



## Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 01:30 pm BST

PDB ID : 9QC6 / pdb\_00009qc6  
EMDB ID : EMD-53004  
Title : Structure of eIF2B decamer bound to (P)eIF2 alpha and Compound A-(S)  
Authors : Shilliday, F.; Maia de Oliveira, T.; Gancedo-Rodrigo, M.  
Deposited on : 2025-03-04  
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

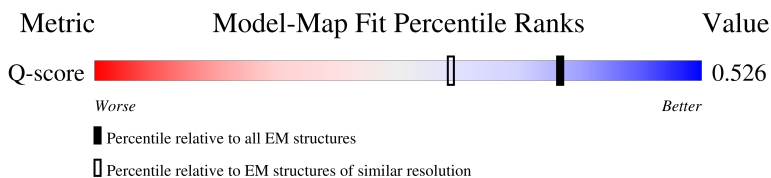
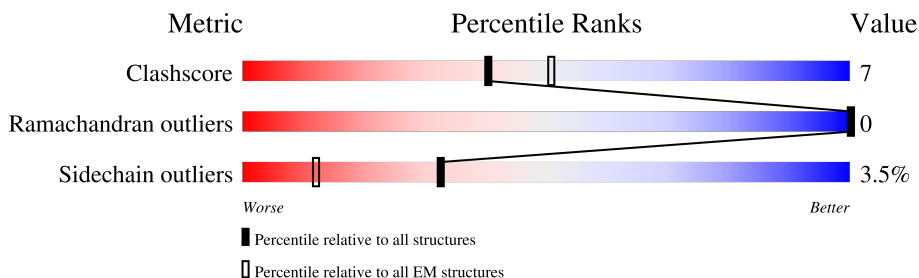
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 2.83 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	11847 ( 2.33 - 3.33 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div>6%</div> <div>69%</div> <div>20%</div> <div>12%</div> </div>
1	B	326	<div> <div>10%</div> <div>70%</div> <div>17%</div> <div>12%</div> </div>
2	C	351	<div> <div>•</div> <div>70%</div> <div>20%</div> <div>• 10%</div> </div>
2	D	351	<div> <div>•</div> <div>72%</div> <div>18%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	452	
3	F	452	
4	G	523	
4	H	523	
5	I	742	
5	J	742	
6	K	210	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24390 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 eIF2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	0
			2094	1355	351	378	10		
1	B	286	Total	C	N	O	S	0	0
			2108	1366	352	380	10		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q14232
A	-19	GLY	-	expression tag	UNP Q14232
A	-18	SER	-	expression tag	UNP Q14232
A	-17	SER	-	expression tag	UNP Q14232
A	-16	HIS	-	expression tag	UNP Q14232
A	-15	HIS	-	expression tag	UNP Q14232
A	-14	HIS	-	expression tag	UNP Q14232
A	-13	HIS	-	expression tag	UNP Q14232
A	-12	HIS	-	expression tag	UNP Q14232
A	-11	HIS	-	expression tag	UNP Q14232
A	-10	SER	-	expression tag	UNP Q14232
A	-9	SER	-	expression tag	UNP Q14232
A	-8	GLY	-	expression tag	UNP Q14232
A	-7	LEU	-	expression tag	UNP Q14232
A	-6	GLU	-	expression tag	UNP Q14232
A	-5	VAL	-	expression tag	UNP Q14232
A	-4	LEU	-	expression tag	UNP Q14232
A	-3	PHE	-	expression tag	UNP Q14232
A	-2	GLN	-	expression tag	UNP Q14232
A	-1	GLY	-	expression tag	UNP Q14232
A	0	PRO	-	expression tag	UNP Q14232
B	-20	MET	-	initiating methionine	UNP Q14232
B	-19	GLY	-	expression tag	UNP Q14232
B	-18	SER	-	expression tag	UNP Q14232
B	-17	SER	-	expression tag	UNP Q14232
B	-16	HIS	-	expression tag	UNP Q14232

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q14232
B	-14	HIS	-	expression tag	UNP Q14232
B	-13	HIS	-	expression tag	UNP Q14232
B	-12	HIS	-	expression tag	UNP Q14232
B	-11	HIS	-	expression tag	UNP Q14232
B	-10	SER	-	expression tag	UNP Q14232
B	-9	SER	-	expression tag	UNP Q14232
B	-8	GLY	-	expression tag	UNP Q14232
B	-7	LEU	-	expression tag	UNP Q14232
B	-6	GLU	-	expression tag	UNP Q14232
B	-5	VAL	-	expression tag	UNP Q14232
B	-4	LEU	-	expression tag	UNP Q14232
B	-3	PHE	-	expression tag	UNP Q14232
B	-2	GLN	-	expression tag	UNP Q14232
B	-1	GLY	-	expression tag	UNP Q14232
B	0	PRO	-	expression tag	UNP Q14232

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	317	Total	C	N	O	S	0	0
			2397	1528	426	429	14		
2	D	316	Total	C	N	O	S	0	0
			2373	1511	419	428	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	278	Total	C	N	O	S	0	0
			1745	1106	312	320	7		
3	F	285	Total	C	N	O	S	0	0
			1711	1082	311	314	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	335	Total	C	N	O	S	0	0
			2337	1483	418	424	12		
4	H	341	Total	C	N	O	S	0	0
			2494	1597	444	442	11		

- Molecule 5 is a protein called Translation initiation factor eIF2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	415	Total	C	N	O	S	0	0
			3167	2009	556	587	15		
5	J	418	Total	C	N	O	S	0	0
			3151	1999	561	576	15		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-20	MET	-	initiating methionine	UNP Q13144
I	-19	GLY	-	expression tag	UNP Q13144
I	-18	SER	-	expression tag	UNP Q13144
I	-17	SER	-	expression tag	UNP Q13144
I	-16	HIS	-	expression tag	UNP Q13144
I	-15	HIS	-	expression tag	UNP Q13144
I	-14	HIS	-	expression tag	UNP Q13144
I	-13	HIS	-	expression tag	UNP Q13144
I	-12	HIS	-	expression tag	UNP Q13144
I	-11	HIS	-	expression tag	UNP Q13144
I	-10	SER	-	expression tag	UNP Q13144
I	-9	SER	-	expression tag	UNP Q13144
I	-8	GLY	-	expression tag	UNP Q13144
I	-7	LEU	-	expression tag	UNP Q13144
I	-6	GLU	-	expression tag	UNP Q13144
I	-5	VAL	-	expression tag	UNP Q13144
I	-4	LEU	-	expression tag	UNP Q13144
I	-3	PHE	-	expression tag	UNP Q13144
I	-2	GLN	-	expression tag	UNP Q13144
I	-1	GLY	-	expression tag	UNP Q13144
I	0	PRO	-	expression tag	UNP Q13144
J	-20	MET	-	initiating methionine	UNP Q13144
J	-19	GLY	-	expression tag	UNP Q13144
J	-18	SER	-	expression tag	UNP Q13144
J	-17	SER	-	expression tag	UNP Q13144
J	-16	HIS	-	expression tag	UNP Q13144
J	-15	HIS	-	expression tag	UNP Q13144
J	-14	HIS	-	expression tag	UNP Q13144
J	-13	HIS	-	expression tag	UNP Q13144
J	-12	HIS	-	expression tag	UNP Q13144
J	-11	HIS	-	expression tag	UNP Q13144
J	-10	SER	-	expression tag	UNP Q13144
J	-9	SER	-	expression tag	UNP Q13144
J	-8	GLY	-	expression tag	UNP Q13144
J	-7	LEU	-	expression tag	UNP Q13144

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-6	GLU	-	expression tag	UNP Q13144
J	-5	VAL	-	expression tag	UNP Q13144
J	-4	LEU	-	expression tag	UNP Q13144
J	-3	PHE	-	expression tag	UNP Q13144
J	-2	GLN	-	expression tag	UNP Q13144
J	-1	GLY	-	expression tag	UNP Q13144
J	0	PRO	-	expression tag	UNP Q13144

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

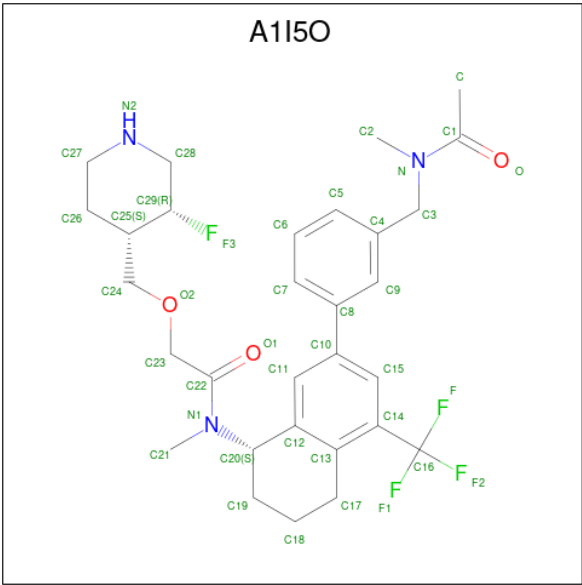
Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	125	Total	C	N	O	P	S	0	0
			773	484	137	149	1	2		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP P05198
K	-1	SER	-	expression tag	UNP P05198
K	187	LEU	-	expression tag	UNP P05198
K	188	GLU	-	expression tag	UNP P05198
K	189	ARG	-	expression tag	UNP P05198
K	190	ALA	-	expression tag	UNP P05198
K	191	PRO	-	expression tag	UNP P05198
K	192	GLY	-	expression tag	UNP P05198
K	193	GLY	-	expression tag	UNP P05198
K	194	LEU	-	expression tag	UNP P05198
K	195	ASN	-	expression tag	UNP P05198
K	196	ASP	-	expression tag	UNP P05198
K	197	ILE	-	expression tag	UNP P05198
K	198	PHE	-	expression tag	UNP P05198
K	199	GLU	-	expression tag	UNP P05198
K	200	ALA	-	expression tag	UNP P05198
K	201	GLN	-	expression tag	UNP P05198
K	202	LYS	-	expression tag	UNP P05198
K	203	ILE	-	expression tag	UNP P05198
K	204	GLU	-	expression tag	UNP P05198
K	205	TRP	-	expression tag	UNP P05198
K	206	HIS	-	expression tag	UNP P05198
K	207	GLU	-	expression tag	UNP P05198

- Molecule 7 is {N}-[(1 {S})-7-[3-[[ethanoyl(methyl)amino]methyl]phenyl]-5-(trifluoromethyl

)-1,2,3,4-tetrahydronaphthalen-1-yl]-2-[[[(3 {R},4 {S})-3-fluoranyl]piperidin-4-yl]methoxy]- {N}-methyl-ethanamide (CCD ID: A1I5O) (formula: C<sub>30</sub>H<sub>37</sub>F<sub>4</sub>N<sub>3</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



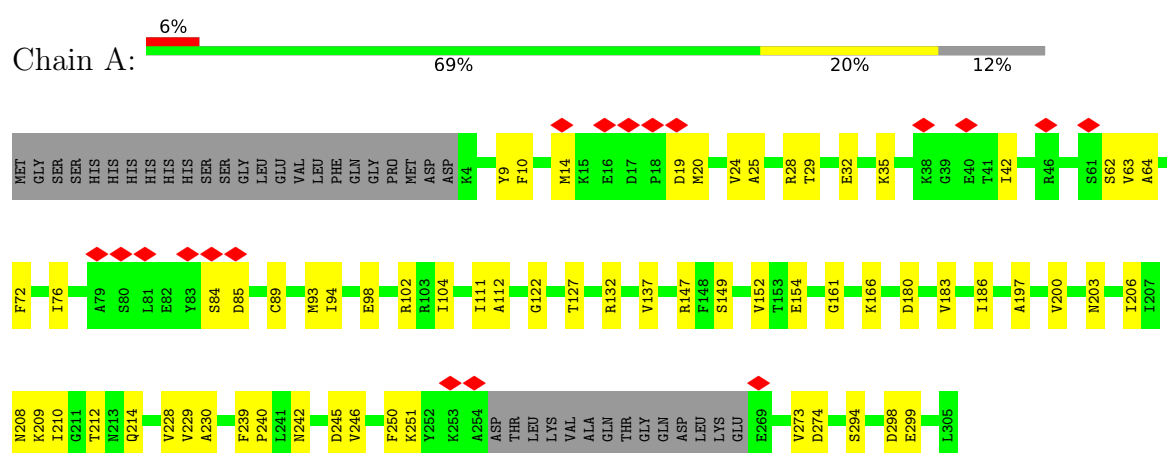
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
7	C	1	40	30	4	3	3	0



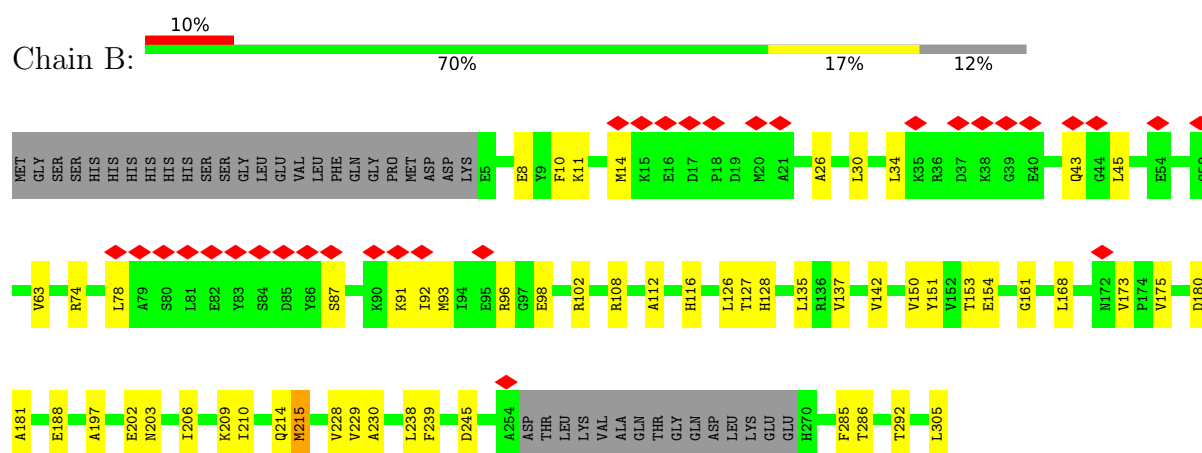
### 3 Residue-property plots

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.

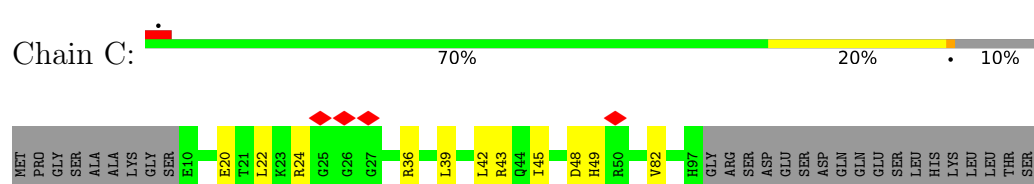
- Molecule 1: Translation initiation factor eIF2B subunit alpha

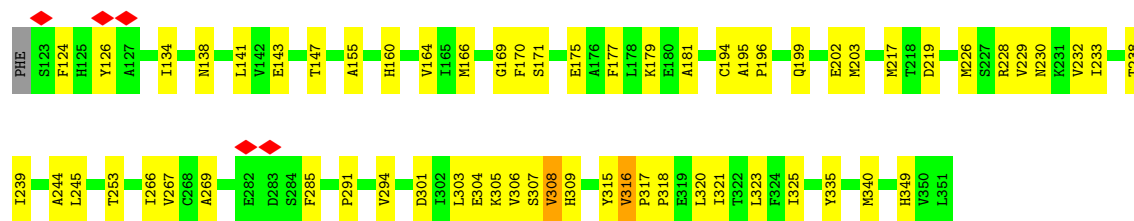


- Molecule 1: Translation initiation factor eIF2B subunit alpha

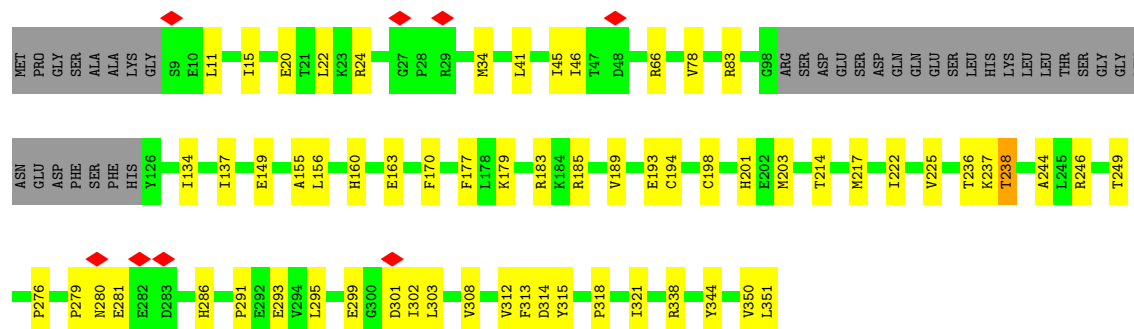


- Molecule 2: Translation initiation factor eIF2B subunit beta

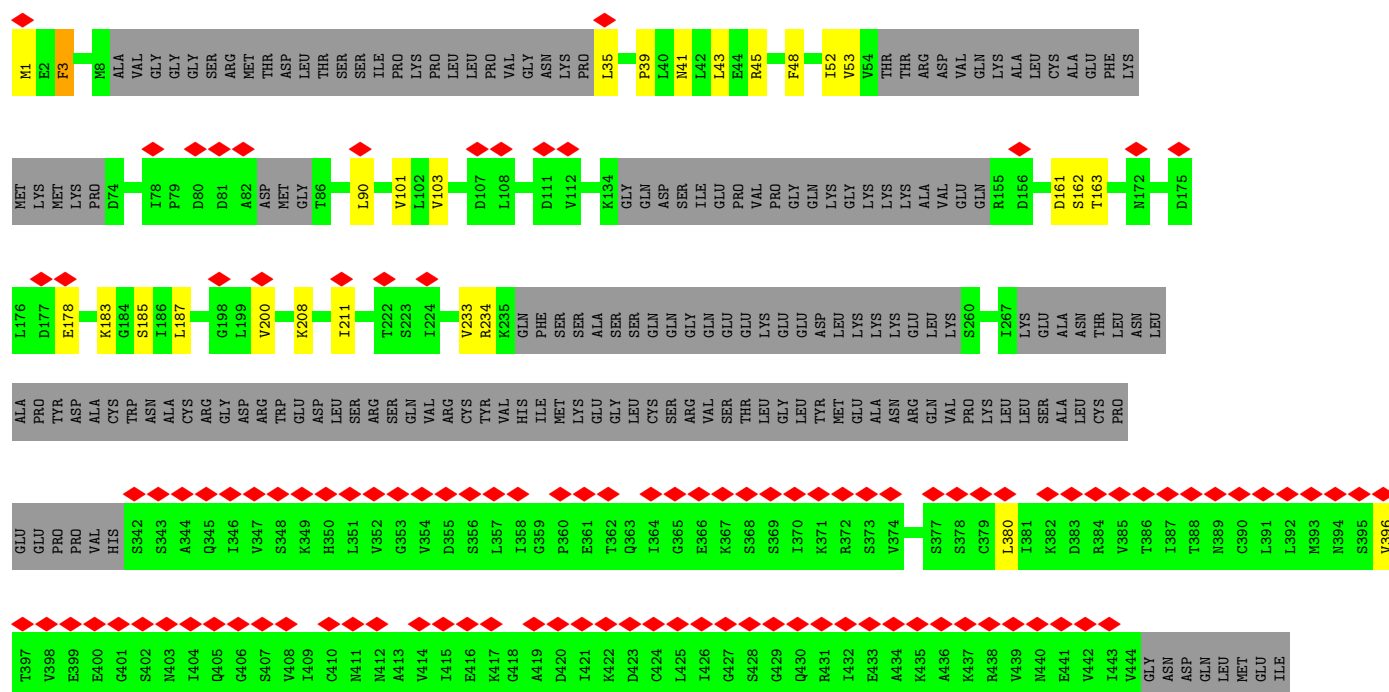




• Molecule 2: Translation initiation factor eIF2B subunit beta



• Molecule 3: Translation initiation factor eIF-2B subunit gamma

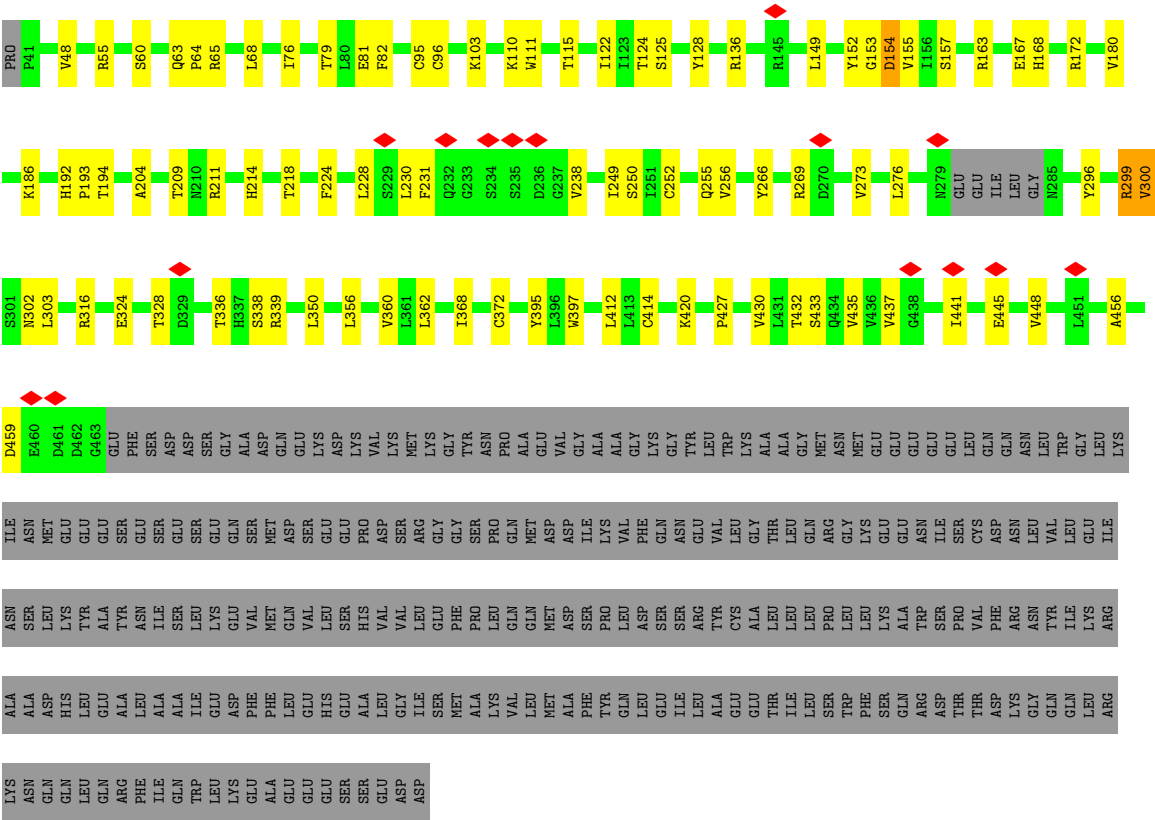


• Molecule 3: Translation initiation factor eIF-2B subunit gamma









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18192	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.281	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	324.9, 324.9, 324.9	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85499996, 0.85499996, 0.85499996	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, A1I5O

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	0.15	0/2130	0.34	0/2898
1	B	0.31	0/2143	0.48	0/2910
2	C	0.35	0/2444	0.51	0/3317
2	D	0.38	0/2418	0.51	0/3283
3	E	0.18	0/1761	0.42	0/2410
3	F	0.13	0/1727	0.35	0/2376
4	G	0.40	0/2380	0.55	0/3264
4	H	0.39	0/2543	0.53	0/3480
5	I	0.33	0/3234	0.48	0/4415
5	J	0.30	0/3217	0.45	0/4395
6	K	0.20	0/768	0.36	0/1059
All	All	0.31	0/24765	0.47	0/33807

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	B	0	1
2	C	0	1
4	G	0	1
4	H	0	3
5	J	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	108	ARG	Sidechain
2	C	36	ARG	Sidechain
4	G	344	ARG	Sidechain
4	H	301	ARG	Sidechain
4	H	344	ARG	Sidechain
4	H	370	ARG	Sidechain
5	J	299	ARG	Sidechain

## 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	2094	0	2059	36	0
1	B	2108	0	2118	38	0
2	C	2397	0	2383	50	0
2	D	2373	0	2355	40	0
3	E	1745	0	1388	17	0
3	F	1711	0	1261	14	0
4	G	2337	0	2163	36	0
4	H	2494	0	2466	32	0
5	I	3167	0	3086	38	0
5	J	3151	0	3062	51	0
6	K	773	0	595	7	0
7	C	40	0	0	3	0
All	All	24390	0	22936	330	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 7.

All (330) 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:206:ILE:HG21	1:A:228:VAL:HG11	1.64	0.77
5:J:155:VAL:HG22	5:J:299:ARG:HB2	1.68	0.76
2:C:169:GLY:HA2	2:C:194:CYS:HB2	1.69	0.74
5:I:66:VAL:HG13	5:I:76:ILE:HB	1.71	0.73
5:J:192:HIS:HD2	5:J:194:THR:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:HD12	5:J:192:HIS:HE1	1.58	0.69
4:G:448:GLN:HG3	4:G:453:VAL:HB	1.77	0.67
5:J:432:THR:HG22	5:J:433:SER:H	1.60	0.67
3:E:52:ILE:HG22	3:E:53:VAL:HG23	1.77	0.66
2:D:295:LEU:HG	2:D:299:GLU:HG3	1.81	0.63
2:D:249:THR:HG23	4:H:389:PRO:HB2	1.81	0.62
3:F:168:LEU:HD12	3:F:234:ARG:HH22	1.63	0.62
2:C:39:LEU:HD13	2:C:141:LEU:HD12	1.80	0.62
4:G:225:ARG:HB3	4:G:273:MET:HE2	1.80	0.62
1:B:150:VAL:HG21	1:B:168:LEU:HD23	1.82	0.62
2:C:171:SER:H	2:C:203:MET:HE2	1.65	0.62
5:I:300:VAL:HA	5:I:305:MET:HB3	1.82	0.61
6:K:73:ILE:HD13	6:K:85:SER:HB2	1.83	0.61
3:F:48:PHE:H	4:G:199:PRO:HG2	1.66	0.61
1:A:239:PHE:O	4:G:326:LYS:NZ	2.33	0.60
2:C:196:PRO:HG3	4:G:387:LEU:HD12	1.82	0.60
2:D:15:ILE:HG12	2:D:41:LEU:HD11	1.82	0.60
3:E:183:LYS:NZ	3:E:185:SER:OG	2.35	0.60
2:C:155:ALA:HB1	2:C:181:ALA:HB2	1.83	0.60
4:H:448:GLN:NE2	4:H:450:ASP:O	2.33	0.60
5:J:136:ARG:NH2	5:J:266:TYR:O	2.35	0.60
4:H:499:LEU:HD11	4:H:506:MET:HB3	1.84	0.60
2:D:293:GLU:HG3	4:H:467:ARG:HH22	1.66	0.59
4:G:395:LEU:HD12	4:G:432:VAL:HG11	1.84	0.59
5:I:138:VAL:HG23	5:I:143:LEU:HD12	1.83	0.59
2:D:338:ARG:NH2	4:G:514:VAL:O	2.35	0.59
2:D:193:GLU:OE2	2:D:201:HIS:NE2	2.27	0.59
2:D:249:THR:HA	2:D:314:ASP:HB2	1.85	0.59
1:B:74:ARG:HB2	1:B:74:ARG:NH1	2.18	0.59
2:C:196:PRO:HG3	2:C:294:VAL:HG12	1.84	0.59
2:C:266:ILE:HD13	2:C:325:ILE:HD12	1.85	0.59
1:B:78:LEU:HD23	1:B:305:LEU:HD13	1.83	0.58
3:F:188:GLN:HB2	3:F:189:LYS:HE2	1.85	0.58
1:A:298:ASP:OD2	1:A:299:GLU:N	2.36	0.57
1:B:206:ILE:HG21	1:B:228:VAL:HG11	1.85	0.57
2:D:291:PRO:HB3	2:D:308:VAL:HB	1.86	0.57
5:I:135:LEU:HA	5:I:138:VAL:HG12	1.86	0.57
4:G:416:SER:OG	4:G:417:ARG:N	2.36	0.57
1:A:9:TYR:CE2	1:A:32:GLU:HG2	2.40	0.57
5:J:350:LEU:HA	5:J:368:ILE:HB	1.87	0.56
5:J:186:LYS:HE2	5:J:296:TYR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:HD12	5:J:192:HIS:CE1	2.39	0.56
4:H:435:LEU:HD22	4:H:499:LEU:HB3	1.88	0.56
2:C:285:PHE:CZ	2:C:315:TYR:HB2	2.40	0.56
2:C:219:ASP:O	4:G:422:GLN:NE2	2.33	0.56
4:G:455:ASN:OD1	4:G:456:GLU:N	2.37	0.56
1:A:251:LYS:HA	1:A:273:VAL:HG22	1.86	0.56
1:B:8:GLU:CD	1:B:8:GLU:H	2.15	0.55
2:C:143:GLU:O	2:C:147:THR:HG23	2.06	0.55
5:I:222:ARG:C	5:I:222:ARG:HD2	2.31	0.55
1:B:112:ALA:HA	1:B:137:VAL:HG22	1.88	0.55
4:H:233:LEU:HD13	4:H:280:LEU:HD23	1.87	0.55
5:J:316:ARG:NH2	5:J:324:GLU:OE2	2.31	0.55
2:D:156:LEU:HD22	2:D:185:ARG:HE	1.72	0.54
5:I:426:LYS:HG2	5:I:443:LEU:O	2.07	0.54
1:A:210:ILE:HA	1:A:274:ASP:HB2	1.88	0.54
2:D:160:HIS:HA	2:D:185:ARG:HH11	1.73	0.54
1:B:11:LYS:HA	1:B:14:MET:SD	2.48	0.53
1:B:229:VAL:HG12	1:B:285:PHE:HB2	1.89	0.53
4:G:386:LEU:HD22	4:G:394:VAL:HB	1.90	0.53
5:J:65:ARG:HA	5:J:68:LEU:HG	1.90	0.53
5:J:63:GLN:HG3	5:J:64:PRO:HD2	1.90	0.53
1:A:208:ASN:ND2	1:A:209:LYS:H	2.06	0.53
1:A:180:ASP:HB2	1:B:180:ASP:HB2	1.90	0.53
5:I:389:VAL:HG13	5:I:406:ALA:HB3	1.91	0.53
2:D:24:ARG:NH2	5:J:81:GLU:OE2	2.40	0.52
5:I:357:GLU:HB3	5:I:375:THR:HB	1.90	0.52
1:B:74:ARG:HB2	1:B:74:ARG:HH11	1.74	0.52
4:G:446:ARG:NH2	4:G:448:GLN:OE1	2.32	0.52
5:I:141:LYS:HB2	5:I:143:LEU:HG	1.92	0.52
1:A:154:GLU:HA	1:A:161:GLY:HA3	1.92	0.52
1:B:98:GLU:O	1:B:102:ARG:HG3	2.08	0.52
3:F:194:ARG:HH22	5:I:237:GLY:HA3	1.75	0.52
2:C:309:HIS:HB2	4:G:386:LEU:HD11	1.92	0.52
4:H:403:LEU:HD13	4:H:420:THR:HG23	1.92	0.51
5:J:356:LEU:HG	5:J:360:VAL:HG11	1.92	0.51
3:F:234:ARG:HD3	3:F:234:ARG:N	2.25	0.51
4:G:180:PHE:HA	4:G:183:LEU:HD13	1.92	0.51
5:J:180:VAL:HG23	5:J:255:GLN:HB2	1.92	0.51
5:J:149:LEU:HD11	5:J:249:ILE:HG22	1.93	0.51
4:G:455:ASN:ND2	4:G:489:TYR:O	2.43	0.51
5:J:103:LYS:HZ3	5:J:122:ILE:HB	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:358:GLU:HG3	5:I:359:ASN:ND2	2.25	0.51
5:J:154:ASP:HB2	5:J:300:VAL:HG22	1.93	0.51
1:B:87:SER:O	1:B:91:LYS:NZ	2.31	0.51
1:B:197:ALA:HB3	1:B:230:ALA:HB2	1.93	0.51
3:F:187:LEU:HD12	5:I:224:PHE:HD2	1.75	0.51
4:G:335:VAL:HG21	4:G:346:LEU:HD11	1.93	0.50
2:D:301:ASP:HA	5:J:193:PRO:HD3	1.94	0.50
5:J:435:VAL:HG23	5:J:459:ASP:HA	1.94	0.50
5:I:346:PRO:HD2	5:I:364:SER:HB3	1.92	0.50
5:I:137:ASP:O	5:I:141:LYS:HG2	2.11	0.50
3:F:101:VAL:HG21	3:F:212:VAL:HG21	1.92	0.50
2:D:170:PHE:CD1	2:D:203:MET:HB2	2.47	0.49
7:C:401:A1I5O:C18	2:D:163:GLU:HG2	2.42	0.49
5:J:448:VAL:O	5:J:456:ALA:HB3	2.11	0.49
1:A:112:ALA:HA	1:A:137:VAL:HG22	1.94	0.49
3:F:157:PHE:C	3:F:158:ILE:HD13	2.37	0.49
4:H:327:ILE:O	4:H:354:ARG:NE	2.45	0.49
2:C:43:ARG:NH1	2:C:138:ASN:OD1	2.44	0.49
2:C:340:MET:HE3	2:C:349:HIS:NE2	2.27	0.49
5:J:338:SER:OG	5:J:339:ARG:N	2.46	0.49
3:E:41:ASN:O	3:E:45:ARG:N	2.42	0.49
2:C:42:LEU:HD11	2:C:82:VAL:HG22	1.95	0.49
4:G:231:ARG:HH22	4:G:308:VAL:HG11	1.78	0.48
4:H:320:SER:HA	4:H:345:ILE:HG12	1.95	0.48
2:D:217:MET:HE1	2:D:222:ILE:HA	1.96	0.48
3:E:3:PHE:HB3	3:E:48:PHE:HZ	1.78	0.48
4:G:435:LEU:HD23	4:G:501:ILE:HD11	1.93	0.48
4:H:319:ILE:HG21	4:H:341:LEU:HD21	1.95	0.48
1:A:127:THR:HG23	1:A:152:VAL:HG23	1.93	0.48
2:C:155:ALA:HA	2:C:177:PHE:CZ	2.49	0.48
2:C:170:PHE:HB3	2:C:199:GLN:HB3	1.95	0.48
2:C:335:TYR:HD1	4:H:514:VAL:HG12	1.77	0.48
1:A:122:GLY:N	1:A:147:ARG:O	2.37	0.48
5:I:201:VAL:HG12	5:I:217:LYS:HD2	1.95	0.48
1:B:10:PHE:HE1	1:B:26:ALA:HB2	1.78	0.48
1:B:128:HIS:CD2	1:B:209:LYS:HB3	2.49	0.48
2:C:42:LEU:HD11	2:C:82:VAL:HA	1.96	0.48
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.79	0.48
2:C:301:ASP:N	2:C:301:ASP:OD1	2.46	0.48
5:J:356:LEU:HD21	5:J:362:LEU:HD11	1.95	0.48
6:K:127:GLU:O	6:K:131:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:90:LEU:HD22	3:E:103:VAL:HG21	1.96	0.47
1:B:14:MET:C	1:B:14:MET:HE2	2.40	0.47
2:D:11:LEU:HD11	2:D:45:ILE:HG12	1.97	0.47
3:E:1:MET:HE1	4:H:199:PRO:HB3	1.96	0.47
2:C:245:LEU:HB2	2:C:316:VAL:HG13	1.96	0.47
2:D:155:ALA:HA	2:D:177:PHE:CZ	2.49	0.47
2:D:20:GLU:HA	2:D:20:GLU:OE2	2.14	0.47
5:J:252:CYS:HB3	5:J:256:VAL:HG21	1.96	0.47
1:A:197:ALA:HB3	1:A:230:ALA:HB2	1.96	0.47
2:C:20:GLU:O	2:C:24:ARG:HG2	2.15	0.47
4:H:313:VAL:HG22	4:H:317:GLN:HE21	1.80	0.47
5:I:168:HIS:CE1	5:I:172:ARG:HD2	2.50	0.47
4:H:388:ILE:N	4:H:389:PRO:HD2	2.29	0.47
4:H:415:MET:HE2	4:H:415:MET:HB3	1.83	0.47
1:A:89:CYS:O	1:A:93:MET:HG3	2.14	0.47
2:D:193:GLU:OE1	4:H:364:ARG:NH1	2.48	0.47
2:C:317:PRO:HD2	2:C:320:LEU:HD12	1.97	0.46
4:G:269:LEU:HD22	4:G:273:MET:SD	2.55	0.46
5:I:168:HIS:HB2	5:I:182:THR:HG21	1.97	0.46
5:J:218:THR:O	5:J:218:THR:OG1	2.30	0.46
1:A:214:GLN:OE1	1:B:181:ALA:HA	2.15	0.46
2:C:228:ARG:NH2	7:C:401:AIIO:F2	2.28	0.46
2:C:244:ALA:HB2	2:C:318:PRO:HD3	1.97	0.46
2:D:280:ASN:O	2:D:281:GLU:HG3	2.15	0.46
3:E:39:PRO:O	3:E:43:LEU:HD23	2.16	0.46
5:J:76:ILE:HA	5:J:79:THR:HG22	1.96	0.46
5:J:276:LEU:HD23	5:J:276:LEU:HA	1.81	0.46
5:J:111:TRP:CZ3	5:J:328:THR:HG23	2.50	0.46
3:E:183:LYS:NZ	3:E:183:LYS:HB3	2.30	0.46
2:C:285:PHE:HZ	2:C:315:TYR:HB2	1.80	0.46
4:G:493:PRO:HD2	4:G:496:LEU:HD12	1.96	0.46
5:J:149:LEU:HD11	5:J:249:ILE:CG2	2.45	0.46
2:C:291:PRO:HB3	2:C:308:VAL:HG22	1.98	0.46
3:E:233:VAL:HG23	3:E:233:VAL:O	2.16	0.46
1:B:74:ARG:HD3	1:B:305:LEU:HD12	1.96	0.46
1:B:245:ASP:OD1	1:B:245:ASP:N	2.48	0.46
4:G:388:ILE:N	4:G:389:PRO:HD2	2.30	0.46
5:J:79:THR:HG21	5:J:153:GLY:HA2	1.97	0.46
1:A:24:VAL:HG22	1:A:104:ILE:HD12	1.98	0.46
6:K:102:THR:O	6:K:106:THR:HG23	2.15	0.46
1:A:10:PHE:CE2	1:A:14:MET:HE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASP:HA	1:A:132:ARG:NH1	2.31	0.46
1:B:230:ALA:O	1:B:286:THR:HA	2.15	0.45
5:J:125:SER:HB3	5:J:128:TYR:CE2	2.50	0.45
1:A:72:PHE:CZ	1:A:76:ILE:HD11	2.51	0.45
5:J:432:THR:O	5:J:435:VAL:HG12	2.17	0.45
4:G:326:LYS:O	4:G:400:LYS:HE3	2.17	0.45
1:A:20:MET:CB	1:A:28:ARG:HH22	2.29	0.45
5:I:253:SER:HB2	5:I:254:PRO:HD2	1.99	0.45
1:A:9:TYR:CD2	1:A:32:GLU:HG2	2.52	0.45
2:D:22:LEU:HD11	2:D:78:VAL:HG11	1.99	0.45
2:D:318:PRO:HA	2:D:321:ILE:HD12	1.98	0.45
3:E:52:ILE:N	3:E:52:ILE:HD12	2.32	0.45
3:F:166:ARG:HD3	3:F:263:ILE:O	2.17	0.45
5:J:437:VAL:HG13	5:J:441:ILE:HD11	1.99	0.45
1:A:208:ASN:OD1	1:A:212:THR:HG21	2.17	0.45
1:B:92:ILE:O	1:B:96:ARG:HG3	2.17	0.45
1:B:168:LEU:HB3	1:B:175:VAL:HG21	1.98	0.45
2:C:160:HIS:NE2	4:H:453:VAL:HG22	2.32	0.45
3:E:161:ASP:OD1	3:E:162:SER:N	2.50	0.45
3:F:357:LEU:O	3:F:375:ILE:N	2.40	0.45
4:H:415:MET:HG3	4:H:491:VAL:HG22	1.99	0.44
1:A:84:SER:OG	1:A:85:ASP:N	2.46	0.44
1:A:183:VAL:HB	1:B:214:GLN:HE22	1.81	0.44
3:E:380:LEU:N	3:E:396:VAL:O	2.50	0.44
6:K:9:GLN:HA	6:K:131:GLN:HE22	1.82	0.44
1:B:126:LEU:HD12	1:B:151:TYR:O	2.18	0.44
1:A:94:ILE:O	1:A:98:GLU:HG2	2.18	0.44
1:A:102:ARG:HG3	1:A:102:ARG:NH1	2.32	0.44
2:C:318:PRO:HA	2:C:321:ILE:HD12	1.99	0.44
2:D:149:GLU:OE1	2:D:149:GLU:N	2.49	0.44
4:G:391:ALA:HA	4:G:394:VAL:HG12	1.99	0.44
4:H:335:VAL:HG11	4:H:346:LEU:HD11	1.98	0.44
5:I:57:PHE:CE1	5:I:61:LYS:HD2	2.53	0.44
5:J:420:LYS:HG2	5:J:437:VAL:O	2.17	0.44
1:B:127:THR:O	1:B:153:THR:HG23	2.18	0.44
1:B:135:LEU:HD12	1:B:168:LEU:HD13	2.00	0.44
4:H:417:ARG:HA	4:H:417:ARG:HD3	1.87	0.44
2:C:45:ILE:O	2:C:49:HIS:HB2	2.18	0.44
4:G:319:ILE:HG21	4:G:341:LEU:HD21	1.97	0.44
4:G:463:LEU:HD12	4:G:463:LEU:HA	1.83	0.44
2:C:304:GLU:HB2	5:I:193:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ARG:HE	2:D:351:LEU:C	2.25	0.44
1:A:29:THR:O	1:A:32:GLU:HG3	2.17	0.44
4:H:270:SER:H	4:H:273:MET:HE3	1.81	0.44
1:B:43:GLN:N	1:B:43:GLN:CD	2.75	0.43
1:B:45:LEU:HD11	1:B:93:MET:HE1	2.00	0.43
2:D:194:CYS:O	2:D:198:CYS:N	2.36	0.43
2:D:299:GLU:HB3	2:D:302:ILE:HD11	1.99	0.43
4:G:354:ARG:O	4:G:355:ARG:NH1	2.44	0.43
3:F:194:ARG:NH1	5:I:237:GLY:O	2.50	0.43
4:G:437:CYS:SG	4:G:501:ILE:HD12	2.58	0.43
1:A:25:ALA:HA	1:A:28:ARG:HE	1.84	0.43
1:A:240:PRO:HA	1:A:245:ASP:HB3	2.00	0.43
4:H:440:THR:HG21	4:H:504:LEU:HG	2.00	0.43
1:A:35:LYS:HG2	1:A:94:ILE:HD13	2.00	0.43
4:G:314:LEU:HD23	6:K:62:ILE:HG12	2.00	0.43
2:C:164:VAL:H	2:C:230:ASN:HD21	1.67	0.43
2:D:244:ALA:HB2	2:D:318:PRO:HD3	2.00	0.43
4:G:355:ARG:HD3	4:G:355:ARG:HA	1.68	0.43
3:E:233:VAL:C	3:E:234:ARG:HD2	2.43	0.43
3:F:182:ILE:HD11	3:F:195:PHE:HZ	1.84	0.43
5:I:259:LEU:HD13	5:I:259:LEU:HA	1.80	0.43
5:J:228:LEU:HA	5:J:231:PHE:HD2	1.84	0.43
1:B:203:ASN:HB3	1:B:239:PHE:CZ	2.54	0.43
2:D:83:ARG:HD3	2:D:276:PRO:HG2	2.00	0.43
2:D:238:THR:HG21	2:D:246:ARG:HH11	1.84	0.43
1:B:128:HIS:HB2	1:B:215:MET:CE	2.49	0.43
1:B:202:GLU:HG3	1:B:238:LEU:O	2.19	0.43
5:J:192:HIS:CD2	5:J:194:THR:HG22	2.54	0.43
1:A:111:ILE:HG21	1:A:229:VAL:HG13	2.01	0.42
2:C:233:ILE:HG23	2:C:266:ILE:HD11	1.99	0.42
2:C:305:LYS:HE3	2:C:305:LYS:HB2	1.95	0.42
4:G:183:LEU:HB3	4:G:457:LEU:HG	2.01	0.42
5:I:269:ARG:HE	5:I:269:ARG:HB3	1.72	0.42
2:C:169:GLY:CA	2:C:194:CYS:HB2	2.44	0.42
3:E:187:LEU:HD23	3:E:187:LEU:HA	1.86	0.42
5:I:61:LYS:NZ	5:I:61:LYS:HB3	2.35	0.42
5:J:209:THR:HG23	5:J:211:ARG:H	1.83	0.42
5:I:218:THR:O	5:I:218:THR:OG1	2.35	0.42
2:C:303:LEU:HD12	5:I:192:HIS:HE2	1.85	0.42
4:H:411:ASN:HD22	4:H:411:ASN:H	1.68	0.42
5:I:105:HIS:O	5:I:108:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:289:MET:HE3	5:I:291:VAL:HG23	2.00	0.42
6:K:46:LEU:HD23	6:K:46:LEU:HA	1.82	0.42
1:B:93:MET:HB3	1:B:93:MET:HE3	1.83	0.42
2:C:39:LEU:HD23	2:C:39:LEU:HA	1.77	0.42
2:C:175:GLU:OE2	2:C:179:LYS:HE2	2.20	0.42
4:G:321:ARG:NE	4:G:321:ARG:HA	2.35	0.42
4:G:403:LEU:HD13	4:G:420:THR:HG23	2.02	0.42
5:I:436:VAL:H	5:I:460:GLU:C	2.28	0.42
2:C:166:MET:HB3	2:C:229:VAL:HG11	2.01	0.42
5:J:192:HIS:CD2	5:J:193:PRO:HD2	2.55	0.42
5:J:303:LEU:HD11	5:J:412:LEU:HD22	2.02	0.42
1:B:154:GLU:HA	1:B:161:GLY:HA3	2.02	0.42
4:H:411:ASN:HB3	4:H:447:VAL:HG23	2.02	0.42
5:I:125:SER:HB3	5:I:128:TYR:CE2	2.55	0.42
2:C:228:ARG:HD2	7:C:401:A1I5O:O1	2.20	0.42
4:H:386:LEU:HD12	4:H:390:ALA:HB3	2.01	0.42
5:J:60:SER:HA	5:J:63:GLN:O	2.19	0.42
5:J:218:THR:HB	5:J:224:PHE:CE1	2.55	0.42
1:B:215:MET:HE2	1:B:215:MET:HB2	1.85	0.42
2:D:34:MET:HE2	2:D:34:MET:HB2	1.85	0.42
3:E:161:ASP:OD1	3:E:163:THR:HG22	2.20	0.42
5:I:161:ILE:HD11	5:I:184:ILE:HG13	2.01	0.42
5:J:204:ALA:HB3	5:J:214:HIS:HB3	2.01	0.42
5:J:269:ARG:O	5:J:273:VAL:HG12	2.20	0.42
1:A:242:ASN:HB2	1:B:188:GLU:OE1	2.20	0.41
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.87	0.41
2:C:43:ARG:HG3	2:C:134:ILE:HD13	2.02	0.41
2:C:245:LEU:HD11	2:C:267:VAL:HG21	2.01	0.41
6:K:8:TYR:O	6:K:9:GLN:C	2.62	0.41
2:C:239:ILE:HD11	2:C:269:ALA:HB3	2.01	0.41
2:D:189:VAL:HB	2:D:214:THR:HG22	2.02	0.41
3:E:208:LYS:O	3:E:211:ILE:HG13	2.21	0.41
5:I:443:LEU:HD11	5:I:449:ILE:HD11	2.03	0.41
2:D:279:PRO:HB3	2:D:315:TYR:CE1	2.56	0.41
5:J:230:LEU:H	5:J:230:LEU:HD23	1.85	0.41
5:J:427:PRO:O	5:J:445:GLU:HG2	2.20	0.41
3:F:7:VAL:N	3:F:52:ILE:O	2.43	0.41
4:G:499:LEU:HD23	4:G:500:VAL:N	2.35	0.41
1:A:62:SER:O	1:A:64:ALA:N	2.47	0.41
2:D:276:PRO:HG3	2:D:344:TYR:CD2	2.56	0.41
5:J:55:ARG:HH11	5:J:302:ASN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ALA:HB1	2:C:196:PRO:HD2	2.02	0.41
4:H:216:GLN:HB2	4:H:218:LEU:HG	2.03	0.41
5:I:127:LEU:HD12	5:I:127:LEU:HA	1.88	0.41
5:J:82:PHE:HB2	5:J:157:SER:O	2.20	0.41
1:B:34:LEU:HD12	1:B:34:LEU:O	2.21	0.41
5:J:163:ARG:HH21	5:J:167:GLU:HG3	1.85	0.41
5:J:395:TYR:HB2	5:J:412:LEU:HD12	2.02	0.41
2:C:22:LEU:HD23	2:C:22:LEU:HA	1.82	0.41
2:C:48:ASP:OD1	2:C:48:ASP:N	2.53	0.41
2:C:124:PHE:CZ	2:C:126:TYR:HB3	2.56	0.41
2:D:179:LYS:O	2:D:183:ARG:HG3	2.21	0.41
3:E:178:GLU:C	5:J:228:LEU:HD23	2.46	0.41
3:F:160:VAL:HG23	3:F:167:LEU:HD23	2.03	0.41
4:G:417:ARG:HD3	4:G:417:ARG:HA	1.90	0.41
4:H:391:ALA:HA	4:H:394:VAL:HG12	2.03	0.41
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.83	0.41
4:H:269:LEU:HD22	4:H:273:MET:SD	2.61	0.41
5:I:83:LEU:O	5:I:86:THR:HG22	2.21	0.41
5:J:397:TRP:CE3	5:J:414:CYS:HA	2.56	0.41
2:C:170:PHE:HA	2:C:203:MET:HB2	2.03	0.40
5:I:103:LYS:O	5:I:107:LEU:HG	2.21	0.40
5:I:241:ARG:HE	5:I:241:ARG:HB3	1.62	0.40
1:A:203:ASN:HB3	1:A:239:PHE:CE1	2.56	0.40
2:D:134:ILE:HD13	2:D:137:ILE:HD12	2.04	0.40
5:J:168:HIS:NE2	5:J:172:ARG:HD2	2.36	0.40
2:C:291:PRO:HD2	5:I:317:TRP:HA	2.04	0.40
2:C:303:LEU:HA	2:C:306:VAL:HG12	2.02	0.40
2:D:225:VAL:HG12	4:H:452:PHE:HZ	1.85	0.40
2:D:237:LYS:HE3	2:D:313:PHE:CZ	2.56	0.40
4:G:402:LEU:HD11	4:G:437:CYS:SG	2.61	0.40
1:A:63:VAL:HG22	1:A:250:PHE:HB3	2.04	0.40
2:C:226:MET:HE1	2:C:232:VAL:CG2	2.52	0.40
4:G:344:ARG:O	4:G:348:GLU:HG2	2.22	0.40
4:H:202:VAL:HG22	4:H:203:ILE:HG13	2.03	0.40
4:H:452:PHE:CZ	4:H:487:LEU:HD11	2.56	0.40
5:I:181:MET:HG2	5:I:287:ILE:HG23	2.03	0.40
2:D:46:ILE:HD12	2:D:137:ILE:HD11	2.03	0.40
4:H:463:LEU:HD22	4:H:484:LEU:HG	2.02	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/326 (87%)	276 (97%)	8 (3%)	0	100	100
1	B	282/326 (86%)	275 (98%)	7 (2%)	0	100	100
2	C	313/351 (89%)	304 (97%)	9 (3%)	0	100	100
2	D	312/351 (89%)	302 (97%)	10 (3%)	0	100	100
3	E	264/452 (58%)	251 (95%)	13 (5%)	0	100	100
3	F	271/452 (60%)	256 (94%)	15 (6%)	0	100	100
4	G	329/523 (63%)	324 (98%)	5 (2%)	0	100	100
4	H	339/523 (65%)	330 (97%)	9 (3%)	0	100	100
5	I	411/742 (55%)	398 (97%)	13 (3%)	0	100	100
5	J	414/742 (56%)	394 (95%)	20 (5%)	0	100	100
6	K	120/210 (57%)	116 (97%)	4 (3%)	0	100	100
All	All	3339/4998 (67%)	3226 (97%)	113 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/278 (74%)	199 (97%)	7 (3%)	32	57
1	B	214/278 (77%)	207 (97%)	7 (3%)	33	58
2	C	248/298 (83%)	240 (97%)	8 (3%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	245/298 (82%)	240 (98%)	5 (2%)	48	72
3	E	115/398 (29%)	111 (96%)	4 (4%)	32	57
3	F	93/398 (23%)	90 (97%)	3 (3%)	34	59
4	G	219/444 (49%)	211 (96%)	8 (4%)	30	55
4	H	255/444 (57%)	247 (97%)	8 (3%)	35	59
5	I	345/644 (54%)	332 (96%)	13 (4%)	29	54
5	J	337/644 (52%)	323 (96%)	14 (4%)	26	51
6	K	52/189 (28%)	48 (92%)	4 (8%)	12	26
All	All	2329/4313 (54%)	2248 (96%)	81 (4%)	32	57

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	149	SER
1	A	166	LYS
1	A	186	ILE
1	A	200	VAL
1	A	246	VAL
1	A	294	SER
1	B	63	VAL
1	B	116	HIS
1	B	142	VAL
1	B	173	VAL
1	B	210	ILE
1	B	215	MET
1	B	292	THR
2	C	202	GLU
2	C	217	MET
2	C	238	THR
2	C	253	THR
2	C	307	SER
2	C	308	VAL
2	C	316	VAL
2	C	323	LEU
2	D	236	THR
2	D	238	THR
2	D	286	HIS
2	D	312	VAL

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Mol	Chain	Res	Type
2	D	350	VAL
3	E	3	PHE
3	E	35	LEU
3	E	101	VAL
3	E	200	VAL
3	F	6	VAL
3	F	51	VAL
3	F	231	TYR
4	G	266	CYS
4	G	313	VAL
4	G	359	VAL
4	G	418	VAL
4	G	432	VAL
4	G	463	LEU
4	G	465	CYS
4	G	514	VAL
4	H	202	VAL
4	H	220	SER
4	H	308	VAL
4	H	313	VAL
4	H	371	HIS
4	H	414	VAL
4	H	434	VAL
4	H	488	VAL
5	I	66	VAL
5	I	91	THR
5	I	124	THR
5	I	127	LEU
5	I	182	THR
5	I	230	LEU
5	I	259	LEU
5	I	300	VAL
5	I	348	VAL
5	I	378	VAL
5	I	400	VAL
5	I	408	ILE
5	I	436	VAL
5	J	48	VAL
5	J	95	CYS
5	J	96	CYS
5	J	110	LYS
5	J	115	THR

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Mol	Chain	Res	Type
5	J	124	THR
5	J	152	TYR
5	J	154	ASP
5	J	238	VAL
5	J	250	SER
5	J	300	VAL
5	J	336	THR
5	J	372	CYS
5	J	430	VAL
6	K	45	ILE
6	K	70	VAL
6	K	84	LEU
6	K	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS
1	A	208	ASN
1	B	214	GLN
2	C	44	GLN
2	C	97	HIS
2	C	252	HIS
2	C	260	HIS
2	C	309	HIS
2	C	331	ASN
2	D	138	ASN
2	D	158	HIS
2	D	199	GLN
3	E	190	HIS
4	G	274	HIS
4	G	309	GLN
4	G	329	ASN
4	H	317	GLN
4	H	329	ASN
5	I	101	GLN
5	I	168	HIS
5	I	197	HIS
5	I	279	ASN
5	I	304	HIS
5	I	359	ASN
5	I	376	ASN

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Mol	Chain	Res	Type
5	J	192	HIS
5	J	248	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SEP	K	51	6	8,9,10	1.54	1 (12%)	8,12,14	1.51	2 (25%)

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	SEP	K	51	6	-	4/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	51	SEP	P-O1P	3.36	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	51	SEP	P-OG-CB	-2.87	110.39	118.30
6	K	51	SEP	OG-CB-CA	2.53	110.61	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	51	SEP	CB-OG-P-O1P
6	K	51	SEP	CB-OG-P-O2P
6	K	51	SEP	CB-OG-P-O3P
6	K	51	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
7	A1I5O	C	401	-	41,43,43	0.44	1 (2%)	51,62,62	0.59	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
7	A1I5O	C	401	-	-	4/32/53/53	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	A1I5O	C1-N	2.57	1.42	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

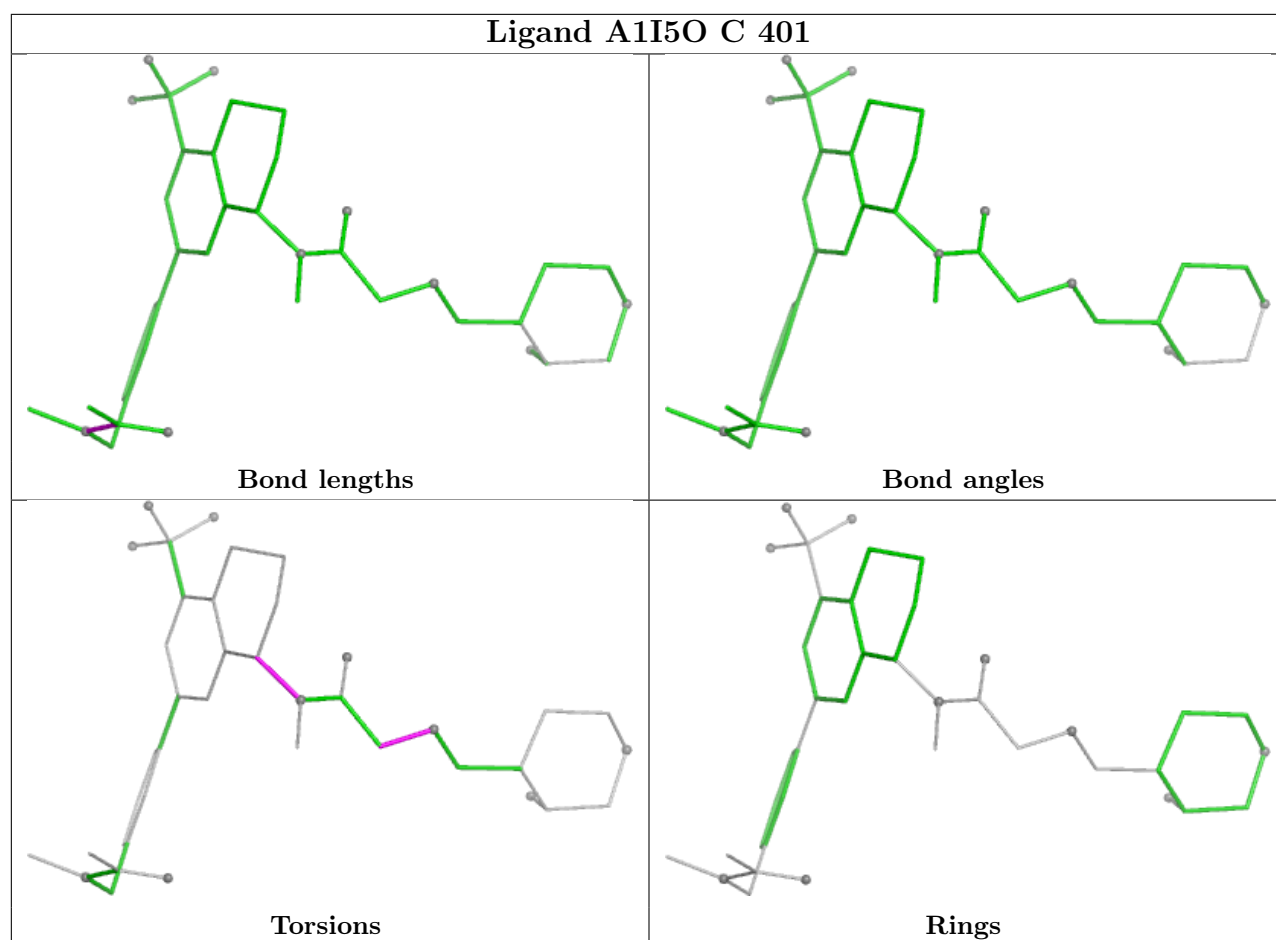
Mol	Chain	Res	Type	Atoms
7	C	401	A1I5O	C12-C20-N1-C21
7	C	401	A1I5O	C19-C20-N1-C21
7	C	401	A1I5O	C22-C23-O2-C24
7	C	401	A1I5O	C19-C20-N1-C22

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	A1I5O	3	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



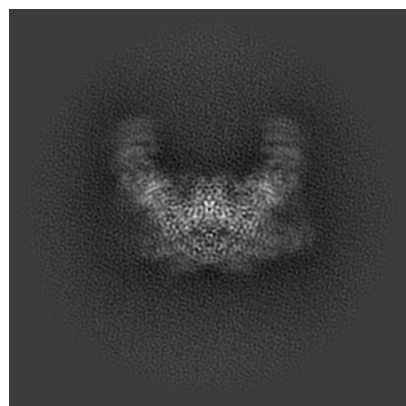
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53004. These allow visual inspection of the internal detail of the map and identification of artifacts.

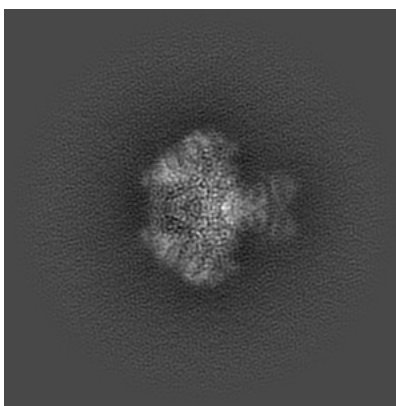
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

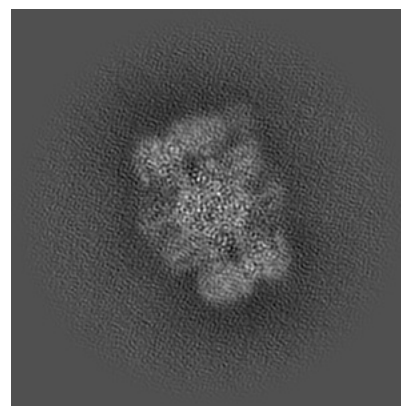
#### 6.1.1 Primary map



X

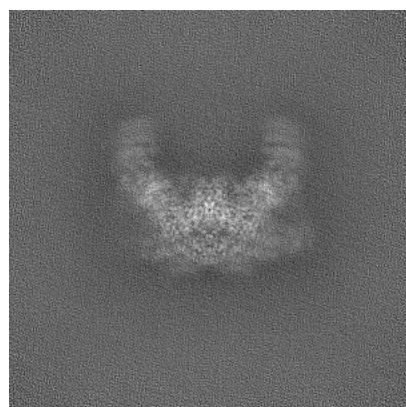


Y

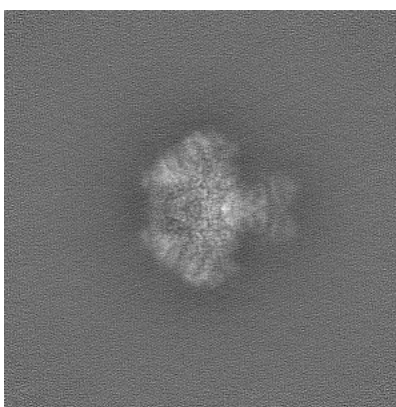


Z

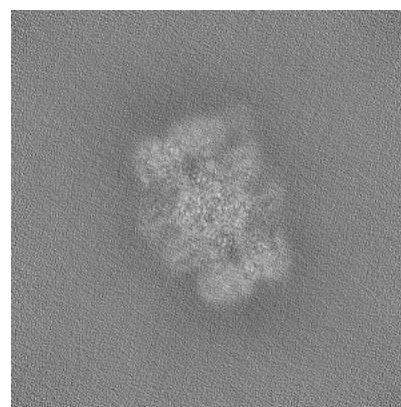
#### 6.1.2 Raw map



X



Y

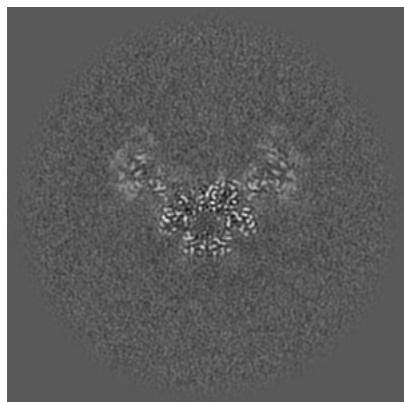


Z

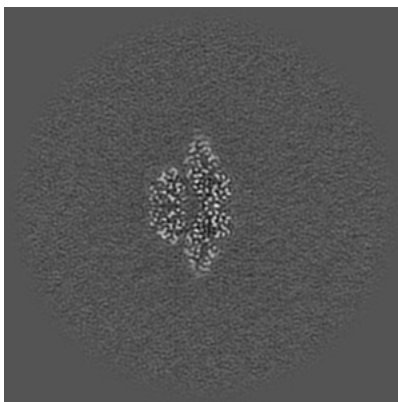
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

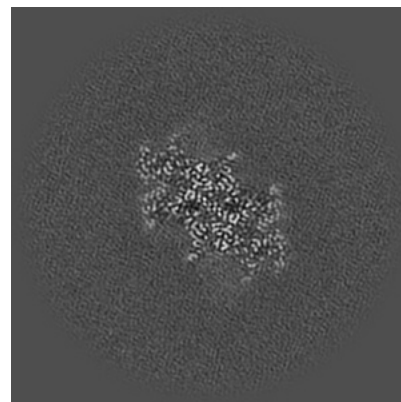
### 6.2.1 Primary map



X Index: 190

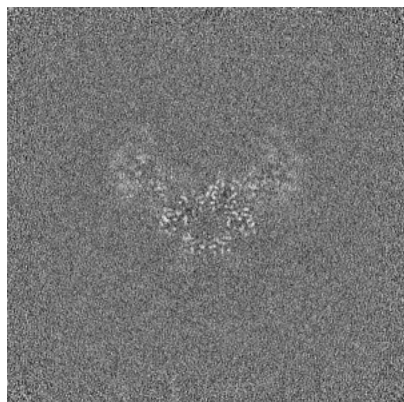


Y Index: 190

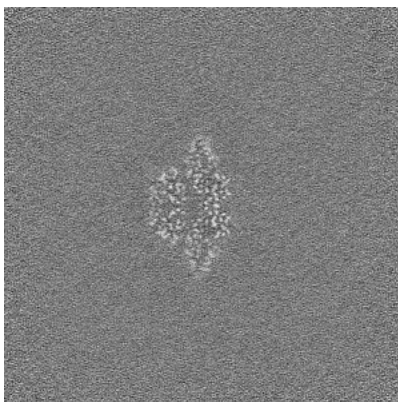


Z Index: 190

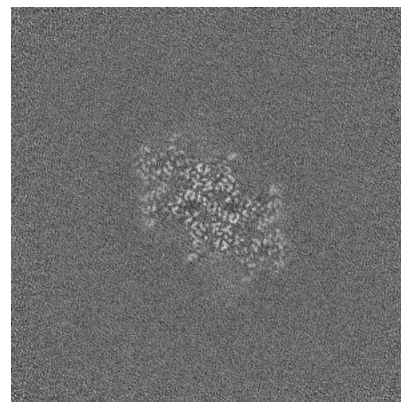
### 6.2.2 Raw map



X Index: 190



Y Index: 190

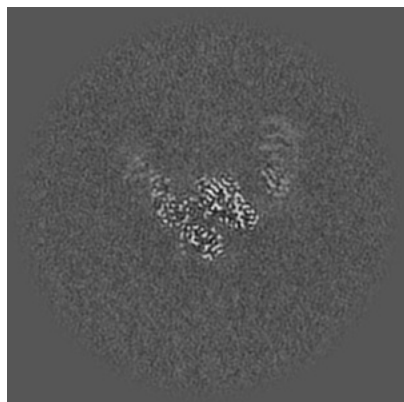


Z Index: 190

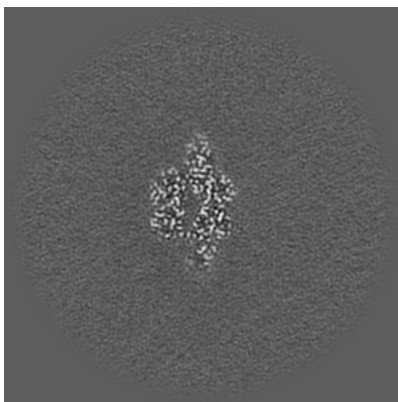
The images above show central slices of the map in three orthogonal directions.

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

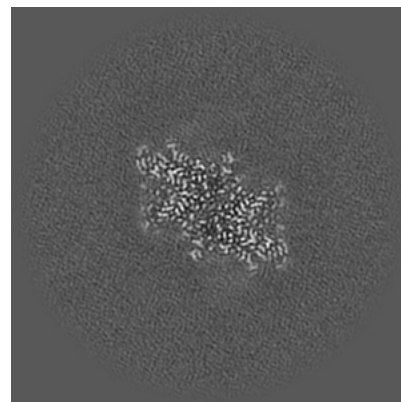
### 6.3.1 Primary map



X Index: 178

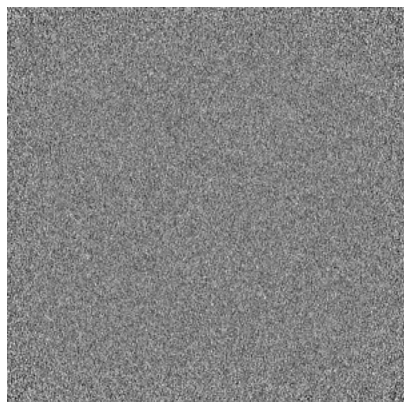


Y Index: 192

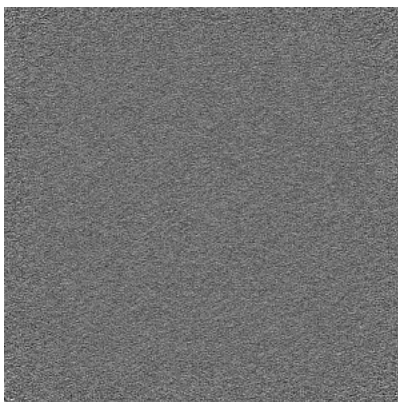


Z Index: 186

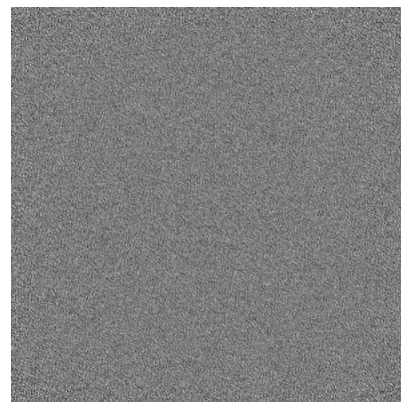
### 6.3.2 Raw map



X Index: 0



Y Index: 0



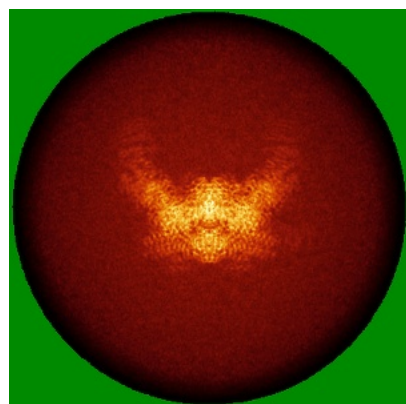
Z Index: 0

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

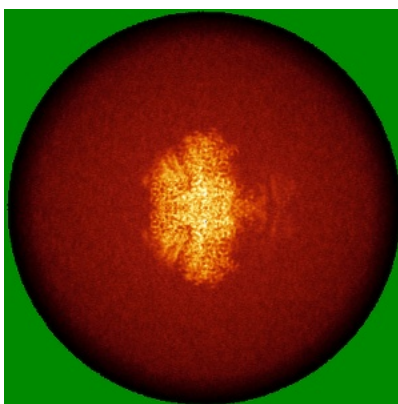


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

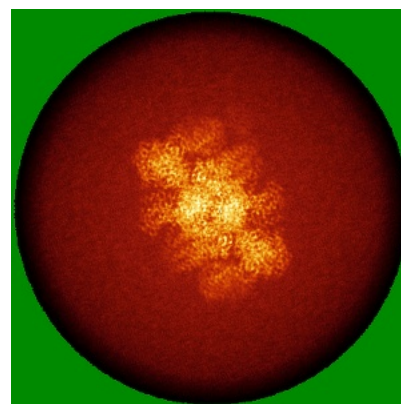
### 6.4.1 Primary map



X

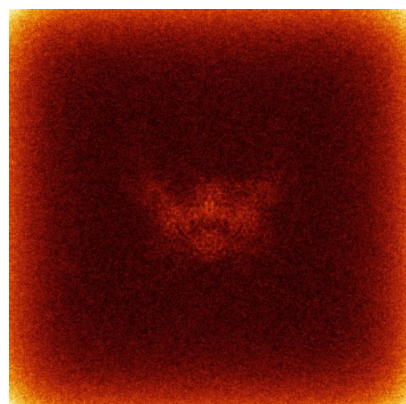


Y

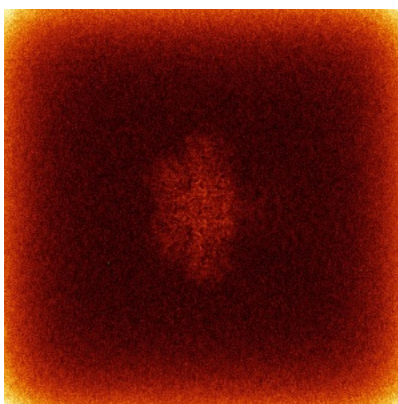


Z

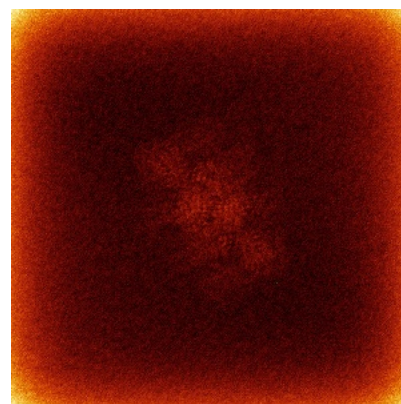
### 6.4.2 Raw map



X



Y

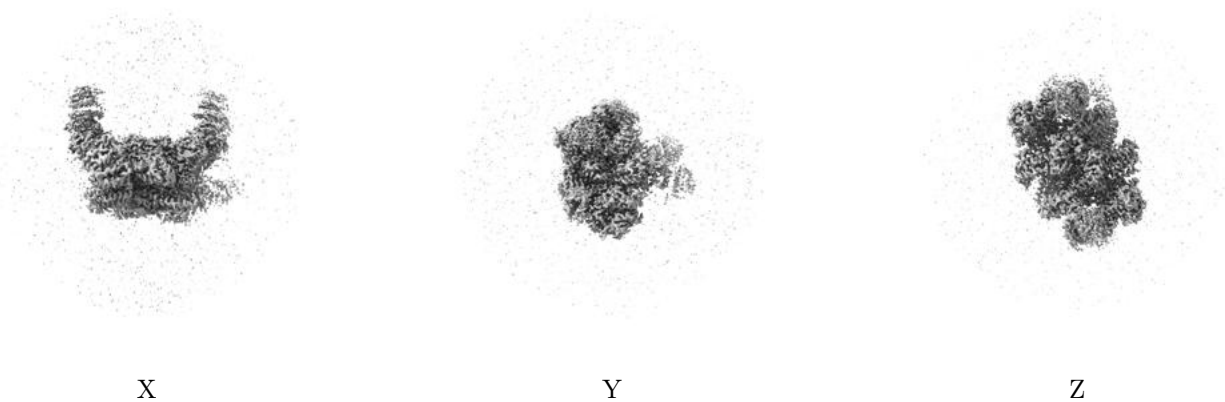


Z

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.

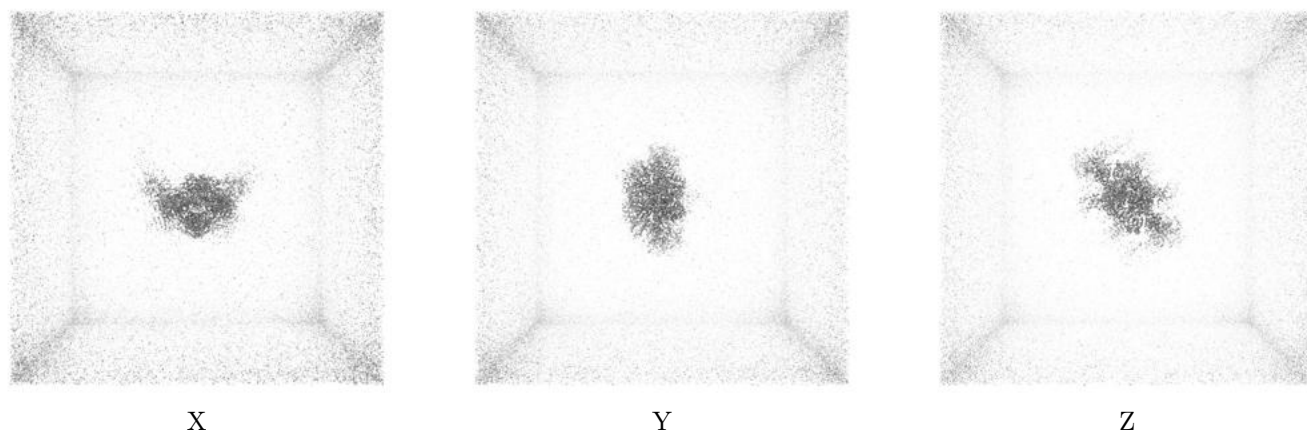
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

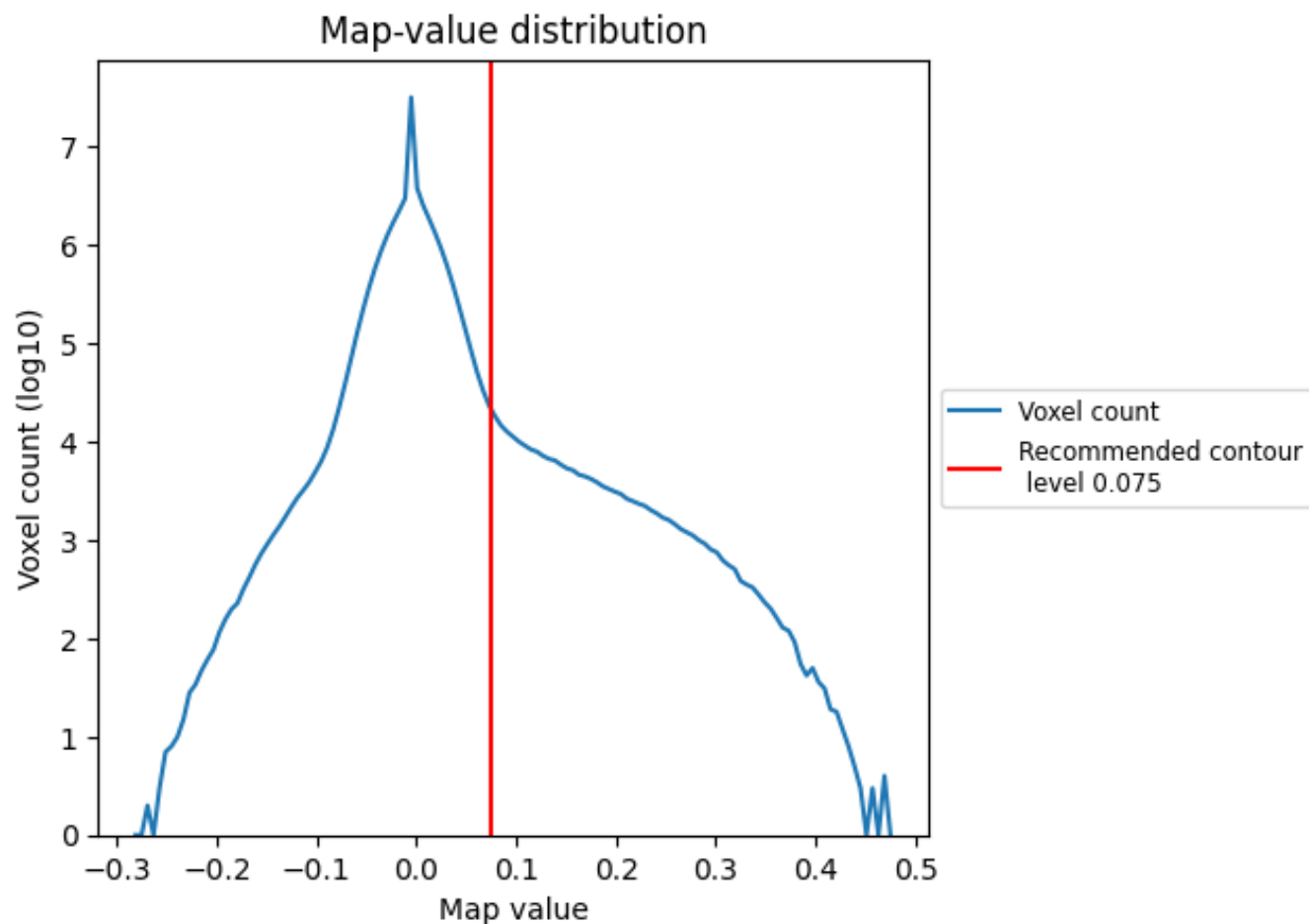
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

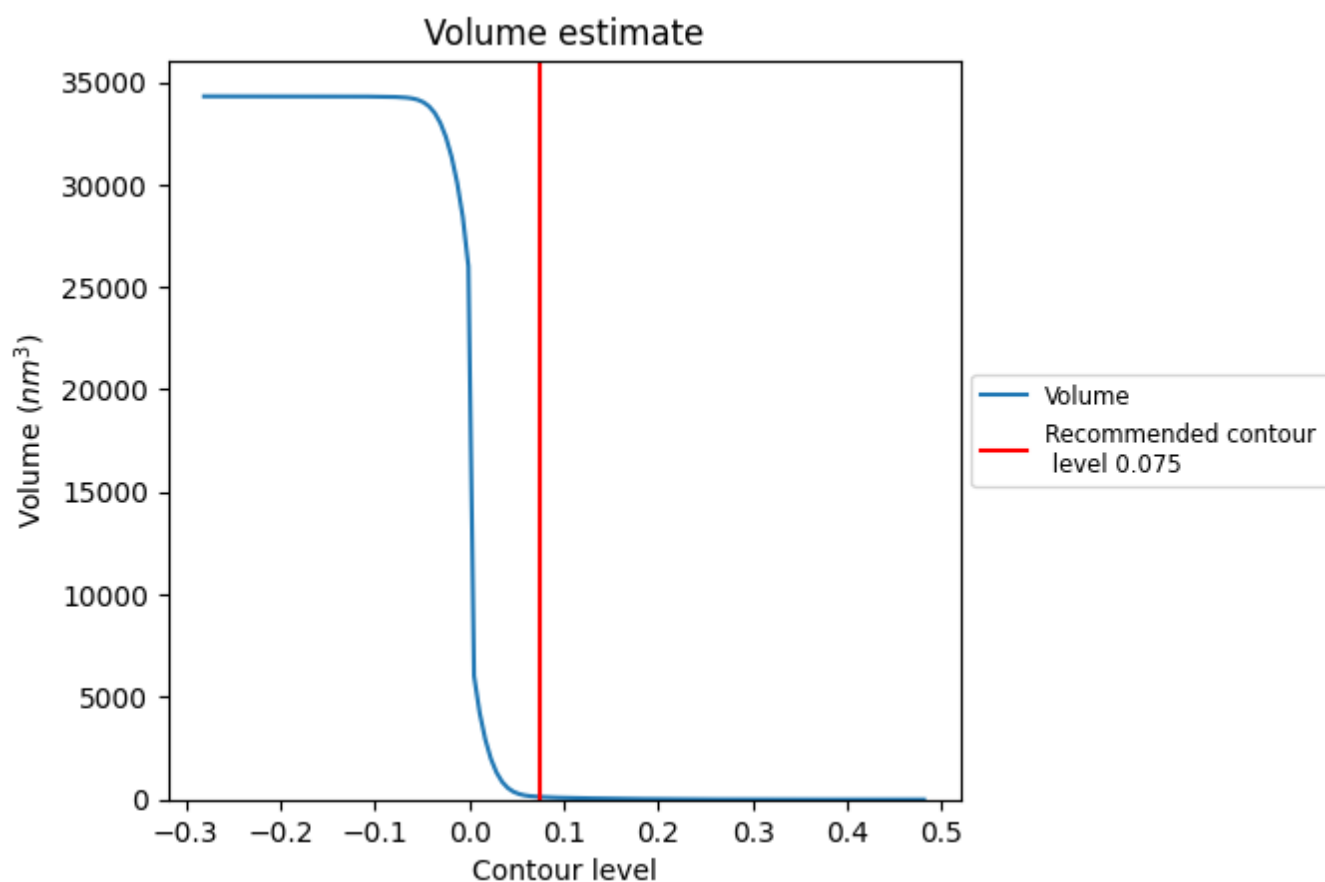
This section contains the results of statistical analysis of the map.

### 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.

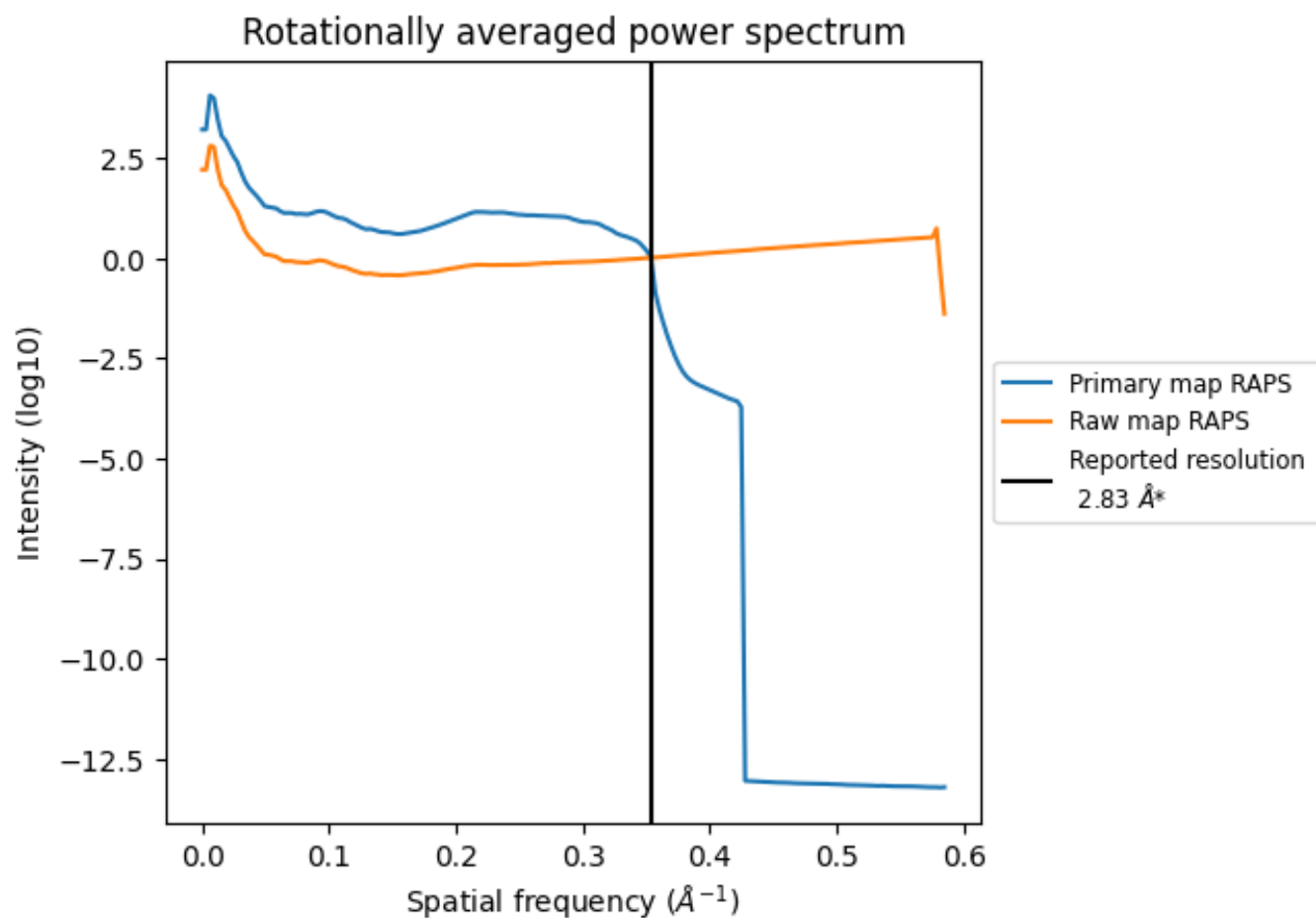
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm<sup>3</sup>; this corresponds to an approximate mass of 116 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 ⓘ



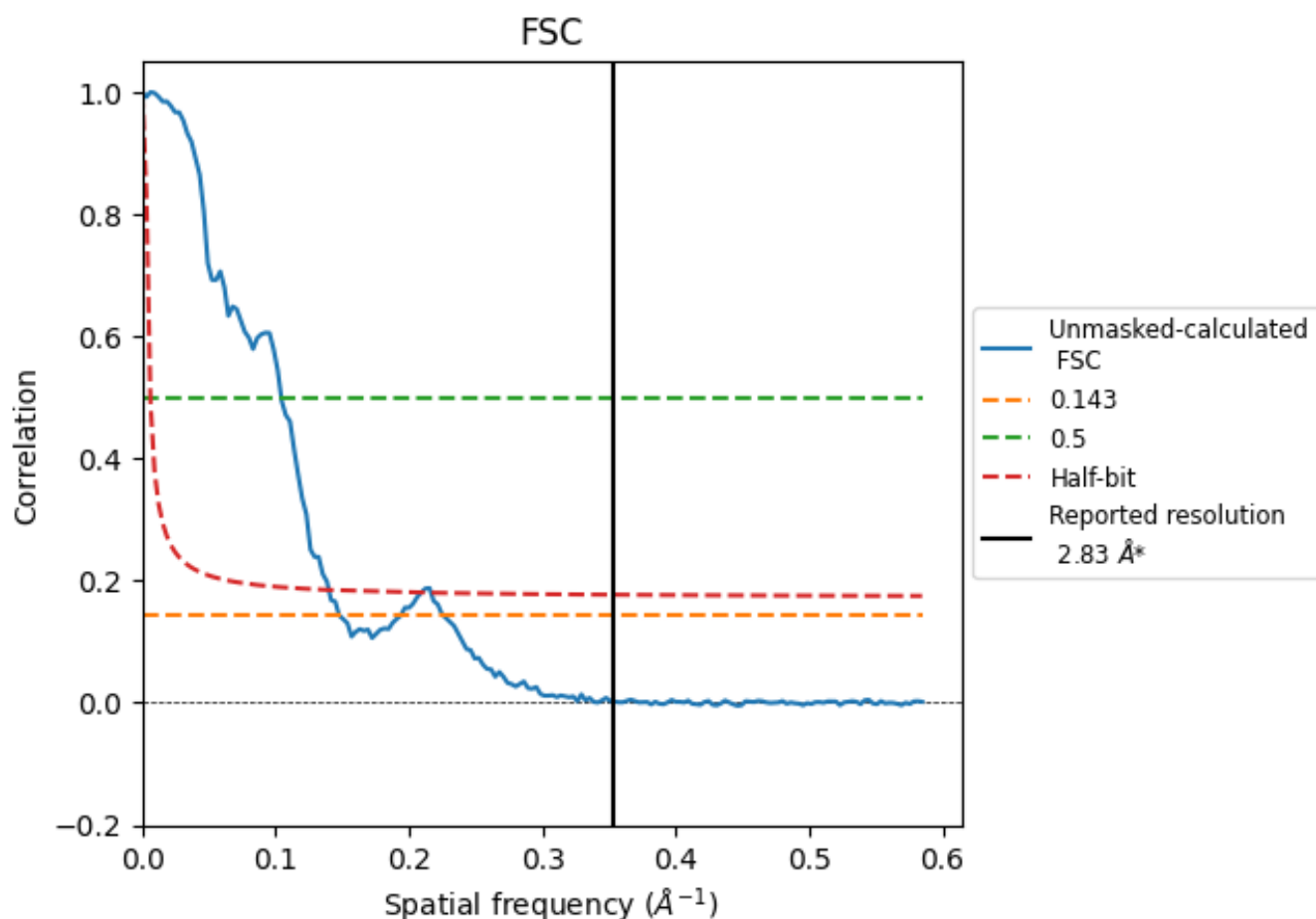
\*Reported resolution corresponds to spatial frequency of 0.353  $\text{\AA}^{-1}$



## 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 0.353  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

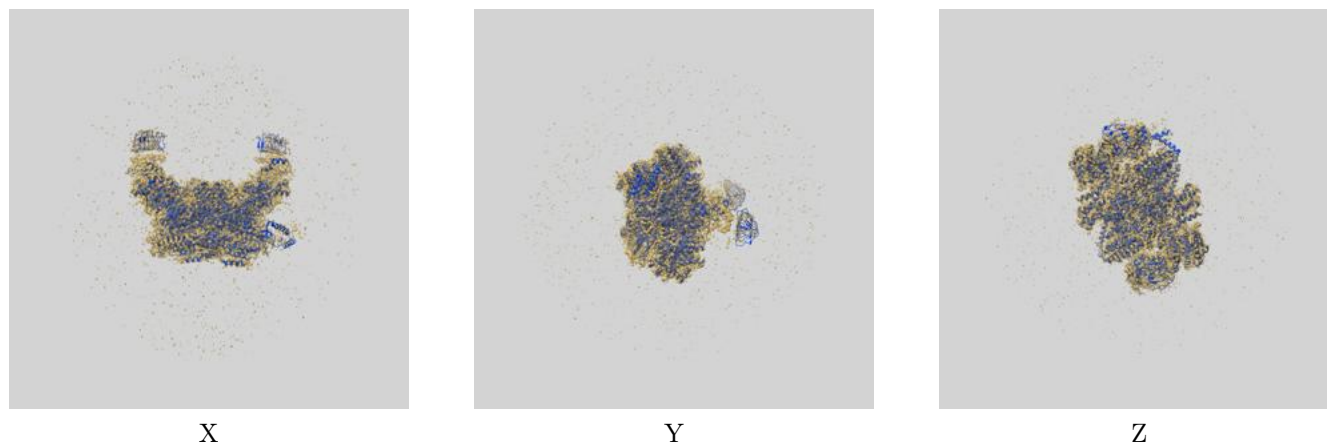
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.77	9.60	7.15

\*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 6.77 differs from the reported value 2.83 by more than 10 %

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

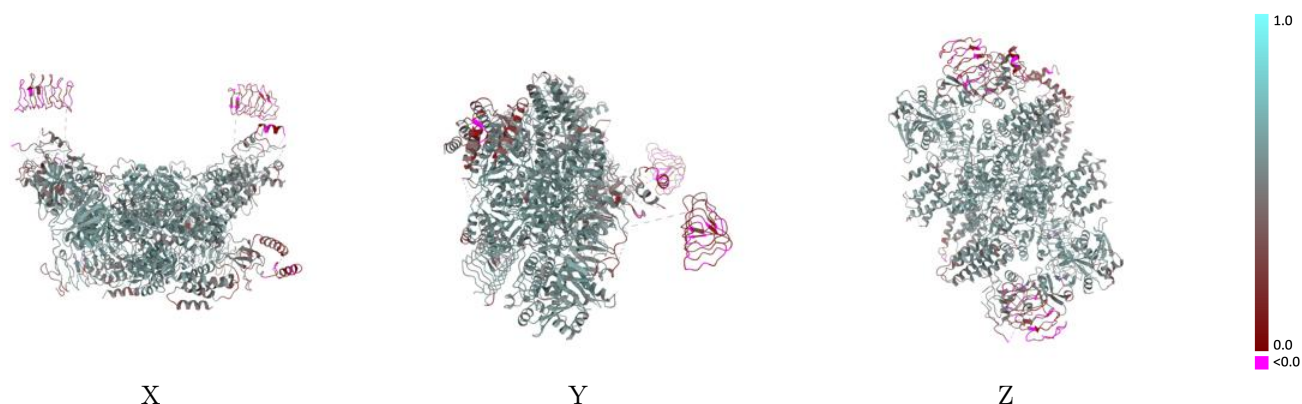
This section contains information regarding the fit between EMDB map EMD-53004 and PDB model 9QC6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



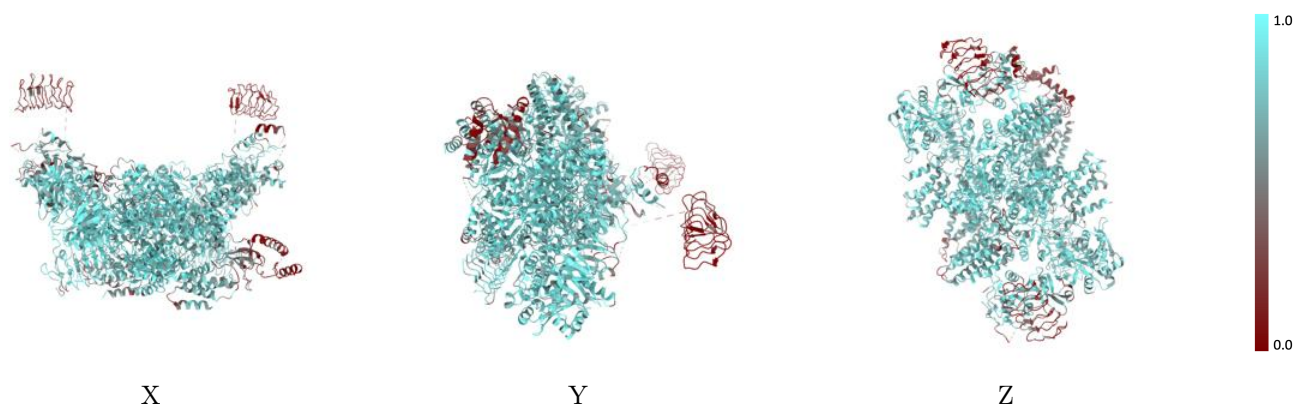
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



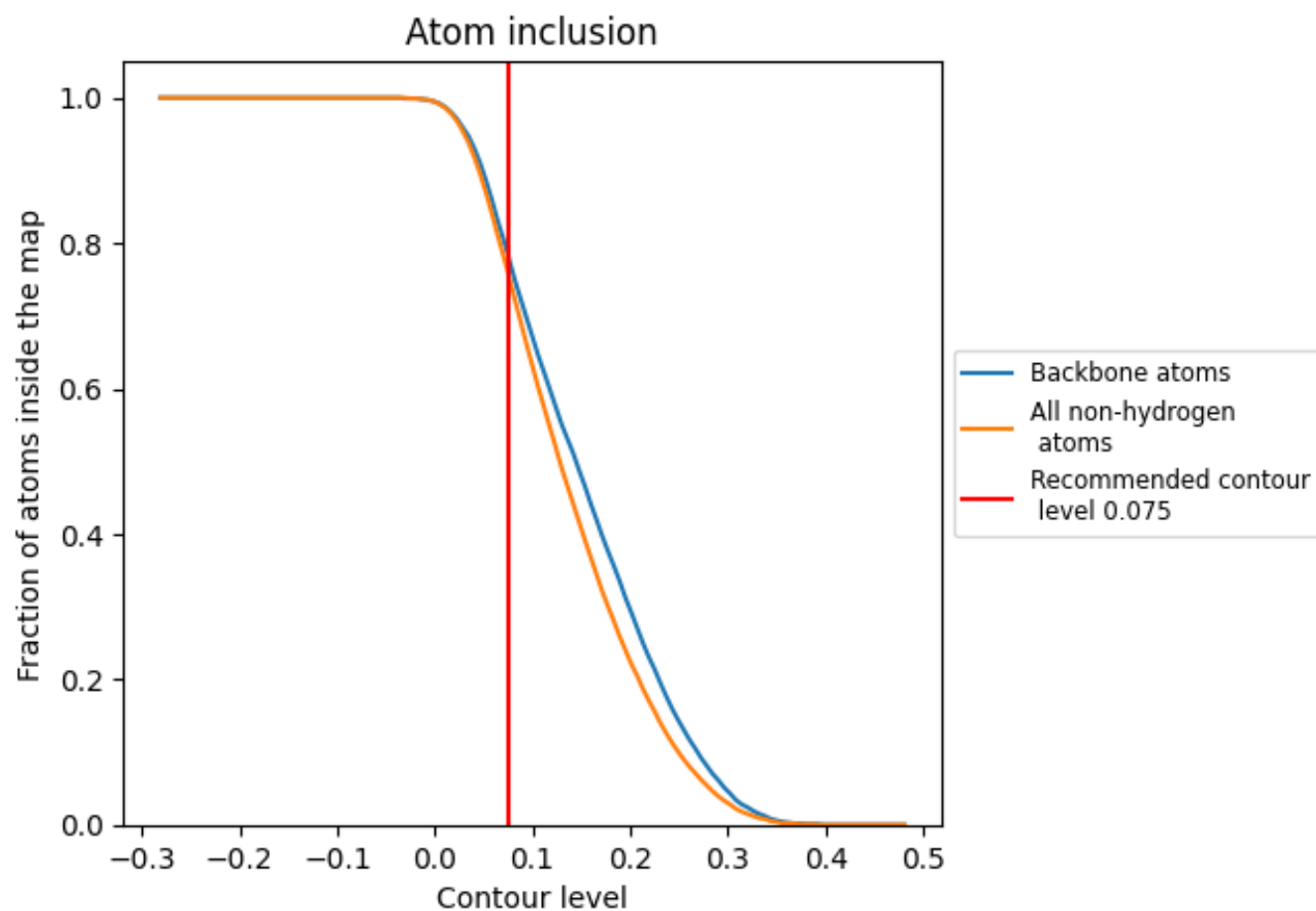
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7600	<div></div> 0.5260
A	<div></div> 0.8080	<div></div> 0.5510
B	<div></div> 0.7690	<div></div> 0.5340
C	<div></div> 0.8530	<div></div> 0.5720
D	<div></div> 0.8500	<div></div> 0.5770
E	<div></div> 0.5420	<div></div> 0.3870
F	<div></div> 0.4880	<div></div> 0.3580
G	<div></div> 0.8630	<div></div> 0.5730
H	<div></div> 0.7810	<div></div> 0.5520
I	<div></div> 0.8170	<div></div> 0.5580
J	<div></div> 0.8080	<div></div> 0.5530
K	<div></div> 0.3210	<div></div> 0.3540

1.0

0.0

<0.0