



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:54 AM UTC

PDB ID : 6EZO / pdb_00006ezo
EMDB ID : EMD-4162
Title : Eukaryotic initiation factor EIF2B in complex with ISRIB
Authors : Faille, A.; Weis, F.; Zyryanova, A.; Warren, A.J.; Ron, D.
Deposited on : 2017-11-16
Resolution : 4.10 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:

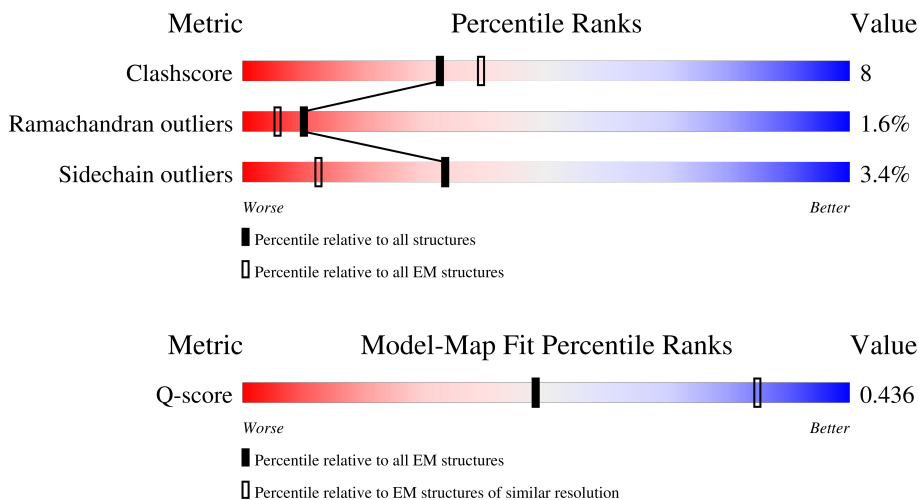
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	305	 81% 10% 8%
1	B	305	 80% 11% 8%
2	C	373	 69% 11% 18%
2	D	373	 72% 11% 17%

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Mol	Chain	Length	Quality of chain
3	E	452	 72%5%23%
3	F	452	 72%5%23%
4	G	523	 60%6%32%
4	H	523	 59%7%33%
5	I	721	 52%45%
5	J	721	 51%45%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18758 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	280	Total	C	N	O	S	0	0
			1624	1033	287	300	4		
1	B	280	Total	C	N	O	S	0	0
			1627	1036	287	299	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	307	Total	C	N	O	S	0	0
			1857	1174	349	327	7		
2	D	308	Total	C	N	O	S	0	0
			1816	1150	342	319	5		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	initiating methionine	UNP P49770
C	-20	PRO	-	expression tag	UNP P49770
C	-19	GLY	-	expression tag	UNP P49770
C	-18	SER	-	expression tag	UNP P49770
C	-17	ASP	-	expression tag	UNP P49770
C	-16	TYR	-	expression tag	UNP P49770
C	-15	LYS	-	expression tag	UNP P49770
C	-14	ASP	-	expression tag	UNP P49770
C	-13	HIS	-	expression tag	UNP P49770
C	-12	ASP	-	expression tag	UNP P49770
C	-11	GLY	-	expression tag	UNP P49770
C	-10	ASP	-	expression tag	UNP P49770
C	-9	TYR	-	expression tag	UNP P49770
C	-8	LYS	-	expression tag	UNP P49770
C	-7	ASP	-	expression tag	UNP P49770
C	-6	HIS	-	expression tag	UNP P49770
C	-5	ASP	-	expression tag	UNP P49770

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ILE	-	expression tag	UNP P49770
C	-3	ASP	-	expression tag	UNP P49770
C	-2	TYR	-	expression tag	UNP P49770
C	-1	LYS	-	expression tag	UNP P49770
C	0	ASP	-	expression tag	UNP P49770
C	1	ASP	-	expression tag	UNP P49770
C	2	ASP	-	expression tag	UNP P49770
C	3	ASP	-	expression tag	UNP P49770
C	4	LYS	-	expression tag	UNP P49770
D	-21	MET	-	initiating methionine	UNP P49770
D	-20	PRO	-	expression tag	UNP P49770
D	-19	GLY	-	expression tag	UNP P49770
D	-18	SER	-	expression tag	UNP P49770
D	-17	ASP	-	expression tag	UNP P49770
D	-16	TYR	-	expression tag	UNP P49770
D	-15	LYS	-	expression tag	UNP P49770
D	-14	ASP	-	expression tag	UNP P49770
D	-13	HIS	-	expression tag	UNP P49770
D	-12	ASP	-	expression tag	UNP P49770
D	-11	GLY	-	expression tag	UNP P49770
D	-10	ASP	-	expression tag	UNP P49770
D	-9	TYR	-	expression tag	UNP P49770
D	-8	LYS	-	expression tag	UNP P49770
D	-7	ASP	-	expression tag	UNP P49770
D	-6	HIS	-	expression tag	UNP P49770
D	-5	ASP	-	expression tag	UNP P49770
D	-4	ILE	-	expression tag	UNP P49770
D	-3	ASP	-	expression tag	UNP P49770
D	-2	TYR	-	expression tag	UNP P49770
D	-1	LYS	-	expression tag	UNP P49770
D	0	ASP	-	expression tag	UNP P49770
D	1	ASP	-	expression tag	UNP P49770
D	2	ASP	-	expression tag	UNP P49770
D	3	ASP	-	expression tag	UNP P49770
D	4	LYS	-	expression tag	UNP P49770

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	347	Total	C	N	O	0	0
			1812	1108	353	351		
3	F	347	Total	C	N	O	0	0
			1806	1102	353	351		

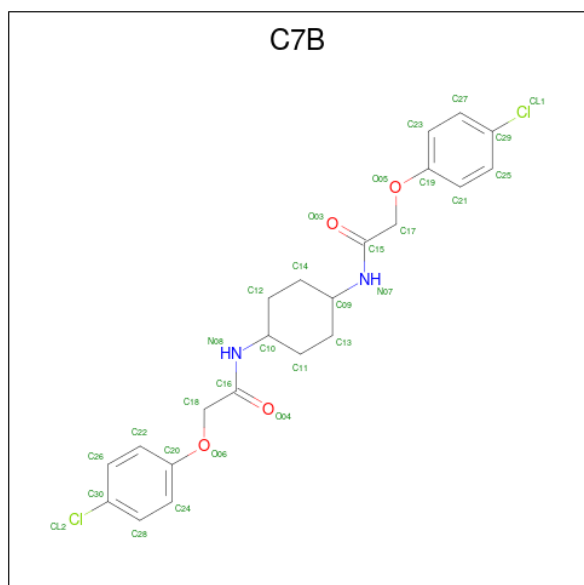
- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	355	Total	C	N	O	S	0	0
			2013	1257	386	369	1		
4	H	353	Total	C	N	O	S	0	0
			1993	1245	379	368	1		

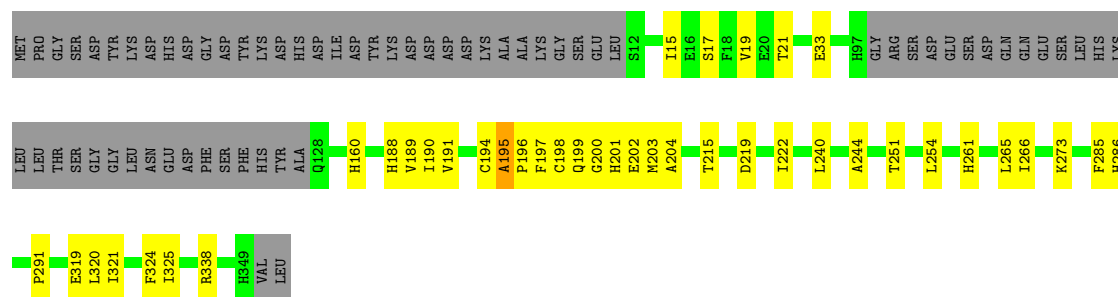
- Molecule 5 is a protein called Human eukaryotic initiation factor EIF2B epsilon subunits.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	396	Total	C	N	O	S	0	0
			2117	1291	417	408	1		
5	J	394	Total	C	N	O		0	0
			2063	1258	403	402			

- Molecule 6 is 2-(4-chloranylphenoxy)- {N}-[4-[2-(4-chloranylphenoxy)ethanoylamino]cyclohexyl]ethanamide (CCD ID: C7B) (formula: C₂₂H₂₄Cl₂N₂O₄).

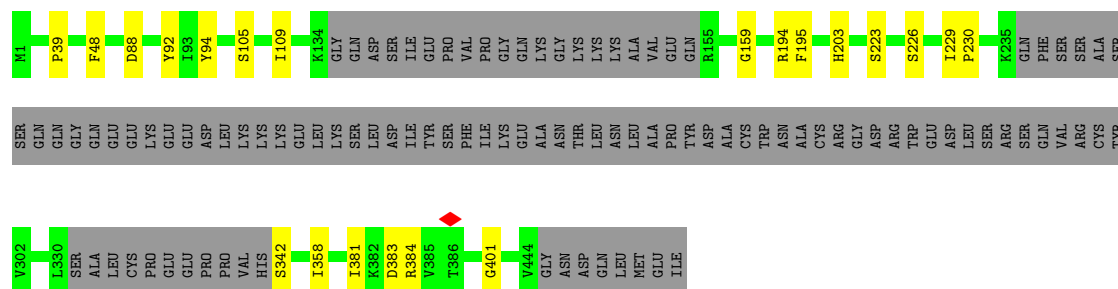


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	Cl	N	O	0
			30	22	2	2	4	



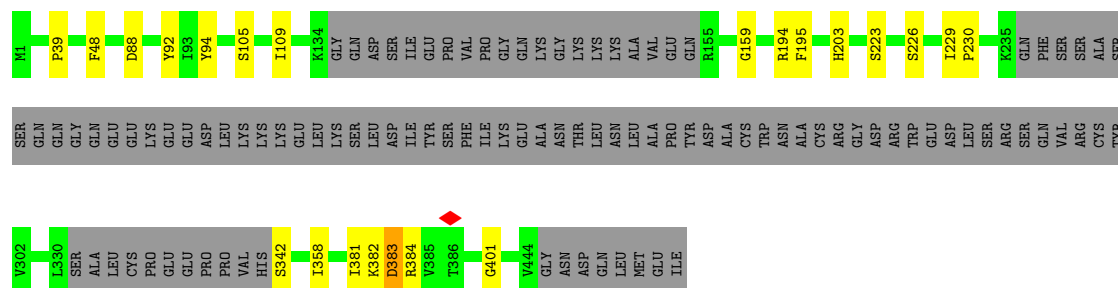
- Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain E: 72% 5% 23%



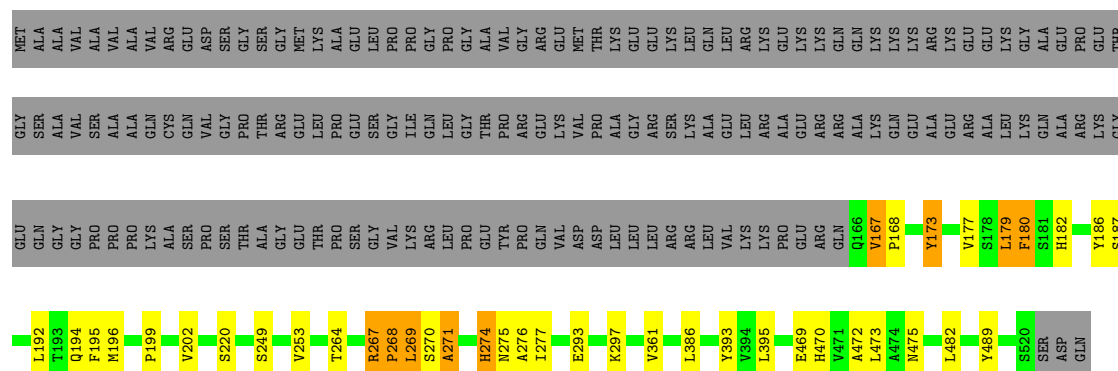
- Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain F: 72% 5% 23%



- Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain G: 60% 6% 32%



L192	F195	S196	S197	I198	P199	S200	S201	V202	S220	Q235	Q238	S249	V253	R267	P268	L269	S270	E293	K297	V361	L386	Y393	I394	L395	T420	A421	Q422	E456	E469	H470	A471	A472	L473	A474	N475	W476	V518	LYS	SER	SER	ASP	GLN		
GLU	GLN	GLY	GLY	PRO	PRO	LYS	ALA	SER	PRO	THR	ALA	THR	THR	THR	ARG	LEU	PRO	GLU	THR	ASP	ASP	LEU	LEU	ARG	VAL	VAL	LYS	PRO	GLU	ARG	GLN	Q166	V167	P168	Y173	G174	V177	S178	L179	F180	Q189	N190	S191	
GLY	SER	ALA	VAL	SER	ALA	GLN	CYS	GLN	VAL	GLY	PRO	GLY	GLY	ILE	GLN	LEU	GLY	THR	PRO	GLU	GLU	LYS	VAL	PRO	ALA	GLY	ARG	ALA	GLN	LYS	LYS	GLN	GLY	ALA	ARG	GLU	ALA	LEU	LYS	GLY	ALA	GLU	PRO	THR
MET	ALA	VAL	ALA	VAL	ALA	VAL	GLU	ASP	SER	GLY	SER	GLY	THR	SER	GLY	GLY	GLY	ALA	VAL	GLU	GLU	GLY	THR	THR	LYS	LYS	LYS	LYS	LYS	LYS	GLN	LYS	LYS	LYS	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY		

[illegible]

ASP	K141	MET
ASP	L149	ALA
SER	I156	ALA
GLY	S157	PRO
ALA	L165	VAL
ASP	L169	VAL
Gln	E175	ALA
GLN	K176	VAL
LYS	N177	VAL
ASP	E239	SER
LYS	S250	ARG
TYR	T268	ALA
ASN	Y296	ASN
PRO	A297	LYS
ALA	A298	ARG
ALA	R299	GLY
GLY	V300	GLY
LYS	S301	SER
GLY	M305	GLY
TYR	Y306	GLY
LEU	W317	GLY
TRP	N326	ALA
LYS	PHE	ARG
ALA	THR	GLY
ALA	THR	ALA
GLY	ASP	ALA
MET	THR	ALA
ASN	ASP	GLU
MET	SER	GLU
GLU	THR	GLU
GLU	THR	PRO
GLU	Gln	F40
GLU	S334	I47
GLU	S450	VAL
LEU	LEU	ALA
Gln	GLN	ASP
GLN	HIS	SER
ASN	PRO	PHE
LEU	PRO	ASP
TRP	ASP	ASP
GLY	ALA	ARG
LEU	GLU	PHE
LYS	GLU	PHE
ILE	ASP	P58
ASN	GLU	
MET	ASP	P69
GLU	ASP	
GLU	GLY	R136
GLU	GLU	D137
SER	PHE	
LEU	SER	I140

ILE	ALA	GLN	TRP	LEU	LYS	GLU	ALA	GLU	GLU	SER	SER	GLU	ASP	ASP	ILE	SER	LEU	GLU	THR	ILE	LEU	SER	TRP	PHE	SER	GLN	LEU	GLU	GLU	THR	ILE	LEU	ALA	GLU	GLU	THR	ILE	LEU	PRO	LEU	LYS	ALA	TRP	SER	PRO	VAL	PHE	ASN	ASN	LEU	TYR	ILE	LYS	ARG	ALA	ASP	HIS	LEU	GLU	ALA	TYR	ASN
ILE	ALA	GLN	TRP	LEU	LYS	GLU	ALA	GLU	GLU	SER	SER	GLU	ASP	ASP	ILE	SER	LEU	GLU	THR	ILE	LEU	SER	TRP	PHE	SER	GLN	LEU	GLU	GLU	THR	ILE	LEU	ALA	GLU	GLU	THR	ILE	LEU	PRO	LEU	LYS	ALA	TRP	SER	PRO	VAL	PHE	ASN	ASN	LEU	TYR	ILE	LYS	ARG	ALA	ASP	HIS	LEU	GLU	ALA	TYR	ASN
ILE	ALA	GLN	TRP	LEU	LYS	GLU	ALA	GLU	GLU	SER	SER	GLU	ASP	ASP	ILE	SER	LEU	GLU	THR	ILE	LEU	SER	TRP	PHE	SER	GLN	LEU	GLU	GLU	THR	ILE	LEU	ALA	GLU	GLU	THR	ILE	LEU	PRO	LEU	LYS	ALA	TRP	SER	PRO	VAL	PHE	ASN	ASN	LEU	TYR	ILE	LYS	ARG	ALA	ASP	HIS	LEU	GLU	ALA	TYR	ASN
ILE	ALA	GLN	TRP	LEU	LYS	GLU	ALA	GLU	GLU	SER	SER	GLU	ASP	ASP	ILE	SER	LEU	GLU	THR	ILE	LEU	SER	TRP	PHE	SER	GLN	LEU	GLU	GLU	THR	ILE	LEU	ALA	GLU	GLU	THR	ILE	LEU	PRO	LEU	LYS	ALA	TRP	SER	PRO	VAL	PHE	ASN	ASN	LEU	TYR	ILE	LYS	ARG	ALA	ASP	HIS	LEU	GLU	ALA	TYR	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	41750	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	80000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.253	Depositor
Minimum map value	-0.769	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.75, 1.75, 1.75	Depositor

5 Model quality

5.1 Standard geometry

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	0.50	0/1644	0.86	3/2283 (0.1%)
1	B	0.50	0/1646	0.87	5/2284 (0.2%)
2	C	0.58	0/1897	0.98	6/2619 (0.2%)
2	D	0.59	0/1855	0.94	5/2568 (0.2%)
3	E	0.48	0/1831	0.83	3/2547 (0.1%)
3	F	0.49	0/1824	0.86	6/2539 (0.2%)
4	G	0.57	0/2053	1.08	13/2854 (0.5%)
4	H	0.60	1/2033 (0.0%)	1.07	14/2828 (0.5%)
5	I	0.50	0/2143	0.82	0/2981
5	J	0.49	0/2085	0.88	4/2903 (0.1%)
All	All	0.53	1/19011 (0.0%)	0.93	59/26406 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	267	ARG	N-CA	5.14	1.50	1.45

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200	GLY	N-CA-C	10.05	124.79	112.73
2	C	201	HIS	N-CA-C	10.03	121.80	111.07
1	A	22	SER	N-CA-C	-9.28	101.17	111.28
4	G	267	ARG	CA-C-N	-8.99	110.31	119.93
4	G	267	ARG	C-N-CA	-8.99	110.31	119.93
5	J	301	SER	N-CA-C	8.36	120.16	111.14
4	G	271	ALA	N-CA-C	-8.34	94.73	108.49
4	G	270	SER	N-CA-C	7.90	121.08	109.07
3	F	383	ASP	CA-C-N	-7.86	109.82	120.90
3	F	383	ASP	C-N-CA	-7.86	109.82	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	N-CA-C	-7.53	103.15	111.36
3	F	382	LYS	N-CA-C	7.44	123.07	113.18
4	G	269	LEU	N-CA-C	7.42	119.37	111.28
1	A	96	ARG	N-CA-C	-7.41	103.29	111.36
4	H	422	GLN	N-CA-C	-7.33	104.34	113.28
2	C	196	PRO	N-CA-C	-7.11	100.03	111.19
2	C	203	MET	O-C-N	-7.03	114.50	122.09
4	G	473	LEU	N-CA-C	-6.99	103.78	112.72
4	G	268	PRO	N-CA-C	-6.75	100.26	111.26
1	B	23	ALA	N-CA-C	-6.55	104.14	111.28
5	J	169	ARG	N-CA-C	-6.47	103.27	112.13
4	H	195	PHE	N-CA-C	6.46	118.40	111.36
1	B	98	GLU	N-CA-C	-6.44	104.26	111.28
4	G	167	VAL	CA-C-N	6.44	127.89	119.84
4	G	167	VAL	C-N-CA	6.44	127.89	119.84
4	H	196	MET	N-CA-C	6.38	119.48	110.23
4	H	267	ARG	CA-C-N	-6.15	113.42	119.76
4	H	267	ARG	C-N-CA	-6.15	113.42	119.76
4	H	198	ILE	N-CA-C	5.84	121.49	108.88
4	H	189	GLN	CA-C-N	5.74	132.51	121.54
4	H	189	GLN	C-N-CA	5.74	132.51	121.54
2	D	33	GLU	N-CA-C	-5.72	105.97	113.12
2	C	33	GLU	N-CA-C	-5.68	106.02	113.12
3	F	381	ILE	N-CA-C	-5.46	100.53	108.17
5	J	298	ALA	N-CA-C	-5.37	100.58	108.79
4	G	202	VAL	N-CA-C	5.34	120.45	109.34
4	H	202	VAL	N-CA-C	5.32	120.42	109.34
1	B	99	LEU	N-CA-C	-5.26	105.54	111.28
2	D	195	ALA	CA-C-N	-5.25	114.35	119.76
2	D	195	ALA	C-N-CA	-5.25	114.35	119.76
2	C	208	SER	N-CA-C	5.24	118.45	111.75
4	H	192	LEU	N-CA-C	5.23	118.93	112.54
1	B	129	ALA	N-CA-C	5.21	114.71	107.73
3	E	381	ILE	N-CA-C	-5.21	100.15	107.75
3	E	94	TYR	CA-C-N	-5.20	115.52	120.83
3	E	94	TYR	C-N-CA	-5.20	115.52	120.83
4	H	395	LEU	CA-C-N	-5.20	114.97	121.00
4	H	395	LEU	C-N-CA	-5.20	114.97	121.00
3	F	94	TYR	CA-C-N	-5.19	115.54	120.83
3	F	94	TYR	C-N-CA	-5.19	115.54	120.83
4	G	220	SER	N-CA-C	5.18	117.50	111.02
4	G	395	LEU	CA-C-N	-5.18	115.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	395	LEU	C-N-CA	-5.18	115.00	121.00
1	A	129	ALA	N-CA-C	5.17	114.66	107.73
4	H	220	SER	N-CA-C	5.10	117.39	111.02
2	C	240	LEU	N-CA-C	5.10	117.10	110.53
2	D	199	GLN	N-CA-C	-5.08	106.77	113.17
5	J	268	THR	N-CA-C	5.03	117.17	110.53
4	H	475	ASN	N-CA-C	5.00	119.01	113.01

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	1624	0	1171	19	0
1	B	1627	0	1200	17	0
2	C	1857	0	1344	52	0
2	D	1816	0	1250	42	0
3	E	1812	0	924	13	0
3	F	1806	0	914	12	0
4	G	2013	0	1187	49	0
4	H	1993	0	1156	39	0
5	I	2117	0	1110	15	0
5	J	2063	0	1030	17	0
6	D	30	0	0	7	0
All	All	18758	0	11286	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:PHE:CD2	2:C:203:MET:HB3	1.74	1.22
2:C:170:PHE:HD2	2:C:203:MET:CB	1.72	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:PHE:HD2	2:C:203:MET:HB3	0.88	1.01
4:G:274:HIS:O	4:G:277:ILE:N	1.94	1.01
2:D:160:HIS:CE1	4:G:179:LEU:HD21	2.00	0.96
2:D:160:HIS:HE1	4:G:179:LEU:HD21	1.32	0.95
4:G:274:HIS:O	4:G:276:ALA:N	2.00	0.94
2:D:222:ILE:HD11	2:D:254:LEU:HD13	1.46	0.94
4:G:274:HIS:O	4:G:275:ASN:C	2.09	0.90
5:J:300:VAL:CB	5:J:305:MET:CB	2.50	0.90
2:D:190:ILE:HD11	6:D:401:C7B:C28	2.03	0.88
2:C:195:ALA:O	2:C:197:PHE:O	1.92	0.87
4:G:267:ARG:HD2	4:G:268:PRO:HD2	1.56	0.87
2:D:196:PRO:HA	2:D:197:PHE:C	2.00	0.86
2:C:265:LEU:O	2:C:265:LEU:HD12	1.75	0.86
2:D:265:LEU:HD12	2:D:265:LEU:O	1.76	0.86
2:C:170:PHE:HB2	2:C:203:MET:HG2	1.57	0.84
5:I:298:ALA:HA	5:I:299:ARG:CB	2.08	0.83
4:G:192:LEU:O	4:G:195:PHE:N	2.09	0.83
4:G:267:ARG:CD	4:G:268:PRO:HD2	2.07	0.83
5:J:156:ILE:O	5:J:297:GLY:HA2	1.78	0.83
1:B:183:VAL:HG11	1:B:215:MET:HG2	1.62	0.81
4:H:196:MET:HA	4:H:196:MET:CE	2.11	0.81
2:D:240:LEU:HD12	2:D:244:ALA:HB3	1.62	0.80
1:A:183:VAL:HG11	1:A:215:MET:HG2	1.64	0.80
5:J:157:SER:CB	5:J:297:GLY:HA3	2.13	0.79
2:C:201:HIS:O	2:C:202:GLU:C	2.26	0.79
2:C:190:ILE:HD11	6:D:401:C7B:C27	2.13	0.79
3:E:383:ASP:O	3:E:384:ARG:C	2.24	0.78
2:C:28:PRO:HB2	2:C:33:GLU:CB	2.14	0.77
2:D:201:HIS:O	2:D:204:ALA:N	2.16	0.77
5:I:155:VAL:HA	5:I:298:ALA:O	1.86	0.76
5:J:298:ALA:HA	5:J:299:ARG:CB	2.16	0.76
4:G:472:ALA:HB1	4:G:475:ASN:CB	2.16	0.76
4:H:196:MET:HA	4:H:196:MET:HE2	1.67	0.75
5:I:156:ILE:O	5:I:297:GLY:HA2	1.87	0.75
4:G:267:ARG:HD2	4:G:268:PRO:CD	2.17	0.74
5:I:165:LEU:O	5:I:169:ARG:HB2	1.88	0.74
2:C:201:HIS:O	2:C:203:MET:N	2.21	0.73
4:H:361:VAL:HA	4:H:386:LEU:O	1.89	0.73
5:J:175:GLU:O	5:J:177:ASN:N	2.21	0.73
2:D:190:ILE:CD1	6:D:401:C7B:C28	2.66	0.72
4:G:271:ALA:HB2	4:G:489:TYR:OH	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:361:VAL:HA	4:G:386:LEU:O	1.89	0.72
2:D:215:THR:HG21	4:H:177:VAL:CG2	2.20	0.72
2:D:190:ILE:HD11	6:D:401:C7B:C24	2.19	0.72
4:G:269:LEU:HD12	4:G:269:LEU:O	1.90	0.71
2:D:160:HIS:CE1	4:G:179:LEU:CD2	2.73	0.71
4:G:274:HIS:C	4:G:276:ALA:N	2.49	0.70
4:G:267:ARG:O	4:G:268:PRO:C	2.32	0.69
3:F:383:ASP:O	3:F:384:ARG:C	2.34	0.69
5:I:147:ASP:H	5:I:254:PRO:HD3	1.58	0.67
4:G:192:LEU:C	4:G:195:PHE:H	2.01	0.67
4:H:199:PRO:HG2	4:H:200:SER:H	1.60	0.66
1:A:21:ALA:HB3	1:A:24:VAL:H	1.61	0.66
2:D:222:ILE:CD1	2:D:254:LEU:HD13	2.24	0.66
2:D:196:PRO:HA	2:D:198:CYS:N	2.12	0.65
4:G:192:LEU:CB	4:G:196:MET:HB2	2.26	0.65
4:G:180:PHE:HD1	4:G:180:PHE:H	1.41	0.65
2:D:215:THR:HG21	4:H:177:VAL:HG21	1.77	0.65
2:C:195:ALA:O	2:C:197:PHE:C	2.40	0.64
4:H:472:ALA:HB1	4:H:475:ASN:CB	2.27	0.64
2:D:160:HIS:HA	4:G:182:HIS:HE1	1.63	0.63
2:C:196:PRO:HA	2:C:197:PHE:C	2.23	0.63
2:D:201:HIS:O	2:D:203:MET:N	2.32	0.63
2:C:156:LEU:HA	2:C:184:LYS:HZ1	1.62	0.63
4:G:192:LEU:HA	4:G:195:PHE:CB	2.29	0.63
5:J:175:GLU:C	5:J:177:ASN:H	2.05	0.63
1:A:128:HIS:HD1	1:A:153:THR:HG1	1.47	0.62
1:B:93:MET:HA	1:B:96:ARG:CB	2.30	0.62
3:F:229:ILE:HG13	3:F:230:PRO:HD3	1.83	0.61
4:H:473:LEU:O	4:H:476:TRP:HD1	1.82	0.61
4:G:482:LEU:HD23	4:G:482:LEU:O	2.01	0.61
3:F:88:ASP:O	3:F:92:TYR:HB2	2.01	0.60
3:E:48:PHE:HA	4:H:199:PRO:HB3	1.83	0.60
3:E:229:ILE:HG13	3:E:230:PRO:HD3	1.83	0.60
4:G:274:HIS:H	4:G:274:HIS:CD2	2.19	0.60
1:B:282:THR:HG22	1:B:283:LEU:H	1.67	0.60
2:D:201:HIS:O	2:D:202:GLU:C	2.43	0.60
4:H:173:TYR:CG	4:H:174:GLY:N	2.69	0.59
2:D:188:HIS:CE1	6:D:401:C7B:O04	2.55	0.59
3:E:88:ASP:O	3:E:92:TYR:HB2	2.01	0.59
4:G:192:LEU:CB	4:G:196:MET:CG	2.81	0.58
1:A:282:THR:HG22	1:A:283:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:240:LEU:HD12	2:C:244:ALA:HB3	1.86	0.58
4:H:267:ARG:O	4:H:268:PRO:C	2.41	0.58
1:B:97:GLY:O	1:B:101:LEU:N	2.35	0.58
3:F:48:PHE:HA	4:G:199:PRO:HB3	1.85	0.58
4:G:177:VAL:O	4:G:177:VAL:HG13	2.04	0.58
4:H:196:MET:HE2	4:H:196:MET:CA	2.34	0.58
4:H:173:TYR:OH	4:H:476:TRP:CZ2	2.55	0.58
4:H:177:VAL:HG22	4:H:177:VAL:O	2.04	0.58
3:E:342:SER:N	3:E:358:ILE:O	2.38	0.57
4:H:177:VAL:O	4:H:177:VAL:HG13	2.04	0.57
3:F:342:SER:N	3:F:358:ILE:O	2.38	0.57
4:H:180:PHE:CD1	4:H:180:PHE:N	2.73	0.57
1:A:19:ASP:O	1:A:20:MET:CB	2.53	0.56
3:F:223:SER:O	3:F:226:SER:N	2.37	0.56
5:I:154:ASP:O	5:I:298:ALA:O	2.22	0.56
4:G:177:VAL:O	4:G:177:VAL:HG22	2.04	0.56
2:C:226:MET:HE1	2:C:232:VAL:HG21	1.87	0.56
2:C:170:PHE:HB2	2:C:203:MET:CG	2.31	0.56
2:C:194:CYS:SG	2:C:195:ALA:N	2.78	0.56
4:H:196:MET:HA	4:H:196:MET:HE3	1.88	0.56
5:J:298:ALA:CA	5:J:299:ARG:CB	2.84	0.56
5:I:298:ALA:CA	5:I:299:ARG:CB	2.83	0.55
2:C:197:PHE:H	2:C:197:PHE:HD1	1.53	0.55
5:J:296:TYR:C	5:J:296:TYR:CD1	2.84	0.55
3:E:159:GLY:HA2	3:E:195:PHE:HA	1.89	0.55
4:G:192:LEU:CB	4:G:196:MET:CB	2.85	0.55
2:C:265:LEU:HD11	2:C:321:ILE:HA	1.89	0.54
2:C:170:PHE:CD1	2:C:170:PHE:C	2.85	0.54
1:A:93:MET:HA	1:A:96:ARG:CB	2.37	0.54
2:D:15:ILE:O	2:D:19:VAL:N	2.36	0.54
2:C:197:PHE:CD1	2:C:197:PHE:N	2.72	0.54
1:A:128:HIS:ND1	1:A:153:THR:OG1	2.39	0.54
3:E:223:SER:O	3:E:226:SER:N	2.37	0.54
1:A:21:ALA:HB3	1:A:24:VAL:CB	2.38	0.54
4:G:173:TYR:CD1	4:G:173:TYR:C	2.85	0.54
3:F:88:ASP:O	3:F:92:TYR:CB	2.56	0.54
4:H:173:TYR:CD1	4:H:173:TYR:C	2.86	0.53
4:H:180:PHE:HD1	4:H:180:PHE:H	1.53	0.53
2:D:240:LEU:HD12	2:D:244:ALA:CB	2.34	0.53
2:C:15:ILE:O	2:C:19:VAL:N	2.36	0.53
4:H:167:VAL:N	4:H:168:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:268:PRO:HG2	4:H:456:GLU:CB	2.38	0.53
3:F:159:GLY:HA2	3:F:195:PHE:HA	1.89	0.53
3:E:88:ASP:O	3:E:92:TYR:CB	2.56	0.53
4:G:167:VAL:N	4:G:168:PRO:HD3	2.23	0.53
2:D:291:PRO:HB2	5:J:317:TRP:HE1	1.73	0.52
2:C:201:HIS:O	2:C:204:ALA:N	2.43	0.52
1:A:21:ALA:CB	1:A:24:VAL:H	2.23	0.52
4:G:180:PHE:CD1	4:G:180:PHE:N	2.73	0.52
5:J:156:ILE:O	5:J:297:GLY:CA	2.54	0.52
2:C:286:HIS:NE2	4:G:393:TYR:OH	2.42	0.52
2:C:156:LEU:CA	2:C:184:LYS:HZ1	2.22	0.51
2:C:285:PHE:HB3	2:C:286:HIS:CE1	2.46	0.51
2:C:190:ILE:CD1	6:D:401:C7B:C27	2.87	0.51
2:D:285:PHE:HB3	2:D:286:HIS:CE1	2.45	0.51
4:H:197:SER:O	4:H:201:SER:CB	2.59	0.51
3:E:39:PRO:HG3	3:E:109:ILE:HA	1.93	0.51
5:J:165:LEU:O	5:J:169:ARG:CB	2.58	0.51
4:G:192:LEU:CB	4:G:196:MET:HG2	2.41	0.51
4:G:192:LEU:C	4:G:194:GLN:H	2.20	0.50
4:H:199:PRO:CG	4:H:200:SER:H	2.23	0.50
2:C:196:PRO:CA	2:C:197:PHE:C	2.85	0.50
4:H:471:VAL:O	4:H:472:ALA:C	2.53	0.50
4:H:199:PRO:HG2	4:H:200:SER:N	2.27	0.50
1:B:128:HIS:ND1	1:B:153:THR:OG1	2.39	0.49
2:D:194:CYS:O	2:D:195:ALA:HB3	2.12	0.49
1:B:119:ILE:HG23	1:B:125:ILE:HD11	1.95	0.49
2:C:196:PRO:HA	2:C:198:CYS:N	2.26	0.49
4:G:167:VAL:N	4:G:168:PRO:CD	2.75	0.49
2:C:291:PRO:HB2	5:I:317:TRP:HE1	1.78	0.49
2:D:266:ILE:HG21	2:D:325:ILE:HD12	1.94	0.49
4:G:192:LEU:C	4:G:194:GLN:N	2.67	0.49
3:F:39:PRO:HG3	3:F:109:ILE:HA	1.93	0.48
2:C:156:LEU:CB	2:C:184:LYS:HZ1	2.26	0.48
2:D:240:LEU:HB2	2:D:244:ALA:HB3	1.95	0.48
3:E:194:ARG:HA	5:J:239:GLU:HA	1.95	0.48
2:D:194:CYS:CB	2:D:219:ASP:CB	2.92	0.48
5:I:69:PRO:O	5:I:306:TYR:OH	2.31	0.48
4:G:192:LEU:O	4:G:194:GLN:N	2.47	0.48
1:B:215:MET:O	1:B:218:CYS:N	2.46	0.48
1:A:21:ALA:HB3	1:A:24:VAL:N	2.28	0.48
2:D:286:HIS:NE2	4:H:393:TYR:OH	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:420:THR:O	4:H:421:ALA:HB3	2.13	0.48
5:I:149:LEU:HA	5:I:250:SER:O	2.15	0.47
1:B:298:ASP:OD2	2:C:338:ARG:HD3	2.15	0.47
2:C:167:THR:HG22	2:C:233:ILE:O	2.15	0.47
4:G:274:HIS:O	4:G:276:ALA:C	2.54	0.47
1:A:73:LEU:O	1:A:77:SER:CB	2.63	0.47
1:B:30:LEU:O	1:B:34:LEU:CB	2.63	0.46
3:E:383:ASP:O	3:E:384:ARG:O	2.33	0.46
5:I:157:SER:CB	5:I:297:GLY:HA3	2.46	0.46
2:C:28:PRO:CB	2:C:33:GLU:CB	2.92	0.46
4:H:469:GLU:O	4:H:470:HIS:C	2.59	0.46
5:J:69:PRO:O	5:J:306:TYR:OH	2.30	0.46
1:A:48:ASN:O	1:A:52:ALA:N	2.48	0.46
5:J:149:LEU:HA	5:J:250:SER:O	2.15	0.46
1:A:215:MET:O	1:A:218:CYS:N	2.47	0.46
1:A:298:ASP:OD2	2:D:338:ARG:HD3	2.16	0.46
1:A:30:LEU:O	1:A:34:LEU:CB	2.63	0.45
1:B:73:LEU:O	1:B:77:SER:CB	2.63	0.45
5:I:136:ARG:O	5:I:140:ALA:CB	2.65	0.45
3:E:105:SER:H	3:E:203:HIS:HD2	1.64	0.45
4:G:186:TYR:CD2	4:G:187:SER:O	2.69	0.45
2:C:240:LEU:HB2	2:C:244:ALA:HB3	1.99	0.45
4:H:198:ILE:N	4:H:199:PRO:HD2	2.32	0.45
2:C:262:SER:OG	2:D:261:HIS:ND1	2.50	0.45
1:A:92:ILE:O	1:A:96:ARG:CB	2.65	0.44
5:J:137:ASP:O	5:J:141:LYS:CB	2.65	0.44
4:G:469:GLU:O	4:G:470:HIS:C	2.59	0.44
2:D:321:ILE:HG21	2:D:324:PHE:CE1	2.52	0.44
4:G:173:TYR:CD1	4:G:173:TYR:O	2.70	0.44
5:I:137:ASP:O	5:I:141:LYS:CB	2.65	0.44
2:C:170:PHE:CD1	2:C:170:PHE:O	2.70	0.44
2:C:201:HIS:C	2:C:203:MET:N	2.74	0.44
2:D:160:HIS:ND1	4:G:179:LEU:CD2	2.80	0.44
2:D:251:THR:O	2:D:254:LEU:HB3	2.17	0.44
3:E:384:ARG:O	3:E:401:GLY:N	2.46	0.44
2:D:265:LEU:HD11	2:D:321:ILE:HA	1.99	0.44
1:B:48:ASN:O	1:B:52:ALA:N	2.47	0.44
2:D:215:THR:HG21	4:H:177:VAL:HG23	1.98	0.44
5:J:136:ARG:O	5:J:140:ALA:CB	2.65	0.44
4:G:274:HIS:CD2	4:G:274:HIS:N	2.84	0.44
2:C:184:LYS:HG2	2:C:185:ARG:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:PHE:O	2:C:197:PHE:CG	2.71	0.44
3:F:105:SER:H	3:F:203:HIS:HD2	1.64	0.44
2:C:167:THR:HG22	2:C:233:ILE:HB	2.00	0.43
4:G:293:GLU:O	4:G:297:LYS:CB	2.66	0.43
4:H:293:GLU:O	4:H:297:LYS:CB	2.66	0.43
2:C:230:ASN:OD1	2:C:230:ASN:C	2.61	0.43
3:F:384:ARG:O	3:F:401:GLY:N	2.46	0.43
1:B:164:MET:O	1:B:168:LEU:HB2	2.19	0.43
2:C:170:PHE:HB2	2:C:203:MET:HB3	1.99	0.43
4:H:198:ILE:N	4:H:199:PRO:CD	2.81	0.43
1:A:187:MET:HE1	1:A:219:ALA:HA	2.00	0.43
4:H:267:ARG:HG2	4:H:268:PRO:HD2	1.99	0.43
2:C:207:LEU:HD23	2:C:214:THR:HG21	2.00	0.43
2:D:201:HIS:C	2:D:203:MET:N	2.76	0.43
4:H:199:PRO:CG	4:H:200:SER:N	2.82	0.43
4:G:267:ARG:NE	4:G:268:PRO:HD2	2.33	0.42
2:C:208:SER:CB	4:G:482:LEU:HD12	2.50	0.42
2:C:332:ALA:HB1	2:C:333:PRO:HD2	2.02	0.42
4:G:264:THR:HA	4:G:269:LEU:HB2	1.99	0.42
1:A:164:MET:O	1:A:168:LEU:HB2	2.19	0.42
2:C:17:SER:O	2:C:21:THR:N	2.53	0.42
1:B:92:ILE:O	1:B:96:ARG:CB	2.68	0.42
2:D:321:ILE:HG21	2:D:324:PHE:HE1	1.85	0.42
4:H:196:MET:CE	4:H:196:MET:CA	2.85	0.42
1:B:187:MET:HE1	1:B:219:ALA:HA	2.00	0.42
3:F:194:ARG:HA	5:I:239:GLU:HA	2.00	0.42
1:B:128:HIS:HD1	1:B:153:THR:HG1	1.66	0.41
1:B:228:VAL:HG23	1:B:284:LEU:HB2	2.02	0.41
4:H:472:ALA:CB	4:H:475:ASN:CB	2.97	0.41
2:C:239:ILE:HG22	2:C:245:LEU:HA	2.02	0.41
2:D:190:ILE:HD12	6:D:401:C7B:C28	2.47	0.41
1:A:228:VAL:HG23	1:A:284:LEU:HB2	2.03	0.41
2:C:246:ARG:HD2	2:C:285:PHE:CE1	2.56	0.41
2:D:17:SER:O	2:D:21:THR:N	2.53	0.41
2:D:189:VAL:HG12	2:D:191:VAL:HG23	2.03	0.41
1:B:49:LEU:O	1:B:52:ALA:HB3	2.21	0.41
2:C:189:VAL:HG12	2:C:191:VAL:HG23	2.03	0.41
4:G:179:LEU:CD2	4:G:179:LEU:C	2.94	0.40
2:D:291:PRO:HD2	5:J:317:TRP:CD1	2.56	0.40
4:G:249:SER:O	4:G:253:VAL:CB	2.70	0.40
4:H:249:SER:O	4:H:253:VAL:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:GLU:O	2:D:320:LEU:HD23	2.22	0.40
2:C:84:ARG:HH12	2:C:272:PHE:HB3	1.85	0.40
2:C:278:PHE:O	2:C:280:ASN:N	2.54	0.40
4:H:235:GLN:O	4:H:238:GLN:C	2.65	0.40
4:H:196:MET:HE2	4:H:197:SER:H	1.86	0.40
5:I:317:TRP:HD1	5:I:317:TRP:HA	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	77/373 (21%)	72 (94%)	5 (6%)	0	100	100
3	E	91/452 (20%)	68 (75%)	23 (25%)	0	100	100
4	G	7/523 (1%)	7 (100%)	0	0	100	100
4	H	96/523 (18%)	68 (71%)	23 (24%)	5 (5%)	1	17
5	J	48/721 (7%)	36 (75%)	12 (25%)	0	100	100
All	All	319/2592 (12%)	251 (79%)	63 (20%)	5 (2%)	10	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	179	LEU
4	H	202	VAL
4	H	269	LEU
4	H	270	SER
4	H	191	SER

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	77/260 (30%)	74 (96%)	3 (4%)	28	51
1	B	82/260 (32%)	79 (96%)	3 (4%)	30	52
2	C	96/319 (30%)	92 (96%)	4 (4%)	26	49
2	D	80/319 (25%)	79 (99%)	1 (1%)	61	72
3	E	25/398 (6%)	25 (100%)	0	100	100
3	F	23/398 (6%)	23 (100%)	0	100	100
4	G	56/444 (13%)	52 (93%)	4 (7%)	13	37
4	H	53/444 (12%)	49 (92%)	4 (8%)	12	35
5	I	38/626 (6%)	38 (100%)	0	100	100
5	J	28/626 (4%)	28 (100%)	0	100	100
All	All	558/4094 (14%)	539 (97%)	19 (3%)	33	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	177	VAL
1	A	229	VAL
1	B	126	LEU
1	B	177	VAL
1	B	229	VAL
2	C	170	PHE
2	C	184	LYS
2	C	239	ILE
2	C	254	LEU
2	D	273	LYS
4	G	173	TYR
4	G	179	LEU
4	G	180	PHE
4	G	274	HIS
4	H	173	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	179	LEU
4	H	180	PHE
4	H	196	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	201	HIS
2	D	158	HIS
2	D	188	HIS
3	E	203	HIS
3	F	203	HIS
4	G	182	HIS
4	G	274	HIS
4	H	182	HIS
4	H	477	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	C7B	D	401	-	32,32,32	0.75	2 (6%)	42,42,42	1.00	3 (7%)

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	C7B	D	401	-	-	5/18/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	C7B	O06-C20	2.47	1.43	1.37
6	D	401	C7B	O05-C19	2.41	1.43	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	401	C7B	C13-C11-C10	-3.18	108.00	111.49
6	D	401	C7B	C11-C13-C09	-2.68	108.55	111.49
6	D	401	C7B	C12-C14-C09	-2.28	109.00	111.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	401	C7B	C13-C09-N07-C15
6	D	401	C7B	N08-C16-C18-O06
6	D	401	C7B	O04-C16-C18-O06
6	D	401	C7B	C24-C20-O06-C18
6	D	401	C7B	C22-C20-O06-C18

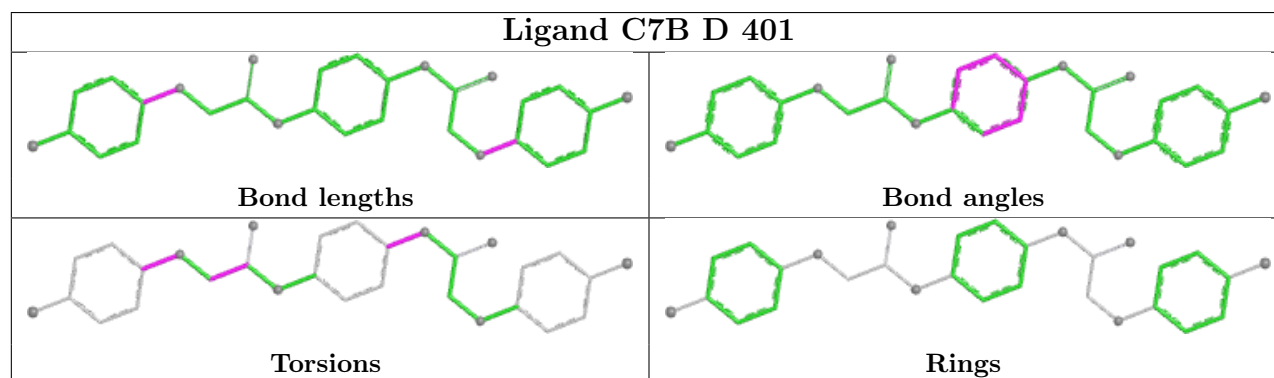
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	C7B	7	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.

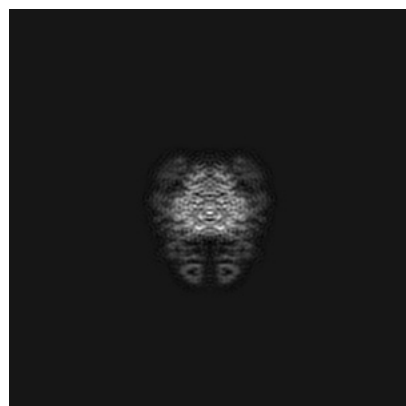
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4162. These allow visual inspection of the internal detail of the map and identification of artifacts.

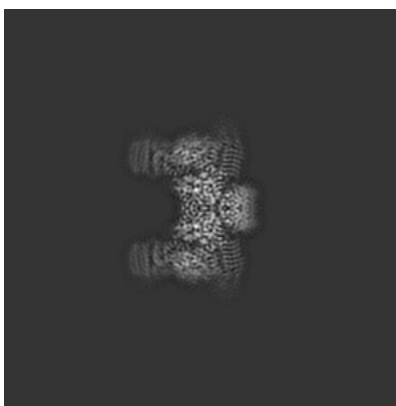
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

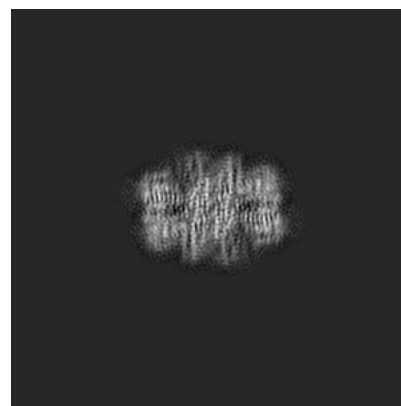
6.1.1 Primary map



X

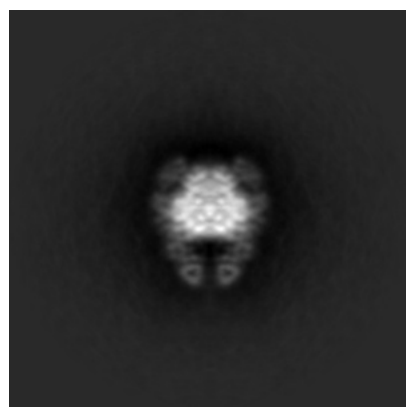


Y

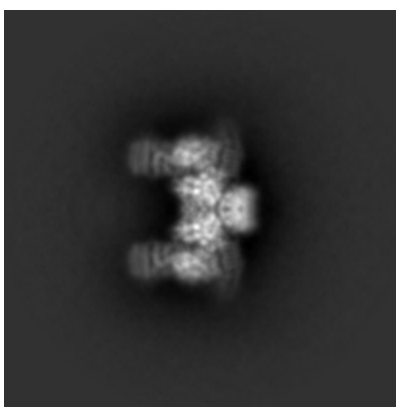


Z

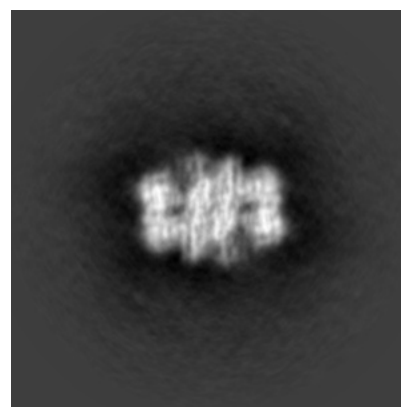
6.1.2 Raw map



X



Y



Z

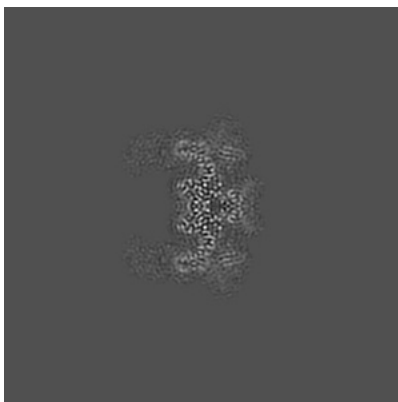
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

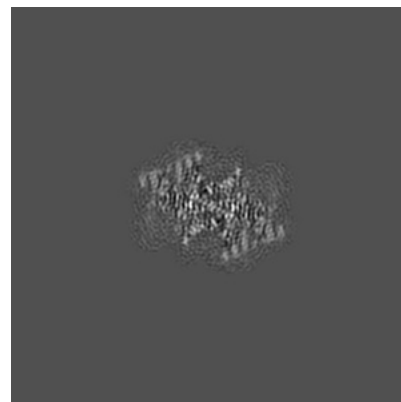
6.2.1 Primary map



X Index: 120

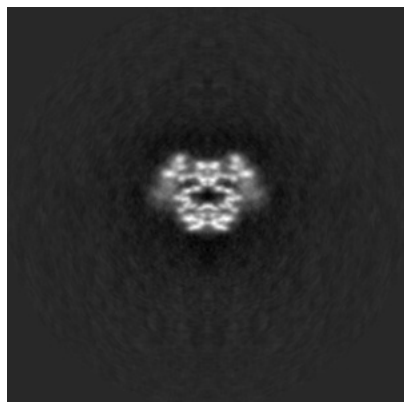


Y Index: 120

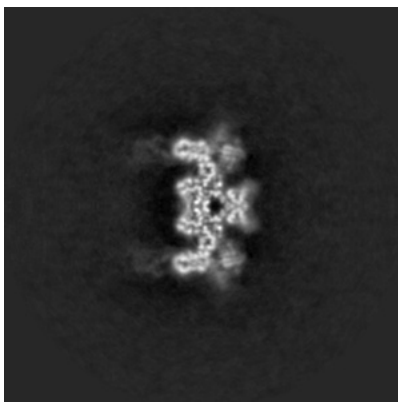


Z Index: 120

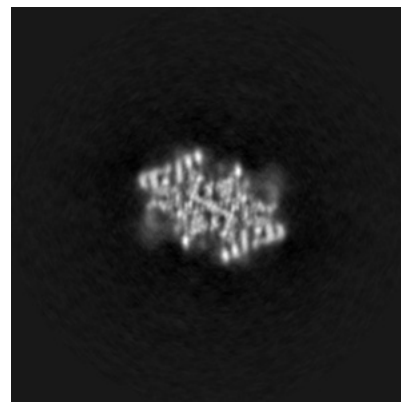
6.2.2 Raw map



X Index: 120



Y Index: 120

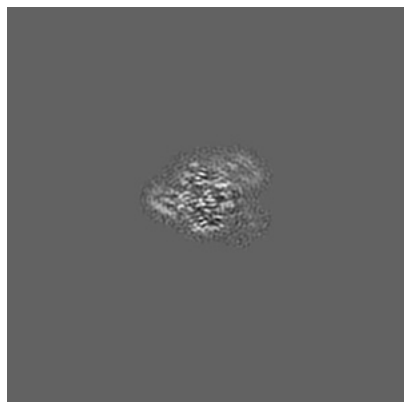


Z Index: 120

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

6.3 Largest variance slices [i](#)

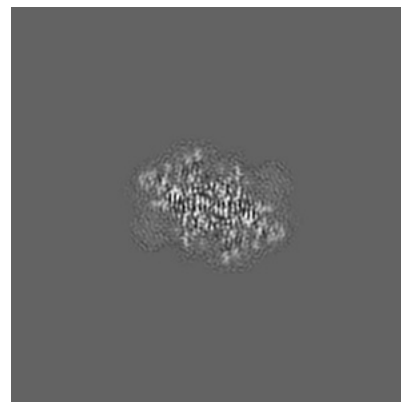
6.3.1 Primary map



X Index: 128

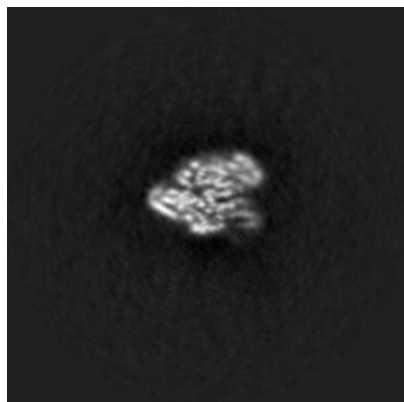


Y Index: 125

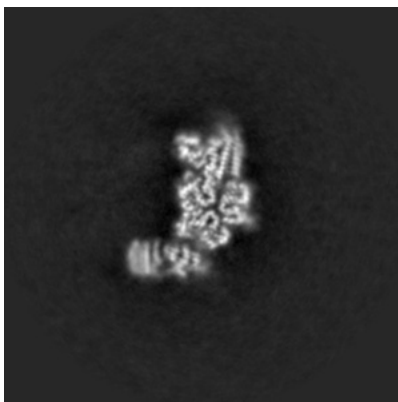


Z Index: 121

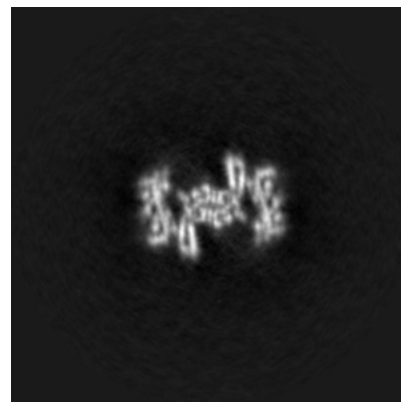
6.3.2 Raw map



X Index: 128



Y Index: 113

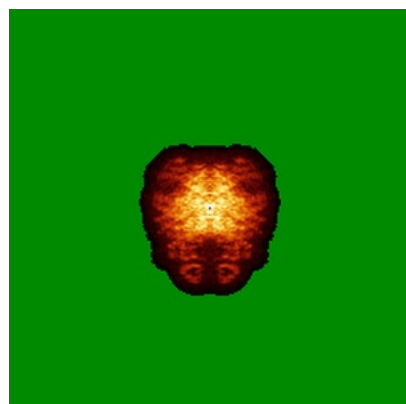


Z Index: 109

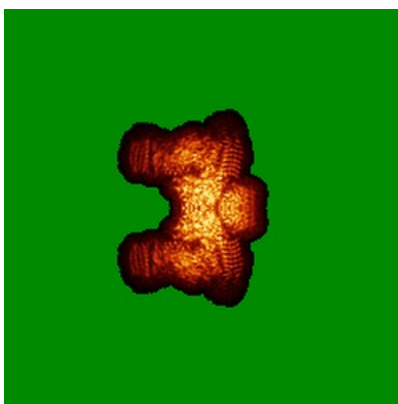
The images above show the largest variance slices of the map in three orthogonal directions.

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

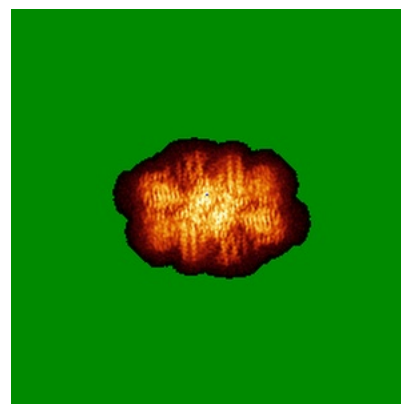
6.4.1 Primary map



X



Y



Z

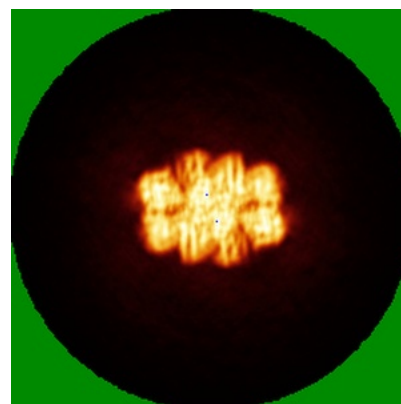
6.4.2 Raw map



X



Y



Z

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

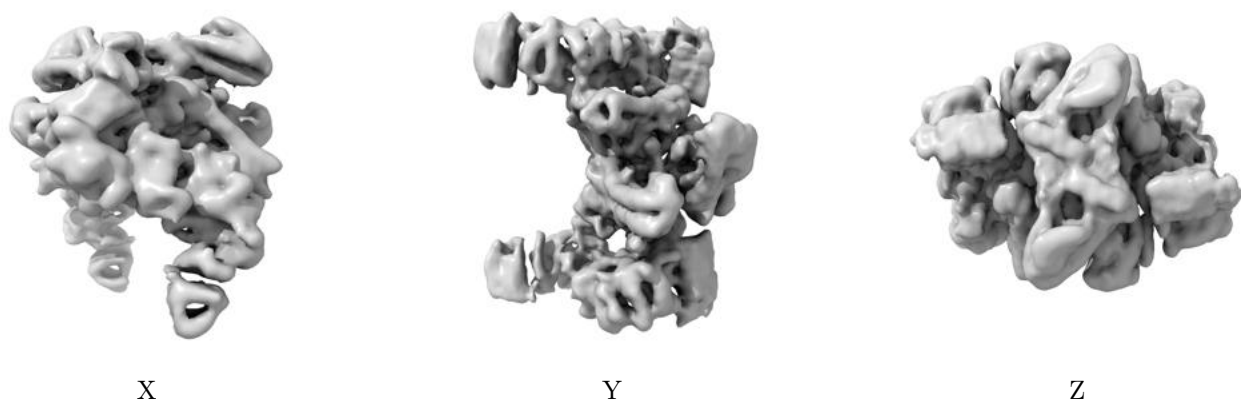
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

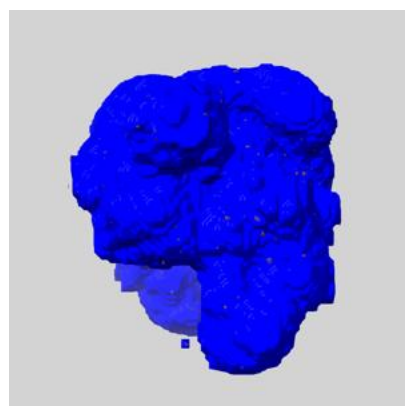
6.6 Mask visualisation [i](#)

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

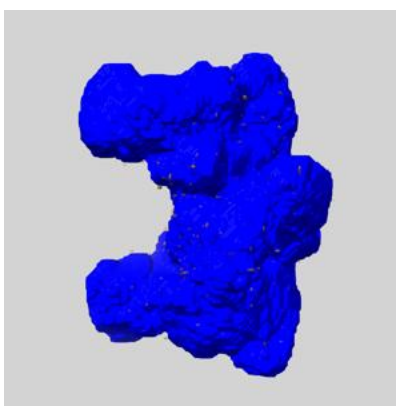
A mask typically either:

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

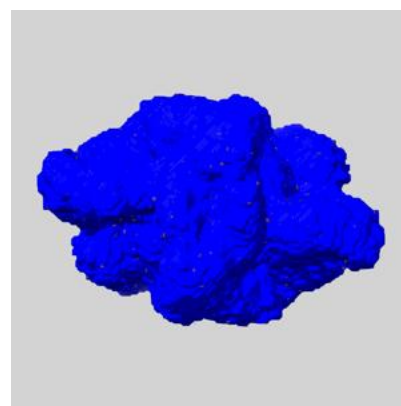
6.6.1 emd_4162_msk_1.map [i](#)



X



Y

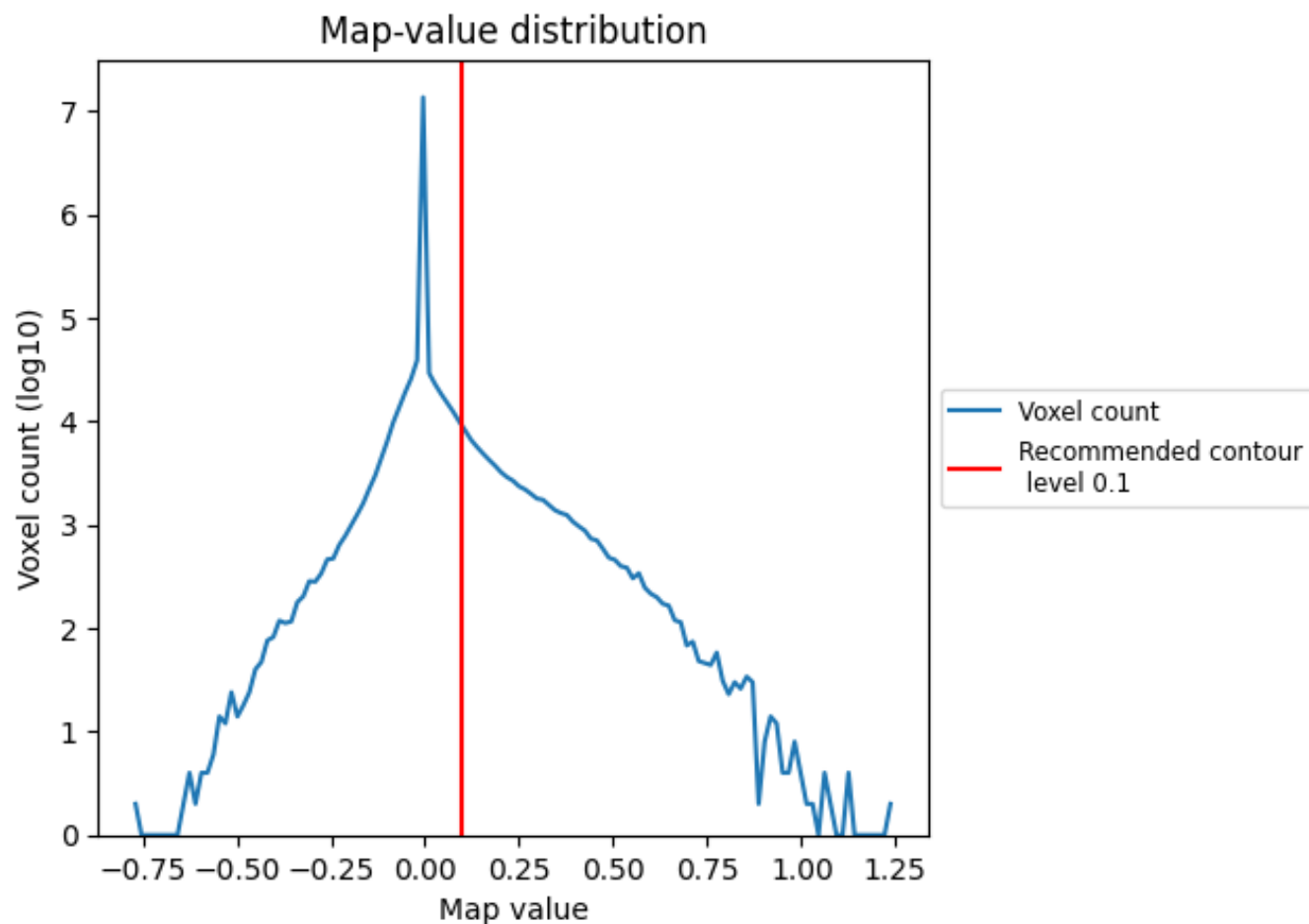


Z

7 Map analysis [i](#)

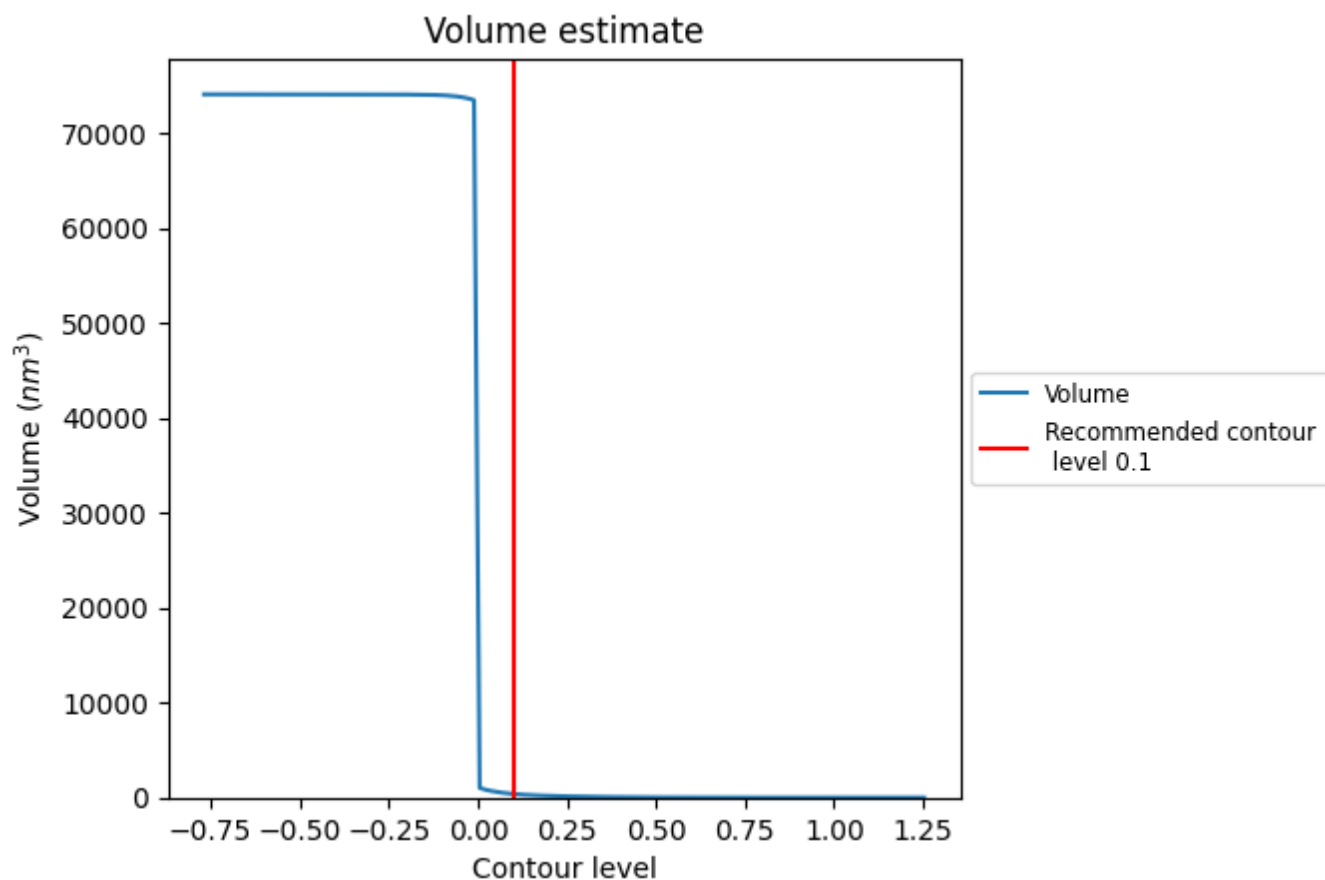
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

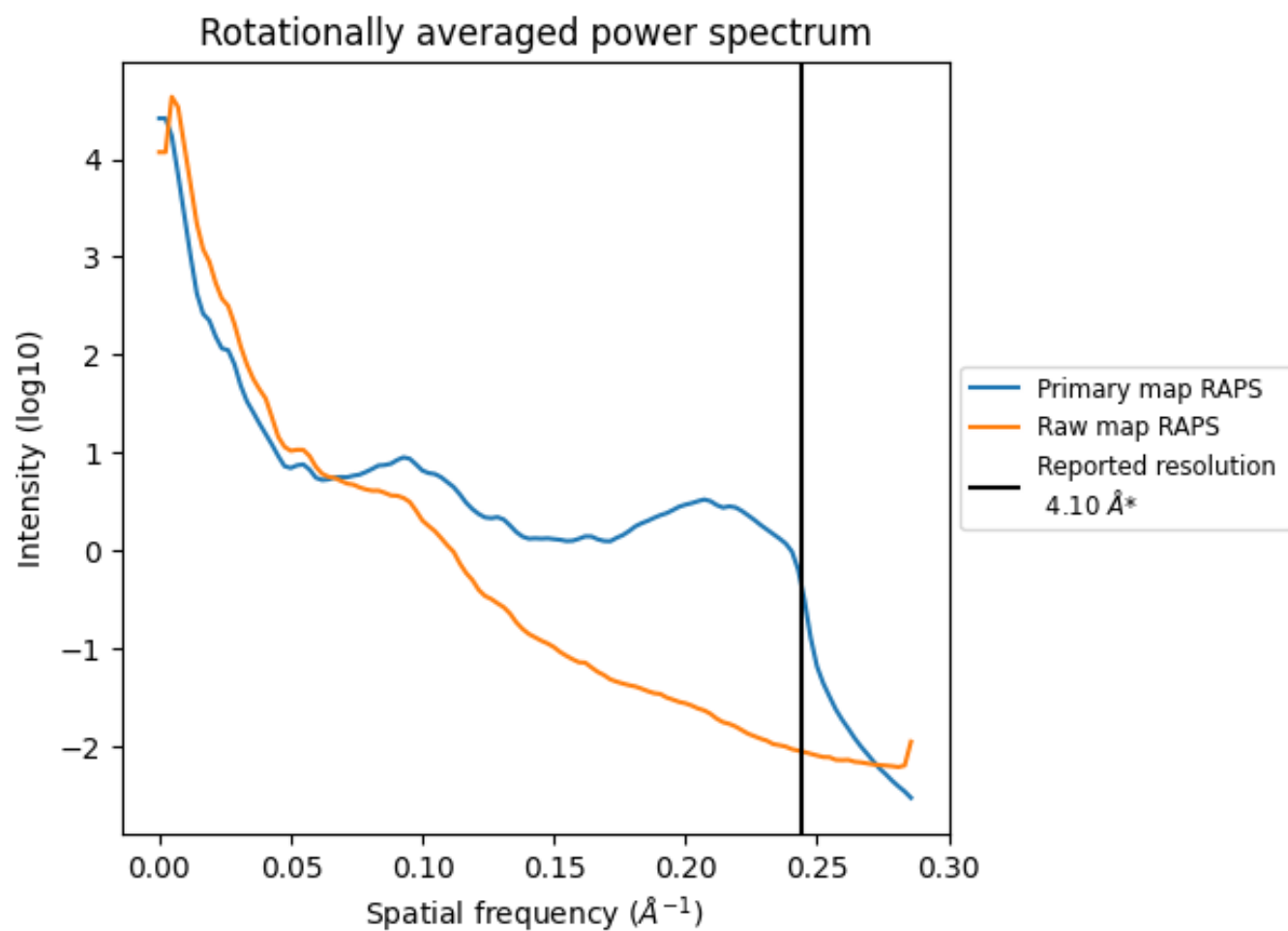
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 342 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 ⓘ

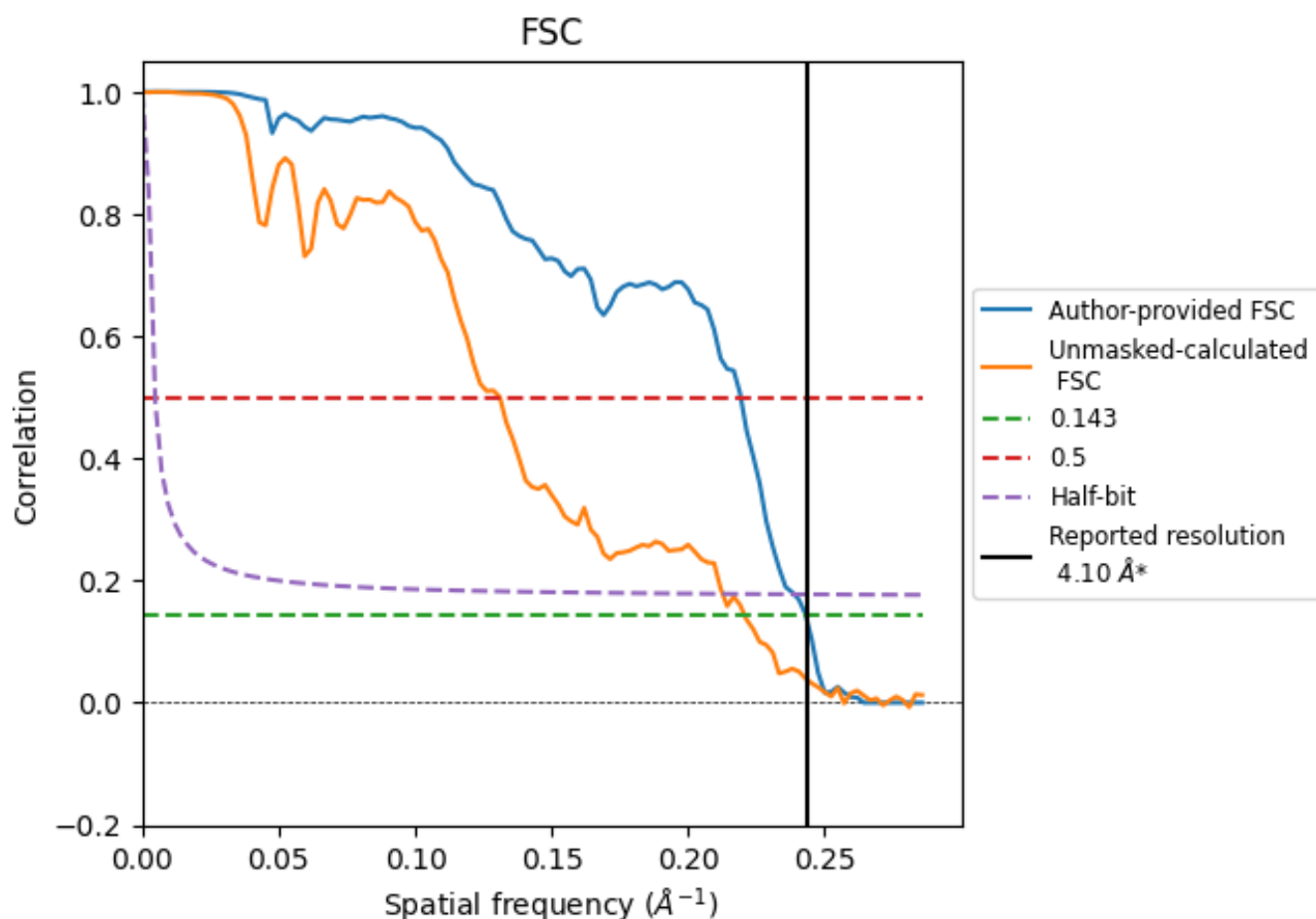


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates

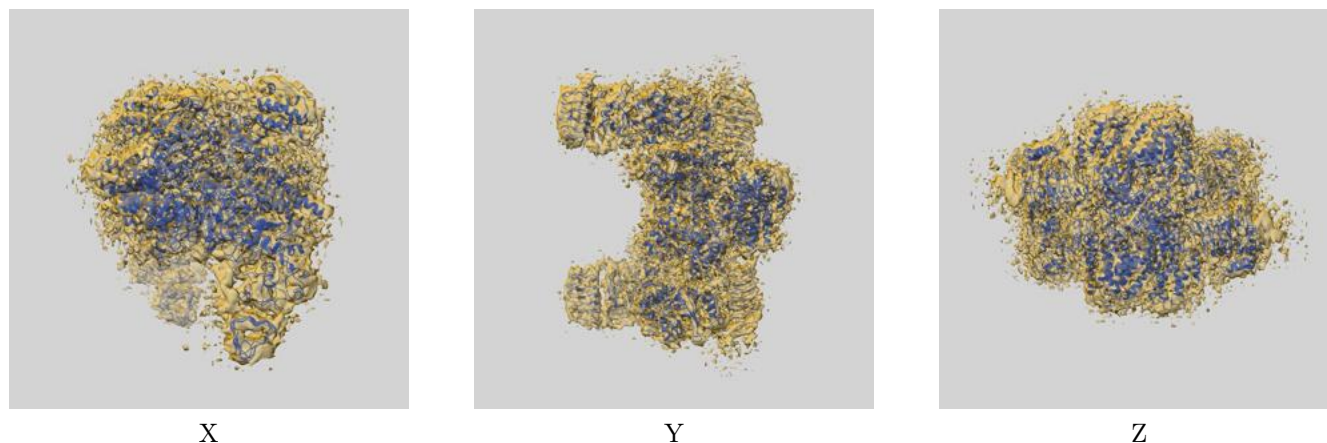
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.56	4.19
Unmasked-calculated*	4.53	7.63	4.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

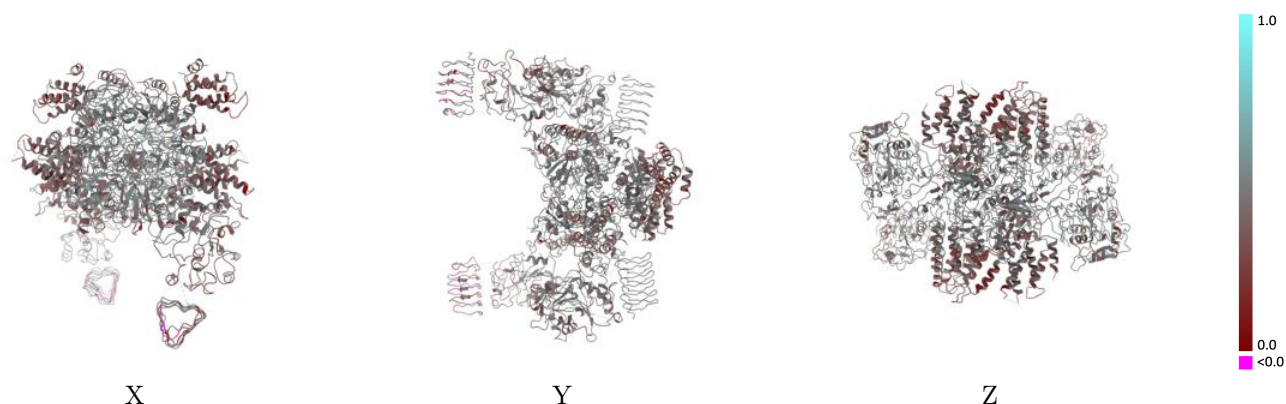
This section contains information regarding the fit between EMDB map EMD-4162 and PDB model 6EZO. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

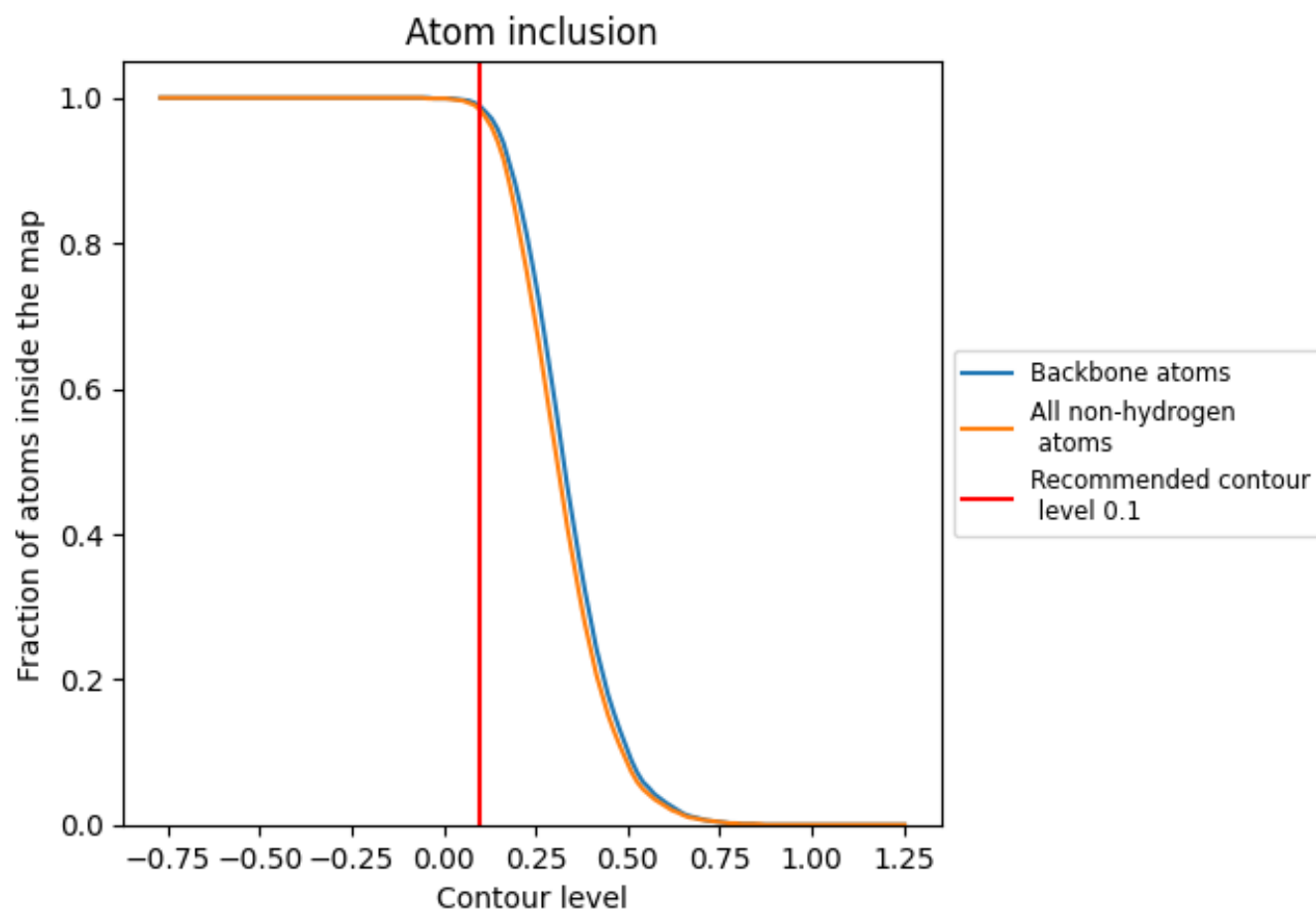


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.4360
A	0.9710	0.4140
B	0.9690	0.4130
C	0.9790	0.4430
D	0.9820	0.4440
E	0.9800	0.3990
F	0.9800	0.3980
G	0.9900	0.4590
H	0.9890	0.4590
I	0.9920	0.4590
J	0.9920	0.4580

1.0

0.0

<0.0