



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 09:05 AM EDT

PDB ID : 7KMF
EMDB ID : EMD-22924
Title : Sugar phosphate activation of the stress sensor eIF2B
Authors : Nocek, B.; Hao, Q.; Wong, Y.; Stoll, V.; Sidrauski, C.
Deposited on : 2020-11-02
Resolution : 2.91 Å(reported)
Based on initial model : 6CAJ

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

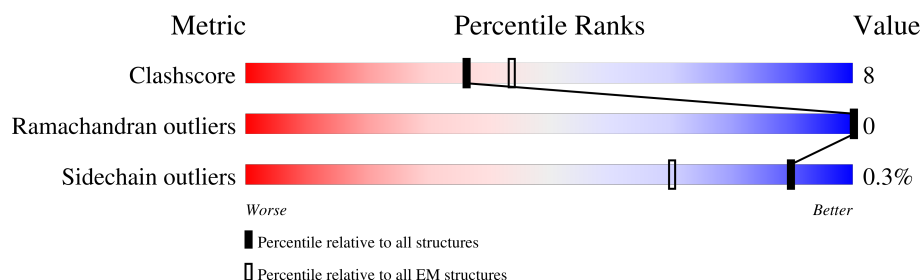
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	367	
1	D	367	
2	E	523	
2	F	523	
3	G	377	
3	H	377	
4	B	721	
4	I	721	

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Mol	Chain	Length	Quality of chain
5	J	452	<div><div><div>14%</div><div>32%</div><div></div></div><div></div><div>64%</div></div>
5	K	452	<div><div><div>14%</div><div>32%</div><div></div></div><div></div><div>64%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22875 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 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	315	Total	C	N	O	S	0	0
			2468	1561	433	459	15		
1	D	314	Total	C	N	O	S	0	0
			2440	1547	434	444	15		

There are 32 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ASN	-	expression tag	UNP P49770
D	-4	LEU	-	expression tag	UNP P49770
D	-3	TYR	-	expression tag	UNP P49770
D	-2	PHE	-	expression tag	UNP P49770
D	-1	GLN	-	expression tag	UNP P49770
D	0	SER	-	expression tag	UNP P49770

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	325	Total	C	N	O	S	1	0
			2414	1539	434	428	13		
2	E	330	Total	C	N	O	S	0	0
			2466	1572	438	442	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	280	Total	C	N	O	S	1	0
			2151	1386	364	391	10		
3	G	287	Total	C	N	O	S	1	0
			2201	1416	371	404	10		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	306	GLY	-	expression tag	UNP Q14232
H	307	GLY	-	expression tag	UNP Q14232
H	308	GLU	-	expression tag	UNP Q14232
H	309	ASN	-	expression tag	UNP Q14232
H	310	LEU	-	expression tag	UNP Q14232
H	311	TYR	-	expression tag	UNP Q14232
H	312	PHE	-	expression tag	UNP Q14232
H	313	GLN	-	expression tag	UNP Q14232
H	314	ALA	-	expression tag	UNP Q14232
H	315	GLU	-	expression tag	UNP Q14232
H	316	ASP	-	expression tag	UNP Q14232
H	317	LYS	-	expression tag	UNP Q14232
H	318	GLY	-	expression tag	UNP Q14232
H	319	GLY	-	expression tag	UNP Q14232
H	320	GLY	-	expression tag	UNP Q14232
H	321	SER	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
H	322	GLY	-	expression tag	UNP Q14232
H	323	GLY	-	expression tag	UNP Q14232
H	324	GLY	-	expression tag	UNP Q14232
H	325	GLY	-	expression tag	UNP Q14232
H	326	SER	-	expression tag	UNP Q14232
H	327	GLY	-	expression tag	UNP Q14232
H	328	GLY	-	expression tag	UNP Q14232
H	329	GLY	-	expression tag	UNP Q14232
H	330	GLY	-	expression tag	UNP Q14232
H	331	SER	-	expression tag	UNP Q14232
H	332	ALA	-	expression tag	UNP Q14232
H	333	SER	-	expression tag	UNP Q14232
H	334	GLN	-	expression tag	UNP Q14232
H	335	GLY	-	expression tag	UNP Q14232
H	336	GLY	-	expression tag	UNP Q14232
H	337	LEU	-	expression tag	UNP Q14232
H	338	ASN	-	expression tag	UNP Q14232
H	339	ASP	-	expression tag	UNP Q14232
H	340	ILE	-	expression tag	UNP Q14232
H	341	PHE	-	expression tag	UNP Q14232
H	342	GLU	-	expression tag	UNP Q14232
H	343	ALA	-	expression tag	UNP Q14232
H	344	GLN	-	expression tag	UNP Q14232
H	345	LYS	-	expression tag	UNP Q14232
H	346	ILE	-	expression tag	UNP Q14232
H	347	GLU	-	expression tag	UNP Q14232
H	348	TRP	-	expression tag	UNP Q14232
H	349	HIS	-	expression tag	UNP Q14232
H	350	GLU	-	expression tag	UNP Q14232
H	351	GLY	-	expression tag	UNP Q14232
H	352	GLY	-	expression tag	UNP Q14232
H	353	GLY	-	expression tag	UNP Q14232
H	354	GLY	-	expression tag	UNP Q14232
H	355	SER	-	expression tag	UNP Q14232
H	356	GLY	-	expression tag	UNP Q14232
H	357	GLY	-	expression tag	UNP Q14232
H	358	GLY	-	expression tag	UNP Q14232
H	359	GLY	-	expression tag	UNP Q14232
H	360	SER	-	expression tag	UNP Q14232
H	361	GLY	-	expression tag	UNP Q14232
H	362	GLY	-	expression tag	UNP Q14232
H	363	GLY	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
H	364	GLY	-	expression tag	UNP Q14232
H	365	SER	-	expression tag	UNP Q14232
H	366	GLY	-	expression tag	UNP Q14232
H	367	ARG	-	expression tag	UNP Q14232
H	368	ASP	-	expression tag	UNP Q14232
H	369	GLN	-	expression tag	UNP Q14232
H	370	ASP	-	expression tag	UNP Q14232
H	371	TYR	-	expression tag	UNP Q14232
H	372	LYS	-	expression tag	UNP Q14232
H	373	ASP	-	expression tag	UNP Q14232
H	374	ASP	-	expression tag	UNP Q14232
H	375	ASP	-	expression tag	UNP Q14232
H	376	ASP	-	expression tag	UNP Q14232
H	377	LYS	-	expression tag	UNP Q14232
G	306	GLY	-	expression tag	UNP Q14232
G	307	GLY	-	expression tag	UNP Q14232
G	308	GLU	-	expression tag	UNP Q14232
G	309	ASN	-	expression tag	UNP Q14232
G	310	LEU	-	expression tag	UNP Q14232
G	311	TYR	-	expression tag	UNP Q14232
G	312	PHE	-	expression tag	UNP Q14232
G	313	GLN	-	expression tag	UNP Q14232
G	314	ALA	-	expression tag	UNP Q14232
G	315	GLU	-	expression tag	UNP Q14232
G	316	ASP	-	expression tag	UNP Q14232
G	317	LYS	-	expression tag	UNP Q14232
G	318	GLY	-	expression tag	UNP Q14232
G	319	GLY	-	expression tag	UNP Q14232
G	320	GLY	-	expression tag	UNP Q14232
G	321	SER	-	expression tag	UNP Q14232
G	322	GLY	-	expression tag	UNP Q14232
G	323	GLY	-	expression tag	UNP Q14232
G	324	GLY	-	expression tag	UNP Q14232
G	325	GLY	-	expression tag	UNP Q14232
G	326	SER	-	expression tag	UNP Q14232
G	327	GLY	-	expression tag	UNP Q14232
G	328	GLY	-	expression tag	UNP Q14232
G	329	GLY	-	expression tag	UNP Q14232
G	330	GLY	-	expression tag	UNP Q14232
G	331	SER	-	expression tag	UNP Q14232
G	332	ALA	-	expression tag	UNP Q14232
G	333	SER	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
G	334	GLN	-	expression tag	UNP Q14232
G	335	GLY	-	expression tag	UNP Q14232
G	336	GLY	-	expression tag	UNP Q14232
G	337	LEU	-	expression tag	UNP Q14232
G	338	ASN	-	expression tag	UNP Q14232
G	339	ASP	-	expression tag	UNP Q14232
G	340	ILE	-	expression tag	UNP Q14232
G	341	PHE	-	expression tag	UNP Q14232
G	342	GLU	-	expression tag	UNP Q14232
G	343	ALA	-	expression tag	UNP Q14232
G	344	GLN	-	expression tag	UNP Q14232
G	345	LYS	-	expression tag	UNP Q14232
G	346	ILE	-	expression tag	UNP Q14232
G	347	GLU	-	expression tag	UNP Q14232
G	348	TRP	-	expression tag	UNP Q14232
G	349	HIS	-	expression tag	UNP Q14232
G	350	GLU	-	expression tag	UNP Q14232
G	351	GLY	-	expression tag	UNP Q14232
G	352	GLY	-	expression tag	UNP Q14232
G	353	GLY	-	expression tag	UNP Q14232
G	354	GLY	-	expression tag	UNP Q14232
G	355	SER	-	expression tag	UNP Q14232
G	356	GLY	-	expression tag	UNP Q14232
G	357	GLY	-	expression tag	UNP Q14232
G	358	GLY	-	expression tag	UNP Q14232
G	359	GLY	-	expression tag	UNP Q14232
G	360	SER	-	expression tag	UNP Q14232
G	361	GLY	-	expression tag	UNP Q14232
G	362	GLY	-	expression tag	UNP Q14232
G	363	GLY	-	expression tag	UNP Q14232
G	364	GLY	-	expression tag	UNP Q14232
G	365	SER	-	expression tag	UNP Q14232
G	366	GLY	-	expression tag	UNP Q14232
G	367	ARG	-	expression tag	UNP Q14232
G	368	ASP	-	expression tag	UNP Q14232
G	369	GLN	-	expression tag	UNP Q14232
G	370	ASP	-	expression tag	UNP Q14232
G	371	TYR	-	expression tag	UNP Q14232
G	372	LYS	-	expression tag	UNP Q14232
G	373	ASP	-	expression tag	UNP Q14232
G	374	ASP	-	expression tag	UNP Q14232
G	375	ASP	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
G	376	ASP	-	expression tag	UNP Q14232
G	377	LYS	-	expression tag	UNP Q14232

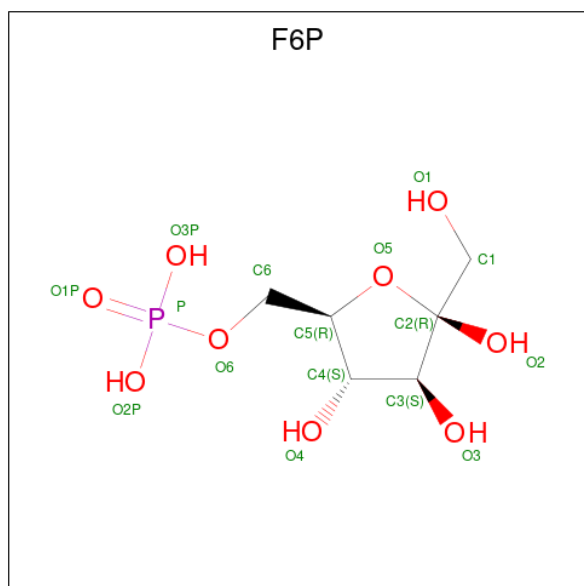
- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	413	Total	C	N	O	S	0	0
			3165	2005	558	587	15		
4	I	416	Total	C	N	O	S	0	0
			3192	2020	562	595	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	162	Total	C	N	O	S	0	0
			1159	755	203	196	5		
5	K	163	Total	C	N	O	S	0	0
			1169	762	200	202	5		

- Molecule 6 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	H	1	Total	C	O	P	0
			16	6	9	1	

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Mol	Chain	Residues	Atoms				AltConf
6	G	1	Total	C	O	P	0
			16	6	9	1	

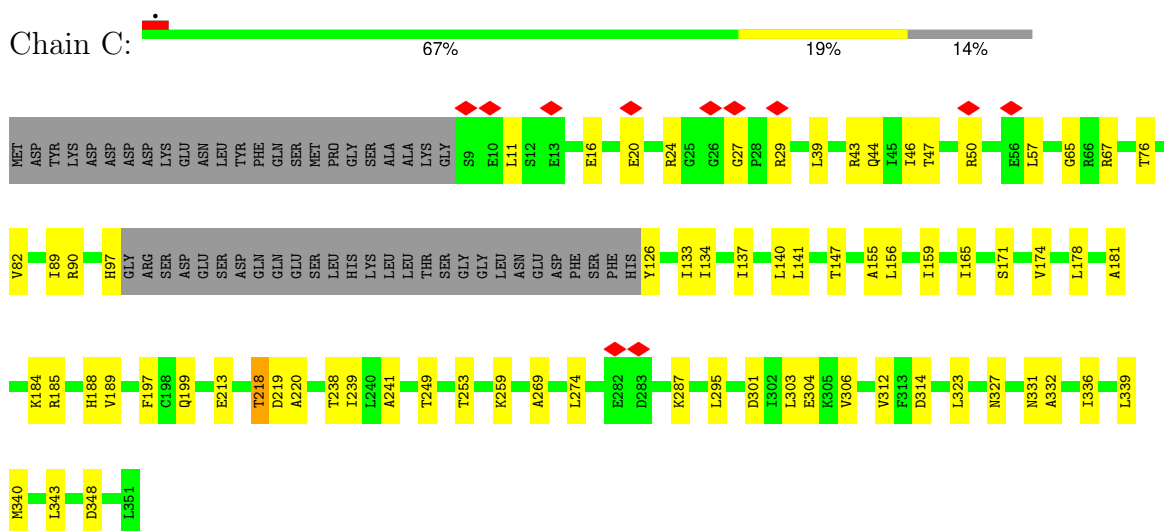
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	C	5	Total	O	0
			5	5	
7	D	3	Total	O	0
			3	3	
7	F	1	Total	O	0
			1	1	
7	E	2	Total	O	0
			2	2	
7	H	3	Total	O	0
			3	3	
7	G	3	Total	O	0
			3	3	
7	B	1	Total	O	0
			1	1	

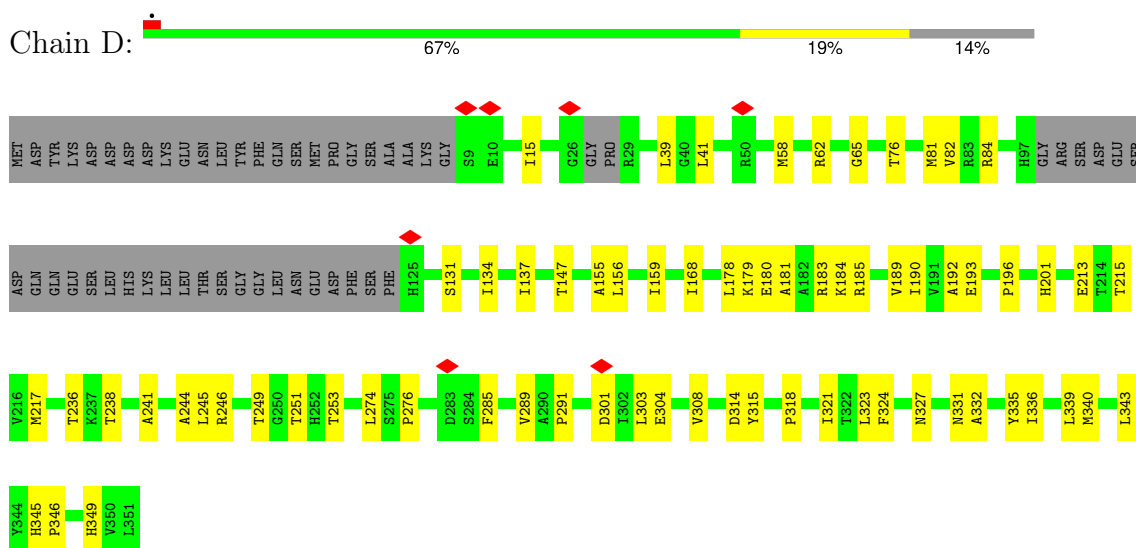
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

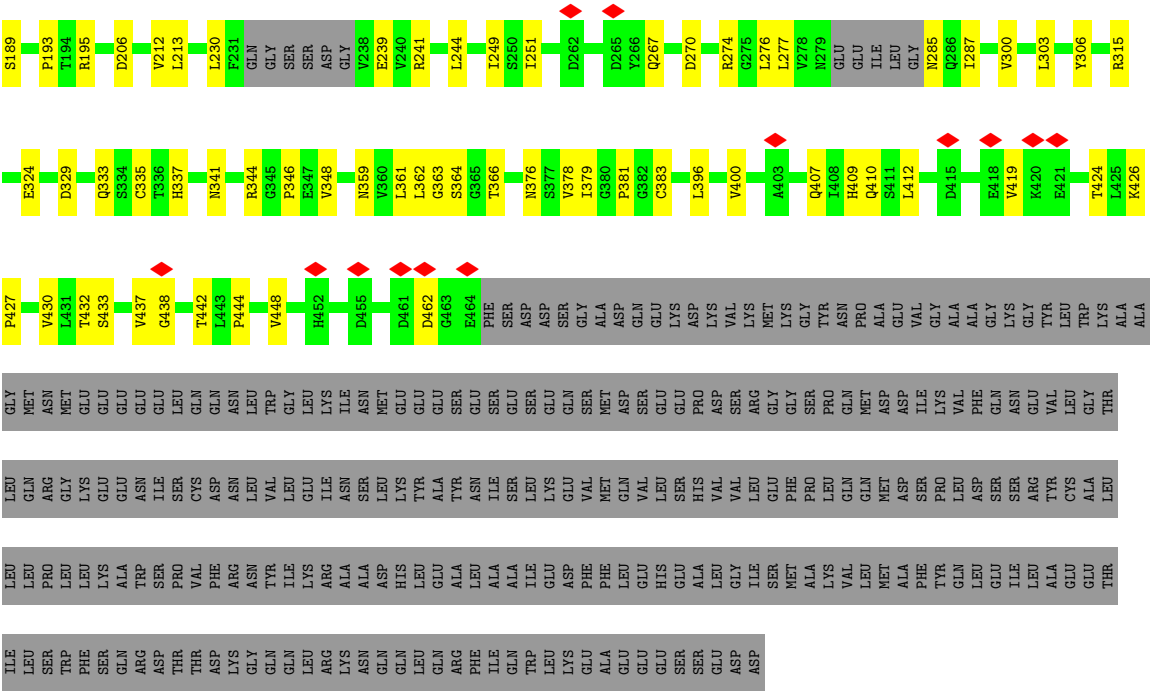
- Molecule 1: Translation initiation factor eIF-2B subunit beta



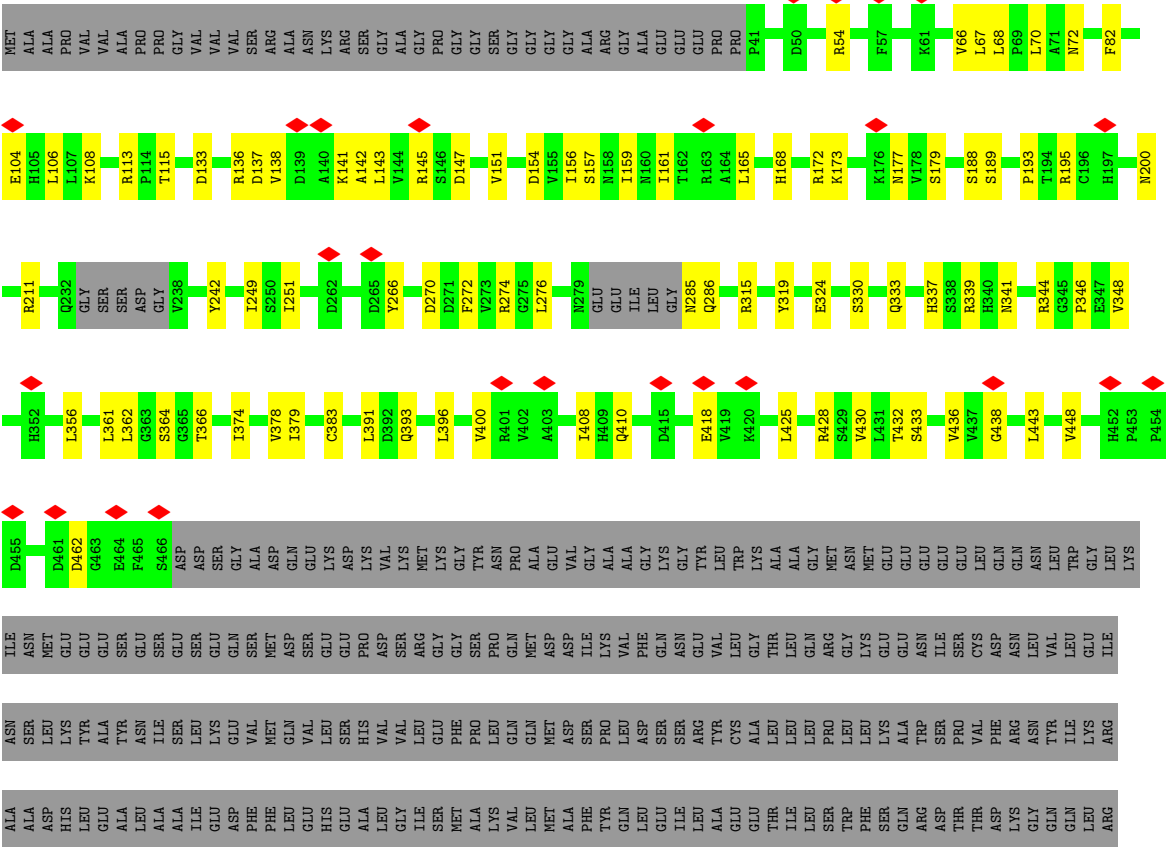
- Molecule 1: Translation initiation factor eIF-2B subunit beta



- Molecule 2: Translation initiation factor eIF-2B subunit delta



• Molecule 4: Translation initiation factor eIF-2B subunit epsilon



VAL	SER	VAL	LYS	LEU	ASP	ASN	ASN	VAL	GLY	VAL	ASP	SER	LEU	ILE	GLY	PRO	GLU	THR	GLN	THR	GLY	GLU	LYS	SER	SER	ILE	LYS	ARG	SER	SER	CYS	ILE	ILE	LYS	ASP	ARG	VAL	GLY	ILE	GLY	LYS	SER	SER	GLN	ASN	ASN	VAL	THR	GLU	GLY	SER	ASN	ILE	GLN	GLY
SER	VAL	ILE	CYS	ASN	ASN	ALA	VAL	VAL	ILE	GLU	GLY	GLY	LYS	ALA	ASP	ASP	ILE	ILE	GLN	GLY	ILE	ILE	GLY	SER	SER	GLN	GLY	ILE	ARG	ARG	ILE	GLU	VAL	ASN	ASN	GLU	VAL	ILE	ILE	LYS	ALA	GLU	GLY	LYS	LYS	ARG	VAL	VAL	LEU	MET	LEU	GLU	ILE		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	73704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.33	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.432	Depositor
Minimum map value	-1.651	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.4534	Depositor
Map size (\AA)	353.59998, 353.59998, 353.59998	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6P

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	C	0.46	0/2514	0.59	2/3401 (0.1%)
1	D	0.46	0/2485	0.56	0/3362
2	E	0.47	0/2507	0.67	7/3418 (0.2%)
2	F	0.46	0/2458	0.63	2/3352 (0.1%)
3	G	0.47	0/2235	0.62	1/3020 (0.0%)
3	H	0.46	0/2183	0.59	1/2948 (0.0%)
4	B	0.40	0/3230	0.64	1/4404 (0.0%)
4	I	0.41	0/3259	0.62	3/4444 (0.1%)
5	J	0.32	0/1175	0.52	0/1591
5	K	0.30	0/1184	0.52	0/1605
All	All	0.43	0/23230	0.61	17/31545 (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
3	G	0	1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ASP	CB-CG-OD1	7.73	125.25	118.30
2	E	346	LEU	CA-CB-CG	7.39	132.31	115.30
2	E	376	LEU	CA-CB-CG	7.39	132.29	115.30
2	E	504	LEU	CA-CB-CG	6.67	130.65	115.30
1	C	218	THR	C-N-CA	6.57	138.13	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	128	HIS	Peptide

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	C	2468	0	2486	42	0
1	D	2440	0	2457	45	0
2	E	2466	0	2451	44	0
2	F	2414	0	2371	47	0
3	G	2201	0	2254	28	0
3	H	2151	0	2223	27	0
4	B	3165	0	3089	56	0
4	I	3192	0	3100	50	0
5	J	1159	0	1030	13	0
5	K	1169	0	1035	13	0
6	G	16	0	11	1	0
6	H	16	0	11	1	0
7	B	1	0	0	0	0
7	C	5	0	0	0	0
7	D	3	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	3	0	0	0	0
7	H	3	0	0	0	0
All	All	22875	0	22518	341	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 8.

The worst 5 of 341 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)
2:F:435:LEU:HD23	2:F:501:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD12	1:D:137:ILE:HG23	1.77	0.66
1:D:193:GLU:OE1	1:D:201:HIS:NE2	2.29	0.66
2:F:332:VAL:HG12	2:F:357:ARG:HB3	1.78	0.66
1:D:192:ALA:HA	1:D:217:MET:HB2	1.79	0.65

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	C	311/367 (85%)	294 (94%)	17 (6%)	0	100	100
1	D	308/367 (84%)	296 (96%)	12 (4%)	0	100	100
2	E	320/523 (61%)	301 (94%)	19 (6%)	0	100	100
2	F	316/523 (60%)	301 (95%)	15 (5%)	0	100	100
3	G	282/377 (75%)	266 (94%)	16 (6%)	0	100	100
3	H	273/377 (72%)	261 (96%)	12 (4%)	0	100	100
4	B	407/721 (56%)	356 (88%)	51 (12%)	0	100	100
4	I	410/721 (57%)	357 (87%)	53 (13%)	0	100	100
5	J	144/452 (32%)	136 (94%)	8 (6%)	0	100	100
5	K	145/452 (32%)	137 (94%)	8 (6%)	0	100	100
All	All	2916/4880 (60%)	2705 (93%)	211 (7%)	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	C	269/314 (86%)	269 (100%)	0	100	100
1	D	262/314 (83%)	262 (100%)	0	100	100
2	E	257/444 (58%)	257 (100%)	0	100	100
2	F	245/444 (55%)	245 (100%)	0	100	100
3	G	235/301 (78%)	232 (99%)	3 (1%)	65	86
3	H	231/301 (77%)	228 (99%)	3 (1%)	65	86
4	B	345/626 (55%)	344 (100%)	1 (0%)	91	97
4	I	349/626 (56%)	347 (99%)	2 (1%)	84	94
5	J	95/398 (24%)	95 (100%)	0	100	100
5	K	97/398 (24%)	97 (100%)	0	100	100
All	All	2385/4166 (57%)	2376 (100%)	9 (0%)	90	96

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

Mol	Chain	Res	Type
4	I	173	LYS
4	I	211	ARG
3	G	91	LYS
3	G	136[A]	ARG
3	G	136[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	331	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 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	F6P	H	401	-	15,16,16	3.44	4 (26%)	16,25,25	0.81	0
6	F6P	G	401	-	15,16,16	3.43	4 (26%)	16,25,25	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	F6P	H	401	-	-	5/9/28/28	0/1/1/1
6	F6P	G	401	-	-	5/9/28/28	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	401	F6P	O5-C2	10.18	1.59	1.43
6	G	401	F6P	O5-C2	10.18	1.59	1.43
6	H	401	F6P	C4-C5	-6.40	1.36	1.53
6	G	401	F6P	C4-C5	-6.28	1.37	1.53
6	H	401	F6P	O5-C5	4.42	1.53	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

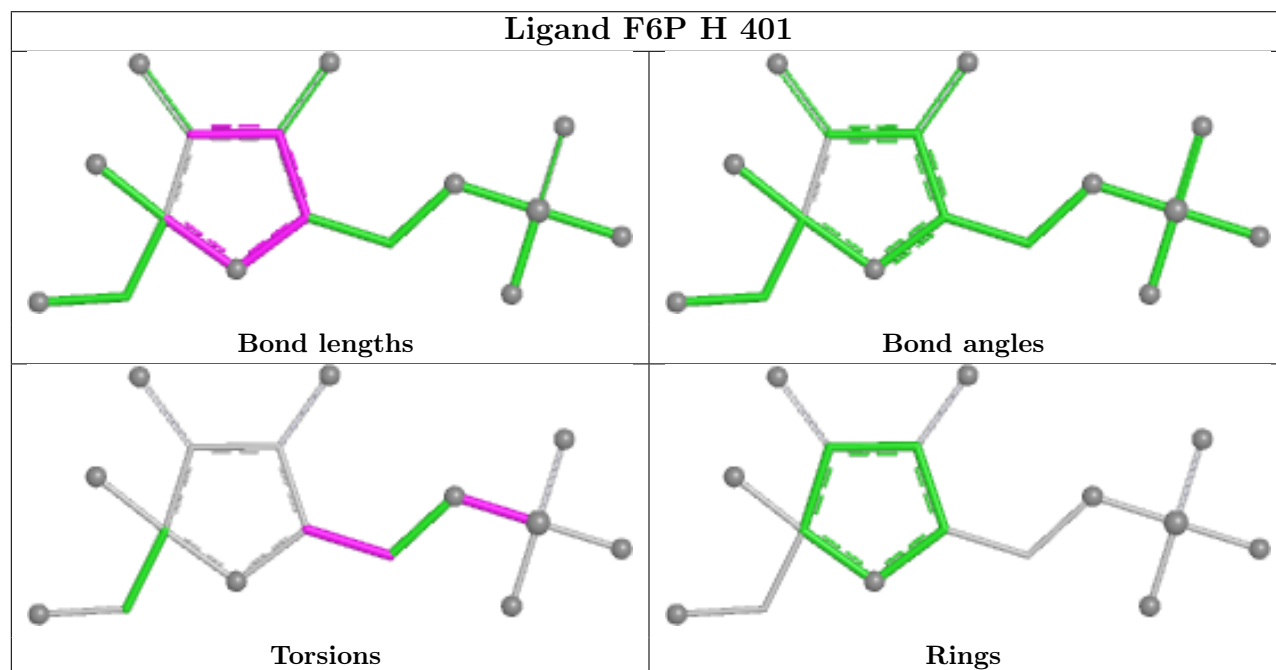
Mol	Chain	Res	Type	Atoms
6	H	401	F6P	O5-C5-C6-O6
6	H	401	F6P	C6-O6-P-O2P
6	H	401	F6P	C6-O6-P-O3P
6	G	401	F6P	O5-C5-C6-O6
6	G	401	F6P	C6-O6-P-O1P

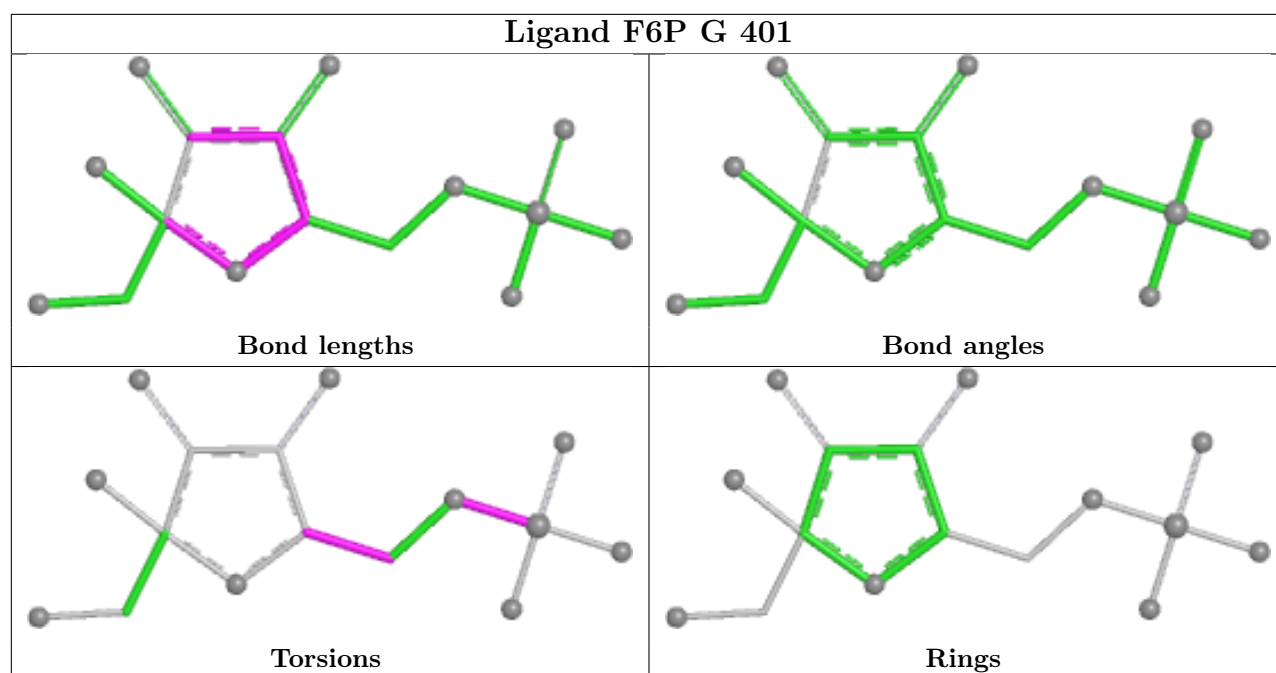
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	401	F6P	1	0
6	G	401	F6P	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.

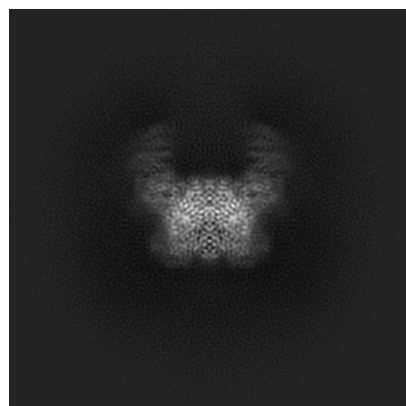
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22924. These allow visual inspection of the internal detail of the map and identification of artifacts.

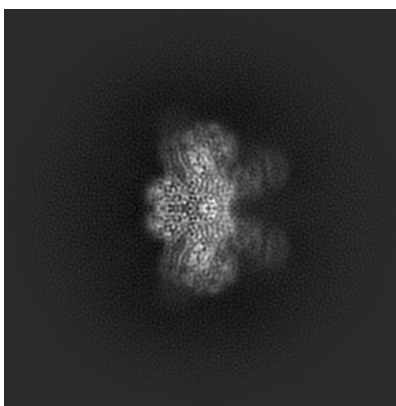
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

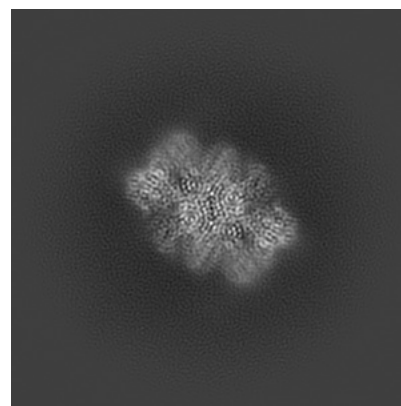
6.1.1 Primary map



X

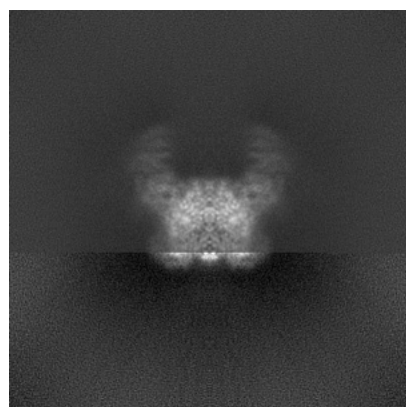


Y

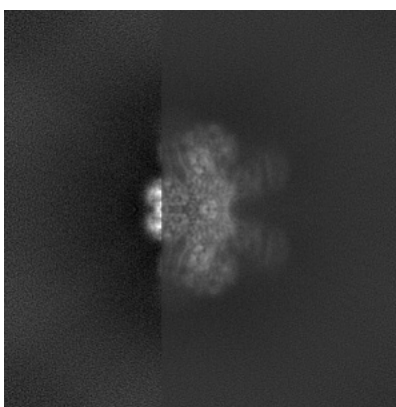


Z

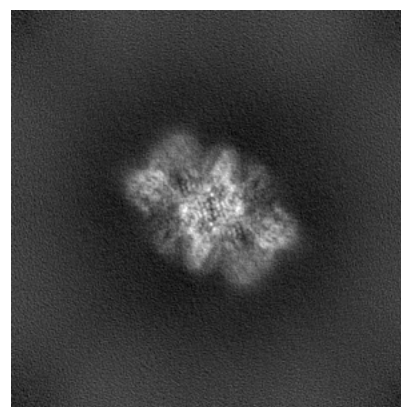
6.1.2 Raw map



X



Y

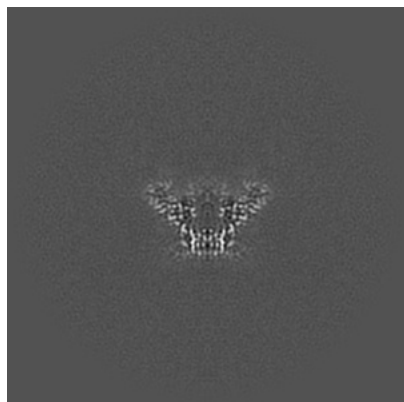


Z

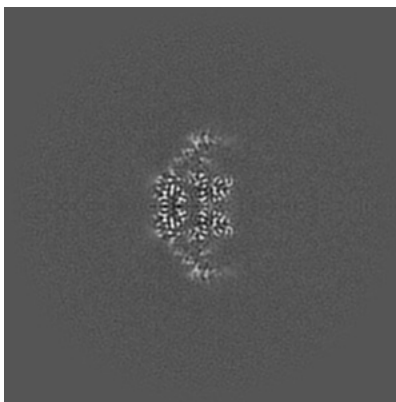
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

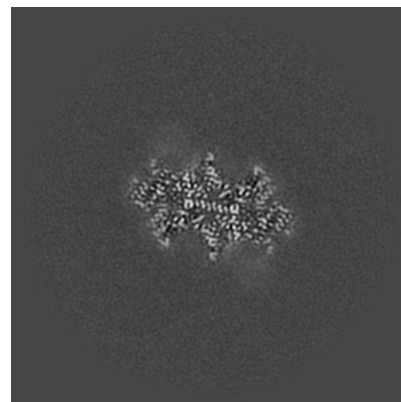
6.2.1 Primary map



X Index: 170

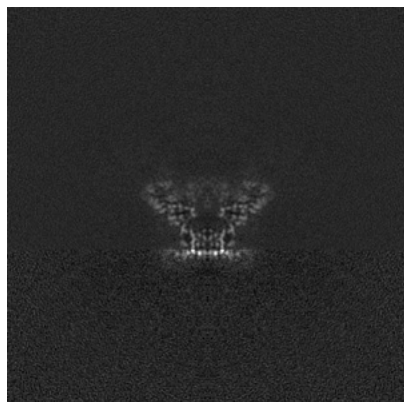


Y Index: 170

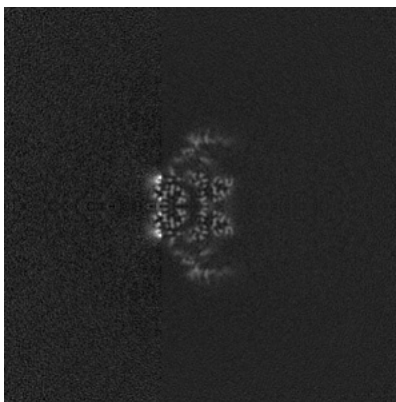


Z Index: 170

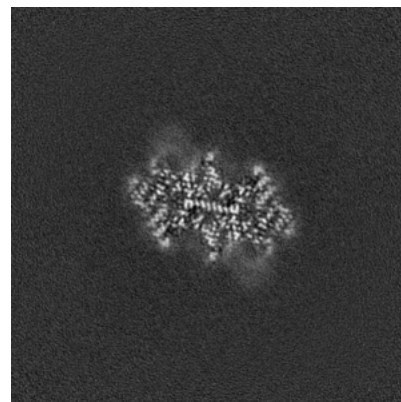
6.2.2 Raw map



X Index: 170



Y Index: 170

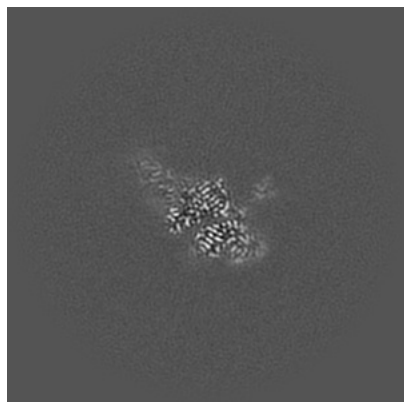


Z Index: 170

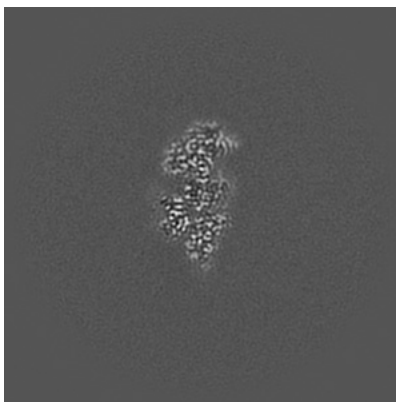
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

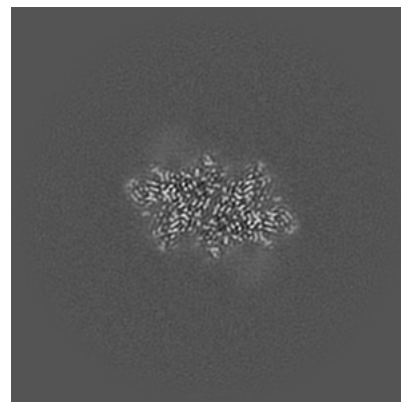
6.3.1 Primary map



X Index: 182

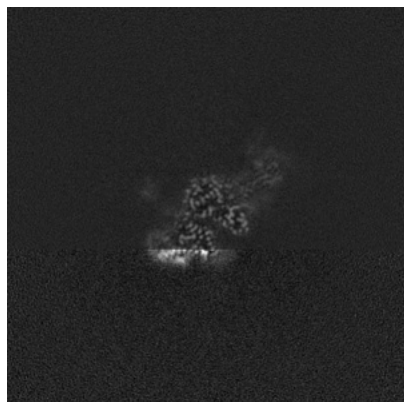


Y Index: 156

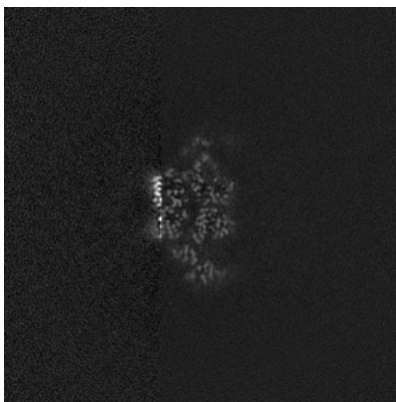


Z Index: 167

6.3.2 Raw map



X Index: 155



Y Index: 173

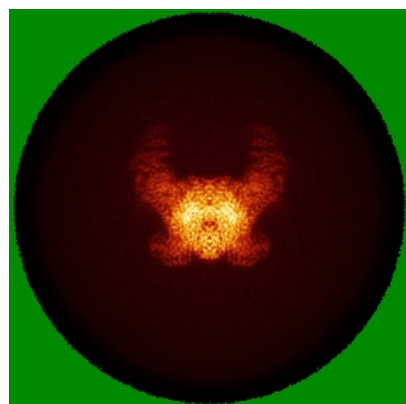


Z Index: 132

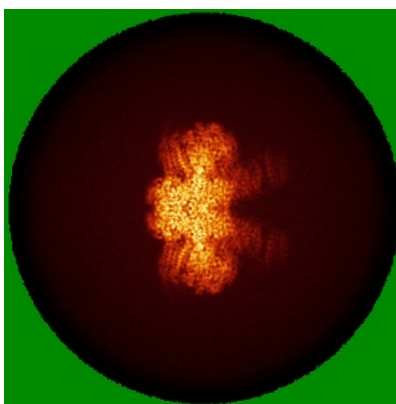
The images above show the largest variance slices of the map in three orthogonal directions.

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

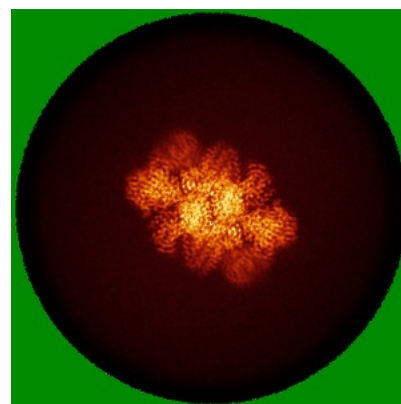
6.4.1 Primary map



X

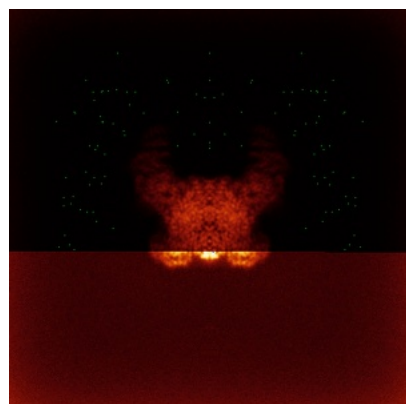


Y

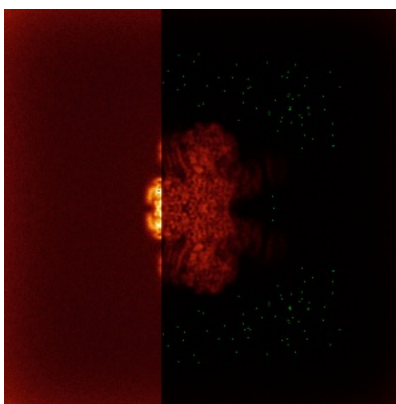


Z

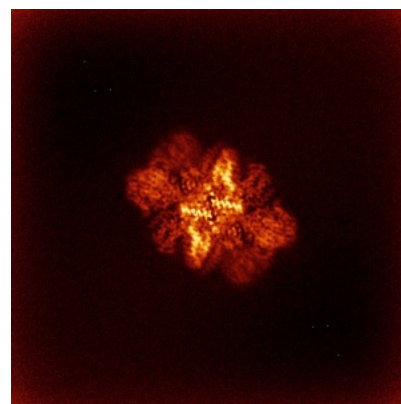
6.4.2 Raw map



X



Y

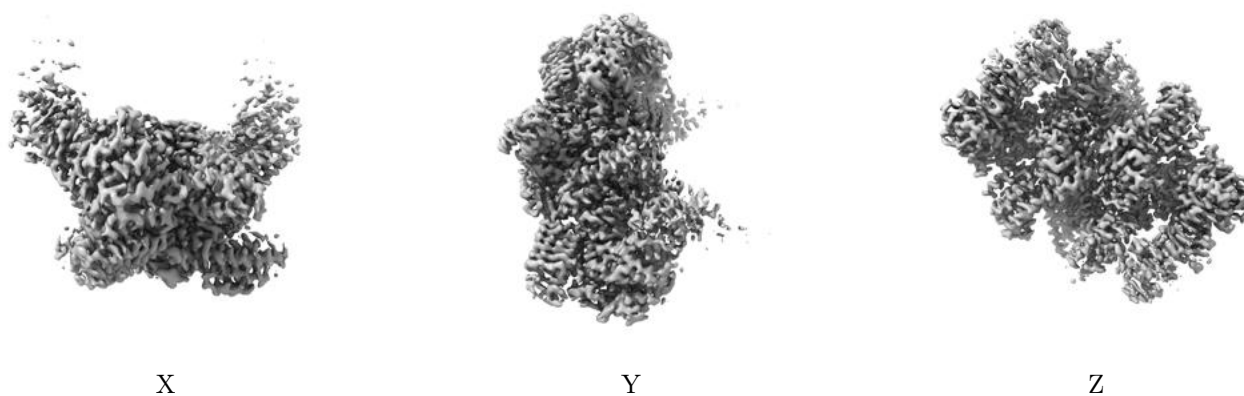


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

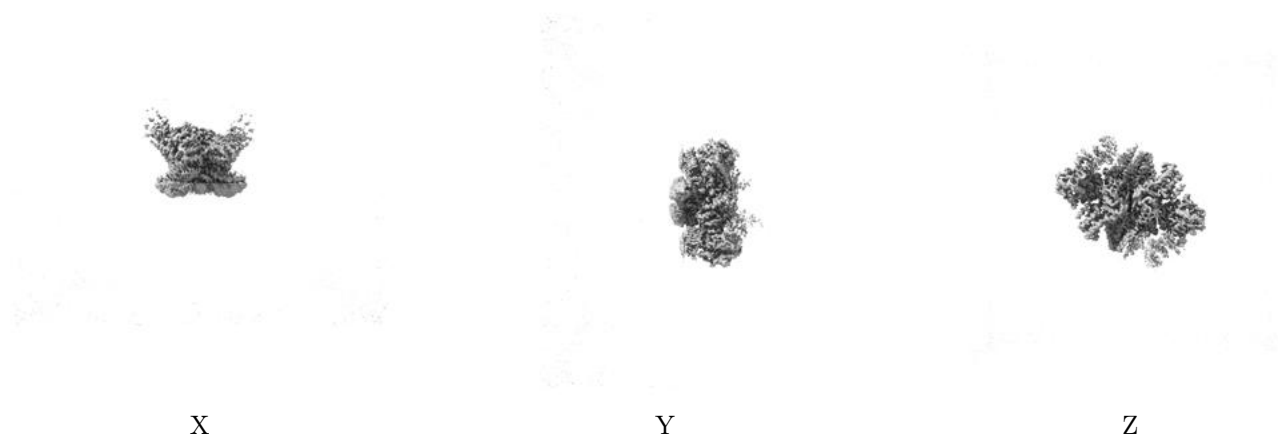
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4534. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

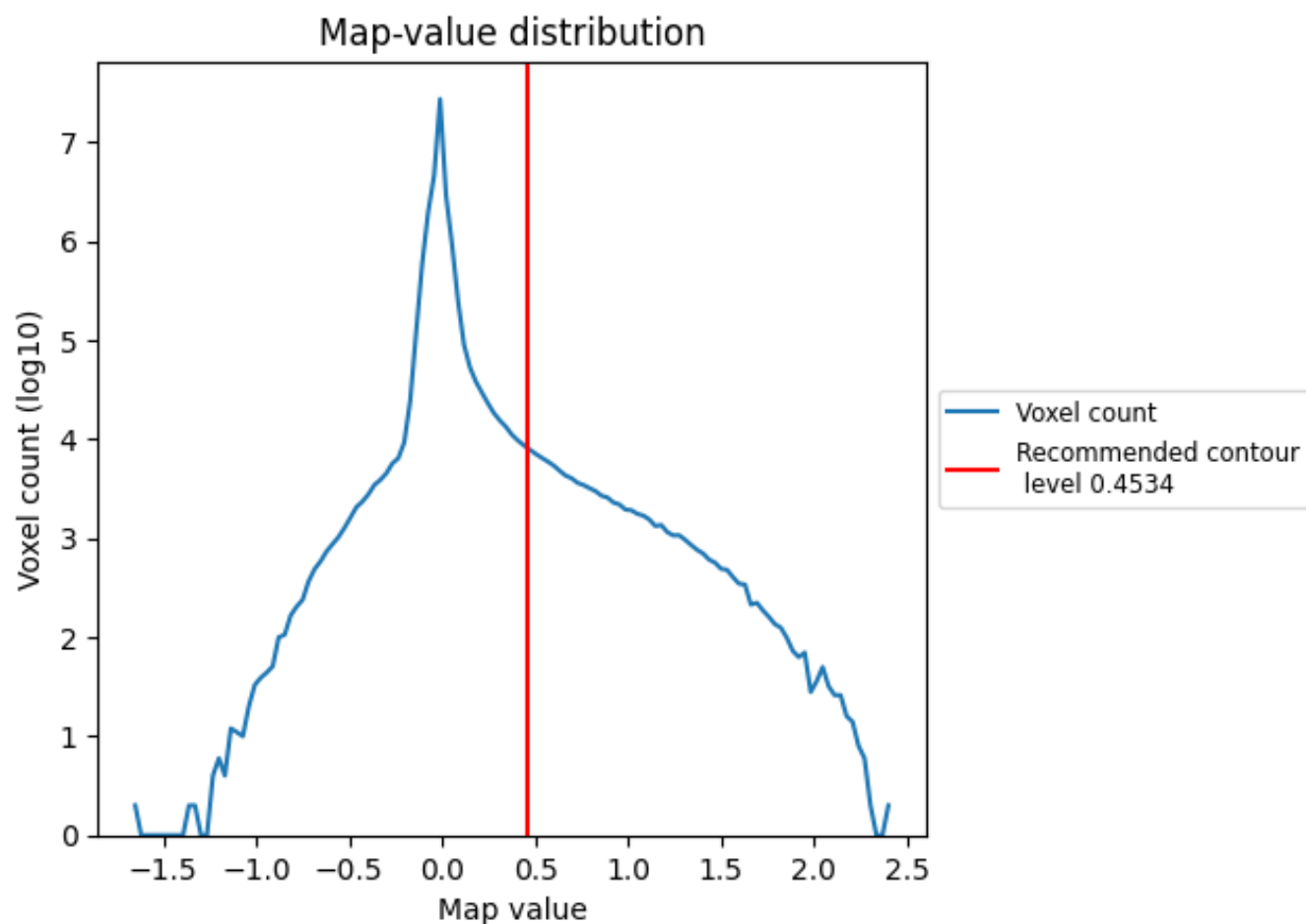
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

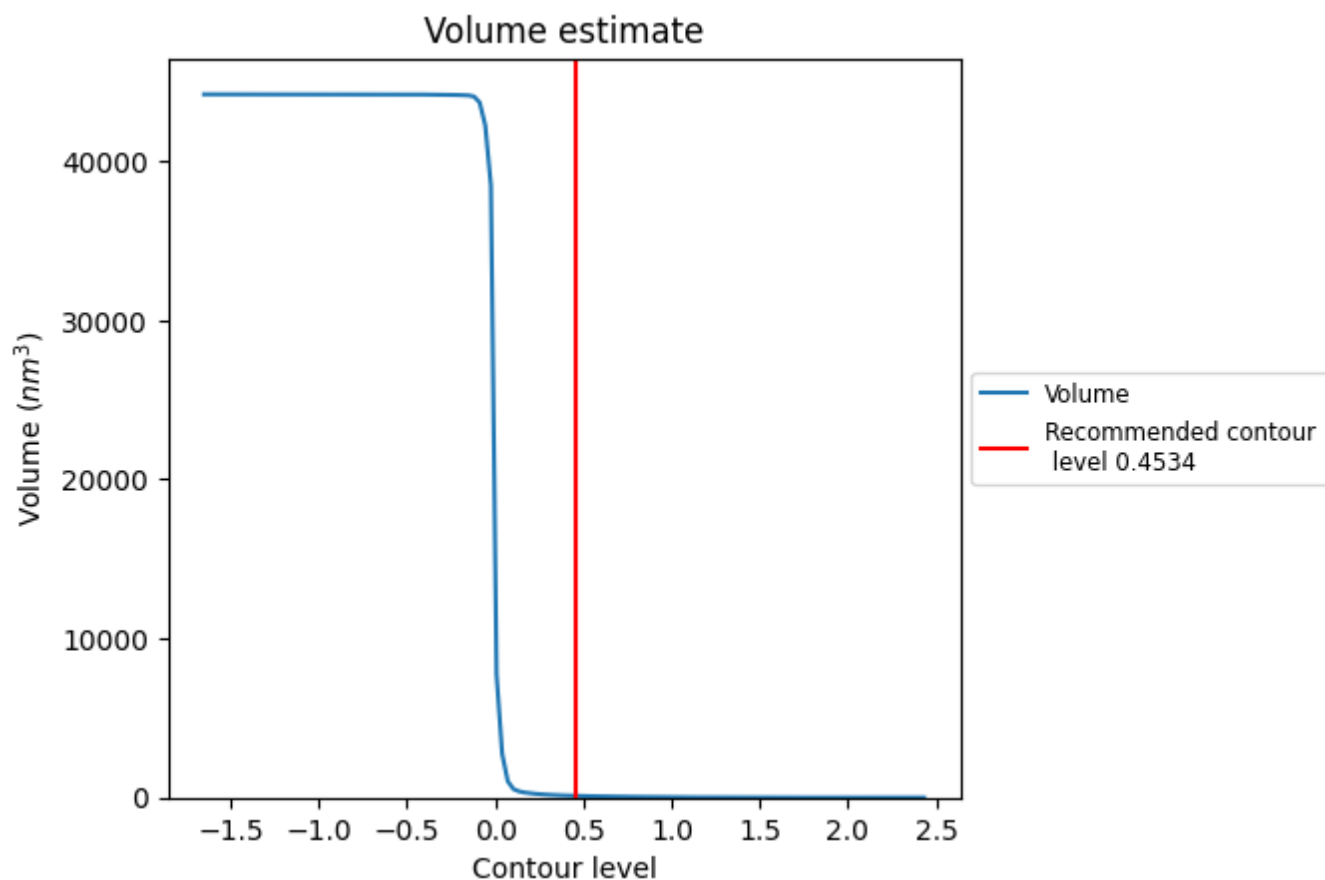
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

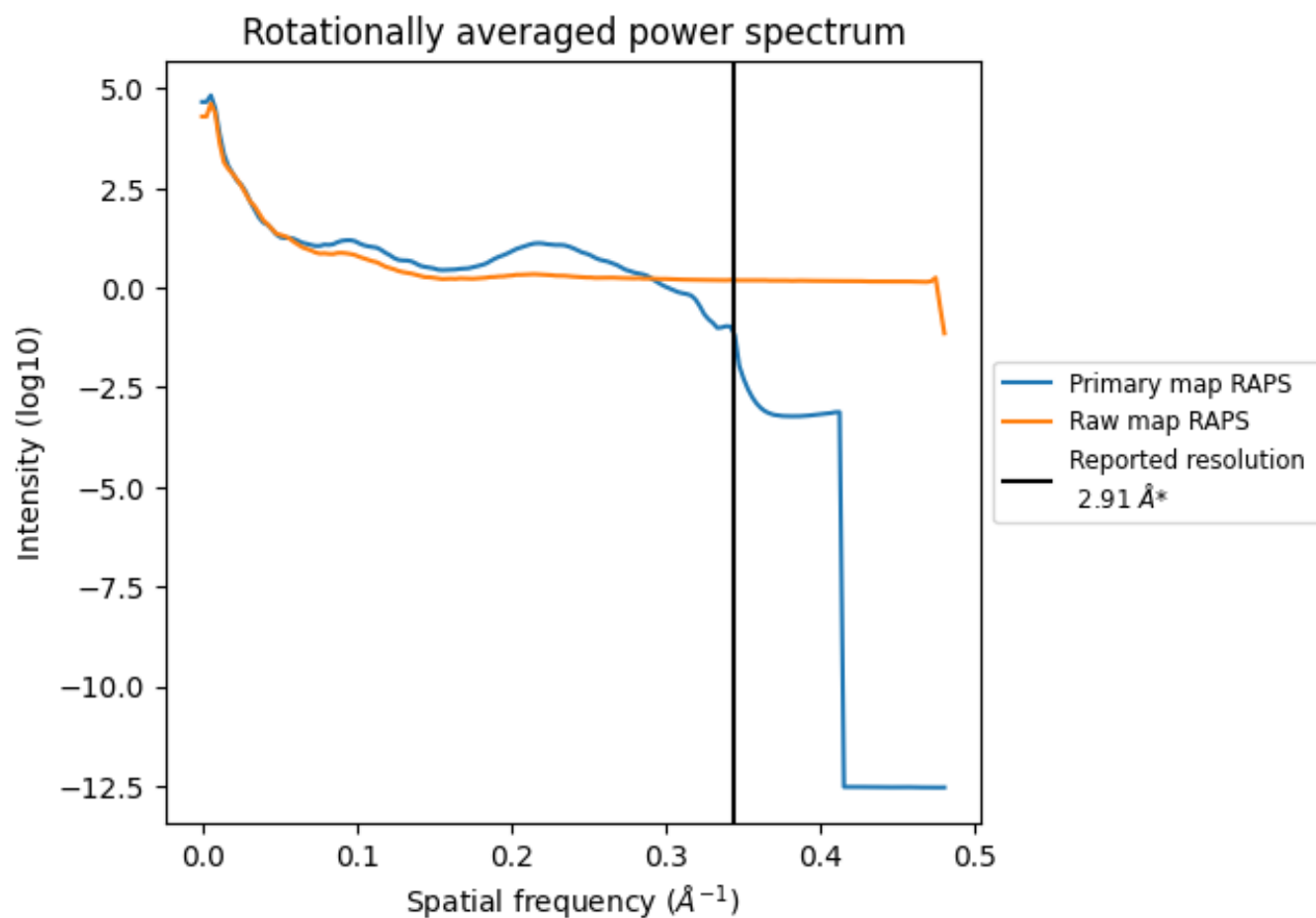
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ

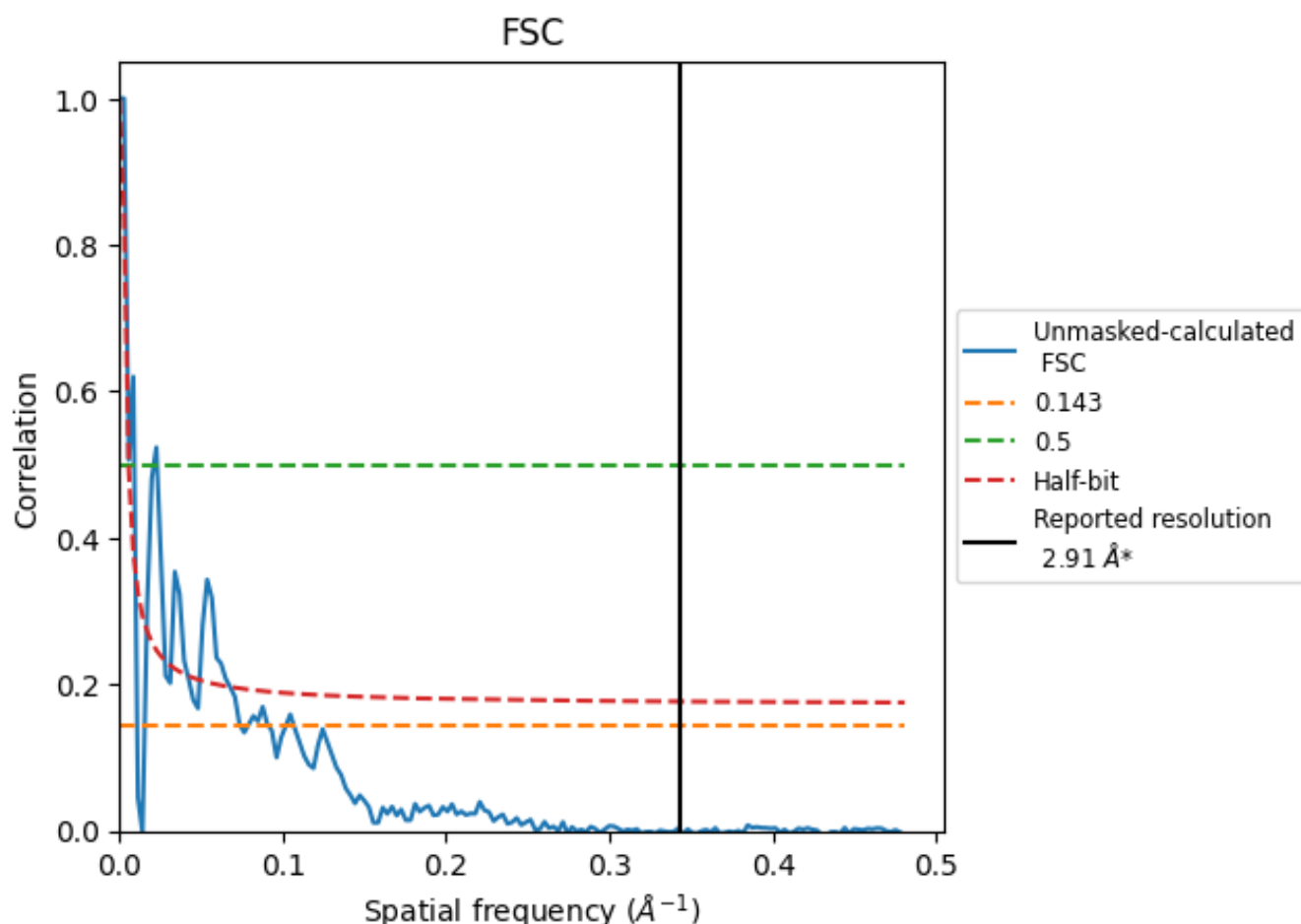


*Reported resolution corresponds to spatial frequency of 0.344 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

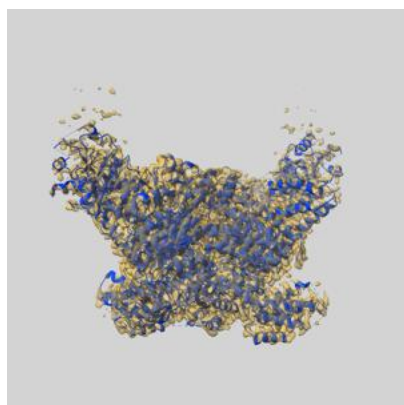
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	92.59	109.89	102.04

*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 92.59 differs from the reported value 2.91 by more than 10 %

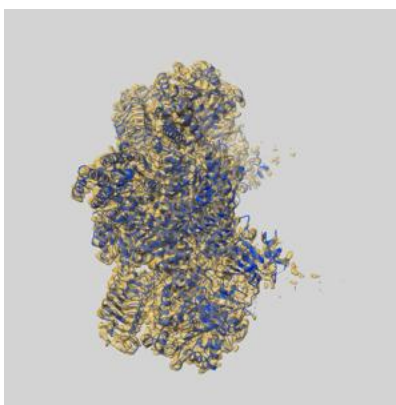
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22924 and PDB model 7KMF. Per-residue inclusion information can be found in section [3](#) on page [11](#).

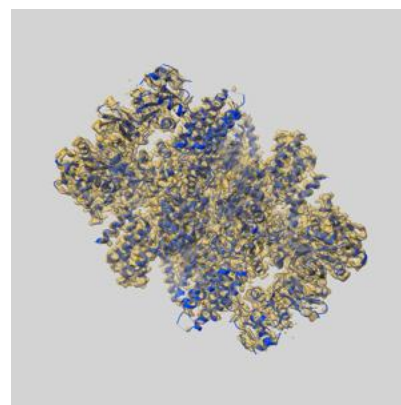
9.1 Map-model overlay [i](#)



X



Y



Z

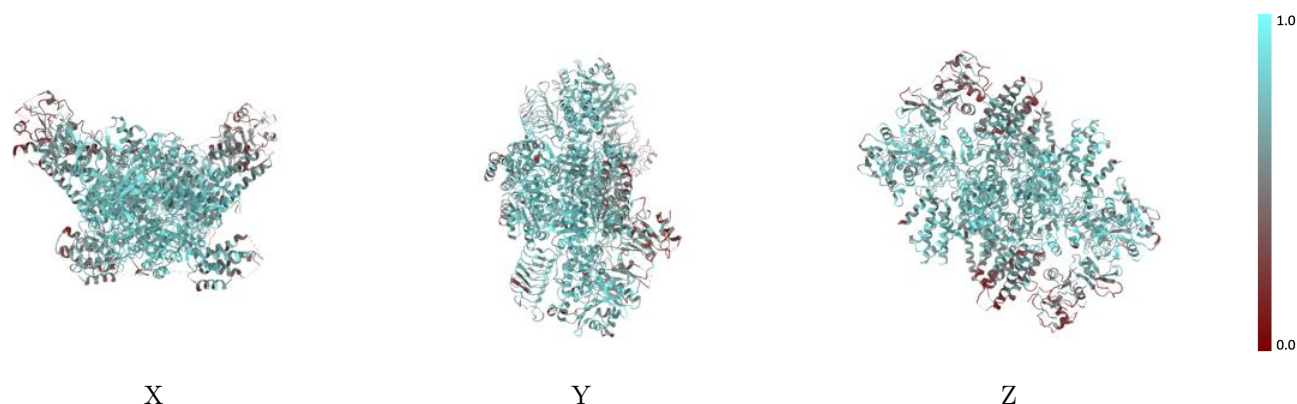
The images above show the 3D surface view of the map at the recommended contour level 0.4534 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



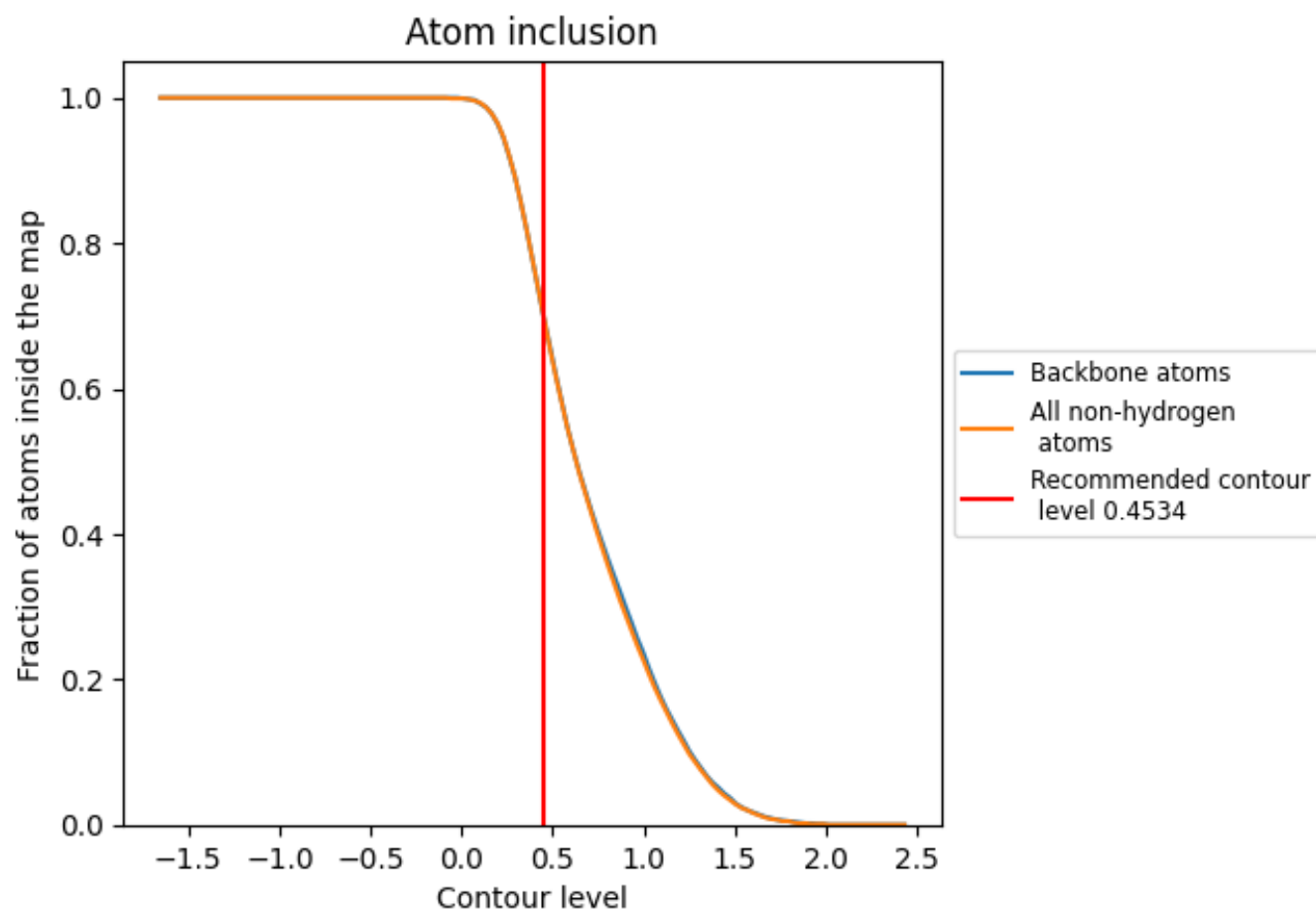
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.4534).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.4534) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6950</div>	<div><div></div>0.5270</div>
B	<div><div></div>0.7180</div>	<div><div></div>0.5190</div>
C	<div><div></div>0.7760</div>	<div><div></div>0.5480</div>
D	<div><div></div>0.7840</div>	<div><div></div>0.5500</div>
E	<div><div></div>0.6830</div>	<div><div></div>0.5380</div>
F	<div><div></div>0.6970</div>	<div><div></div>0.5390</div>
G	<div><div></div>0.7290</div>	<div><div></div>0.5210</div>
H	<div><div></div>0.7450</div>	<div><div></div>0.5270</div>
I	<div><div></div>0.7100</div>	<div><div></div>0.5200</div>
J	<div><div></div>0.4870</div>	<div><div></div>0.4800</div>
K	<div><div></div>0.4810</div>	<div><div></div>0.4810</div>

1.0

0.0

<0.0