



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 04:25 PM EDT

PDB ID : 9Y5S / pdb_00009y5s
EMDB ID : EMD-72521
Title : eIF2B lacking the latch helix bound to ISRACT-01 (Inactive state)
Authors : Dalwadi, U.; Croll, T.; Subramanian, A.; Lee, D.J.; Arthur, C.; Walter, P.; Frost, A.
Deposited on : 2025-09-05
Resolution : 3.10 Å(reported)
Based on initial model : 7L7G

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

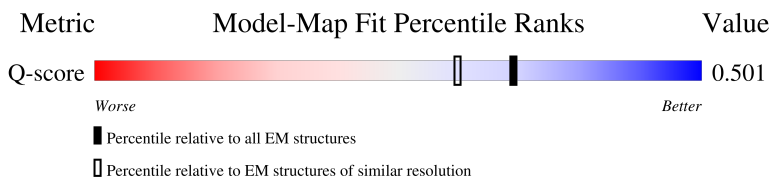
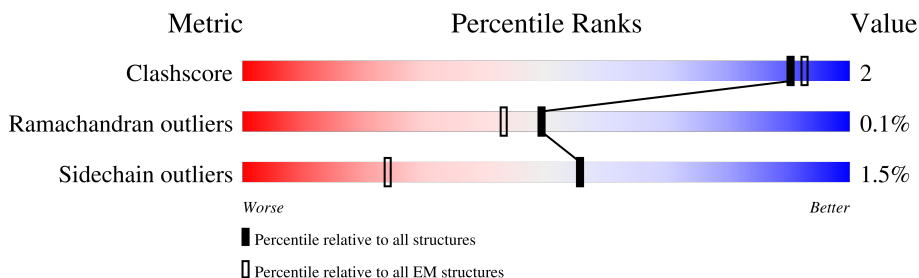
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.10 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	14724 (2.60 - 3.60)

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	721	
1	B	721	
2	C	355	
2	D	355	

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Mol	Chain	Length	Quality of chain
3	E	523	
3	F	523	
4	G	305	
4	H	305	
5	I	452	
5	J	452	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ZN	E	601	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 28748 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 Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		
1	B	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		

- Molecule 2 is a protein called Translation initiation factor eIF2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	331	Total	C	N	O	S	0	0
			2583	1629	455	484	15		
2	D	331	Total	C	N	O	S	0	0
			2583	1629	455	484	15		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P49770
C	-15	HIS	-	expression tag	UNP P49770
C	-14	HIS	-	expression tag	UNP P49770
C	-13	HIS	-	expression tag	UNP P49770
C	-12	HIS	-	expression tag	UNP P49770
C	-11	HIS	-	expression tag	UNP P49770
C	-10	HIS	-	expression tag	UNP P49770
C	-9	GLY	-	expression tag	UNP P49770
C	-8	GLY	-	expression tag	UNP P49770
C	-7	GLY	-	expression tag	UNP P49770
C	-6	SER	-	expression tag	UNP P49770
C	-5	GLU	-	expression tag	UNP P49770
C	-4	ASN	-	expression tag	UNP P49770
C	-3	LEU	-	expression tag	UNP P49770
C	-2	TYR	-	expression tag	UNP P49770
C	-1	PHE	-	expression tag	UNP P49770
C	0	GLN	-	expression tag	UNP P49770

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP P49770
C	100	GLY	SER	conflict	UNP P49770
C	101	SER	ASP	conflict	UNP P49770
C	102	GLY	GLU	conflict	UNP P49770
C	?	-	ASP	deletion	UNP P49770
C	?	-	GLN	deletion	UNP P49770
C	?	-	GLN	deletion	UNP P49770
C	?	-	GLU	deletion	UNP P49770
C	?	-	SER	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	HIS	deletion	UNP P49770
C	?	-	LYS	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	THR	deletion	UNP P49770
C	?	-	SER	deletion	UNP P49770
C	?	-	GLY	deletion	UNP P49770
D	-16	MET	-	initiating methionine	UNP P49770
D	-15	HIS	-	expression tag	UNP P49770
D	-14	HIS	-	expression tag	UNP P49770
D	-13	HIS	-	expression tag	UNP P49770
D	-12	HIS	-	expression tag	UNP P49770
D	-11	HIS	-	expression tag	UNP P49770
D	-10	HIS	-	expression tag	UNP P49770
D	-9	GLY	-	expression tag	UNP P49770
D	-8	GLY	-	expression tag	UNP P49770
D	-7	GLY	-	expression tag	UNP P49770
D	-6	SER	-	expression tag	UNP P49770
D	-5	GLU	-	expression tag	UNP P49770
D	-4	ASN	-	expression tag	UNP P49770
D	-3	LEU	-	expression tag	UNP P49770
D	-2	TYR	-	expression tag	UNP P49770
D	-1	PHE	-	expression tag	UNP P49770
D	0	GLN	-	expression tag	UNP P49770
D	1	SER	-	expression tag	UNP P49770
D	100	GLY	SER	conflict	UNP P49770
D	101	SER	ASP	conflict	UNP P49770
D	102	GLY	GLU	conflict	UNP P49770
D	?	-	ASP	deletion	UNP P49770
D	?	-	GLN	deletion	UNP P49770
D	?	-	GLN	deletion	UNP P49770
D	?	-	GLU	deletion	UNP P49770

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	HIS	deletion	UNP P49770
D	?	-	LYS	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	THR	deletion	UNP P49770
D	?	-	SER	deletion	UNP P49770
D	?	-	GLY	deletion	UNP P49770

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	356	Total	C	N	O	S	0	0
			2770	1751	493	512	14		
3	F	356	Total	C	N	O	S	0	0
			2770	1751	493	512	14		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		
4	H	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	421	Total	C	N	O	S	0	0
			3268	2068	561	613	26		
5	J	421	Total	C	N	O	S	0	0
			3268	2068	561	613	26		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

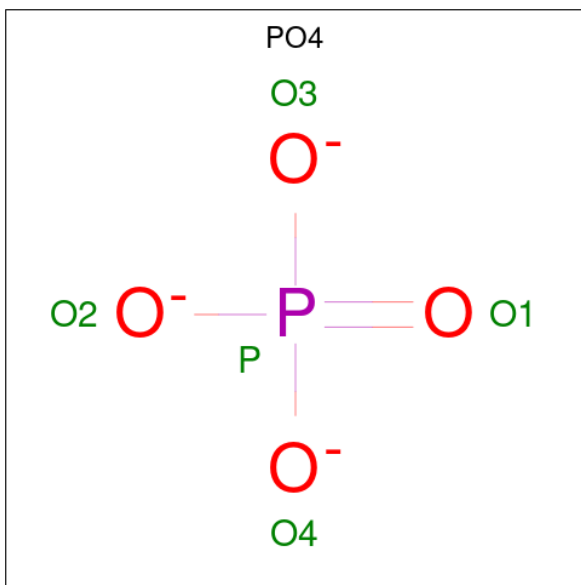
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total	Zn
			1	1
6	B	1	Total	Zn
			1	1

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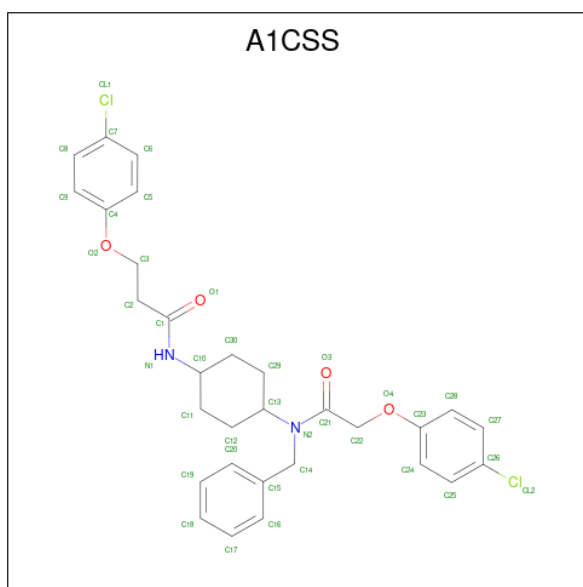
Mol	Chain	Residues	Atoms		AltConf
6	E	2	Total	Zn	0
			2	2	
6	F	2	Total	Zn	0
			2	2	

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	

- Molecule 8 is N-((1r,4r)-4-[N-benzyl-2-(4-chlorophenoxy)acetamido]cyclohexyl)-3-(4-chlorophenoxy)propanamide (CCD ID: A1CSS) (formula: C₃₀H₃₂Cl₂N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
8	D	1	38	30	2	2	4	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
9	E	1	1	1	0
9	F	1	1	1	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.473	Depositor
Minimum map value	-0.254	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	357.44, 357.44, 357.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8936, 0.8936, 0.8936	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: PO4, A1CSS, CL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	0/3497	1.13	5/4758 (0.1%)
1	B	0.66	0/3497	1.13	2/4758 (0.0%)
2	C	0.72	1/2633 (0.0%)	1.17	4/3559 (0.1%)
2	D	0.72	0/2633	1.22	7/3559 (0.2%)
3	E	0.70	0/2822	1.17	5/3835 (0.1%)
3	F	0.68	0/2822	1.18	6/3835 (0.2%)
4	G	0.65	0/2338	1.18	8/3155 (0.3%)
4	H	0.65	0/2338	1.16	6/3155 (0.2%)
5	I	0.60	0/3318	1.04	4/4481 (0.1%)
5	J	0.57	0/3318	1.01	5/4481 (0.1%)
All	All	0.66	1/29216 (0.0%)	1.14	52/39576 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
2	C	0	6
2	D	0	3
3	E	0	8
3	F	0	7
4	G	0	3
5	J	0	1
All	All	0	36

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	317	PRO	CA-CB	-5.08	1.49	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	188	GLU	N-CA-CB	-7.52	98.26	110.14
3	F	490	ASP	CA-CB-CG	7.04	119.64	112.60
2	D	317	PRO	CB-CA-C	-7.00	104.59	111.17
3	E	490	ASP	CA-CB-CG	6.78	119.38	112.60
3	E	351	THR	CA-CB-OG1	-6.67	99.59	109.60
2	D	197	PHE	CA-CB-CG	-6.65	107.15	113.80
2	D	271	MET	CG-SD-CE	-6.51	86.58	100.90
1	A	366	THR	CA-CB-OG1	-6.50	99.85	109.60
4	H	245	ASP	CA-CB-CG	6.49	119.09	112.60
2	C	309	HIS	CA-CB-CG	-6.43	107.37	113.80
3	E	423	LEU	N-CA-CB	6.41	119.54	110.12
5	I	175	ASP	CA-CB-CG	6.33	118.93	112.60
4	H	229	VAL	N-CA-CB	-6.28	103.28	111.82
4	H	136	ARG	CB-CA-C	-6.27	100.38	110.79
4	G	274	ASP	CA-CB-CG	6.22	118.82	112.60
4	H	202	GLU	N-CA-CB	-6.16	99.84	110.32
3	F	499	LEU	N-CA-CB	6.05	120.13	111.05
4	G	214	GLN	N-CA-CB	-6.03	100.94	110.28
2	C	317	PRO	CB-CA-C	-5.98	105.55	111.17
1	B	289	MET	CB-CA-C	-5.95	99.99	109.80
3	F	172	ASP	CA-CB-CG	5.94	118.54	112.60
4	G	202	GLU	N-CA-CB	-5.86	100.14	110.39
4	G	3	ASP	CA-CB-CG	5.81	118.41	112.60
2	D	213	GLU	N-CA-CB	5.68	118.48	109.51
2	C	144	LEU	N-CA-CB	5.62	118.31	109.94
5	J	423	ASP	CA-CB-CG	5.55	118.15	112.60
4	G	243	GLN	CB-CA-C	-5.54	101.43	110.85
5	J	180	LEU	N-CA-CB	-5.51	101.43	110.52
2	D	177	PHE	CA-CB-CG	5.50	119.30	113.80
3	E	247	GLU	N-CA-CB	-5.48	101.96	110.57
5	I	156	ASP	CA-CB-CG	5.47	118.07	112.60
5	J	292	ASP	CA-CB-CG	5.42	118.02	112.60
3	E	487	LEU	N-CA-CB	-5.41	102.02	109.97
1	A	84	THR	CA-CB-OG1	-5.35	101.57	109.60
4	H	237	ARG	CD-NE-CZ	5.35	131.89	124.40
4	G	269	GLU	CB-CG-CD	5.29	121.60	112.60
2	D	289	VAL	N-CA-CB	-5.27	102.54	111.23
4	G	124	THR	CA-CB-OG1	-5.27	101.70	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	357	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	D	317	PRO	N-CA-CB	5.25	105.95	103.22
1	A	256	VAL	N-CA-CB	5.25	116.69	110.55
5	I	49	GLU	CB-CG-CD	5.21	121.46	112.60
5	I	201	ASP	CA-CB-CG	5.21	117.81	112.60
5	J	201	ASP	CA-CB-CG	5.20	117.80	112.60
4	G	229	VAL	N-CA-CB	-5.20	104.88	111.64
1	A	53	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	152	TYR	N-CA-CB	5.11	118.21	110.45
1	B	194	THR	CA-CB-OG1	-5.08	101.97	109.60
2	C	259	LYS	CB-CA-C	-5.08	100.92	110.67
3	F	517	ARG	NE-CZ-NH1	-5.06	116.44	121.50
5	J	156	ASP	CA-CB-CG	5.05	117.65	112.60
3	F	402	LEU	N-CA-CB	-5.02	102.82	110.65

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Peptide
1	A	211	ARG	Sidechain
1	A	232	GLN	Peptide
1	A	339	ARG	Sidechain
1	B	169	ARG	Sidechain
1	B	195	ARG	Sidechain
1	B	299	ARG	Sidechain
1	B	422	ARG	Sidechain
2	C	185	ARG	Sidechain
2	C	245	LEU	Peptide
2	C	284	SER	Peptide
2	C	338	ARG	Sidechain
2	C	43	ARG	Sidechain
2	C	95	ARG	Sidechain
2	D	183	ARG	Sidechain
2	D	185	ARG	Sidechain
2	D	338	ARG	Sidechain
3	E	209	ARG	Sidechain
3	E	267	ARG	Sidechain
3	E	306	ARG	Sidechain
3	E	364	ARG	Sidechain
3	E	446	ARG	Sidechain
3	E	483	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	E	499	LEU	Peptide
3	E	517	ARG	Sidechain
3	F	225	ARG	Sidechain
3	F	267	ARG	Sidechain
3	F	321	ARG	Sidechain
3	F	355	ARG	Sidechain
3	F	446	ARG	Sidechain
3	F	470	HIS	Peptide
3	F	499	LEU	Peptide
4	G	136	ARG	Sidechain
4	G	147	ARG	Sidechain
4	G	192	LEU	Peptide
5	J	276	ALA	Peptide

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	3423	0	3418	16	0
1	B	3423	0	3418	15	0
2	C	2583	0	2583	13	0
2	D	2583	0	2583	9	0
3	E	2770	0	2829	10	0
3	F	2770	0	2828	10	0
4	G	2302	0	2378	13	0
4	H	2302	0	2378	13	0
5	I	3268	0	3368	3	0
5	J	3268	0	3368	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	E	2	0	0	2	0
6	F	2	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	D	38	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	28748	0	29151	96	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 2.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG13	1:A:76:ILE:HB	1.73	0.70
1:B:70:LEU:C	1:B:70:LEU:HD23	2.21	0.66
3:E:465:CYS:SG	6:E:601:ZN:ZN	1.87	0.64
4:H:237:ARG:NE	4:H:305:LEU:OXT	2.29	0.61
1:A:318:VAL:HG22	1:A:318:VAL:O	2.01	0.60
3:E:465:CYS:HG	6:E:601:ZN:ZN	1.18	0.58
1:B:396:LEU:HG	1:B:400:VAL:HG11	1.85	0.58
4:G:111:ILE:HG21	4:G:229:VAL:HG13	1.86	0.57
4:G:237:ARG:NE	4:G:305:LEU:O	2.40	0.55
2:D:217:MET:HE1	2:D:222:ILE:HA	1.89	0.54
1:A:156:ILE:HG13	1:A:309:VAL:HG11	1.89	0.54
1:B:66:VAL:HG13	1:B:76:ILE:HB	1.90	0.54
3:F:395:LEU:N	3:F:396:PRO:CD	2.71	0.53
2:C:194:CYS:SG	2:C:248:VAL:CG1	2.98	0.52
2:C:236:THR:HG21	2:C:245:LEU:HD22	1.92	0.52
3:E:499:LEU:CD2	4:G:239:PHE:CE1	2.93	0.52
2:D:62:ARG:NH1	2:D:348:ASP:OD1	2.42	0.51
3:E:177:VAL:HG21	3:E:485:LEU:HB2	1.93	0.51
4:H:202:GLU:HB2	4:H:238:LEU:O	2.11	0.51
1:A:186:LYS:HE3	2:D:297:PHE:CD2	2.46	0.51
2:C:194:CYS:SG	2:C:248:VAL:HG13	2.51	0.51
4:G:178:VAL:HG11	4:G:186:ILE:HG13	1.93	0.51
4:G:237:ARG:HE	4:G:305:LEU:C	2.18	0.51
3:E:405:ALA:HA	3:E:416:SER:OG	2.12	0.50
2:C:62:ARG:NH2	2:C:351:LEU:O	2.42	0.50
1:A:234:SER:OG	1:A:236:ASP:OD1	2.30	0.49
2:C:165:ILE:HG21	2:C:233:ILE:HD12	1.94	0.49
4:H:108:ARG:HG2	4:H:136:ARG:HG3	1.94	0.49
2:C:188:HIS:ND1	2:C:213:GLU:HG2	2.27	0.49
3:E:269:LEU:HD22	3:E:273:MET:HE2	1.94	0.49
1:B:302:ASN:OD1	1:B:302:ASN:C	2.57	0.48
3:F:499:LEU:CD2	4:H:239:PHE:CE1	2.96	0.48
4:H:237:ARG:HB2	4:H:237:ARG:HH21	1.79	0.48
3:F:443:PHE:HB2	3:F:516:LEU:HD23	1.97	0.47
3:E:374:ARG:NH1	5:I:288:ASP:HA	2.29	0.47
4:G:70:GLU:OE2	4:G:237:ARG:NH1	2.47	0.47
3:E:257:LYS:HB2	3:E:258:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:199:LEU:HD21	5:J:304:ILE:HD11	1.96	0.46
1:A:97:TRP:O	1:A:97:TRP:CE3	2.68	0.46
2:D:170:PHE:C	2:D:170:PHE:CD1	2.93	0.46
4:H:108:ARG:HG3	4:H:133:VAL:HG23	1.98	0.46
5:I:229:ILE:HB	5:I:230:PRO:HD3	1.98	0.46
4:H:186:ILE:HD13	4:H:186:ILE:HA	1.84	0.45
1:A:318:VAL:O	1:A:318:VAL:CG2	2.65	0.45
4:G:111:ILE:CG2	4:G:229:VAL:HG13	2.47	0.44
4:H:71:LEU:HG	4:H:305:LEU:HD13	1.99	0.44
1:B:432:THR:HG22	1:B:433:SER:H	1.82	0.44
2:D:281:GLU:CG	4:H:120:LYS:HB3	2.47	0.44
3:F:326:LYS:HD3	3:F:326:LYS:HA	1.84	0.44
2:D:281:GLU:HG3	4:H:120:LYS:HB3	1.99	0.44
1:A:47:LEU:C	1:A:47:LEU:HD23	2.42	0.44
4:G:236:VAL:HA	4:G:305:LEU:HD21	2.00	0.43
1:A:432:THR:HG22	1:A:433:SER:H	1.84	0.43
2:C:160:HIS:O	2:C:163:GLU:HB2	2.19	0.43
2:C:236:THR:HG22	2:C:245:LEU:HD13	2.01	0.43
1:A:279:ASN:HA	1:A:282:ILE:HD12	1.99	0.43
3:F:512:VAL:N	3:F:513:PRO:CD	2.82	0.43
1:B:389:VAL:HG12	1:B:390:VAL:N	2.34	0.43
2:C:271:MET:SD	2:C:328:ILE:HD13	2.59	0.43
1:A:47:LEU:HD21	1:A:153:GLY:HA3	2.01	0.42
2:C:350:VAL:O	2:C:351:LEU:HB3	2.18	0.42
2:D:271:MET:HE1	2:D:339:LEU:HD13	2.00	0.42
4:G:203:ASN:O	4:G:278:PRO:HG3	2.19	0.42
4:G:237:ARG:HE	4:G:305:LEU:HG	1.83	0.42
3:F:348:GLU:O	3:F:349:ALA:C	2.63	0.42
1:B:394:THR:HG22	1:B:396:LEU:HD13	1.99	0.42
3:F:193:THR:HA	3:F:196:MET:HG2	2.00	0.42
3:F:499:LEU:HD23	4:H:239:PHE:CE1	2.55	0.42
1:A:161:ILE:O	1:A:162:THR:C	2.63	0.42
1:A:296:TYR:OH	1:A:312:ASP:OD2	2.34	0.42
2:D:193:GLU:HA	2:D:200:GLY:HA3	2.02	0.42
5:J:158:ILE:HD12	5:J:170:MET:HE2	2.02	0.42
1:B:186:LYS:HE3	2:C:297:PHE:CD2	2.55	0.42
3:F:388:ILE:HG22	3:F:389:PRO:HD3	2.01	0.42
4:G:27:ILE:HG23	4:G:72:PHE:CD1	2.55	0.42
4:G:203:ASN:HB3	4:G:239:PHE:CZ	2.55	0.42
1:B:156:ILE:HG13	1:B:309:VAL:HG11	2.02	0.42
5:J:326:VAL:N	5:J:327:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:C	1:B:70:LEU:CD2	2.93	0.41
1:B:171:ARG:HD3	1:B:288:HIS:CD2	2.55	0.41
1:B:386:GLY:O	1:B:389:VAL:HG23	2.19	0.41
4:H:236:VAL:HA	4:H:305:LEU:HD21	2.01	0.41
1:B:319:TYR:CD1	1:B:320:PRO:HA	2.56	0.41
2:D:81:MET:HE2	2:D:81:MET:HA	2.03	0.41
3:E:180:PHE:CZ	3:E:452:PHE:CD2	3.09	0.41
3:F:422:GLN:O	3:F:426:VAL:HG23	2.21	0.41
4:G:185:TYR:HA	4:H:243:GLN:HG3	2.03	0.41
3:E:248:LEU:C	3:E:248:LEU:HD23	2.46	0.40
1:B:432:THR:HG22	1:B:433:SER:N	2.36	0.40
1:A:454:PRO:HA	1:A:497:TRP:CE2	2.56	0.40
2:C:204:ALA:CB	2:C:216:VAL:HG22	2.52	0.40
1:A:419:VAL:CG1	1:A:423:VAL:HB	2.51	0.40
1:B:192:HIS:CE1	1:B:194:THR:HG1	2.40	0.40
2:C:62:ARG:NH1	2:C:348:ASP:OD1	2.54	0.40
5:I:326:VAL:N	5:I:327:PRO:CD	2.84	0.40
1:A:319:TYR:CG	1:A:320:PRO:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/721 (60%)	417 (96%)	16 (4%)	0	100	100
1	B	433/721 (60%)	412 (95%)	21 (5%)	0	100	100
2	C	329/355 (93%)	318 (97%)	11 (3%)	0	100	100
2	D	329/355 (93%)	321 (98%)	7 (2%)	1 (0%)	36	67
3	E	354/523 (68%)	345 (98%)	9 (2%)	0	100	100
3	F	354/523 (68%)	343 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
4	H	292/305 (96%)	280 (96%)	12 (4%)	0	100	100
5	I	417/452 (92%)	398 (95%)	17 (4%)	2 (0%)	24	57
5	J	417/452 (92%)	390 (94%)	27 (6%)	0	100	100
All	All	3650/4712 (78%)	3510 (96%)	137 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	50	GLU
2	D	248	VAL
5	I	10	VAL

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	384/626 (61%)	377 (98%)	7 (2%)	51	73
1	B	384/626 (61%)	379 (99%)	5 (1%)	61	77
2	C	280/298 (94%)	272 (97%)	8 (3%)	37	66
2	D	280/298 (94%)	275 (98%)	5 (2%)	51	73
3	E	312/444 (70%)	306 (98%)	6 (2%)	50	73
3	F	312/444 (70%)	309 (99%)	3 (1%)	68	79
4	G	253/260 (97%)	250 (99%)	3 (1%)	63	78
4	H	253/260 (97%)	249 (98%)	4 (2%)	55	75
5	I	370/398 (93%)	366 (99%)	4 (1%)	65	78
5	J	370/398 (93%)	367 (99%)	3 (1%)	73	81
All	All	3198/4052 (79%)	3150 (98%)	48 (2%)	55	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	66	VAL
1	A	151	VAL
1	A	289	MET
1	A	338	SER
1	A	394	THR
1	A	447	SER
1	B	39	PRO
1	B	47	LEU
1	B	221	LEU
1	B	250	SER
1	B	394	THR
2	C	163	GLU
2	C	225	VAL
2	C	248	VAL
2	C	249	THR
2	C	271	MET
2	C	274	LEU
2	C	292	GLU
2	C	334	SER
2	D	29	ARG
2	D	163	GLU
2	D	248	VAL
2	D	292	GLU
2	D	350	VAL
3	E	236	VAL
3	E	261	SER
3	E	351	THR
3	E	386	LEU
3	E	392	SER
3	E	396	PRO
3	F	386	LEU
3	F	428	ARG
3	F	435	LEU
4	G	136	ARG
4	G	186	ILE
4	G	209	LYS
4	H	171	LEU
4	H	186	ILE
4	H	229	VAL
4	H	237	ARG
5	I	1	MET
5	I	128	LEU

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Mol	Chain	Res	Type
5	I	175	ASP
5	I	233	VAL
5	J	81	ASP
5	J	128	LEU
5	J	153	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	89	GLN
1	A	371	ASN
1	A	416	ASN
1	B	89	GLN
1	B	210	ASN
1	B	279	ASN
1	B	337	HIS
1	B	416	ASN
2	C	154	GLN
2	C	160	HIS
2	C	252	HIS
2	C	261	HIS
2	D	128	GLN
2	D	162	ASN
2	D	280	ASN
3	E	309	GLN
3	F	431	ASN
4	G	116	HIS
4	G	170	HIS
4	G	222	GLN
4	G	223	ASN
4	H	208	ASN
5	I	136	GLN
5	I	363	GLN
5	J	196	HIS

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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
8	A1CSS	D	402	-	41,41,41	1.69	10 (24%)	52,54,54	1.48	7 (13%)
7	PO4	C	1000	-	4,4,4	0.90	0	6,6,6	0.58	0
7	PO4	D	401	-	4,4,4	1.37	1 (25%)	6,6,6	0.27	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1CSS	D	402	-	-	8/27/37/37	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	402	A1CSS	O1-C1	3.45	1.30	1.23
8	D	402	A1CSS	O3-C21	3.26	1.30	1.23
8	D	402	A1CSS	O4-C23	-3.23	1.30	1.37
8	D	402	A1CSS	O2-C4	-2.98	1.30	1.37
8	D	402	A1CSS	C8-C7	2.77	1.43	1.38
8	D	402	A1CSS	C9-C4	2.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	402	A1CSS	C1-N1	2.37	1.39	1.34
8	D	402	A1CSS	C17-C16	2.18	1.42	1.38
7	D	401	PO4	P-O1	2.17	1.55	1.50
8	D	402	A1CSS	C19-C20	2.08	1.42	1.38
8	D	402	A1CSS	C28-C23	2.06	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	402	A1CSS	C8-C7-CL1	4.47	125.95	119.36
8	D	402	A1CSS	C22-O4-C23	3.11	123.21	117.63
8	D	402	A1CSS	C3-O2-C4	2.92	125.51	117.93
8	D	402	A1CSS	C8-C7-C6	-2.85	117.71	121.24
8	D	402	A1CSS	C5-C6-C7	2.49	121.75	119.24
8	D	402	A1CSS	C12-C13-N2	2.40	115.16	111.83
8	D	402	A1CSS	C6-C7-CL1	-2.05	116.33	119.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

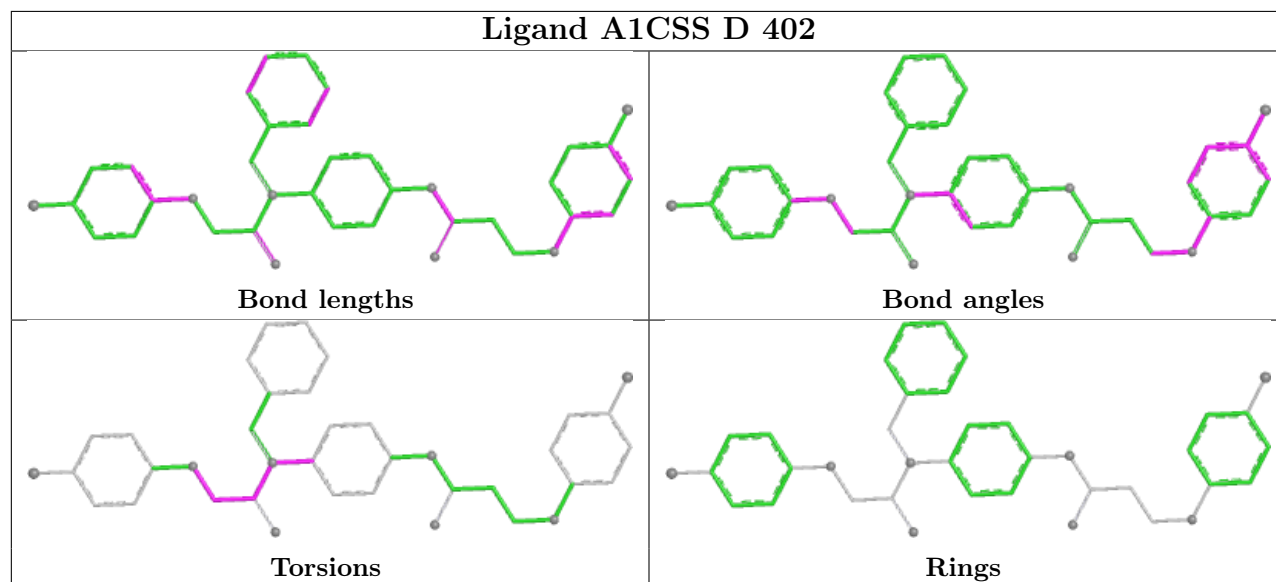
Mol	Chain	Res	Type	Atoms
8	D	402	A1CSS	C22-C21-N2-C13
8	D	402	A1CSS	O3-C21-N2-C13
8	D	402	A1CSS	O3-C21-N2-C14
8	D	402	A1CSS	O3-C21-C22-O4
8	D	402	A1CSS	C22-C21-N2-C14
8	D	402	A1CSS	N2-C21-C22-O4
8	D	402	A1CSS	C12-C13-N2-C14
8	D	402	A1CSS	C21-C22-O4-C23

There are no ring outliers.

No monomer is involved in short contacts.

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.

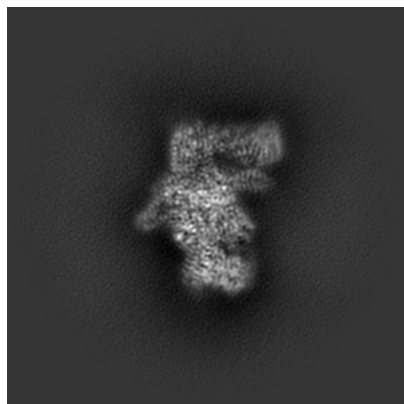
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72521. These allow visual inspection of the internal detail of the map and identification of artifacts.

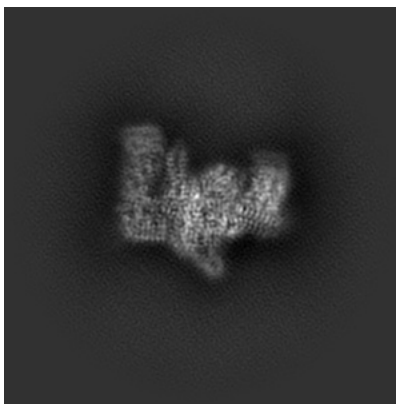
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

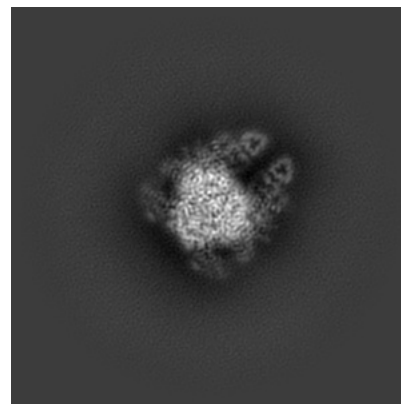
6.1.1 Primary map



X

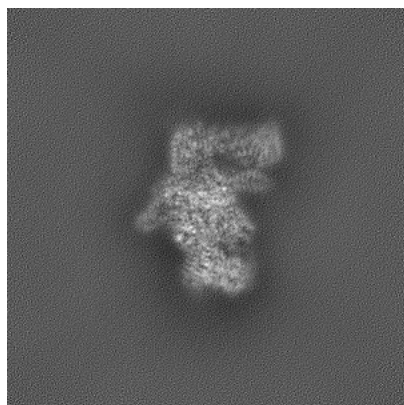


Y

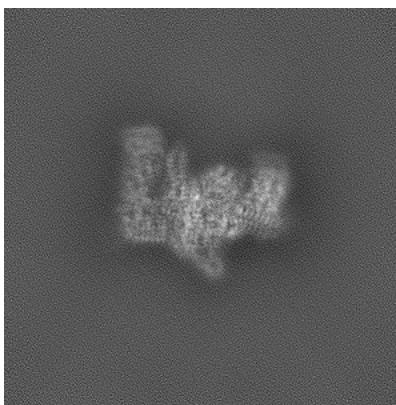


Z

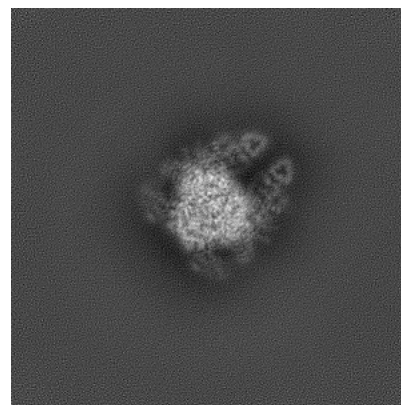
6.1.2 Raw map



X



Y

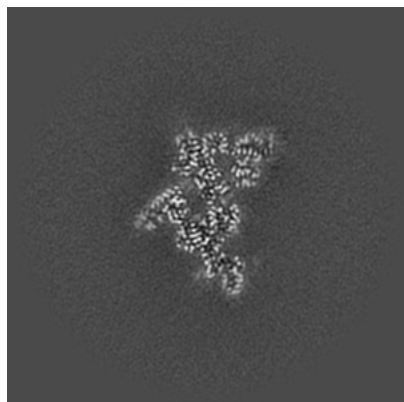


Z

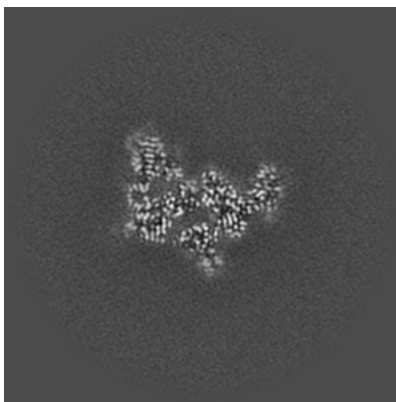
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

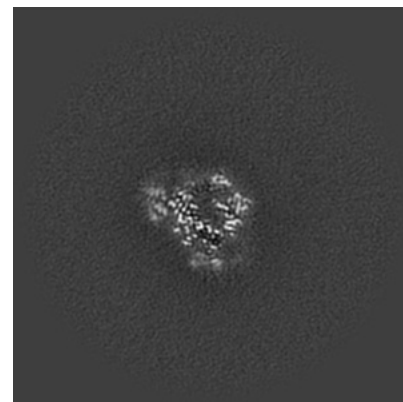
6.2.1 Primary map



X Index: 200

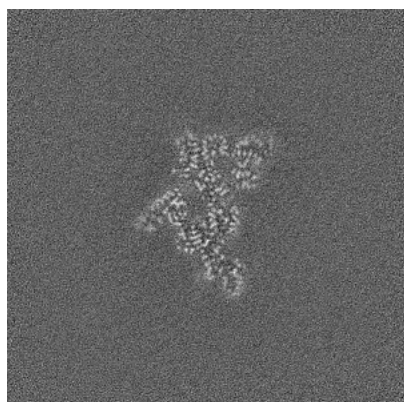


Y Index: 200

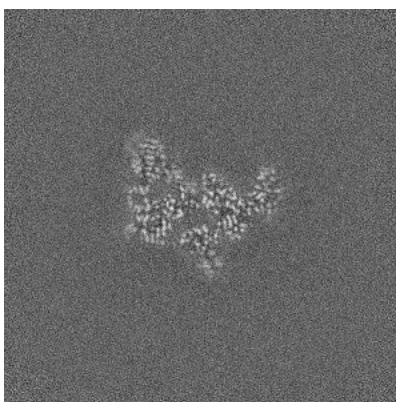


Z Index: 200

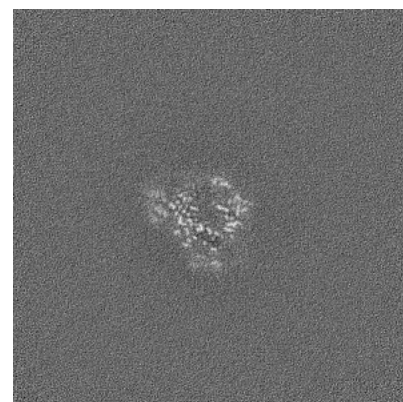
6.2.2 Raw map



X Index: 200



Y Index: 200

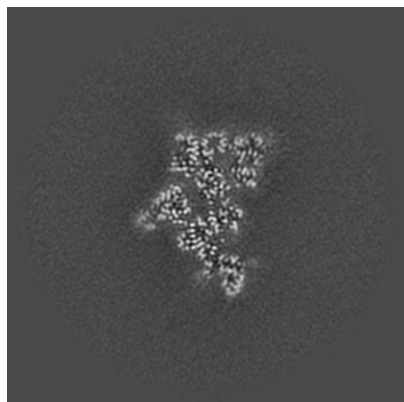


Z Index: 200

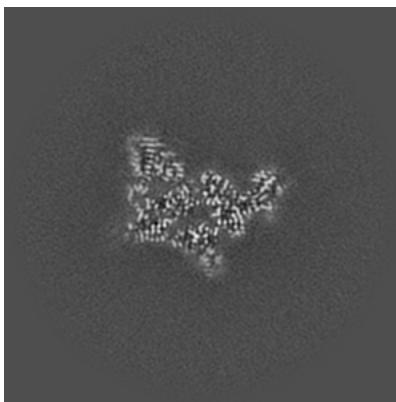
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

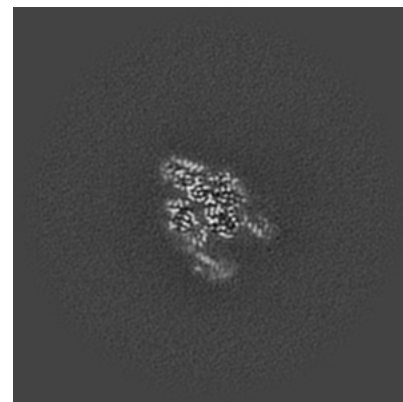
6.3.1 Primary map



X Index: 198

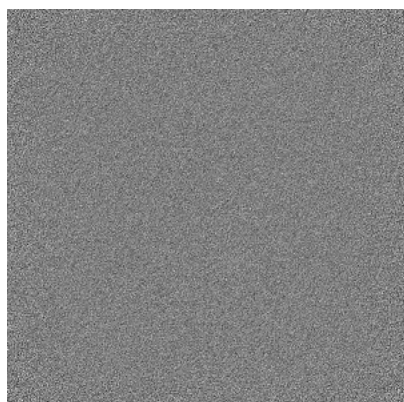


Y Index: 198

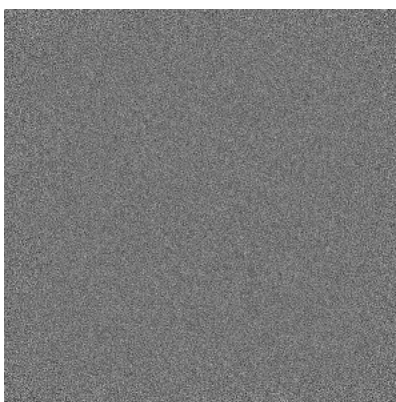


Z Index: 182

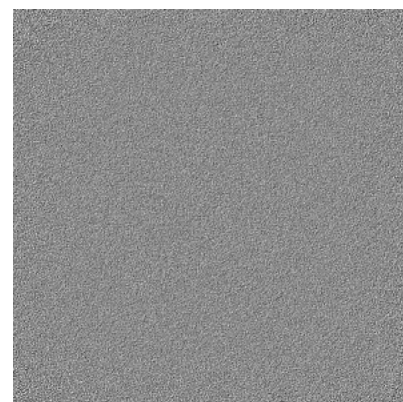
6.3.2 Raw map



X Index: 0



Y Index: 0

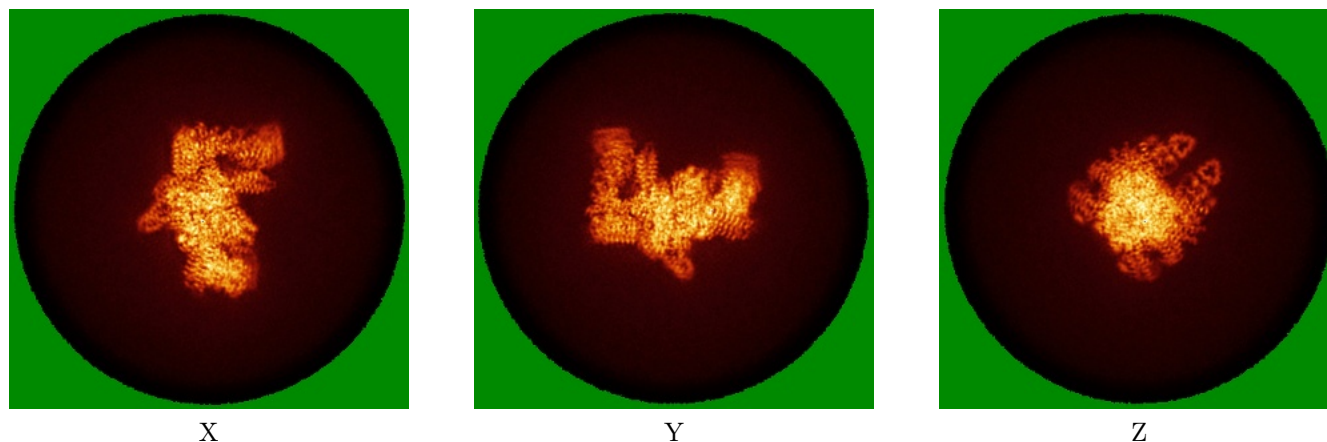


Z Index: 399

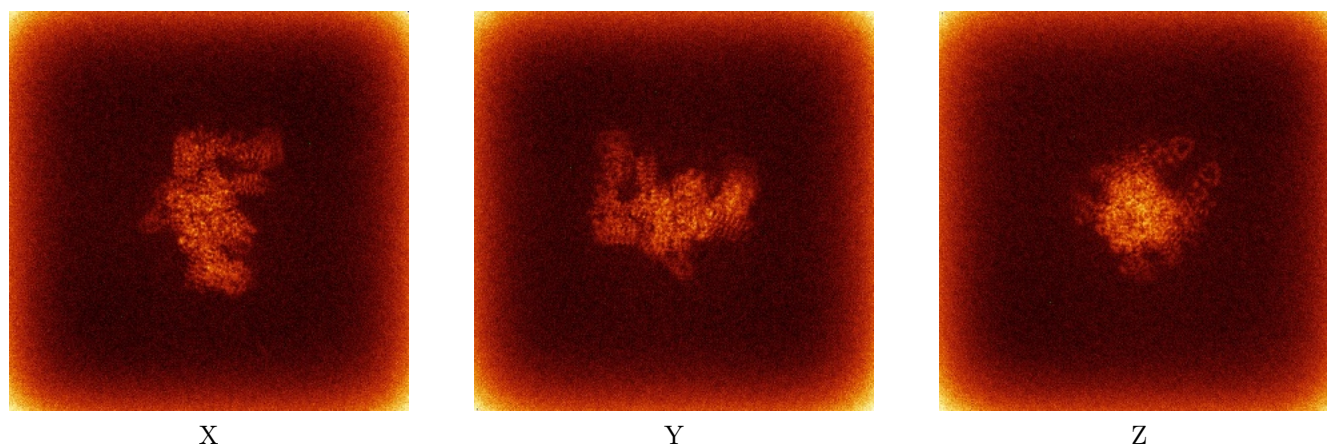
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



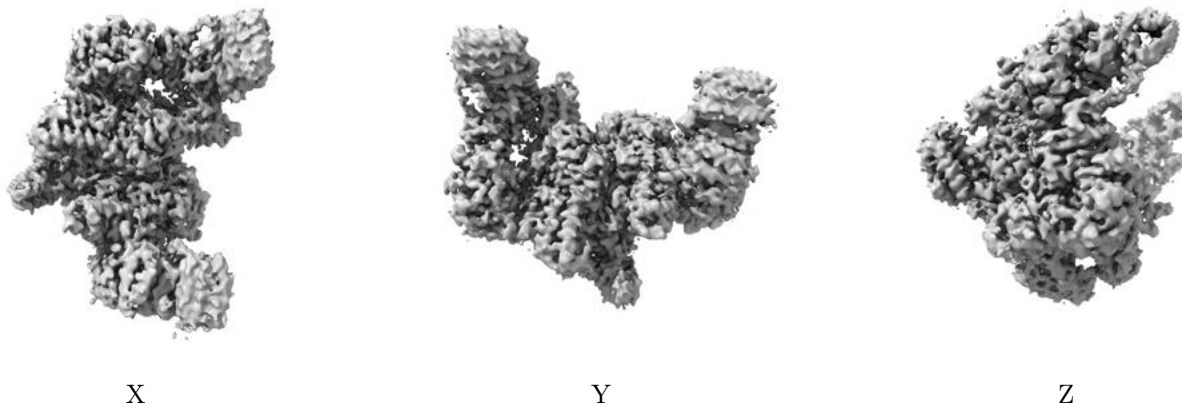
6.4.2 Raw map



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.

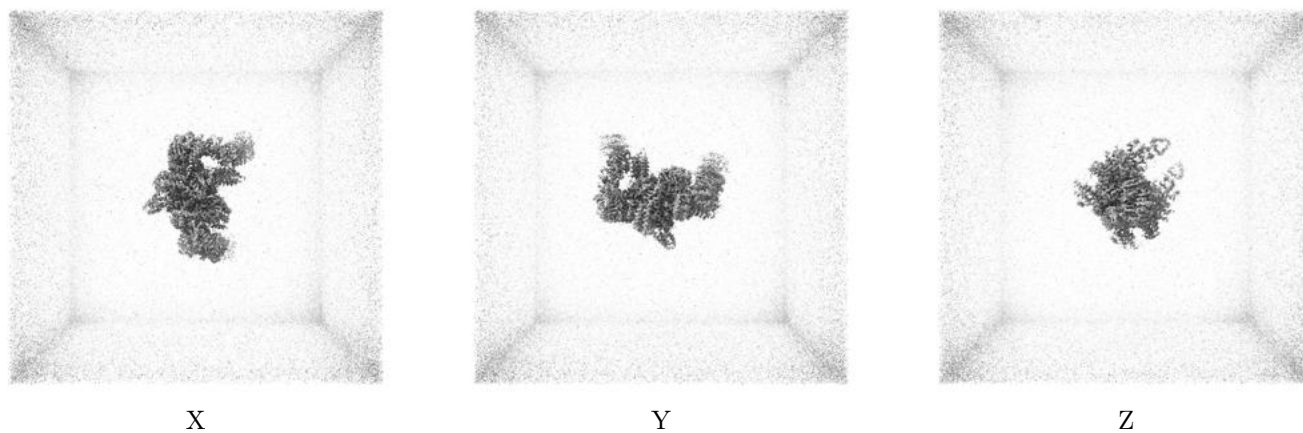
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

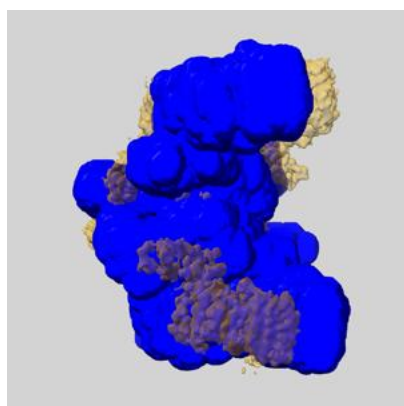
6.6 Mask visualisation [i](#)

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

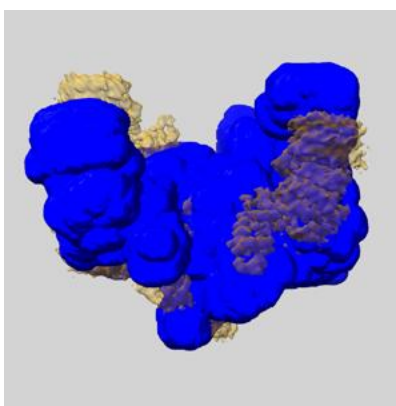
A mask typically either:

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

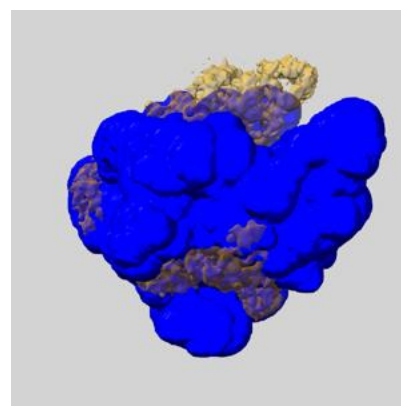
6.6.1 emd_72521_msk_1.map [i](#)



X



Y

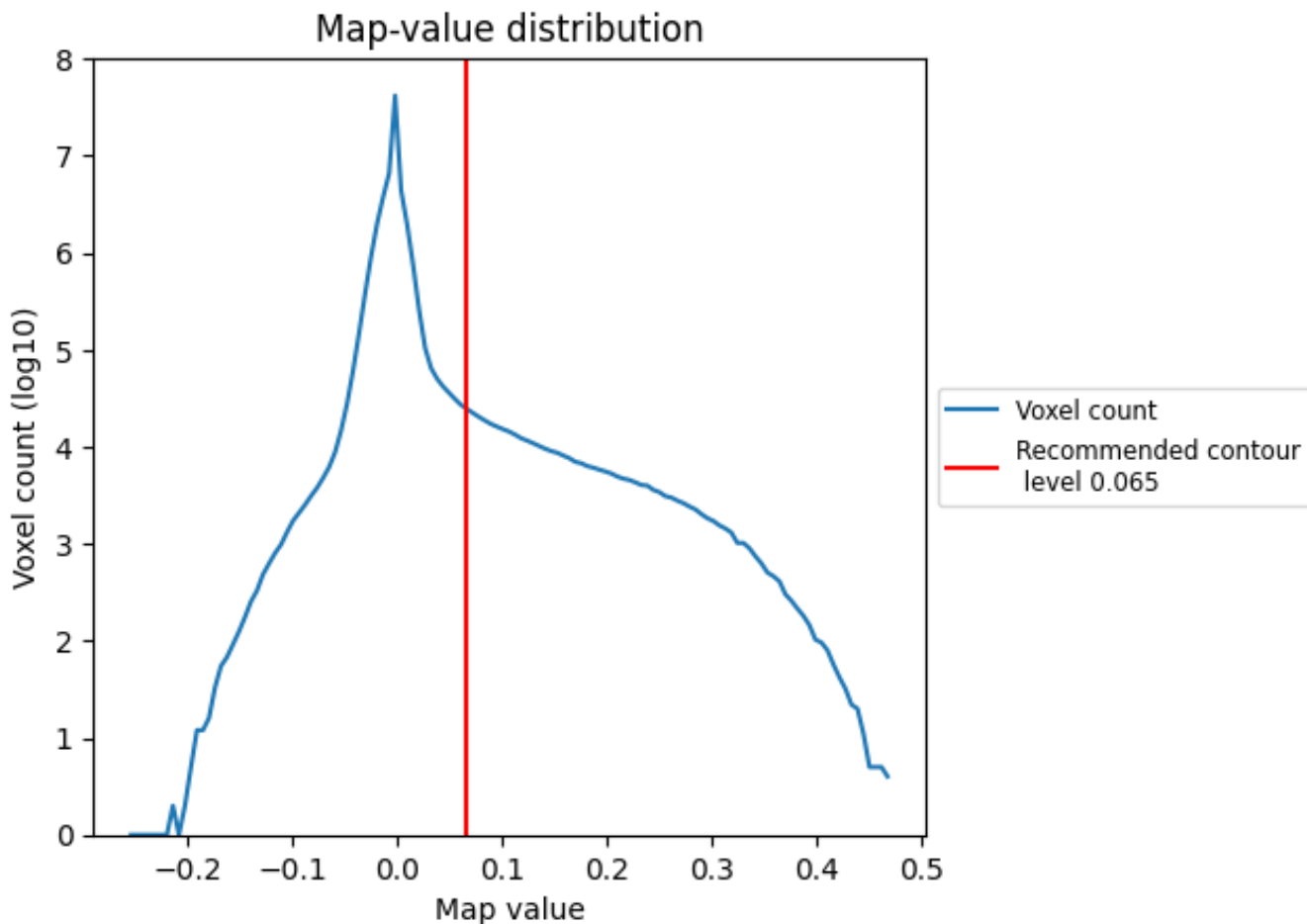


Z

7 Map analysis [i](#)

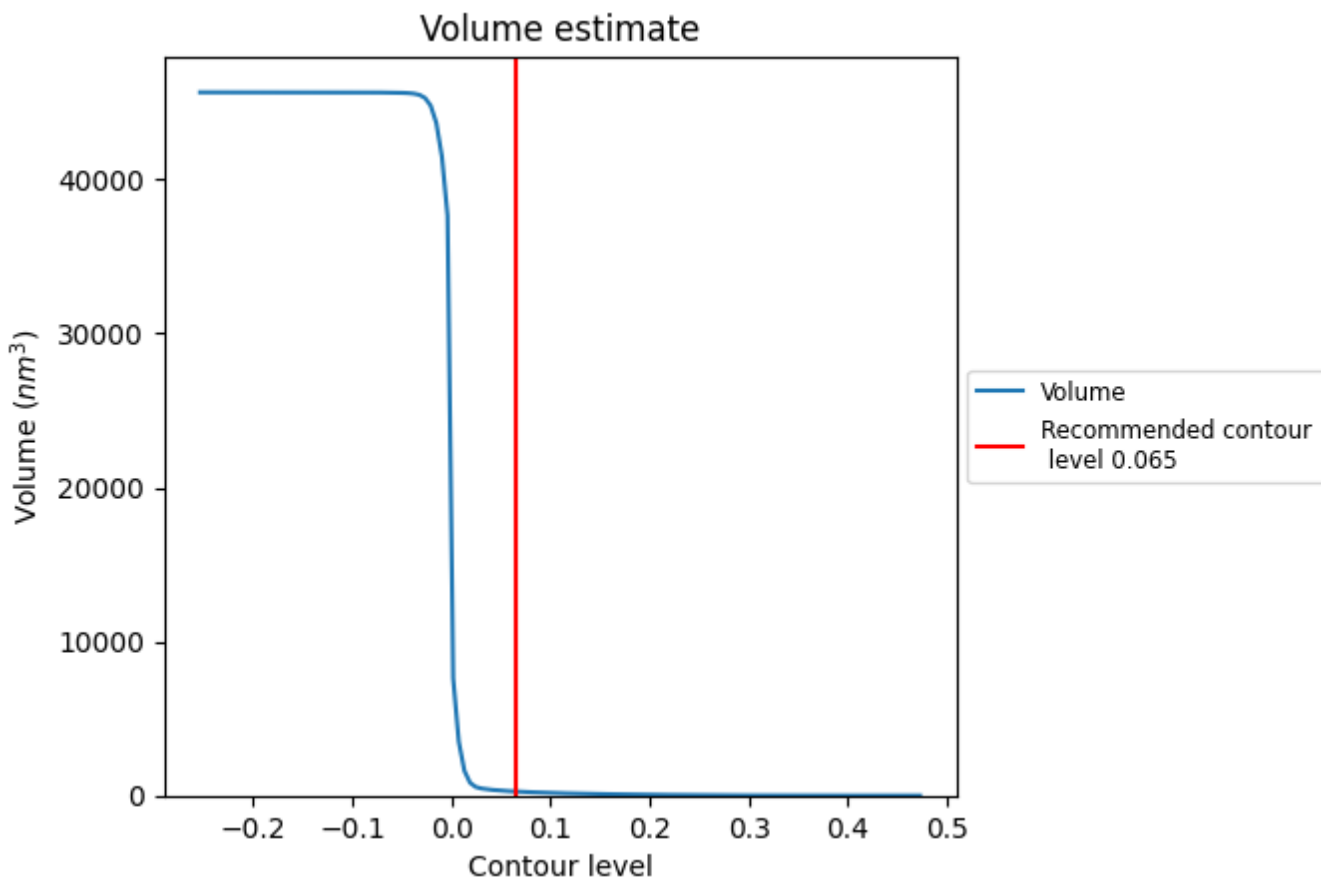
This section contains the results of statistical analysis of the map.

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.

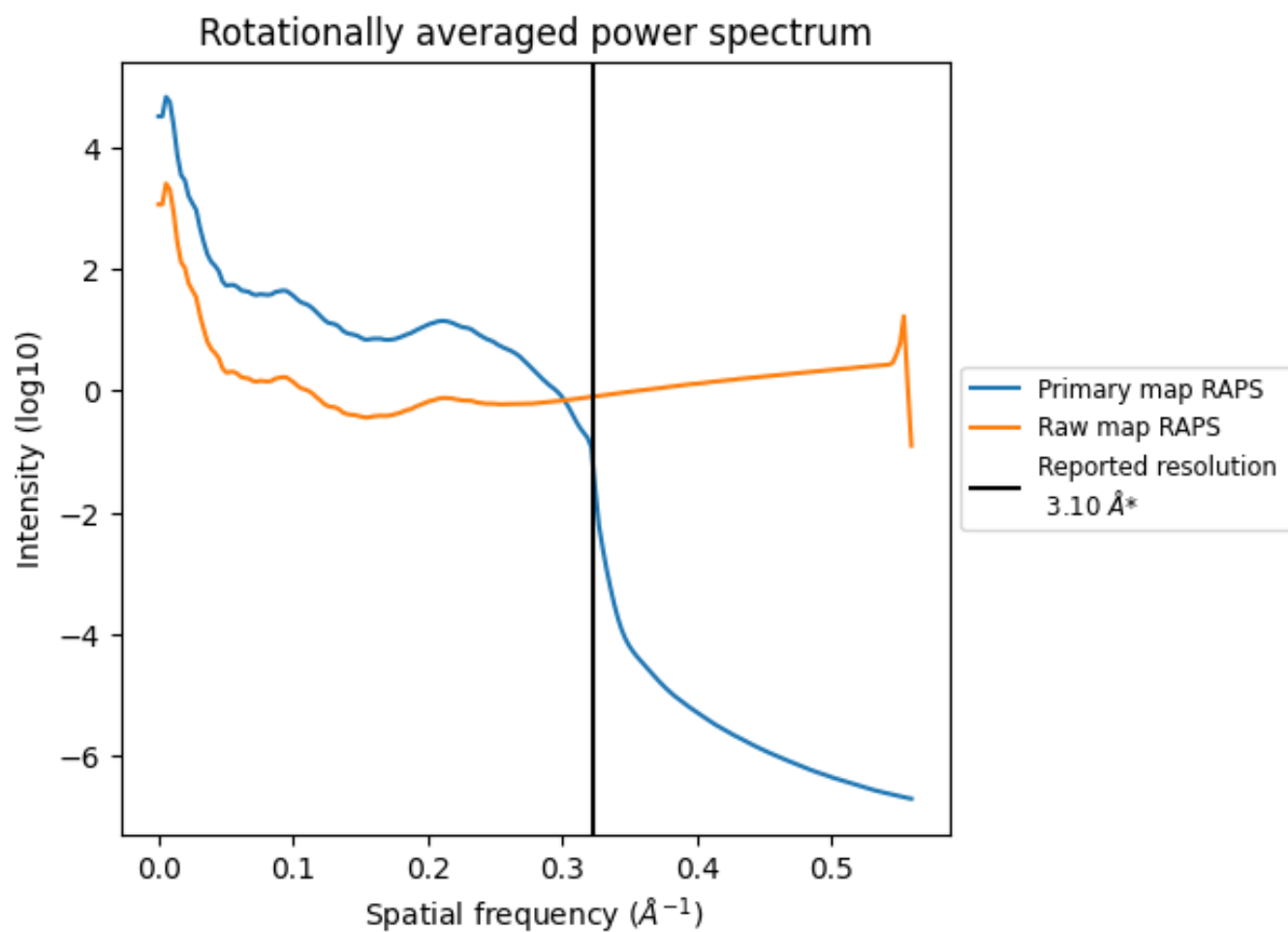
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm³; this corresponds to an approximate mass of 237 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](#)

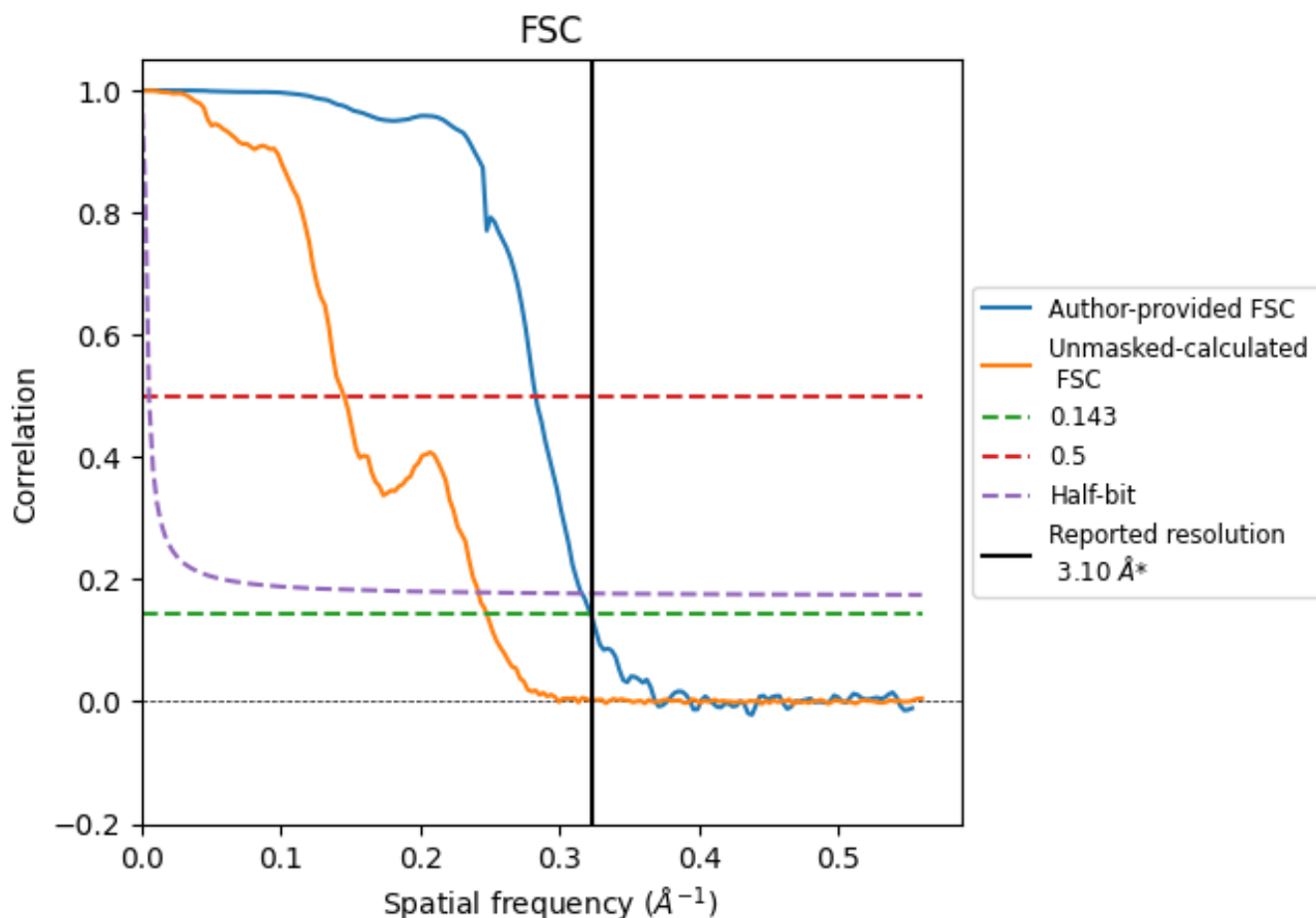


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323\AA^{-1}

8.2 Resolution estimates [i](#)

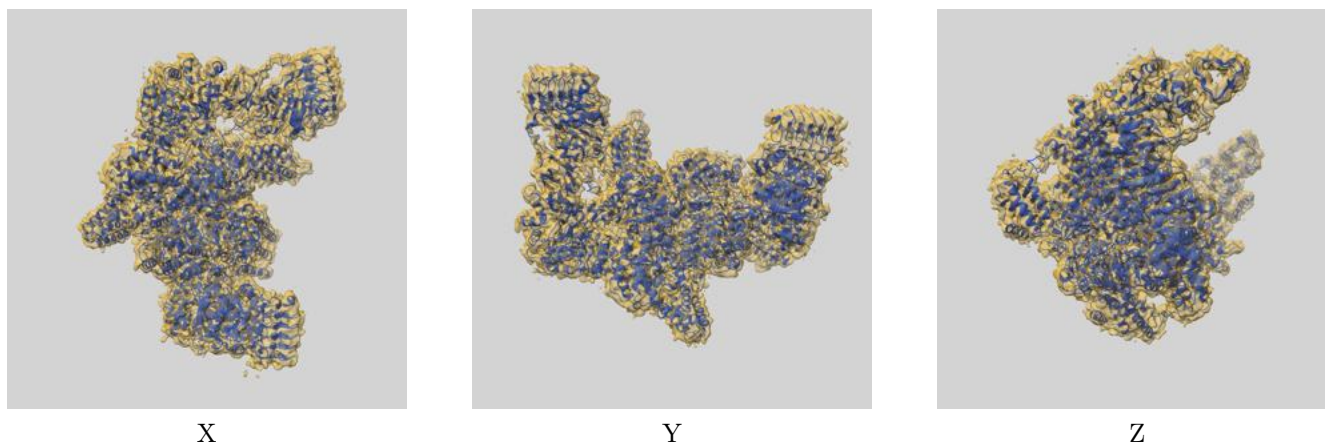
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.54	3.17
Unmasked-calculated*	4.04	6.88	4.14

*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 4.04 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72521 and PDB model 9Y5S. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



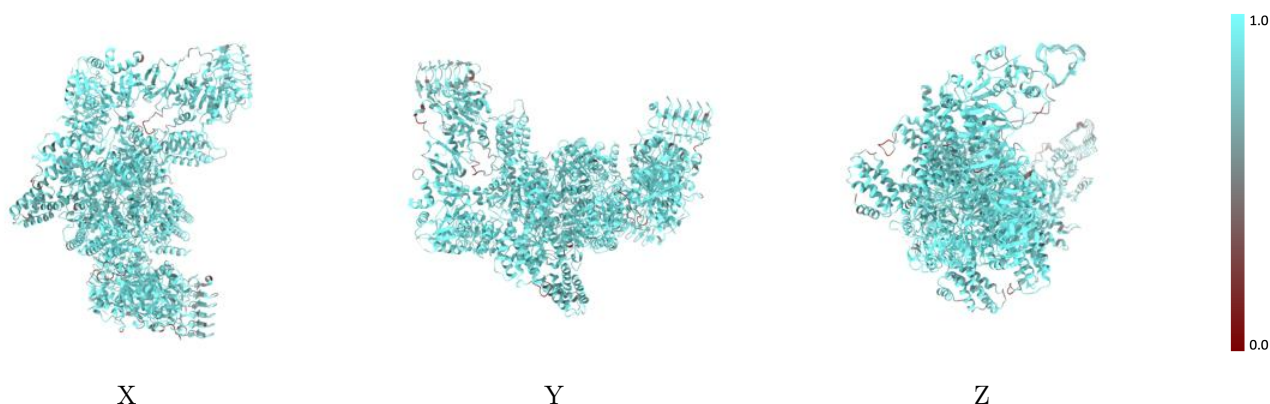
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



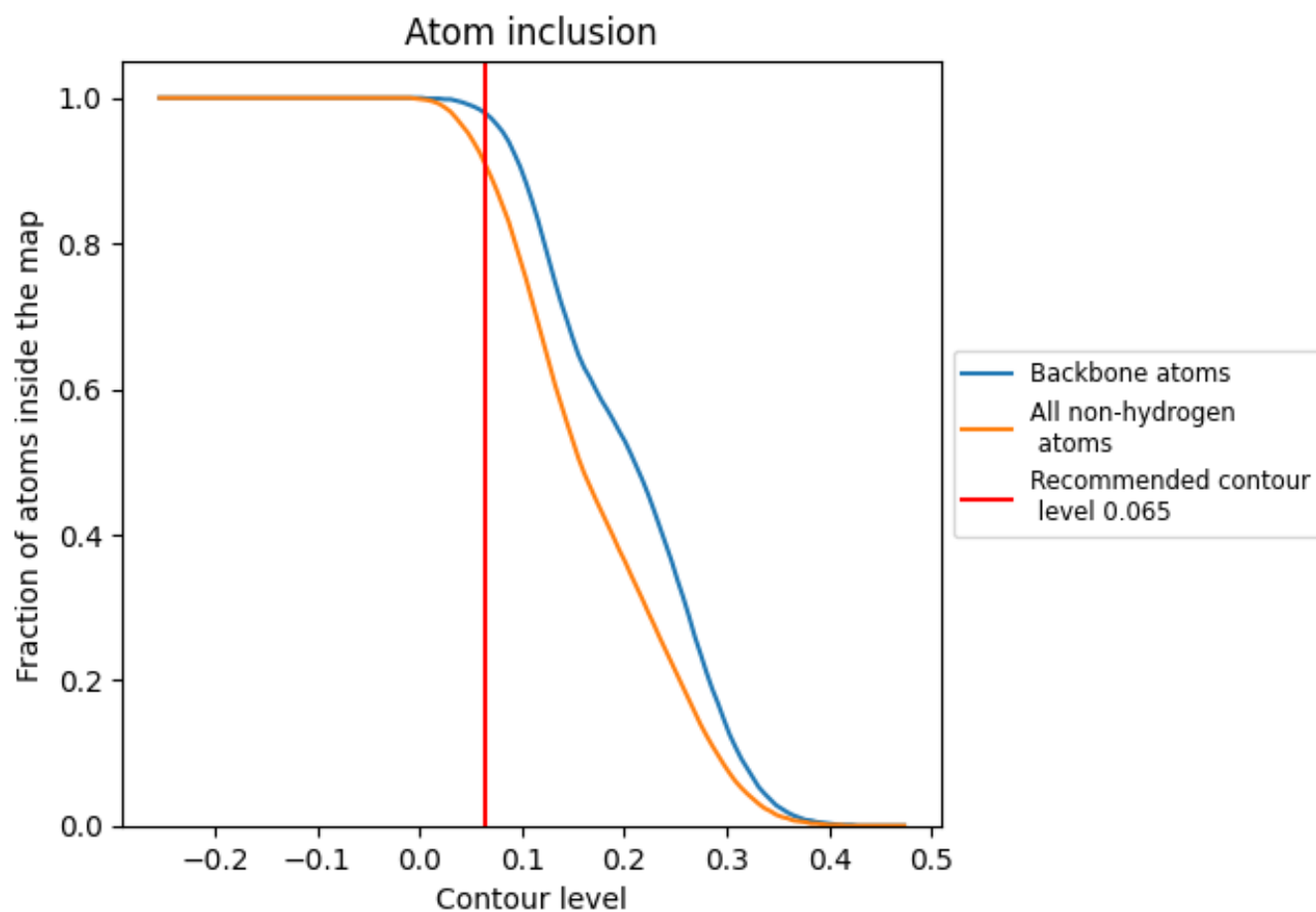
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5010
A	 0.9400	 0.5310
B	 0.9360	 0.5290
C	 0.9310	 0.5250
D	 0.9340	 0.5270
E	 0.9360	 0.5290
F	 0.9340	 0.5280
G	 0.9260	 0.4960
H	 0.9230	 0.4970
I	 0.8330	 0.4320
J	 0.7940	 0.4240

