



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 11:12 PM EST

PDB ID : 6O85
EMDB ID : EMD-0651
Title : Electron cryo-microscopy of the eukaryotic translation initiation factor 2B bound to eukaryotic translation initiation factor 2 from Homo sapiens
Authors : Nguyen, H.C.; Kenner, L.R.; Frost, A.S.
Deposited on : 2019-03-08
Resolution : 3.03 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

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

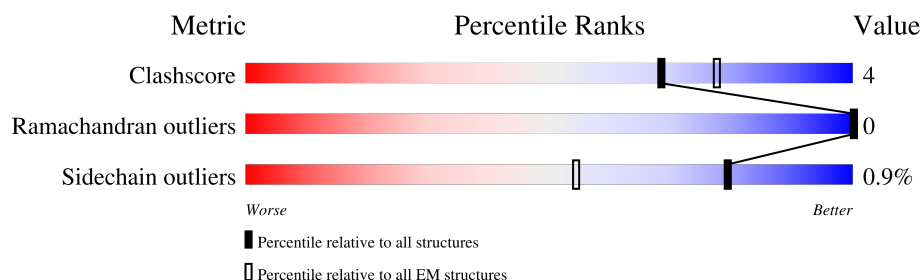
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	721	<div> <div>7%</div> <div>52%</div> <div>7%</div> <div>41%</div> </div>
1	B	721	<div> <div>20%</div> <div>75%</div> <div>6%</div> <div>18%</div> </div>
2	C	368	<div> <div>7%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
2	D	368	<div> <div>10%</div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
3	E	523	<div> <div>•</div> <div>59%</div> <div>9%</div> <div>32%</div> </div>
3	F	523	<div> <div>5%</div> <div>59%</div> <div>9%</div> <div>32%</div> </div>
4	G	305	<div> <div>6%</div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div>
4	H	305	<div> <div>15%</div> <div>79%</div> <div>14%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	452	<div><div></div><div>18%</div><div>50%</div><div></div><div>47%</div></div>
5	J	452	<div><div></div><div>16%</div><div>50%</div><div></div><div>47%</div></div>
6	L	314	<div><div></div><div>11%</div><div>84%</div><div></div><div>12%</div></div>
7	S	472	<div><div></div><div>22%</div><div>86%</div><div></div><div>13%</div></div>
8	d	14	<div><div></div><div>29%</div><div>100%</div><div></div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28576 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3172	2043	524	590	15		
1	B	590	Total	C	N	O	S	0	0
			3994	2536	689	754	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	317	Total	C	N	O	S	0	0
			2415	1558	394	448	15		
2	D	318	Total	C	N	O	S	0	0
			2425	1564	397	449	15		

There are 36 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	357	Total	C	N	O	S	0	0
			2712	1751	447	500	14		
3	F	357	Total	C	N	O	S	0	0
			2713	1752	447	500	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	285	Total	C	N	O	S	0	0
			2025	1324	328	365	8		
4	H	285	Total	C	N	O	S	0	0
			2025	1324	328	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	240	Total	C	N	O	S	0	0
			1609	1050	266	285	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	240	Total	C	N	O	S	0	0
			1609	1050	266	285	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	275	Total	C	N	O	S	0	0
			1651	1047	307	294	3		

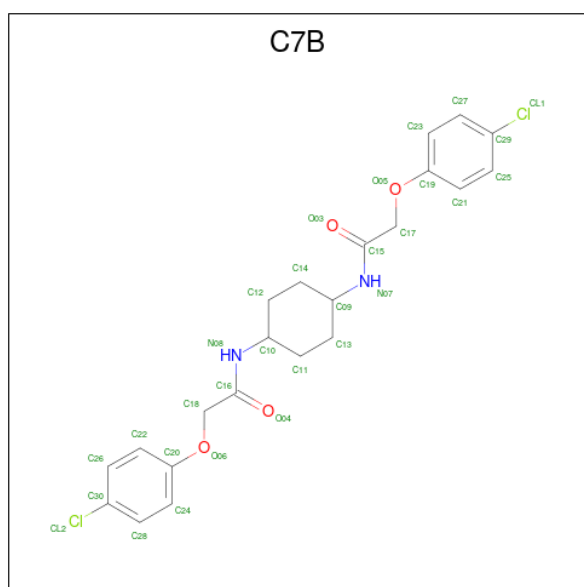
- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	410	Total	C	N	O	S	0	0
			2096	1264	421	410	1		

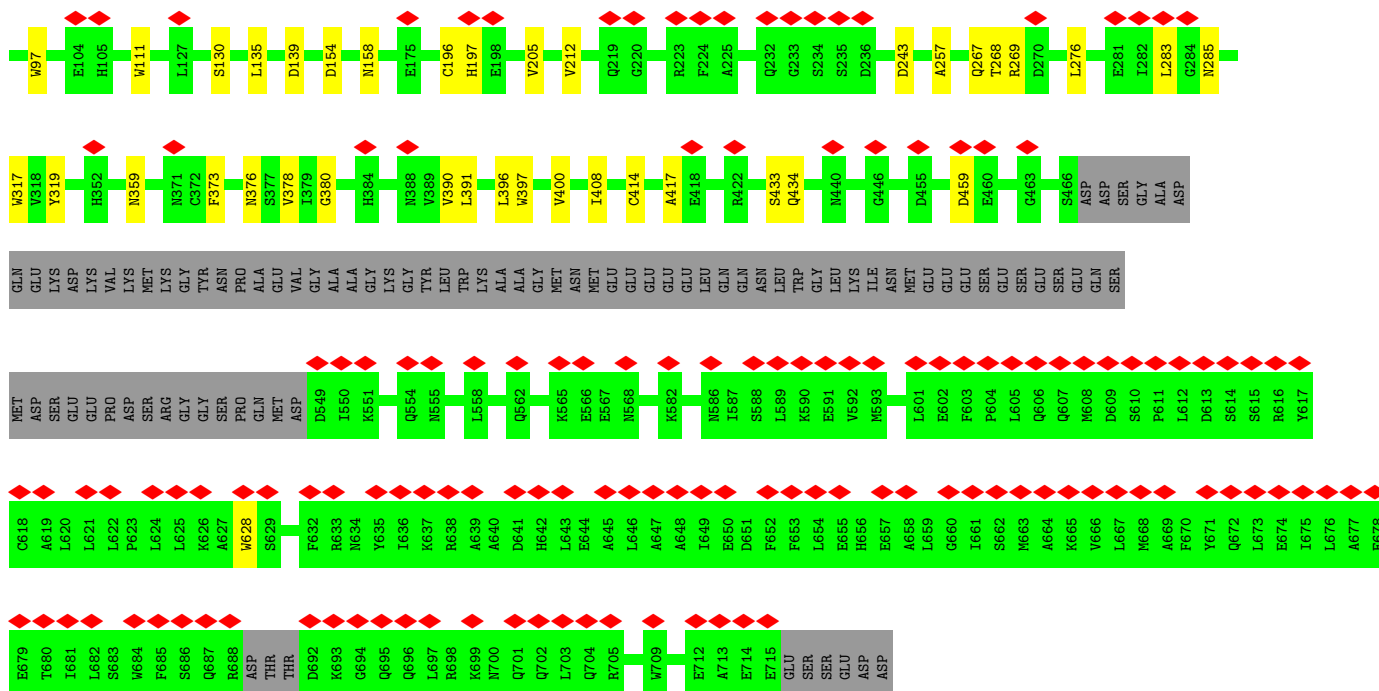
- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	d	14	Total	C	N	O	0	0
			70	42	14	14		

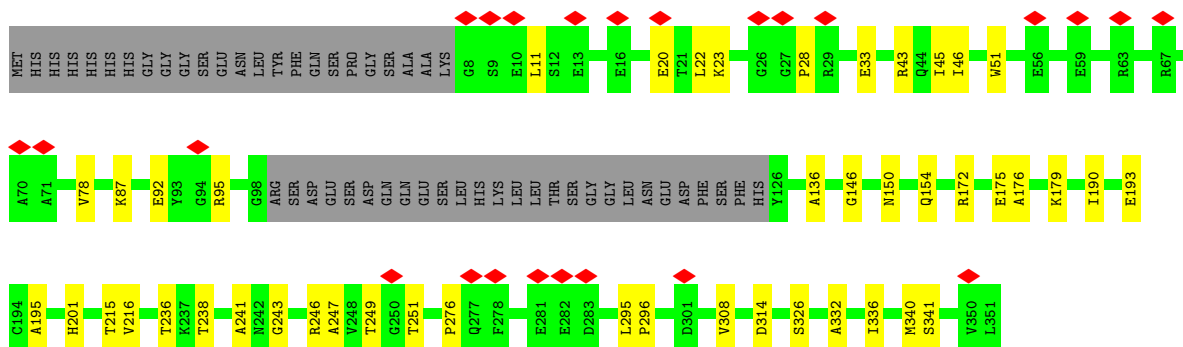
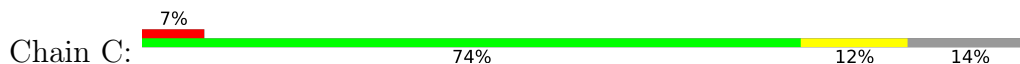
- Molecule 9 is 2-(4-chloranylphenoxy)- {N}-[4-[2-(4-chloranylphenoxy)ethanoylamino]cyclohexyl]ethanamide (three-letter code: C7B) (formula: C₂₂H₂₄Cl₂N₂O₄).



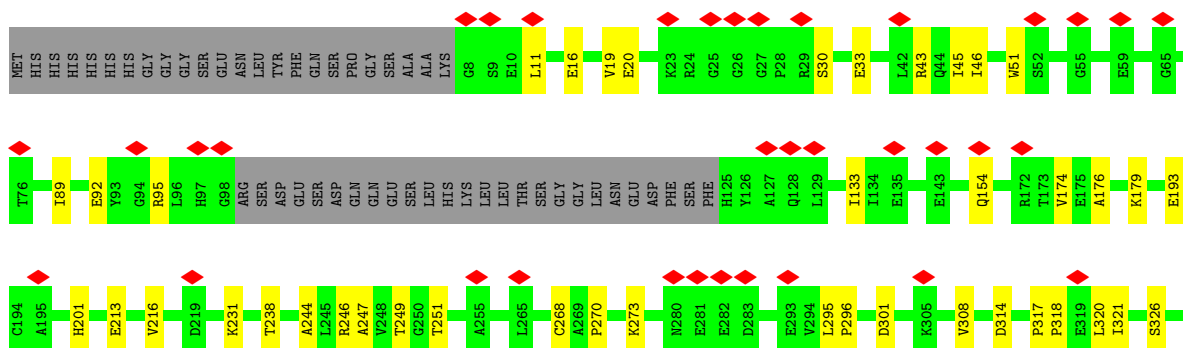
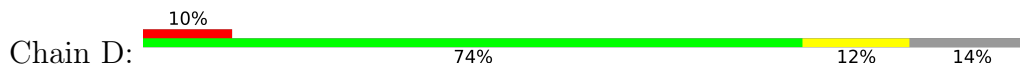
Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	Cl	N	O	1
			60	44	4	4	8	



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

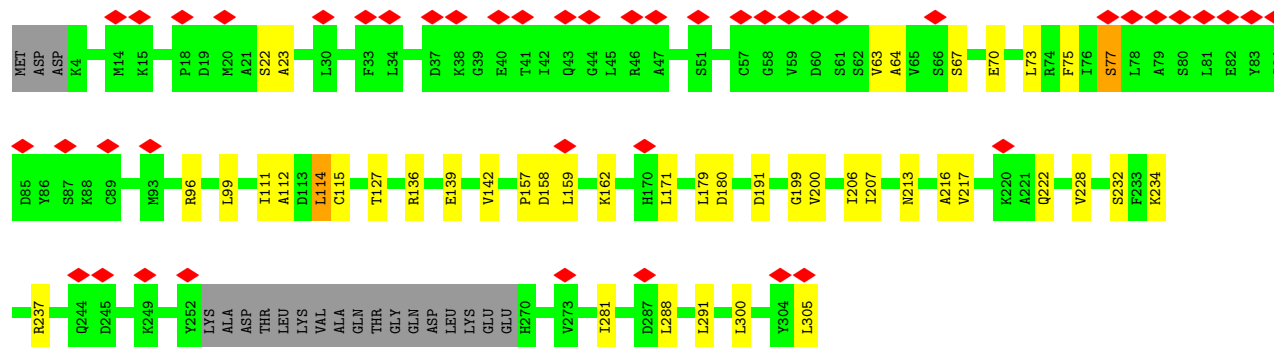
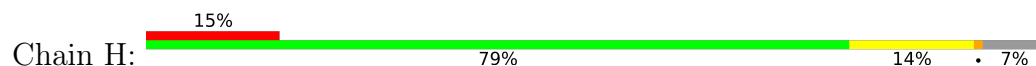


• Molecule 2: Translation initiation factor eIF-2B subunit beta

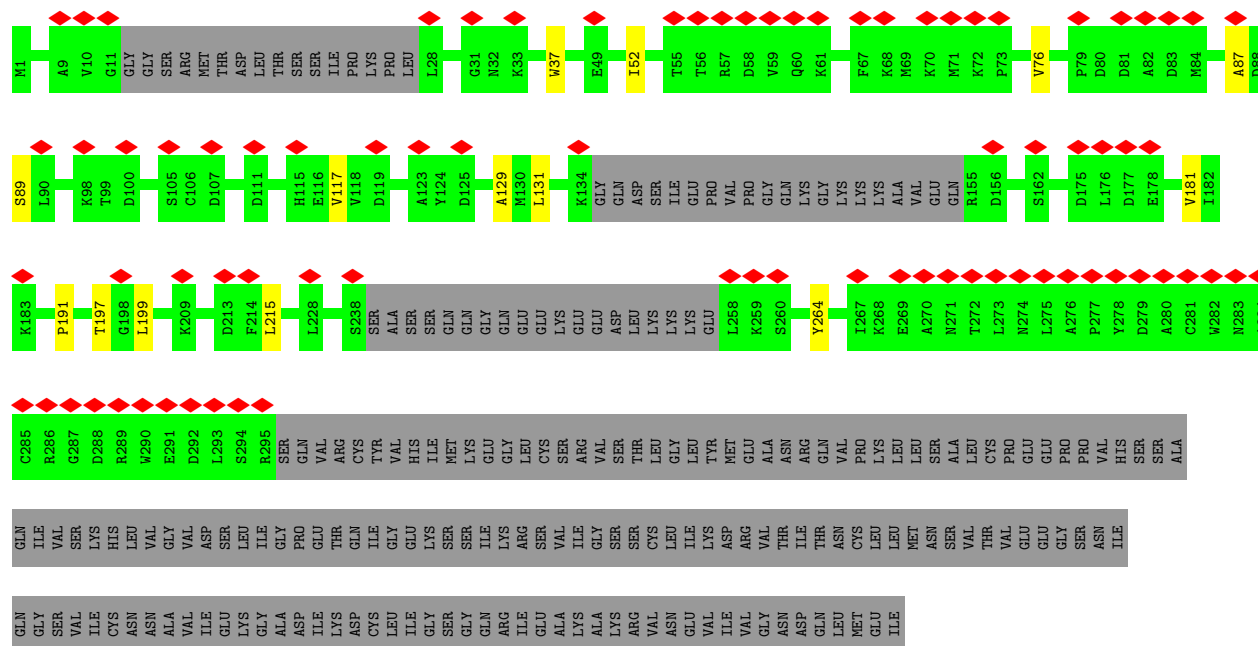




• Molecule 4: Translation initiation factor eIF-2B subunit alpha

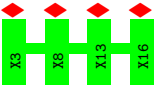


• Molecule 5: Translation initiation factor eIF-2B subunit gamma



• Molecule 5: 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	44157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	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	2.372	Depositor
Minimum map value	-1.177	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	394.56, 394.56, 394.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82199997, 0.82199997, 0.82199997	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C7B

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	0.39	4/3236 (0.1%)	0.69	9/4403 (0.2%)
1	B	0.39	5/4057 (0.1%)	0.63	11/5546 (0.2%)
2	C	0.32	1/2460 (0.0%)	0.54	2/3318 (0.1%)
2	D	0.32	1/2471 (0.0%)	0.54	2/3333 (0.1%)
3	E	0.37	3/2761 (0.1%)	0.61	6/3736 (0.2%)
3	F	0.38	3/2762 (0.1%)	0.61	6/3738 (0.2%)
4	G	0.28	0/2061	0.59	3/2798 (0.1%)
4	H	0.28	0/2061	0.59	3/2798 (0.1%)
5	I	0.34	1/1630 (0.1%)	0.59	2/2219 (0.1%)
5	J	0.34	1/1630 (0.1%)	0.59	2/2219 (0.1%)
6	L	0.32	1/1670 (0.1%)	0.51	2/2282 (0.1%)
7	S	0.35	2/2100 (0.1%)	0.56	4/2896 (0.1%)
All	All	0.35	22/28899 (0.1%)	0.60	52/39286 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	628	TRP	CD2-CE2	6.24	1.48	1.41
1	A	111	TRP	CD2-CE2	6.22	1.48	1.41
7	S	456	TRP	CD2-CE2	6.22	1.48	1.41
1	A	97	TRP	CD2-CE2	6.20	1.48	1.41
2	C	51	TRP	CD2-CE2	6.18	1.48	1.41
5	J	37	TRP	CD2-CE2	6.18	1.48	1.41
1	B	97	TRP	CD2-CE2	6.16	1.48	1.41
5	I	37	TRP	CD2-CE2	6.16	1.48	1.41
2	D	51	TRP	CD2-CE2	6.15	1.48	1.41
1	A	317	TRP	CD2-CE2	6.14	1.48	1.41
1	B	317	TRP	CD2-CE2	6.14	1.48	1.41
1	B	397	TRP	CD2-CE2	6.14	1.48	1.41
3	F	350	TRP	CD2-CE2	6.14	1.48	1.41
7	S	451	TRP	CD2-CE2	6.14	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	366	TRP	CD2-CE2	6.13	1.48	1.41
1	A	397	TRP	CD2-CE2	6.12	1.48	1.41
1	B	111	TRP	CD2-CE2	6.11	1.48	1.41
3	F	366	TRP	CD2-CE2	6.10	1.48	1.41
6	L	135	TRP	CD2-CE2	6.07	1.48	1.41
3	E	350	TRP	CD2-CE2	6.07	1.48	1.41
3	E	476	TRP	CD2-CE2	6.05	1.48	1.41
3	F	476	TRP	CD2-CE2	5.99	1.48	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	TRP	CD2-CE3-CZ3	8.19	129.45	118.80
1	A	397	TRP	CD2-CE3-CZ3	8.18	129.44	118.80
3	F	476	TRP	CD2-CE3-CZ3	8.18	129.43	118.80
3	F	350	TRP	CD2-CE3-CZ3	8.17	129.42	118.80
6	L	135	TRP	CD2-CE3-CZ3	8.17	129.42	118.80
2	D	51	TRP	CD2-CE3-CZ3	8.15	129.40	118.80
1	A	97	TRP	CD2-CE3-CZ3	8.15	129.40	118.80
3	E	366	TRP	CD2-CE3-CZ3	8.15	129.40	118.80
1	B	397	TRP	CD2-CE3-CZ3	8.14	129.39	118.80
3	E	476	TRP	CD2-CE3-CZ3	8.13	129.37	118.80
1	B	317	TRP	CD2-CE3-CZ3	8.13	129.37	118.80
1	B	628	TRP	CD2-CE3-CZ3	8.11	129.34	118.80
5	I	37	TRP	CD2-CE3-CZ3	8.11	129.34	118.80
3	F	366	TRP	CD2-CE3-CZ3	8.10	129.33	118.80
7	S	456	TRP	CD2-CE3-CZ3	8.10	129.33	118.80
7	S	451	TRP	CD2-CE3-CZ3	8.10	129.33	118.80
2	C	51	TRP	CD2-CE3-CZ3	8.10	129.33	118.80
3	E	350	TRP	CD2-CE3-CZ3	8.10	129.32	118.80
1	B	111	TRP	CD2-CE3-CZ3	8.09	129.32	118.80
5	J	37	TRP	CD2-CE3-CZ3	8.08	129.31	118.80
1	B	97	TRP	CD2-CE3-CZ3	8.07	129.29	118.80
1	A	111	TRP	CD2-CE3-CZ3	8.05	129.27	118.80
1	A	283	LEU	CA-CB-CG	8.01	133.72	115.30
1	B	283	LEU	CA-CB-CG	7.79	133.21	115.30
4	G	114	LEU	CA-CB-CG	7.65	132.90	115.30
4	H	114	LEU	CA-CB-CG	7.64	132.86	115.30
4	G	180	ASP	CB-CG-OD1	6.17	123.86	118.30
4	H	180	ASP	CB-CG-OD1	6.17	123.85	118.30
4	G	114	LEU	CB-CG-CD1	5.55	120.43	111.00
4	H	114	LEU	CB-CG-CD1	5.53	120.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	TRP	CE2-CD2-CE3	5.20	124.94	118.70
5	J	37	TRP	CE2-CD2-CE3	5.19	124.93	118.70
7	S	456	TRP	CE2-CD2-CE3	5.18	124.92	118.70
7	S	451	TRP	CE2-CD2-CE3	5.16	124.89	118.70
1	A	97	TRP	CE2-CD2-CE3	5.16	124.89	118.70
1	B	317	TRP	CE2-CD2-CE3	5.16	124.89	118.70
3	E	366	TRP	CE2-CD2-CE3	5.16	124.89	118.70
5	I	37	TRP	CE2-CD2-CE3	5.16	124.89	118.70
3	E	350	TRP	CE2-CD2-CE3	5.15	124.88	118.70
3	F	366	TRP	CE2-CD2-CE3	5.15	124.88	118.70
3	F	476	TRP	CE2-CD2-CE3	5.15	124.88	118.70
3	E	476	TRP	CE2-CD2-CE3	5.15	124.88	118.70
1	A	397	TRP	CE2-CD2-CE3	5.14	124.87	118.70
1	A	317	TRP	CE2-CD2-CE3	5.13	124.86	118.70
2	D	51	TRP	CE2-CD2-CE3	5.12	124.85	118.70
3	F	350	TRP	CE2-CD2-CE3	5.12	124.85	118.70
2	C	51	TRP	CE2-CD2-CE3	5.12	124.84	118.70
1	A	111	TRP	CE2-CD2-CE3	5.11	124.83	118.70
1	B	628	TRP	CE2-CD2-CE3	5.11	124.83	118.70
1	B	397	TRP	CE2-CD2-CE3	5.10	124.82	118.70
1	B	111	TRP	CE2-CD2-CE3	5.09	124.81	118.70
6	L	135	TRP	CE2-CD2-CE3	5.08	124.80	118.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3172	0	3018	30	0
1	B	3994	0	3386	22	0
2	C	2415	0	2390	27	0
2	D	2425	0	2397	26	0
3	E	2712	0	2718	26	0
3	F	2713	0	2719	30	0
4	G	2025	0	1909	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2025	0	1909	23	0
5	I	1609	0	1377	6	0
5	J	1609	0	1377	6	0
6	L	1651	0	1123	7	0
7	S	2096	0	1026	1	0
8	d	70	0	16	0	0
9	C	60	0	0	0	0
All	All	28576	0	25365	207	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 4.

All (207) 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)
4:H:206:ILE:HG21	4:H:228:VAL:HG11	1.79	0.64
4:G:206:ILE:HG21	4:G:228:VAL:HG11	1.79	0.64
3:F:407:ALA:HB3	3:F:415:MET:HB3	1.81	0.62
1:B:72:ASN:HD21	1:B:380:GLY:HA2	1.65	0.61
1:A:214:HIS:HB2	1:A:230:LEU:HD21	1.83	0.61
1:A:168:HIS:ND1	1:A:182:THR:OG1	2.35	0.60
1:A:211:ARG:HA	1:A:288:HIS:HA	1.83	0.60
3:E:513:PRO:O	3:E:516:LEU:HB2	2.01	0.59
6:L:5:CYS:SG	6:L:6:ARG:N	2.76	0.58
1:B:205:VAL:HG12	1:B:212:VAL:HA	1.86	0.58
2:C:154:GLN:NE2	2:C:326:SER:O	2.36	0.58
3:F:405:ALA:HB3	3:F:438:CYS:HB2	1.85	0.57
4:G:179:LEU:HD21	4:H:157:PRO:HG3	1.86	0.57
2:D:154:GLN:NE2	2:D:326:SER:O	2.38	0.57
3:E:405:ALA:HB3	3:E:438:CYS:HB2	1.86	0.57
3:F:431:ASN:ND2	4:G:222:GLN:O	2.37	0.57
3:E:403:LEU:HD13	3:E:420:THR:HG23	1.88	0.56
4:H:111:ILE:O	4:H:115:CYS:HB3	2.06	0.56
1:B:276:LEU:HD11	1:B:285:ASN:HB2	1.87	0.56
1:A:51:SER:HB2	1:A:65:ARG:HD2	1.87	0.55
4:H:112:ALA:HB2	4:H:136:ARG:HG3	1.88	0.55
2:D:249:THR:HA	2:D:314:ASP:HB2	1.89	0.55
3:E:407:ALA:HB3	3:E:415:MET:HB3	1.88	0.55
3:E:431:ASN:ND2	4:H:222:GLN:O	2.37	0.55
4:G:111:ILE:O	4:G:115:CYS:HB3	2.06	0.55
4:H:73:LEU:O	4:H:77:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:157:PRO:HG3	4:H:179:LEU:HD21	1.89	0.55
4:G:73:LEU:O	4:G:77:SER:OG	2.25	0.54
4:G:112:ALA:HB2	4:G:136:ARG:HG3	1.88	0.54
2:C:332:ALA:HB2	3:E:411:ASN:HA	1.88	0.54
2:D:231:LYS:NZ	3:F:449:THR:OG1	2.41	0.54
1:A:168:HIS:HD1	1:A:182:THR:HG1	1.49	0.54
1:B:139:ASP:HB2	1:B:257:ALA:HB1	1.89	0.54
3:E:245:ASN:HB2	6:L:79:LYS:HA	1.90	0.54
1:B:243:ASP:HB3	5:J:191:PRO:HB2	1.89	0.53
2:D:193:GLU:OE1	2:D:201:HIS:NE2	2.37	0.53
3:F:513:PRO:O	3:F:516:LEU:HB2	2.08	0.53
1:A:65:ARG:HA	1:A:68:LEU:HD23	1.90	0.53
2:D:332:ALA:HB2	3:F:411:ASN:HA	1.91	0.53
1:A:70:LEU:HD22	1:A:310:CYS:HB2	1.90	0.52
1:B:196:CYS:SG	1:B:197:HIS:N	2.82	0.52
2:C:238:THR:HB	2:C:246:ARG:HG2	1.91	0.52
1:A:368:ILE:HA	1:A:385:ILE:HB	1.90	0.52
3:F:368:GLU:O	3:F:371:HIS:HB2	2.10	0.52
3:F:210:LEU:HD12	3:F:213:GLN:HE21	1.75	0.52
1:B:130:SER:OG	1:B:267:GLN:O	2.27	0.51
2:C:249:THR:HA	2:C:314:ASP:HB2	1.92	0.51
3:E:311:LYS:HD3	3:E:441:TYR:HB3	1.92	0.51
3:E:168:PRO:O	3:E:265:GLN:NE2	2.35	0.51
2:D:308:VAL:HG22	3:E:385:TYR:HB3	1.91	0.51
3:E:319:ILE:HG22	3:E:345:ILE:HD11	1.93	0.50
1:A:414:CYS:HB2	1:A:432:THR:HA	1.91	0.50
3:E:332:VAL:HG13	3:E:399:SER:H	1.75	0.50
1:A:139:ASP:HB2	1:A:257:ALA:HB1	1.93	0.50
2:D:11:LEU:HD21	2:D:45:ILE:HA	1.92	0.49
5:I:52:ILE:HA	5:I:76:VAL:HB	1.94	0.49
2:D:216:VAL:HB	3:E:484:LEU:HD13	1.94	0.49
2:D:30:SER:OG	2:D:33:GLU:OE1	2.24	0.49
1:B:414:CYS:HB2	1:B:433:SER:H	1.77	0.49
2:C:43:ARG:HA	2:C:46:ILE:HG12	1.93	0.49
2:C:87:LYS:NZ	2:C:341:SER:O	2.45	0.49
2:C:146:GLY:O	2:C:150:ASN:ND2	2.45	0.49
3:E:413:SER:HB3	3:E:491:VAL:HB	1.93	0.49
3:F:305:ASP:HA	3:F:308:VAL:HG12	1.95	0.49
3:E:177:VAL:HG21	3:E:485:LEU:HD22	1.95	0.49
2:C:172:ARG:HA	2:C:175:GLU:HG2	1.95	0.48
1:A:66:VAL:HG12	1:A:76:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:473:LEU:HD13	3:E:484:LEU:HD11	1.95	0.48
2:D:244:ALA:HB2	2:D:318:PRO:HD3	1.94	0.48
5:J:52:ILE:HA	5:J:76:VAL:HB	1.94	0.48
4:H:158:ASP:OD1	4:H:158:ASP:N	2.46	0.48
4:G:158:ASP:N	4:G:158:ASP:OD1	2.46	0.48
3:E:234:GLN:NE2	3:E:305:ASP:OD1	2.45	0.48
4:H:159:LEU:HD23	4:H:162:LYS:HD2	1.96	0.48
1:A:243:ASP:HB3	5:I:191:PRO:HB2	1.96	0.47
2:C:190:ILE:HG23	2:C:215:THR:HB	1.95	0.47
2:C:193:GLU:OE1	2:C:201:HIS:NE2	2.47	0.47
1:A:356:LEU:HD22	1:A:360:VAL:HG11	1.96	0.47
1:A:213:LEU:HB3	1:A:230:LEU:HG	1.97	0.47
1:B:417:ALA:HA	1:B:434:GLN:HA	1.97	0.47
2:C:11:LEU:HD11	2:C:45:ILE:HA	1.96	0.47
1:B:391:LEU:HD23	1:B:408:ILE:HB	1.97	0.47
2:C:195:ALA:HB1	3:F:387:LEU:HD13	1.96	0.47
2:D:174:VAL:HG22	2:D:268:CYS:HB2	1.96	0.47
3:F:334:LEU:HB3	3:F:401:VAL:HG22	1.96	0.47
6:L:23:VAL:HB	6:L:64:ILE:HA	1.97	0.47
3:F:473:LEU:HD13	3:F:484:LEU:HD11	1.97	0.47
4:G:206:ILE:HG12	4:G:281:ILE:HD11	1.97	0.47
4:G:159:LEU:HD23	4:G:162:LYS:HD2	1.96	0.46
2:C:20:GLU:HA	2:C:23:LYS:HB2	1.97	0.46
3:F:202:VAL:HG23	3:F:203:ILE:HG12	1.97	0.46
4:G:142:VAL:HG21	4:G:171:LEU:HD21	1.97	0.46
4:G:288:LEU:HB2	4:G:291:LEU:HD11	1.98	0.46
1:A:407:GLN:HB3	1:A:409:HIS:HE1	1.80	0.46
2:C:308:VAL:HG22	3:F:385:TYR:HB3	1.97	0.46
4:H:142:VAL:HG21	4:H:171:LEU:HD21	1.97	0.46
3:F:167:VAL:HG21	3:F:203:ILE:HD11	1.98	0.46
4:G:191:ASP:N	4:G:191:ASP:OD1	2.48	0.46
4:H:191:ASP:OD1	4:H:191:ASP:N	2.48	0.46
1:B:459:ASP:OD1	1:B:459:ASP:N	2.47	0.46
2:D:295:LEU:HD12	2:D:296:PRO:HD2	1.98	0.46
4:H:237:ARG:HG3	4:H:305:LEU:HA	1.98	0.46
2:C:92:GLU:OE2	6:L:53:ARG:NH2	2.49	0.46
4:G:237:ARG:HG3	4:G:305:LEU:HA	1.98	0.46
4:H:206:ILE:HG12	4:H:281:ILE:HD11	1.97	0.46
4:H:288:LEU:HB2	4:H:291:LEU:HD11	1.98	0.46
3:F:180:PHE:HD1	3:F:183:LEU:HD12	1.80	0.45
3:F:450:ASP:OD1	3:F:450:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ARG:HA	2:D:46:ILE:HG12	1.97	0.45
4:H:200:VAL:HG22	4:H:206:ILE:HG22	1.99	0.45
4:G:217:VAL:HG23	4:H:217:VAL:HG23	1.98	0.45
2:D:92:GLU:HA	2:D:95:ARG:HG2	1.99	0.45
4:G:63:VAL:HG21	4:G:207:ILE:HG21	1.99	0.45
3:F:461:ASP:OD1	3:F:476:TRP:NE1	2.40	0.45
2:D:89:ILE:HD13	2:D:133:ILE:HD12	1.99	0.45
4:H:139:GLU:HA	4:H:142:VAL:HG22	1.99	0.45
3:E:334:LEU:HB3	3:E:401:VAL:HG22	1.99	0.44
3:E:409:LEU:HD12	3:E:413:SER:HB2	1.99	0.44
4:G:200:VAL:HG22	4:G:206:ILE:HG22	1.99	0.44
1:B:158:ASN:ND2	1:B:319:TYR:O	2.46	0.44
4:H:199:GLY:HA2	4:H:234:LYS:HB3	1.99	0.44
1:A:356:LEU:HB3	1:A:360:VAL:HG21	1.98	0.44
1:B:47:LEU:HD22	1:B:93:VAL:HG13	1.99	0.44
3:E:256:LEU:HD23	3:E:259:TYR:HD2	1.82	0.44
3:F:319:ILE:HG22	3:F:345:ILE:HD11	1.98	0.44
6:L:36:LEU:HD23	6:L:40:ASN:HD21	1.81	0.44
1:A:131:LEU:HD21	1:A:150:LEU:HD11	2.00	0.44
3:F:233:LEU:HD13	3:F:280:LEU:HD22	1.98	0.44
3:F:256:LEU:HD23	3:F:259:TYR:HD2	1.82	0.44
3:F:391:ALA:HA	3:F:394:VAL:HG12	2.00	0.44
1:A:135:LEU:HD11	1:A:150:LEU:HD12	1.99	0.44
4:H:63:VAL:HG21	4:H:207:ILE:HG21	1.99	0.43
1:A:268:THR:OG1	1:A:269:ARG:N	2.50	0.43
2:C:22:LEU:HD21	2:C:78:VAL:HG21	2.01	0.43
2:D:301:ASP:OD1	2:D:301:ASP:N	2.52	0.43
2:C:176:ALA:HA	2:C:179:LYS:HG2	1.99	0.43
1:A:133:ASP:HA	1:A:136:ARG:HG2	1.99	0.43
2:C:241:ALA:HA	2:C:340:MET:HE3	1.99	0.43
3:E:519:LYS:HD2	3:E:519:LYS:HA	1.80	0.43
4:G:213:ASN:O	4:G:216:ALA:HB3	2.18	0.43
5:I:199:LEU:HD23	5:I:199:LEU:HA	1.91	0.43
2:C:92:GLU:HA	2:C:95:ARG:HG2	2.00	0.43
1:B:154:ASP:N	1:B:154:ASP:OD1	2.52	0.43
1:B:268:THR:OG1	1:B:269:ARG:N	2.52	0.43
2:D:16:GLU:HA	2:D:19:VAL:HG12	2.00	0.43
4:G:199:GLY:HA2	4:G:234:LYS:HB3	1.99	0.43
4:H:213:ASN:O	4:H:216:ALA:HB3	2.18	0.43
1:A:154:ASP:OD1	1:A:154:ASP:N	2.51	0.43
1:B:373:PHE:HB3	1:B:390:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:LEU:HD12	2:C:296:PRO:HD2	2.00	0.42
2:D:247:ALA:HB3	2:D:251:THR:HG21	2.00	0.42
3:E:408:LEU:HD12	3:E:443:PHE:HE1	1.83	0.42
2:C:28:PRO:HG3	2:C:33:GLU:HG3	2.00	0.42
2:C:247:ALA:HB3	2:C:251:THR:HG21	2.01	0.42
2:D:317:PRO:HD2	2:D:320:LEU:HD12	2.01	0.42
4:G:139:GLU:HA	4:G:142:VAL:HG22	1.99	0.42
2:C:216:VAL:HB	3:F:484:LEU:HD13	2.01	0.42
2:D:176:ALA:HA	2:D:179:LYS:HG2	2.02	0.42
2:D:16:GLU:O	2:D:20:GLU:HG2	2.18	0.42
3:F:440:THR:HG21	3:F:519:LYS:HE3	2.01	0.42
1:A:413:LEU:HG	1:A:431:LEU:HD11	2.02	0.42
1:B:359:ASN:HB2	1:B:376:ASN:HA	2.01	0.42
3:F:416:SER:O	3:F:489:TYR:HA	2.20	0.42
5:I:87:ALA:HB1	5:I:215:LEU:HD11	2.02	0.42
5:I:117:VAL:HG21	5:I:131:LEU:HB2	2.02	0.42
2:C:241:ALA:HB2	2:C:276:PRO:HA	2.02	0.42
2:D:213:GLU:H	3:E:481:SER:HB2	1.85	0.42
7:S:372:GLU:HA	7:S:426:LYS:HA	2.01	0.42
2:C:136:ALA:HB2	6:L:53:ARG:HH21	1.84	0.42
2:D:318:PRO:HA	2:D:321:ILE:HD12	2.01	0.42
1:A:53:ASP:HB3	1:A:55:ARG:HG2	2.02	0.41
2:D:238:THR:HB	2:D:246:ARG:HG2	2.02	0.41
3:F:416:SER:OG	3:F:417:ARG:N	2.52	0.41
1:A:155:VAL:HG11	1:A:249:ILE:HD11	2.01	0.41
1:A:354:SER:HA	1:A:372:CYS:H	1.85	0.41
1:B:83:LEU:HD22	1:B:88:VAL:HG21	2.02	0.41
2:C:236:THR:OG1	2:C:246:ARG:O	2.38	0.41
3:F:348:GLU:O	3:F:352:GLU:HB2	2.20	0.41
1:A:77:ASP:HB3	1:A:328:THR:HG21	2.01	0.41
1:B:71:ALA:HA	1:B:378:VAL:HG11	2.02	0.41
3:F:252:LEU:HD12	3:F:252:LEU:HA	1.94	0.41
3:F:428:ARG:HE	3:F:496:LEU:HA	1.85	0.41
4:H:75:PHE:HZ	4:H:96:ARG:HB3	1.85	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.94	0.41
3:E:180:PHE:HD1	3:E:183:LEU:HD12	1.85	0.41
4:G:23:ALA:HB2	4:G:64:ALA:HB1	2.02	0.41
1:A:243:ASP:OD1	1:A:243:ASP:N	2.53	0.41
6:L:52:ARG:HG3	6:L:87:ARG:HG3	2.02	0.41
4:H:23:ALA:HB2	4:H:64:ALA:HB1	2.02	0.41
1:A:389:VAL:HG12	1:A:406:ALA:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LEU:HD23	1:B:400:VAL:HG21	2.02	0.41
5:J:117:VAL:HG21	5:J:131:LEU:HB2	2.02	0.41
5:J:167:LEU:HD23	5:J:265:SER:HB2	2.03	0.40
3:E:440:THR:OG1	3:E:503:GLU:OE2	2.34	0.40
4:H:300:LEU:HD23	4:H:300:LEU:HA	1.95	0.40
5:I:129:ALA:HA	5:I:264:TYR:O	2.21	0.40
5:J:129:ALA:HA	5:J:264:TYR:O	2.21	0.40
3:E:205:PRO:HA	3:E:208:VAL:HG12	2.03	0.40
1:A:106:LEU:HD22	1:A:122:ILE:HD11	2.03	0.40
1:A:380:GLY:N	1:A:396:LEU:O	2.55	0.40
2:D:270:PRO:HD2	2:D:273:LYS:HD2	2.03	0.40
2:D:338:ARG:HA	2:D:338:ARG:HD2	1.93	0.40
3:F:362:ASP:HB3	3:F:387:LEU:HD23	2.04	0.40
4:G:75:PHE:HZ	4:G:96:ARG:HB3	1.85	0.40
5:J:87:ALA:HB1	5:J:215:LEU:HD11	2.02	0.40
1:B:56:PHE:O	1:B:60:SER:N	2.50	0.40
2:C:243:GLY:HA2	2:C:336:ILE:HG13	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	424/721 (59%)	400 (94%)	24 (6%)	0	100	100
1	B	584/721 (81%)	554 (95%)	30 (5%)	0	100	100
2	C	313/368 (85%)	304 (97%)	9 (3%)	0	100	100
2	D	314/368 (85%)	300 (96%)	14 (4%)	0	100	100
3	E	355/523 (68%)	339 (96%)	16 (4%)	0	100	100
3	F	355/523 (68%)	343 (97%)	12 (3%)	0	100	100
4	G	281/305 (92%)	270 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	281/305 (92%)	270 (96%)	11 (4%)	0	100	100
5	I	232/452 (51%)	221 (95%)	11 (5%)	0	100	100
5	J	232/452 (51%)	221 (95%)	11 (5%)	0	100	100
6	L	273/314 (87%)	261 (96%)	12 (4%)	0	100	100
7	S	402/472 (85%)	377 (94%)	25 (6%)	0	100	100
All	All	4046/5524 (73%)	3860 (95%)	186 (5%)	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	347/626 (55%)	347 (100%)	0	100	100
1	B	348/626 (56%)	348 (100%)	0	100	100
2	C	265/312 (85%)	265 (100%)	0	100	100
2	D	266/312 (85%)	266 (100%)	0	100	100
3	E	312/444 (70%)	312 (100%)	0	100	100
3	F	312/444 (70%)	312 (100%)	0	100	100
4	G	193/260 (74%)	185 (96%)	8 (4%)	30	65
4	H	193/260 (74%)	185 (96%)	8 (4%)	30	65
5	I	127/398 (32%)	124 (98%)	3 (2%)	49	78
5	J	127/398 (32%)	124 (98%)	3 (2%)	49	78
6	L	75/279 (27%)	75 (100%)	0	100	100
7	S	16/397 (4%)	16 (100%)	0	100	100
All	All	2581/4756 (54%)	2559 (99%)	22 (1%)	79	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	22	SER
4	G	67	SER
4	G	70	GLU
4	G	77	SER
4	G	99	LEU
4	G	114	LEU
4	G	127	THR
4	G	232	SER
4	H	22	SER
4	H	67	SER
4	H	70	GLU
4	H	77	SER
4	H	99	LEU
4	H	114	LEU
4	H	127	THR
4	H	232	SER
5	I	89	SER
5	I	181	VAL
5	I	197	THR
5	J	89	SER
5	J	181	VAL
5	J	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	409	HIS
1	B	63	GLN
1	B	72	ASN
2	D	138	ASN
2	D	158	HIS
3	F	213	GLN
3	F	234	GLN
3	F	254	ASN
6	L	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
9	C7B	C	401[B]	-	32,32,32	1.72	6 (18%)	42,42,42	0.92	2 (4%)
9	C7B	C	401[A]	-	32,32,32	1.72	4 (12%)	42,42,42	0.94	2 (4%)

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
9	C7B	C	401[B]	-	-	6/18/28/28	0/3/3/3
9	C7B	C	401[A]	-	-	7/18/28/28	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401[B]	C7B	C16-N08	5.97	1.46	1.34
9	C	401[A]	C7B	C16-N08	5.94	1.46	1.34
9	C	401[A]	C7B	C15-N07	5.52	1.45	1.34
9	C	401[B]	C7B	C15-N07	5.49	1.45	1.34
9	C	401[A]	C7B	O03-C15	-2.15	1.18	1.23
9	C	401[B]	C7B	O03-C15	-2.12	1.19	1.23

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	401[B]	C7B	O04-C16	-2.05	1.19	1.23
9	C	401[B]	C7B	C30-CL2	2.04	1.79	1.74
9	C	401[B]	C7B	C29-CL1	2.01	1.78	1.74
9	C	401[A]	C7B	O04-C16	-2.00	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	401[A]	C7B	C10-N08-C16	2.60	126.75	122.92
9	C	401[B]	C7B	C10-N08-C16	2.59	126.74	122.92
9	C	401[B]	C7B	C18-O06-C20	-2.17	113.86	117.67
9	C	401[A]	C7B	C18-O06-C20	-2.00	114.14	117.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

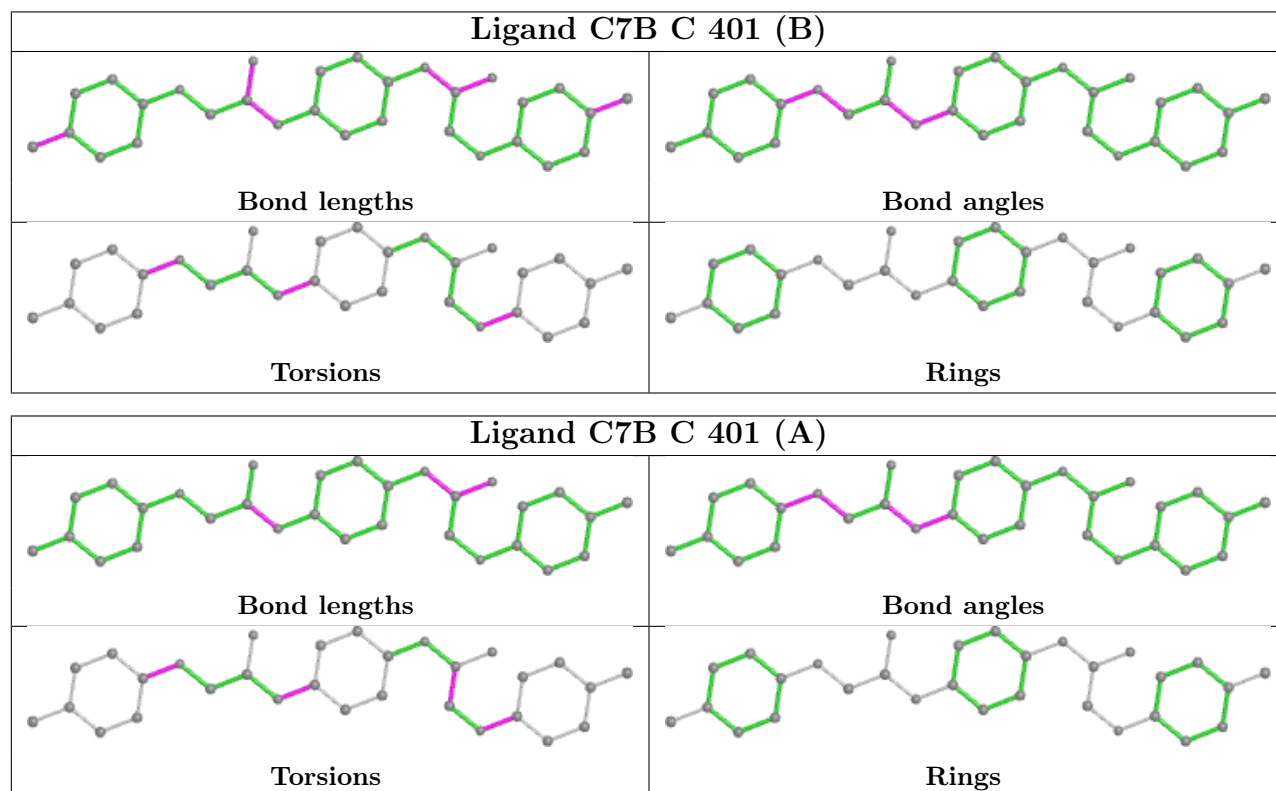
Mol	Chain	Res	Type	Atoms
9	C	401[B]	C7B	C22-C20-O06-C18
9	C	401[A]	C7B	C22-C20-O06-C18
9	C	401[B]	C7B	C24-C20-O06-C18
9	C	401[A]	C7B	C24-C20-O06-C18
9	C	401[A]	C7B	C21-C19-O05-C17
9	C	401[A]	C7B	C23-C19-O05-C17
9	C	401[B]	C7B	C21-C19-O05-C17
9	C	401[B]	C7B	C23-C19-O05-C17
9	C	401[B]	C7B	C12-C10-N08-C16
9	C	401[A]	C7B	C11-C10-N08-C16
9	C	401[A]	C7B	C12-C10-N08-C16
9	C	401[B]	C7B	C11-C10-N08-C16
9	C	401[A]	C7B	O03-C15-C17-O05

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

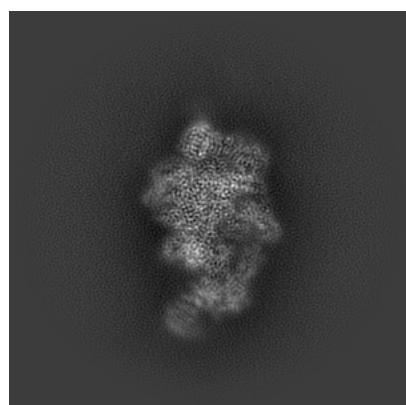
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0651. These allow visual inspection of the internal detail of the map and identification of artifacts.

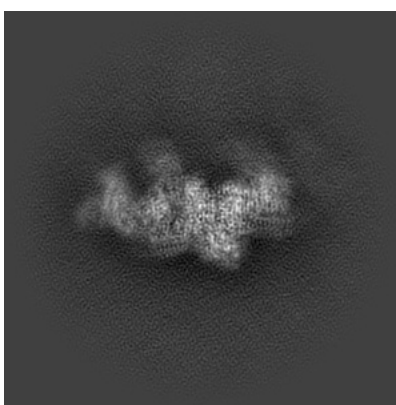
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

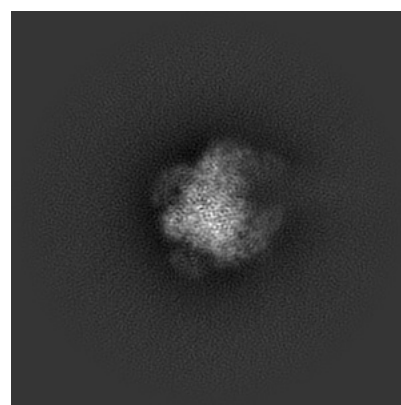
6.1.1 Primary map



X



Y

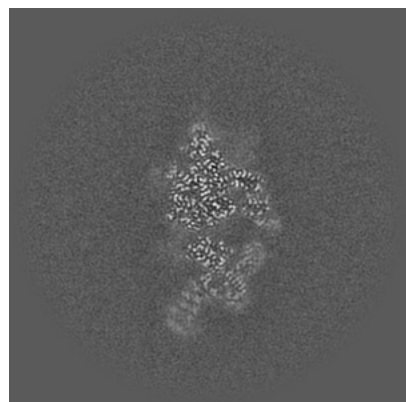


Z

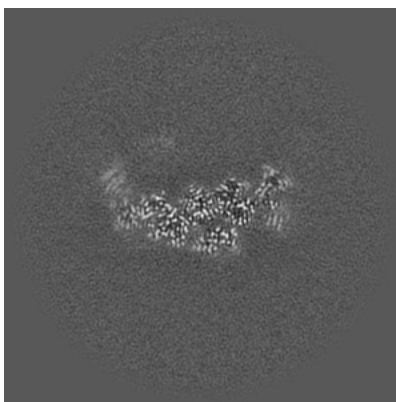
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

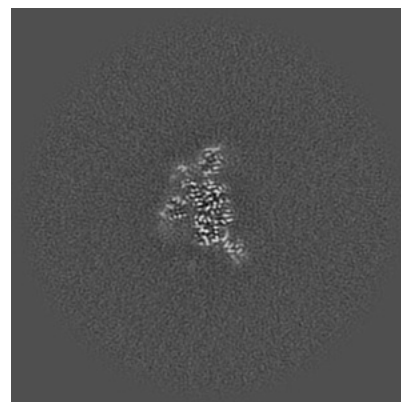
6.2.1 Primary map



X Index: 240



Y Index: 240

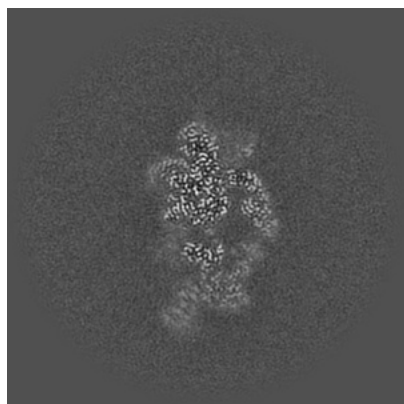


Z Index: 240

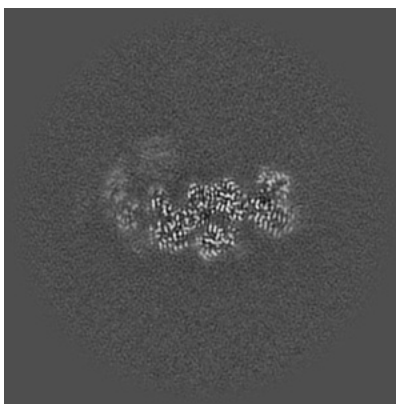
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

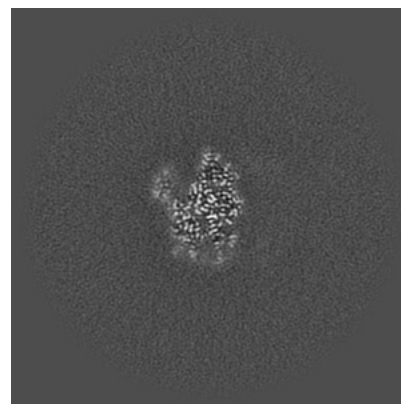
6.3.1 Primary map



X Index: 246



Y Index: 232



Z Index: 274

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

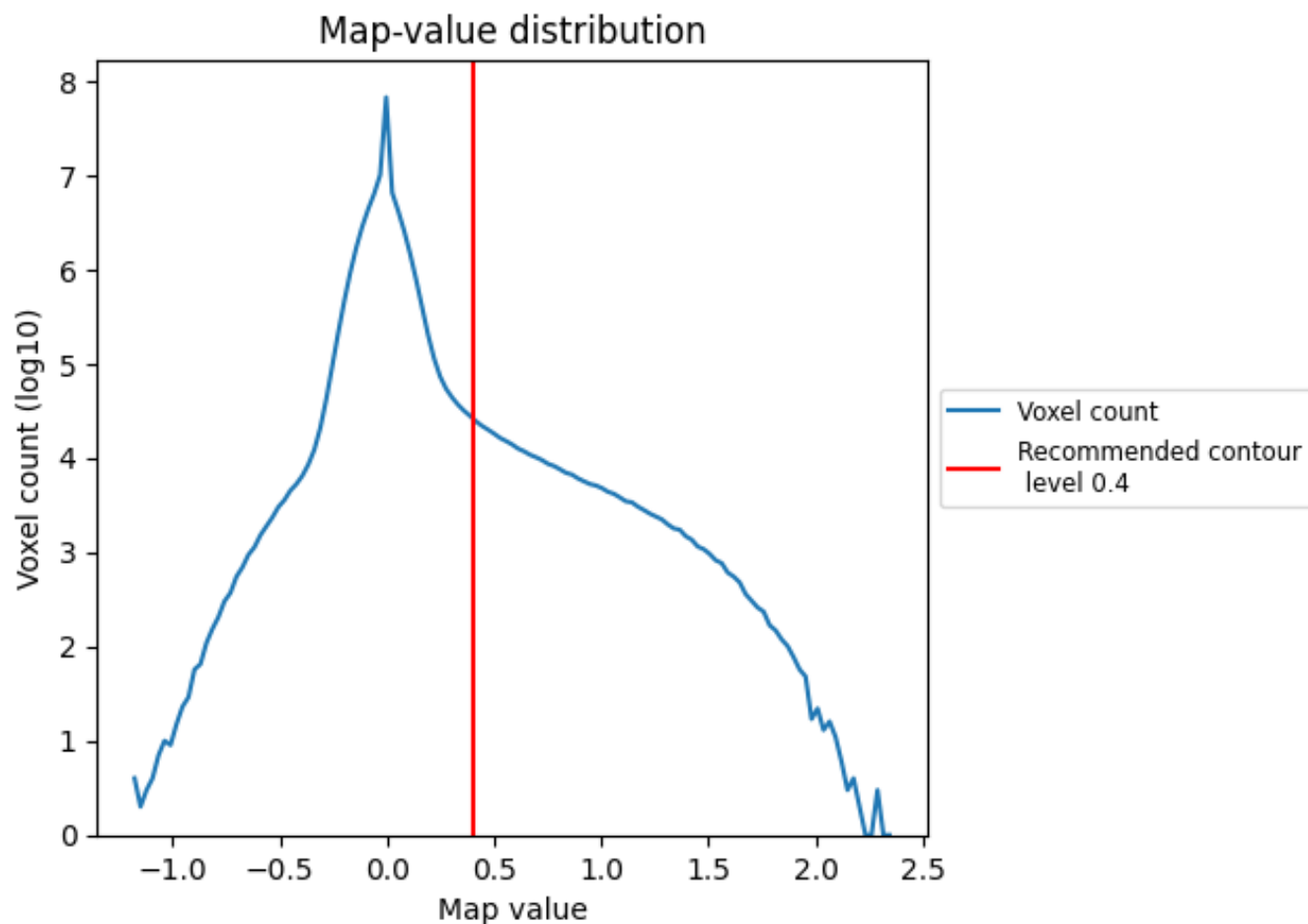
6.5 Mask visualisation

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

7 Map analysis [i](#)

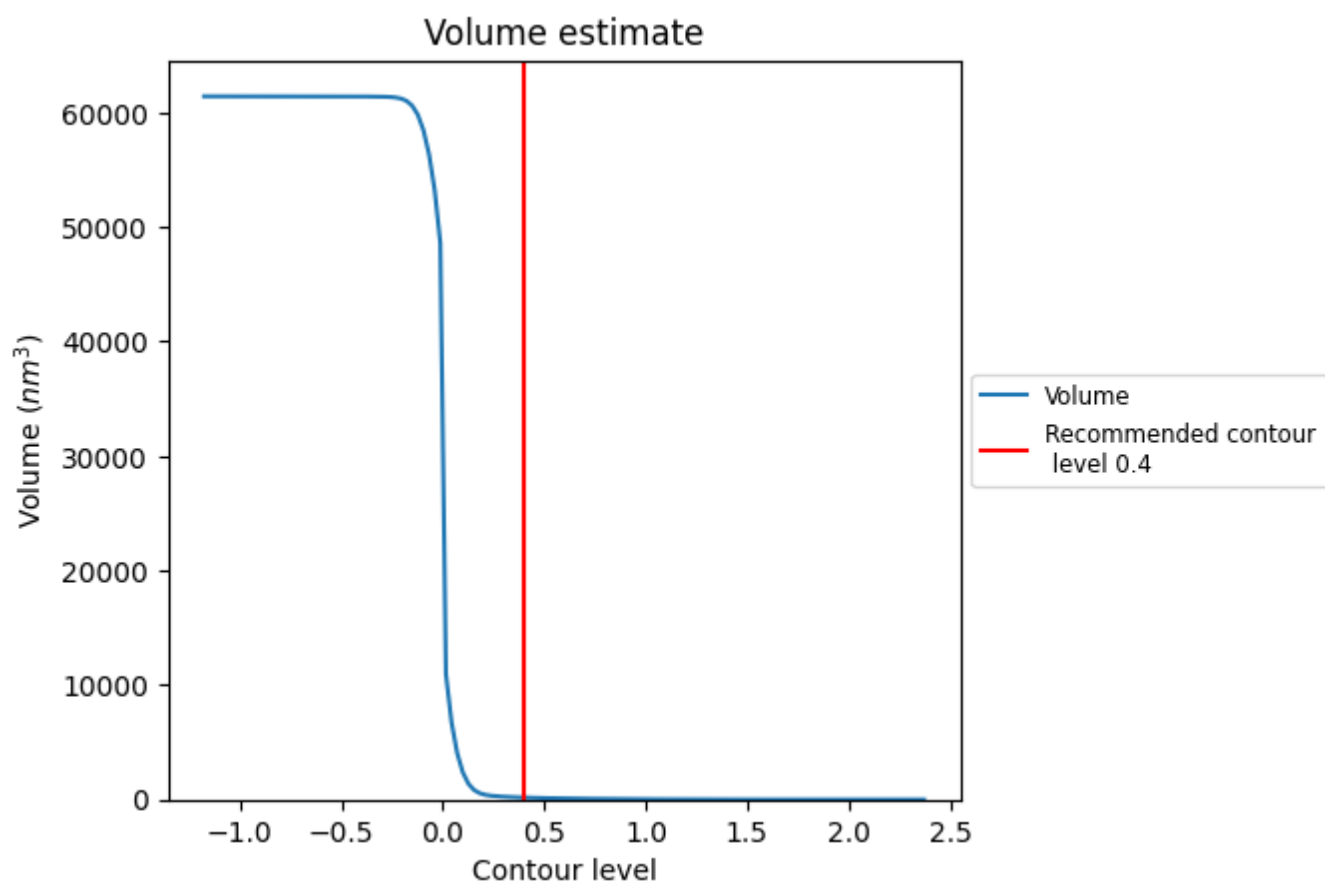
This section contains the results of statistical analysis of the map.

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.

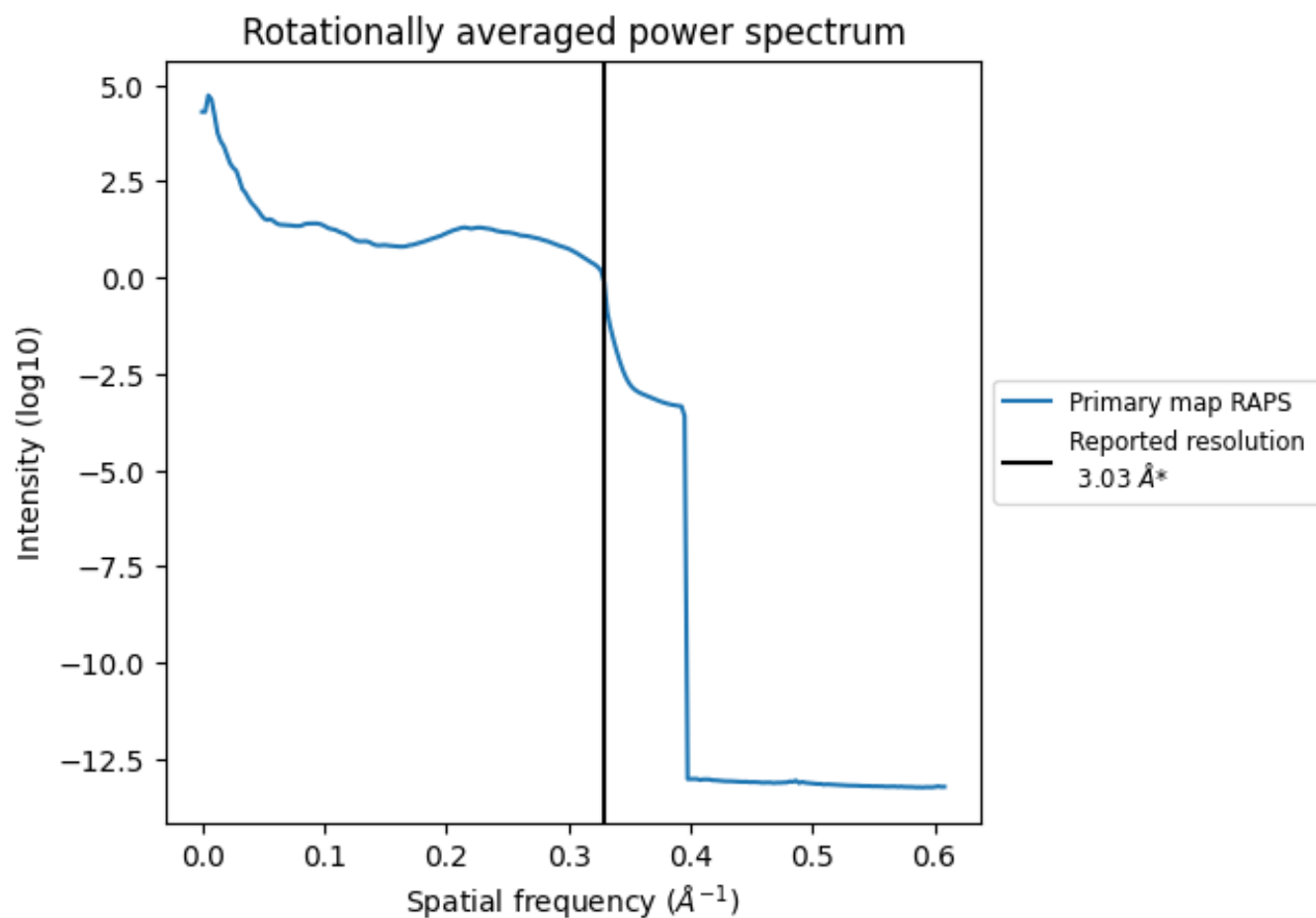
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 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 0.330 Å⁻¹

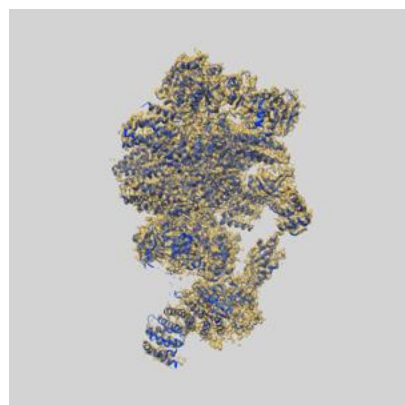
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

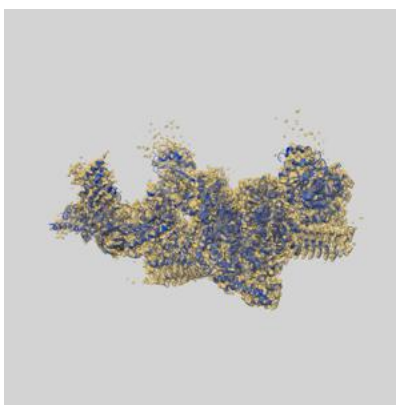
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0651 and PDB model 6O85. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

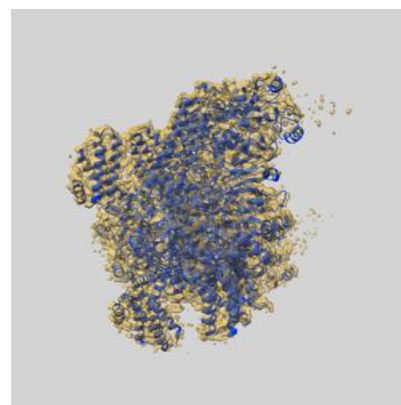
9.1 Map-model overlay [i](#)



X



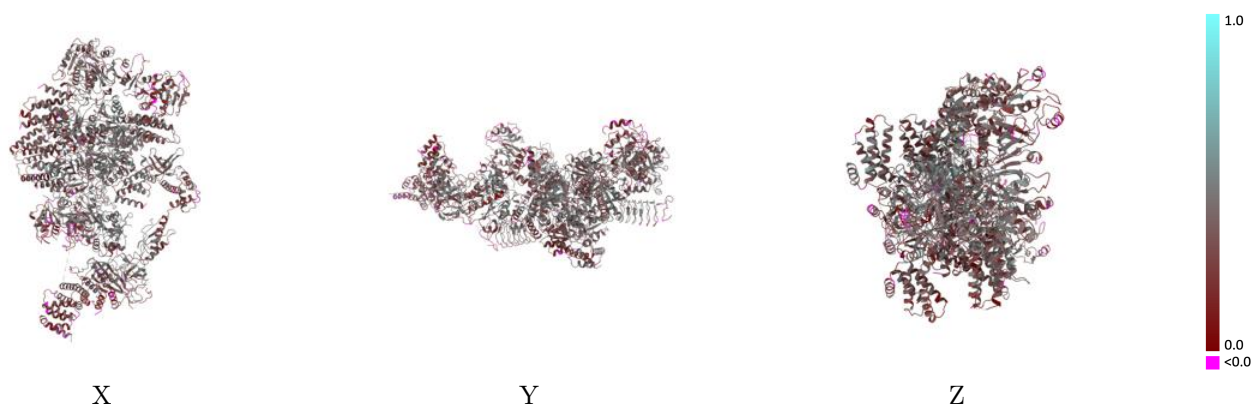
Y



Z

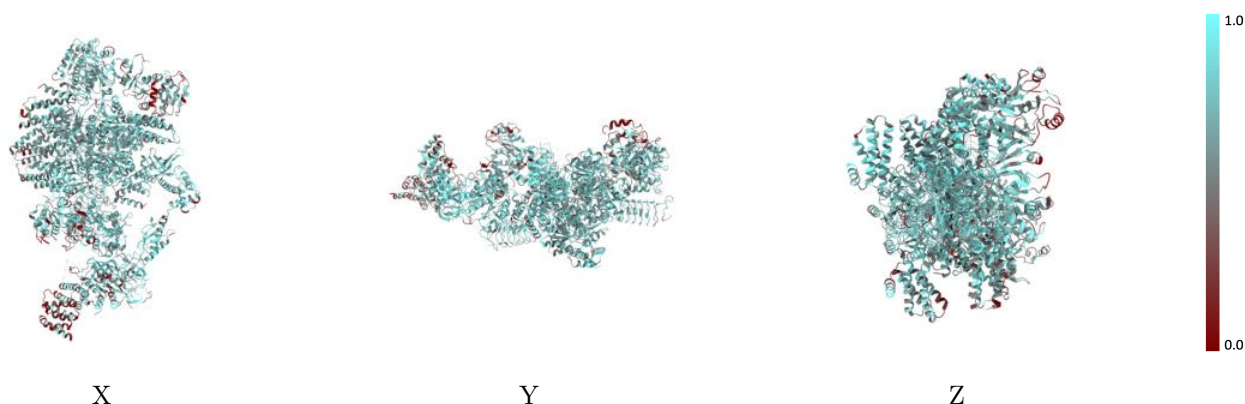
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



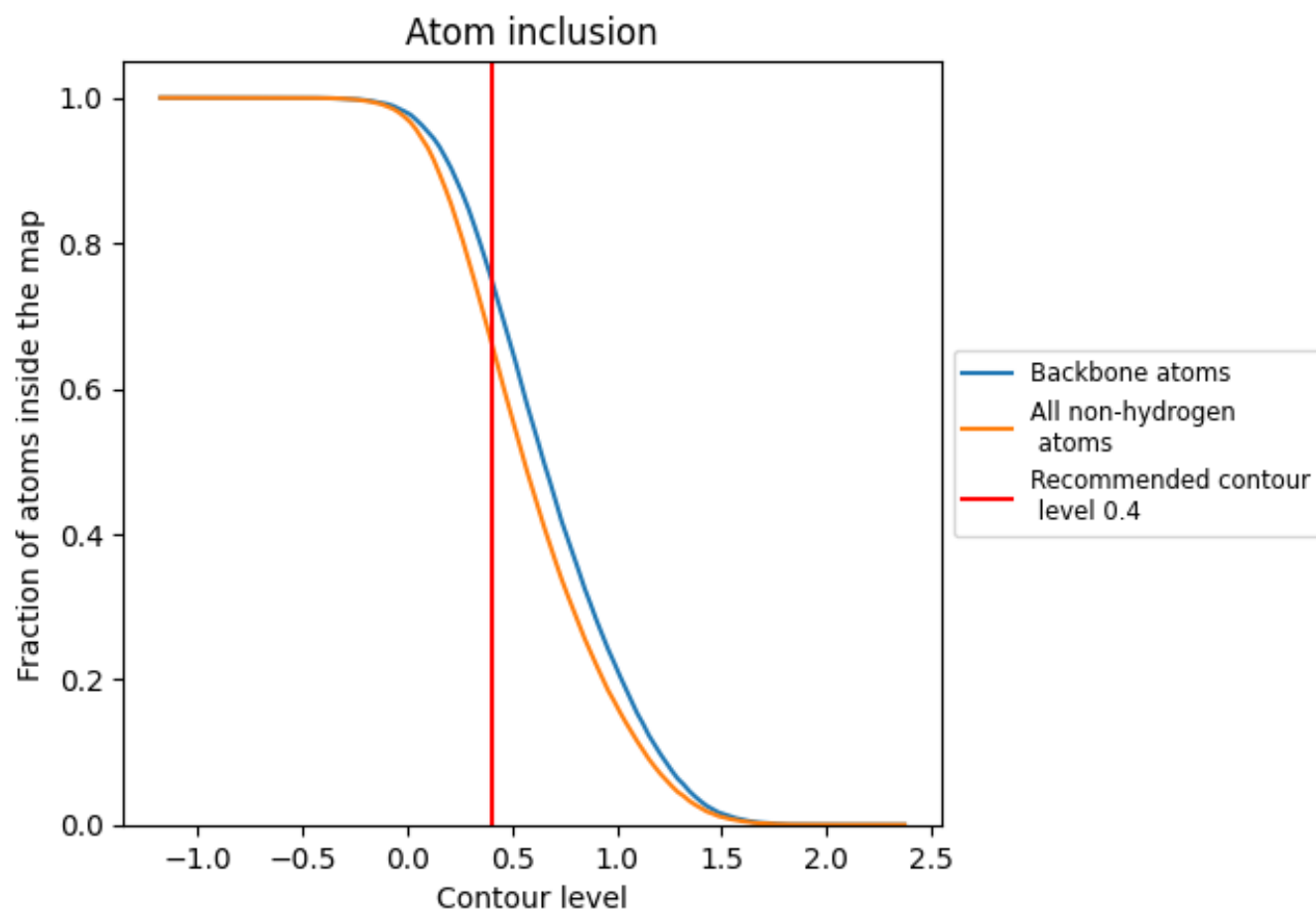
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6658	 0.3590
A	 0.6668	 0.3680
B	 0.6580	 0.3590
C	 0.7190	 0.3990
D	 0.6437	 0.3450
E	 0.7216	 0.3950
F	 0.6871	 0.3710
G	 0.7080	 0.3580
H	 0.6709	 0.3420
I	 0.5277	 0.2980
J	 0.5786	 0.3300
L	 0.6969	 0.3560
S	 0.6479	 0.3480
d	 0.6143	 0.1810

