Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:24 pm GMT

PDB ID	:	7AOH
EMDB ID	:	EMD-11844
Title	:	Atomic structure of the poxvirus late initially transcribing complex
Authors	:	Grimm, C.; Bartuli, J.; Fischer, U.
Deposited on	:	2020-10-14
Resolution	:	2.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

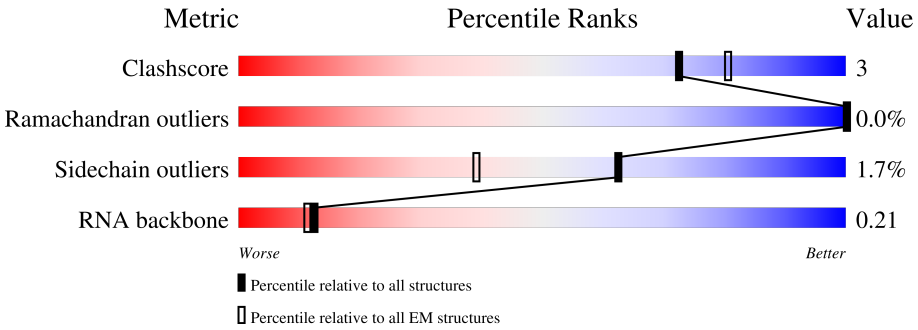
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.70 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
RNA backbone	4643	859

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	1286	91% 7% •
2	B	1164	89% 8% •
3	C	305	90% 9% •
4	E	185	93% 6% •
5	F	164	58% 5% 37%
6	G	161	88% 9% • •
7	I	795	10% 81% 13% 6%

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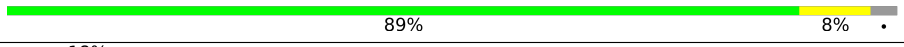
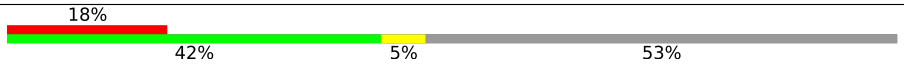
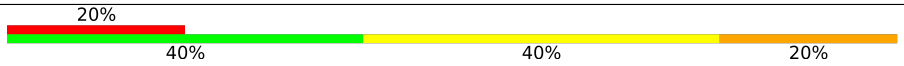
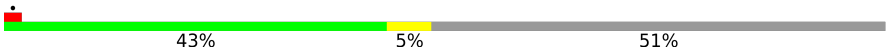
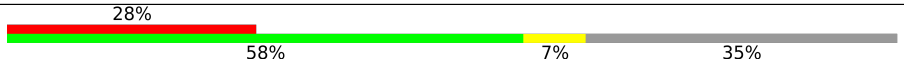
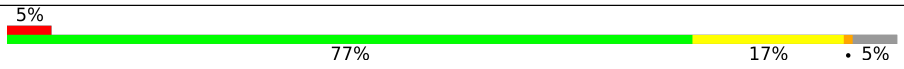
Mol	Chain	Length	Quality of chain
8	J	63	
9	N	60	
10	P	10	
11	S	259	
12	T	60	
13	Y	631	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 39496 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 147 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1263	10145	6530	1670	1900	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1134	9130	5819	1559	1704	48	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	conflict	UNP Q49PH2

- Molecule 3 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	303	2475	1603	397	462	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	184	1495	966	248	276	5	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	103	849	545	148	153	3	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	158	Total	C	N	O	S	0	0
			1233	778	204	245	6		

- Molecule 7 is a protein called Protein H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	746	Total	C	N	O	S	0	0
			6234	4075	991	1147	21		

- Molecule 8 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	61	Total	C	N	O	S	0	0
			490	310	88	88	4		

- Molecule 9 is a DNA chain called Synthetic promoter DNA oligomer, non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	28	Total	C	N	O	P	0	0
			575	274	104	169	28		

- Molecule 10 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*UP*CP*UP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	10	Total	C	N	O	P	0	0
			212	96	39	67	10		

- Molecule 11 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	126	Total	C	N	O	S	0	0
			1036	659	169	204	4		

- Molecule 12 is a DNA chain called Synthetic promoter DNA oligomer, template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	39	Total	C	N	O	P	0	0
			800	383	142	236	39		

- Molecule 13 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	597	Total	C	N	O	S	0	0
			4817	3088	822	882	25		

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

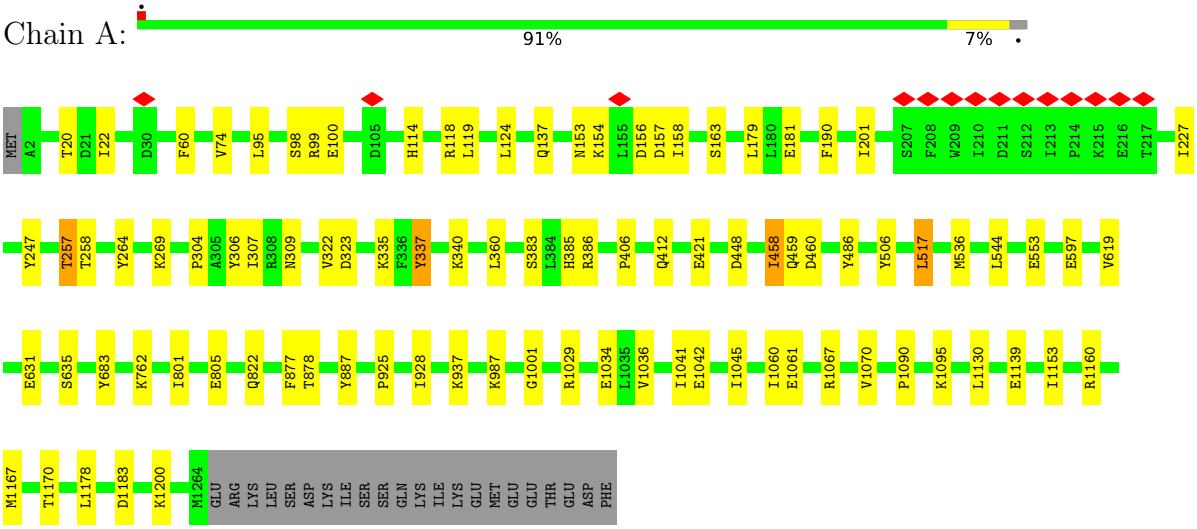
Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	J	1	Total	Zn	0
			1	1	

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.

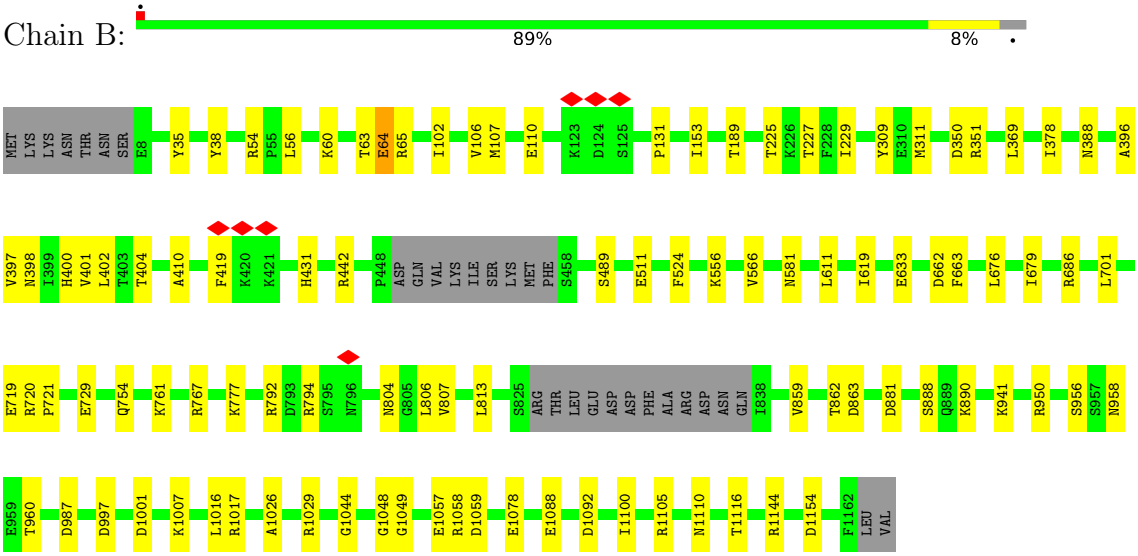
• Molecule 1: DNA-directed RNA polymerase 147 kDa polypeptide

Chain A:



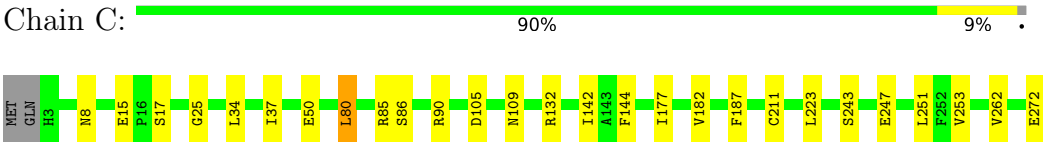
• Molecule 2: DNA-directed RNA polymerase

Chain B:



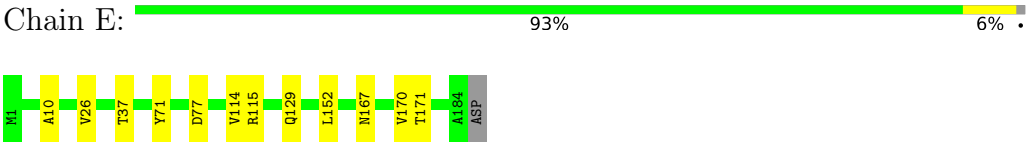
• Molecule 3: DNA-directed RNA polymerase 35 kDa subunit

Chain C:



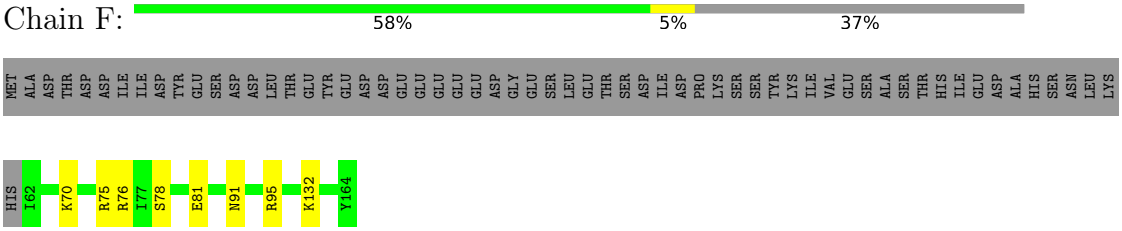
• Molecule 4: DNA-directed RNA polymerase subunit

Chain E:



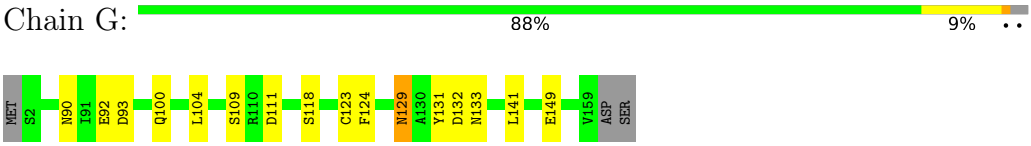
• Molecule 5: DNA-directed RNA polymerase 19 kDa subunit

Chain F:



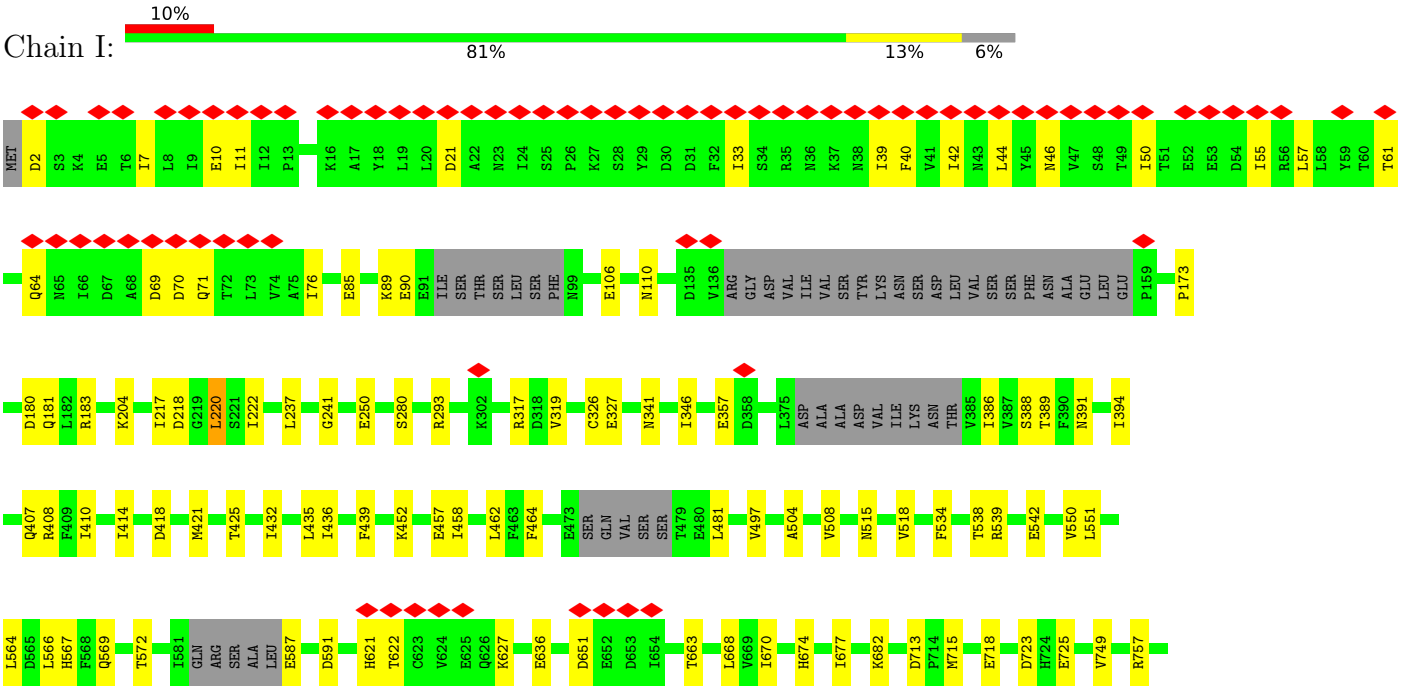
• Molecule 6: DNA-directed RNA polymerase 18 kDa subunit

Chain G:



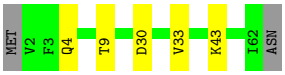
• Molecule 7: Protein H4

Chain I:



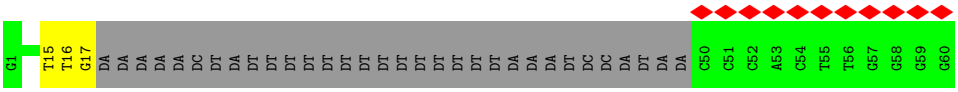
• Molecule 8: DNA-directed RNA polymerase 7 kDa subunit

Chain J:



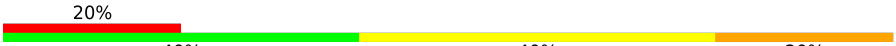
• Molecule 9: Synthetic promoter DNA oligomer, non-template strand

Chain N:



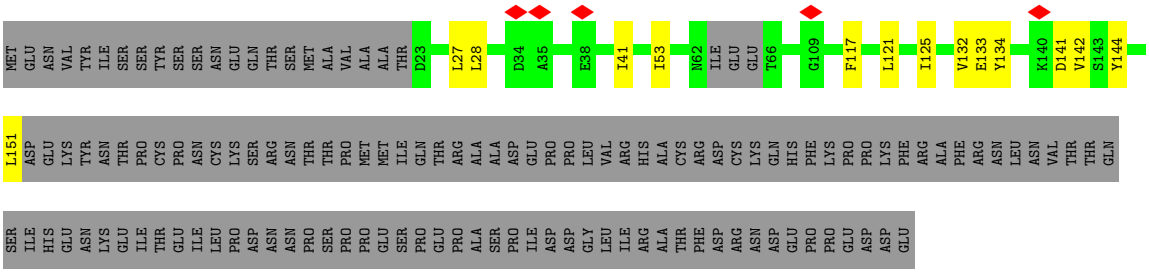
• Molecule 10: RNA (5'-R(P*AP*AP*AP*AP*UP*CP*UP*AP*UP*A)-3')

Chain P:



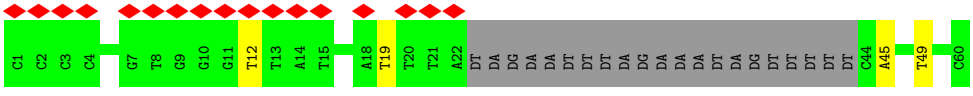
• Molecule 11: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S:



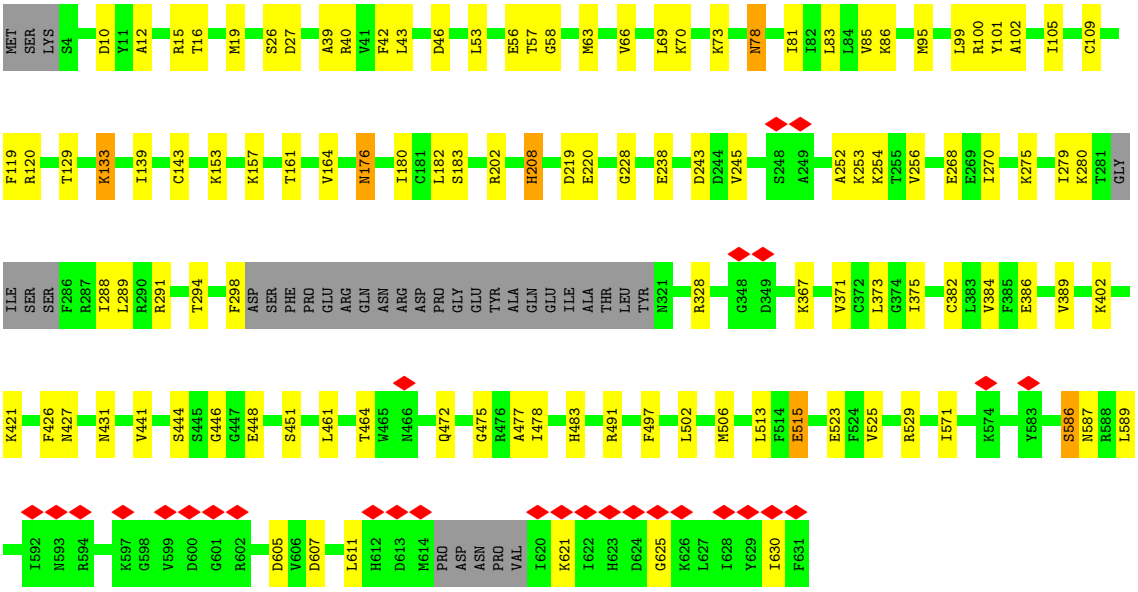
• Molecule 12: Synthetic promoter DNA oligomer, template strand

Chain T:



• Molecule 13: Nucleoside triphosphatase I

Chain Y:


MET SER LYS S4 D10 Y11 A12 R15 T16 M19 S26 D27 A39 R40 V41 F42 L43 D46 L53 E56 T57 G58 M63 V66 L69 K70 K73 N78 I81 I82 L83 L84 V85 K86 M95 L99 R100 Y101 A102 I105 C109
F119 R120 T129 K133 I139 C143 K153 K157 T161 V164 N176 I180 C181 L182 S183 R202 H208 D219 E220 G228 E238 D243 D244 V245 S248 A249 A252 K253 K254 T255 V256 E268 E269 I270 K275 I279 K280 T281 GLY
ILE SER SER F286 R287 I288 L289 R290 R291 T294 F298 ASP SER PHE PRO GLU ARG GLN ASN ARG ASP PRO GLY GLU TYR ALA GLN GLU ILE ALA THR LEU TYR N321 R328 G348 D349 K367 V371 C372 L373 G374 I375 C382 L383 V384 F385 E386 V389 K402
K421 F426 N427 N431 V441 S444 S445 G446 G447 E448 S451 L461 T464 W465 N466 Q472 G475 R476 A477 I478 H483 R491 F497 L502 M506 L513 F514 E515 E523 F524 V525 R529 I571 K574 Y583 S586 N587 R588 L589
I592 N593 R594 K597 G598 V599 D600 G601 R602 D605 V606 D607 L611 H612 D613 M614 PRO ASP ASN PRO VAL I620 K621 I622 H623 D624 G625 K626 L627 I628 Y629 I630 F631

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278260	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 ($e^-/Å^2$)	78.90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	12.209	Depositor
Minimum map value	-5.800	Depositor
Average map value	0.271	Depositor
Map value standard deviation	1.084	Depositor
Recommended contour level	1.35	Depositor
Map size (Å)	160.99997, 156.32484, 159.83167	wwPDB
Map dimensions	241, 232, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.67083323, 0.673814, 0.6632019	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/10351	0.48	0/13996
2	B	0.31	0/9321	0.50	0/12591
3	C	0.30	0/2531	0.48	0/3428
4	E	0.29	0/1522	0.50	0/2069
5	F	0.30	0/863	0.53	0/1158
6	G	0.28	0/1252	0.51	0/1698
7	I	0.30	0/6374	0.53	1/8622 (0.0%)
8	J	0.30	0/494	0.51	0/663
9	N	0.80	0/643	0.96	0/988
10	P	0.25	0/237	0.82	0/366
11	S	0.27	0/1051	0.46	0/1407
12	T	0.71	0/895	1.02	0/1377
13	Y	0.28	0/4908	0.57	1/6603 (0.0%)
All	All	0.33	0/40442	0.54	2/54966 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	651	ASP	CB-CG-OD1	6.55	124.19	118.30
13	Y	589	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	458	ILE	Peptide

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	10145	0	10265	56	0
2	B	9130	0	9180	57	0
3	C	2475	0	2462	16	0
4	E	1495	0	1548	9	0
5	F	849	0	874	5	0
6	G	1233	0	1218	10	0
7	I	6234	0	6275	66	0
8	J	490	0	528	4	0
9	N	575	0	318	3	0
10	P	212	0	107	3	0
11	S	1036	0	1037	10	0
12	T	800	0	444	4	0
13	Y	4817	0	4863	66	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	J	1	0	0	0	0
All	All	39496	0	39119	267	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 3.

All (267) 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:720:ARG:NH2	2:B:729:GLU:OE1	2.18	0.77
2:B:369:LEU:HD11	2:B:410:ALA:HB1	1.68	0.76
9:N:15:DT:OP2	13:Y:157:LYS:NZ	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LYS:O	2:B:63:THR:OG1	2.06	0.73
1:A:269:LYS:NZ	12:T:12:DT:OP1	2.21	0.73
2:B:1154:ASP:O	5:F:75:ARG:NH1	2.22	0.72
4:E:10:ALA:HB1	4:E:37:THR:HG21	1.73	0.71
13:Y:288:ILE:HG23	13:Y:289:LEU:HD22	1.73	0.71
7:I:436:ILE:HG13	7:I:497:VAL:HG21	1.73	0.70
2:B:890:LYS:NZ	10:P:10:A:OP1	2.24	0.70
2:B:941:LYS:O	2:B:950:ARG:NH1	2.25	0.68
1:A:98:SER:OG	1:A:100:GLU:OE1	2.11	0.68
13:Y:81:ILE:HD12	13:Y:105:ILE:HG21	1.75	0.68
4:E:170:VAL:HG23	4:E:171:THR:HG23	1.75	0.68
1:A:822:GLN:NE2	4:E:167:ASN:OD1	2.27	0.67
4:E:129:GLN:O	5:F:70:LYS:NZ	2.27	0.67
10:P:1:A:O2'	10:P:2:A:O5'	2.11	0.67
7:I:250:GLU:OE2	7:I:280:SER:OG	2.13	0.67
2:B:1058:ARG:NH2	2:B:1059:ASP:OD1	2.27	0.67
13:Y:386:GLU:OE1	13:Y:444:SER:OG	2.04	0.67
3:C:132:ARG:NH1	7:I:591:ASP:O	2.28	0.66
7:I:414:ILE:HD11	7:I:432:ILE:HG21	1.76	0.66
2:B:110:GLU:N	2:B:110:GLU:OE1	2.28	0.66
7:I:418:ASP:OD1	7:I:425:THR:OG1	2.15	0.65
3:C:34:LEU:HD12	3:C:182:VAL:HG12	1.78	0.65
7:I:85:GLU:OE2	7:I:204:LYS:N	2.30	0.65
2:B:1088:GLU:OE2	2:B:1116:THR:OG1	2.15	0.64
7:I:346:ILE:HG21	7:I:386:ILE:HD13	1.80	0.64
7:I:388:SER:OG	7:I:391:ASN:OD1	2.10	0.64
2:B:792:ARG:O	2:B:794:ARG:NH2	2.31	0.63
13:Y:83:LEU:HD13	13:Y:139:ILE:HB	1.81	0.63
7:I:2:ASP:O	7:I:46:ASN:ND2	2.32	0.62
7:I:407:GLN:HG3	13:Y:129:THR:HG22	1.79	0.62
13:Y:69:LEU:O	13:Y:73:LYS:NZ	2.32	0.62
1:A:386:ARG:NE	1:A:448:ASP:OD2	2.31	0.62
13:Y:56:GLU:OE1	13:Y:58:GLY:N	2.32	0.62
6:G:118:SER:HG	6:G:123:CYS:HG	1.41	0.62
7:I:50:ILE:HD12	7:I:55:ILE:HD11	1.82	0.62
7:I:408:ARG:HB3	13:Y:129:THR:HG21	1.82	0.62
7:I:621:HIS:ND1	7:I:622:THR:HG23	2.14	0.62
1:A:1061:GLU:OE2	1:A:1067:ARG:NH1	2.33	0.61
6:G:92:GLU:N	6:G:92:GLU:OE1	2.33	0.61
1:A:163:SER:OG	7:I:183:ARG:NH2	2.34	0.61
1:A:406:PRO:HB3	1:A:458:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:719:GLU:OE2	8:J:43:LYS:NZ	2.25	0.61
13:Y:143:CYS:SG	13:Y:183:SER:OG	2.50	0.60
11:S:28:LEU:CD2	11:S:125:ILE:HD11	2.32	0.60
2:B:1092:ASP:OD2	2:B:1105:ARG:NH2	2.35	0.60
7:I:106:GLU:N	7:I:106:GLU:OE1	2.35	0.60
3:C:105:ASP:O	3:C:109:ASN:N	2.35	0.59
2:B:35:TYR:OH	2:B:153:ILE:O	2.15	0.59
7:I:636:GLU:N	7:I:636:GLU:OE1	2.35	0.59
7:I:457:GLU:HB2	7:I:551:LEU:HD21	1.85	0.59
2:B:767:ARG:O	8:J:4:GLN:NE2	2.36	0.59
4:E:26:VAL:HG22	4:E:114:VAL:CG1	2.33	0.59
13:Y:427:ASN:ND2	13:Y:451:SER:O	2.36	0.59
1:A:304:PRO:HD2	1:A:307:ILE:HD12	1.83	0.59
1:A:323:ASP:OD1	7:I:317:ARG:NH1	2.36	0.59
13:Y:270:ILE:HD13	13:Y:298:PHE:H	1.67	0.58
13:Y:70:LYS:NZ	13:Y:101:TYR:O	2.36	0.58
13:Y:586:SER:O	13:Y:630:ILE:HD12	2.03	0.58
7:I:458:ILE:HD11	7:I:464:PHE:CE2	2.38	0.58
13:Y:16:THR:O	13:Y:40:ARG:NE	2.37	0.58
1:A:340:LYS:NZ	2:B:1078:GLU:OE2	2.37	0.58
5:F:91:ASN:OD1	5:F:95:ARG:NH1	2.37	0.58
7:I:76:ILE:HD11	13:Y:625:GLY:O	2.04	0.58
2:B:309:TYR:OH	7:I:725:GLU:OE2	2.17	0.57
7:I:715:MET:O	7:I:757:ARG:NH2	2.37	0.57
1:A:1160:ARG:NH1	1:A:1183:ASP:OD1	2.37	0.57
2:B:987:ASP:OD2	2:B:1007:LYS:NZ	2.37	0.57
1:A:762:LYS:NZ	1:A:1200:LYS:O	2.37	0.57
2:B:107:MET:SD	7:I:674:HIS:ND1	2.77	0.57
3:C:251:LEU:HD21	3:C:262:VAL:HG11	1.86	0.57
1:A:99:ARG:NH2	7:I:218:ASP:O	2.37	0.57
3:C:243:SER:O	3:C:251:LEU:HD12	2.05	0.57
7:I:410:ILE:HD12	7:I:436:ILE:HD13	1.86	0.57
13:Y:243:ASP:O	13:Y:254:LYS:NZ	2.33	0.57
1:A:60:PHE:HA	1:A:201:ILE:HD12	1.87	0.56
1:A:1060:ILE:HG21	11:S:132:VAL:HG11	1.86	0.56
2:B:38:TYR:OH	2:B:131:PRO:O	2.21	0.56
2:B:761:LYS:NZ	8:J:9:THR:O	2.34	0.56
13:Y:100:ARG:NH2	13:Y:101:TYR:OH	2.39	0.56
13:Y:119:PHE:CE2	13:Y:164:VAL:HG11	2.40	0.56
1:A:309:ASN:O	1:A:335:LYS:NZ	2.39	0.56
7:I:414:ILE:HD11	7:I:432:ILE:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:HD11	3:C:142:ILE:HD11	1.89	0.55
1:A:412:GLN:NE2	1:A:421:GLU:OE2	2.38	0.55
6:G:109:SER:OG	6:G:111:ASP:OD1	2.22	0.55
13:Y:56:GLU:OE1	13:Y:57:THR:N	2.39	0.55
1:A:486:TYR:O	1:A:506:TYR:OH	2.13	0.55
1:A:460:ASP:OD1	2:B:754:GLN:NE2	2.40	0.55
4:E:26:VAL:HG22	4:E:114:VAL:HG11	1.89	0.55
13:Y:477:ALA:O	13:Y:483:HIS:NE2	2.39	0.55
2:B:388:ASN:ND2	2:B:396:ALA:O	2.40	0.54
7:I:668:LEU:HD13	7:I:677:ILE:HD13	1.89	0.54
10:P:1:A:HO2'	10:P:2:A:C5'	2.20	0.54
13:Y:291:ARG:O	13:Y:294:THR:OG1	2.25	0.54
11:S:141:ASP:OD1	11:S:142:VAL:N	2.41	0.54
3:C:8:ASN:HB3	3:C:305:LEU:HD11	1.89	0.54
1:A:1034:GLU:OE2	1:A:1034:GLU:N	2.40	0.54
7:I:64:GLN:OE1	13:Y:621:LYS:N	2.41	0.54
1:A:114:HIS:O	1:A:118:ARG:N	2.41	0.54
3:C:25:GLY:HA3	3:C:223:LEU:HD21	1.89	0.54
6:G:118:SER:OG	6:G:123:CYS:SG	2.59	0.54
1:A:619:VAL:O	11:S:144:TYR:OH	2.23	0.53
7:I:436:ILE:CG1	7:I:497:VAL:HG21	2.37	0.53
2:B:369:LEU:HD13	2:B:419:PHE:CE1	2.44	0.53
11:S:28:LEU:HD22	11:S:125:ILE:HD11	1.89	0.53
1:A:805:GLU:N	1:A:805:GLU:OE1	2.41	0.53
13:Y:220:GLU:OE2	13:Y:529:ARG:NH1	2.42	0.53
7:I:7:ILE:HD12	7:I:42:ILE:HD12	1.90	0.53
7:I:508:VAL:HG12	7:I:518:VAL:HG21	1.91	0.53
1:A:181:GLU:OE1	1:A:181:GLU:N	2.42	0.53
1:A:257:THR:O	1:A:258:THR:OG1	2.24	0.52
2:B:442:ARG:NH2	2:B:489:SER:O	2.41	0.52
7:I:497:VAL:HG12	7:I:564:LEU:HD21	1.91	0.52
13:Y:586:SER:OG	13:Y:587:ASN:N	2.41	0.52
7:I:723:ASP:OD1	7:I:723:ASP:N	2.43	0.52
13:Y:78:ASN:OD1	13:Y:133:LYS:NZ	2.43	0.52
4:E:26:VAL:HA	4:E:114:VAL:HG12	1.92	0.52
7:I:346:ILE:CG2	7:I:386:ILE:HD13	2.39	0.52
1:A:801:ILE:O	1:A:887:TYR:OH	2.10	0.52
7:I:504:ALA:O	7:I:508:VAL:HG13	2.10	0.52
9:N:17:DG:H1	13:Y:153:LYS:CE	2.23	0.52
13:Y:105:ILE:O	13:Y:109:CYS:N	2.40	0.51
1:A:156:ASP:OD1	1:A:157:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:GLU:OE1	3:C:247:GLU:N	2.43	0.51
13:Y:69:LEU:HD13	13:Y:81:ILE:HG21	1.92	0.51
1:A:337:TYR:HD1	1:A:360:LEU:HD21	1.74	0.51
2:B:881:ASP:OD2	2:B:1017:ARG:NH2	2.44	0.50
13:Y:268:GLU:HG3	13:Y:502:LEU:HD22	1.94	0.50
7:I:33:ILE:HD12	7:I:40:PHE:HE2	1.76	0.50
13:Y:448:GLU:O	13:Y:472:GLN:NE2	2.45	0.50
13:Y:605:ASP:HB3	13:Y:611:LEU:HD21	1.94	0.50
7:I:11:ILE:HG12	7:I:39:ILE:HD12	1.93	0.50
2:B:581:ASN:ND2	2:B:633:GLU:OE1	2.45	0.49
11:S:28:LEU:CD1	11:S:41:ILE:HD11	2.42	0.49
3:C:37:ILE:HG23	3:C:177:ILE:HD13	1.94	0.49
1:A:337:TYR:CD1	1:A:360:LEU:HD21	2.47	0.49
2:B:400:HIS:O	2:B:404:THR:HG22	2.13	0.49
2:B:777:LYS:NZ	12:T:19:DT:OP1	2.35	0.49
2:B:229:ILE:HG23	2:B:311:MET:SD	2.53	0.49
2:B:1110:ASN:ND2	7:I:110:ASN:OD1	2.41	0.49
7:I:33:ILE:HD12	7:I:40:PHE:CE2	2.48	0.49
13:Y:275:LYS:O	13:Y:279:ILE:HG23	2.13	0.48
2:B:431:HIS:HB3	2:B:701:LEU:HD21	1.95	0.48
13:Y:253:LYS:NZ	13:Y:491:ARG:O	2.44	0.48
7:I:569:GLN:O	7:I:572:THR:OG1	2.28	0.48
13:Y:53:LEU:HD12	13:Y:182:LEU:HD11	1.94	0.48
7:I:515:ASN:O	7:I:515:ASN:ND2	2.46	0.48
1:A:227:ILE:HD11	1:A:247:TYR:CB	2.44	0.48
2:B:102:ILE:HG13	2:B:397:VAL:HG11	1.95	0.48
13:Y:102:ALA:HB1	13:Y:105:ILE:HD13	1.94	0.48
13:Y:426:PHE:O	13:Y:431:ASN:ND2	2.46	0.48
1:A:306:TYR:OH	2:B:1026:ALA:HB1	2.14	0.47
1:A:322:VAL:HG23	7:I:319:VAL:HG23	1.96	0.47
2:B:679:ILE:N	2:B:956:SER:O	2.47	0.47
13:Y:46:ASP:OD1	13:Y:176:ASN:ND2	2.47	0.47
6:G:104:LEU:HD21	6:G:141:LEU:HD21	1.96	0.47
5:F:76:ARG:O	5:F:132:LYS:NZ	2.48	0.47
7:I:217:ILE:O	7:I:220:LEU:HD23	2.14	0.47
11:S:117:PHE:CE2	11:S:121:LEU:HD11	2.49	0.47
7:I:341:ASN:O	7:I:341:ASN:ND2	2.48	0.47
13:Y:12:ALA:O	13:Y:16:THR:OG1	2.18	0.47
7:I:237:LEU:O	7:I:241:GLY:N	2.48	0.46
13:Y:571:ILE:HG23	13:Y:571:ILE:O	2.16	0.46
1:A:257:THR:HG22	1:A:258:THR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:ILE:HG23	7:I:42:ILE:HD12	1.97	0.46
7:I:21:ASP:OD1	7:I:21:ASP:N	2.48	0.46
1:A:20:THR:HG22	1:A:22:ILE:H	1.80	0.46
1:A:153:ASN:OD1	1:A:154:LYS:N	2.49	0.46
13:Y:119:PHE:CD2	13:Y:161:THR:HG22	2.51	0.46
12:T:49:DT:OP1	13:Y:446:GLY:N	2.48	0.46
7:I:57:LEU:O	7:I:61:THR:HG23	2.16	0.46
9:N:16:DT:O3'	13:Y:464:THR:HG21	2.16	0.46
1:A:383:SER:OG	2:B:1057:GLU:OE2	2.21	0.46
7:I:89:LYS:NZ	13:Y:607:ASP:OD2	2.29	0.46
13:Y:53:LEU:HD12	13:Y:182:LEU:CD1	2.45	0.46
1:A:517:LEU:HD13	1:A:544:LEU:HD11	1.98	0.45
2:B:720:ARG:NH1	2:B:721:PRO:O	2.49	0.45
12:T:45:DA:N3	13:Y:288:ILE:HG21	2.31	0.45
13:Y:42:PHE:CZ	13:Y:180:ILE:HD11	2.50	0.45
2:B:401:VAL:HG23	2:B:402:LEU:HD12	1.98	0.45
2:B:862:THR:HG22	2:B:863:ASP:H	1.80	0.45
2:B:350:ASP:OD1	2:B:351:ARG:N	2.49	0.45
1:A:987:LYS:NZ	1:A:1139:GLU:O	2.43	0.45
7:I:326:CYS:SG	7:I:327:GLU:N	2.90	0.45
13:Y:252:ALA:N	13:Y:478:ILE:O	2.42	0.45
13:Y:475:GLY:HA2	13:Y:478:ILE:HG22	1.97	0.45
13:Y:515:GLU:OE1	13:Y:515:GLU:N	2.49	0.45
1:A:137:GLN:N	1:A:137:GLN:OE1	2.50	0.45
1:A:631:GLU:OE1	1:A:635:SER:OG	2.34	0.45
7:I:670:ILE:HG21	7:I:718:GLU:OE2	2.17	0.45
1:A:1167:MET:O	1:A:1170:THR:OG1	2.35	0.44
7:I:391:ASN:O	7:I:394:ILE:HG22	2.16	0.44
2:B:1100:ILE:HD11	6:G:149:GLU:HG3	1.98	0.44
7:I:542:GLU:OE1	7:I:542:GLU:N	2.40	0.44
1:A:158:ILE:HD11	7:I:173:PRO:HA	1.98	0.44
2:B:54:ARG:HD2	2:B:378:ILE:HD13	1.98	0.44
11:S:133:GLU:OE1	11:S:134:TYR:N	2.51	0.44
1:A:1130:LEU:HD12	1:A:1153:ILE:HD11	1.99	0.44
2:B:524:PHE:CE2	7:I:749:VAL:HG21	2.53	0.44
2:B:662:ASP:OD1	2:B:663:PHE:N	2.49	0.44
3:C:253:VAL:O	3:C:272:GLU:N	2.51	0.44
7:I:180:ASP:OD1	7:I:181:GLN:N	2.51	0.44
4:E:115:ARG:NH1	4:E:152:LEU:O	2.49	0.44
13:Y:371:VAL:CG2	13:Y:461:LEU:HD11	2.48	0.44
1:A:1036:VAL:HG13	11:S:53:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:132:ASP:OD1	6:G:133:ASN:N	2.51	0.43
7:I:435:LEU:HD12	7:I:564:LEU:CD1	2.48	0.43
13:Y:502:LEU:HD12	13:Y:506:MET:CG	2.48	0.43
13:Y:384:VAL:HB	13:Y:441:VAL:HG12	2.00	0.43
7:I:69:ASP:OD1	7:I:70:ASP:N	2.52	0.43
13:Y:367:LYS:CG	13:Y:461:LEU:HD12	2.49	0.43
1:A:124:LEU:HD23	1:A:124:LEU:O	2.19	0.43
1:A:1041:ILE:HG22	1:A:1045:ILE:HD12	2.01	0.43
2:B:611:LEU:CD1	2:B:619:ILE:HD11	2.48	0.43
2:B:806:LEU:CD1	2:B:859:VAL:HG21	2.48	0.43
6:G:124:PHE:O	6:G:131:TYR:N	2.51	0.43
13:Y:27:ASP:N	13:Y:100:ARG:O	2.51	0.43
1:A:1029:ARG:NH2	11:S:144:TYR:OH	2.47	0.43
2:B:958:ASN:ND2	2:B:960:THR:O	2.48	0.43
2:B:1088:GLU:OE2	2:B:1144:ARG:NH2	2.51	0.43
7:I:534:PHE:O	7:I:538:THR:HG22	2.18	0.43
13:Y:85:VAL:HG12	13:Y:86:LYS:H	1.83	0.43
3:C:50:GLU:OE1	3:C:50:GLU:N	2.49	0.43
3:C:80:LEU:HD12	3:C:144:PHE:CE2	2.53	0.43
7:I:407:GLN:CG	13:Y:129:THR:HG22	2.49	0.43
1:A:937:LYS:HG2	1:A:1178:LEU:HD11	2.00	0.42
2:B:686:ARG:NH2	2:B:888:SER:O	2.49	0.42
8:J:30:ASP:O	8:J:33:VAL:HG12	2.19	0.42
13:Y:63:MET:HA	13:Y:66:VAL:HG22	2.02	0.42
1:A:553:GLU:OE1	1:A:553:GLU:N	2.53	0.42
3:C:251:LEU:CD2	3:C:262:VAL:HG11	2.49	0.42
2:B:997:ASP:O	2:B:1001:ASP:N	2.48	0.42
6:G:129:ASN:N	6:G:129:ASN:OD1	2.52	0.42
13:Y:256:VAL:HG13	13:Y:497:PHE:HE2	1.85	0.42
13:Y:375:ILE:HG23	13:Y:382:CYS:SG	2.59	0.42
13:Y:502:LEU:HD12	13:Y:506:MET:HG2	2.01	0.42
13:Y:39:ALA:O	13:Y:43:LEU:HD23	2.19	0.42
1:A:306:TYR:CZ	2:B:1026:ALA:HB1	2.55	0.42
2:B:398:ASN:OD1	2:B:400:HIS:ND1	2.53	0.41
2:B:807:VAL:HG21	2:B:813:LEU:HD21	2.02	0.41
4:E:71:TYR:OH	4:E:77:ASP:OD2	2.32	0.41
6:G:93:ASP:N	6:G:93:ASP:OD1	2.53	0.41
7:I:718:GLU:OE1	7:I:718:GLU:N	2.48	0.41
13:Y:208:HIS:ND1	13:Y:208:HIS:O	2.53	0.41
1:A:877:PHE:O	1:A:878:THR:OG1	2.32	0.41
1:A:1001:GLY:N	1:A:1090:PRO:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:LYS:NZ	2:B:566:VAL:O	2.38	0.41
7:I:61:THR:HG22	13:Y:621:LYS:HG2	2.01	0.41
1:A:95:LEU:HD22	7:I:222:ILE:HD13	2.02	0.41
2:B:1044:GLY:O	2:B:1049:GLY:N	2.47	0.41
2:B:64:GLU:HB2	2:B:106:VAL:HG22	2.02	0.41
5:F:78:SER:N	5:F:81:GLU:OE1	2.47	0.41
3:C:15:GLU:OE1	3:C:17:SER:N	2.51	0.41
7:I:386:ILE:HD12	7:I:386:ILE:N	2.35	0.41
13:Y:202:ARG:NH2	13:Y:228:GLY:O	2.47	0.41
1:A:925:PRO:HB2	1:A:928:ILE:HG22	2.03	0.41
7:I:435:LEU:HD12	7:I:564:LEU:HD12	2.02	0.41
13:Y:95:MET:O	13:Y:99:LEU:HD23	2.21	0.41
7:I:713:ASP:N	7:I:713:ASP:OD1	2.54	0.41
1:A:74:VAL:HG12	1:A:190:PHE:CE2	2.55	0.40
1:A:1045:ILE:HD13	1:A:1070:VAL:HG11	2.02	0.40
3:C:85:ARG:NH1	3:C:86:SER:O	2.54	0.40
2:B:227:THR:O	2:B:227:THR:OG1	2.38	0.40
2:B:1029:ARG:NH1	2:B:1048:GLY:O	2.54	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	1261/1286 (98%)	1231 (98%)	30 (2%)	0	100	100
2	B	1128/1164 (97%)	1099 (97%)	29 (3%)	0	100	100
3	C	301/305 (99%)	291 (97%)	10 (3%)	0	100	100
4	E	182/185 (98%)	179 (98%)	3 (2%)	0	100	100
5	F	101/164 (62%)	100 (99%)	1 (1%)	0	100	100
6	G	156/161 (97%)	146 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	734/795 (92%)	708 (96%)	26 (4%)	0	100	100
8	J	59/63 (94%)	59 (100%)	0	0	100	100
11	S	122/259 (47%)	119 (98%)	3 (2%)	0	100	100
13	Y	589/631 (93%)	558 (95%)	30 (5%)	1 (0%)	47	73
All	All	4633/5013 (92%)	4490 (97%)	142 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	Y	389	VAL

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	1134/1157 (98%)	1121 (99%)	13 (1%)	73	90
2	B	1035/1064 (97%)	1026 (99%)	9 (1%)	78	92
3	C	285/287 (99%)	281 (99%)	4 (1%)	67	86
4	E	174/175 (99%)	174 (100%)	0	100	100
5	F	94/151 (62%)	94 (100%)	0	100	100
6	G	141/144 (98%)	138 (98%)	3 (2%)	53	80
7	I	709/755 (94%)	688 (97%)	21 (3%)	41	70
8	J	60/62 (97%)	60 (100%)	0	100	100
11	S	117/240 (49%)	115 (98%)	2 (2%)	60	84
13	Y	538/573 (94%)	516 (96%)	22 (4%)	30	59
All	All	4287/4608 (93%)	4213 (98%)	74 (2%)	62	84

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	257	THR
1	A	264	TYR
1	A	337	TYR
1	A	385	HIS
1	A	459	GLN
1	A	517	LEU
1	A	536	MET
1	A	597	GLU
1	A	683	TYR
1	A	1042	GLU
1	A	1095	LYS
2	B	56	LEU
2	B	64	GLU
2	B	65	ARG
2	B	189	THR
2	B	225	THR
2	B	511	GLU
2	B	676	LEU
2	B	804	ASN
2	B	1016	LEU
3	C	80	LEU
3	C	90	ARG
3	C	187	PHE
3	C	211	CYS
6	G	90	ASN
6	G	100	GLN
6	G	129	ASN
7	I	10	GLU
7	I	44	LEU
7	I	71	GLN
7	I	90	GLU
7	I	220	LEU
7	I	293	ARG
7	I	357	GLU
7	I	389	THR
7	I	421	MET
7	I	439	PHE
7	I	452	LYS
7	I	462	LEU
7	I	481	LEU
7	I	539	ARG

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Mol	Chain	Res	Type
7	I	550	VAL
7	I	566	LEU
7	I	567	HIS
7	I	587	GLU
7	I	627	LYS
7	I	663	THR
7	I	682	LYS
11	S	27	LEU
11	S	151	LEU
13	Y	10	ASP
13	Y	15	ARG
13	Y	19	MET
13	Y	26	SER
13	Y	78	ASN
13	Y	120	ARG
13	Y	133	LYS
13	Y	176	ASN
13	Y	208	HIS
13	Y	219	ASP
13	Y	238	GLU
13	Y	245	VAL
13	Y	280	LYS
13	Y	328	ARG
13	Y	373	LEU
13	Y	402	LYS
13	Y	421	LYS
13	Y	513	LEU
13	Y	515	GLU
13	Y	523	GLU
13	Y	525	VAL
13	Y	586	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	10/10 (100%)	4 (40%)	2 (20%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	P	2	A
10	P	4	A
10	P	5	U
10	P	7	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	P	1	A
10	P	4	A

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 5 ligands modelled in this entry, 5 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.

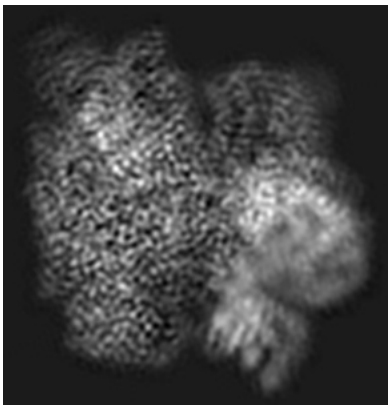
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11844. These allow visual inspection of the internal detail of the map and identification of artifacts.

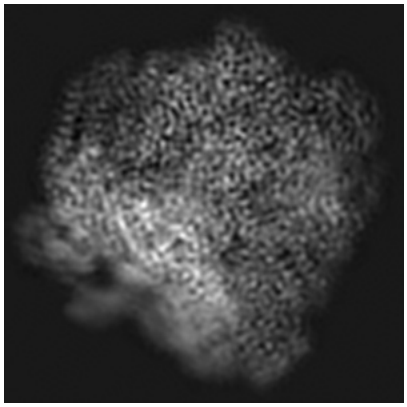
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

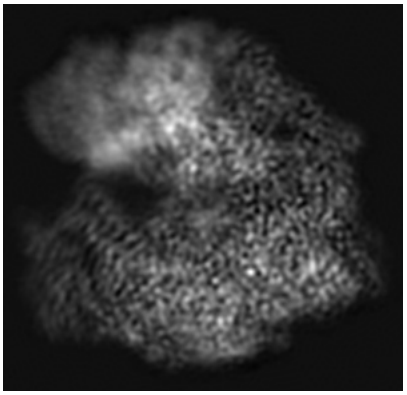
6.1.1 Primary map



X



Y

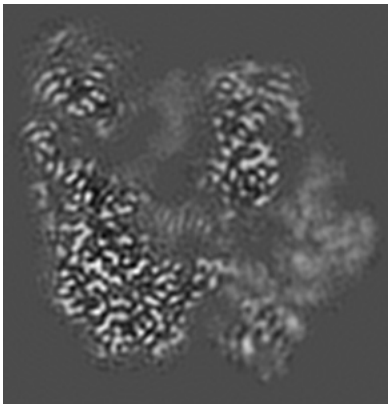


Z

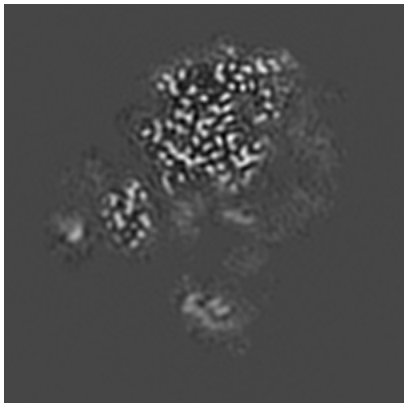
The images above show the map projected in three orthogonal directions.

6.2 Central slices

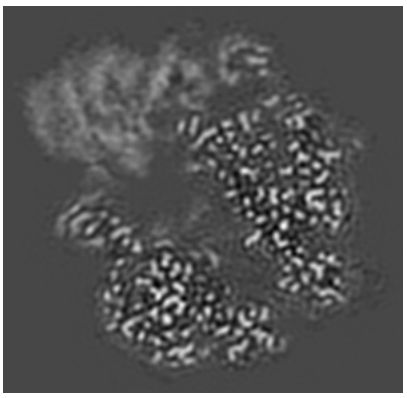
6.2.1 Primary map



X Index: 120



Y Index: 116

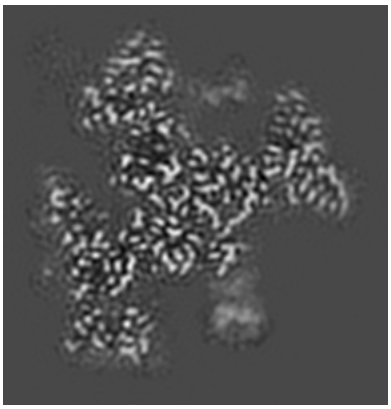


Z Index: 120

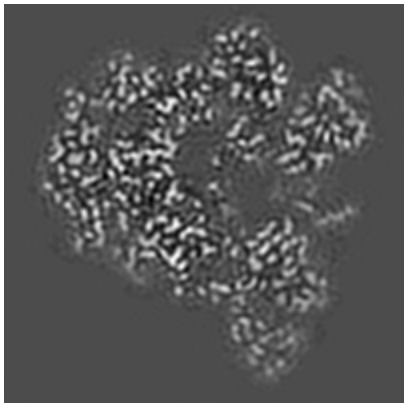
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

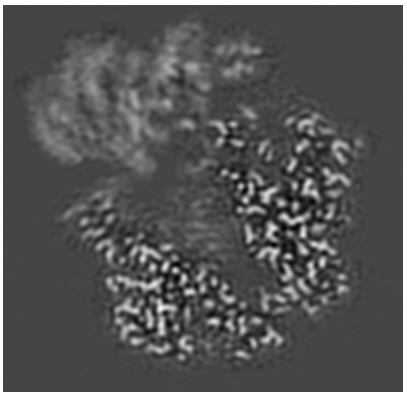
6.3.1 Primary map



X Index: 154



Y Index: 71

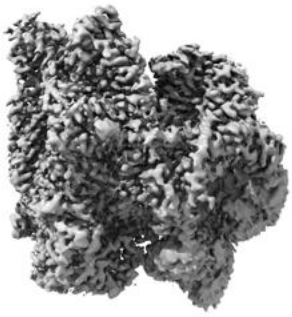


Z Index: 115

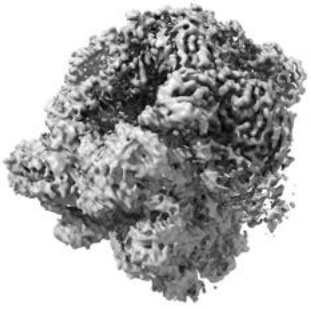
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

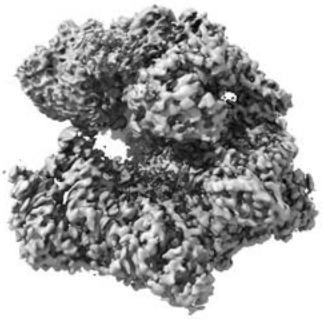
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

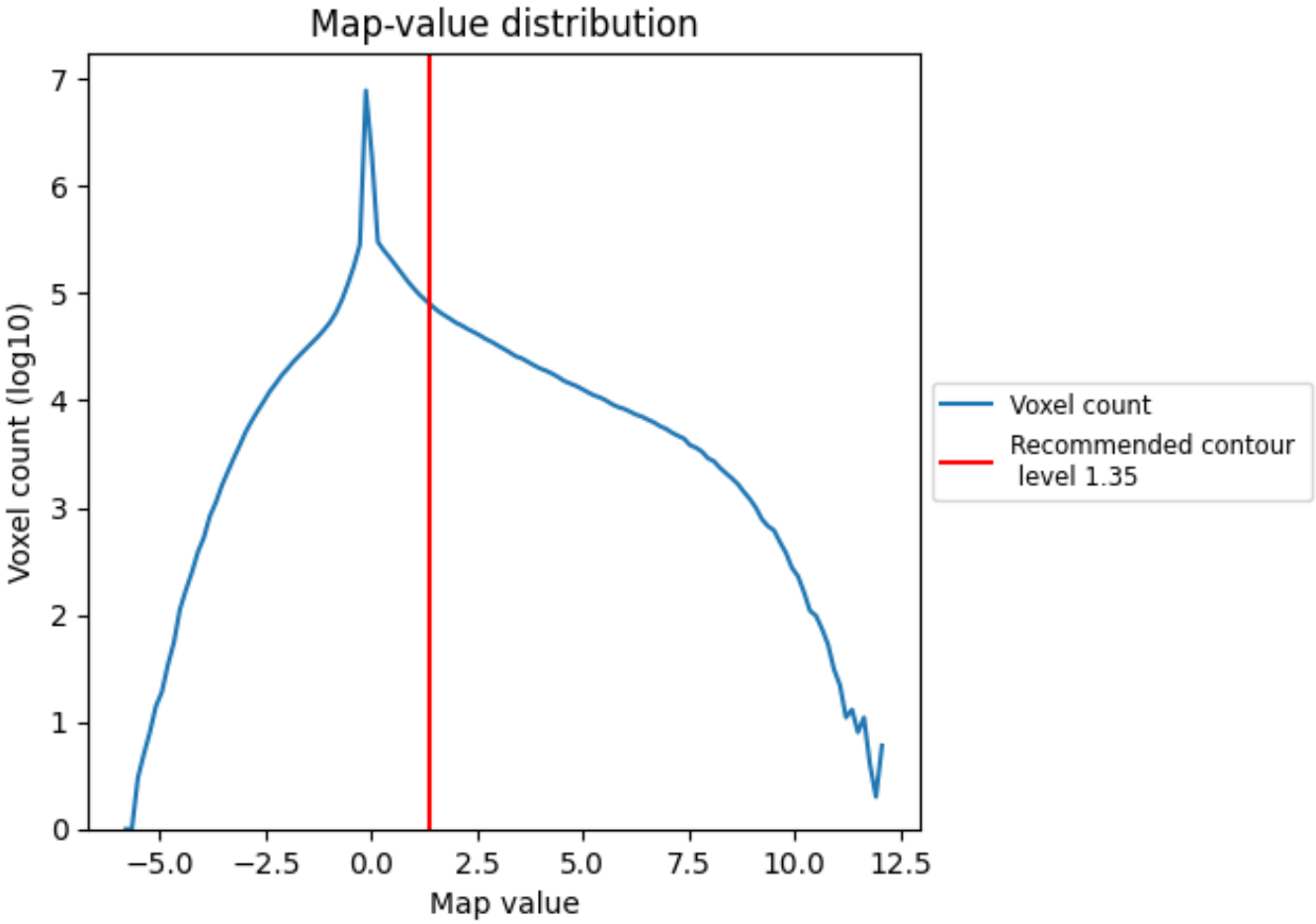
6.5 Mask visualisation (i)

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

7 Map analysis

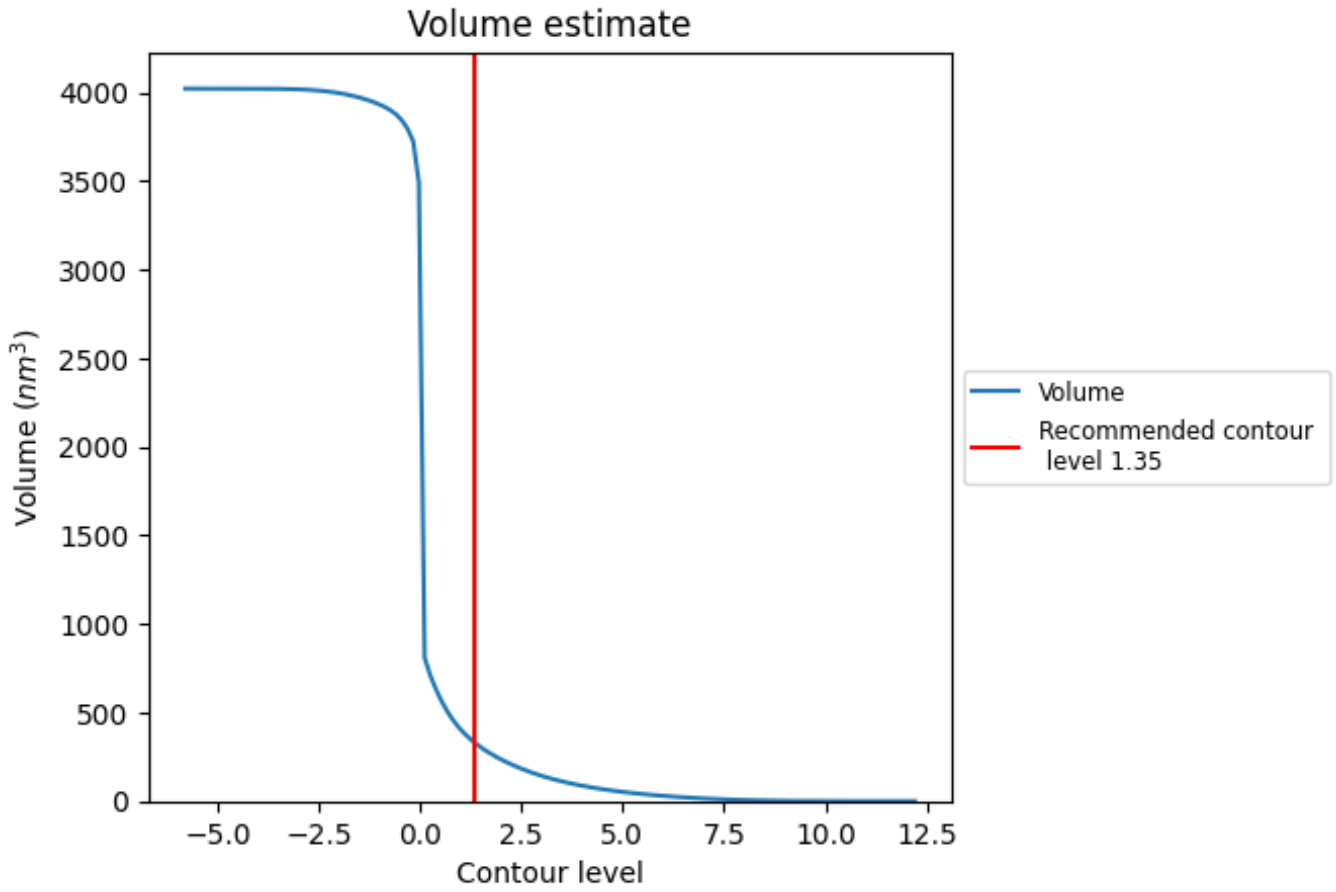
This section contains the results of statistical analysis of the map.

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 329 nm^3; this corresponds to an approximate mass of 298 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

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

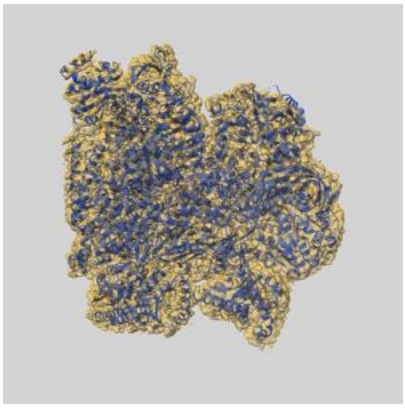
8 Fourier-Shell correlation

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

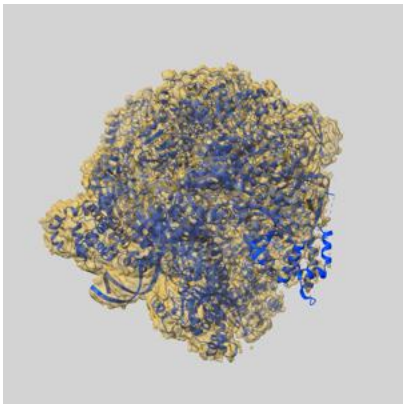
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11844 and PDB model 7AOH. Per-residue inclusion information can be found in section 3 on page 7.

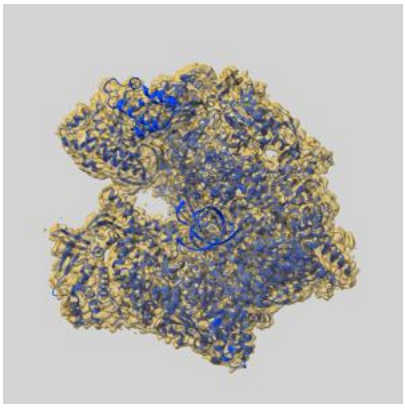
9.1 Map-model overlay



X



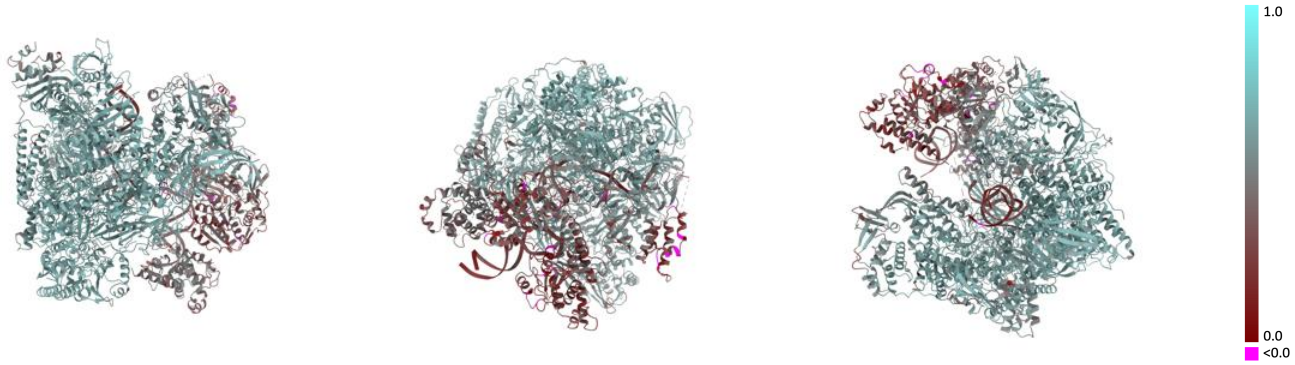
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.35 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.

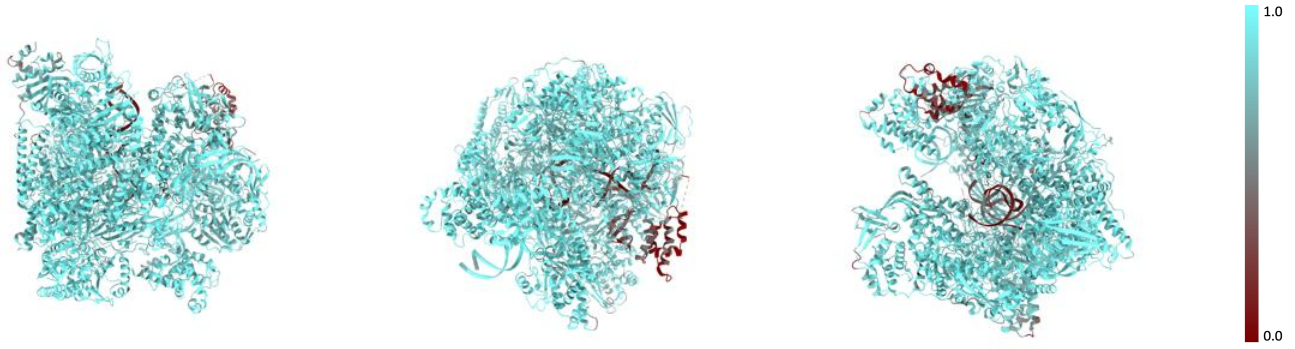
9.2 Q-score mapped to coordinate model (i)



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.

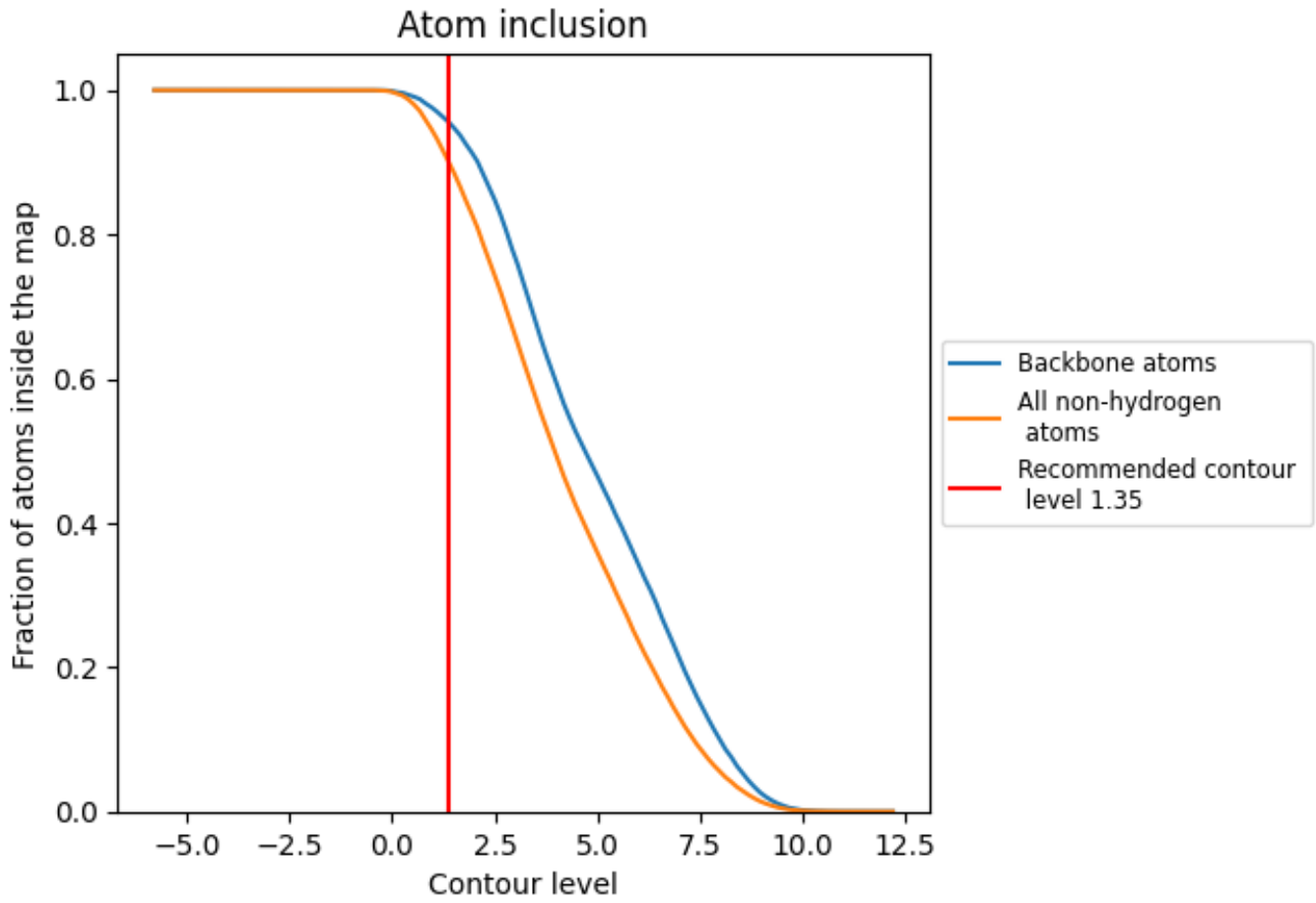
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.35).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (1.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9038	0.5430
A	0.9433	0.6190
B	0.9496	0.6220
C	0.9648	0.6320
E	0.9686	0.6280
F	0.9807	0.6450
G	0.9340	0.5880
I	0.8225	0.4810
J	0.9813	0.6490
N	0.6087	0.2200
P	0.5613	0.3700
S	0.7915	0.5510
T	0.5787	0.2700
Y	0.8885	0.2940