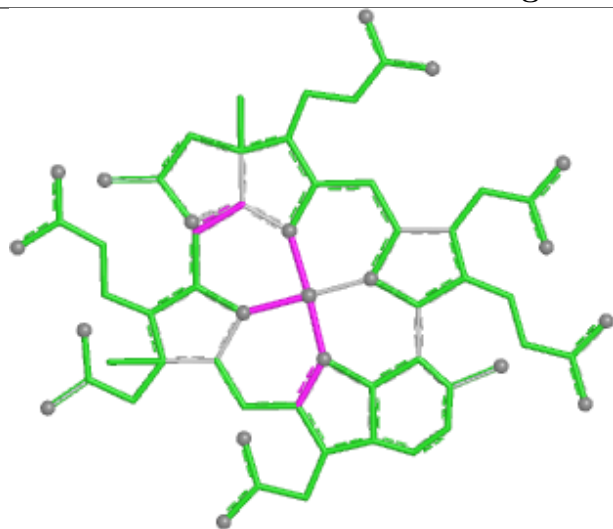
There are no ring outliers.

3 monomers are involved in 7 short contacts:

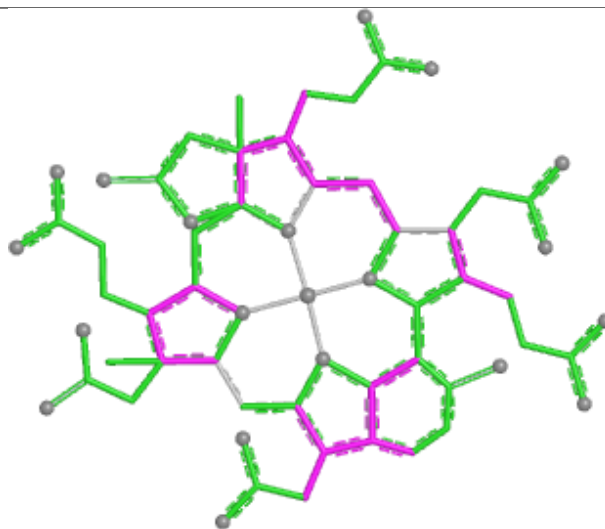
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	F43	5	0
5	A	601	COM	1	0
7	B	601	TP7	1	0

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.

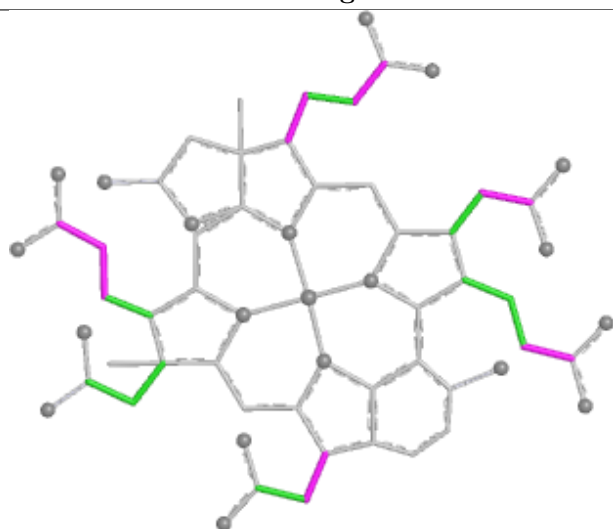
Ligand F43 A 602



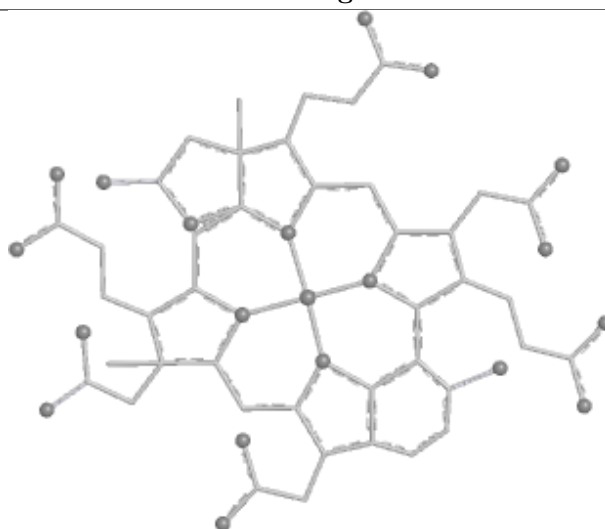
Bond lengths



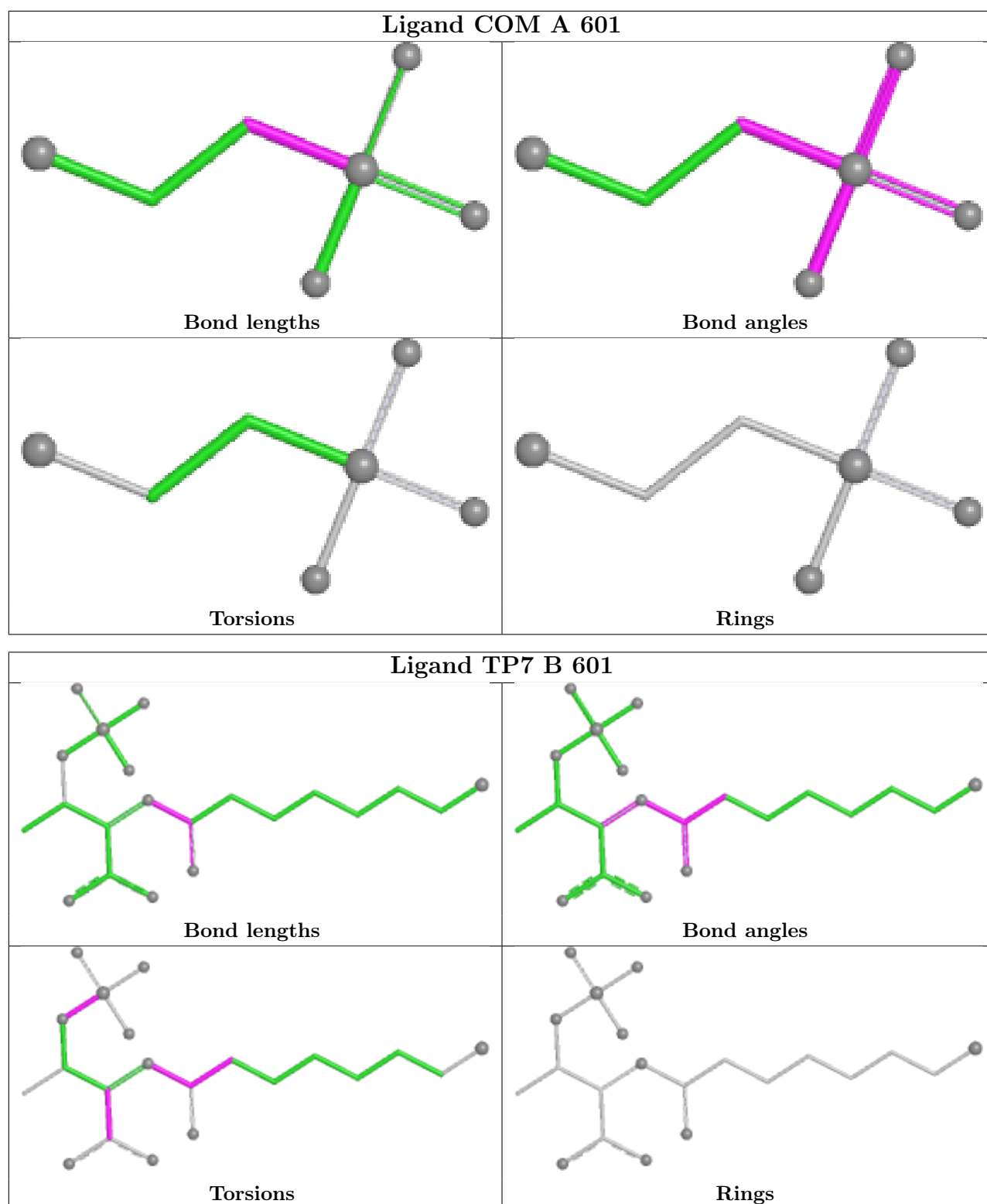
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

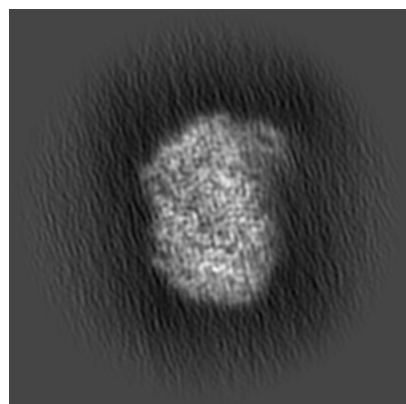
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29978. These allow visual inspection of the internal detail of the map and identification of artifacts.

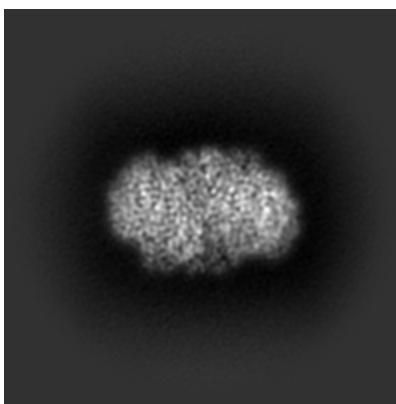
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

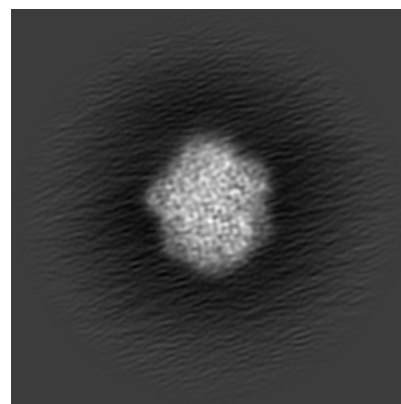
6.1.1 Primary map



X

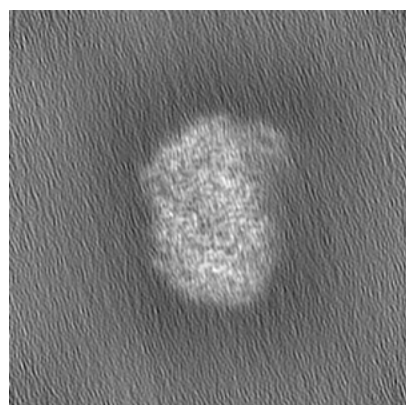


Y

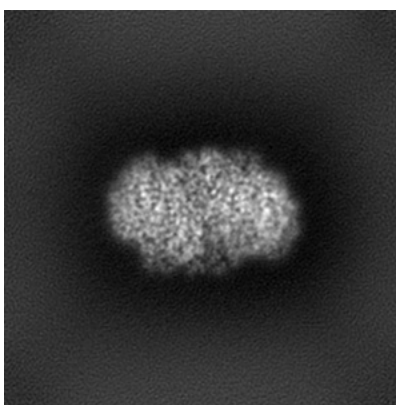


Z

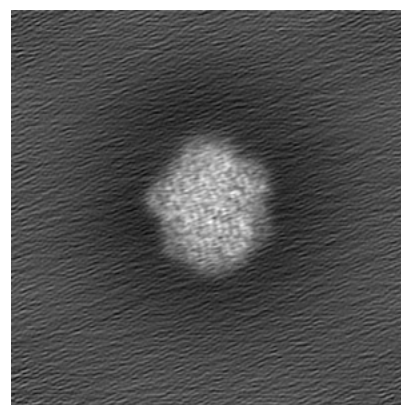
6.1.2 Raw map



X



Y

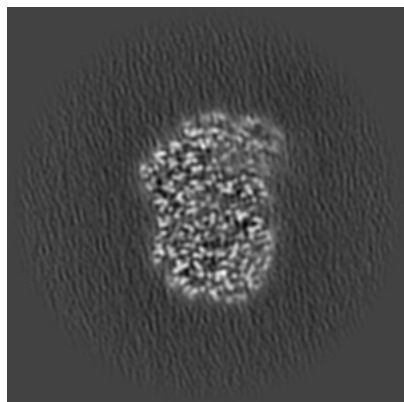


Z

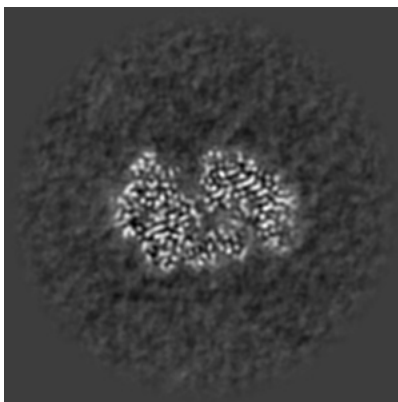
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

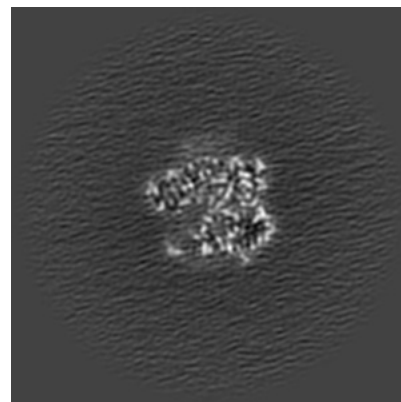
6.2.1 Primary map



X Index: 112

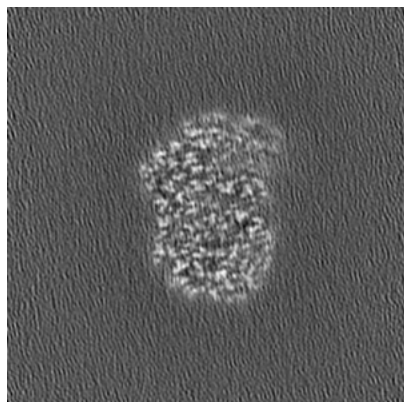


Y Index: 112

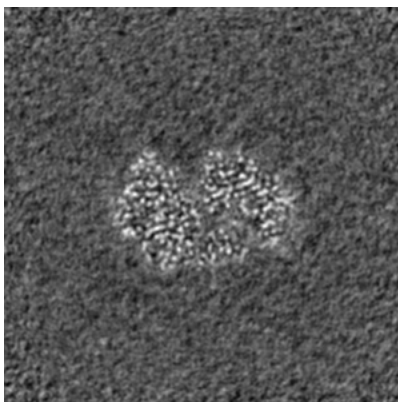


Z Index: 112

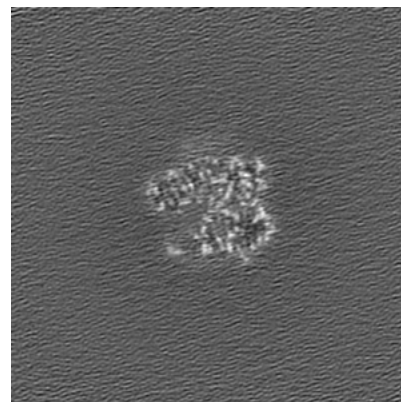
6.2.2 Raw map



X Index: 112



Y Index: 112

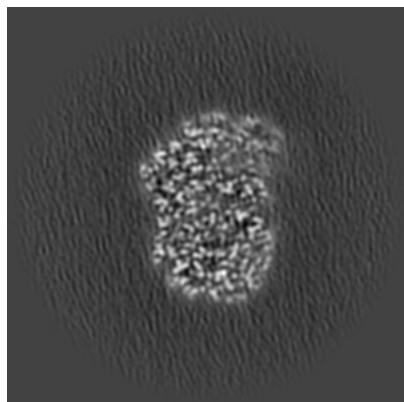


Z Index: 112

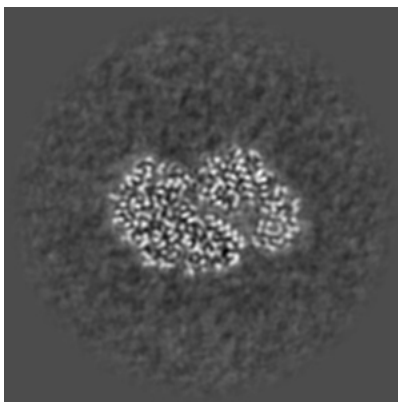
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

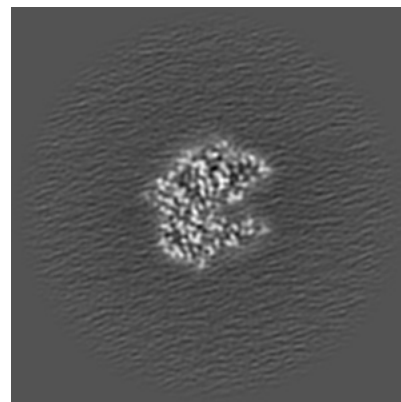
6.3.1 Primary map



X Index: 112

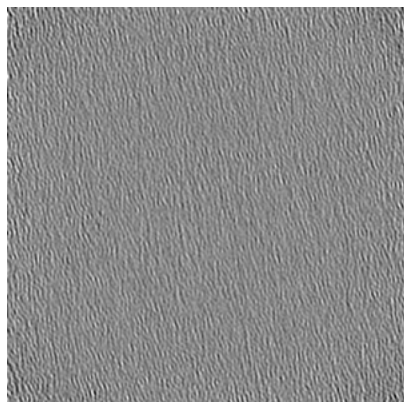


Y Index: 119

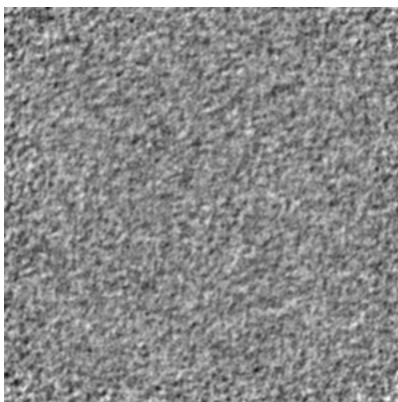


Z Index: 101

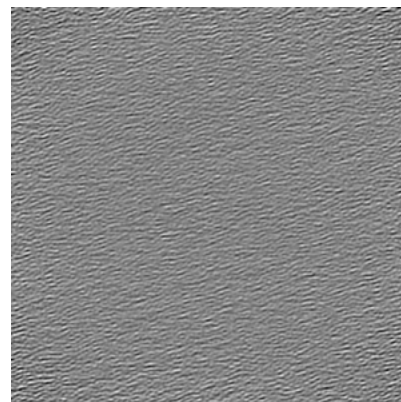
6.3.2 Raw map



X Index: 0



Y Index: 0

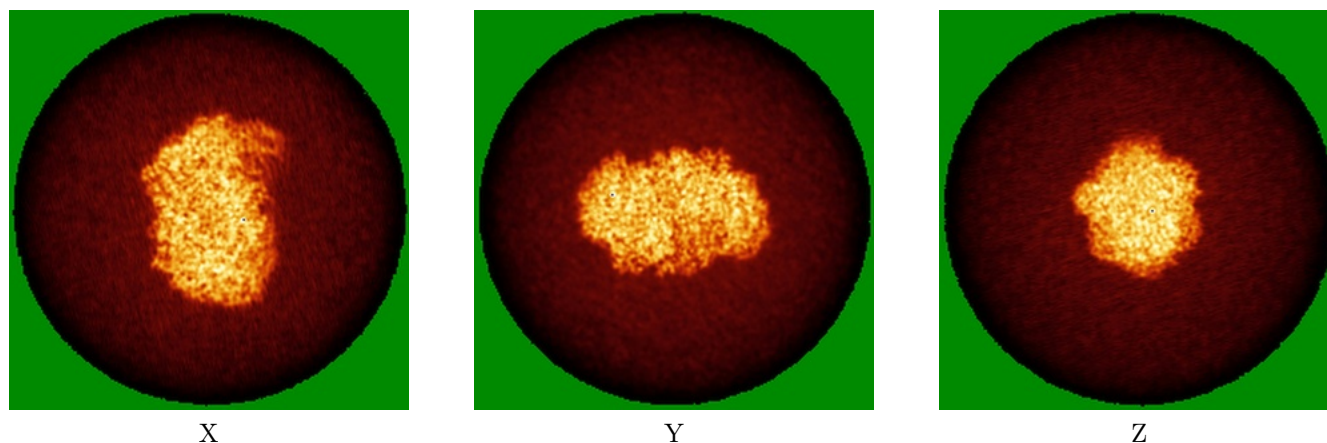


Z Index: 0

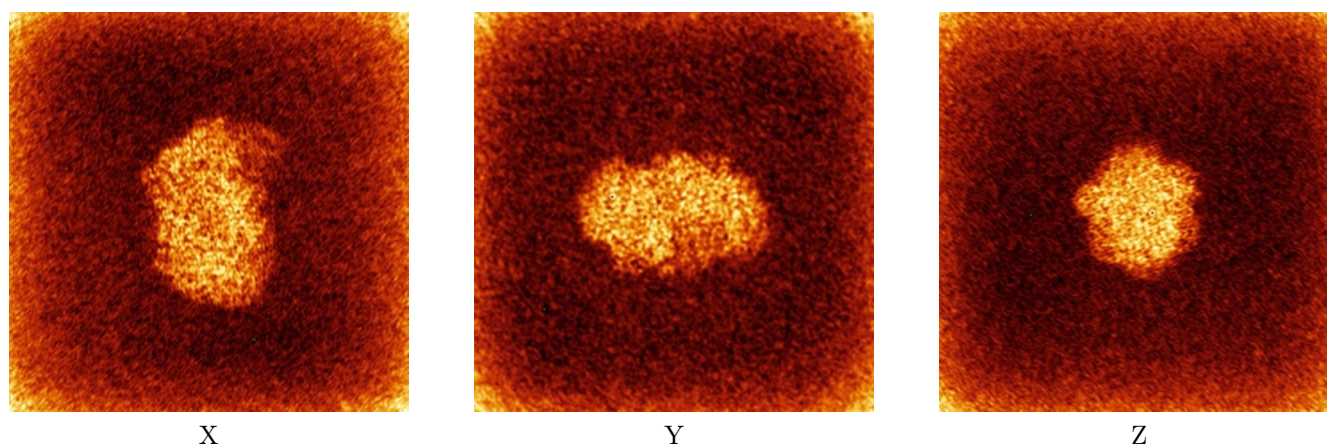
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

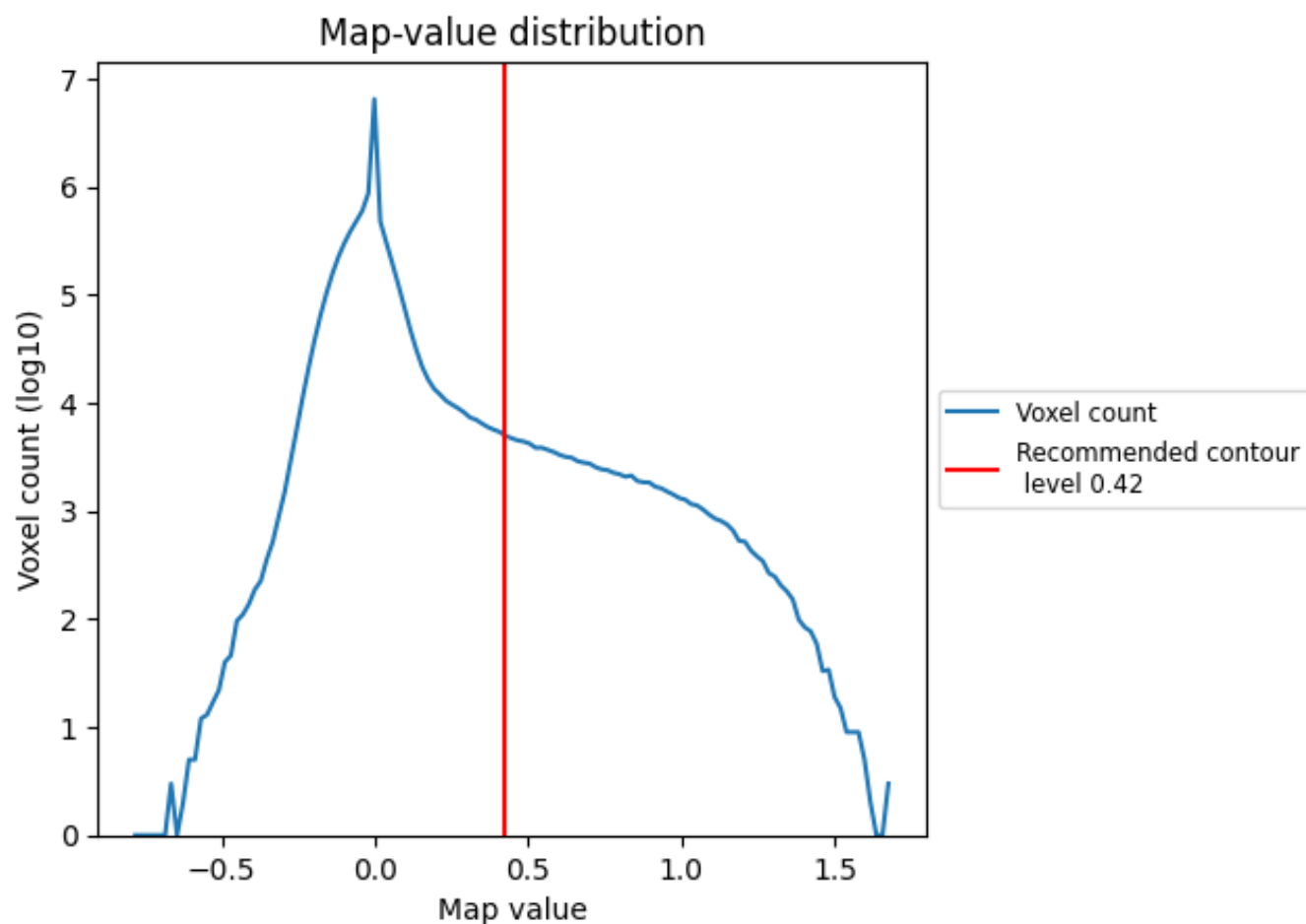
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

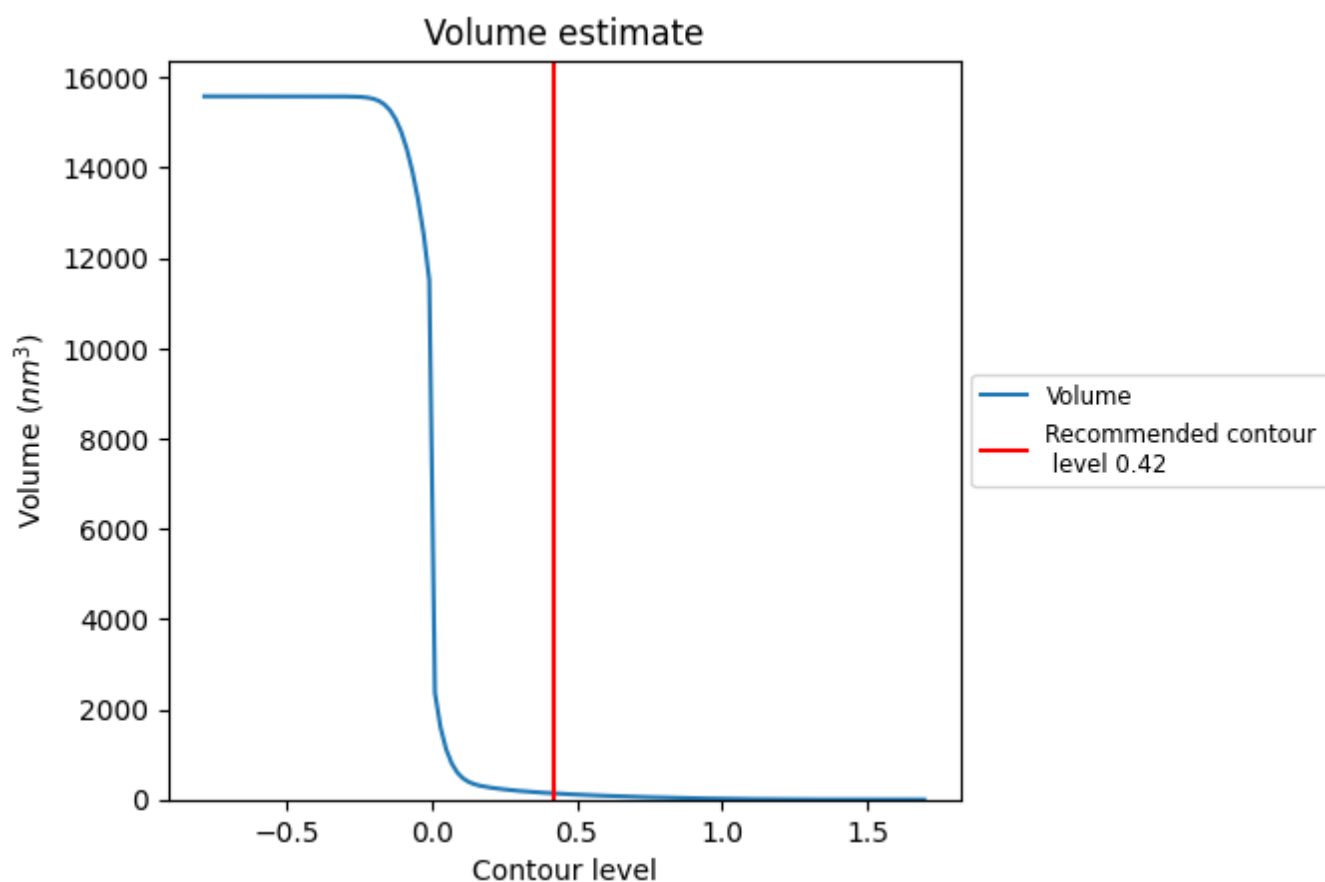
This section contains the results of statistical analysis of the map.

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.

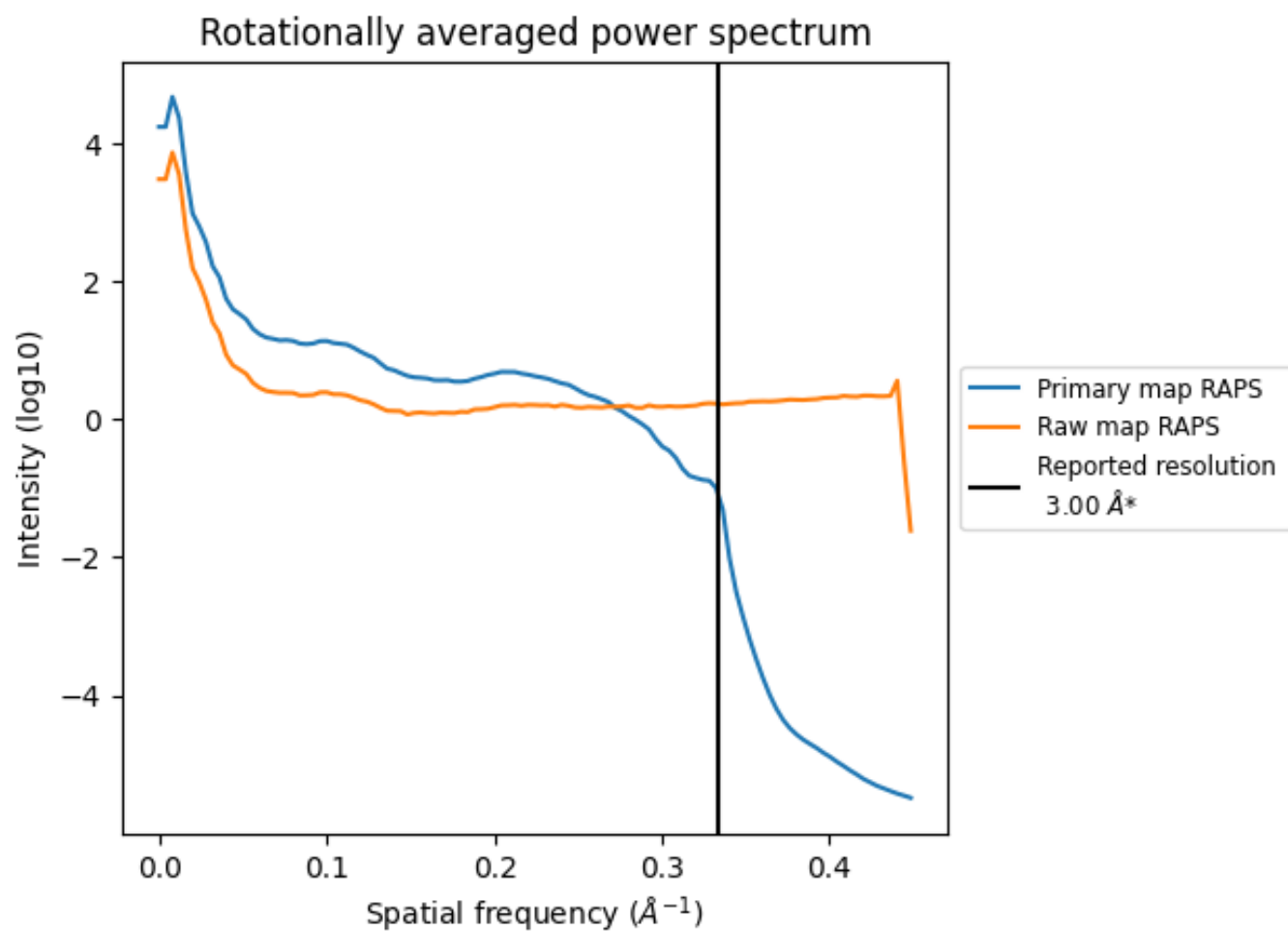
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 ⓘ

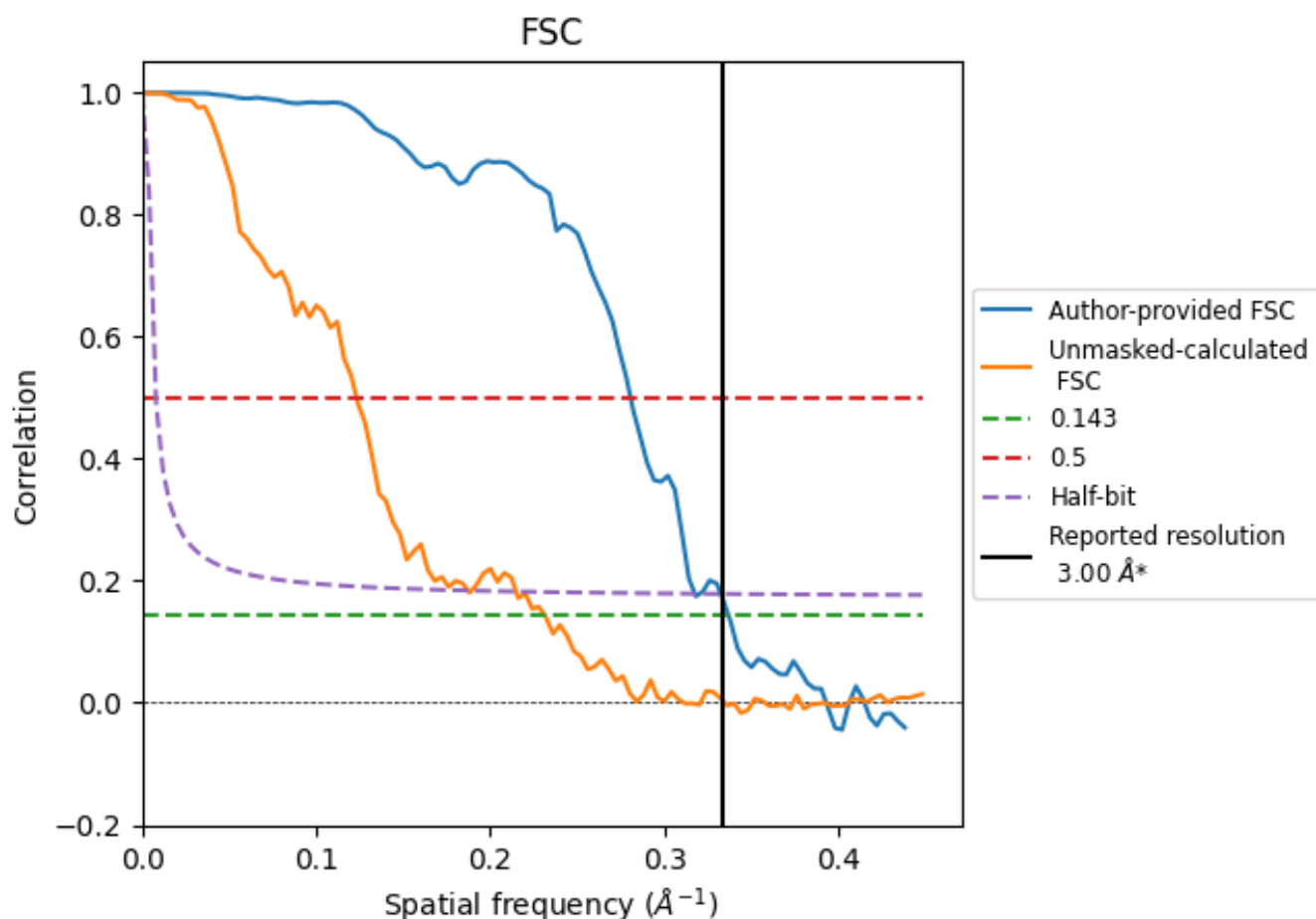


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

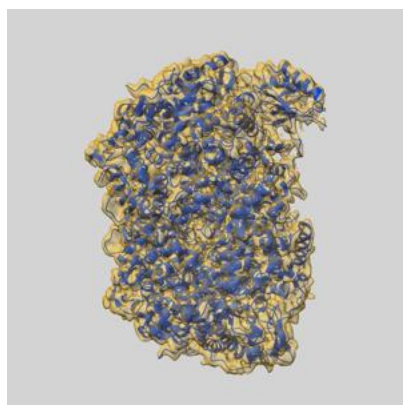
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.56	3.15
Unmasked-calculated*	4.32	8.11	5.34

*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 4.32 differs from the reported value 3.0 by more than 10 %

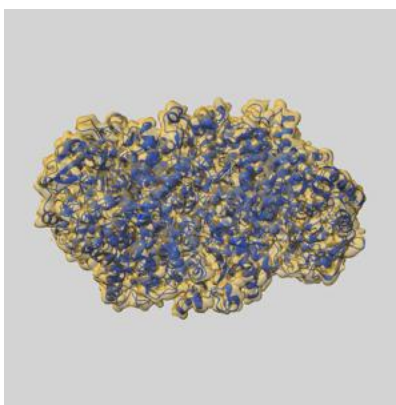
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29978 and PDB model 8GF5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

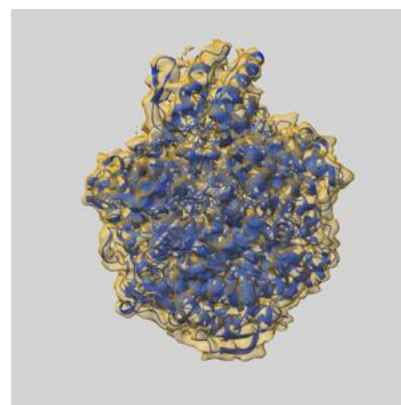
9.1 Map-model overlay [i](#)



X



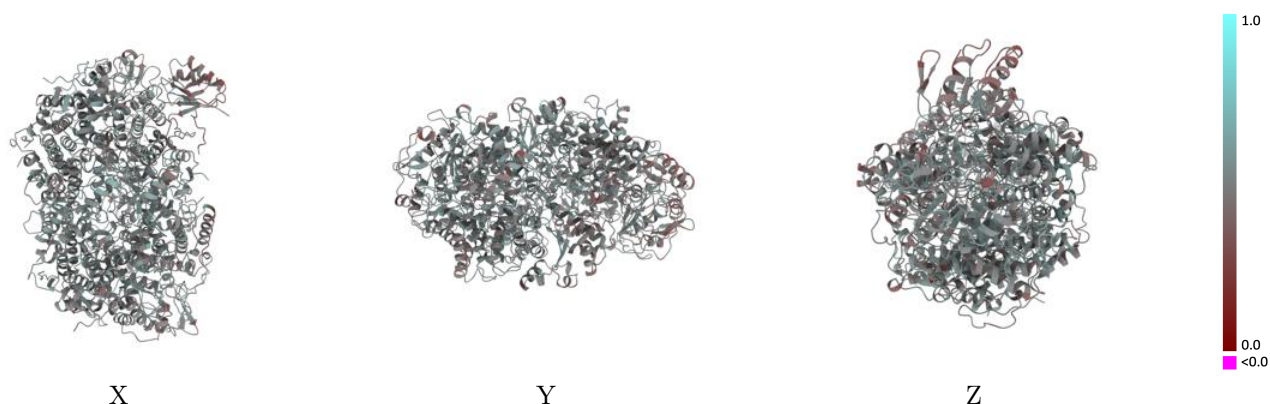
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

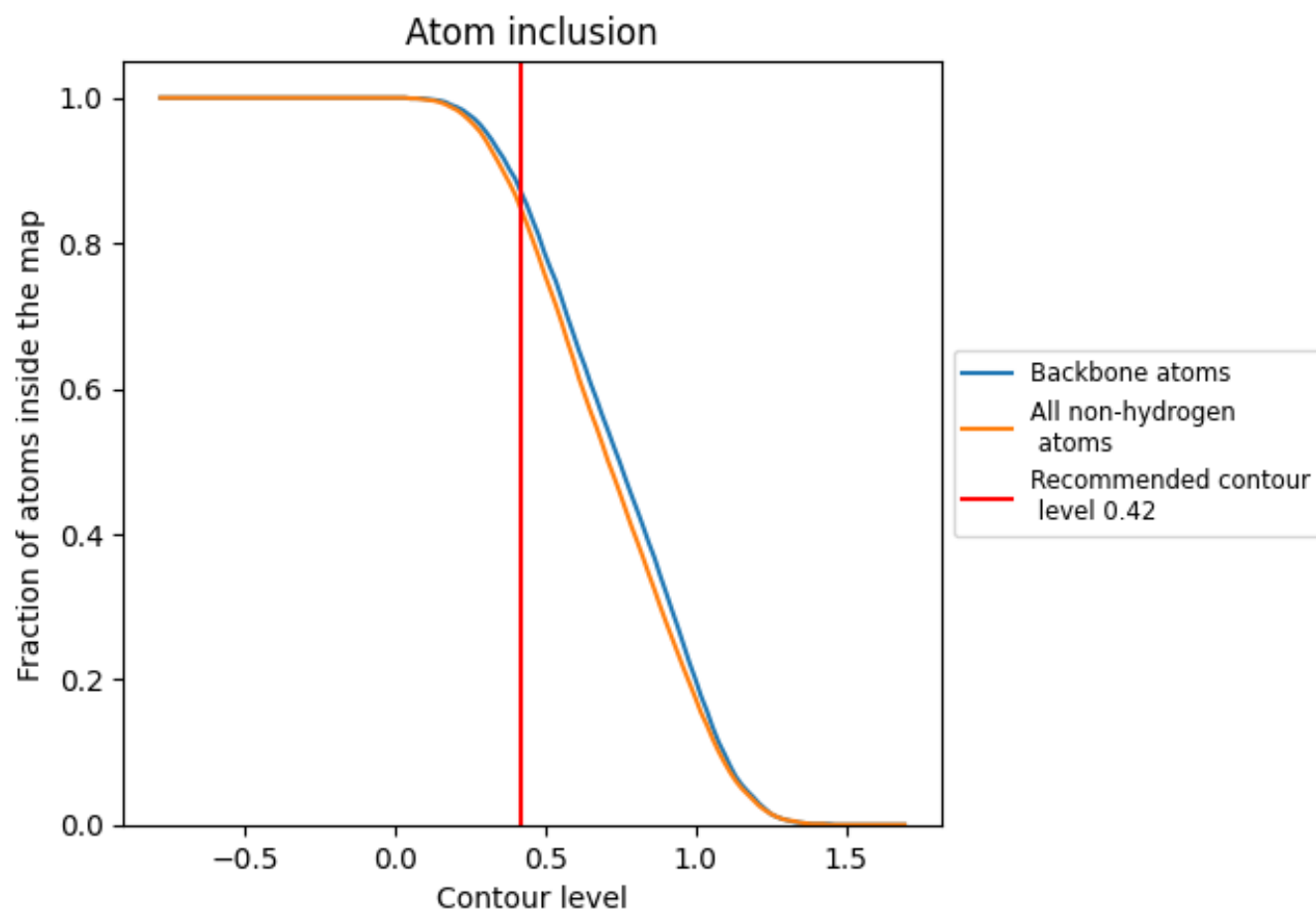


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.5020
A	0.8250	0.4970
B	0.8430	0.5070
C	0.8770	0.5170
D	0.8570	0.5050
E	0.8920	0.5060
F	0.8910	0.5010
X	0.6660	0.4350

1.0

0.0

<0.0