Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 07:53 am GMT

PDB ID	:	7ZF2
EMDB ID	:	EMD-14696
Title	:	Protomeric substructure from an octameric assembly of M. tuberculosis RNA polymerase in complex with sigma-b initiation factor
Authors	:	Trapani, S.; Bron, P.; Lai Kee Him, J.; Brodolin, K.; Morichaud, Z.; Vishwakarma, R.
Deposited on	:	2022-03-31
Resolution	:	3.86 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:

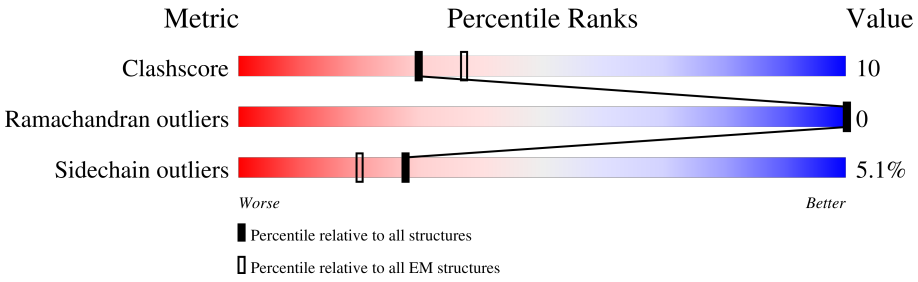
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.86 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	347	47% 15% 35%
1	B	347	50% 17% 32%
2	C	1174	5% 74% 21%
3	D	1319	7% 69% 25%
4	E	110	5% 60% 12% 26%
5	F	343	10% 29% 12% 59%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23822 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	224	Total	C	N	O	S	0	0
			1704	1072	295	335	2		
1	B	235	Total	C	N	O	S	0	0
			1781	1121	303	354	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1122	Total	C	N	O	S	0	0
			8699	5445	1524	1691	39		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY8
C	6	VAL	-	expression tag	UNP P9WGY8

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1264	Total	C	N	O	S	0	0
			9879	6184	1792	1863	40		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP P9WGY7
D	1318	HIS	-	expression tag	UNP P9WGY7
D	1319	HIS	-	expression tag	UNP P9WGY7
D	1320	HIS	-	expression tag	UNP P9WGY7
D	1321	HIS	-	expression tag	UNP P9WGY7
D	1322	HIS	-	expression tag	UNP P9WGY7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	81	Total	C	N	O	0	0
			637	408	106	123		

- Molecule 5 is a protein called RNA polymerase sigma factor SigB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P9WGI4
F	-18	GLY	-	expression tag	UNP P9WGI4
F	-17	SER	-	expression tag	UNP P9WGI4
F	-16	SER	-	expression tag	UNP P9WGI4
F	-15	HIS	-	expression tag	UNP P9WGI4
F	-14	HIS	-	expression tag	UNP P9WGI4
F	-13	HIS	-	expression tag	UNP P9WGI4
F	-12	HIS	-	expression tag	UNP P9WGI4
F	-11	HIS	-	expression tag	UNP P9WGI4
F	-10	HIS	-	expression tag	UNP P9WGI4
F	-9	SER	-	expression tag	UNP P9WGI4
F	-8	SER	-	expression tag	UNP P9WGI4
F	-7	GLY	-	expression tag	UNP P9WGI4
F	-6	LEU	-	expression tag	UNP P9WGI4
F	-5	VAL	-	expression tag	UNP P9WGI4
F	-4	PRO	-	expression tag	UNP P9WGI4
F	-3	ARG	-	expression tag	UNP P9WGI4
F	-2	GLY	-	expression tag	UNP P9WGI4
F	-1	SER	-	expression tag	UNP P9WGI4
F	0	HIS	-	expression tag	UNP P9WGI4

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total	Zn	0
			2	2	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

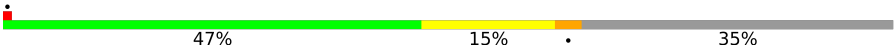
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	D	1	1	1	0

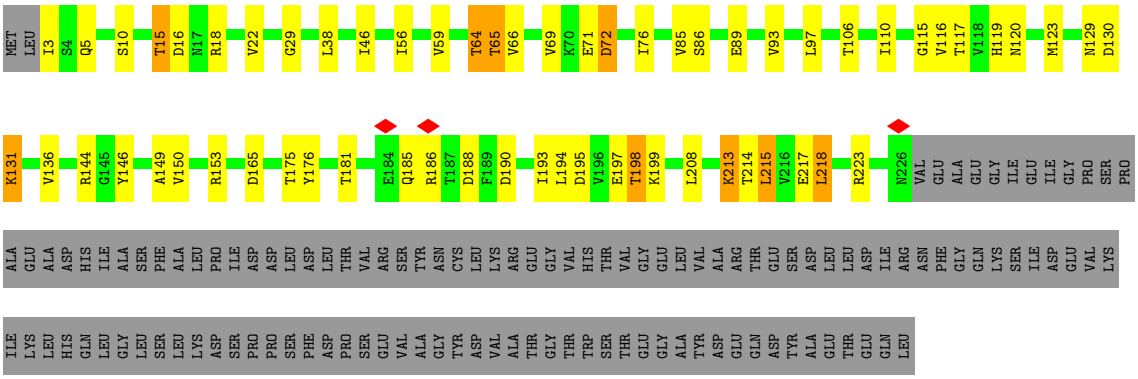
3 Residue-property plots (i)

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: DNA-directed RNA polymerase subunit alpha

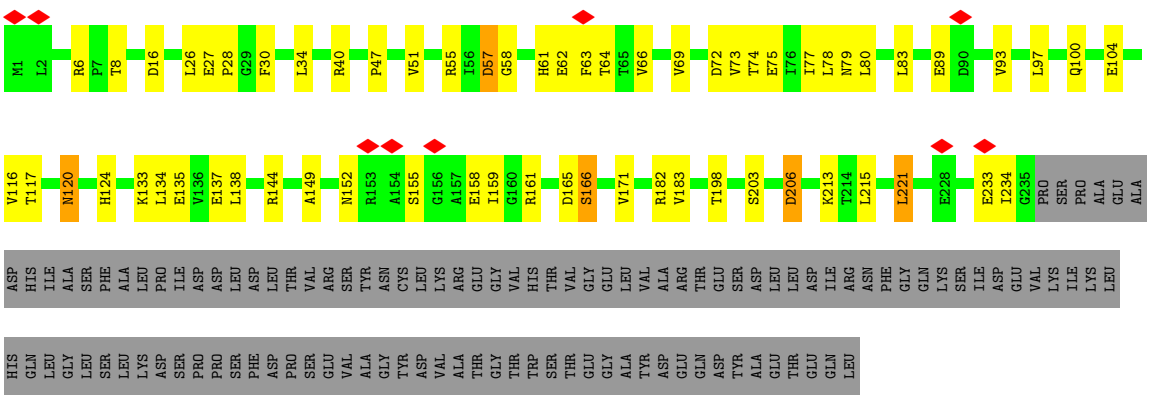
Chain A:





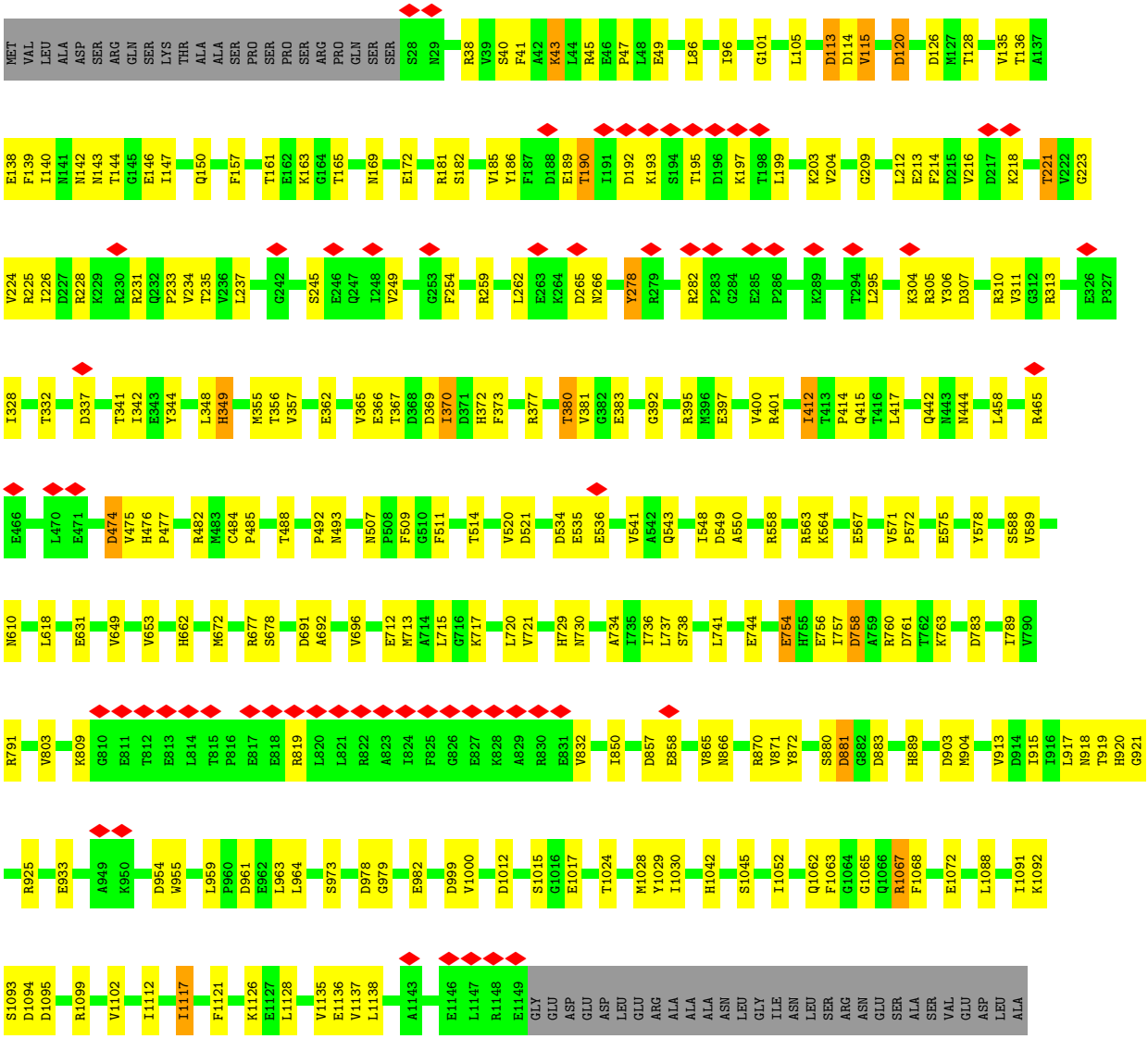
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



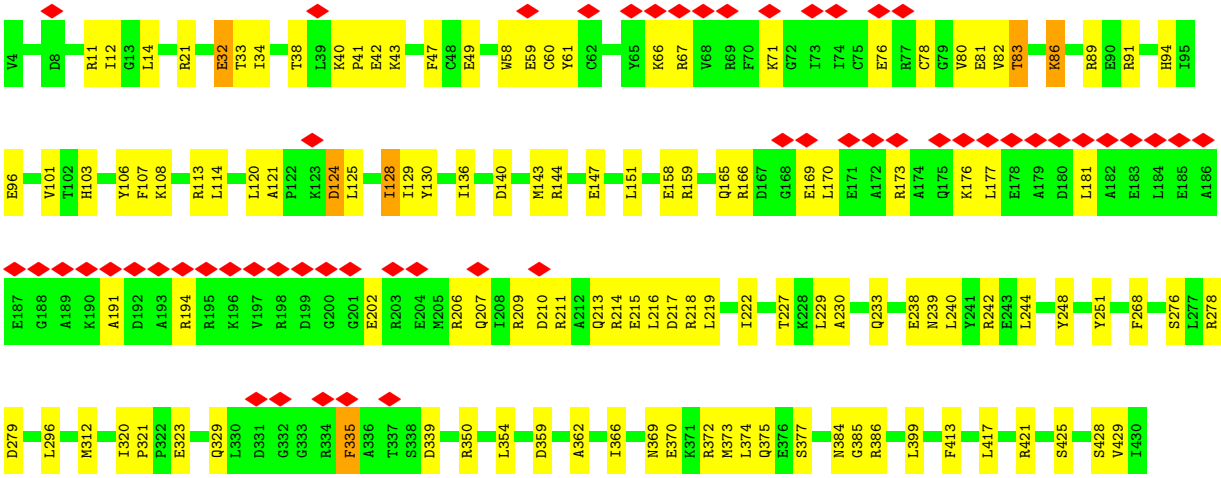
• Molecule 2: DNA-directed RNA polymerase subunit beta

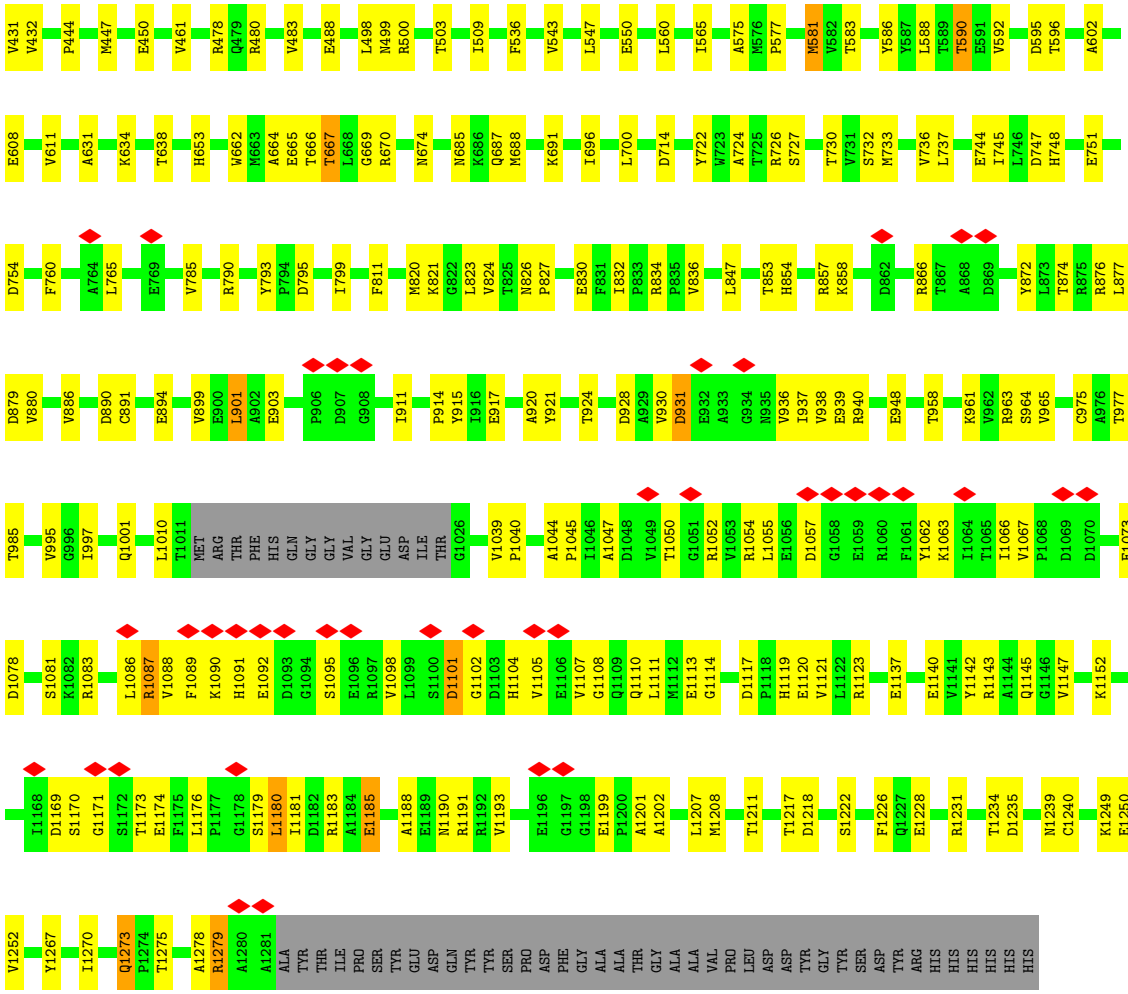
Chain C:



• Molecule 3: DNA-directed RNA polymerase subunit beta'

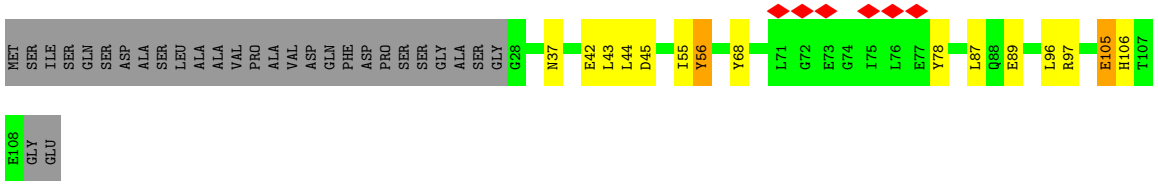
Chain D:





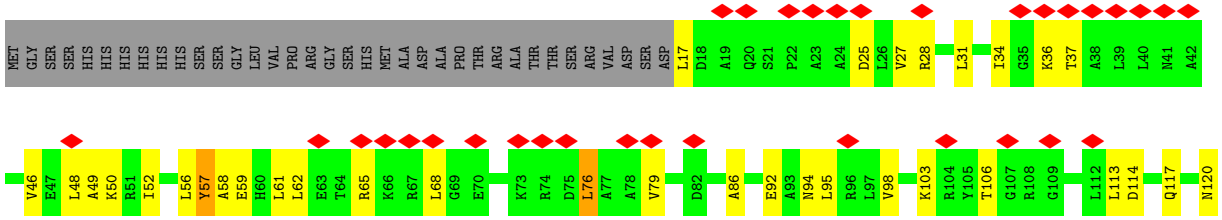
• Molecule 4: DNA-directed RNA polymerase subunit omega

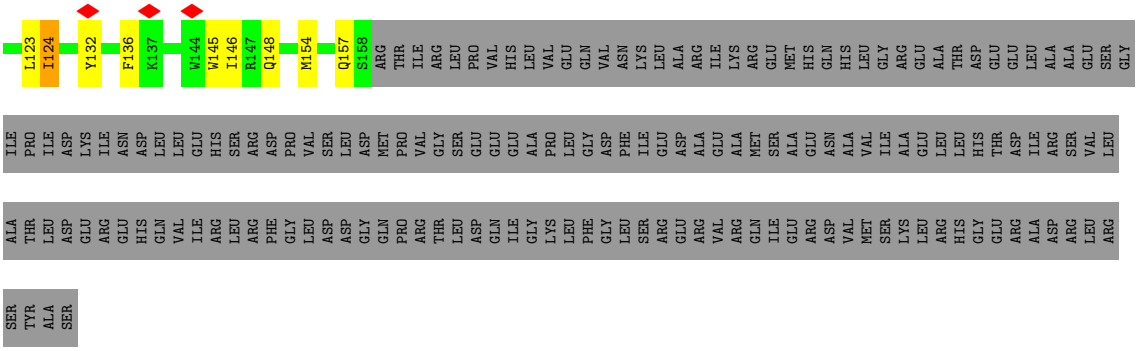
Chain E:



• Molecule 5: RNA polymerase sigma factor SigB

Chain F:




L123
I124
Y132
F136
K137
W144
W145
I146
R147
Q148
M154
Q157
S158
ARG THR ILE ARG LEU PRO VAL HIS LEU VAL GLU GLN VAL ASN LYS LEU ALA ARG ILE LYS ARG GLU MET HIS GLN HIS LEU GLY ARG GLU ALA THR ASP GLU GLU LEU ALA ALA GLU SER GLY
ILE PRO ILE ASP LYS ILE ASN ASP LEU LEU GLU HIS SER ARG ASP PRO VAL SER LEU ASP MET PRO VAL GLY SER GLU GLU GLU ALA PRO LEU GLY ASP PHE ILE GLU ASP ALA GLU ALA MET SER ALA GLU ASN ALA VAL ILE ALA GLU LEU LEU HIS THR ASP ILE ARG SER VAL LEU
ALA THR LEU ASP GLU ARG GLU HIS GLN VAL ILE ARG LEU ARG PHE GLY LEU ASP ASP GLY GLN PRO ARG THR LEU ASP GLN ILE GLY LYS LEU PHE GLY LEU SER ARG GLU ARG VAL ARG GLN ILE GLU ARG ASP VAL MET SER LYS LEU ARG HIS GLY GLU ARG ALA ASP ARG LEU ARG
SER TYR ALA SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	267457	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 ($e^-/Å^2$)	49.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.246	Depositor
Minimum map value	-0.155	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	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: MG, ZN

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	0.37	0/1730	0.56	0/2354
1	B	0.35	0/1807	0.53	0/2458
2	C	0.37	0/8858	0.52	0/12010
3	D	0.36	0/10044	0.54	0/13580
4	E	0.39	0/650	0.52	0/886
5	F	0.25	0/1134	0.53	0/1525
All	All	0.36	0/24223	0.53	0/32813

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	1704	0	1741	38	0
1	B	1781	0	1817	47	0
2	C	8699	0	8631	155	0
3	D	9879	0	9939	229	0
4	E	637	0	635	9	0
5	F	1119	0	1155	29	0
6	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
All	All	23822	0	23918	483	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 10.

All (483) 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:B:149:ALA:HA	1:B:165:ASP:HB3	1.59	0.85
3:D:1066:ILE:O	3:D:1074:GLU:HA	1.83	0.78
3:D:101:VAL:HG13	3:D:375:GLN:HG2	1.68	0.75
3:D:1087:ARG:HG3	3:D:1098:VAL:HA	1.68	0.75
1:A:181:THR:O	1:A:188:ASP:HA	1.89	0.72
2:C:96:ILE:HG23	2:C:401:ARG:HH21	1.56	0.71
3:D:362:ALA:HB1	3:D:366:ILE:HD11	1.73	0.70
2:C:1065:GLY:O	3:D:421:ARG:NH1	2.24	0.70
2:C:304:LYS:HG3	2:C:305:ARG:HG3	1.74	0.69
3:D:59:GLU:HG2	3:D:66:LYS:HG2	1.75	0.69
2:C:181:ARG:HH21	2:C:370:ILE:HG13	1.58	0.69
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.58	0.69
3:D:60:CYS:HB2	3:D:78:CYS:SG	2.32	0.68
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.26	0.68
3:D:595:ASP:OD1	3:D:596:THR:N	2.27	0.68
2:C:380:THR:OG1	2:C:381:VAL:N	2.25	0.68
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.27	0.68
3:D:58:TRP:HA	3:D:82:VAL:HG23	1.76	0.68
3:D:165:GLN:NE2	3:D:169:GLU:OE1	2.26	0.68
2:C:45:ARG:HH11	2:C:47:PRO:HD2	1.59	0.67
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.76	0.67
2:C:1138:LEU:HD11	3:D:11:ARG:HD2	1.77	0.67
1:B:89:GLU:OE1	1:B:89:GLU:N	2.29	0.66
3:D:1279:ARG:O	3:D:1279:ARG:NH1	2.29	0.66
5:F:62:LEU:HG	5:F:76:LEU:HD12	1.77	0.66
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.28	0.66
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.76	0.66
2:C:961:ASP:HA	2:C:964:LEU:HD13	1.78	0.66
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.28	0.66
2:C:730:ASN:HA	2:C:734:ALA:HB3	1.77	0.66
1:A:130:ASP:OD1	1:A:131:LYS:N	2.29	0.65
1:B:8:THR:H	1:B:234:ILE:HD11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG21	1:A:116:VAL:HG11	1.79	0.65
2:C:38:ARG:NH2	2:C:712:GLU:OE1	2.26	0.64
3:D:722:TYR:O	3:D:726:ARG:NH1	2.30	0.64
2:C:43:LYS:NZ	2:C:43:LYS:O	2.29	0.64
1:B:6:ARG:HG3	1:B:183:VAL:HG21	1.79	0.64
2:C:507:ASN:HD21	2:C:511:PHE:HB2	1.62	0.64
1:A:86:SER:OG	1:A:119:HIS:NE2	2.26	0.64
3:D:89:ARG:HG2	3:D:323:GLU:HG3	1.78	0.64
3:D:1101:ASP:N	3:D:1101:ASP:OD1	2.29	0.64
1:B:74:THR:OG1	1:B:75:GLU:OE1	2.16	0.63
3:D:478:ARG:HD3	3:D:480:ARG:HH21	1.61	0.63
1:B:171:VAL:HG22	1:B:198:THR:HG22	1.80	0.63
3:D:876:ARG:NH2	3:D:1211:THR:OG1	2.32	0.62
5:F:58:ALA:HB1	5:F:76:LEU:HD13	1.82	0.62
1:A:64:THR:OG1	1:A:65:THR:N	2.33	0.62
2:C:558:ARG:HH21	2:C:571:VAL:HA	1.65	0.62
3:D:914:PRO:HB2	3:D:1143:ARG:HH22	1.65	0.62
3:D:670:ARG:O	3:D:674:ASN:ND2	2.30	0.62
3:D:11:ARG:NH2	3:D:1240:CYS:SG	2.71	0.61
5:F:31:LEU:HD13	5:F:34:ILE:HD11	1.82	0.61
1:A:18:ARG:NE	1:A:197:GLU:OE2	2.33	0.61
3:D:191:ALA:HA	3:D:194:ARG:HD2	1.82	0.61
3:D:278:ARG:HH21	3:D:296:LEU:HD11	1.65	0.61
3:D:930:VAL:HB	3:D:936:VAL:HG12	1.83	0.61
3:D:665:GLU:N	3:D:665:GLU:OE1	2.33	0.60
2:C:369:ASP:HB3	2:C:372:HIS:HB2	1.83	0.60
2:C:691:ASP:OD1	2:C:692:ALA:N	2.33	0.60
3:D:239:ASN:OD1	3:D:242:ARG:NH2	2.35	0.60
1:B:75:GLU:OE1	1:B:75:GLU:N	2.35	0.60
5:F:65:ARG:HE	5:F:68:LEU:HB2	1.65	0.60
1:B:75:GLU:O	1:B:79:ASN:ND2	2.34	0.60
2:C:311:VAL:HG12	2:C:509:PHE:HB3	1.84	0.60
3:D:1117:ASP:OD1	3:D:1119:HIS:ND1	2.25	0.59
2:C:313:ARG:NH2	2:C:332:THR:O	2.34	0.59
3:D:499:ASN:OD1	3:D:500:ARG:N	2.36	0.59
3:D:1110:GLN:NE2	3:D:1114:GLY:O	2.34	0.59
1:A:97:LEU:HB2	1:A:110:ILE:HD13	1.85	0.58
2:C:737:LEU:HD13	2:C:741:LEU:HD12	1.85	0.58
2:C:754:GLU:HB2	2:C:872:TYR:CE1	2.38	0.58
3:D:821:LYS:HB3	3:D:836:VAL:HB	1.85	0.58
1:A:10:SER:HB2	1:B:221:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:534:ASP:OD1	2:C:535:GLU:N	2.37	0.58
2:C:1136:GLU:N	2:C:1136:GLU:OE1	2.36	0.58
3:D:214:ARG:O	3:D:218:ARG:HG2	2.04	0.58
3:D:1235:ASP:O	3:D:1239:ASN:ND2	2.37	0.58
1:B:27:GLU:HG2	1:B:28:PRO:HD2	1.85	0.58
2:C:223:GLY:HA2	2:C:233:PRO:HA	1.84	0.58
3:D:81:GLU:OE2	3:D:83:THR:OG1	2.21	0.58
3:D:928:ASP:OD1	3:D:940:ARG:N	2.30	0.58
2:C:758:ASP:N	2:C:758:ASP:OD1	2.37	0.57
2:C:278:TYR:HE1	2:C:282:ARG:HD2	1.68	0.57
3:D:634:LYS:HG2	3:D:665:GLU:HG3	1.86	0.57
1:A:16:ASP:OD1	1:A:16:ASP:N	2.36	0.57
3:D:1050:THR:HB	3:D:1107:VAL:HB	1.86	0.57
2:C:355:MET:N	2:C:362:GLU:OE2	2.38	0.57
3:D:147:GLU:HG3	3:D:151:LEU:HG	1.86	0.57
3:D:238:GLU:OE2	5:F:36:LYS:NZ	2.36	0.57
3:D:1250:GLU:N	3:D:1250:GLU:OE1	2.36	0.57
5:F:27:VAL:HG22	5:F:113:LEU:HD13	1.86	0.57
1:A:3:ILE:O	1:A:5:GLN:NE2	2.38	0.57
1:B:152:ASN:HB2	1:B:155:SER:HB2	1.85	0.57
2:C:397:GLU:HA	2:C:400:VAL:HG12	1.87	0.57
3:D:827:PRO:HD3	3:D:854:HIS:NE2	2.20	0.57
4:E:56:TYR:OH	4:E:105:GLU:O	2.21	0.57
2:C:216:VAL:HG11	2:C:349:HIS:CD2	2.39	0.56
3:D:586:TYR:O	3:D:590:THR:OG1	2.23	0.56
3:D:1174:GLU:OE1	3:D:1174:GLU:N	2.39	0.56
3:D:444:PRO:HD2	3:D:447:MET:HE3	1.87	0.56
3:D:602:ALA:N	3:D:608:GLU:OE2	2.37	0.56
2:C:114:ASP:OD1	2:C:115:VAL:N	2.37	0.56
2:C:356:THR:OG1	2:C:362:GLU:OE1	2.21	0.56
1:A:217:GLU:HG3	1:B:234:ILE:HG22	1.88	0.56
2:C:1094:ASP:N	2:C:1094:ASP:OD1	2.38	0.56
3:D:1088:VAL:HG11	3:D:1105:VAL:HG12	1.88	0.56
4:E:43:LEU:HD21	4:E:96:LEU:HD22	1.87	0.56
2:C:631:GLU:HB2	2:C:713:MET:HB3	1.88	0.56
1:A:218:LEU:HD12	1:B:34:LEU:HD11	1.87	0.56
2:C:507:ASN:ND2	2:C:511:PHE:HB2	2.19	0.55
3:D:144:ARG:NH2	3:D:227:THR:O	2.36	0.55
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.87	0.55
3:D:209:ARG:HH12	3:D:213:GLN:HB2	1.71	0.55
2:C:43:LYS:NZ	2:C:45:ARG:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:880:SER:N	2:C:883:ASP:OD2	2.36	0.55
1:A:185:GLN:HG2	1:A:186:ARG:H	1.72	0.55
5:F:94:ASN:HB2	5:F:123:LEU:HD11	1.88	0.55
1:A:29:GLY:O	1:B:40:ARG:NH1	2.39	0.55
2:C:857:ASP:O	2:C:858:GLU:HG3	2.06	0.54
2:C:1102:VAL:HG23	2:C:1112:ILE:HG23	1.88	0.54
5:F:98:VAL:HG23	5:F:146:ILE:HD13	1.90	0.54
2:C:444:ASN:N	2:C:444:ASN:OD1	2.39	0.54
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.73	0.54
3:D:1120:GLU:OE1	3:D:1123:ARG:NH1	2.34	0.54
1:A:149:ALA:N	1:A:165:ASP:OD1	2.40	0.54
3:D:209:ARG:NH2	3:D:210:ASP:OD1	2.30	0.54
5:F:95:LEU:HA	5:F:98:VAL:HG12	1.89	0.54
1:A:129:ASN:OD1	1:A:130:ASP:N	2.40	0.54
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.88	0.54
3:D:498:LEU:HD22	3:D:543:VAL:HG22	1.89	0.54
5:F:25:ASP:HB2	5:F:28:ARG:HB3	1.90	0.54
3:D:903:GLU:O	3:D:911:ILE:N	2.27	0.54
2:C:140:ILE:HG23	2:C:147:ILE:HG22	1.89	0.54
3:D:1180:LEU:H	3:D:1180:LEU:HD23	1.73	0.54
1:A:89:GLU:OE2	1:A:115:GLY:HA3	2.08	0.53
1:B:93:VAL:HG21	1:B:116:VAL:HG21	1.89	0.53
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.89	0.53
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.90	0.53
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.90	0.53
2:C:138:GLU:OE1	2:C:138:GLU:N	2.41	0.53
2:C:142:ASN:OD1	2:C:143:ASN:N	2.42	0.53
3:D:1057:ASP:OD1	3:D:1057:ASP:N	2.39	0.53
3:D:1067:VAL:HA	3:D:1074:GLU:HG2	1.91	0.53
2:C:1017:GLU:N	2:C:1017:GLU:OE1	2.40	0.53
3:D:1045:PRO:HD3	3:D:1083:ARG:HH21	1.73	0.53
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	1.91	0.53
2:C:120:ASP:OD1	2:C:120:ASP:N	2.41	0.53
3:D:480:ARG:O	3:D:483:VAL:HG12	2.08	0.53
5:F:114:ASP:O	5:F:117:GLN:HG2	2.09	0.53
2:C:474:ASP:OD1	2:C:474:ASP:N	2.36	0.53
3:D:1267:TYR:HB3	4:E:55:ILE:HD12	1.90	0.53
2:C:549:ASP:OD1	2:C:550:ALA:N	2.42	0.52
1:A:56:ILE:HG12	1:A:136:VAL:HG12	1.91	0.52
2:C:1024:THR:H	3:D:730:THR:HG21	1.73	0.52
3:D:1052:ARG:HG3	3:D:1067:VAL:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NE	3:D:488:GLU:OE2	2.42	0.52
2:C:214:PHE:HE2	2:C:341:THR:HG23	1.75	0.52
2:C:978:ASP:OD1	2:C:979:GLY:N	2.40	0.52
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.45	0.52
2:C:225:ARG:HD3	2:C:228:ARG:HA	1.92	0.52
2:C:881:ASP:N	2:C:881:ASP:OD1	2.41	0.52
3:D:826:ASN:ND2	3:D:830:GLU:OE2	2.41	0.52
2:C:161:THR:HG23	2:C:163:LYS:H	1.74	0.52
3:D:1275:THR:HB	4:E:105:GLU:HB3	1.91	0.52
5:F:62:LEU:HD11	5:F:76:LEU:HB3	1.92	0.52
5:F:114:ASP:HA	5:F:117:GLN:HE21	1.73	0.52
1:A:69:VAL:HG12	1:A:71:GLU:H	1.74	0.52
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.45	0.52
3:D:1090:LYS:HG3	3:D:1104:HIS:H	1.75	0.52
3:D:1044:ALA:HA	3:D:1083:ARG:HH21	1.75	0.51
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.92	0.51
2:C:224:VAL:HG11	2:C:237:LEU:HD23	1.92	0.51
1:B:61:HIS:CE1	1:B:63:PHE:HB3	2.45	0.51
3:D:1047:ALA:O	3:D:1108:GLY:N	2.37	0.51
1:A:106:THR:HB	1:A:123:MET:O	2.11	0.51
2:C:789:ILE:HG21	2:C:850:ILE:HG21	1.93	0.51
3:D:1275:THR:HG23	3:D:1278:ALA:H	1.75	0.51
2:C:203:LYS:HA	2:C:213:GLU:HB2	1.92	0.51
2:C:982:GLU:N	2:C:982:GLU:OE1	2.44	0.51
2:C:49:GLU:N	2:C:49:GLU:OE1	2.41	0.51
2:C:150:GLN:NE2	2:C:415:GLN:OE1	2.44	0.51
3:D:14:LEU:HD11	3:D:106:TYR:HE2	1.76	0.51
3:D:1062:TYR:O	3:D:1078:ASP:HA	2.11	0.51
3:D:577:PRO:HB3	3:D:581:MET:HB2	1.92	0.51
1:B:171:VAL:HG22	1:B:198:THR:CG2	2.39	0.50
4:E:89:GLU:OE2	4:E:97:ARG:NH2	2.44	0.50
1:A:213:LYS:NZ	1:B:233:GLU:OE2	2.44	0.50
1:A:223:ARG:HH21	1:B:213:LYS:HG3	1.76	0.50
3:D:248:TYR:HB3	3:D:251:TYR:HB2	1.93	0.50
3:D:108:LYS:HG2	3:D:386:ARG:HG3	1.93	0.50
3:D:826:ASN:HB2	3:D:830:GLU:HG3	1.93	0.50
3:D:924:THR:HG23	3:D:963:ARG:HB2	1.94	0.50
1:B:78:LEU:HD21	3:D:611:VAL:HG12	1.93	0.50
1:A:65:THR:OG1	1:A:66:VAL:N	2.44	0.50
2:C:45:ARG:HD2	2:C:47:PRO:HD3	1.94	0.50
2:C:101:GLY:O	2:C:142:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:795:ASP:N	3:D:795:ASP:OD1	2.42	0.50
1:A:86:SER:OG	1:A:117:THR:OG1	2.30	0.50
1:B:16:ASP:N	1:B:16:ASP:OD1	2.43	0.50
1:B:57:ASP:OD1	1:B:58:GLY:N	2.45	0.50
3:D:384:ASN:OD1	3:D:385:GLY:N	2.45	0.50
3:D:1228:GLU:HG3	3:D:1231:ARG:HE	1.76	0.50
1:B:120:ASN:O	1:B:120:ASN:ND2	2.37	0.49
2:C:128:THR:HG22	2:C:169:ASN:H	1.76	0.49
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.92	0.49
3:D:42:GLU:OE1	3:D:42:GLU:N	2.40	0.49
3:D:931:ASP:OD1	3:D:931:ASP:N	2.26	0.49
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.94	0.49
2:C:564:LYS:O	2:C:567:GLU:HG2	2.12	0.49
3:D:1052:ARG:HH21	3:D:1102:GLY:N	2.10	0.49
2:C:197:LYS:HD2	2:C:218:LYS:HA	1.93	0.49
3:D:14:LEU:HD21	3:D:106:TYR:CE2	2.48	0.49
2:C:192:ASP:OD2	2:C:195:THR:N	2.40	0.49
2:C:265:ASP:OD1	2:C:266:ASN:N	2.46	0.49
3:D:890:ASP:OD1	3:D:891:CYS:N	2.45	0.49
2:C:189:GLU:HG2	2:C:367:THR:HG21	1.94	0.49
3:D:121:ALA:HB2	5:F:17:LEU:HD12	1.94	0.49
3:D:939:GLU:CD	3:D:939:GLU:H	2.17	0.49
2:C:484:CYS:SG	2:C:588:SER:N	2.85	0.49
3:D:136:ILE:HD13	3:D:233:GLN:HB2	1.94	0.49
2:C:488:THR:HG21	3:D:857:ARG:HH12	1.77	0.49
3:D:173:ARG:HH12	3:D:176:LYS:HD3	1.78	0.49
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.94	0.48
2:C:520:VAL:HG13	2:C:521:ASP:H	1.78	0.48
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.95	0.48
2:C:1117:ILE:HD11	2:C:1121:PHE:HD2	1.78	0.48
3:D:736:VAL:HG22	3:D:799:ILE:HD11	1.95	0.48
2:C:221:THR:O	2:C:231:ARG:NH2	2.45	0.48
2:C:45:ARG:HD2	2:C:47:PRO:CD	2.42	0.48
3:D:339:ASP:OD2	3:D:399:LEU:HB3	2.13	0.48
1:B:8:THR:HG21	1:B:26:LEU:HD23	1.95	0.48
5:F:76:LEU:HA	5:F:79:VAL:HG12	1.94	0.48
1:B:55:ARG:HB2	1:B:137:GLU:HB2	1.96	0.48
3:D:42:GLU:H	3:D:42:GLU:CD	2.16	0.48
3:D:732:SER:OG	3:D:733:MET:N	2.47	0.48
3:D:903:GLU:N	3:D:911:ILE:O	2.42	0.48
3:D:120:LEU:HB3	3:D:124:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:866:ARG:NH1	3:D:1010:LEU:O	2.47	0.48
1:A:213:LYS:HG3	1:A:214:THR:N	2.28	0.48
1:B:165:ASP:OD1	1:B:165:ASP:N	2.47	0.48
2:C:414:PRO:HA	2:C:417:LEU:HD12	1.94	0.48
3:D:915:TYR:HE1	3:D:1143:ARG:HG3	1.79	0.48
5:F:145:TRP:O	5:F:148:GLN:HG2	2.13	0.48
3:D:924:THR:HG21	3:D:977:THR:O	2.14	0.48
3:D:1054:ARG:HA	3:D:1101:ASP:HA	1.95	0.48
5:F:46:VAL:O	5:F:50:LYS:HG2	2.14	0.48
2:C:465:ARG:HH12	2:C:492:PRO:HG2	1.79	0.47
2:C:999:ASP:OD1	2:C:1000:VAL:N	2.47	0.47
3:D:106:TYR:HD2	3:D:312:MET:HG3	1.78	0.47
3:D:211:ARG:O	3:D:215:GLU:HG2	2.13	0.47
3:D:1086:LEU:HD13	3:D:1113:GLU:HA	1.96	0.47
5:F:37:THR:HG21	5:F:92:GLU:HB2	1.95	0.47
2:C:40:SER:HB3	2:C:973:SER:HB3	1.97	0.47
2:C:1093:SER:O	2:C:1099:ARG:NH2	2.47	0.47
3:D:159:ARG:HH12	3:D:216:LEU:HB2	1.79	0.47
3:D:177:LEU:O	3:D:181:LEU:HG	2.15	0.47
4:E:56:TYR:CE2	4:E:106:HIS:HB2	2.50	0.47
1:B:62:GLU:O	1:B:73:VAL:HG11	2.15	0.47
2:C:249:VAL:HG22	2:C:259:ARG:CZ	2.45	0.47
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.47	0.47
3:D:76:GLU:OE1	3:D:76:GLU:N	2.47	0.47
3:D:1181:ILE:HG23	3:D:1185:GLU:OE1	2.15	0.47
3:D:1279:ARG:HD3	3:D:1279:ARG:N	2.30	0.47
3:D:948:GLU:N	3:D:948:GLU:OE1	2.46	0.47
3:D:1052:ARG:HH12	3:D:1054:ARG:HB2	1.78	0.47
3:D:114:LEU:HD23	3:D:125:LEU:HD21	1.97	0.47
3:D:207:GLN:HG3	3:D:211:ARG:NH1	2.30	0.47
2:C:756:GLU:OE2	2:C:870:ARG:NE	2.40	0.47
3:D:872:TYR:OH	3:D:876:ARG:NH1	2.47	0.46
1:A:72:ASP:OD1	1:A:72:ASP:N	2.28	0.46
1:B:80:LEU:HD21	1:B:138:LEU:HD22	1.97	0.46
1:B:158:GLU:OE1	1:B:158:GLU:N	2.49	0.46
3:D:1117:ASP:O	3:D:1121:VAL:HG23	2.15	0.46
1:B:61:HIS:CE1	1:B:64:THR:H	2.34	0.46
2:C:1128:LEU:HD23	2:C:1128:LEU:HA	1.77	0.46
3:D:329:GLN:HB2	3:D:335:PHE:CZ	2.50	0.46
3:D:350:ARG:HH11	3:D:377:SER:HB2	1.81	0.46
5:F:120:ASN:O	5:F:124:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:O	1:A:153:ARG:HG2	2.15	0.46
2:C:809:LYS:HZ3	2:C:832:VAL:H	1.62	0.46
3:D:790:ARG:HG3	3:D:811:PHE:CZ	2.51	0.46
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.97	0.46
2:C:783:ASP:O	2:C:791:ARG:HG3	2.16	0.46
3:D:43:LYS:NZ	3:D:49:GLU:OE1	2.40	0.46
2:C:918:ASN:OD1	2:C:919:THR:N	2.48	0.46
3:D:369:ASN:HA	3:D:372:ARG:NH1	2.31	0.46
3:D:874:THR:O	3:D:878:VAL:HG23	2.15	0.46
3:D:276:SER:HA	3:D:279:ASP:OD2	2.16	0.46
3:D:320:ILE:HG12	3:D:321:PRO:HD2	1.97	0.46
3:D:1062:TYR:CD1	3:D:1081:SER:HA	2.51	0.46
3:D:1170:SER:O	3:D:1173:THR:OG1	2.25	0.46
2:C:677:ARG:HG2	2:C:678:SER:O	2.16	0.46
2:C:1067:ARG:HG3	2:C:1068:PHE:N	2.31	0.46
2:C:1099:ARG:O	2:C:1102:VAL:HG12	2.16	0.46
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.81	0.46
2:C:181:ARG:NH2	2:C:370:ILE:HG13	2.28	0.45
2:C:344:TYR:OH	2:C:365:VAL:HA	2.16	0.45
3:D:66:LYS:HB2	3:D:67:ARG:HE	1.81	0.45
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.98	0.45
5:F:56:LEU:O	5:F:59:GLU:HG3	2.16	0.45
2:C:482:ARG:NH1	2:C:536:GLU:OE1	2.48	0.45
3:D:158:GLU:HG3	3:D:219:LEU:HD21	1.97	0.45
3:D:724:ALA:O	3:D:727:SER:OG	2.23	0.45
3:D:1044:ALA:HA	3:D:1083:ARG:NH2	2.31	0.45
1:B:100:GLN:HB2	1:B:133:LYS:NZ	2.31	0.45
3:D:760:PHE:HA	3:D:765:LEU:HB2	1.98	0.45
2:C:182:SER:O	2:C:186:TYR:OH	2.26	0.45
3:D:428:SER:OG	3:D:429:VAL:N	2.48	0.45
3:D:785:VAL:HG21	3:D:820:MET:HG2	1.98	0.45
3:D:901:LEU:N	3:D:958:THR:O	2.36	0.45
2:C:618:LEU:HD12	2:C:717:LYS:HE3	1.99	0.45
3:D:827:PRO:HA	3:D:858:LYS:HD2	1.99	0.45
5:F:103:LYS:HA	5:F:106:THR:HG23	1.98	0.45
3:D:106:TYR:HE1	3:D:1234:THR:HG1	1.63	0.45
1:A:198:THR:OG1	1:A:199:LYS:N	2.48	0.45
3:D:903:GLU:HB3	3:D:911:ILE:HB	1.98	0.45
3:D:432:VAL:HB	3:D:536:PHE:CZ	2.52	0.45
3:D:997:ILE:O	3:D:1001:GLN:HG2	2.17	0.45
2:C:715:LEU:N	2:C:1029:TYR:OH	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:ILE:HG21	2:C:803:VAL:HG11	1.98	0.44
3:D:86:LYS:HE3	3:D:86:LYS:HB3	1.86	0.44
2:C:754:GLU:HB2	2:C:872:TYR:HE1	1.82	0.44
5:F:65:ARG:HA	5:F:65:ARG:HD2	1.86	0.44
2:C:224:VAL:HB	2:C:234:VAL:HG12	2.00	0.44
2:C:1045:SER:HB3	3:D:450:GLU:O	2.17	0.44
3:D:33:THR:OG1	3:D:34:ILE:N	2.51	0.44
3:D:140:ASP:OD1	3:D:140:ASP:N	2.35	0.44
3:D:688:MET:HE1	3:D:696:ILE:HD12	1.99	0.44
3:D:1045:PRO:HD3	3:D:1083:ARG:NH2	2.33	0.44
3:D:1052:ARG:HH21	3:D:1102:GLY:H	1.65	0.44
1:A:120:ASN:OD1	1:A:120:ASN:N	2.50	0.44
1:B:72:ASP:OD1	1:B:73:VAL:N	2.45	0.44
2:C:588:SER:OG	2:C:589:VAL:N	2.50	0.44
3:D:744:GLU:HA	3:D:747:ASP:OD2	2.17	0.44
3:D:751:GLU:HA	3:D:754:ASP:OD2	2.18	0.44
2:C:212:LEU:HD13	2:C:226:ILE:HG12	2.00	0.44
2:C:959:LEU:HD21	2:C:963:LEU:HB2	2.00	0.44
2:C:1062:GLN:OE1	2:C:1062:GLN:N	2.50	0.44
3:D:745:ILE:H	3:D:745:ILE:HG13	1.62	0.44
3:D:1250:GLU:H	3:D:1250:GLU:CD	2.20	0.44
1:B:66:VAL:O	1:B:69:VAL:HG22	2.17	0.44
1:B:97:LEU:O	1:B:135:GLU:HA	2.18	0.44
1:B:137:GLU:OE1	1:B:137:GLU:N	2.50	0.44
2:C:41:PHE:CE2	2:C:963:LEU:HD22	2.52	0.44
2:C:105:LEU:HD12	2:C:138:GLU:O	2.17	0.44
3:D:94:HIS:NE2	3:D:96:GLU:HG2	2.33	0.44
3:D:823:LEU:HD23	3:D:823:LEU:HA	1.86	0.44
3:D:877:LEU:HD22	3:D:1157:ILE:HD13	2.00	0.44
3:D:894:GLU:O	3:D:961:LYS:NZ	2.43	0.44
4:E:44:LEU:HD12	4:E:44:LEU:HA	1.76	0.44
2:C:144:THR:OG1	2:C:146:GLU:HG2	2.18	0.44
3:D:230:ALA:N	3:D:233:GLN:OE1	2.43	0.44
2:C:412:ILE:HD13	2:C:412:ILE:HA	1.80	0.43
2:C:921:GLY:O	2:C:925:ARG:HG2	2.18	0.43
3:D:218:ARG:O	3:D:222:ILE:HG12	2.18	0.43
3:D:359:ASP:OD1	3:D:359:ASP:N	2.33	0.43
3:D:917:GLU:HA	3:D:921:TYR:HB2	2.00	0.43
1:A:72:ASP:O	1:A:76:ILE:HG12	2.17	0.43
2:C:310:ARG:HE	2:C:328:ILE:HG21	1.83	0.43
3:D:143:MET:HG2	3:D:251:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:HG23	1:B:234:ILE:HD11	1.99	0.43
2:C:259:ARG:NH2	2:C:262:LEU:HD23	2.32	0.43
2:C:392:GLY:HA2	2:C:395:ARG:HD3	1.98	0.43
3:D:350:ARG:NH1	3:D:377:SER:HB2	2.33	0.43
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.78	0.43
2:C:954:ASP:OD1	2:C:955:TRP:N	2.51	0.43
3:D:1052:ARG:HH22	3:D:1054:ARG:HB2	1.83	0.43
1:B:159:ILE:HG13	1:B:161:ARG:H	1.84	0.43
2:C:209:GLY:HA3	2:C:306:TYR:CD1	2.52	0.43
3:D:666:THR:HG22	3:D:685:ASN:HD21	1.83	0.43
3:D:38:THR:O	3:D:40:LYS:HG2	2.18	0.43
3:D:58:TRP:HE1	3:D:71:LYS:HZ3	1.65	0.43
3:D:832:ILE:HG22	3:D:834:ARG:H	1.84	0.43
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.52	0.43
2:C:738:SER:HB2	2:C:904:MET:HG3	2.01	0.43
3:D:498:LEU:CD2	3:D:543:VAL:HG22	2.49	0.43
1:A:15:THR:HG22	1:A:16:ASP:H	1.84	0.43
2:C:213:GLU:OE2	2:C:225:ARG:HB3	2.19	0.43
2:C:563:ARG:HG2	2:C:564:LYS:H	1.84	0.43
3:D:1120:GLU:HA	3:D:1123:ARG:HG2	2.01	0.43
3:D:1142:TYR:HB3	3:D:1147:VAL:HG23	2.00	0.43
1:B:171:VAL:HA	1:B:198:THR:HG22	2.01	0.42
3:D:213:GLN:O	3:D:216:LEU:HG	2.18	0.42
1:A:22:VAL:HG22	1:A:193:ILE:HG12	2.01	0.42
3:D:166:ARG:HD3	3:D:170:LEU:HG	2.01	0.42
3:D:1176:LEU:O	3:D:1179:SER:OG	2.22	0.42
3:D:209:ARG:NH1	3:D:213:GLN:HB2	2.34	0.42
3:D:373:MET:SD	5:F:117:GLN:NE2	2.91	0.42
2:C:572:PRO:HG2	2:C:575:GLU:OE2	2.20	0.42
2:C:763:LYS:O	2:C:819:ARG:NH1	2.52	0.42
1:A:46:ILE:HD13	1:A:46:ILE:HA	1.91	0.42
3:D:691:LYS:HE3	3:D:691:LYS:HB2	1.90	0.42
3:D:1165:VAL:HG13	3:D:1183:ARG:HG2	2.02	0.42
3:D:1222:SER:HB2	3:D:1250:GLU:OE1	2.20	0.42
1:B:55:ARG:HG2	1:B:161:ARG:HA	2.02	0.42
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.84	0.42
2:C:543:GLN:OE1	3:D:847:LEU:HD23	2.19	0.42
2:C:729:HIS:HB2	2:C:736:ILE:HD11	2.01	0.42
3:D:106:TYR:CD1	3:D:106:TYR:N	2.87	0.42
3:D:211:ARG:HD3	3:D:214:ARG:HH21	1.85	0.42
3:D:159:ARG:HG2	3:D:219:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1054:ARG:HG3	3:D:1101:ASP:HB3	2.01	0.42
2:C:172:GLU:OE1	2:C:442:GLN:NE2	2.53	0.42
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.48	0.42
3:D:937:ILE:HG13	3:D:938:VAL:HG23	2.02	0.42
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.84	0.42
3:D:240:LEU:O	3:D:244:LEU:HG	2.20	0.42
1:B:215:LEU:HA	1:B:215:LEU:HD23	1.84	0.42
2:C:139:PHE:O	2:C:147:ILE:HA	2.20	0.42
2:C:1095:ASP:O	2:C:1099:ARG:HG2	2.20	0.42
3:D:202:GLU:O	3:D:206:ARG:HG2	2.19	0.42
3:D:667:THR:OG1	3:D:669:GLY:N	2.53	0.42
3:D:877:LEU:O	3:D:880:VAL:HG12	2.20	0.42
1:A:18:ARG:NH2	1:A:195:ASP:OD2	2.53	0.41
3:D:125:LEU:HA	3:D:128:ILE:HG22	2.01	0.41
2:C:113:ASP:N	2:C:113:ASP:OD1	2.53	0.41
3:D:129:ILE:HG22	3:D:130:TYR:CD1	2.55	0.41
5:F:48:LEU:HB3	5:F:86:ALA:HB1	2.02	0.41
1:B:51:VAL:O	1:B:166:SER:HB3	2.20	0.41
2:C:337:ASP:O	2:C:341:THR:HG22	2.20	0.41
2:C:344:TYR:CZ	2:C:365:VAL:HG13	2.55	0.41
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.02	0.41
3:D:1117:ASP:OD2	3:D:1120:GLU:HG2	2.20	0.41
5:F:154:MET:O	5:F:157:GLN:HG2	2.20	0.41
2:C:507:ASN:OD1	2:C:511:PHE:N	2.53	0.41
2:C:563:ARG:HB3	2:C:567:GLU:HG3	2.02	0.41
2:C:1072:GLU:OE2	3:D:499:ASN:ND2	2.48	0.41
3:D:886:VAL:HG23	3:D:995:VAL:HG21	2.02	0.41
4:E:42:GLU:OE1	4:E:42:GLU:N	2.53	0.41
1:A:175:THR:O	1:A:194:LEU:HD12	2.21	0.41
2:C:235:THR:HG21	2:C:262:LEU:HA	2.01	0.41
2:C:245:SER:O	2:C:249:VAL:HG23	2.19	0.41
3:D:737:LEU:HD23	3:D:737:LEU:HA	1.83	0.41
2:C:920:HIS:NE2	3:D:583:THR:HG21	2.35	0.41
3:D:91:ARG:H	3:D:91:ARG:HG2	1.68	0.41
3:D:560:LEU:HD12	3:D:560:LEU:HA	1.85	0.41
3:D:595:ASP:HB3	3:D:631:ALA:HB2	2.03	0.41
3:D:1171:GLY:HA3	3:D:1199:GLU:OE2	2.21	0.41
3:D:1273:GLN:O	4:E:105:GLU:HG3	2.21	0.41
5:F:57:TYR:O	5:F:61:LEU:HG	2.21	0.41
1:B:89:GLU:H	1:B:89:GLU:CD	2.24	0.41
2:C:96:ILE:HG12	2:C:397:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:LYS:H	2:C:193:LYS:HG3	1.63	0.41
2:C:366:GLU:HG2	2:C:367:THR:O	2.21	0.41
2:C:1012:ASP:OD2	2:C:1015:SER:OG	2.25	0.41
3:D:21:ARG:NH2	3:D:96:GLU:OE1	2.53	0.41
3:D:129:ILE:HD13	3:D:129:ILE:HA	1.89	0.41
3:D:1173:THR:OG1	3:D:1201:ALA:HB2	2.20	0.41
5:F:49:ALA:HA	5:F:52:ILE:HG22	2.03	0.41
2:C:342:ILE:HD13	2:C:342:ILE:HA	1.95	0.41
3:D:32:GLU:OE1	3:D:33:THR:N	2.54	0.41
3:D:41:PRO:HG2	3:D:49:GLU:OE2	2.20	0.41
3:D:58:TRP:HE1	3:D:71:LYS:NZ	2.19	0.41
3:D:1226:PHE:HE1	3:D:1249:LYS:HE3	1.86	0.41
5:F:65:ARG:HH21	5:F:68:LEU:HA	1.85	0.41
1:B:203:SER:HB3	1:B:206:ASP:OD1	2.21	0.41
2:C:521:ASP:OD1	2:C:521:ASP:N	2.53	0.41
2:C:917:LEU:HD11	2:C:1028:MET:HE1	2.02	0.41
3:D:113:ARG:H	3:D:113:ARG:HD2	1.86	0.41
3:D:592:VAL:HG13	3:D:595:ASP:HB2	2.02	0.41
3:D:1188:ALA:HA	3:D:1191:ARG:NH1	2.36	0.41
5:F:61:LEU:O	5:F:65:ARG:N	2.48	0.41
2:C:575:GLU:OE1	2:C:575:GLU:N	2.54	0.41
3:D:229:LEU:HD12	3:D:229:LEU:HA	1.93	0.41
1:A:175:THR:OG1	1:A:176:TYR:N	2.54	0.40
1:A:215:LEU:HD13	1:A:215:LEU:HA	1.77	0.40
1:B:47:PRO:HD3	1:B:144:ARG:HH12	1.85	0.40
2:C:366:GLU:N	2:C:366:GLU:OE1	2.54	0.40
3:D:590:THR:HG23	3:D:687:GLN:OE1	2.21	0.40
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.96	0.40
3:D:1057:ASP:HA	3:D:1063:LYS:H	1.85	0.40
2:C:760:ARG:HA	2:C:865:VAL:HA	2.02	0.40
2:C:1126:LYS:HD3	2:C:1126:LYS:HA	1.81	0.40
3:D:1152:LYS:HE3	3:D:1152:LYS:HB2	1.88	0.40
1:B:77:ILE:HD13	1:B:77:ILE:HA	1.89	0.40
3:D:339:ASP:CG	3:D:399:LEU:HB3	2.42	0.40
3:D:700:LEU:HD23	3:D:700:LEU:HA	1.83	0.40
1:B:104:GLU:OE2	1:B:124:HIS:ND1	2.53	0.40
2:C:548:ILE:HD12	2:C:548:ILE:HA	2.00	0.40
3:D:41:PRO:HB3	3:D:47:PHE:HB2	2.03	0.40
3:D:354:LEU:N	3:D:370:GLU:OE2	2.54	0.40
3:D:1010:LEU:HD23	3:D:1145:GLN:HG2	2.03	0.40
3:D:1137:GLU:HA	3:D:1140:GLU:OE1	2.22	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	222/347 (64%)	204 (92%)	18 (8%)	0	100	100
1	B	233/347 (67%)	214 (92%)	19 (8%)	0	100	100
2	C	1120/1174 (95%)	1050 (94%)	70 (6%)	0	100	100
3	D	1260/1319 (96%)	1203 (96%)	57 (4%)	0	100	100
4	E	79/110 (72%)	76 (96%)	3 (4%)	0	100	100
5	F	140/343 (41%)	134 (96%)	6 (4%)	0	100	100
All	All	3054/3640 (84%)	2881 (94%)	173 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	192/297 (65%)	177 (92%)	15 (8%)	12	41
1	B	200/297 (67%)	191 (96%)	9 (4%)	27	55
2	C	949/995 (95%)	904 (95%)	45 (5%)	26	54
3	D	1047/1098 (95%)	998 (95%)	49 (5%)	26	54
4	E	68/90 (76%)	61 (90%)	7 (10%)	7	30
5	F	111/284 (39%)	106 (96%)	5 (4%)	27	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2567/3061 (84%)	2437 (95%)	130 (5%)	27 53

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	59	VAL
1	A	64	THR
1	A	65	THR
1	A	72	ASP
1	A	85	VAL
1	A	131	LYS
1	A	144	ARG
1	A	146	TYR
1	A	190	ASP
1	A	198	THR
1	A	208	LEU
1	A	213	LYS
1	A	215	LEU
1	A	218	LEU
1	B	30	PHE
1	B	57	ASP
1	B	83	LEU
1	B	117	THR
1	B	120	ASN
1	B	134	LEU
1	B	166	SER
1	B	206	ASP
1	B	221	LEU
2	C	43	LYS
2	C	113	ASP
2	C	115	VAL
2	C	120	ASP
2	C	126	ASP
2	C	135	VAL
2	C	136	THR
2	C	157	PHE
2	C	165	THR
2	C	190	THR
2	C	221	THR
2	C	254	PHE
2	C	278	TYR

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Mol	Chain	Res	Type
2	C	295	LEU
2	C	307	ASP
2	C	349	HIS
2	C	357	VAL
2	C	370	ILE
2	C	373	PHE
2	C	380	THR
2	C	412	ILE
2	C	458	LEU
2	C	474	ASP
2	C	475	VAL
2	C	514	THR
2	C	610	ASN
2	C	649	VAL
2	C	653	VAL
2	C	662	HIS
2	C	672	MET
2	C	696	VAL
2	C	744	GLU
2	C	754	GLU
2	C	758	ASP
2	C	871	VAL
2	C	881	ASP
2	C	903	ASP
2	C	1030	ILE
2	C	1042	HIS
2	C	1052	ILE
2	C	1063	PHE
2	C	1067	ARG
2	C	1091	ILE
2	C	1117	ILE
2	C	1137	VAL
3	D	32	GLU
3	D	61	TYR
3	D	80	VAL
3	D	83	THR
3	D	86	LYS
3	D	103	HIS
3	D	107	PHE
3	D	124	ASP
3	D	128	ILE
3	D	217	ASP

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Mol	Chain	Res	Type
3	D	268	PHE
3	D	335	PHE
3	D	374	LEU
3	D	413	PHE
3	D	417	LEU
3	D	425	SER
3	D	431	VAL
3	D	461	VAL
3	D	503	THR
3	D	509	ILE
3	D	547	LEU
3	D	550	GLU
3	D	581	MET
3	D	588	LEU
3	D	590	THR
3	D	638	THR
3	D	653	HIS
3	D	667	THR
3	D	714	ASP
3	D	748	HIS
3	D	824	VAL
3	D	879	ASP
3	D	901	LEU
3	D	931	ASP
3	D	964	SER
3	D	965	VAL
3	D	975	CYS
3	D	985	THR
3	D	1073	GLU
3	D	1087	ARG
3	D	1101	ASP
3	D	1180	LEU
3	D	1185	GLU
3	D	1207	LEU
3	D	1208	MET
3	D	1252	VAL
3	D	1270	ILE
3	D	1273	GLN
3	D	1279	ARG
4	E	37	ASN
4	E	45	ASP
4	E	56	TYR

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Mol	Chain	Res	Type
4	E	68	TYR
4	E	78	TYR
4	E	87	LEU
4	E	105	GLU
5	F	57	TYR
5	F	76	LEU
5	F	124	ILE
5	F	132	TYR
5	F	136	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	150	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - 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.

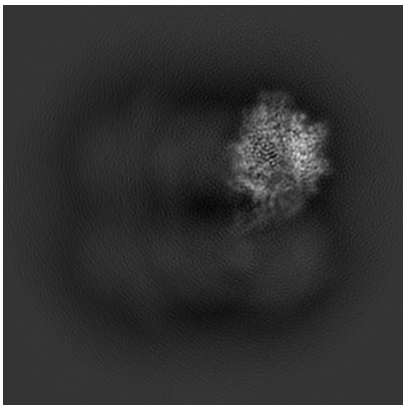
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14696. These allow visual inspection of the internal detail of the map and identification of artifacts.

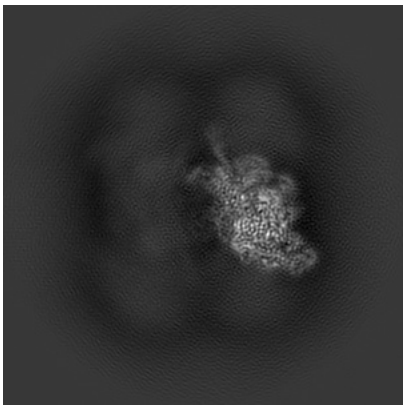
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

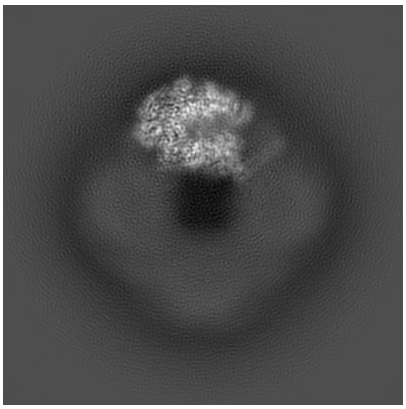
6.1.1 Primary map



X

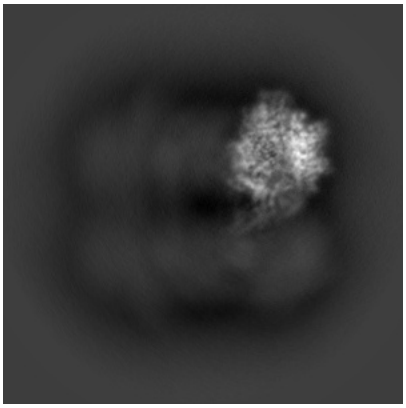


Y

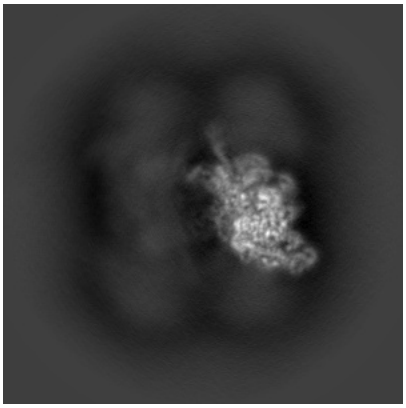


Z

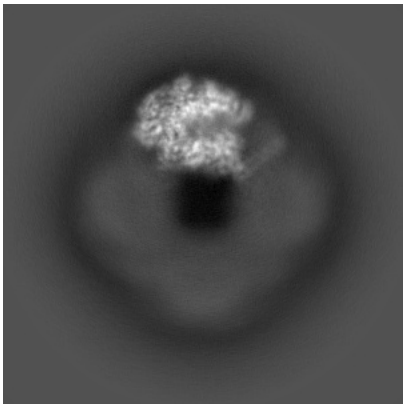
6.1.2 Raw map



X



Y

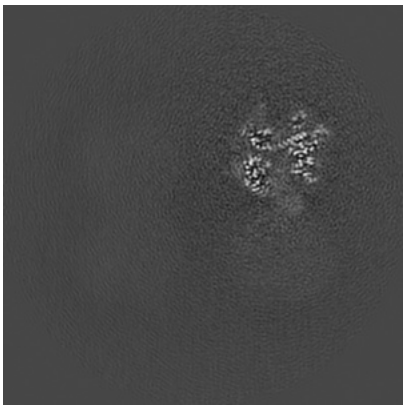


Z

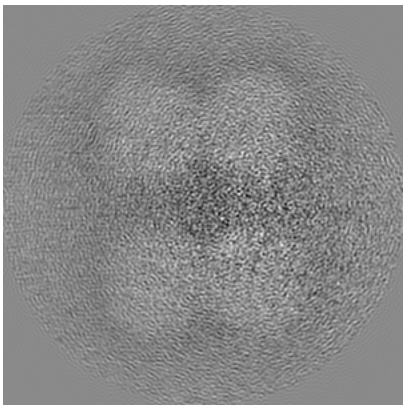
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

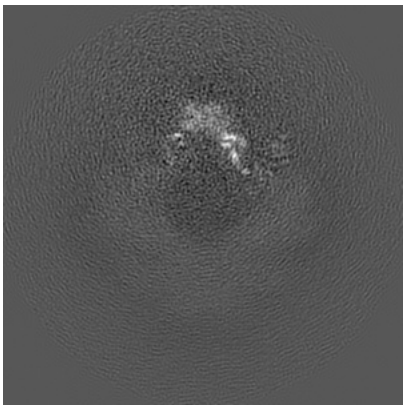
6.2.1 Primary map



X Index: 200

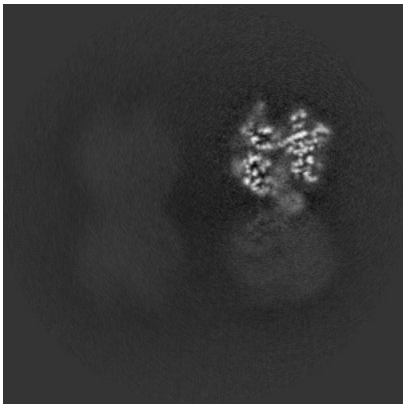


Y Index: 200

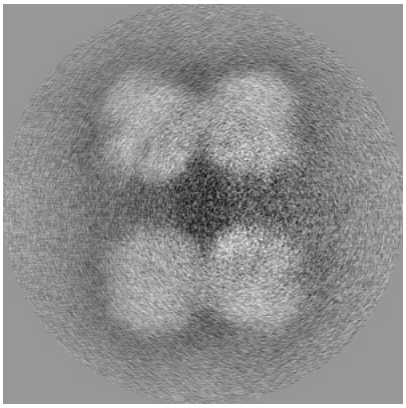


Z Index: 200

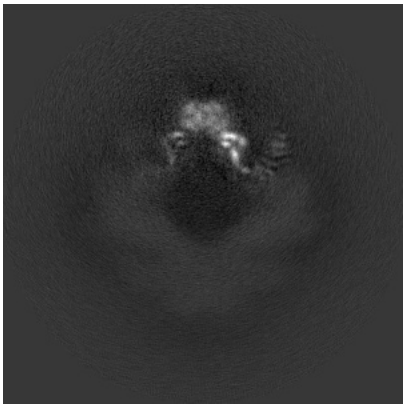
6.2.2 Raw map



X Index: 200



Y Index: 200

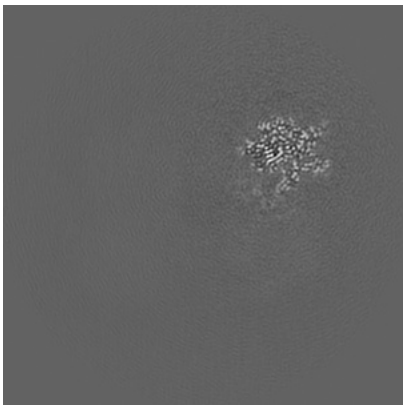


Z Index: 200

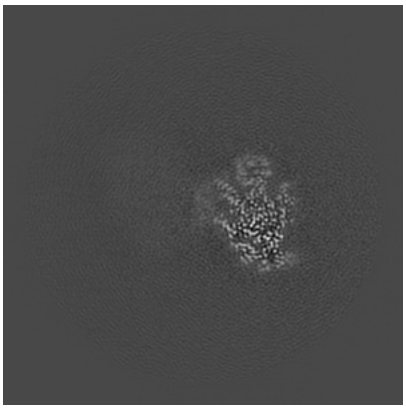
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

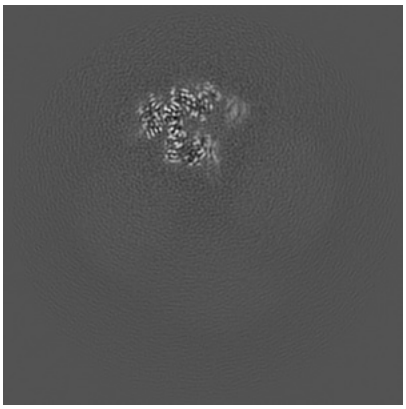
6.3.1 Primary map



X Index: 176

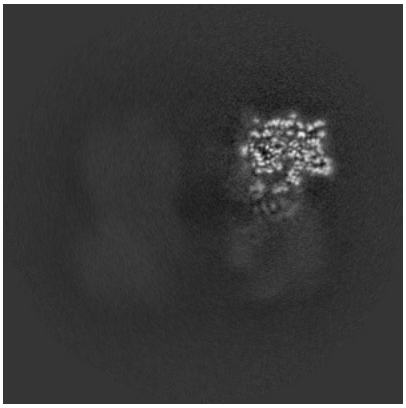


Y Index: 294

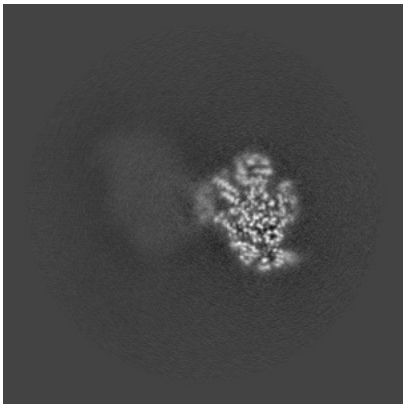


Z Index: 264

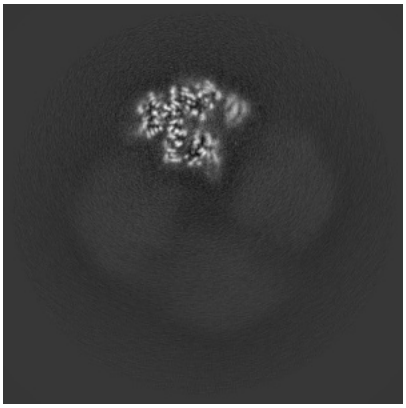
6.3.2 Raw map



X Index: 180



Y Index: 295

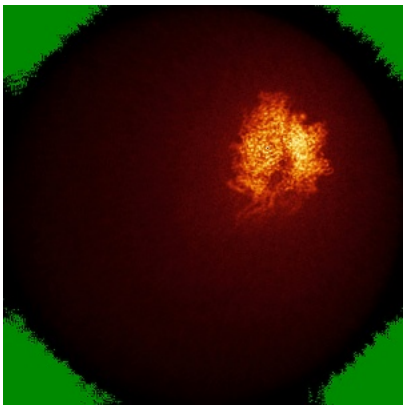


Z Index: 264

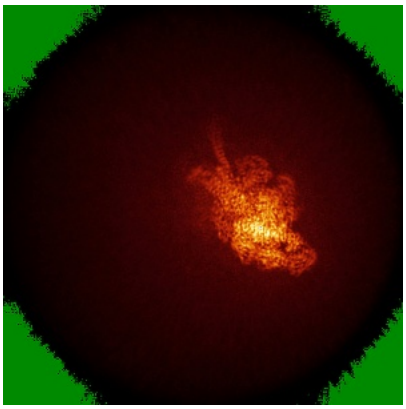
The images above show the largest variance slices of the map in three orthogonal directions.

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

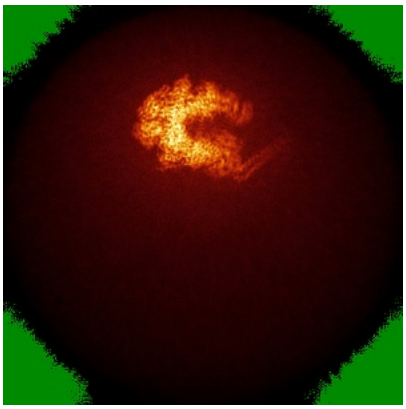
6.4.1 Primary map



X

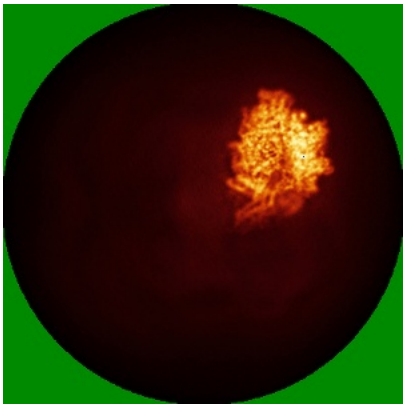


Y

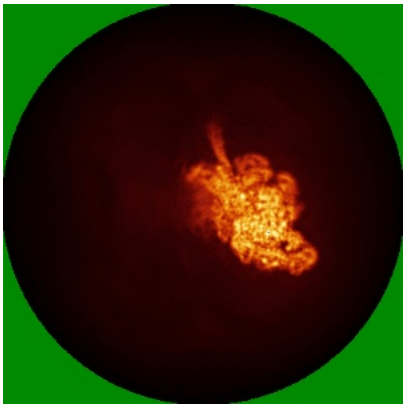


Z

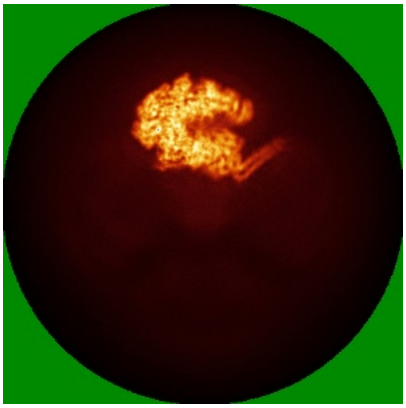
6.4.2 Raw map



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 0.03. 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.

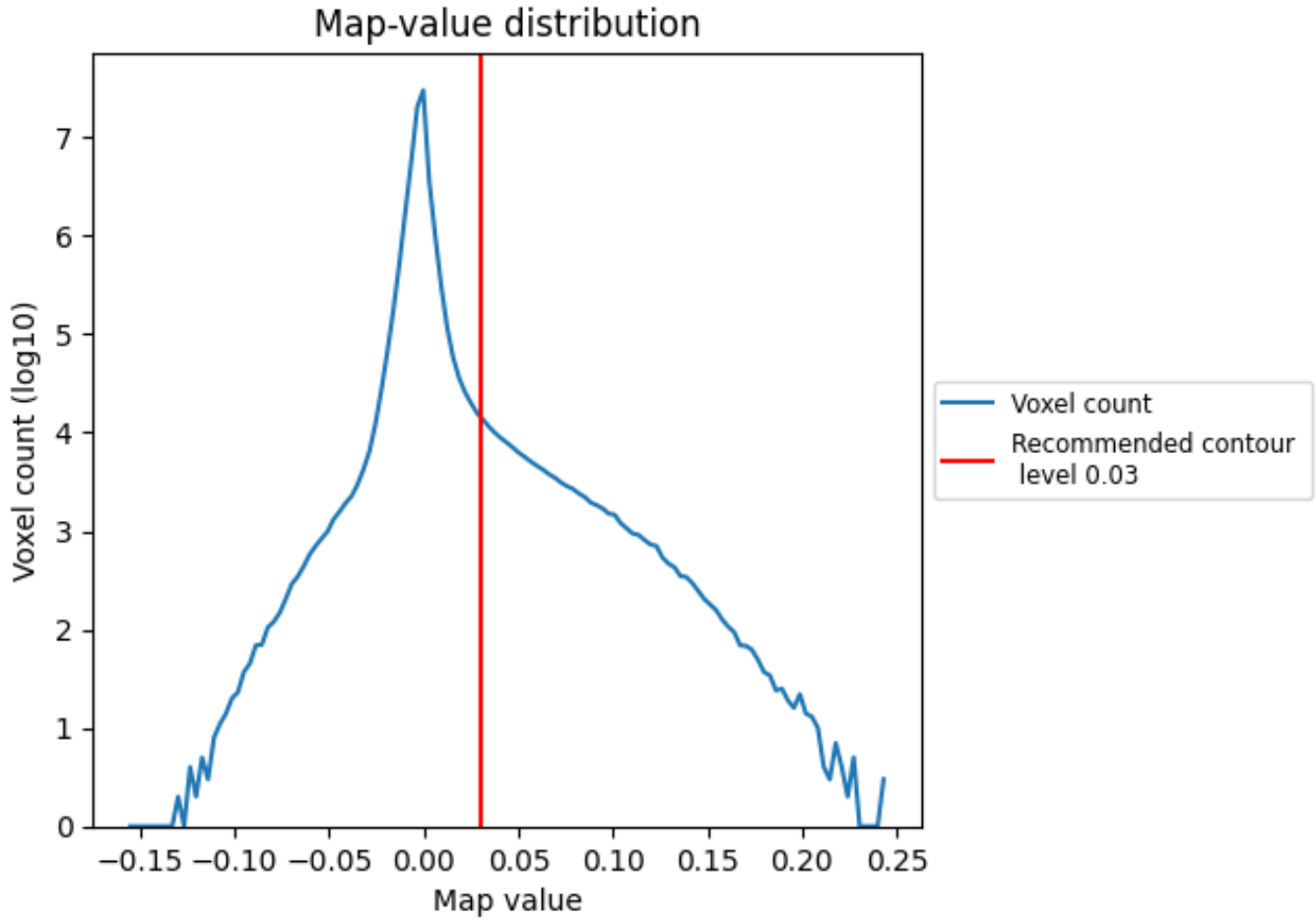
6.6 Mask visualisation (i)

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

7 Map analysis

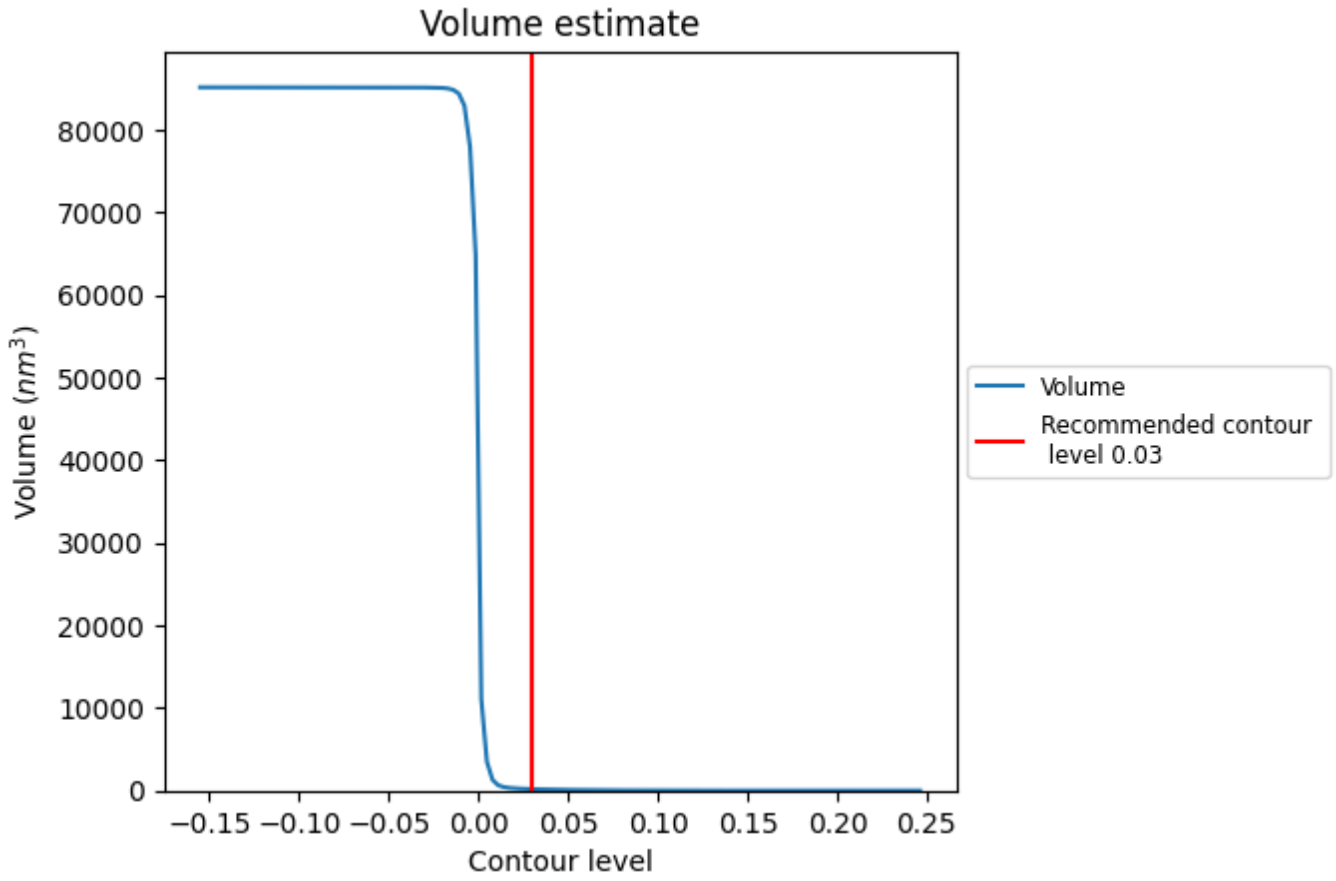
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

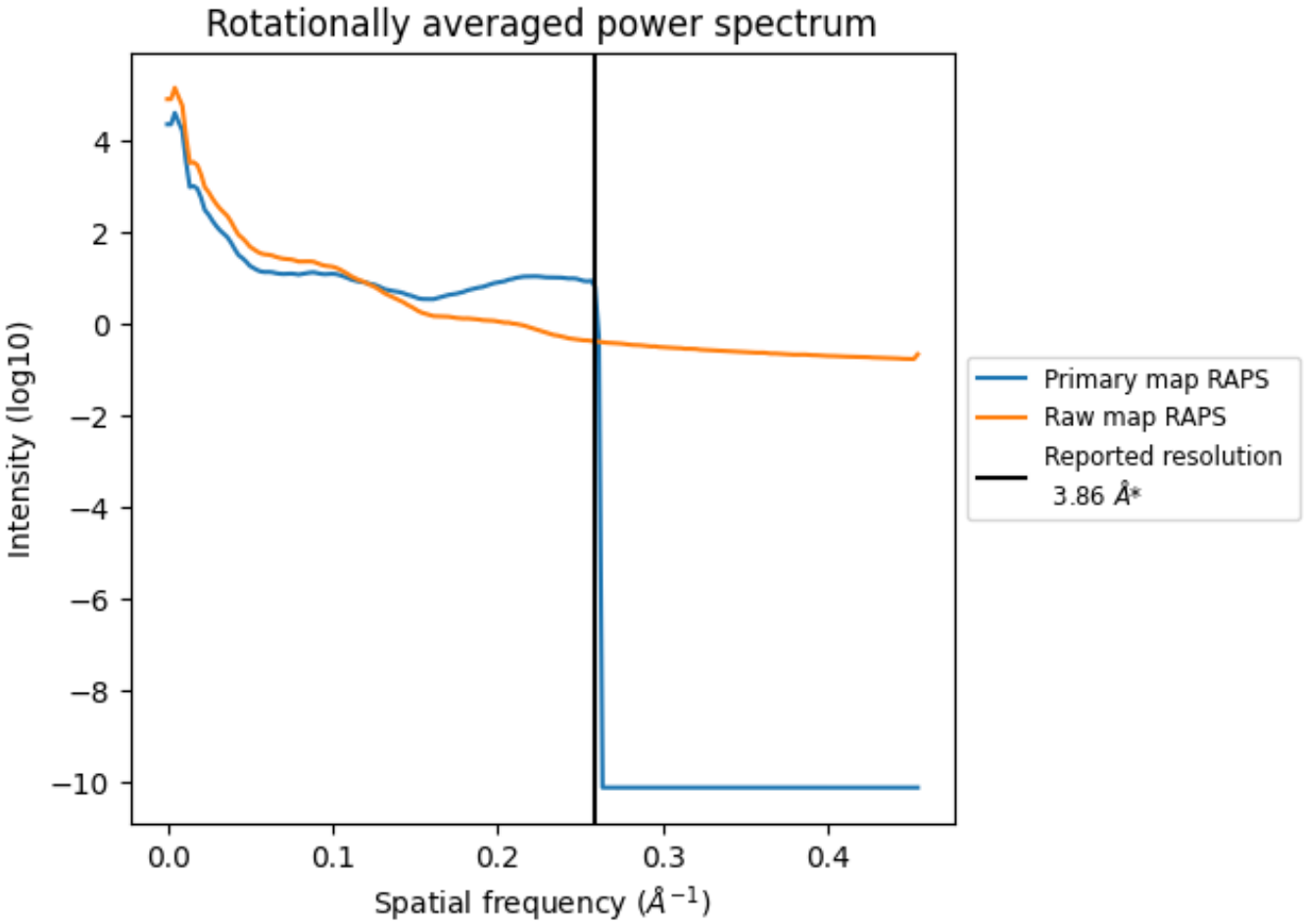
7.2 Volume estimate



The volume at the recommended contour level is 173 nm^3; this corresponds to an approximate mass of 156 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)

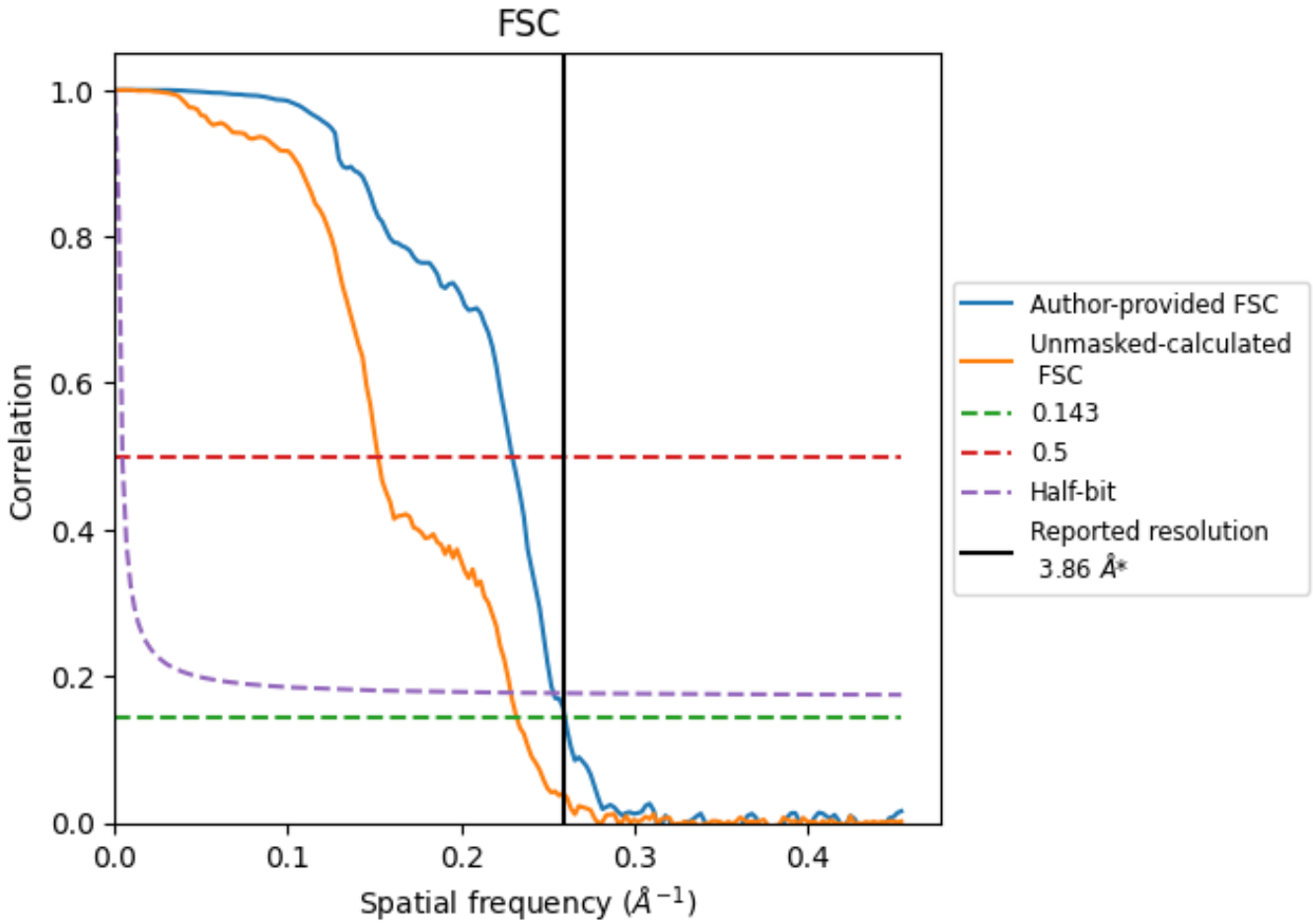


*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8.2 Resolution estimates (i)

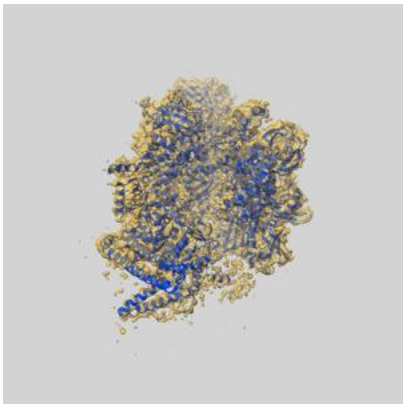
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.84	4.35	3.94
Unmasked-calculated*	4.30	6.57	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.86 by more than 10 %

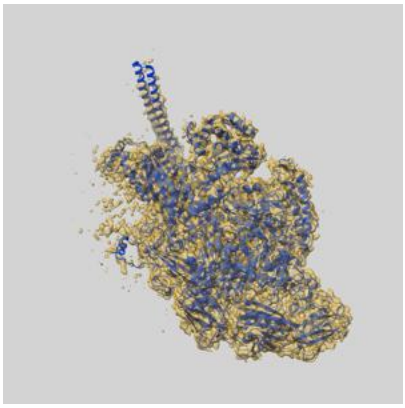
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14696 and PDB model 7ZF2. Per-residue inclusion information can be found in section 3 on page 6.

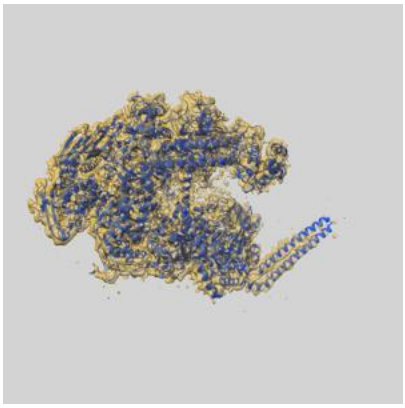
9.1 Map-model overlay



X



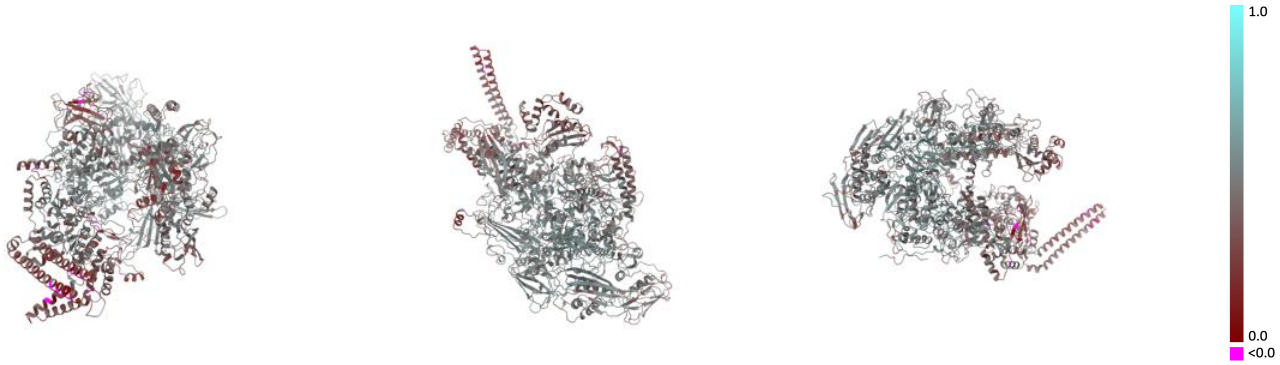
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

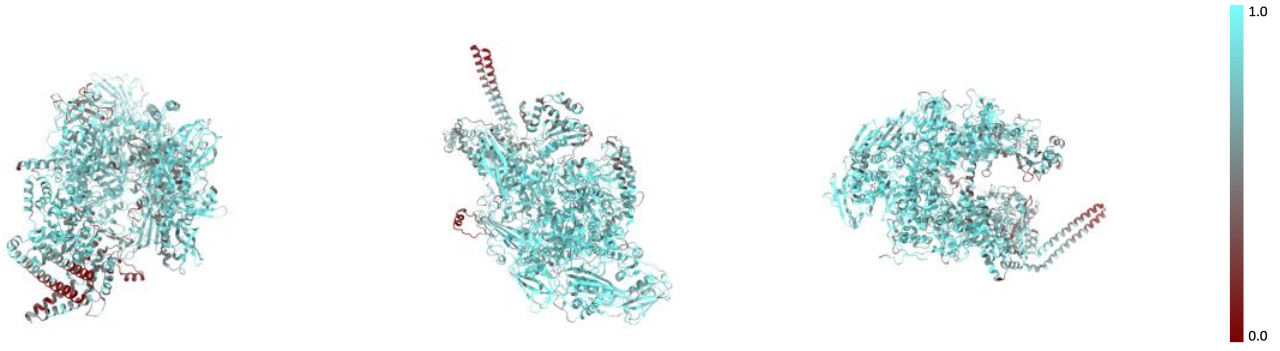
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

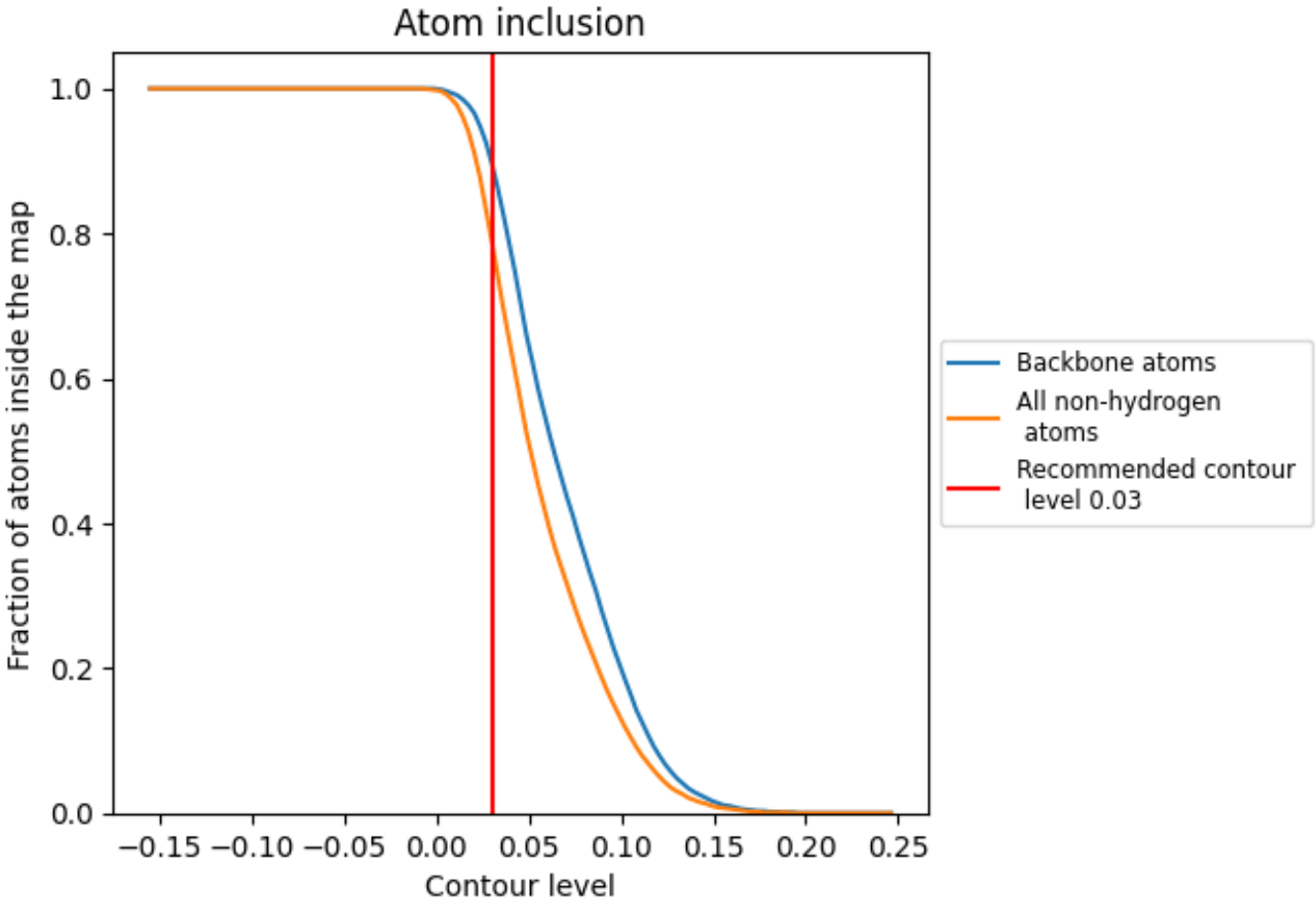
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.4590
A	0.8650	0.4880
B	0.8290	0.4730
C	0.8090	0.4730
D	0.7710	0.4520
E	0.8190	0.4750
F	0.5610	0.3300