Full wwPDB EM Validation Report (i)

Aug 12, 2023 – 02:11 PM EDT

PDB ID	:	8FEF
EMDB ID	:	EMD-29025
Title	:	Structure of Mce1 transporter from Mycobacterium smegmatis (Map0)
Authors	:	Chen, J.; Bhabha, G.; Ekiert, D.C.
Deposited on	:	2022-12-06
Resolution	:	2.71 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 (i) 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 (i)) were used in the production of this report:

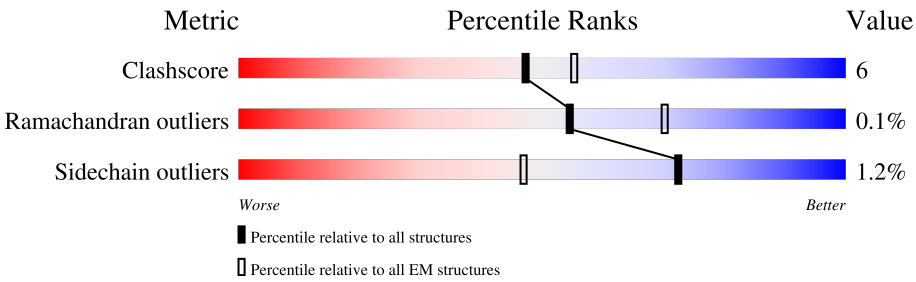
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.71 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	409	9% 81% 13% • •
2	B	343	• 84% 13% • •
3	C	524	9% 50% 9% • 41%
4	D	547	5% 58% 12% 30%
5	E	390	• 77% 14% • 8%
6	F	518	6% 66% 11% 23%
7	G	653	• 37% 8% 54%
7	H	653	• 37% 8% 54%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	266	78% 17% 5%
9	J	289	7% 78% 13% 9%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 25532 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 Virulence factor Mce family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	392	2974	1887	507	573	7	0	0

- Molecule 2 is a protein called Virulence factor Mce family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	335	2588	1645	442	498	3	0	0

- Molecule 3 is a protein called MCE-family protein MCE1c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	310	2344	1464	418	456	6	0	0

- Molecule 4 is a protein called Virulence factor mce family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	385	2943	1864	507	566	6	0	0

- Molecule 5 is a protein called Virulence factor Mce family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	358	2742	1718	488	531	5	0	0

- Molecule 6 is a protein called Mce-family protein mce1f.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	399	2987	1887	512	579	9	0	0

- Molecule 7 is a protein called ABC transporter, ATP-binding protein,Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	299	2297	1454	402	429	12	0	0
7	H	298	2286	1448	398	428	12	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	361	GLY	-	linker	UNP A0QS64
G	362	LEU	-	linker	UNP A0QS64
G	363	SER	-	linker	UNP A0QS64
G	364	GLY	-	linker	UNP A0QS64
G	365	GLN	-	linker	UNP A0QS64
G	366	PRO	-	linker	UNP A0QS64
G	367	PRO	-	linker	UNP A0QS64
G	368	ARG	-	linker	UNP A0QS64
G	369	SER	-	linker	UNP A0QS64
G	370	PRO	-	linker	UNP A0QS64
G	371	SER	-	linker	UNP A0QS64
G	372	SER	-	linker	UNP A0QS64
G	373	GLY	-	linker	UNP A0QS64
G	374	SER	-	linker	UNP A0QS64
G	375	SER	-	linker	UNP A0QS64
G	376	SER	-	linker	UNP A0QS64
G	377	ASN	-	linker	UNP A0QS64
G	378	SER	-	linker	UNP A0QS64
G	379	LEU	-	linker	UNP A0QS64
G	380	GLU	-	linker	UNP A0QS64
G	381	VAL	-	linker	UNP A0QS64
G	382	LEU	-	linker	UNP A0QS64
G	383	PHE	-	linker	UNP A0QS64
G	384	GLN	-	linker	UNP A0QS64
G	385	GLY	-	linker	UNP A0QS64
G	386	PRO	-	linker	UNP A0QS64
G	387	THR	-	linker	UNP A0QS64
G	388	ALA	-	linker	UNP A0QS64
G	389	ALA	-	linker	UNP A0QS64
G	390	ALA	-	linker	UNP A0QS64
G	391	ALA	-	linker	UNP A0QS64
G	392	VAL	-	linker	UNP A0QS64
G	393	SER	-	linker	UNP A0QS64

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	394	LYS	-	linker	UNP A0QS64
G	395	GLY	-	linker	UNP A0QS64
G	396	GLU	-	linker	UNP A0QS64
G	397	GLU	-	linker	UNP A0QS64
G	398	LEU	-	linker	UNP A0QS64
G	399	PHE	-	linker	UNP A0QS64
G	400	THR	-	linker	UNP A0QS64
G	401	GLY	-	linker	UNP A0QS64
G	402	VAL	-	linker	UNP A0QS64
G	403	VAL	-	linker	UNP A0QS64
G	404	PRO	-	linker	UNP A0QS64
G	405	ILE	-	linker	UNP A0QS64
G	406	LEU	-	linker	UNP A0QS64
G	407	VAL	-	linker	UNP A0QS64
G	408	GLU	-	linker	UNP A0QS64
G	409	LEU	-	linker	UNP A0QS64
G	410	ASP	-	linker	UNP A0QS64
G	411	GLY	-	linker	UNP A0QS64
G	412	ASP	-	linker	UNP A0QS64
G	413	VAL	-	linker	UNP A0QS64
G	414	ASN	-	linker	UNP A0QS64
G	415	GLY	-	linker	UNP A0QS64
G	416	HIS	-	linker	UNP A0QS64
G	417	LYS	-	linker	UNP A0QS64
G	418	PHE	-	linker	UNP A0QS64
G	419	SER	-	linker	UNP A0QS64
G	420	VAL	-	linker	UNP A0QS64
G	421	SER	-	linker	UNP A0QS64
G	422	GLY	-	linker	UNP A0QS64
G	423	GLU	-	linker	UNP A0QS64
G	455	LEU	PHE	conflict	UNP P42212
G	456	THR	SER	conflict	UNP P42212
G	622	LEU	HIS	conflict	UNP P42212
G	630	GLY	-	expression tag	UNP P42212
G	631	GLY	-	expression tag	UNP P42212
G	632	GLY	-	expression tag	UNP P42212
G	633	GLY	-	expression tag	UNP P42212
G	634	GLU	-	expression tag	UNP P42212
G	635	ASN	-	expression tag	UNP P42212
G	636	LEU	-	expression tag	UNP P42212
G	637	TYR	-	expression tag	UNP P42212
G	638	PHE	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	639	GLN	-	expression tag	UNP P42212
G	640	ASP	-	expression tag	UNP P42212
G	641	TYR	-	expression tag	UNP P42212
G	642	LYS	-	expression tag	UNP P42212
G	643	ASP	-	expression tag	UNP P42212
G	644	ASP	-	expression tag	UNP P42212
G	645	ASP	-	expression tag	UNP P42212
G	646	ASP	-	expression tag	UNP P42212
G	647	LYS	-	expression tag	UNP P42212
G	648	HIS	-	expression tag	UNP P42212
G	649	HIS	-	expression tag	UNP P42212
G	650	HIS	-	expression tag	UNP P42212
G	651	HIS	-	expression tag	UNP P42212
G	652	HIS	-	expression tag	UNP P42212
G	653	HIS	-	expression tag	UNP P42212
H	361	GLY	-	linker	UNP A0QS64
H	362	LEU	-	linker	UNP A0QS64
H	363	SER	-	linker	UNP A0QS64
H	364	GLY	-	linker	UNP A0QS64
H	365	GLN	-	linker	UNP A0QS64
H	366	PRO	-	linker	UNP A0QS64
H	367	PRO	-	linker	UNP A0QS64
H	368	ARG	-	linker	UNP A0QS64
H	369	SER	-	linker	UNP A0QS64
H	370	PRO	-	linker	UNP A0QS64
H	371	SER	-	linker	UNP A0QS64
H	372	SER	-	linker	UNP A0QS64
H	373	GLY	-	linker	UNP A0QS64
H	374	SER	-	linker	UNP A0QS64
H	375	SER	-	linker	UNP A0QS64
H	376	SER	-	linker	UNP A0QS64
H	377	ASN	-	linker	UNP A0QS64
H	378	SER	-	linker	UNP A0QS64
H	379	LEU	-	linker	UNP A0QS64
H	380	GLU	-	linker	UNP A0QS64
H	381	VAL	-	linker	UNP A0QS64
H	382	LEU	-	linker	UNP A0QS64
H	383	PHE	-	linker	UNP A0QS64
H	384	GLN	-	linker	UNP A0QS64
H	385	GLY	-	linker	UNP A0QS64
H	386	PRO	-	linker	UNP A0QS64
H	387	THR	-	linker	UNP A0QS64

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	388	ALA	-	linker	UNP A0QS64
H	389	ALA	-	linker	UNP A0QS64
H	390	ALA	-	linker	UNP A0QS64
H	391	ALA	-	linker	UNP A0QS64
H	392	VAL	-	linker	UNP A0QS64
H	393	SER	-	linker	UNP A0QS64
H	394	LYS	-	linker	UNP A0QS64
H	395	GLY	-	linker	UNP A0QS64
H	396	GLU	-	linker	UNP A0QS64
H	397	GLU	-	linker	UNP A0QS64
H	398	LEU	-	linker	UNP A0QS64
H	399	PHE	-	linker	UNP A0QS64
H	400	THR	-	linker	UNP A0QS64
H	401	GLY	-	linker	UNP A0QS64
H	402	VAL	-	linker	UNP A0QS64
H	403	VAL	-	linker	UNP A0QS64
H	404	PRO	-	linker	UNP A0QS64
H	405	ILE	-	linker	UNP A0QS64
H	406	LEU	-	linker	UNP A0QS64
H	407	VAL	-	linker	UNP A0QS64
H	408	GLU	-	linker	UNP A0QS64
H	409	LEU	-	linker	UNP A0QS64
H	410	ASP	-	linker	UNP A0QS64
H	411	GLY	-	linker	UNP A0QS64
H	412	ASP	-	linker	UNP A0QS64
H	413	VAL	-	linker	UNP A0QS64
H	414	ASN	-	linker	UNP A0QS64
H	415	GLY	-	linker	UNP A0QS64
H	416	HIS	-	linker	UNP A0QS64
H	417	LYS	-	linker	UNP A0QS64
H	418	PHE	-	linker	UNP A0QS64
H	419	SER	-	linker	UNP A0QS64
H	420	VAL	-	linker	UNP A0QS64
H	421	SER	-	linker	UNP A0QS64
H	422	GLY	-	linker	UNP A0QS64
H	423	GLU	-	linker	UNP A0QS64
H	455	LEU	PHE	conflict	UNP P42212
H	456	THR	SER	conflict	UNP P42212
H	622	LEU	HIS	conflict	UNP P42212
H	630	GLY	-	expression tag	UNP P42212
H	631	GLY	-	expression tag	UNP P42212
H	632	GLY	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	633	GLY	-	expression tag	UNP P42212
H	634	GLU	-	expression tag	UNP P42212
H	635	ASN	-	expression tag	UNP P42212
H	636	LEU	-	expression tag	UNP P42212
H	637	TYR	-	expression tag	UNP P42212
H	638	PHE	-	expression tag	UNP P42212
H	639	GLN	-	expression tag	UNP P42212
H	640	ASP	-	expression tag	UNP P42212
H	641	TYR	-	expression tag	UNP P42212
H	642	LYS	-	expression tag	UNP P42212
H	643	ASP	-	expression tag	UNP P42212
H	644	ASP	-	expression tag	UNP P42212
H	645	ASP	-	expression tag	UNP P42212
H	646	ASP	-	expression tag	UNP P42212
H	647	LYS	-	expression tag	UNP P42212
H	648	HIS	-	expression tag	UNP P42212
H	649	HIS	-	expression tag	UNP P42212
H	650	HIS	-	expression tag	UNP P42212
H	651	HIS	-	expression tag	UNP P42212
H	652	HIS	-	expression tag	UNP P42212
H	653	HIS	-	expression tag	UNP P42212

- Molecule 8 is a protein called Conserved hypothetical integral membrane protein Yrbe1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	253	1844	1216	297	324	7	0	0

- Molecule 9 is a protein called ABC-transporter integral membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	263	1966	1283	323	347	13	0	0

- Molecule 10 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
10	A	3	69	69	0
10	B	6	95	95	0

Continued on next page...

Continued from previous page...

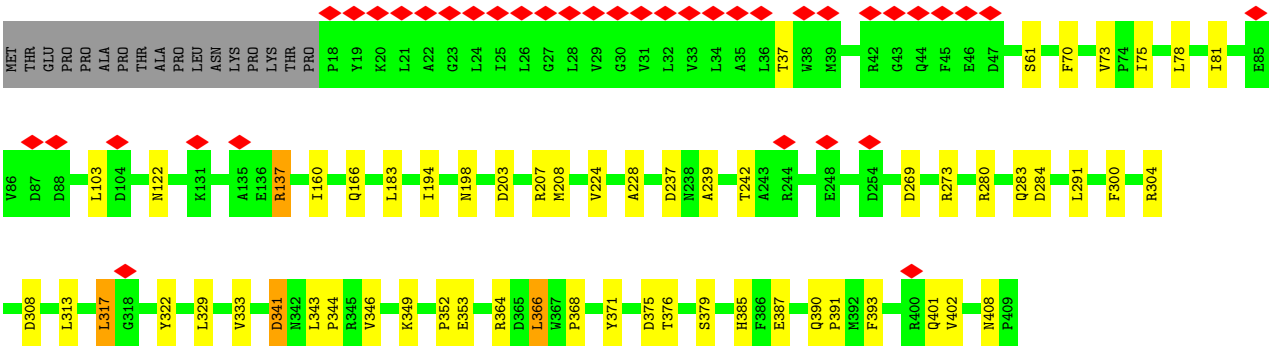
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
10	C	4	59	59	0
			Total	C	
10	D	6	102	102	0
			Total	C	
10	E	7	147	147	0
			Total	C	
10	F	5	89	89	0

3 Residue-property plots (i)

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.

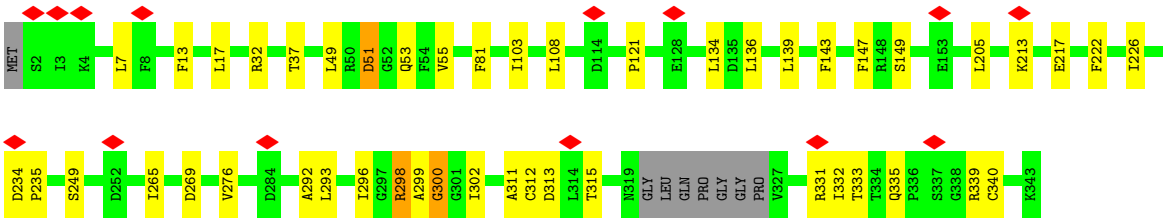
• Molecule 1: Virulence factor Mce family protein

Chain A:



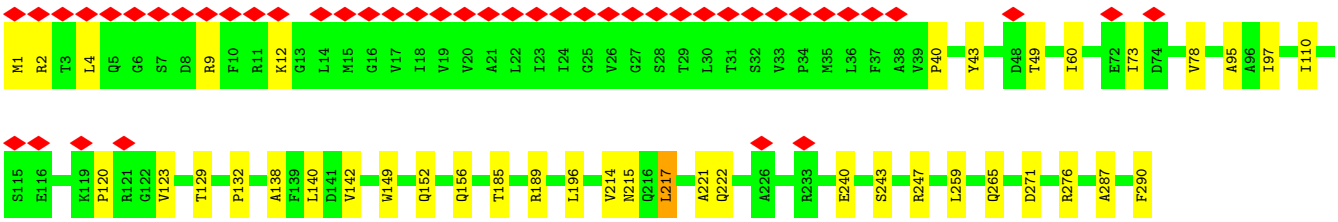
• Molecule 2: Virulence factor Mce family protein

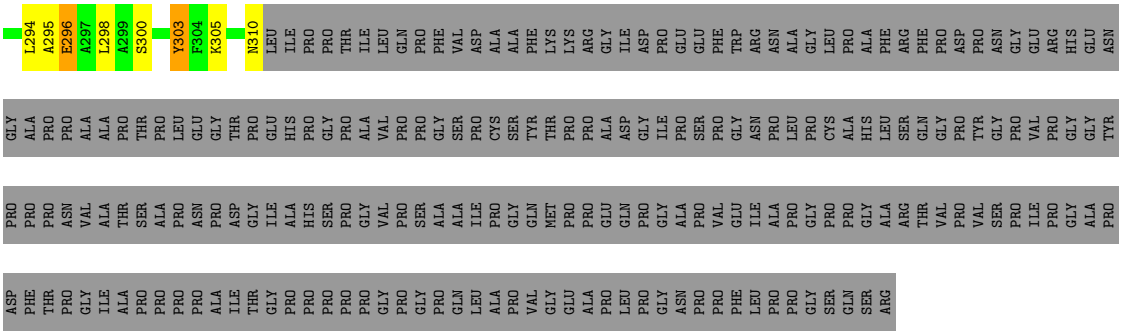
Chain B:



• Molecule 3: MCE-family protein MCE1c

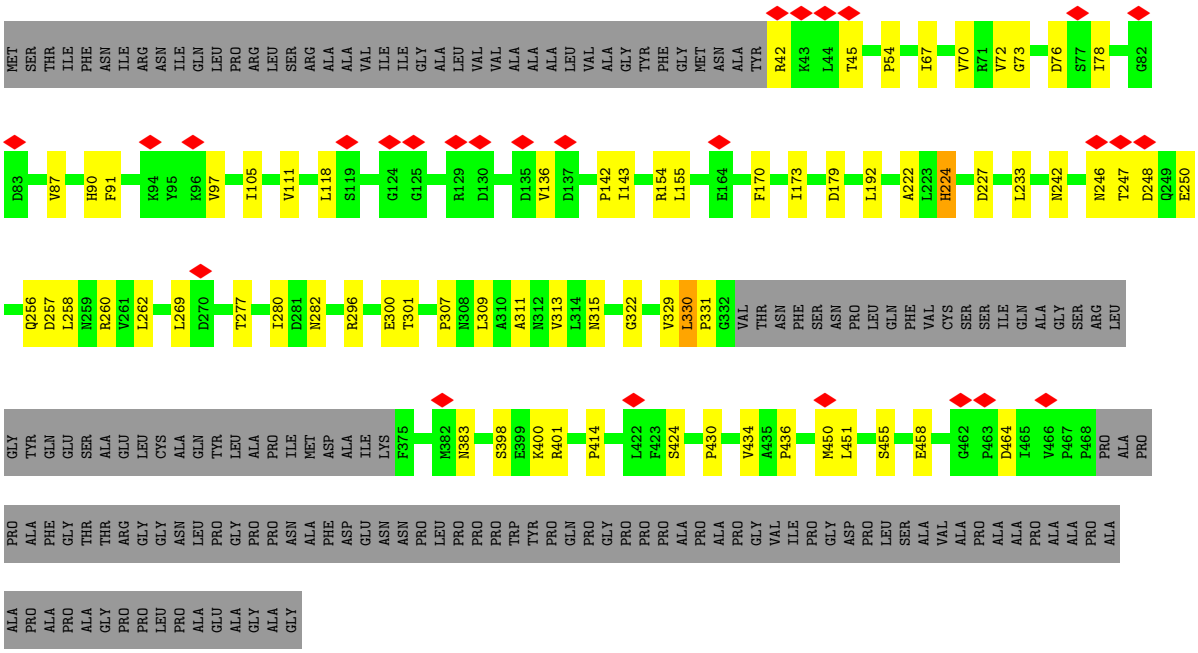
Chain C:





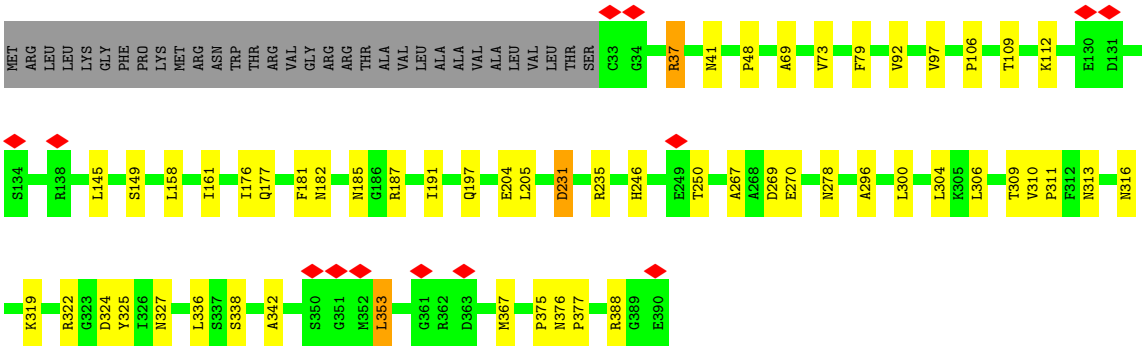
• Molecule 4: Virulence factor mce family protein

Chain D:



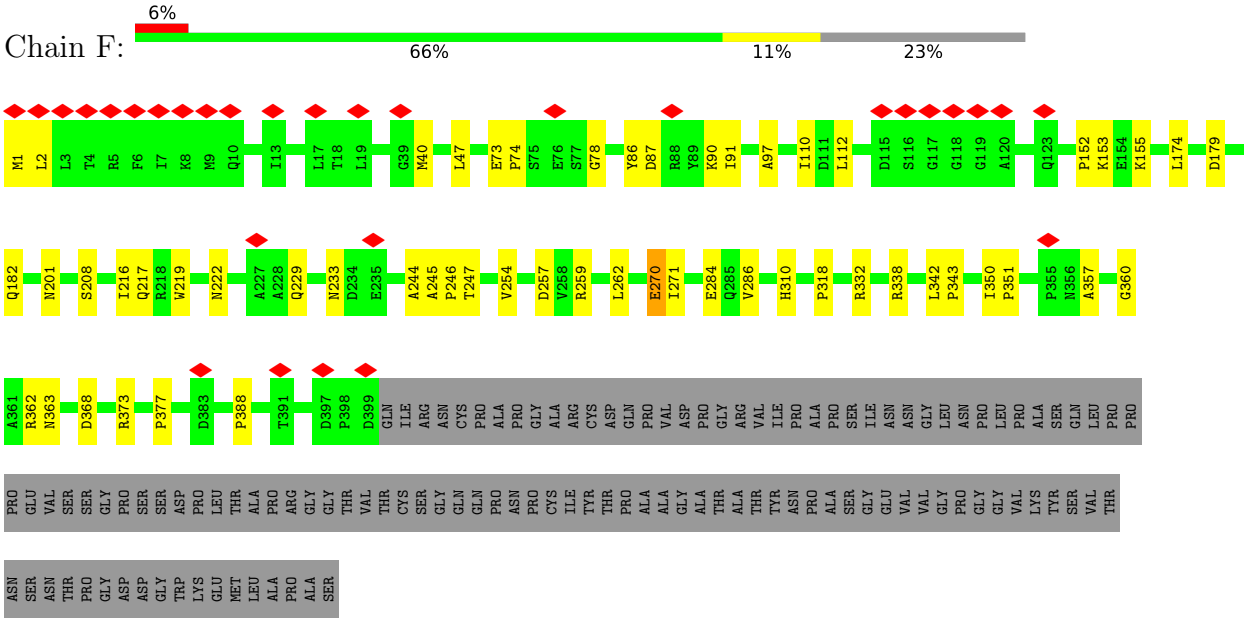
• Molecule 5: Virulence factor Mce family protein

Chain E:



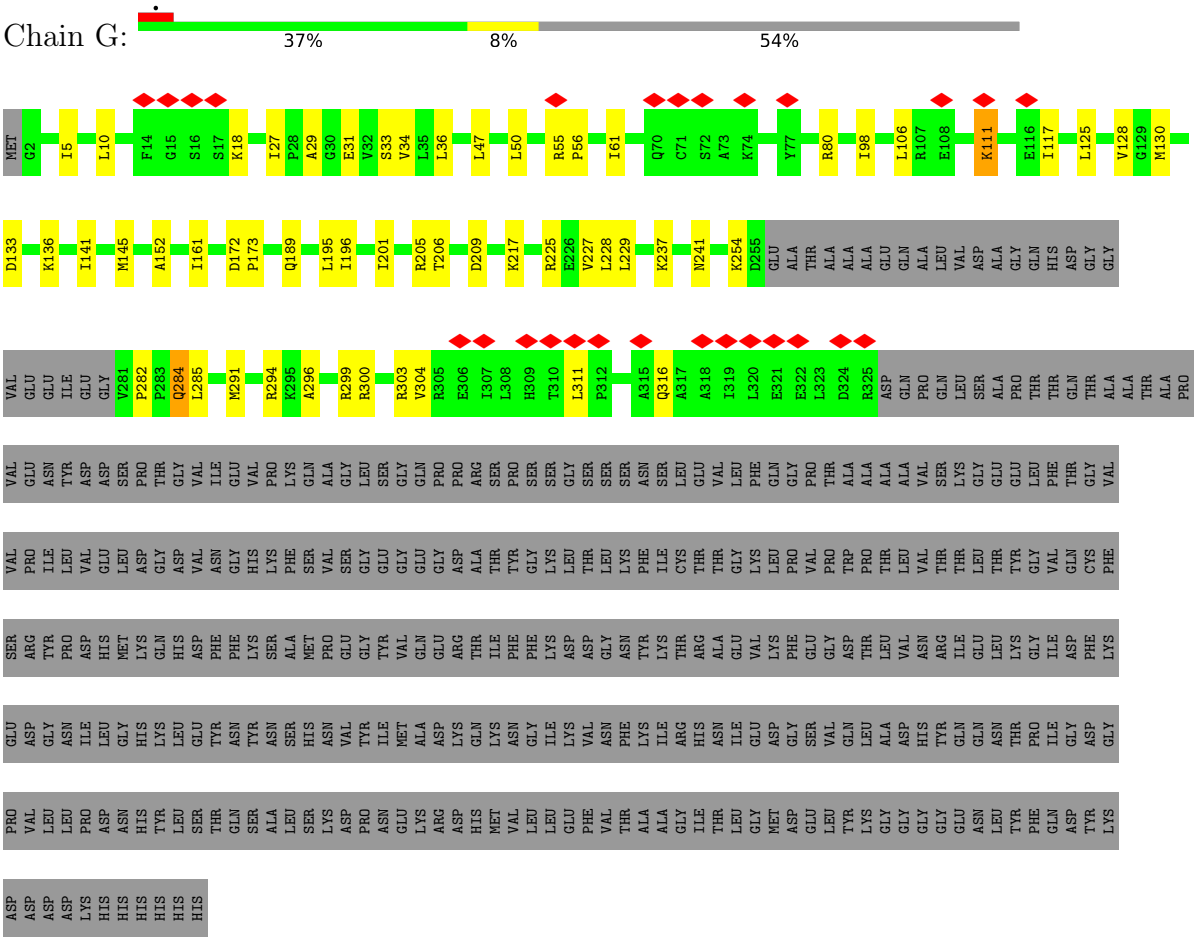
• Molecule 6: Mce-family protein mce1f

Chain F:



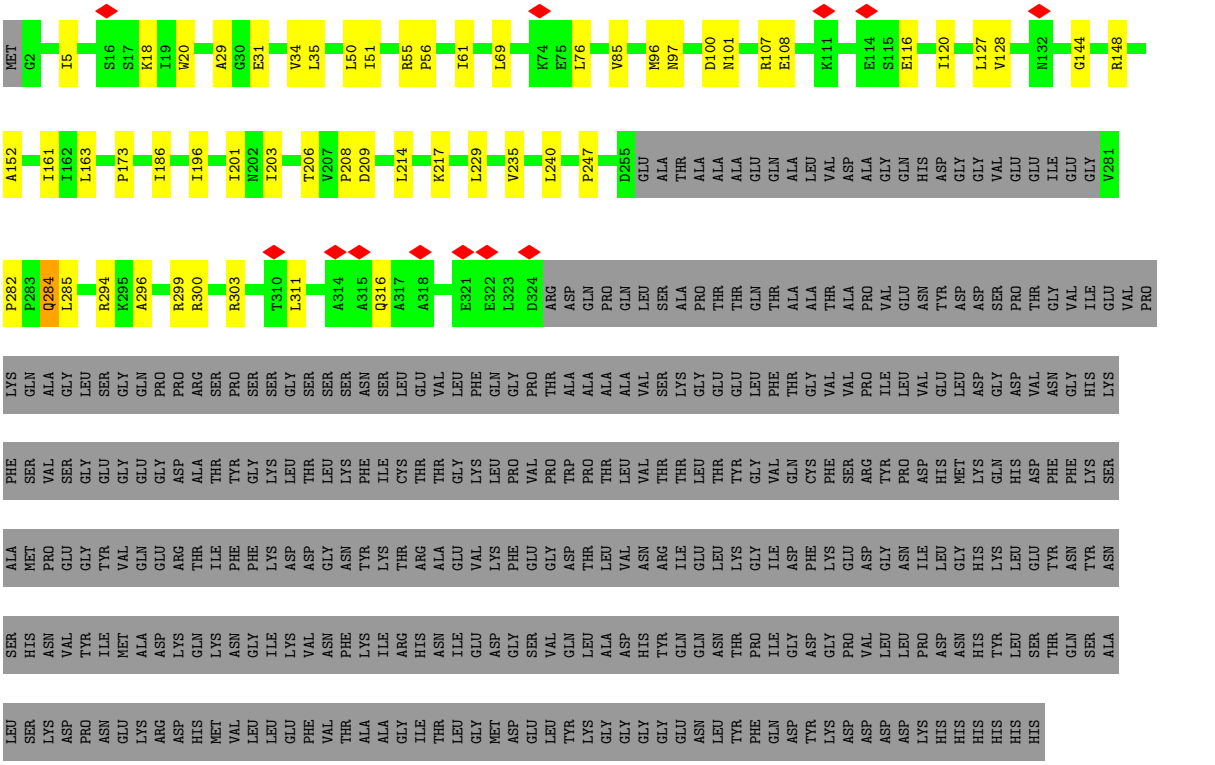
• Molecule 7: ABC transporter, ATP-binding protein,Green fluorescent protein chimera

Chain G:



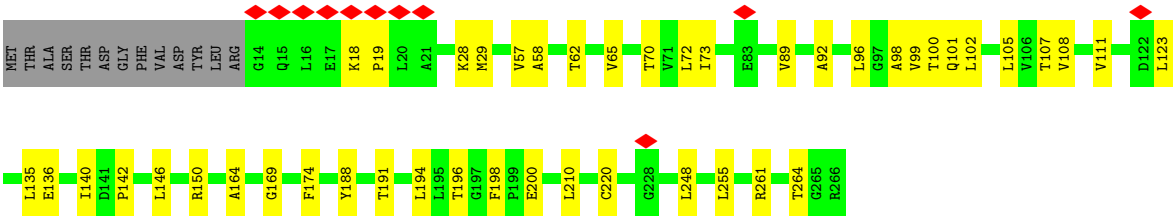
• Molecule 7: ABC transporter, ATP-binding protein,Green fluorescent protein chimera

Chain H:



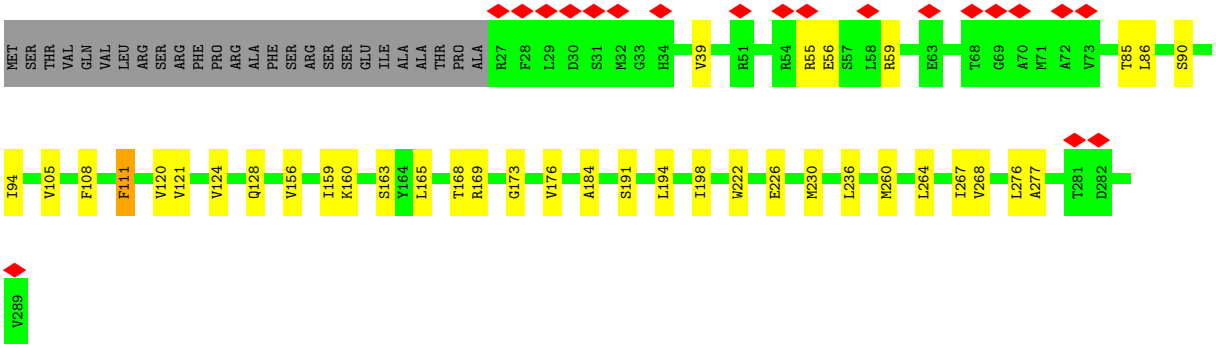
• Molecule 8: Conserved hypothetical integral membrane protein Yrbe1a

Chain I:



• Molecule 9: ABC-transporter integral membrane protein

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	305172	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	62.004	Depositor
Minimum map value	-41.229	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.941	Depositor
Recommended contour level	8.69	Depositor
Map size (Å)	528.32, 528.32, 528.32	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8255, 0.8255, 0.8255	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.28	0/3039	0.51	0/4148
2	B	0.27	0/2624	0.52	1/3556 (0.0%)
3	C	0.27	0/2370	0.52	0/3211
4	D	0.26	0/3007	0.52	1/4105 (0.0%)
5	E	0.25	0/2790	0.51	0/3803
6	F	0.26	0/3050	0.50	0/4170
7	G	0.26	0/2333	0.53	0/3151
7	H	0.26	0/2322	0.50	0/3137
8	I	0.27	0/1876	0.46	0/2558
9	J	0.26	0/2005	0.44	0/2725
All	All	0.26	0/25416	0.50	2/34564 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	330	LEU	CA-CB-CG	7.21	131.88	115.30
2	B	300	GLY	N-CA-C	6.97	130.53	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2974	0	2939	63	0
2	B	2588	0	2650	45	0
3	C	2344	0	2410	51	0
4	D	2943	0	2926	61	0
5	E	2742	0	2768	46	0
6	F	2987	0	2976	63	0
7	G	2297	0	2378	37	0
7	H	2286	0	2365	31	0
8	I	1844	0	1951	29	0
9	J	1966	0	2013	25	0
10	A	69	0	0	0	0
10	B	95	0	0	0	0
10	C	59	0	0	0	0
10	D	102	0	0	0	0
10	E	147	0	0	0	0
10	F	89	0	0	0	0
All	All	25532	0	25376	326	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 6.

All (326) 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:B:300:GLY:HA3	3:C:294:LEU:HD11	1.42	0.99
3:C:298:LEU:HD11	4:D:313:VAL:CG1	1.92	0.98
1:A:343:LEU:HD21	6:F:363:ASN:ND2	1.81	0.95
7:G:206:THR:O	7:G:284:GLN:HG2	1.69	0.92
2:B:298:ARG:HG2	2:B:302:ILE:HD13	1.54	0.89
3:C:298:LEU:HD11	4:D:313:VAL:HG12	1.56	0.87
3:C:298:LEU:CD1	4:D:313:VAL:CG1	2.52	0.87
3:C:298:LEU:CD1	4:D:313:VAL:HG13	2.06	0.85
9:J:90:SER:O	9:J:94:ILE:HG13	1.76	0.84
1:A:343:LEU:CD2	6:F:363:ASN:ND2	2.40	0.83
1:A:166:GLN:HG3	6:F:153:LYS:HB2	1.62	0.81
7:G:229:LEU:HD13	7:G:282:PRO:HD2	1.65	0.77
4:D:262:LEU:HD22	6:F:247:THR:HG21	1.69	0.74
3:C:298:LEU:CD1	4:D:313:VAL:HG12	2.16	0.74
6:F:351:PRO:HB3	6:F:388:PRO:HG3	1.71	0.73
1:A:375:ASP:OD2	4:D:401:ARG:NH2	2.23	0.71
6:F:362:ARG:NH1	6:F:363:ASN:OD1	2.23	0.71
7:G:225:ARG:HH22	7:G:282:PRO:HB2	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG21	3:C:265:GLN:HB2	1.74	0.70
2:B:298:ARG:HG3	2:B:298:ARG:HH11	1.55	0.70
2:B:292:ALA:O	2:B:296:ILE:HG22	1.90	0.69
1:A:343:LEU:HD22	6:F:363:ASN:HB3	1.75	0.69
3:C:298:LEU:HD11	4:D:313:VAL:HG13	1.67	0.68
7:H:284:GLN:OE1	7:H:300:ARG:NH1	2.27	0.67
4:D:242:ASN:OD1	6:F:222:ASN:ND2	2.27	0.67
1:A:343:LEU:CD2	6:F:363:ASN:HD22	2.06	0.67
1:A:273:ARG:NH2	6:F:259:ARG:O	2.28	0.66
7:G:18:LYS:HG3	7:G:217:LYS:HD3	1.77	0.66
2:B:300:GLY:HA3	3:C:294:LEU:CD1	2.22	0.66
1:A:269:ASP:OD2	1:A:273:ARG:NH1	2.29	0.66
7:H:229:LEU:HD13	7:H:282:PRO:HD2	1.79	0.65
2:B:335:GLN:NE2	2:B:340:CYS:SG	2.69	0.64
7:G:205:ARG:O	7:G:225:ARG:NH2	2.31	0.64
1:A:341:ASP:N	1:A:341:ASP:OD1	2.28	0.63
8:I:58:ALA:O	8:I:62:THR:OG1	2.16	0.63
5:E:182:ASN:O	5:E:187:ARG:NH2	2.31	0.63
1:A:349:LYS:O	4:D:398:SER:OG	2.16	0.63
2:B:300:GLY:CA	3:C:294:LEU:HD11	2.23	0.63
7:G:225:ARG:NH2	7:G:282:PRO:HB2	2.14	0.62
1:A:317:LEU:HD12	5:E:316:ASN:HB2	1.82	0.62
2:B:312:CYS:SG	2:B:335:GLN:NE2	2.73	0.62
6:F:332:ARG:NH2	6:F:338:ARG:O	2.33	0.62
7:G:80:ARG:HH12	8:I:136:GLU:HG2	1.65	0.61
2:B:213:LYS:NZ	2:B:217:GLU:OE2	2.34	0.61
3:C:240:GLU:OE2	4:D:246:ASN:ND2	2.33	0.61
1:A:343:LEU:HD22	6:F:363:ASN:HD22	1.64	0.61
7:G:311:LEU:O	7:G:316:GLN:NE2	2.33	0.61
8:I:92:ALA:HB2	8:I:191:THR:HG22	1.83	0.61
7:G:209:ASP:OD2	7:G:294:ARG:NH2	2.34	0.60
1:A:352:PRO:O	5:E:388:ARG:NH2	2.34	0.60
1:A:304:ARG:NH1	1:A:308:ASP:OD1	2.35	0.59
2:B:299:ALA:HA	5:E:324:ASP:O	2.02	0.59
8:I:210:LEU:HD12	8:I:255:LEU:HD11	1.84	0.59
1:A:208:MET:HG2	5:E:204:GLU:HB3	1.83	0.59
3:C:271:ASP:OD1	4:D:282:ASN:ND2	2.36	0.59
6:F:97:ALA:HB1	6:F:110:ILE:HD11	1.85	0.59
7:H:31:GLU:OE1	7:H:303:ARG:NH2	2.36	0.59
7:H:18:LYS:HG3	7:H:217:LYS:HD2	1.85	0.59
7:H:55:ARG:NH1	7:H:69:LEU:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:87:ASP:O	6:F:90:LYS:NZ	2.34	0.59
3:C:303:TYR:OH	6:F:318:PRO:CG	2.51	0.59
1:A:291:LEU:HD11	6:F:284:GLU:HB2	1.85	0.59
6:F:2:LEU:HD21	9:J:59:ARG:HB2	1.85	0.58
2:B:298:ARG:HH11	2:B:298:ARG:CG	2.16	0.58
3:C:303:TYR:OH	6:F:318:PRO:HG3	2.03	0.58
7:G:173:PRO:HG2	7:H:201:ILE:HG12	1.86	0.58
1:A:198:ASN:OD1	5:E:197:GLN:NE2	2.37	0.58
7:G:128:VAL:HG21	7:G:152:ALA:HB2	1.86	0.58
6:F:216:ILE:HA	6:F:219:TRP:CD1	2.38	0.57
2:B:332:ILE:HG22	2:B:333:THR:HG23	1.86	0.57
7:H:311:LEU:O	7:H:316:GLN:NE2	2.36	0.57
7:H:56:PRO:HD2	7:H:69:LEU:HD11	1.87	0.57
8:I:70:THR:HG21	8:I:169:GLY:HA2	1.87	0.57
3:C:138:ALA:O	3:C:142:VAL:HG23	2.05	0.57
8:I:65:VAL:HG13	9:J:268:VAL:HG21	1.87	0.57
3:C:214:VAL:HA	3:C:217:LEU:HD23	1.86	0.57
9:J:160:LYS:HB2	9:J:163:SER:HB3	1.87	0.57
3:C:95:ALA:HB3	3:C:129:THR:HG22	1.86	0.56
7:H:128:VAL:HG21	7:H:152:ALA:HB2	1.87	0.56
1:A:228:ALA:HB2	6:F:217:GLN:HG2	1.87	0.56
4:D:257:ASP:OD1	4:D:260:ARG:NH2	2.37	0.56
5:E:112:LYS:HA	5:E:149:SER:O	2.06	0.56
7:G:33:SER:HB2	7:G:195:LEU:HD12	1.88	0.56
4:D:269:LEU:HD22	6:F:254:VAL:HG21	1.86	0.56
4:D:192:LEU:HD13	6:F:174:LEU:HD21	1.88	0.56
3:C:300:SER:OG	3:C:305:LYS:HE2	2.05	0.56
7:H:97:ASN:O	7:H:101:ASN:ND2	2.32	0.56
4:D:246:ASN:ND2	4:D:250:GLU:OE2	2.39	0.55
5:E:73:VAL:HG21	5:E:97:VAL:HG13	1.89	0.55
7:H:108:GLU:HG3	9:J:159:ILE:HD11	1.86	0.55
4:D:111:VAL:HB	9:J:105:VAL:HG12	1.88	0.55
2:B:17:LEU:HD22	8:I:164:ALA:HB2	1.89	0.55
2:B:51:ASP:N	2:B:51:ASP:OD1	2.39	0.55
7:H:34:VAL:HG22	7:H:196:ILE:HB	1.88	0.55
9:J:120:VAL:HG23	9:J:121:VAL:HG23	1.88	0.55
1:A:385:HIS:CD2	1:A:387:GLU:HG3	2.42	0.55
4:D:54:PRO:HD3	4:D:136:VAL:HG13	1.86	0.55
4:D:301:THR:HG22	6:F:377:PRO:HD2	1.88	0.55
7:H:209:ASP:OD2	7:H:294:ARG:NH2	2.39	0.55
9:J:124:VAL:O	9:J:128:GLN:HG2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:ALA:O	3:C:310:ASN:ND2	2.35	0.54
2:B:339:ARG:NH2	5:E:325:TYR:O	2.39	0.54
1:A:344:PRO:O	6:F:373:ARG:NH2	2.40	0.54
3:C:243:SER:OG	3:C:247:ARG:NH1	2.41	0.54
3:C:152:GLN:HG2	3:C:156:GLN:HE21	1.71	0.54
6:F:73:GLU:HG3	6:F:74:PRO:HD2	1.89	0.54
7:G:31:GLU:HG2	7:G:296:ALA:HB1	1.89	0.54
7:H:235:VAL:HG22	7:H:247:PRO:HG2	1.89	0.54
7:G:31:GLU:OE1	7:G:303:ARG:NH2	2.41	0.53
8:I:100:THR:HG23	8:I:101:GLN:HG2	1.91	0.53
7:G:201:ILE:HG12	7:H:173:PRO:HG2	1.89	0.53
1:A:280:ARG:HG3	6:F:270:GLU:HG3	1.91	0.53
4:D:256:GLN:NE2	6:F:233:ASN:OD1	2.42	0.53
7:H:50:LEU:HA	7:H:61:ILE:HD13	1.89	0.53
4:D:322:GLY:O	6:F:310:HIS:NE2	2.41	0.53
5:E:336:LEU:HD22	5:E:353:LEU:HD12	1.89	0.53
1:A:343:LEU:CD2	6:F:363:ASN:HB3	2.39	0.53
6:F:357:ALA:O	6:F:362:ARG:NH2	2.41	0.53
1:A:70:PHE:HB2	1:A:75:ILE:HD13	1.89	0.53
7:G:237:LYS:O	7:G:241:ASN:ND2	2.34	0.53
1:A:239:ALA:HA	1:A:242:THR:HG22	1.90	0.52
7:H:29:ALA:O	7:H:299:ARG:NH1	2.38	0.52
8:I:96:LEU:O	8:I:100:THR:HG22	2.09	0.52
3:C:185:THR:O	3:C:189:ARG:NH1	2.40	0.52
9:J:39:VAL:HG12	9:J:236:LEU:HD22	1.92	0.52
8:I:98:ALA:HA	8:I:102:LEU:HB3	1.91	0.52
3:C:12:LYS:HG2	8:I:28:LYS:HB2	1.90	0.52
1:A:343:LEU:HD22	6:F:363:ASN:ND2	2.22	0.52
9:J:86:LEU:HD23	9:J:191:SER:HB3	1.91	0.52
6:F:342:LEU:HD23	6:F:342:LEU:H	1.75	0.51
3:C:305:LYS:HD3	4:D:329:VAL:HG11	1.92	0.51
7:G:34:VAL:HG22	7:G:196:ILE:HB	1.92	0.51
7:G:225:ARG:NE	7:G:284:GLN:HG3	2.25	0.51
4:D:179:ASP:OD1	6:F:155:LYS:NZ	2.44	0.51
3:C:60:ILE:HG12	3:C:110:ILE:HB	1.92	0.51
7:G:300:ARG:O	7:G:304:VAL:HG23	2.11	0.51
5:E:319:LYS:O	5:E:322:ARG:NE	2.32	0.51
1:A:364:ARG:NH2	5:E:367:MET:O	2.28	0.51
5:E:309:THR:O	5:E:311:PRO:HD2	2.10	0.51
5:E:231:ASP:OD1	5:E:231:ASP:N	2.44	0.51
4:D:248:ASP:O	6:F:229:GLN:NE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD22	5:E:306:LEU:HD21	1.92	0.50
2:B:298:ARG:CG	2:B:298:ARG:NH1	2.74	0.50
2:B:313:ASP:N	2:B:313:ASP:OD1	2.45	0.50
7:G:5:ILE:HD11	7:G:161:ILE:HD13	1.92	0.50
8:I:123:LEU:HD12	8:I:220:CYS:HA	1.94	0.50
4:D:78:ILE:HG12	4:D:87:VAL:HG22	1.93	0.50
4:D:401:ARG:NH1	4:D:436:PRO:O	2.44	0.50
7:H:206:THR:HG22	7:H:285:LEU:HB2	1.92	0.50
1:A:390:GLN:HB2	1:A:391:PRO:HD3	1.93	0.50
2:B:339:ARG:O	5:E:322:ARG:NH1	2.44	0.49
3:C:1:MET:CE	8:I:142:PRO:HB2	2.42	0.49
7:G:172:ASP:OD1	7:G:172:ASP:N	2.39	0.49
5:E:300:LEU:O	5:E:304:LEU:HG	2.12	0.49
3:C:140:LEU:HD12	4:D:143:ILE:HD13	1.93	0.49
6:F:1:MET:O	9:J:55:ARG:NH1	2.45	0.49
1:A:322:TYR:HD2	2:B:340:CYS:HB2	1.78	0.49
3:C:296:GLU:OE1	3:C:296:GLU:HA	2.13	0.49
7:G:133:ASP:OD1	7:G:136:LYS:NZ	2.38	0.49
4:D:296:ARG:HH21	6:F:271:ILE:HD13	1.78	0.49
3:C:215:ASN:ND2	4:D:222:ALA:O	2.46	0.48
5:E:92:VAL:HG21	5:E:145:LEU:HD11	1.95	0.48
1:A:371:TYR:OH	4:D:315:ASN:OD1	2.31	0.48
3:C:290:PHE:HB3	6:F:342:LEU:HD12	1.94	0.48
9:J:108:PHE:HB3	9:J:111:PHE:HD2	1.78	0.48
2:B:49:LEU:HD12	2:B:53:GLN:OE1	2.14	0.48
5:E:306:LEU:HD13	5:E:313:ASN:HD22	1.78	0.48
7:G:106:LEU:HB3	7:G:117:ILE:HD12	1.96	0.48
3:C:243:SER:OG	4:D:257:ASP:OD2	2.26	0.48
7:G:189:GLN:NE2	7:G:291:MET:SD	2.77	0.48
4:D:329:VAL:HG23	4:D:331:PRO:HD3	1.95	0.48
1:A:300:PHE:HA	5:E:296:ALA:HB2	1.96	0.47
6:F:216:ILE:HA	6:F:219:TRP:NE1	2.29	0.47
4:D:430:PRO:HA	4:D:450:MET:HG3	1.96	0.47
7:H:35:LEU:HD11	7:H:214:LEU:HG	1.96	0.47
1:A:408:ASN:ND2	4:D:424:SER:O	2.46	0.47
3:C:97:ILE:HB	3:C:132:PRO:HD3	1.97	0.47
1:A:166:GLN:CG	6:F:153:LYS:HB2	2.41	0.47
2:B:143:PHE:HB3	2:B:147:PHE:CE2	2.50	0.47
4:D:434:VAL:HG23	4:D:455:SER:HB3	1.96	0.47
2:B:32:ARG:NH2	5:E:37:ARG:O	2.35	0.46
9:J:194:LEU:HG	9:J:198:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:451:LEU:O	4:D:455:SER:HB2	2.15	0.46
7:H:31:GLU:HG2	7:H:296:ALA:HB1	1.97	0.46
8:I:73:ILE:HD12	8:I:102:LEU:HD12	1.97	0.46
9:J:85:THR:HG21	9:J:184:ALA:HB1	1.96	0.46
7:H:5:ILE:HD11	7:H:161:ILE:HD13	1.97	0.46
1:A:353:GLU:O	4:D:400:LYS:NZ	2.48	0.46
3:C:296:GLU:OE2	6:F:360:GLY:CA	2.64	0.46
2:B:269:ASP:HA	3:C:265:GLN:NE2	2.31	0.46
1:A:37:THR:HG23	9:J:277:ALA:HB2	1.97	0.46
6:F:40:MET:HG2	6:F:86:TYR:HA	1.98	0.46
1:A:366:LEU:HB3	5:E:375:PRO:O	2.15	0.46
1:A:368:PRO:HG2	5:E:376:ASN:HB3	1.98	0.46
4:D:458:GLU:HG3	4:D:464:ASP:HA	1.97	0.46
7:H:51:ILE:HD13	9:J:156:VAL:HG22	1.96	0.46
4:D:73:GLY:HA3	4:D:91:PHE:HA	1.98	0.45
4:D:97:VAL:HG11	4:D:118:LEU:HD13	1.98	0.45
1:A:317:LEU:HD11	5:E:313:ASN:HB3	1.97	0.45
1:A:317:LEU:HB2	5:E:316:ASN:HB2	1.97	0.45
2:B:298:ARG:HH12	6:F:343:PRO:HD3	1.82	0.45
1:A:333:VAL:HG23	4:D:383:ASN:HD21	1.81	0.45
3:C:49:THR:HG22	3:C:78:VAL:HG11	1.97	0.45
7:G:227:VAL:HG22	7:G:311:LEU:HD11	1.98	0.45
2:B:293:LEU:HD13	3:C:287:ALA:HB2	1.98	0.45
8:I:135:LEU:CD2	8:I:140:ILE:HD12	2.47	0.45
7:G:50:LEU:HA	7:G:61:ILE:HD13	1.99	0.45
5:E:246:HIS:O	5:E:250:THR:HG22	2.17	0.45
9:J:56:GLU:OE2	9:J:59:ARG:NH2	2.38	0.45
2:B:249:SER:OG	5:E:269:ASP:OD1	2.30	0.45
3:C:296:GLU:OE2	6:F:360:GLY:HA3	2.17	0.45
1:A:379:SER:HB2	4:D:414:PRO:HG3	1.99	0.45
1:A:343:LEU:CD2	6:F:363:ASN:CG	2.86	0.44
1:A:224:VAL:HG12	6:F:216:ILE:HD11	1.99	0.44
3:C:1:MET:HE1	8:I:142:PRO:HB2	1.99	0.44
9:J:222:TRP:O	9:J:226:GLU:HG3	2.17	0.44
1:A:61:SER:HB3	1:A:122:ASN:HA	1.99	0.44
2:B:149:SER:O	5:E:177:GLN:NE2	2.50	0.44
3:C:1:MET:HE2	8:I:142:PRO:HG2	1.97	0.44
7:H:96:MET:HB2	7:H:100:ASP:HB2	1.99	0.44
2:B:226:ILE:HD13	3:C:221:ALA:HB2	1.99	0.44
2:B:298:ARG:NH1	6:F:343:PRO:HD3	2.32	0.44
1:A:322:TYR:CD2	2:B:340:CYS:HB2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD22	5:E:338:SER:HB2	1.98	0.44
2:B:136:LEU:HD12	2:B:139:LEU:HD23	2.00	0.44
2:B:139:LEU:HD22	5:E:158:LEU:HB3	2.00	0.44
6:F:244:ALA:HA	6:F:247:THR:HG22	1.99	0.44
1:A:393:PHE:H	1:A:402:VAL:HG22	1.83	0.44
7:H:116:GLU:O	7:H:120:ILE:HG22	2.18	0.44
6:F:91:ILE:HD13	6:F:112:LEU:HD13	1.99	0.44
1:A:329:LEU:HD13	5:E:342:ALA:HB2	2.00	0.43
1:A:353:GLU:HB2	5:E:388:ARG:HH22	1.83	0.43
4:D:105:ILE:HB	4:D:142:PRO:HD3	2.00	0.43
7:H:203:ILE:O	7:H:208:PRO:HD3	2.17	0.43
2:B:315:THR:HG22	2:B:331:ARG:HA	1.99	0.43
7:G:285:LEU:HD12	7:G:285:LEU:HA	1.77	0.43
1:A:73:VAL:HG21	6:F:74:PRO:HD3	2.00	0.43
2:B:37:THR:HG21	2:B:121:PRO:HB3	2.00	0.43
3:C:4:LEU:O	3:C:9:ARG:NE	2.51	0.43
4:D:224:HIS:HB3	6:F:201:ASN:HB3	2.00	0.43
9:J:173:GLY:HA2	9:J:176:VAL:HG12	1.99	0.43
1:A:137:ARG:HD2	1:A:137:ARG:HA	1.76	0.43
5:E:48:PRO:HD2	5:E:79:PHE:CZ	2.54	0.43
6:F:350:ILE:HD11	6:F:362:ARG:HH21	1.83	0.43
7:H:201:ILE:HD13	7:H:201:ILE:HA	1.80	0.43
1:A:343:LEU:CD2	6:F:363:ASN:CB	2.97	0.43
8:I:89:VAL:HA	8:I:191:THR:HG21	2.00	0.43
1:A:366:LEU:HB2	5:E:377:PRO:HD3	2.00	0.43
3:C:2:ARG:NH1	7:G:55:ARG:HH21	2.16	0.43
3:C:276:ARG:HA	3:C:276:ARG:HD3	1.85	0.43
7:G:98:ILE:HD11	7:G:141:ILE:HD13	2.01	0.43
8:I:174:PHE:HB2	8:I:188:TYR:CE2	2.54	0.43
9:J:56:GLU:HG3	9:J:168:THR:HG21	1.99	0.43
7:H:85:VAL:HG22	7:H:163:LEU:HD12	2.01	0.43
2:B:205:LEU:HD12	3:C:196:LEU:HD12	2.01	0.42
3:C:295:ALA:HB2	4:D:309:LEU:HD12	2.01	0.42
7:G:254:LYS:HE2	7:G:254:LYS:HB3	1.79	0.42
2:B:103:ILE:HD11	8:I:194:LEU:HD11	2.00	0.42
2:B:265:ILE:HD13	3:C:259:LEU:HD13	2.01	0.42
4:D:246:ASN:HD22	4:D:247:THR:HG23	1.84	0.42
6:F:47:LEU:O	6:F:78:GLY:HA3	2.19	0.42
9:J:90:SER:O	9:J:94:ILE:CG1	2.58	0.42
9:J:165:LEU:O	9:J:169:ARG:HG2	2.18	0.42
6:F:179:ASP:O	6:F:182:GLN:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:368:ASP:OD1	6:F:368:ASP:N	2.50	0.42
7:G:47:LEU:HD12	7:G:195:LEU:HD23	2.01	0.42
1:A:194:ILE:HG21	5:E:191:ILE:HG12	2.00	0.42
3:C:73:ILE:HD11	4:D:70:VAL:HB	2.00	0.42
3:C:222:GLN:HB2	4:D:233:LEU:HB2	2.01	0.42
4:D:307:PRO:HG3	6:F:286:VAL:HG23	2.01	0.42
8:I:18:LYS:HB3	8:I:19:PRO:HD3	2.02	0.42
8:I:99:VAL:HG21	8:I:196:THR:HG21	2.01	0.42
1:A:203:ASP:OD1	1:A:207:ARG:NH1	2.52	0.42
7:G:141:ILE:HB	7:G:145:MET:HB2	2.02	0.42
7:H:127:LEU:HD21	7:H:186:ILE:HG12	2.01	0.42
8:I:135:LEU:HD23	8:I:140:ILE:HD12	2.02	0.42
8:I:200:GLU:OE1	8:I:264:THR:OG1	2.32	0.42
3:C:40:PRO:HB3	3:C:120:PRO:HB3	2.00	0.42
4:D:258:LEU:O	4:D:262:LEU:HG	2.20	0.42
6:F:152:PRO:HB2	6:F:155:LYS:HB2	2.01	0.42
1:A:343:LEU:HA	1:A:344:PRO:HD3	1.83	0.42
1:A:160:ILE:HG21	5:E:161:ILE:HD11	2.02	0.42
2:B:205:LEU:HD23	2:B:205:LEU:HA	1.90	0.42
4:D:76:ASP:OD1	4:D:90:HIS:ND1	2.43	0.42
5:E:41:ASN:HA	5:E:69:ALA:HB3	2.02	0.42
7:G:111:LYS:HE2	7:G:111:LYS:HB2	1.92	0.42
7:H:229:LEU:HD23	7:H:240:LEU:HD13	2.01	0.42
8:I:72:LEU:HG	9:J:120:VAL:HG12	2.02	0.42
1:A:283:GLN:OE1	5:E:278:ASN:ND2	2.49	0.42
2:B:134:LEU:HD11	5:E:158:LEU:HB2	2.02	0.42
2:B:340:CYS:HB3	5:E:327:ASN:ND2	2.35	0.42
7:G:29:ALA:O	7:G:299:ARG:NH1	2.45	0.42
2:B:55:VAL:HG21	2:B:81:PHE:HB2	2.02	0.41
4:D:300:GLU:HB3	6:F:377:PRO:HG3	2.02	0.41
5:E:267:ALA:HA	5:E:270:GLU:HG2	2.03	0.41
6:F:1:MET:HG2	7:H:107:ARG:NH1	2.35	0.41
9:J:230:MET:HG3	9:J:267:ILE:HG12	2.01	0.41
3:C:43:TYR:HB2	3:C:123:VAL:HG22	2.01	0.41
8:I:108:VAL:HG22	8:I:248:LEU:HD13	2.00	0.41
2:B:234:ASP:HB3	2:B:235:PRO:HD3	2.02	0.41
9:J:260:MET:O	9:J:264:LEU:HG	2.20	0.41
3:C:149:TRP:O	4:D:154:ARG:NH2	2.54	0.41
5:E:106:PRO:O	5:E:109:THR:OG1	2.25	0.41
8:I:146:LEU:HD22	8:I:150:ARG:HH21	1.85	0.41
4:D:170:PHE:HA	4:D:173:ILE:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:ILE:HD13	6:F:262:LEU:HD13	2.02	0.41
1:A:346:VAL:HG12	1:A:346:VAL:O	2.20	0.41
1:A:376:THR:HG21	4:D:311:ALA:HB1	2.03	0.41
6:F:245:ALA:HB3	6:F:246:PRO:HD3	2.03	0.41
7:H:144:GLY:O	7:H:148:ARG:HG2	2.20	0.41
8:I:107:THR:O	8:I:111:VAL:HB	2.21	0.41
1:A:78:LEU:HD21	1:A:81:ILE:HD11	2.03	0.41
7:G:125:LEU:HB3	7:G:130:MET:O	2.21	0.41
4:D:42:ARG:O	4:D:45:THR:OG1	2.34	0.40
7:G:10:LEU:HD11	7:G:56:PRO:HG2	2.03	0.40
1:A:237:ASP:OD1	5:E:235:ARG:NH1	2.54	0.40
2:B:55:VAL:HG22	2:B:108:LEU:HB3	2.03	0.40
7:G:27:ILE:HD13	7:G:195:LEU:HD13	2.02	0.40
1:A:183:LEU:HD12	5:E:176:ILE:HG23	2.04	0.40
4:D:330:LEU:O	4:D:330:LEU:HD12	2.21	0.40
8:I:105:LEU:HA	8:I:105:LEU:HD23	1.82	0.40
4:D:67:ILE:HG13	4:D:72:VAL:HG21	2.03	0.40
4:D:227:ASP:HB2	6:F:208:SER:HB2	2.04	0.40
4:D:277:THR:HG21	6:F:257:ASP:HB3	2.04	0.40
5:E:181:PHE:O	5:E:185:ASN:HB2	2.21	0.40
5:E:205:LEU:HD23	5:E:205:LEU:HA	1.88	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
1	A	390/409 (95%)	378 (97%)	12 (3%)	0	100 100
2	B	331/343 (96%)	325 (98%)	6 (2%)	0	100 100
3	C	308/524 (59%)	306 (99%)	1 (0%)	1 (0%)	41 65
4	D	381/547 (70%)	369 (97%)	12 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	356/390 (91%)	349 (98%)	6 (2%)	1 (0%)	41	65
6	F	397/518 (77%)	380 (96%)	17 (4%)	0	100	100
7	G	295/653 (45%)	283 (96%)	11 (4%)	1 (0%)	41	65
7	H	294/653 (45%)	288 (98%)	6 (2%)	0	100	100
8	I	251/266 (94%)	247 (98%)	4 (2%)	0	100	100
9	J	261/289 (90%)	253 (97%)	8 (3%)	0	100	100
All	All	3264/4592 (71%)	3178 (97%)	83 (2%)	3 (0%)	54	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	310	VAL
7	G	284	GLN
3	C	303	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/331 (96%)	309 (98%)	7 (2%)	52	78
2	B	285/290 (98%)	280 (98%)	5 (2%)	59	82
3	C	257/421 (61%)	255 (99%)	2 (1%)	81	92
4	D	322/438 (74%)	320 (99%)	2 (1%)	86	94
5	E	303/329 (92%)	300 (99%)	3 (1%)	76	90
6	F	316/409 (77%)	315 (100%)	1 (0%)	92	97
7	G	254/550 (46%)	251 (99%)	3 (1%)	71	88
7	H	253/550 (46%)	250 (99%)	3 (1%)	71	88
8	I	193/205 (94%)	189 (98%)	4 (2%)	53	79
9	J	203/225 (90%)	201 (99%)	2 (1%)	76	90
All	All	2702/3748 (72%)	2670 (99%)	32 (1%)	72	88

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	137	ARG
1	A	284	ASP
1	A	317	LEU
1	A	341	ASP
1	A	366	LEU
1	A	401	GLN
2	B	7	LEU
2	B	13	PHE
2	B	51	ASP
2	B	222	PHE
2	B	298	ARG
3	C	217	LEU
3	C	296	GLU
4	D	155	LEU
4	D	224	HIS
5	E	37	ARG
5	E	231	ASP
5	E	353	LEU
6	F	270	GLU
7	G	36	LEU
7	G	111	LYS
7	G	228	LEU
7	H	20	TRP
7	H	76	LEU
7	H	284	GLN
8	I	29	MET
8	I	57	VAL
8	I	198	PHE
8	I	261	ARG
9	J	111	PHE
9	J	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	72	ASN
2	B	335	GLN
3	C	156	GLN
3	C	220	ASN
5	E	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	292	GLN
5	E	313	ASN
7	H	109	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 31 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

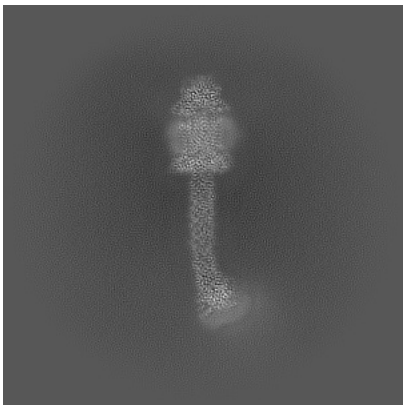
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-29025. These allow visual inspection of the internal detail of the map and identification of artifacts.

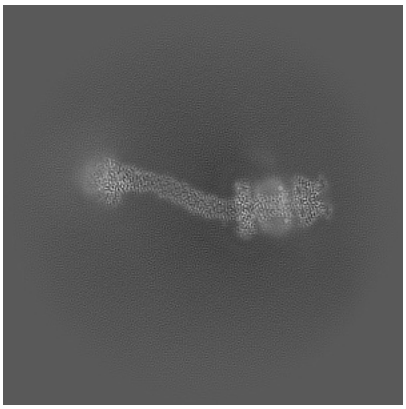
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

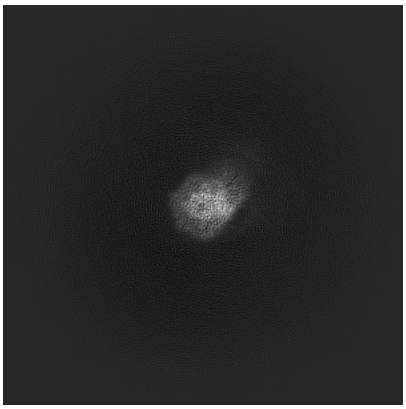
6.1.1 Primary map



X

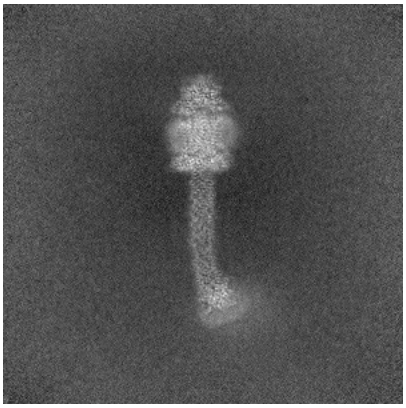


Y

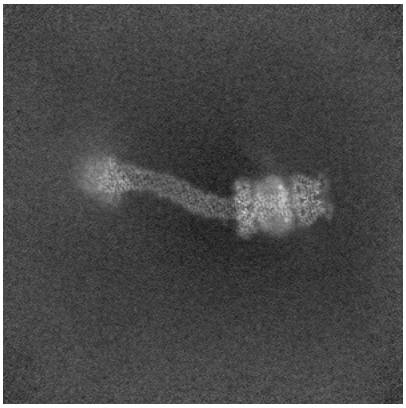


Z

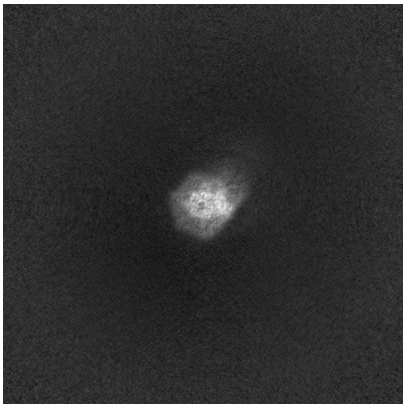
6.1.2 Raw map



X



Y

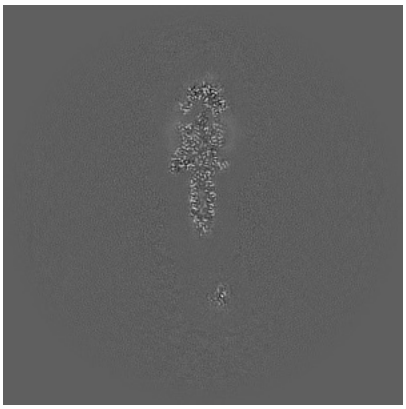


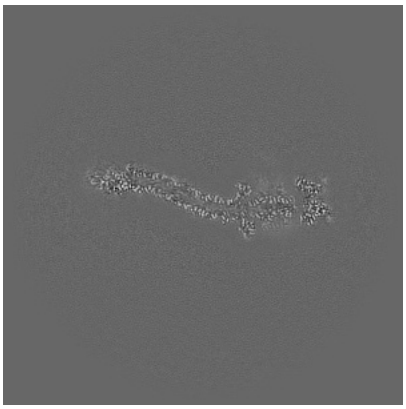
Z

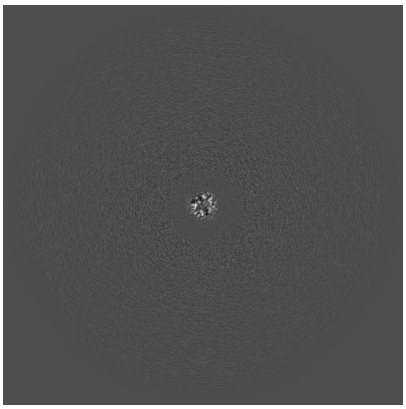
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

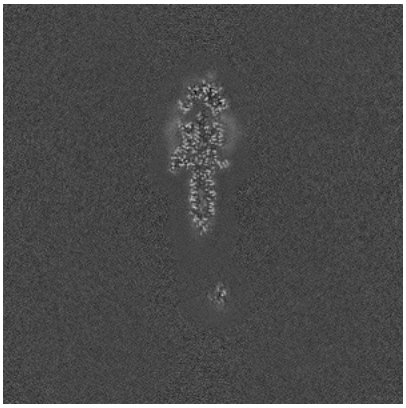
6.2.1 Primary map

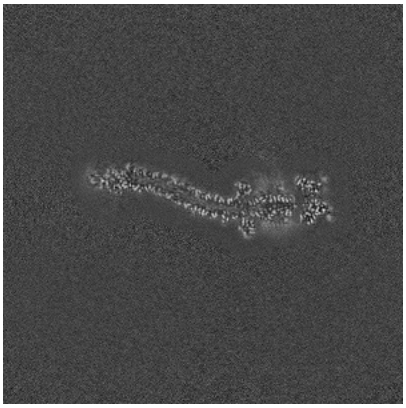

X Index: 320

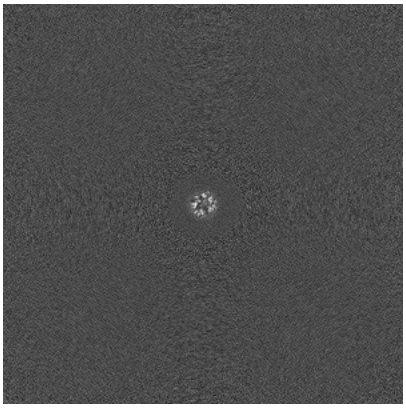

Y Index: 320


Z Index: 320

6.2.2 Raw map


X Index: 320

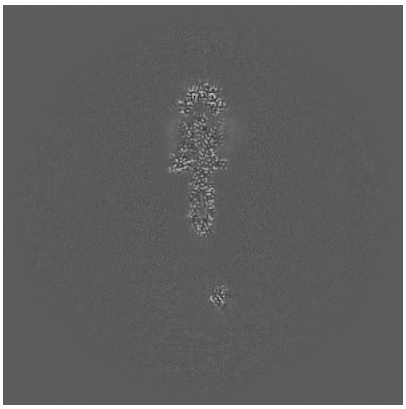

Y Index: 320


Z Index: 320

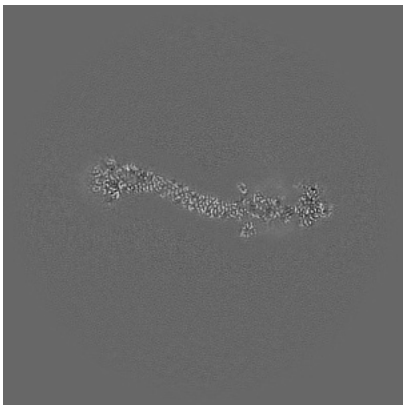
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

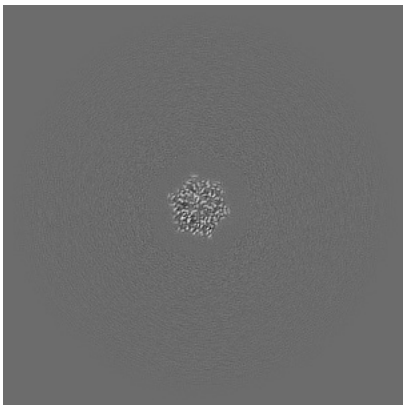
6.3.1 Primary map



X Index: 323

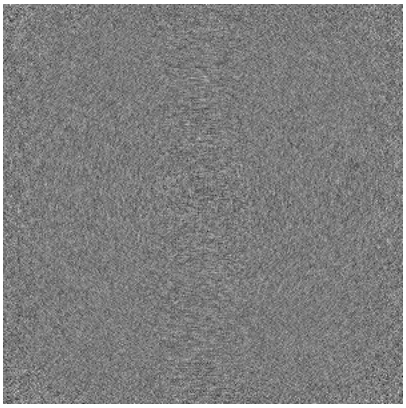


Y Index: 330

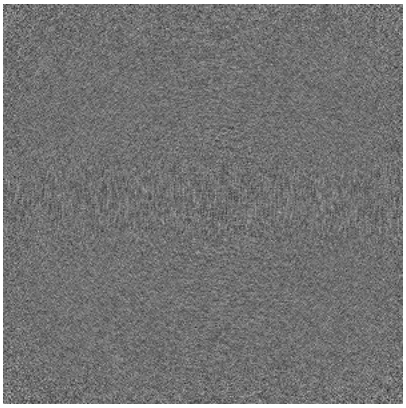


Z Index: 387

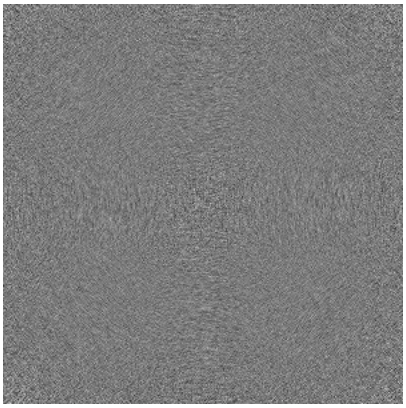
6.3.2 Raw map



X Index: 0



Y Index: 0

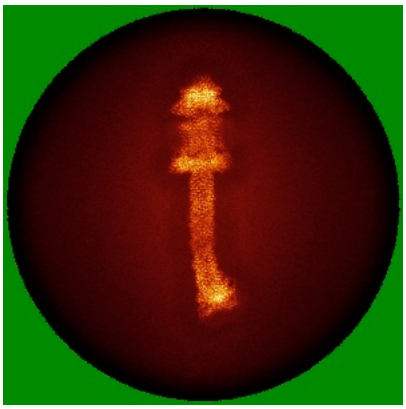


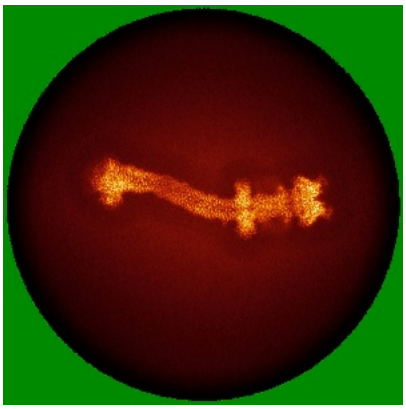
Z Index: 0

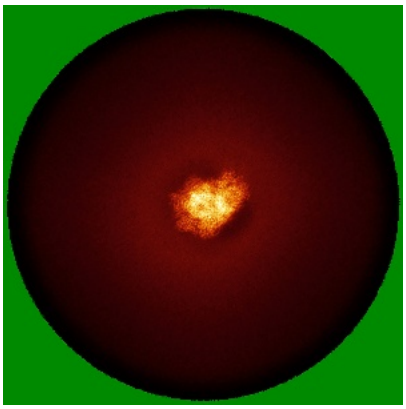
The images above show the largest variance slices of the map in three orthogonal directions.

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

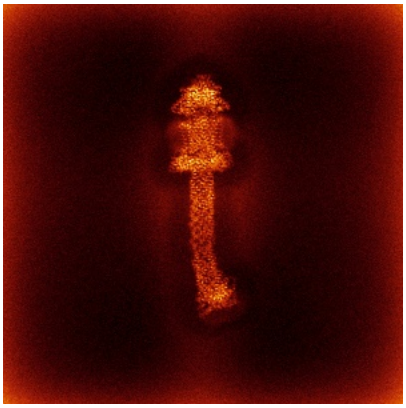
6.4.1 Primary map

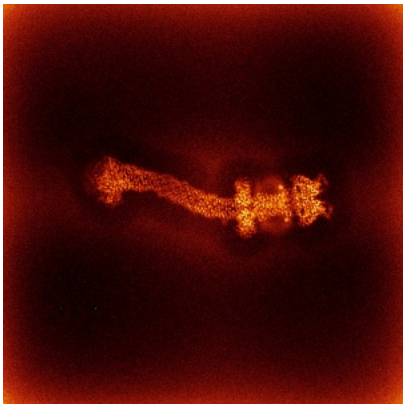

X

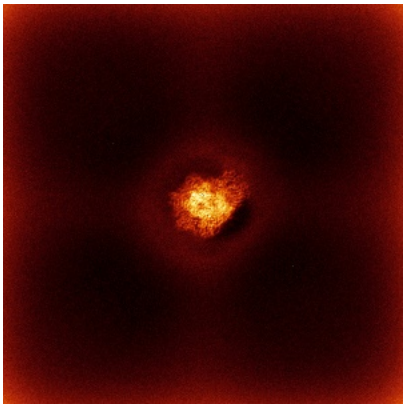

Y


Z

6.4.2 Raw map


X

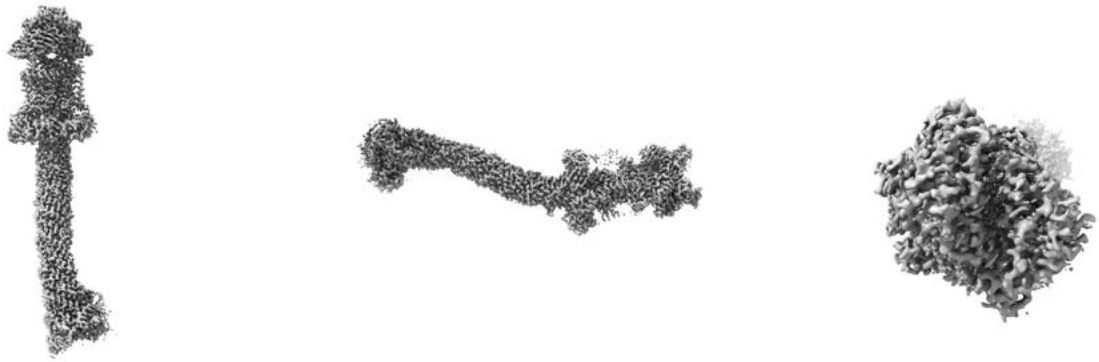

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.69. 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

X Y Z

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

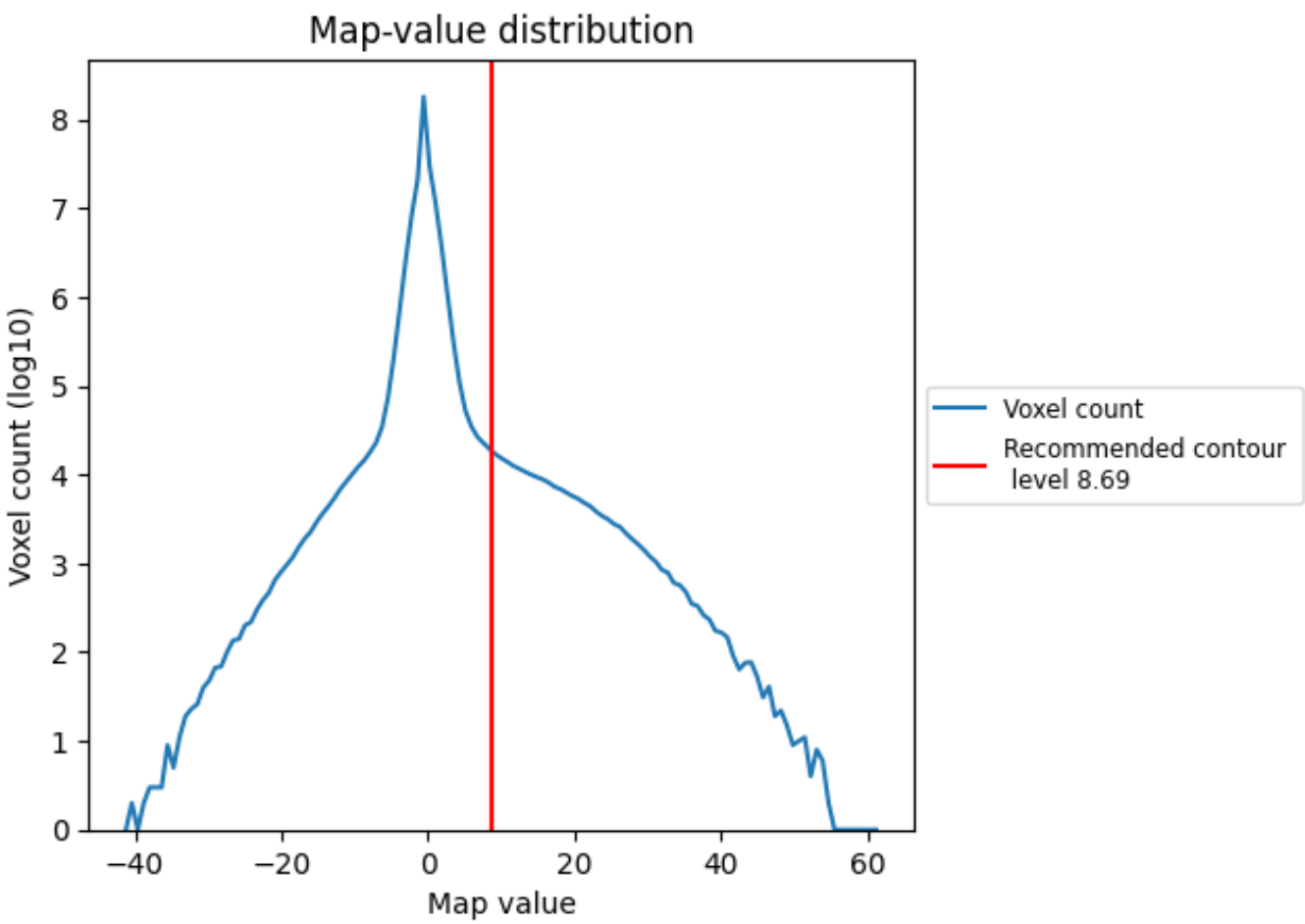
6.6 Mask visualisation (i)

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

7 Map analysis (i)

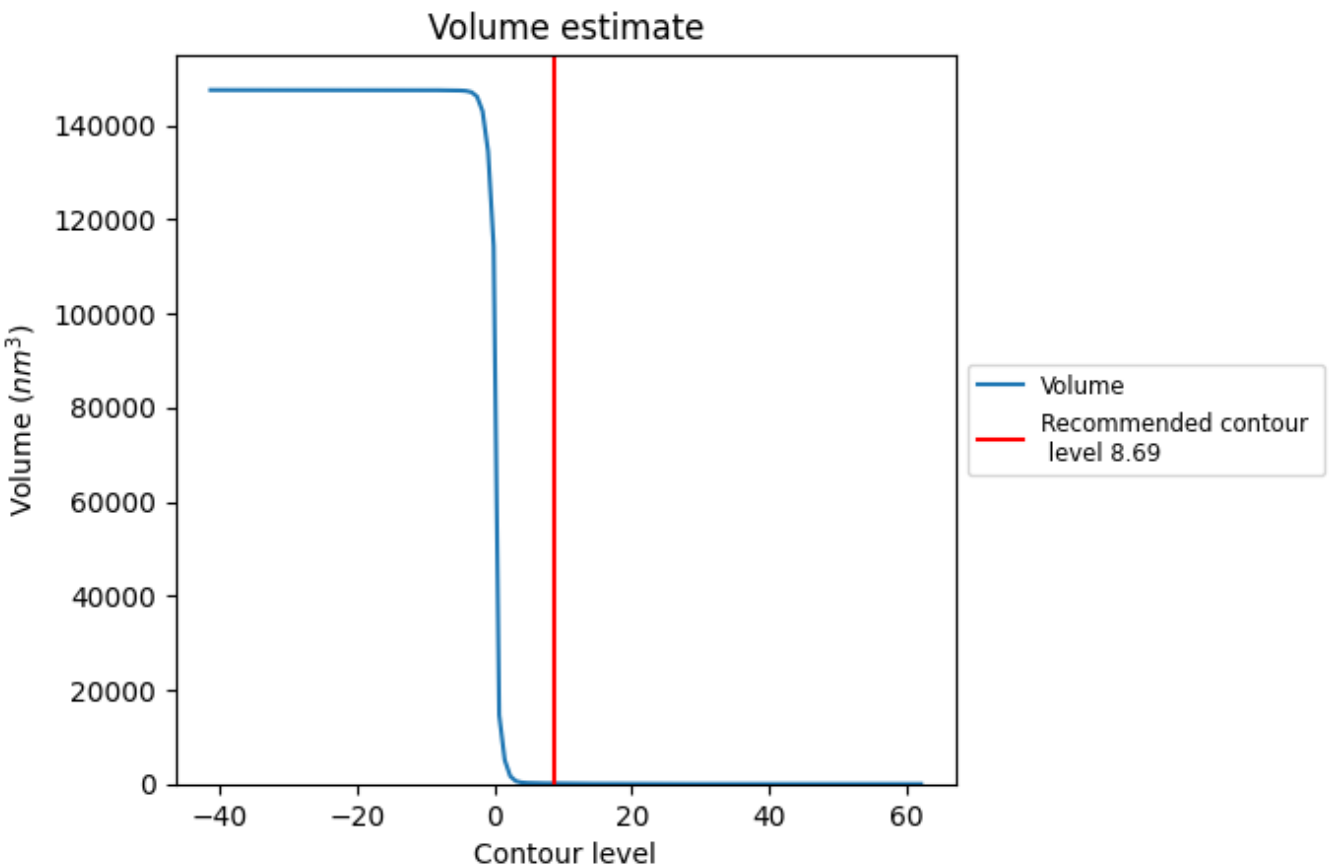
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

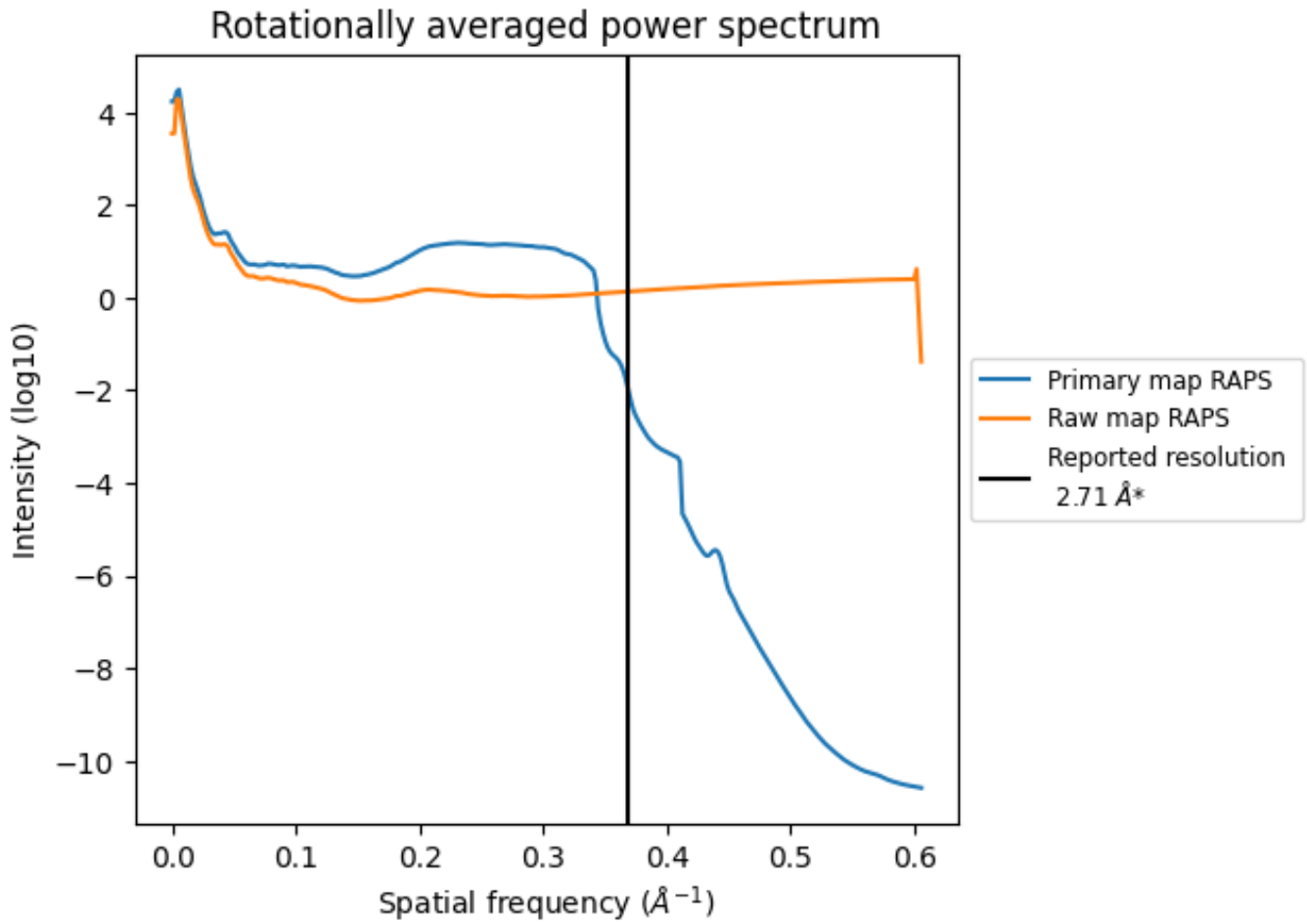
7.2 Volume estimate (i)



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

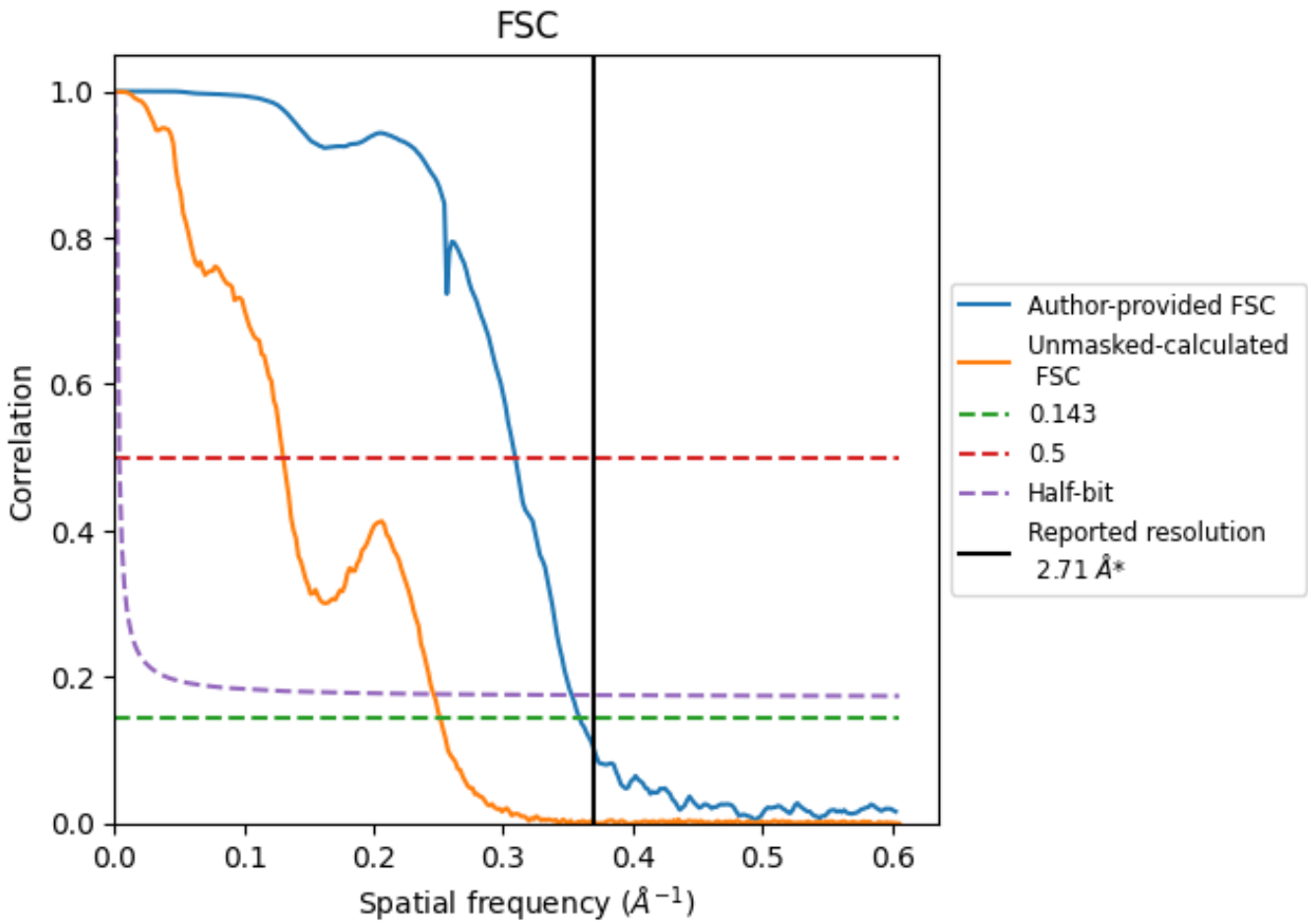


*Reported resolution corresponds to spatial frequency of 0.369 Å^{-1}

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 0.369 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.79	3.23	2.83
Unmasked-calculated*	3.98	7.68	4.06

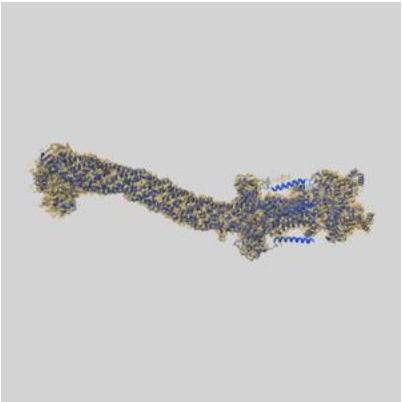
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.71 by more than 10 %

9 Map-model fit (i)

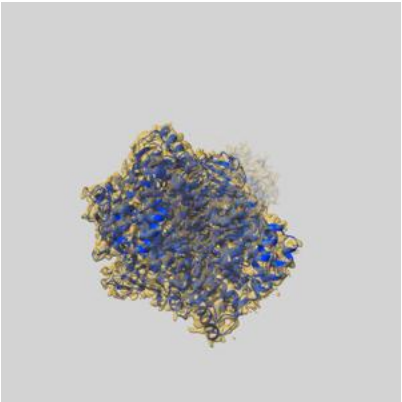
This section contains information regarding the fit between EMDB map EMD-29025 and PDB model 8FEF. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay (i)

X



Y



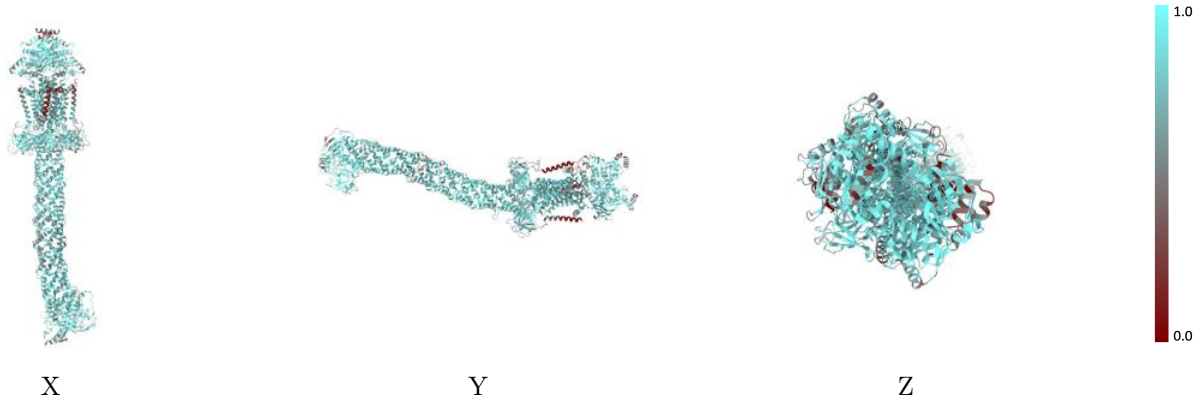
Z

The images above show the 3D surface view of the map at the recommended contour level 8.69 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

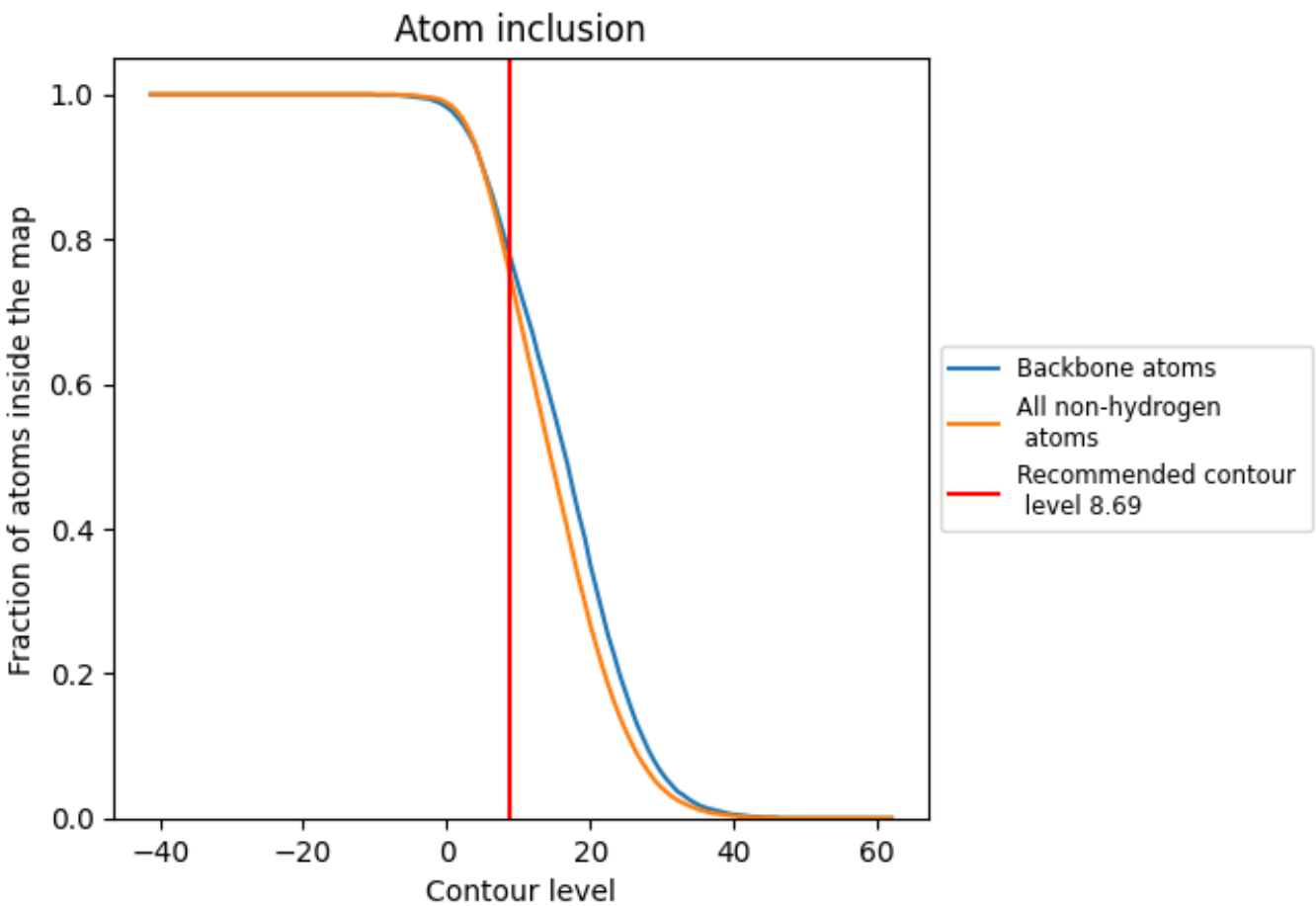
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.69).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8.69) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.5640
A	0.7440	0.5560
B	0.7730	0.5710
C	0.6930	0.5660
D	0.7580	0.5650
E	0.7820	0.5730
F	0.7440	0.5540
G	0.7730	0.5500
H	0.7960	0.5680
I	0.7580	0.5720
J	0.7410	0.5730