



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:14 AM UTC

PDB ID : 7SAR / pdb_00007sar
EMDB ID : EMD-24954
Title : Cryo-EM structure of TMEM106B fibrils extracted from a FTLD-TDP patient, polymorph 2
Authors : Cao, Q.; Jiang, Y.; Sawaya, M.R.; Eisenberg, D.S.
Deposited on : 2021-09-23
Resolution : 3.20 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:

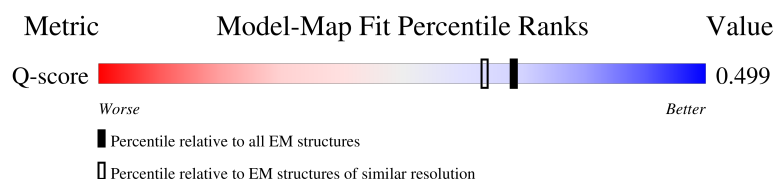
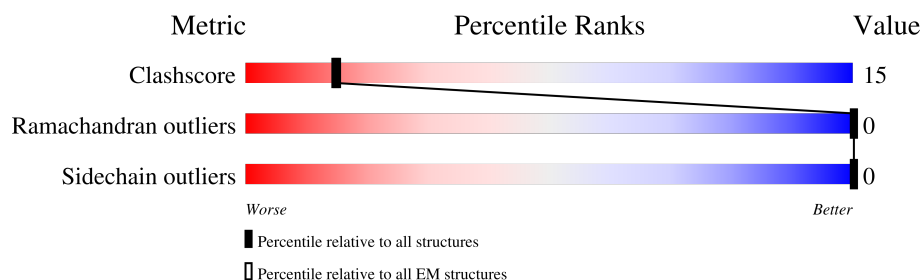
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.20 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	15020 (2.70 - 3.70)

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	274	
1	B	274	
1	C	274	
1	D	274	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	274	37% 12% 51%
1	F	274	37% 12% 51%
1	G	274	5% 38% 11% 51%
1	H	274	38% 11% 51%
1	I	274	39% 11% 51%
1	J	274	38% 12% 51%



2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11420 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 Transmembrane protein 106B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	B	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	C	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	D	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	E	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	F	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	G	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	H	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	I	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		
1	J	135	Total	C	N	O	S	0	0
			1086	694	173	212	7		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	D	1	Total 14	C 8	N 1	O 5	0
2	D	1	Total 14	C 8	N 1	O 5	0
2	E	1	Total 14	C 8	N 1	O 5	0
2	E	1	Total 14	C 8	N 1	O 5	0
2	E	1	Total 14	C 8	N 1	O 5	0
2	E	1	Total 14	C 8	N 1	O 5	0
2	F	1	Total 14	C 8	N 1	O 5	0
2	F	1	Total 14	C 8	N 1	O 5	0
2	F	1	Total 14	C 8	N 1	O 5	0
2	F	1	Total 14	C 8	N 1	O 5	0
2	G	1	Total 14	C 8	N 1	O 5	0
2	G	1	Total 14	C 8	N 1	O 5	0
2	G	1	Total 14	C 8	N 1	O 5	0
2	G	1	Total 14	C 8	N 1	O 5	0
2	H	1	Total 14	C 8	N 1	O 5	0
2	H	1	Total 14	C 8	N 1	O 5	0
2	H	1	Total 14	C 8	N 1	O 5	0
2	H	1	Total 14	C 8	N 1	O 5	0
2	I	1	Total 14	C 8	N 1	O 5	0
2	I	1	Total 14	C 8	N 1	O 5	0
2	I	1	Total 14	C 8	N 1	O 5	0

Continued on next page...

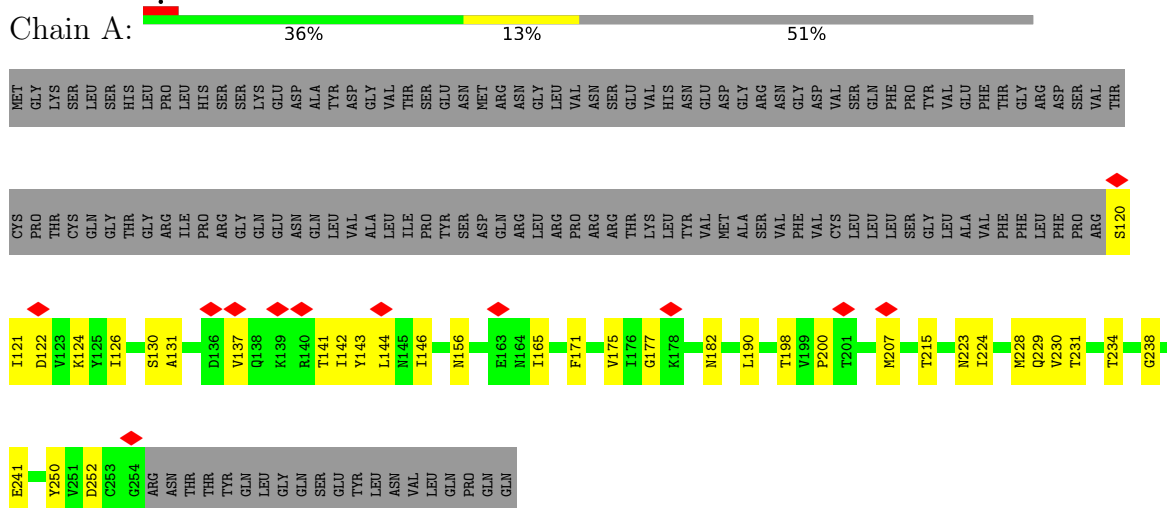
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	I	1	Total	C	N	O	0
			14	8	1	5	
2	J	1	Total	C	N	O	0
			14	8	1	5	
2	J	1	Total	C	N	O	0
			14	8	1	5	
2	J	1	Total	C	N	O	0
			14	8	1	5	
2	J	1	Total	C	N	O	0
			14	8	1	5	

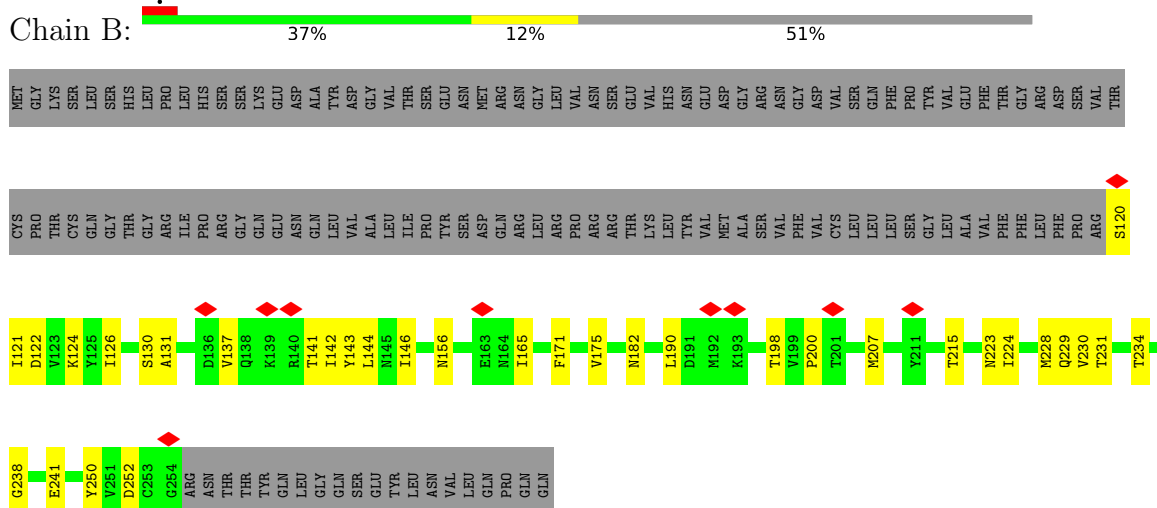
3 Residue-property plots

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.

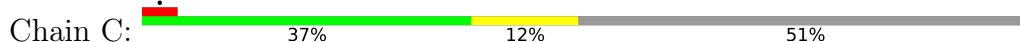
• Molecule 1: Transmembrane protein 106B



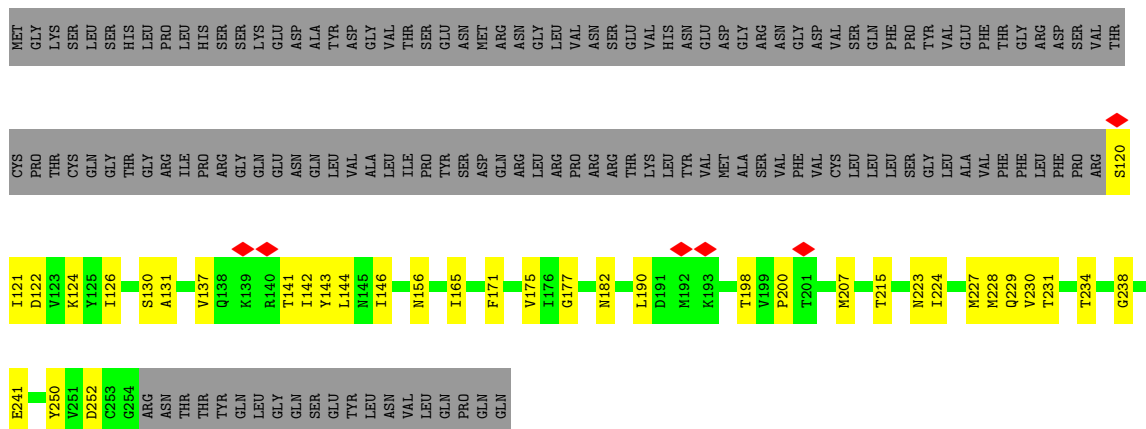
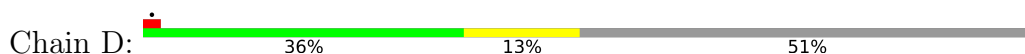
• Molecule 1: Transmembrane protein 106B



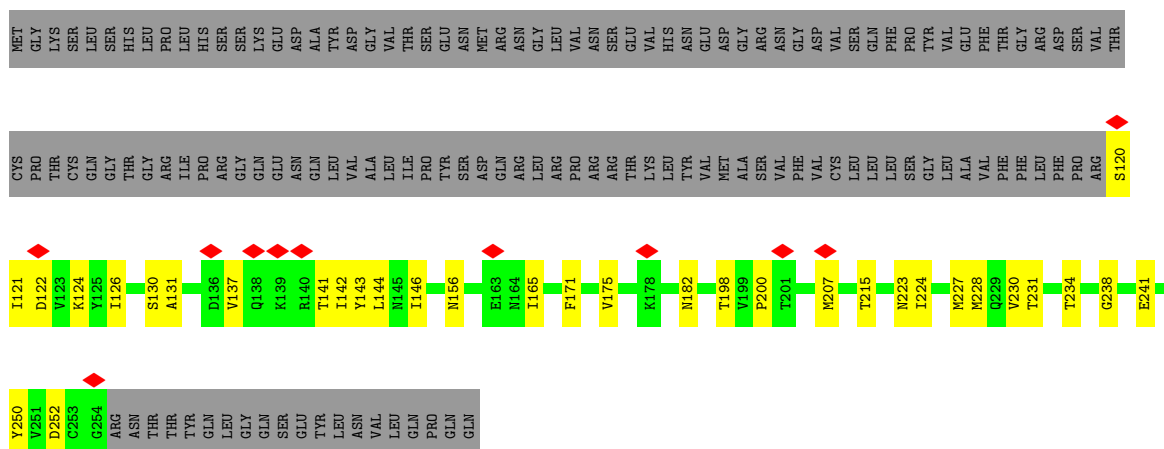
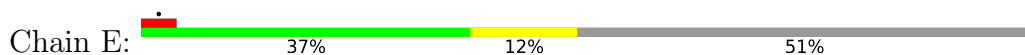
• Molecule 1: Transmembrane protein 106B



- Molecule 1: Transmembrane protein 106B



- Molecule 1: Transmembrane protein 106B



- Molecule 1: Transmembrane protein 106B

Chain F: 

C253		G254		ARG		ASN		THR		TYR		GLN		LEU		GLY		GLN		SER		GLU		TYR		LEU		ASN		VAL		GLN		PRO		GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
I121	D122	V123	K124	Y125	I126	S130	A131	V137	Q138	K139	R140	T141	I142	Y143	L144	N145	I146	N156	I165	F171	V175	N182	M192	K193	T198	V199	P200	T201	M207	T215	N223	I224	M228	Q229	V230	T231	T234	G238	E241	Y250	V251																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
CYS		PRO		THR		CYS		GLN		GLY		THR		GLY		LEU		ILE		PRO		ARG		GLN		GLY		ASN		GLN		VAL		ASP		GLY		THR		SER		PRO		TYR		VAL		GLU		PHE		THR		GLY		ARG		ASP		SER		VAL		THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
S120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	

- Molecule 1: Transmembrane protein 106B

Chain G: 

V251	D252	C253	G254	ARG	ASN	THR	THR	THR	TYR	GLN	LEU	GLY	GLN	SER	GLU	LEU	ASN	VAL	LEU	GLN	PRO	GLN																								
I121	D122	V123	K124	Y125	I126	S130	A131	D136	V137	Q138	K139	R140	T141	I142	Y143	L144	N145	I146	N156	E163	M164	I165	F171	V175	K178	A179	R180	L181	N182	T198	V199	P200	T201	M207	T215	N223	I224	M227	M228	Q229	V230	G238	E241	Y250		
MET	GLY	LYS	SER	LEU	HIS	LEU	PRO	HIS	SER	SER	LYS	GLU	ASP	ALA	TYR	ASP	GLY	VAL	ASN	SER	GLU	VAL	HIS	ASN	GLU	ASP	GLY	ARG	ASN	VAL	PHE	GLN	SER	PRO	TYR	VAL	GLU	PHE	THR	GLY	ARG	ASP	SER	VAL	THR	
CYS	PRO	THR	CYS	GLN	GLY	THR	ARG	ILE	PRO	ARG	GLN	ASN	GLN	LEU	VAL	ALA	LEU	ILE	PRO	TYR	SER	SER	ASP	GLN	ARG	ASN	GLY	VAL	ASN	ASN	ARG	THR	LYS	TYR	VAL	LEU	TYR	LEU	SER	PRO	GLY	LEU	ALA	VAL	ARG	S120

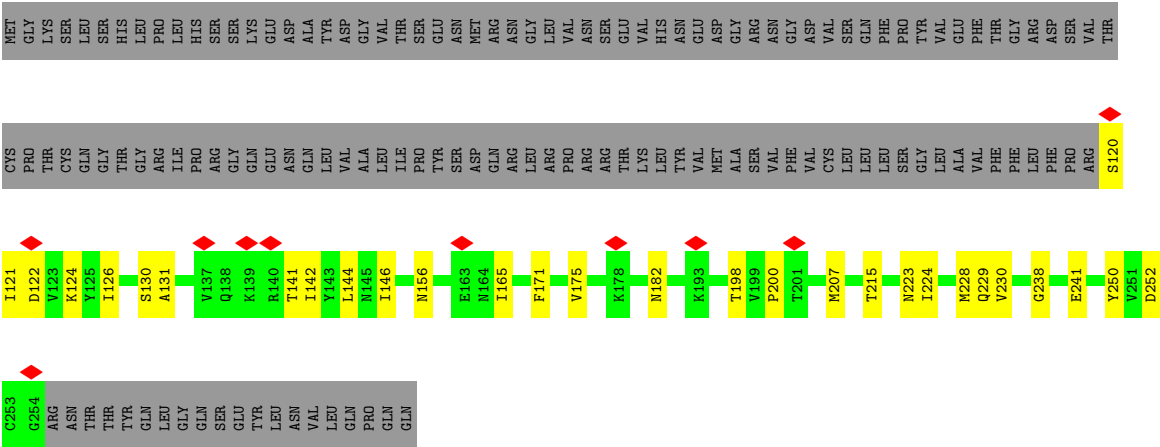
- Molecule 1: Transmembrane protein 106B

Chain H: 

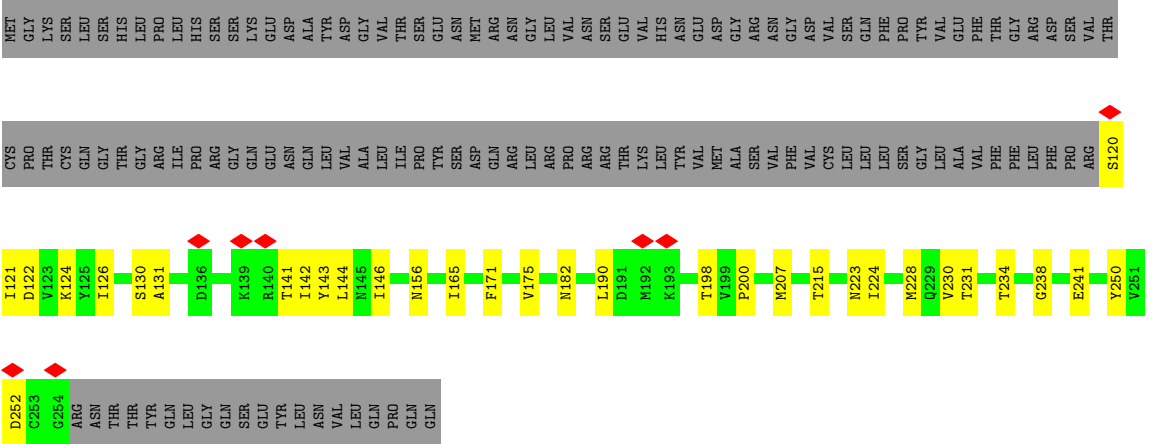
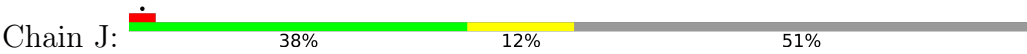
THR	THR	TYR	GLN	LEU	GLN	SER	GLU	TYR	LEU	ASN	VAL	LEU	GLN	PRO	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

- Molecule 1: Transmembrane protein 106B

Chain I: 



● Molecule 1: Transmembrane protein 106B



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.59°, rise=4.91 Å, axial sym=C2	Depositor
Number of segments used	16883	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 ($e^-/\text{Å}^2$)	39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0235	Depositor
Map size (Å)	220.0, 220.0, 55.0	wwPDB
Map dimensions	200, 200, 50	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.24	0/1104	0.48	0/1501
1	B	0.24	0/1104	0.48	0/1501
1	C	0.24	0/1104	0.48	0/1501
1	D	0.24	0/1104	0.48	0/1501
1	E	0.24	0/1104	0.48	0/1501
1	F	0.24	0/1104	0.48	0/1501
1	G	0.24	0/1104	0.48	0/1501
1	H	0.24	0/1104	0.48	0/1501
1	I	0.24	0/1104	0.48	0/1501
1	J	0.24	0/1104	0.48	0/1501
All	All	0.24	0/11040	0.48	0/15010

There are no bond length outliers.

There are no bond angle outliers.

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	1086	0	1080	57	0
1	B	1086	0	1080	56	0
1	C	1086	0	1080	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1086	0	1080	58	0
1	E	1086	0	1080	56	0
1	F	1086	0	1080	55	0
1	G	1086	0	1080	37	0
1	H	1086	0	1080	36	0
1	I	1086	0	1080	35	0
1	J	1086	0	1080	39	0
2	A	56	0	52	5	0
2	B	56	0	52	5	0
2	C	56	0	52	5	0
2	D	56	0	52	5	0
2	E	56	0	52	5	0
2	F	56	0	52	5	0
2	G	56	0	52	5	0
2	H	56	0	52	5	0
2	I	56	0	52	5	0
2	J	56	0	52	5	0
All	All	11420	0	11320	340	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 15.

All (340) 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:182:ASN:ND2	2:A:303:NAG:H82	1.77	0.99
1:F:182:ASN:ND2	2:F:303:NAG:H82	1.77	0.99
1:I:182:ASN:ND2	2:I:303:NAG:H82	1.77	0.99
1:D:182:ASN:ND2	2:D:303:NAG:H82	1.77	0.98
1:G:182:ASN:ND2	2:G:303:NAG:H82	1.77	0.98
1:J:182:ASN:ND2	2:J:303:NAG:H82	1.77	0.98
1:E:182:ASN:ND2	2:E:303:NAG:H82	1.77	0.97
1:B:182:ASN:ND2	2:B:303:NAG:H82	1.77	0.97
1:C:182:ASN:ND2	2:C:303:NAG:H82	1.77	0.97
1:H:182:ASN:ND2	2:H:303:NAG:H82	1.77	0.97
1:B:122:ASP:OD1	1:B:124:LYS:HE3	1.67	0.94
1:C:122:ASP:OD1	1:C:124:LYS:HE3	1.67	0.94
1:H:122:ASP:OD1	1:H:124:LYS:HE3	1.67	0.94
1:E:122:ASP:OD1	1:E:124:LYS:HE3	1.67	0.94
1:J:122:ASP:OD1	1:J:124:LYS:HE3	1.67	0.94
1:I:122:ASP:OD1	1:I:124:LYS:HE3	1.67	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:OD1	1:F:124:LYS:HE3	1.67	0.93
1:A:122:ASP:OD1	1:A:124:LYS:HE3	1.67	0.93
1:G:122:ASP:OD1	1:G:124:LYS:HE3	1.67	0.93
1:D:122:ASP:OD1	1:D:124:LYS:HE3	1.67	0.93
1:B:142:ILE:HG22	1:B:144:LEU:CD1	2.04	0.88
1:E:142:ILE:HG22	1:E:144:LEU:CD1	2.04	0.88
1:J:142:ILE:HG22	1:J:144:LEU:CD1	2.04	0.88
1:C:142:ILE:HG22	1:C:144:LEU:CD1	2.04	0.88
1:H:142:ILE:HG22	1:H:144:LEU:CD1	2.04	0.88
1:A:142:ILE:HG22	1:A:144:LEU:CD1	2.04	0.88
1:F:142:ILE:HG22	1:F:144:LEU:CD1	2.04	0.88
1:I:142:ILE:HG22	1:I:144:LEU:CD1	2.04	0.88
1:D:142:ILE:HG22	1:D:144:LEU:CD1	2.04	0.88
1:G:142:ILE:HG22	1:G:144:LEU:CD1	2.04	0.88
1:E:142:ILE:HG22	1:E:144:LEU:HD12	1.65	0.79
1:J:142:ILE:HG22	1:J:144:LEU:HD12	1.65	0.79
1:B:142:ILE:HG22	1:B:144:LEU:HD12	1.65	0.78
1:C:142:ILE:HG22	1:C:144:LEU:HD12	1.65	0.78
1:H:142:ILE:HG22	1:H:144:LEU:HD12	1.65	0.78
1:G:142:ILE:HG22	1:G:144:LEU:HD12	1.65	0.77
1:C:120:SER:HB2	1:C:241:GLU:OE2	1.84	0.77
1:H:120:SER:HB2	1:H:241:GLU:OE2	1.84	0.77
1:D:142:ILE:HG22	1:D:144:LEU:HD12	1.65	0.77
1:E:120:SER:HB2	1:E:241:GLU:OE2	1.84	0.77
1:B:120:SER:HB2	1:B:241:GLU:OE2	1.84	0.77
1:A:142:ILE:HG22	1:A:144:LEU:HD12	1.65	0.77
1:J:120:SER:HB2	1:J:241:GLU:OE2	1.84	0.77
1:A:230:VAL:HG12	1:D:230:VAL:HG22	1.67	0.77
1:F:142:ILE:HG22	1:F:144:LEU:HD12	1.65	0.77
1:I:120:SER:HB2	1:I:241:GLU:OE2	1.84	0.77
1:F:230:VAL:HG22	1:I:230:VAL:HG12	1.67	0.76
1:F:120:SER:HB2	1:F:241:GLU:OE2	1.84	0.76
1:I:142:ILE:HG22	1:I:144:LEU:HD12	1.65	0.76
1:A:120:SER:HB2	1:A:241:GLU:OE2	1.84	0.76
1:D:230:VAL:HG12	1:G:230:VAL:HG22	1.68	0.76
1:G:120:SER:HB2	1:G:241:GLU:OE2	1.84	0.76
1:D:120:SER:HB2	1:D:241:GLU:OE2	1.84	0.76
1:A:230:VAL:HG22	1:F:230:VAL:HG12	1.68	0.75
1:B:230:VAL:HG22	1:E:230:VAL:HG12	1.67	0.73
1:C:230:VAL:HG12	1:H:230:VAL:HG22	1.67	0.73
1:B:230:VAL:HG12	1:C:230:VAL:HG22	1.67	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:VAL:HG22	1:J:230:VAL:HG12	1.68	0.73
1:G:182:ASN:HD22	2:G:303:NAG:H82	1.54	0.73
1:D:182:ASN:HD22	2:D:303:NAG:H82	1.54	0.73
1:A:182:ASN:HD22	2:A:303:NAG:H82	1.54	0.72
1:F:182:ASN:HD22	2:F:303:NAG:H82	1.54	0.72
1:I:182:ASN:HD22	2:I:303:NAG:H82	1.54	0.72
1:F:231:THR:HG1	1:F:234:THR:HG1	1.38	0.71
1:J:182:ASN:HD22	2:J:303:NAG:H82	1.54	0.71
1:A:231:THR:HG1	1:A:234:THR:HG1	1.38	0.71
1:E:182:ASN:HD22	2:E:303:NAG:H82	1.54	0.71
1:B:143:TYR:O	1:E:144:LEU:HB2	1.91	0.70
1:B:182:ASN:HD22	2:B:303:NAG:H82	1.54	0.70
1:C:144:LEU:HB2	1:H:143:TYR:O	1.92	0.70
1:C:182:ASN:HD22	2:C:303:NAG:H82	1.54	0.70
1:A:143:TYR:O	1:F:144:LEU:HB2	1.91	0.70
1:H:182:ASN:HD22	2:H:303:NAG:H82	1.54	0.70
1:B:144:LEU:HB2	1:C:143:TYR:O	1.93	0.69
1:E:143:TYR:O	1:J:144:LEU:HB2	1.93	0.69
1:F:143:TYR:O	1:I:144:LEU:HB2	1.91	0.69
1:J:126:ILE:HD13	1:J:130:SER:HB2	1.75	0.68
1:E:126:ILE:HD13	1:E:130:SER:HB2	1.75	0.68
1:B:126:ILE:HD13	1:B:130:SER:HB2	1.75	0.68
1:D:144:LEU:HB2	1:G:143:TYR:O	1.93	0.68
1:D:231:THR:HG1	1:D:234:THR:HG1	1.41	0.68
1:C:126:ILE:HD13	1:C:130:SER:HB2	1.75	0.68
1:H:126:ILE:HD13	1:H:130:SER:HB2	1.75	0.68
1:A:144:LEU:HB2	1:D:143:TYR:O	1.93	0.67
1:F:126:ILE:HD13	1:F:130:SER:HB2	1.75	0.66
1:I:126:ILE:HD13	1:I:130:SER:HB2	1.76	0.66
1:A:175:VAL:HG13	1:D:175:VAL:HG23	1.77	0.66
1:A:126:ILE:HD13	1:A:130:SER:HB2	1.75	0.66
1:D:126:ILE:HD13	1:D:130:SER:HB2	1.75	0.66
1:G:126:ILE:HD13	1:G:130:SER:HB2	1.75	0.66
1:D:175:VAL:HG13	1:G:175:VAL:HG23	1.79	0.65
1:F:175:VAL:HG23	1:I:175:VAL:HG13	1.79	0.65
1:B:175:VAL:HG13	1:C:175:VAL:HG23	1.79	0.64
1:B:175:VAL:HG23	1:E:175:VAL:HG13	1.79	0.64
1:C:175:VAL:HG13	1:H:175:VAL:HG23	1.79	0.64
1:E:175:VAL:HG23	1:J:175:VAL:HG13	1.79	0.64
1:A:175:VAL:HG23	1:F:175:VAL:HG13	1.81	0.63
1:D:156:ASN:HD22	1:G:156:ASN:HB2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:THR:HG1	1:J:234:THR:HG1	1.37	0.62
1:A:156:ASN:HB2	1:F:156:ASN:HD22	1.65	0.62
1:A:156:ASN:HD22	1:D:156:ASN:HB2	1.65	0.62
1:F:156:ASN:HB2	1:I:156:ASN:HD22	1.65	0.61
1:B:156:ASN:HD22	1:C:156:ASN:HB2	1.64	0.61
1:E:156:ASN:HB2	1:J:156:ASN:HD22	1.64	0.61
1:C:156:ASN:HD22	1:H:156:ASN:HB2	1.65	0.60
1:D:144:LEU:O	1:D:146:ILE:HD12	2.01	0.60
1:G:144:LEU:O	1:G:146:ILE:HD12	2.01	0.60
1:A:144:LEU:O	1:A:146:ILE:HD12	2.01	0.60
1:B:156:ASN:HB2	1:E:156:ASN:HD22	1.65	0.60
1:F:144:LEU:O	1:F:146:ILE:HD12	2.01	0.60
1:I:144:LEU:O	1:I:146:ILE:HD12	2.01	0.60
1:J:144:LEU:O	1:J:146:ILE:HD12	2.01	0.59
1:H:144:LEU:O	1:H:146:ILE:HD12	2.01	0.59
1:E:144:LEU:O	1:E:146:ILE:HD12	2.01	0.59
1:C:144:LEU:O	1:C:146:ILE:HD12	2.01	0.59
1:A:224:ILE:HB	1:D:224:ILE:HD13	1.85	0.59
1:B:144:LEU:O	1:B:146:ILE:HD12	2.01	0.59
1:B:224:ILE:HB	1:C:224:ILE:HD13	1.85	0.58
1:E:224:ILE:HD13	1:J:224:ILE:HB	1.85	0.58
1:B:224:ILE:HD13	1:E:224:ILE:HB	1.85	0.58
1:C:224:ILE:HB	1:H:224:ILE:HD13	1.85	0.58
1:F:224:ILE:HD13	1:I:224:ILE:HB	1.85	0.58
1:D:224:ILE:HB	1:G:224:ILE:HD13	1.85	0.58
1:A:224:ILE:HD13	1:F:224:ILE:HB	1.86	0.58
1:F:182:ASN:HD21	2:F:303:NAG:H82	1.66	0.58
1:A:182:ASN:HD21	2:A:303:NAG:H82	1.66	0.58
1:I:182:ASN:HD21	2:I:303:NAG:H82	1.67	0.58
1:D:182:ASN:HD21	2:D:303:NAG:H82	1.66	0.57
1:G:182:ASN:HD21	2:G:303:NAG:H82	1.66	0.57
1:G:182:ASN:ND2	2:G:303:NAG:C8	2.62	0.56
1:J:231:THR:OG1	1:J:234:THR:OG1	2.16	0.55
1:E:231:THR:OG1	1:E:234:THR:OG1	2.16	0.55
1:D:182:ASN:ND2	2:D:303:NAG:C8	2.62	0.55
1:B:231:THR:OG1	1:B:234:THR:OG1	2.16	0.55
1:A:182:ASN:ND2	2:A:303:NAG:C8	2.62	0.55
1:C:231:THR:OG1	1:C:234:THR:OG1	2.16	0.55
1:F:182:ASN:ND2	2:F:303:NAG:C8	2.62	0.55
1:J:182:ASN:HD21	2:J:303:NAG:H82	1.66	0.54
1:I:182:ASN:ND2	2:I:303:NAG:C8	2.62	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ASN:HD21	2:E:303:NAG:H82	1.66	0.54
1:E:231:THR:HG1	1:E:234:THR:HG1	1.45	0.54
1:B:182:ASN:HD21	2:B:303:NAG:H82	1.66	0.54
1:B:231:THR:HG1	1:B:234:THR:HG1	1.45	0.54
1:E:182:ASN:ND2	2:E:303:NAG:C8	2.62	0.53
1:J:182:ASN:ND2	2:J:303:NAG:C8	2.62	0.53
1:B:182:ASN:ND2	2:B:303:NAG:C8	2.62	0.53
1:C:182:ASN:ND2	2:C:303:NAG:C8	2.62	0.53
1:C:182:ASN:HD21	2:C:303:NAG:H82	1.67	0.53
1:H:182:ASN:ND2	2:H:303:NAG:C8	2.62	0.53
1:H:182:ASN:HD21	2:H:303:NAG:H82	1.66	0.53
1:A:143:TYR:HD2	1:F:146:ILE:HD11	1.75	0.51
1:F:143:TYR:HD2	1:I:146:ILE:HD11	1.76	0.51
1:J:198:THR:HG22	1:J:200:PRO:HD3	1.93	0.50
1:A:171:PHE:O	1:D:171:PHE:HA	2.10	0.50
1:B:198:THR:HG22	1:B:200:PRO:HD3	1.93	0.50
1:C:198:THR:HG22	1:C:200:PRO:HD3	1.93	0.50
1:E:198:THR:HG22	1:E:200:PRO:HD3	1.93	0.50
1:I:198:THR:HG22	1:I:200:PRO:HD3	1.93	0.50
1:A:198:THR:HG22	1:A:200:PRO:HD3	1.93	0.50
1:F:198:THR:HG22	1:F:200:PRO:HD3	1.93	0.50
1:H:198:THR:HG22	1:H:200:PRO:HD3	1.93	0.50
1:D:198:THR:HG22	1:D:200:PRO:HD3	1.93	0.50
1:G:198:THR:HG22	1:G:200:PRO:HD3	1.93	0.50
1:B:143:TYR:HD2	1:E:146:ILE:HD11	1.76	0.50
1:D:142:ILE:CG2	1:D:144:LEU:CD1	2.85	0.50
1:A:142:ILE:CG2	1:A:144:LEU:CD1	2.85	0.49
1:A:250:TYR:HB3	1:D:250:TYR:O	2.13	0.49
1:C:146:ILE:HD11	1:H:143:TYR:HD2	1.76	0.49
1:A:207:MET:HA	1:F:207:MET:O	2.13	0.49
1:E:171:PHE:HA	1:J:171:PHE:O	2.12	0.49
1:G:142:ILE:CG2	1:G:144:LEU:CD1	2.85	0.49
1:H:142:ILE:CG2	1:H:144:LEU:CD1	2.85	0.49
1:B:171:PHE:O	1:C:171:PHE:HA	2.12	0.49
1:F:142:ILE:CG2	1:F:144:LEU:CD1	2.85	0.49
1:D:250:TYR:HB3	1:G:250:TYR:O	2.13	0.49
1:E:250:TYR:O	1:J:250:TYR:HB3	2.13	0.49
1:A:146:ILE:HD11	1:D:143:TYR:HD2	1.78	0.49
1:B:141:THR:HG21	1:C:137:VAL:HG12	1.93	0.49
1:B:171:PHE:HA	1:E:171:PHE:O	2.12	0.49
1:C:171:PHE:O	1:H:171:PHE:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ILE:HD11	1:G:143:TYR:HD2	1.78	0.49
1:A:250:TYR:O	1:F:250:TYR:HB3	2.13	0.49
1:B:250:TYR:HB3	1:C:250:TYR:O	2.13	0.49
1:E:137:VAL:HG12	1:J:141:THR:HG21	1.93	0.49
1:F:250:TYR:O	1:I:250:TYR:HB3	2.13	0.49
1:C:142:ILE:CG2	1:C:144:LEU:CD1	2.85	0.48
1:D:171:PHE:O	1:G:171:PHE:HA	2.12	0.48
1:I:142:ILE:CG2	1:I:144:LEU:CD1	2.85	0.48
1:B:250:TYR:O	1:E:250:TYR:HB3	2.13	0.48
1:C:250:TYR:HB3	1:H:250:TYR:O	2.13	0.48
1:D:141:THR:HG21	1:G:137:VAL:HG12	1.93	0.48
1:F:171:PHE:HA	1:I:171:PHE:O	2.12	0.48
1:F:207:MET:HA	1:I:207:MET:O	2.13	0.48
1:A:215:THR:O	1:F:215:THR:HA	2.13	0.48
1:F:131:ALA:HA	1:I:131:ALA:O	2.13	0.48
1:A:131:ALA:HA	1:F:131:ALA:O	2.12	0.48
1:D:207:MET:O	1:G:207:MET:HA	2.14	0.48
1:B:142:ILE:CG2	1:B:144:LEU:CD1	2.85	0.48
1:B:146:ILE:HD11	1:C:143:TYR:HD2	1.77	0.48
1:D:215:THR:HA	1:G:215:THR:O	2.13	0.48
1:B:131:ALA:HA	1:E:131:ALA:O	2.13	0.48
1:C:131:ALA:O	1:H:131:ALA:HA	2.13	0.48
1:E:142:ILE:CG2	1:E:144:LEU:CD1	2.85	0.48
1:E:143:TYR:HD2	1:J:146:ILE:HD11	1.77	0.48
1:F:215:THR:O	1:I:215:THR:HA	2.14	0.48
1:A:207:MET:O	1:D:207:MET:HA	2.14	0.47
1:A:131:ALA:O	1:D:131:ALA:HA	2.13	0.47
1:A:165:ILE:HA	1:D:165:ILE:O	2.14	0.47
1:A:215:THR:HA	1:D:215:THR:O	2.14	0.47
1:E:215:THR:O	1:J:215:THR:HA	2.13	0.47
1:B:131:ALA:O	1:C:131:ALA:HA	2.13	0.47
1:B:207:MET:HA	1:E:207:MET:O	2.13	0.47
1:J:142:ILE:CG2	1:J:144:LEU:CD1	2.85	0.47
1:B:215:THR:HA	1:C:215:THR:O	2.13	0.47
1:E:131:ALA:HA	1:J:131:ALA:O	2.13	0.47
1:B:207:MET:O	1:C:207:MET:HA	2.14	0.47
1:B:215:THR:O	1:E:215:THR:HA	2.14	0.47
1:C:207:MET:O	1:H:207:MET:HA	2.13	0.47
1:D:165:ILE:HA	1:G:165:ILE:O	2.15	0.47
1:A:137:VAL:HG12	1:F:141:THR:HG21	1.94	0.47
1:C:215:THR:HA	1:H:215:THR:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ALA:O	1:G:131:ALA:HA	2.14	0.47
1:E:207:MET:HA	1:J:207:MET:O	2.13	0.47
1:B:165:ILE:HA	1:C:165:ILE:O	2.15	0.47
1:E:165:ILE:O	1:J:165:ILE:HA	2.15	0.47
1:H:182:ASN:HD21	2:H:303:NAG:C8	2.27	0.47
1:C:182:ASN:HD21	2:C:303:NAG:C8	2.27	0.47
1:B:182:ASN:HD21	2:B:303:NAG:C8	2.27	0.47
1:E:182:ASN:HD21	2:E:303:NAG:C8	2.27	0.47
1:J:142:ILE:HG22	1:J:144:LEU:HD11	1.93	0.46
1:J:182:ASN:HD21	2:J:303:NAG:C8	2.27	0.46
1:A:171:PHE:HA	1:F:171:PHE:O	2.15	0.46
1:E:142:ILE:HG22	1:E:144:LEU:HD11	1.93	0.46
1:A:182:ASN:O	1:D:182:ASN:HA	2.15	0.46
1:B:142:ILE:HG22	1:B:144:LEU:HD11	1.93	0.46
1:A:141:THR:HG21	1:D:137:VAL:HG12	1.96	0.46
1:I:182:ASN:HD21	2:I:303:NAG:C8	2.27	0.46
1:B:165:ILE:O	1:E:165:ILE:HA	2.16	0.46
1:F:165:ILE:O	1:I:165:ILE:HA	2.16	0.46
1:F:182:ASN:HD21	2:F:303:NAG:C8	2.27	0.46
1:C:142:ILE:HG22	1:C:144:LEU:HD11	1.93	0.45
1:C:165:ILE:HA	1:H:165:ILE:O	2.16	0.45
1:A:182:ASN:HD21	2:A:303:NAG:C8	2.27	0.45
1:B:137:VAL:HG12	1:E:141:THR:HG21	1.97	0.45
1:H:142:ILE:HG22	1:H:144:LEU:HD11	1.93	0.45
1:A:165:ILE:O	1:F:165:ILE:HA	2.16	0.45
1:C:141:THR:HG21	1:H:137:VAL:HG12	1.97	0.45
1:D:182:ASN:HD21	2:D:303:NAG:C8	2.27	0.45
1:H:142:ILE:CG2	1:H:144:LEU:HD11	2.47	0.45
1:C:142:ILE:CG2	1:C:144:LEU:HD11	2.47	0.45
1:B:142:ILE:CG2	1:B:144:LEU:HD11	2.47	0.45
1:E:142:ILE:CG2	1:E:144:LEU:HD11	2.47	0.45
1:G:182:ASN:HD21	2:G:303:NAG:C8	2.27	0.45
1:F:137:VAL:HG12	1:I:141:THR:HG21	1.97	0.44
1:D:182:ASN:O	1:G:182:ASN:HA	2.17	0.44
1:F:182:ASN:HA	1:I:182:ASN:O	2.17	0.44
1:I:142:ILE:HG22	1:I:144:LEU:HD11	1.93	0.44
1:I:142:ILE:CG2	1:I:144:LEU:HD11	2.47	0.44
1:B:182:ASN:O	1:C:182:ASN:HA	2.17	0.43
1:C:182:ASN:O	1:H:182:ASN:HA	2.17	0.43
1:E:182:ASN:HA	1:J:182:ASN:O	2.17	0.43
1:F:142:ILE:CG2	1:F:144:LEU:HD11	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ILE:CG2	1:J:144:LEU:HD11	2.47	0.43
1:A:142:ILE:CG2	1:A:144:LEU:HD11	2.47	0.43
1:B:182:ASN:HA	1:E:182:ASN:O	2.17	0.43
1:D:142:ILE:CG2	1:D:144:LEU:HD11	2.47	0.43
1:F:121:ILE:N	1:F:121:ILE:HD12	2.34	0.43
1:F:142:ILE:HG22	1:F:144:LEU:HD11	1.93	0.43
1:G:142:ILE:CG2	1:G:144:LEU:HD11	2.47	0.43
1:A:121:ILE:N	1:A:121:ILE:HD12	2.34	0.43
1:A:142:ILE:HG22	1:A:144:LEU:HD11	1.93	0.43
1:I:121:ILE:N	1:I:121:ILE:HD12	2.34	0.43
1:B:228:MET:HE3	1:C:228:MET:HG3	2.01	0.43
1:D:121:ILE:N	1:D:121:ILE:HD12	2.34	0.43
1:E:228:MET:HG3	1:J:228:MET:HE3	2.01	0.43
1:G:121:ILE:N	1:G:121:ILE:HD12	2.34	0.43
1:J:121:ILE:HD12	1:J:121:ILE:N	2.34	0.43
1:B:228:MET:HG3	1:E:228:MET:HE3	2.01	0.43
1:C:228:MET:HE3	1:H:228:MET:HG3	2.01	0.43
1:E:121:ILE:HD12	1:E:121:ILE:N	2.34	0.43
1:D:142:ILE:HG22	1:D:144:LEU:HD11	1.93	0.43
1:F:231:THR:OG1	1:F:234:THR:OG1	2.16	0.43
1:B:121:ILE:N	1:B:121:ILE:HD12	2.34	0.43
1:A:231:THR:OG1	1:A:234:THR:OG1	2.16	0.43
1:C:121:ILE:HD12	1:C:121:ILE:N	2.34	0.43
1:H:121:ILE:HD12	1:H:121:ILE:N	2.34	0.43
1:A:228:MET:HE3	1:D:228:MET:HG3	2.01	0.42
1:D:231:THR:OG1	1:D:234:THR:OG1	2.16	0.42
1:D:228:MET:HE3	1:G:228:MET:HG3	2.01	0.42
1:A:144:LEU:HA	1:F:144:LEU:HD22	2.02	0.42
1:G:142:ILE:HG22	1:G:144:LEU:HD11	1.93	0.42
1:F:228:MET:HG3	1:I:228:MET:HE3	2.01	0.42
1:A:228:MET:HG3	1:F:228:MET:HE3	2.01	0.42
1:D:144:LEU:HD22	1:G:144:LEU:HA	2.02	0.42
1:B:144:LEU:HD22	1:C:144:LEU:HA	2.02	0.42
1:A:182:ASN:HA	1:F:182:ASN:O	2.19	0.42
1:D:228:MET:HG2	1:D:229:GLN:HG3	2.02	0.42
1:A:238:GLY:O	1:D:238:GLY:HA3	2.19	0.42
1:E:144:LEU:HA	1:J:144:LEU:HD22	2.02	0.42
1:G:228:MET:HG2	1:G:229:GLN:HG3	2.02	0.42
1:I:228:MET:HG2	1:I:229:GLN:HG3	2.02	0.42
1:A:228:MET:HG2	1:A:229:GLN:HG3	2.02	0.42
1:F:228:MET:HG2	1:F:229:GLN:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD11	1:D:227:MET:HE1	2.01	0.41
1:B:252:ASP:O	1:E:252:ASP:HA	2.21	0.41
1:A:223:ASN:ND2	1:A:224:ILE:HG12	2.36	0.41
1:C:252:ASP:HA	1:H:252:ASP:O	2.21	0.41
1:D:223:ASN:ND2	1:D:224:ILE:HG12	2.36	0.41
1:F:223:ASN:ND2	1:F:224:ILE:HG12	2.36	0.41
1:G:223:ASN:ND2	1:G:224:ILE:HG12	2.36	0.41
1:B:238:GLY:O	1:C:238:GLY:HA3	2.20	0.41
1:D:238:GLY:O	1:G:238:GLY:HA3	2.20	0.41
1:E:238:GLY:HA3	1:J:238:GLY:O	2.20	0.41
1:F:238:GLY:HA3	1:I:238:GLY:O	2.20	0.41
1:F:252:ASP:O	1:I:252:ASP:HA	2.21	0.41
1:I:223:ASN:ND2	1:I:224:ILE:HG12	2.36	0.41
1:J:223:ASN:ND2	1:J:224:ILE:HG12	2.36	0.41
1:A:252:ASP:O	1:F:252:ASP:HA	2.21	0.41
1:B:223:ASN:ND2	1:B:224:ILE:HG12	2.36	0.41
1:D:190:LEU:HD11	1:G:227:MET:HE1	2.02	0.41
1:E:223:ASN:ND2	1:E:224:ILE:HG12	2.36	0.41
1:C:223:ASN:ND2	1:C:224:ILE:HG12	2.36	0.41
1:E:227:MET:HE1	1:J:190:LEU:HD11	2.01	0.41
1:H:223:ASN:ND2	1:H:224:ILE:HG12	2.36	0.41
1:B:190:LEU:HD11	1:C:227:MET:HE1	2.02	0.41
1:B:238:GLY:HA3	1:E:238:GLY:O	2.20	0.41
1:C:238:GLY:O	1:H:238:GLY:HA3	2.20	0.41
1:A:238:GLY:HA3	1:F:238:GLY:O	2.21	0.41
1:B:252:ASP:HA	1:C:252:ASP:O	2.21	0.41
1:E:252:ASP:O	1:J:252:ASP:HA	2.21	0.41
1:A:177:GLY:O	1:D:177:GLY:HA2	2.21	0.40
1:A:252:ASP:HA	1:D:252:ASP:O	2.21	0.40
1:H:228:MET:HG2	1:H:229:GLN:HG3	2.02	0.40
1:C:228:MET:HG2	1:C:229:GLN:HG3	2.02	0.40
1:D:252:ASP:HA	1:G:252:ASP:O	2.21	0.40
1:B:228:MET:HG2	1:B:229:GLN:HG3	2.02	0.40
1:C:143:TYR:CE2	1:C:146:ILE:HD13	2.57	0.40
1:E:143:TYR:CE2	1:E:146:ILE:HD13	2.57	0.40
1:H:143:TYR:CE2	1:H:146:ILE:HD13	2.57	0.40
1:J:143:TYR:CE2	1:J:146:ILE:HD13	2.57	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	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	B	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	C	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	D	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	E	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	F	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	G	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	H	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	I	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
1	J	133/274 (48%)	118 (89%)	15 (11%)	0	100	100
All	All	1330/2740 (48%)	1180 (89%)	150 (11%)	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	126/250 (50%)	126 (100%)	0	100	100
1	B	126/250 (50%)	126 (100%)	0	100	100
1	C	126/250 (50%)	126 (100%)	0	100	100
1	D	126/250 (50%)	126 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	126/250 (50%)	126 (100%)	0	100	100
1	F	126/250 (50%)	126 (100%)	0	100	100
1	G	126/250 (50%)	126 (100%)	0	100	100
1	H	126/250 (50%)	126 (100%)	0	100	100
1	I	126/250 (50%)	126 (100%)	0	100	100
1	J	126/250 (50%)	126 (100%)	0	100	100
All	All	1260/2500 (50%)	1260 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	182	ASN
1	A	194	GLN
1	A	223	ASN
1	B	156	ASN
1	B	182	ASN
1	B	194	GLN
1	B	223	ASN
1	C	156	ASN
1	C	182	ASN
1	C	194	GLN
1	C	223	ASN
1	D	156	ASN
1	D	182	ASN
1	D	194	GLN
1	D	223	ASN
1	E	156	ASN
1	E	182	ASN
1	E	194	GLN
1	E	223	ASN
1	F	156	ASN
1	F	182	ASN
1	F	194	GLN
1	F	223	ASN
1	G	156	ASN
1	G	182	ASN
1	G	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	223	ASN
1	H	156	ASN
1	H	182	ASN
1	H	194	GLN
1	H	223	ASN
1	I	156	ASN
1	I	182	ASN
1	I	223	ASN
1	I	239	HIS
1	J	156	ASN
1	J	182	ASN
1	J	194	GLN
1	J	223	ASN
1	J	239	HIS

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](#)

40 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
2	NAG	B	302	1	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	F	301	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	B	304	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	F	304	1	14,14,15	0.22	0	17,19,21	0.35	0
2	NAG	E	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	F	303	1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	C	304	1	14,14,15	0.23	0	17,19,21	0.34	0
2	NAG	D	301	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	H	301	1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	A	302	1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	A	301	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	C	302	1	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	I	301	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	D	304	1	14,14,15	0.21	0	17,19,21	0.34	0
2	NAG	J	302	1	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	E	301	1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	A	304	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	E	304	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	J	301	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	J	304	1	14,14,15	0.23	0	17,19,21	0.34	0
2	NAG	A	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	I	304	1	14,14,15	0.20	0	17,19,21	0.34	0
2	NAG	G	304	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	D	302	1	14,14,15	0.22	0	17,19,21	0.38	0
2	NAG	H	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	H	304	1	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	B	301	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	E	302	1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	H	302	1	14,14,15	0.23	0	17,19,21	0.37	0
2	NAG	J	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	C	301	1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	D	303	1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	I	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	G	301	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	I	302	1	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	G	302	1	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	F	302	1	14,14,15	0.21	0	17,19,21	0.38	0
2	NAG	C	303	1	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	G	303	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	B	303	1	14,14,15	0.25	0	17,19,21	0.48	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
2	NAG	B	302	1	-	1/6/23/26	0/1/1/1
2	NAG	F	301	1	-	2/6/23/26	0/1/1/1
2	NAG	B	304	1	-	2/6/23/26	0/1/1/1
2	NAG	F	304	1	-	2/6/23/26	0/1/1/1
2	NAG	E	303	1	-	1/6/23/26	0/1/1/1
2	NAG	F	303	1	-	1/6/23/26	0/1/1/1
2	NAG	C	304	1	-	2/6/23/26	0/1/1/1
2	NAG	D	301	1	-	2/6/23/26	0/1/1/1
2	NAG	H	301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	302	1	-	1/6/23/26	0/1/1/1
2	NAG	A	301	1	-	2/6/23/26	0/1/1/1
2	NAG	C	302	1	-	1/6/23/26	0/1/1/1
2	NAG	I	301	1	-	2/6/23/26	0/1/1/1
2	NAG	D	304	1	-	2/6/23/26	0/1/1/1
2	NAG	J	302	1	-	1/6/23/26	0/1/1/1
2	NAG	E	301	1	-	2/6/23/26	0/1/1/1
2	NAG	A	304	1	-	2/6/23/26	0/1/1/1
2	NAG	E	304	1	-	2/6/23/26	0/1/1/1
2	NAG	J	301	1	-	2/6/23/26	0/1/1/1
2	NAG	J	304	1	-	2/6/23/26	0/1/1/1
2	NAG	A	303	1	-	1/6/23/26	0/1/1/1
2	NAG	I	304	1	-	2/6/23/26	0/1/1/1
2	NAG	G	304	1	-	2/6/23/26	0/1/1/1
2	NAG	D	302	1	-	1/6/23/26	0/1/1/1
2	NAG	H	303	1	-	1/6/23/26	0/1/1/1
2	NAG	H	304	1	-	2/6/23/26	0/1/1/1
2	NAG	B	301	1	-	2/6/23/26	0/1/1/1
2	NAG	E	302	1	-	1/6/23/26	0/1/1/1
2	NAG	H	302	1	-	1/6/23/26	0/1/1/1
2	NAG	J	303	1	-	1/6/23/26	0/1/1/1
2	NAG	C	301	1	-	2/6/23/26	0/1/1/1
2	NAG	D	303	1	-	1/6/23/26	0/1/1/1
2	NAG	I	303	1	-	1/6/23/26	0/1/1/1
2	NAG	G	301	1	-	2/6/23/26	0/1/1/1
2	NAG	I	302	1	-	1/6/23/26	0/1/1/1
2	NAG	G	302	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	302	1	-	1/6/23/26	0/1/1/1
2	NAG	C	303	1	-	1/6/23/26	0/1/1/1
2	NAG	G	303	1	-	1/6/23/26	0/1/1/1
2	NAG	B	303	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	304	NAG	O5-C5-C6-O6
2	B	304	NAG	O5-C5-C6-O6
2	C	304	NAG	O5-C5-C6-O6
2	D	304	NAG	O5-C5-C6-O6
2	E	304	NAG	O5-C5-C6-O6
2	F	304	NAG	O5-C5-C6-O6
2	G	304	NAG	O5-C5-C6-O6
2	H	304	NAG	O5-C5-C6-O6
2	I	304	NAG	O5-C5-C6-O6
2	J	304	NAG	O5-C5-C6-O6
2	A	304	NAG	C4-C5-C6-O6
2	B	304	NAG	C4-C5-C6-O6
2	C	304	NAG	C4-C5-C6-O6
2	D	304	NAG	C4-C5-C6-O6
2	E	304	NAG	C4-C5-C6-O6
2	F	304	NAG	C4-C5-C6-O6
2	G	304	NAG	C4-C5-C6-O6
2	H	304	NAG	C4-C5-C6-O6
2	I	304	NAG	C4-C5-C6-O6
2	J	304	NAG	C4-C5-C6-O6
2	A	301	NAG	O5-C5-C6-O6
2	B	301	NAG	O5-C5-C6-O6
2	C	301	NAG	O5-C5-C6-O6
2	D	301	NAG	O5-C5-C6-O6
2	E	301	NAG	O5-C5-C6-O6
2	F	301	NAG	O5-C5-C6-O6
2	G	301	NAG	O5-C5-C6-O6
2	H	301	NAG	O5-C5-C6-O6
2	I	301	NAG	O5-C5-C6-O6
2	J	301	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	301	NAG	C4-C5-C6-O6
2	C	301	NAG	C4-C5-C6-O6
2	D	301	NAG	C4-C5-C6-O6
2	E	301	NAG	C4-C5-C6-O6
2	G	301	NAG	C4-C5-C6-O6
2	H	301	NAG	C4-C5-C6-O6
2	J	301	NAG	C4-C5-C6-O6
2	B	301	NAG	C4-C5-C6-O6
2	F	301	NAG	C4-C5-C6-O6
2	I	301	NAG	C4-C5-C6-O6
2	B	303	NAG	O5-C5-C6-O6
2	D	303	NAG	O5-C5-C6-O6
2	E	303	NAG	O5-C5-C6-O6
2	F	303	NAG	O5-C5-C6-O6
2	G	303	NAG	O5-C5-C6-O6
2	H	303	NAG	O5-C5-C6-O6
2	I	303	NAG	O5-C5-C6-O6
2	J	303	NAG	O5-C5-C6-O6
2	A	303	NAG	O5-C5-C6-O6
2	C	303	NAG	O5-C5-C6-O6
2	A	302	NAG	O5-C5-C6-O6
2	B	302	NAG	O5-C5-C6-O6
2	C	302	NAG	O5-C5-C6-O6
2	D	302	NAG	O5-C5-C6-O6
2	E	302	NAG	O5-C5-C6-O6
2	F	302	NAG	O5-C5-C6-O6
2	G	302	NAG	O5-C5-C6-O6
2	H	302	NAG	O5-C5-C6-O6
2	I	302	NAG	O5-C5-C6-O6
2	J	302	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	303	NAG	5	0
2	F	303	NAG	5	0
2	A	303	NAG	5	0
2	H	303	NAG	5	0
2	J	303	NAG	5	0
2	D	303	NAG	5	0
2	I	303	NAG	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	NAG	5	0
2	G	303	NAG	5	0
2	B	303	NAG	5	0

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.

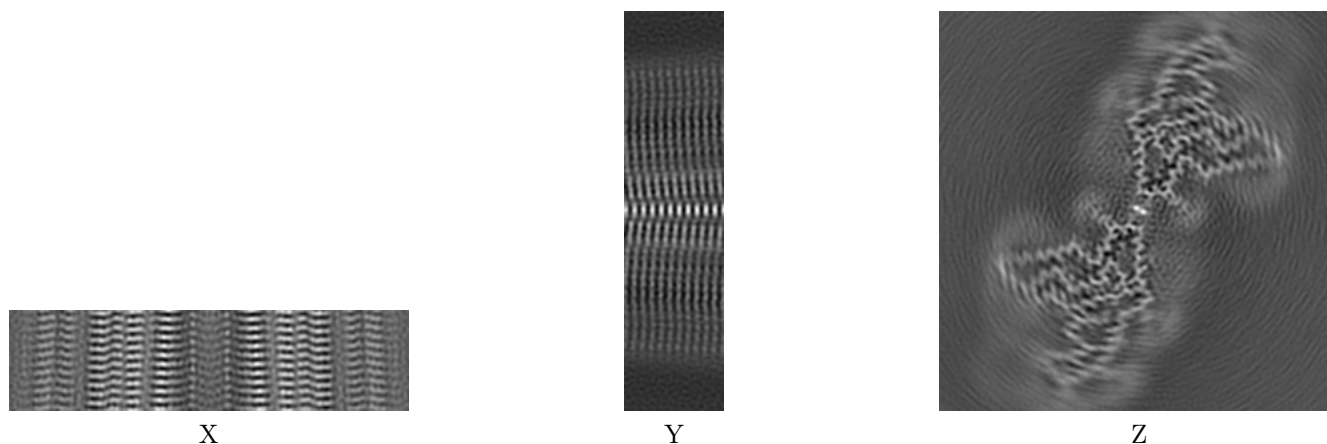
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24954. 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



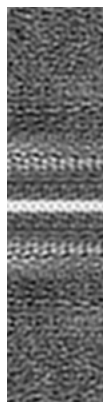
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

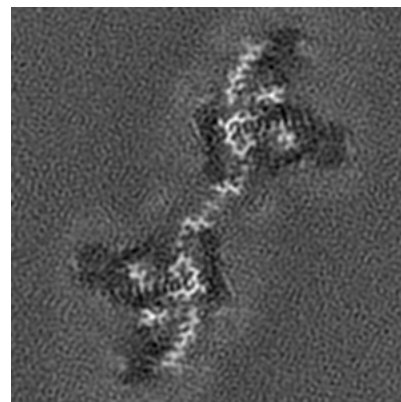
6.2.1 Primary map



X Index: 100



Y Index:
100



Z Index: 25

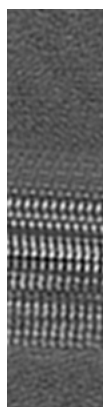
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

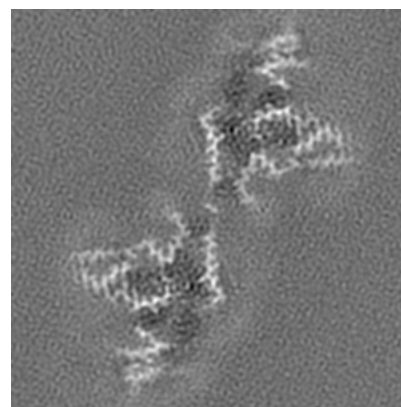
6.3.1 Primary map



X Index: 100



Y Index:
64

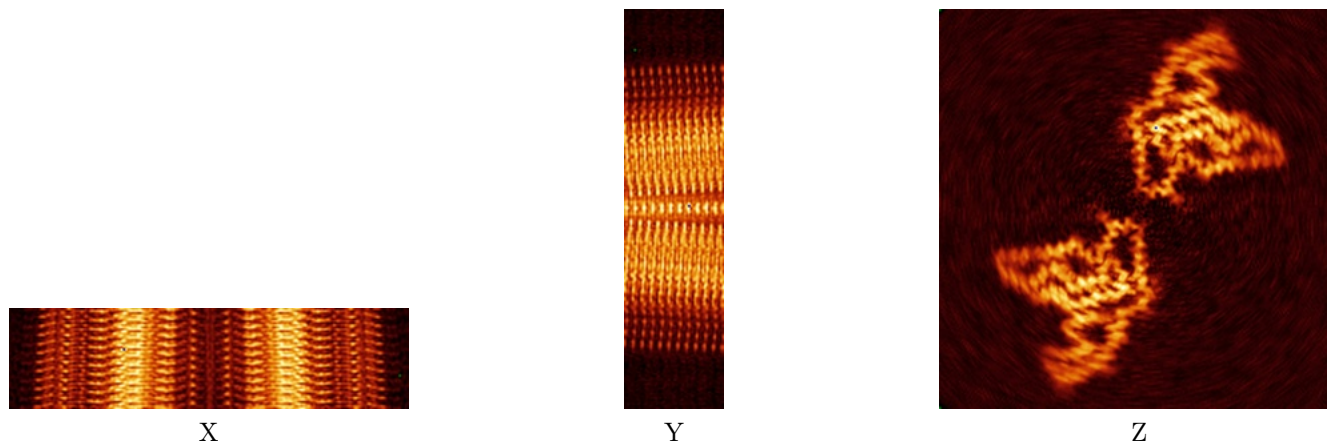


Z Index: 32

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



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](#)

This section was not generated.

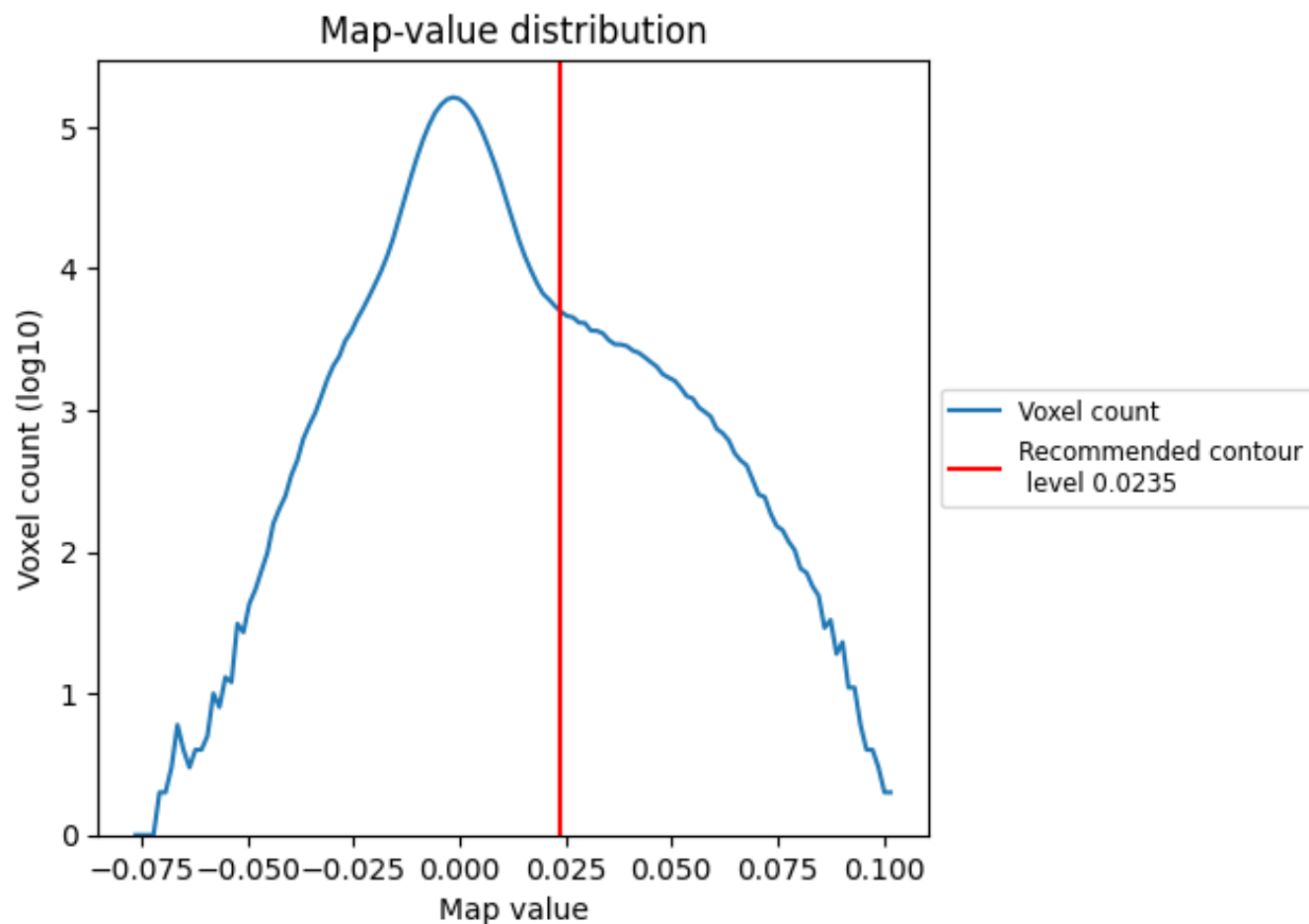
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

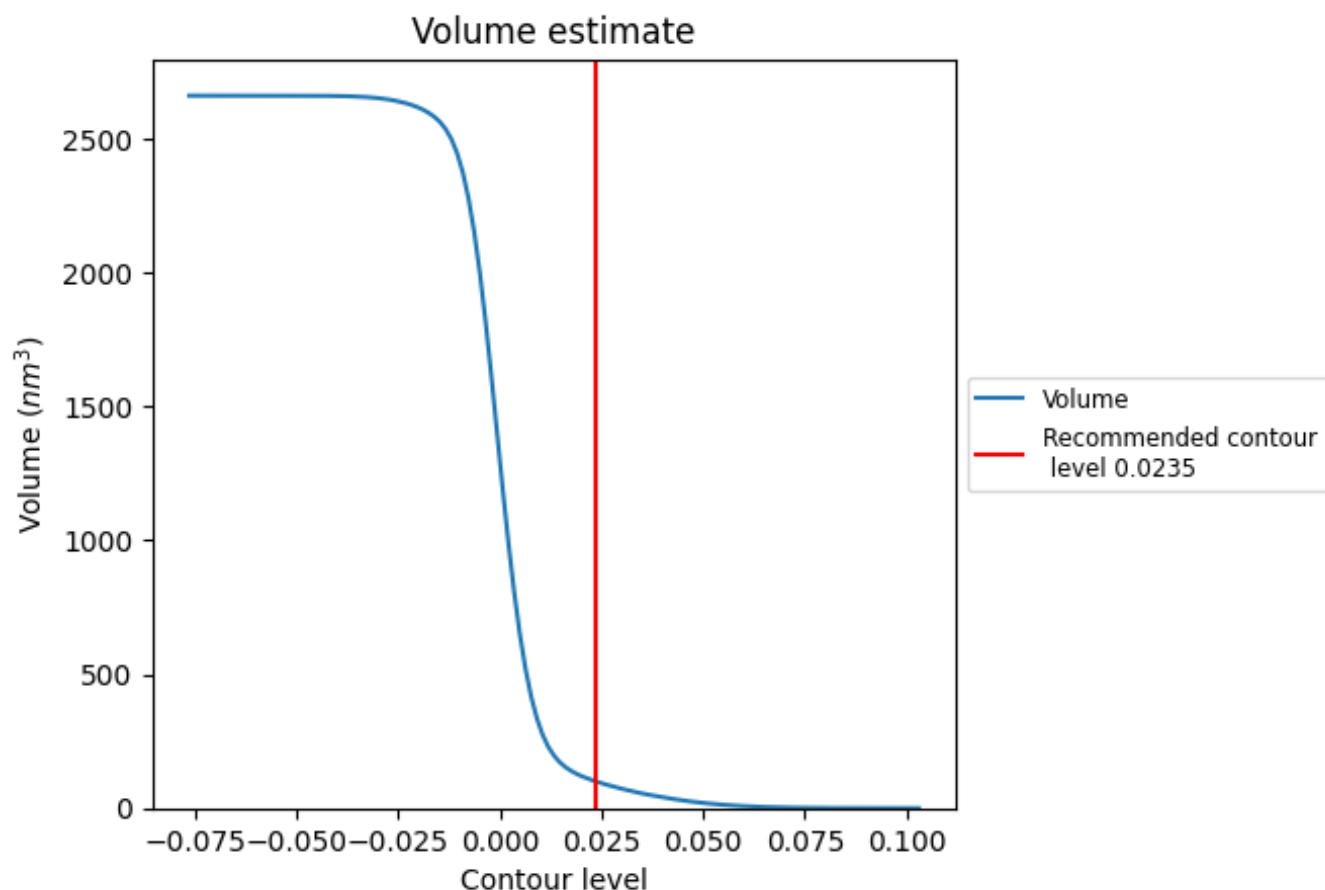
This section contains the results of statistical analysis of the map.

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 100 nm³; this corresponds to an approximate mass of 91 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

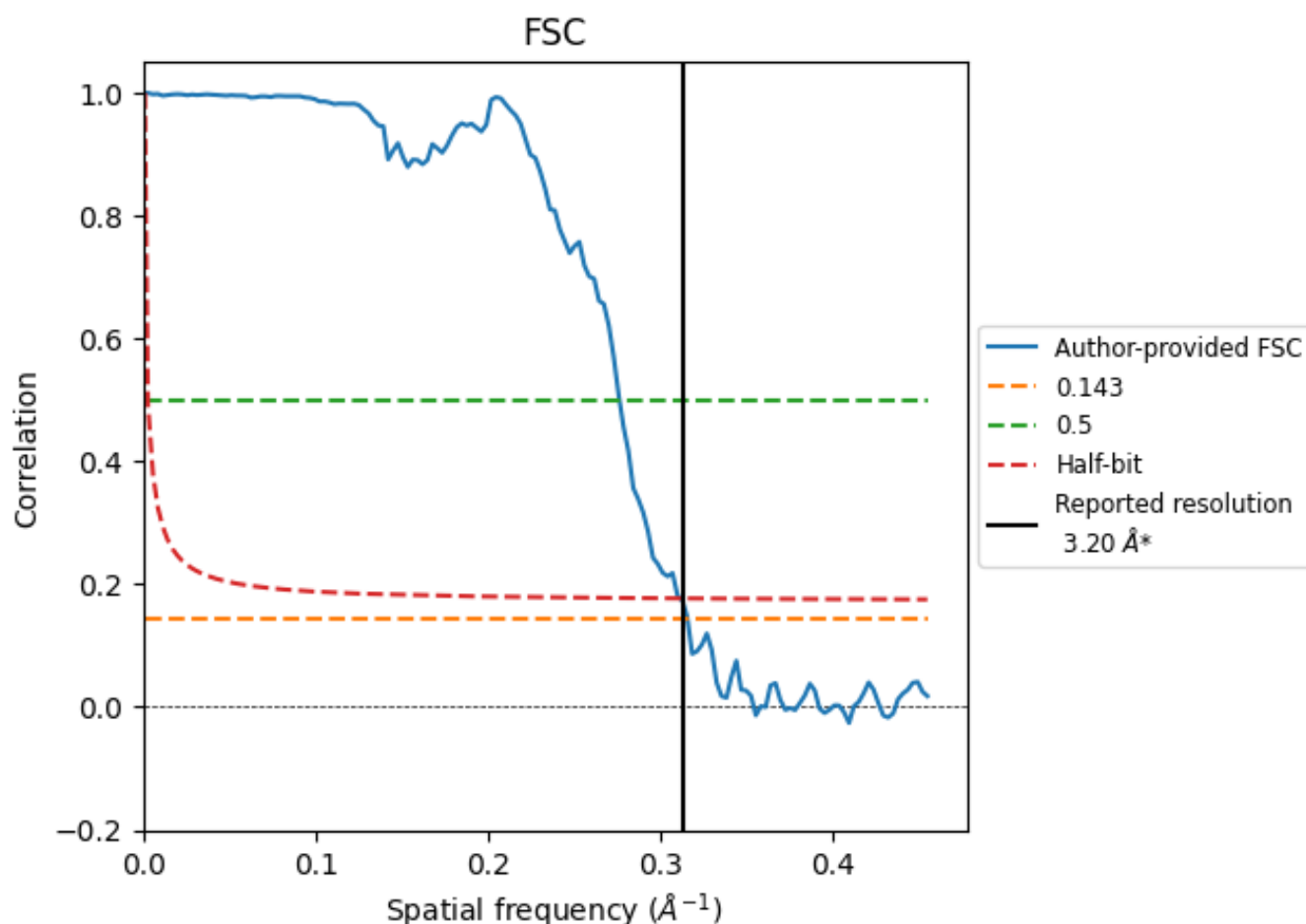
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.62	3.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

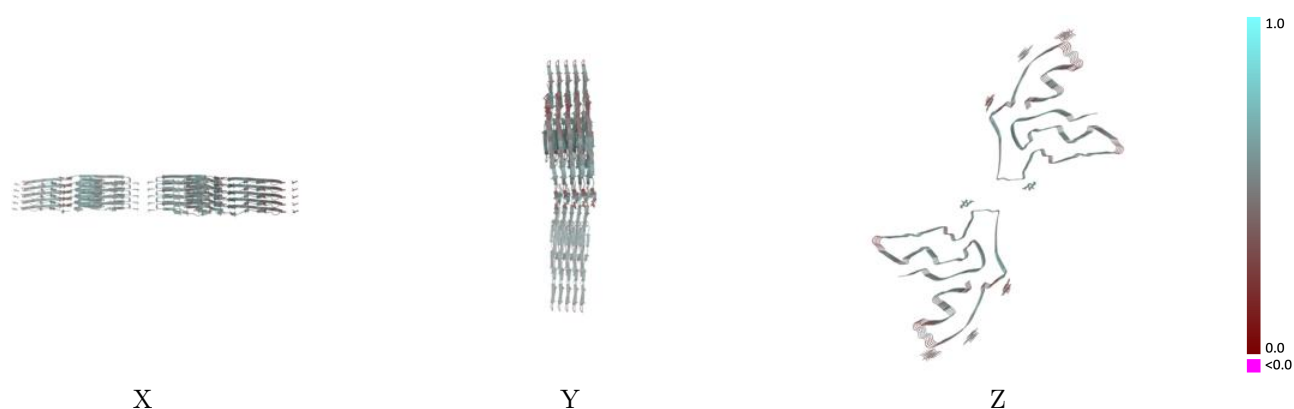
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24954 and PDB model 7SAR. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

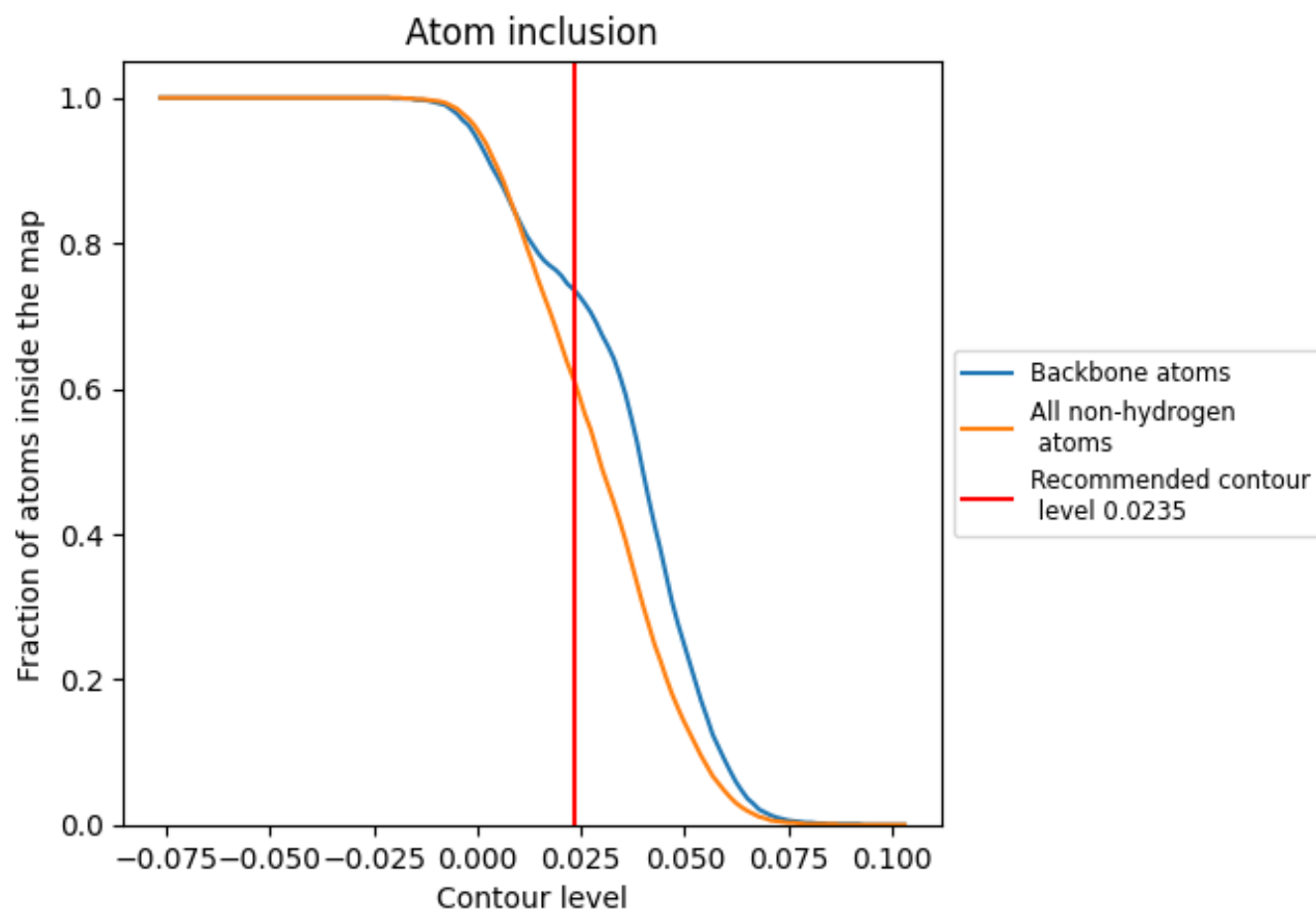


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 61% 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 (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.4990
A	0.6080	0.5030
B	0.6090	0.4950
C	0.6120	0.5010
D	0.6020	0.4980
E	0.6140	0.5000
F	0.6090	0.4970
G	0.6170	0.5030
H	0.6030	0.4950
I	0.6130	0.5010
J	0.6030	0.4930

1.0

0.0

<0.0