Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 01:13 pm GMT

PDB ID	:	9FNE
EMDB ID	:	EMD-50591
Title	:	Mycobacterial PafBC-bound transcription initiation complex
Authors	:	Zdanowicz, R.; Schilling, C.M.; Rabl, J.; Mueller, A.U.; Boehringer, D.; Glockshuber, R.; Weber-Ban, E.
Deposited on	:	2024-06-10
Resolution	:	4.00 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:

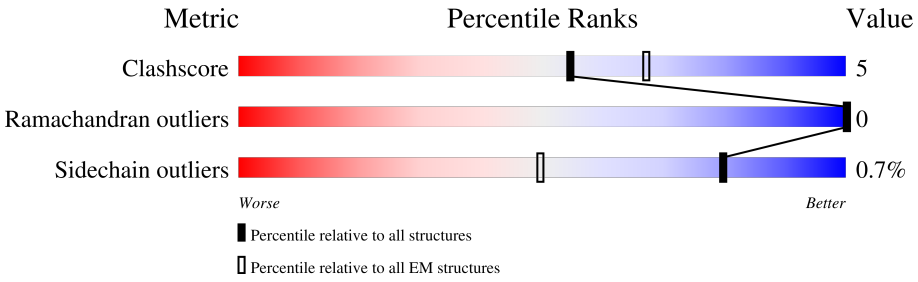
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 4.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	350	54% 11% 36%
1	B	350	60% 8% 33%
2	C	1169	82% 13%
3	D	1317	9% 83% 13%
4	E	107	6% 73% 10% 17%
5	F	466	59% 9% 32%
6	J	114	39% 71% 7% 22%
7	O	68	7% 51% 12% 37%

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Mol	Chain	Length	Quality of chain
8	P	68	32% 31% 37%
9	Y	318	15% 85% 15%
10	X	333	14% 82% 17%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 32706 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	225	Total	C	N	O	S	0	0
			1708	1075	295	336	2		
1	B	236	Total	C	N	O	S	0	0
			1790	1125	308	354	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0
			8678	5424	1521	1697	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0
			9897	6199	1794	1862	42		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	89	Total	C	N	O	0	0
			684	433	114	137		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	318	Total	C	N	O	S	0	0
			2543	1588	461	487	7		

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	89	Total	C	N	O	S	0	0
			726	454	132	138	2		

- Molecule 7 is a DNA chain called recA-op non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	43	Total	C	N	O	P	0	0
			879	417	159	260	43		

- Molecule 8 is a DNA chain called recA-op template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	43	Total	C	N	O	P	0	0
			884	418	173	250	43		

- Molecule 9 is a protein called PafC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	317	Total	C	N	O	S	0	0
			2383	1498	408	467	10		

- Molecule 10 is a protein called Transcriptional regulator-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	330	Total	C	N	O	S	0	0
			2531	1559	481	489	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-1	GLY	-	expression tag	UNP I7G3U5
X	0	LEU	-	expression tag	UNP I7G3U5
X	1	SER	-	expression tag	UNP I7G3U5

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

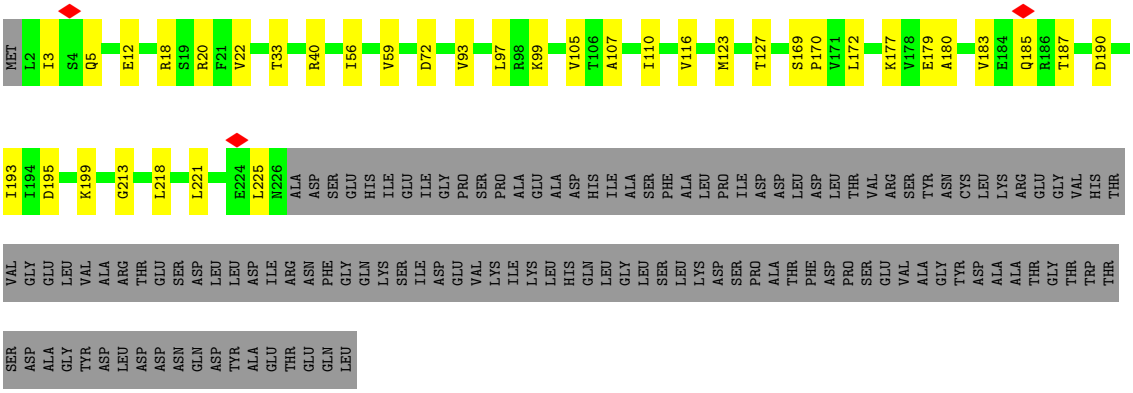
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	D	1	1	1	0

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.

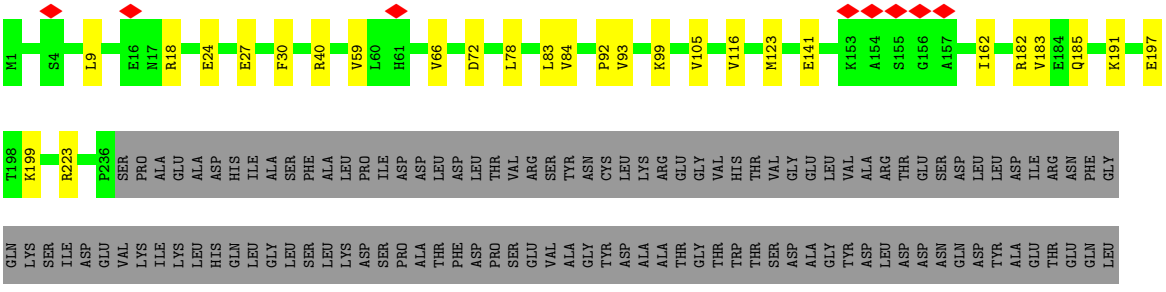
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



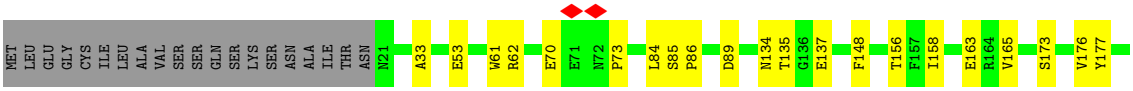
• Molecule 1: DNA-directed RNA polymerase subunit alpha

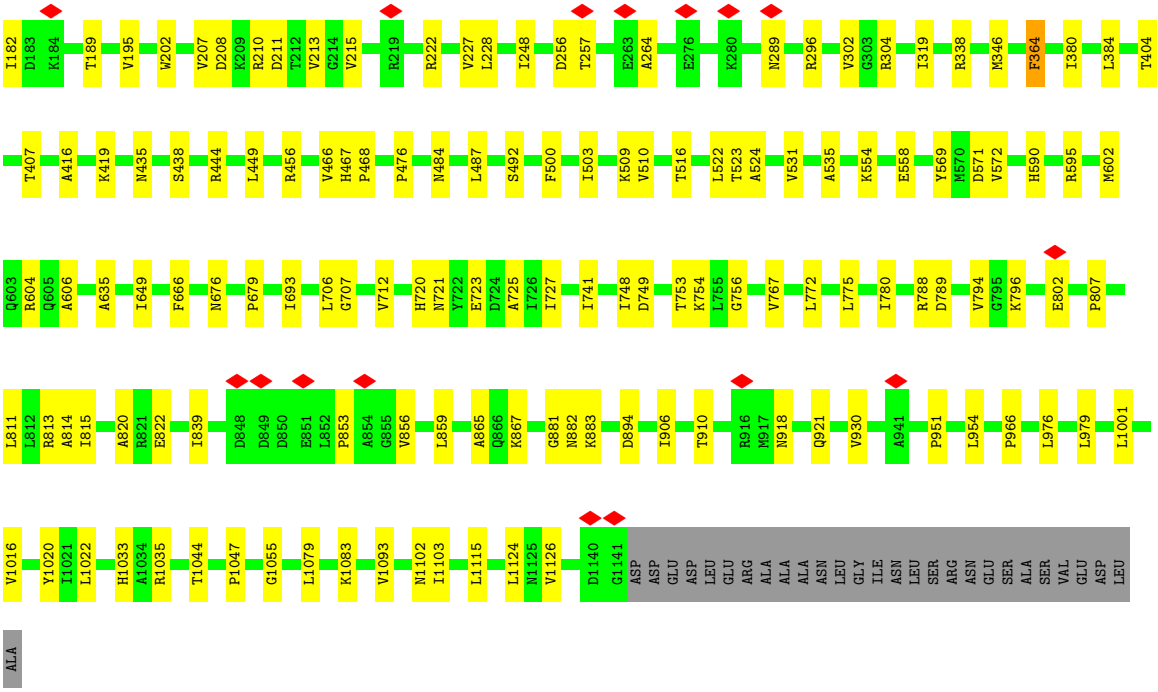
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

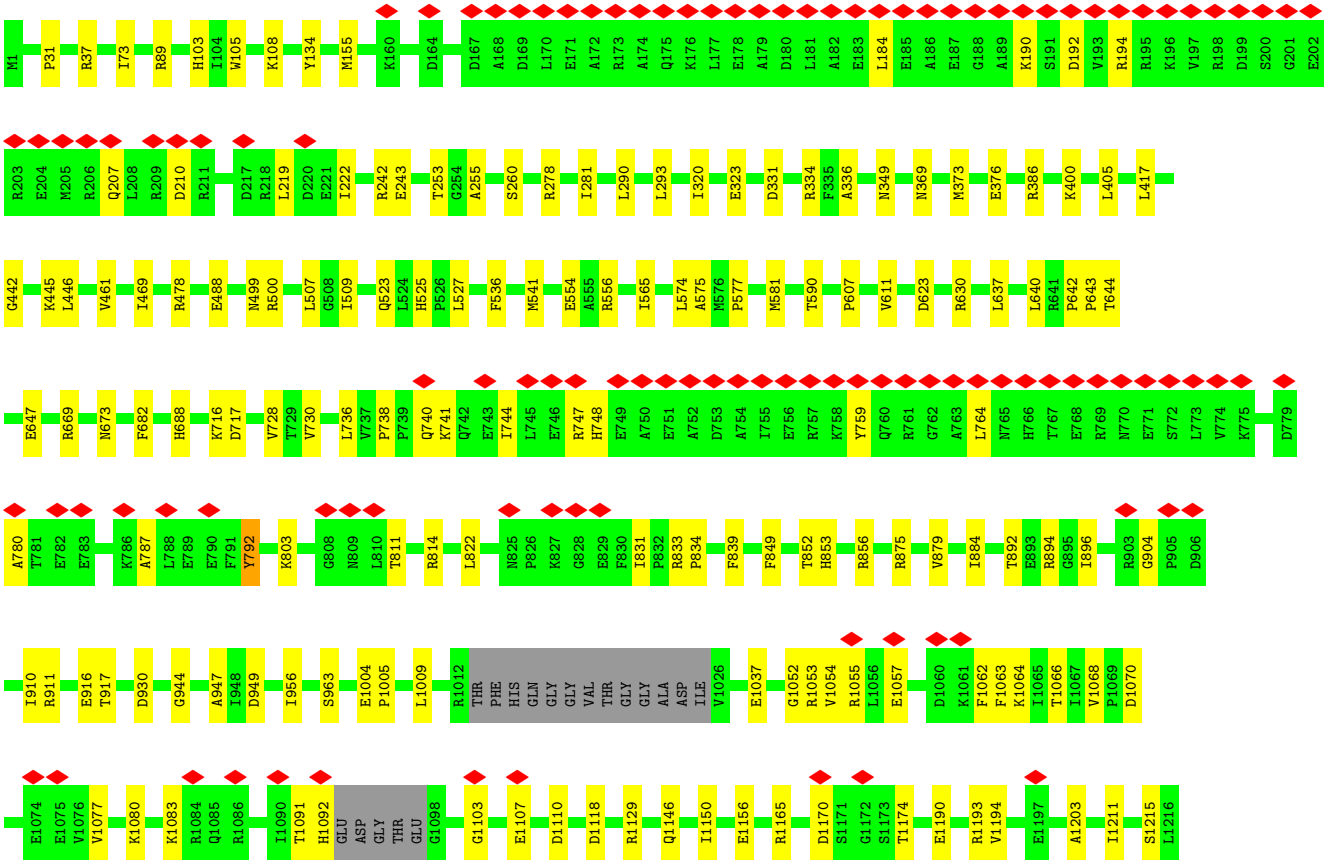
Chain C:

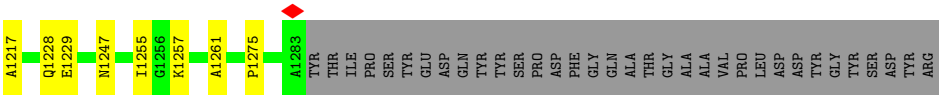




• Molecule 3: DNA-directed RNA polymerase subunit beta'

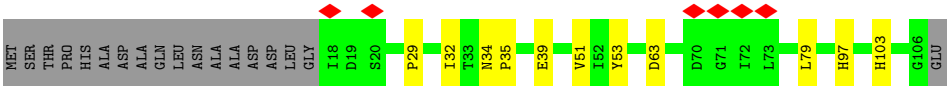
Chain D:





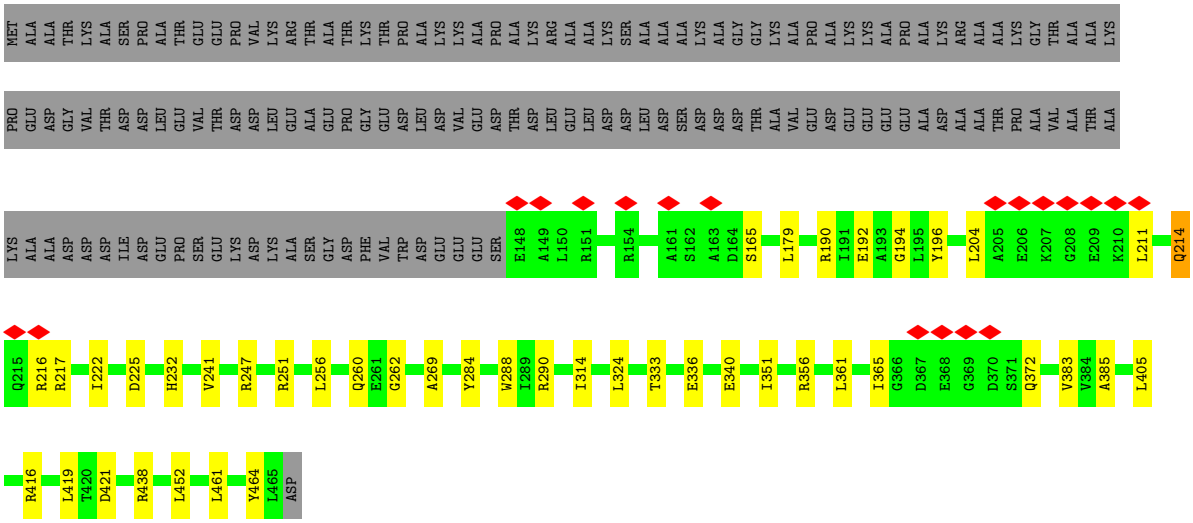
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



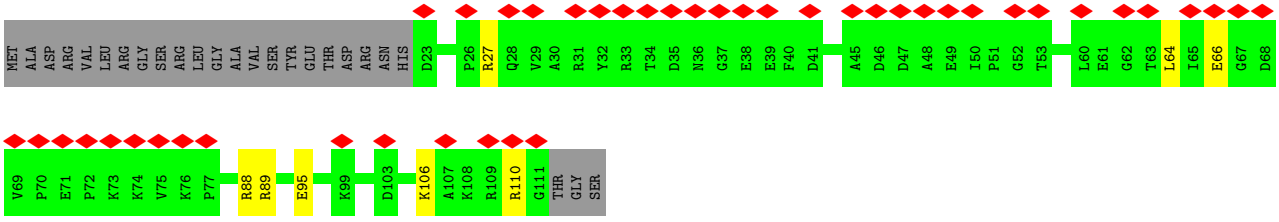
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



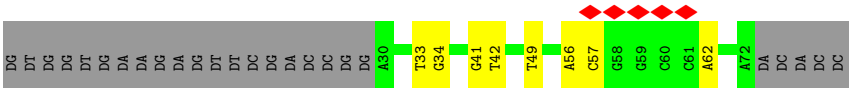
• Molecule 6: RNA polymerase-binding protein RbpA

Chain J:



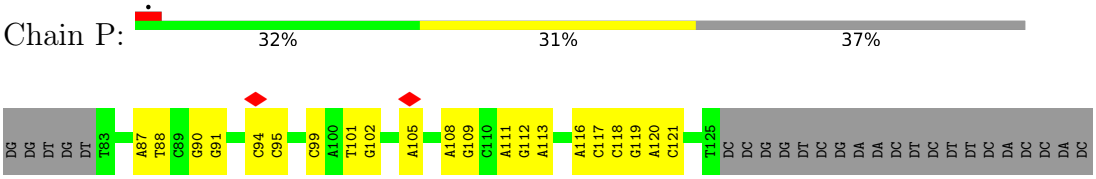
• Molecule 7: recA-op non-template strand

Chain O:



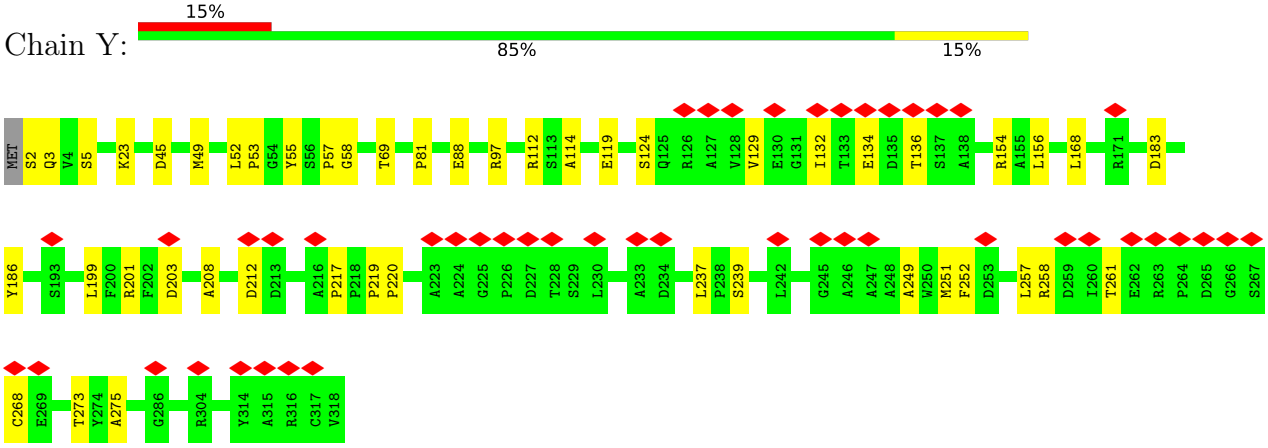
• Molecule 8: recA-op template strand

Chain P:



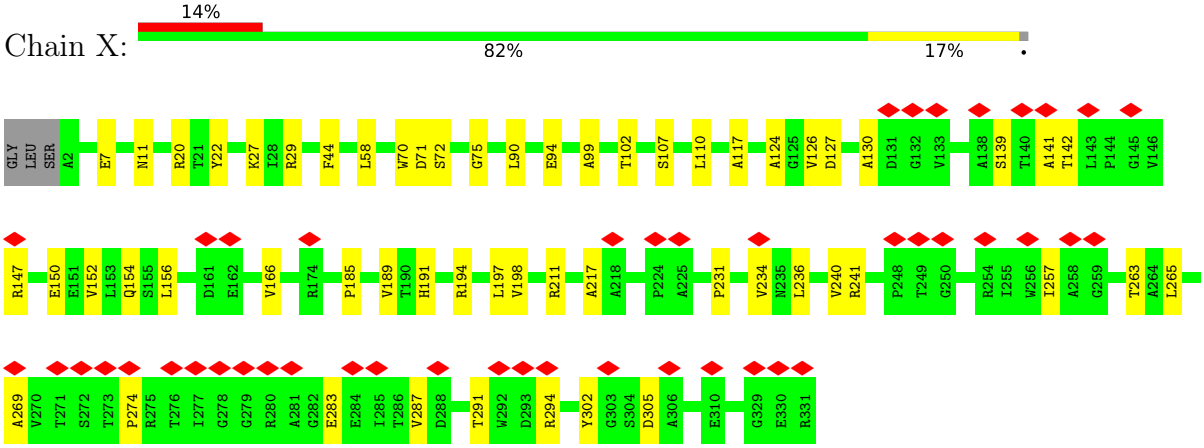
• Molecule 9: PafC

Chain Y:



• Molecule 10: Transcriptional regulator-like protein

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470245	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	66.076	Depositor
Minimum map value	-48.435	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.3	Depositor
Map size (Å)	403.2, 403.2, 403.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	0.24	0/1734	0.51	0/2360
1	B	0.24	0/1818	0.49	0/2474
2	C	0.24	0/8831	0.49	0/11965
3	D	0.24	0/10055	0.49	0/13584
4	E	0.25	0/697	0.46	0/949
5	F	0.23	0/2574	0.48	0/3468
6	J	0.23	0/740	0.50	0/999
7	O	0.51	0/984	0.88	0/1516
8	P	0.48	0/994	0.79	0/1531
9	Y	0.24	0/2430	0.48	0/3322
10	X	0.23	0/2572	0.52	0/3494
All	All	0.26	0/33429	0.52	0/45662

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	1708	0	1747	22	0
1	B	1790	0	1824	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8678	0	8618	90	0
3	D	9897	0	10037	102	0
4	E	684	0	677	7	0
5	F	2543	0	2590	34	0
6	J	726	0	723	6	0
7	O	879	0	484	5	0
8	P	884	0	480	20	0
9	Y	2383	0	2348	33	0
10	X	2531	0	2528	38	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	32706	0	32056	317	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 5.

All (317) 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)
9:Y:112:ARG:HH22	9:Y:136:THR:HG23	1.52	0.75
2:C:754:LYS:HG3	10:X:70:TRP:HB2	1.76	0.68
3:D:1055:ARG:HB3	3:D:1066:THR:HB	1.75	0.68
2:C:554:LYS:HB2	2:C:558:GLU:HB2	1.76	0.67
2:C:1102:ASN:ND2	4:E:63:ASP:OD1	2.27	0.67
9:Y:88:GLU:HB2	10:X:117:ALA:HB2	1.77	0.66
1:A:93:VAL:HG21	1:A:116:VAL:HG21	1.78	0.66
3:D:1053:ARG:HB3	3:D:1068:VAL:HB	1.79	0.65
5:F:405:LEU:HD11	5:F:452:LEU:HD11	1.78	0.65
2:C:208:ASP:HB3	2:C:222:ARG:HH12	1.61	0.64
3:D:334:ARG:HH22	8:P:101:DT:H5"	1.61	0.64
2:C:449:LEU:HD21	2:C:487:LEU:HD13	1.80	0.63
2:C:590:HIS:ND1	3:D:839:PHE:O	2.29	0.63
2:C:535:ALA:HB2	2:C:571:ASP:HB2	1.80	0.63
3:D:740:GLN:HE21	3:D:787:ALA:HB1	1.63	0.63
2:C:951:PRO:HD2	2:C:954:LEU:HD12	1.79	0.63
3:D:1165:ARG:NH2	3:D:1217:ALA:O	2.32	0.63
2:C:84:LEU:HD22	2:C:384:LEU:HB3	1.80	0.62
3:D:822:LEU:HD23	3:D:834:PRO:HB3	1.82	0.62
3:D:1053:ARG:NH1	3:D:1054:VAL:O	2.32	0.62
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.80	0.62
2:C:211:ASP:HB3	2:C:248:ILE:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HB2	1:A:110:ILE:HG12	1.82	0.61
9:Y:2:SER:N	9:Y:5:SER:HG	1.98	0.61
4:E:39:GLU:OE1	4:E:97:HIS:NE2	2.32	0.61
10:X:302:TYR:HB3	10:X:305:ASP:HB2	1.83	0.61
3:D:369:ASN:ND2	5:F:260:GLN:OE1	2.34	0.60
3:D:1275:PRO:HB3	4:E:79:LEU:HD11	1.83	0.60
1:A:225:LEU:HD23	1:B:9:LEU:H	1.66	0.60
3:D:1064:LYS:HZ3	3:D:1066:THR:HG1	1.50	0.60
2:C:882:ASN:ND2	2:C:921:GLN:OE1	2.35	0.59
3:D:1057:GLU:HB3	3:D:1064:LYS:HB3	1.85	0.59
3:D:89:ARG:HB3	3:D:323:GLU:HB2	1.85	0.59
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.83	0.59
3:D:637:LEU:HD13	3:D:640:LEU:HD12	1.85	0.59
1:A:177:LYS:NZ	1:A:179:GLU:OE2	2.35	0.59
2:C:741:ILE:HG12	2:C:867:LYS:HG2	1.85	0.59
9:Y:239:SER:HA	9:Y:273:THR:HA	1.84	0.59
3:D:1174:THR:HG22	3:D:1194:VAL:HG21	1.85	0.58
2:C:1035:ARG:HH11	2:C:1055:GLY:HA2	1.69	0.58
9:Y:156:LEU:HD11	9:Y:208:ALA:HB1	1.85	0.58
3:D:875:ARG:NH1	3:D:1037:GLU:OE2	2.37	0.58
1:A:172:LEU:HG	1:A:199:LYS:HG2	1.85	0.58
3:D:669:ARG:O	3:D:673:ASN:ND2	2.30	0.58
2:C:1079:LEU:HD23	2:C:1083:LYS:HD2	1.86	0.57
2:C:338:ARG:HD2	2:C:346:MET:HG3	1.85	0.57
3:D:879:VAL:HG22	3:D:1215:SER:HB3	1.87	0.57
5:F:251:ARG:NH1	8:P:105:DA:OP2	2.37	0.57
8:P:90:DG:H2'	8:P:91:DG:C8	2.39	0.57
2:C:176:VAL:HG12	2:C:195:VAL:HG22	1.85	0.57
4:E:29:PRO:HB2	4:E:34:ASN:HA	1.87	0.57
10:X:90:LEU:HD22	10:X:126:VAL:HG21	1.87	0.57
2:C:822:GLU:O	10:X:20:ARG:NH2	2.37	0.57
3:D:892:THR:HG22	3:D:894:ARG:H	1.70	0.56
1:B:162:ILE:HG23	3:D:607:PRO:HG2	1.86	0.56
3:D:911:ARG:NH2	3:D:949:ASP:OD1	2.39	0.56
2:C:173:SER:O	2:C:177:TYR:OH	2.21	0.56
5:F:333:THR:OG1	5:F:336:GLU:OE1	2.23	0.56
1:B:78:LEU:HD21	3:D:611:VAL:HG12	1.88	0.56
3:D:738:PRO:HG2	3:D:741:LYS:HB2	1.87	0.56
10:X:139:SER:HG	10:X:142:THR:HG1	1.49	0.55
1:A:107:ALA:HB2	1:A:123:MET:HG2	1.87	0.55
5:F:190:ARG:NH2	5:F:225:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NH2	1:A:195:ASP:OD2	2.35	0.55
2:C:227:VAL:HG13	2:C:264:ALA:HB1	1.88	0.55
8:P:116:DA:H2"	8:P:117:DC:H5"	1.88	0.55
5:F:438:ARG:NH1	9:Y:49:MET:SD	2.81	0.54
9:Y:261:THR:HB	9:Y:268:CYS:HB3	1.89	0.54
3:D:879:VAL:HG21	3:D:1211:ILE:HB	1.90	0.54
1:B:93:VAL:HG11	1:B:116:VAL:HG21	1.90	0.54
2:C:70:GLU:HG3	2:C:73:PRO:HG3	1.89	0.54
5:F:211:LEU:HB2	5:F:216:ARG:HE	1.73	0.54
1:A:40:ARG:NH1	2:C:894:ASP:OD1	2.38	0.54
2:C:649:ILE:HD11	2:C:679:PRO:HB3	1.90	0.53
8:P:120:DA:H2"	8:P:121:DC:H5'	1.89	0.53
2:C:1033:HIS:NE2	2:C:1055:GLY:O	2.38	0.53
2:C:364:PHE:HE2	2:C:503:ILE:HD12	1.72	0.53
10:X:166:VAL:HG22	10:X:185:PRO:HD3	1.90	0.53
3:D:500:ARG:HB2	3:D:541:MET:HG2	1.89	0.53
2:C:910:THR:HG23	3:D:730:VAL:HG23	1.90	0.53
3:D:290:LEU:HA	3:D:293:LEU:HD12	1.91	0.53
10:X:7:GLU:O	10:X:11:ASN:ND2	2.34	0.53
2:C:853:PRO:HG2	2:C:856:VAL:HG21	1.91	0.53
1:A:33:THR:HG21	1:B:40:ARG:HG3	1.91	0.53
9:Y:258:ARG:HH12	9:Y:273:THR:H	1.56	0.52
10:X:90:LEU:HD13	10:X:126:VAL:HG11	1.90	0.52
7:O:56:DA:H2'	7:O:57:DC:C6	2.44	0.52
1:A:183:VAL:HG22	1:A:187:THR:HA	1.92	0.52
2:C:182:ILE:HG12	2:C:189:THR:HG22	1.92	0.52
5:F:324:LEU:HD21	5:F:340:GLU:HG2	1.91	0.52
1:B:59:VAL:HG21	1:B:66:VAL:HG22	1.92	0.52
5:F:290:ARG:HH12	8:P:105:DA:H62	1.58	0.52
9:Y:217:PRO:HB2	9:Y:219:PRO:HD2	1.92	0.52
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.75	0.52
3:D:1063:PHE:HE1	3:D:1083:LYS:HA	1.74	0.52
3:D:759:TYR:HA	3:D:764:LEU:HB2	1.92	0.51
1:A:170:PRO:HA	1:A:199:LYS:HE2	1.90	0.51
9:Y:237:LEU:HD11	9:Y:275:ALA:HA	1.92	0.51
10:X:141:ALA:HA	10:X:147:ARG:HG2	1.92	0.51
3:D:811:THR:HG23	3:D:814:ARG:HH21	1.75	0.51
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.93	0.51
1:B:99:LYS:HG2	1:B:105:VAL:HG22	1.93	0.51
3:D:376:GLU:OE2	5:F:165:SER:OG	2.28	0.51
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:438:SER:OG	2:C:604:ARG:O	2.28	0.51
3:D:716:LYS:NZ	3:D:717:ASP:OD1	2.43	0.51
3:D:134:TYR:OH	3:D:242:ARG:NH1	2.43	0.50
1:A:72:ASP:OD1	1:A:72:ASP:N	2.40	0.50
3:D:1009:LEU:HD12	3:D:1146:GLN:HG3	1.92	0.50
3:D:643:PRO:HG3	3:D:682:PHE:HB3	1.94	0.50
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.94	0.50
2:C:815:ILE:HD11	5:F:452:LEU:HD23	1.92	0.50
2:C:1093:VAL:HG22	2:C:1103:ILE:HG23	1.92	0.50
3:D:400:LYS:HE2	3:D:405:LEU:HD23	1.94	0.50
3:D:688:HIS:NE2	3:D:803:LYS:O	2.41	0.50
2:C:606:ALA:HB2	2:C:1022:LEU:HD23	1.93	0.50
2:C:749:ASP:HB3	2:C:859:LEU:HD13	1.94	0.50
3:D:849:PHE:O	3:D:852:THR:OG1	2.23	0.50
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.94	0.49
3:D:445:LYS:HG3	3:D:446:LEU:HD12	1.94	0.49
9:Y:168:LEU:HD21	10:X:263:THR:HG21	1.93	0.49
1:B:18:ARG:NH1	1:B:197:GLU:OE1	2.45	0.49
2:C:444:ARG:NH2	2:C:492:SER:O	2.44	0.49
3:D:916:GLU:HG3	3:D:917:THR:HG23	1.94	0.49
5:F:204:LEU:HB3	5:F:211:LEU:HD11	1.94	0.49
9:Y:97:ARG:HD2	9:Y:129:VAL:HG22	1.94	0.49
1:A:3:ILE:HG22	1:A:5:GLN:H	1.77	0.49
3:D:334:ARG:NH1	8:P:101:DT:OP2	2.46	0.49
5:F:269:ALA:HB2	5:F:288:TRP:HB2	1.94	0.49
9:Y:52:LEU:HD12	9:Y:53:PRO:HD2	1.95	0.49
9:Y:217:PRO:HG2	9:Y:220:PRO:HG2	1.95	0.49
8:P:111:DA:H2"	8:P:112:DG:H8	1.78	0.49
1:B:72:ASP:OD1	1:B:72:ASP:N	2.45	0.49
2:C:780:ILE:HG23	2:C:794:VAL:HG22	1.95	0.49
5:F:194:GLY:HA2	5:F:222:ILE:HG22	1.94	0.49
6:J:88:ARG:HG3	6:J:89:ARG:HG2	1.94	0.49
2:C:135:THR:HG23	2:C:137:GLU:H	1.78	0.48
2:C:435:ASN:OD1	2:C:435:ASN:N	2.46	0.48
2:C:707:GLY:N	2:C:1020:TYR:OH	2.40	0.48
2:C:811:LEU:HD13	5:F:419:LEU:HD11	1.94	0.48
2:C:456:ARG:NH1	2:C:484:ASN:OD1	2.46	0.48
2:C:712:VAL:HG23	2:C:906:ILE:HG23	1.95	0.48
3:D:507:LEU:HD22	3:D:574:LEU:HD12	1.93	0.48
3:D:461:VAL:HG21	3:D:469:ILE:HD13	1.94	0.48
5:F:416:ARG:NH1	9:Y:55:TYR:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:87:DA:H2'	8:P:88:DT:H71	1.94	0.48
10:X:269:ALA:HA	10:X:287:VAL:HG12	1.95	0.48
2:C:134:ASN:OD1	2:C:135:THR:N	2.46	0.48
9:Y:183:ASP:OD2	10:X:194:ARG:NH1	2.40	0.48
10:X:231:PRO:HB2	10:X:234:VAL:HG23	1.95	0.48
10:X:274:PRO:HA	10:X:283:GLU:HA	1.94	0.48
2:C:302:VAL:HG22	2:C:500:PHE:HB3	1.96	0.48
10:X:152:VAL:HG22	10:X:217:ALA:HA	1.96	0.48
9:Y:201:ARG:NE	9:Y:203:ASP:OD1	2.45	0.48
2:C:456:ARG:HH22	2:C:484:ASN:HD21	1.61	0.48
2:C:918:ASN:O	2:C:921:GLN:HG2	2.14	0.48
1:A:180:ALA:HA	1:A:190:ASP:HA	1.96	0.48
2:C:304:ARG:HG2	2:C:319:ILE:HG23	1.95	0.48
2:C:53:GLU:HG3	2:C:61:TRP:HB2	1.96	0.48
10:X:29:ARG:HB2	10:X:44:PHE:CZ	2.49	0.48
2:C:635:ALA:HB2	2:C:693:ILE:HD11	1.95	0.47
2:C:721:ASN:HA	2:C:725:ALA:HB3	1.96	0.47
4:E:34:ASN:HB3	4:E:35:PRO:HD3	1.96	0.47
2:C:720:HIS:HB2	2:C:727:ILE:HD11	1.96	0.47
3:D:904:GLY:HA2	3:D:910:ILE:HG22	1.95	0.47
2:C:807:PRO:HB2	5:F:419:LEU:HD23	1.97	0.47
3:D:1247:ASN:O	3:D:1247:ASN:ND2	2.47	0.47
1:A:213:GLY:HA2	1:B:223:ARG:HD3	1.96	0.47
2:C:476:PRO:O	3:D:856:ARG:NH2	2.47	0.47
3:D:1107:GLU:HB2	3:D:1110:ASP:HB2	1.96	0.47
5:F:416:ARG:HG3	9:Y:57:PRO:HD3	1.95	0.47
2:C:723:GLU:HB3	3:D:536:PHE:HD2	1.80	0.47
3:D:736:LEU:HB2	3:D:792:TYR:HE1	1.80	0.47
3:D:748:HIS:CD2	3:D:780:ALA:HB2	2.50	0.47
2:C:522:LEU:HD11	2:C:569:TYR:CZ	2.50	0.47
3:D:31:PRO:HG3	3:D:349:ASN:OD1	2.15	0.47
3:D:1064:LYS:HE2	3:D:1077:VAL:HG13	1.96	0.47
2:C:772:LEU:HA	2:C:775:LEU:HD13	1.97	0.47
3:D:331:ASP:OD1	3:D:331:ASP:N	2.48	0.47
10:X:107:SER:N	10:X:150:GLU:OE2	2.39	0.46
2:C:1124:LEU:HD11	3:D:105:TRP:HZ3	1.79	0.46
3:D:896:ILE:HG23	3:D:1129:ARG:NH2	2.29	0.46
3:D:1229:GLU:HG2	8:P:90:DG:H4'	1.97	0.46
5:F:421:ASP:OD1	5:F:421:ASP:N	2.48	0.46
9:Y:81:PRO:HG2	10:X:124:ALA:HA	1.97	0.46
2:C:1001:LEU:HD21	2:C:1016:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1118:ASP:N	3:D:1118:ASP:OD1	2.46	0.46
7:O:33:DT:H2"	7:O:34:DG:C8	2.51	0.46
2:C:813:ARG:HD3	2:C:820:ALA:HB2	1.98	0.46
3:D:577:PRO:HB3	3:D:581:MET:HB2	1.98	0.46
8:P:118:DC:H2'	8:P:119:DG:C8	2.50	0.46
2:C:930:VAL:HG11	2:C:979:LEU:HB3	1.98	0.46
2:C:467:HIS:CG	2:C:468:PRO:HD2	2.51	0.45
2:C:789:ASP:O	3:D:478:ARG:NH2	2.49	0.45
2:C:802:GLU:OE1	10:X:27:LYS:NZ	2.38	0.45
3:D:1053:ARG:HH12	3:D:1103:GLY:H	1.63	0.45
8:P:112:DG:H2"	8:P:113:DA:H8	1.81	0.45
9:Y:23:LYS:HE2	9:Y:69:THR:HG21	1.98	0.45
1:B:40:ARG:HH12	3:D:623:ASP:HB3	1.81	0.45
2:C:207:VAL:HG22	2:C:213:VAL:HG12	1.99	0.45
8:P:108:DA:H2"	8:P:109:DG:H8	1.81	0.45
9:Y:114:ALA:HB2	10:X:94:GLU:HG3	1.98	0.45
10:X:22:TYR:HB3	10:X:75:GLY:HA3	1.97	0.45
2:C:202:TRP:HH2	7:O:62:DA:H8	1.65	0.45
9:Y:112:ARG:NE	9:Y:134:GLU:O	2.48	0.45
2:C:148:PHE:HE1	2:C:380:ILE:HD11	1.82	0.45
9:Y:132:ILE:HG12	10:X:191:HIS:HD2	1.81	0.45
2:C:839:ILE:HD13	2:C:865:ALA:HB2	1.98	0.45
3:D:373:MET:SD	5:F:256:LEU:HB3	2.57	0.45
3:D:590:THR:HG23	3:D:630:ARG:HD2	1.99	0.45
1:A:3:ILE:HD11	1:A:185:GLN:HG2	1.99	0.44
1:B:182:ARG:NH2	3:D:488:GLU:OE1	2.51	0.44
3:D:930:ASP:HB3	3:D:956:ILE:HG12	1.98	0.44
3:D:944:GLY:H	3:D:947:ALA:HB3	1.81	0.44
3:D:1005:PRO:HG2	3:D:1150:ILE:HD11	1.99	0.44
9:Y:249:ALA:HA	9:Y:252:PHE:HD1	1.83	0.44
1:A:99:LYS:HD3	1:A:105:VAL:HG22	1.98	0.44
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.99	0.44
3:D:1052:GLY:HA2	3:D:1070:ASP:HB2	1.98	0.44
10:X:127:ASP:OD1	10:X:127:ASP:N	2.50	0.44
3:D:278:ARG:HA	3:D:281:ILE:HG22	1.99	0.44
2:C:33:ALA:HB2	2:C:966:PRO:HG2	1.99	0.44
2:C:62:ARG:NH1	2:C:73:PRO:O	2.51	0.44
3:D:642:PRO:HB2	3:D:647:GLU:HB2	1.98	0.44
7:O:41:DG:C8	7:O:42:DT:H72	2.53	0.44
2:C:753:THR:OG1	2:C:756:GLY:O	2.27	0.44
3:D:525:HIS:CE1	3:D:527:LEU:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:290:ARG:NH1	8:P:105:DA:N7	2.65	0.44
9:Y:186:TYR:HB3	9:Y:199:LEU:HB3	2.00	0.44
2:C:85:SER:OG	2:C:86:PRO:HD3	2.18	0.44
2:C:666:PHE:H	2:C:676:ASN:HB3	1.82	0.44
3:D:744:ILE:HG12	3:D:747:ARG:HH21	1.82	0.43
3:D:1228:GLN:HG2	3:D:1229:GLU:HG3	2.00	0.43
5:F:247:ARG:HH11	8:P:105:DA:N6	2.16	0.43
2:C:89:ASP:OD1	2:C:89:ASP:N	2.49	0.43
5:F:314:ILE:HG12	5:F:351:ILE:HG23	2.00	0.43
10:X:156:LEU:HD13	10:X:197:LEU:HD13	1.99	0.43
2:C:416:ALA:HB1	8:P:102:DG:H1'	2.00	0.43
5:F:241:VAL:HG13	5:F:262:GLY:HA3	2.01	0.43
9:Y:2:SER:OG	9:Y:3:GLN:N	2.52	0.43
1:B:27:GLU:HB2	1:B:30:PHE:CD2	2.54	0.43
2:C:1035:ARG:CZ	2:C:1047:PRO:HB3	2.48	0.43
3:D:184:LEU:HD13	3:D:194:ARG:HG2	1.99	0.43
10:X:99:ALA:O	10:X:102:THR:HG22	2.18	0.43
3:D:792:TYR:HD1	3:D:792:TYR:HA	1.74	0.43
10:X:189:VAL:HB	10:X:240:VAL:HG21	2.00	0.43
2:C:523:THR:OG1	2:C:524:ALA:N	2.52	0.43
2:C:215:VAL:HG21	2:C:228:LEU:HD22	2.01	0.43
2:C:435:ASN:HD22	2:C:706:LEU:HD22	1.84	0.43
3:D:155:MET:HE3	3:D:219:LEU:HB3	2.00	0.43
3:D:207:GLN:HA	3:D:210:ASP:OD2	2.19	0.43
1:B:27:GLU:HB2	1:B:30:PHE:HD2	1.83	0.42
3:D:37:ARG:NE	10:X:72:SER:OG	2.52	0.42
5:F:214:GLN:HA	5:F:217:ARG:HE	1.84	0.42
9:Y:119:GLU:HG3	9:Y:124:SER:HB2	2.01	0.42
2:C:158:ILE:HG13	2:C:163:GLU:HG2	2.00	0.42
2:C:466:VAL:HB	3:D:853:HIS:CD2	2.54	0.42
6:J:106:LYS:O	6:J:110:ARG:HG2	2.19	0.42
10:X:194:ARG:CZ	10:X:211:ARG:HH21	2.32	0.42
10:X:257:ILE:HG21	10:X:265:LEU:HD23	2.02	0.42
1:B:182:ARG:HH11	1:B:185:GLN:H	1.68	0.42
3:D:554:GLU:HG3	4:E:51:VAL:HG11	2.02	0.42
3:D:255:ALA:HB3	3:D:260:SER:HB3	2.01	0.42
3:D:1004:GLU:HB3	3:D:1005:PRO:HD3	2.01	0.42
8:P:94:DC:H2'	8:P:95:DC:H6	1.84	0.42
2:C:256:ASP:OD1	2:C:257:THR:N	2.53	0.42
3:D:884:ILE:HD13	3:D:1261:ALA:HB2	2.02	0.42
5:F:196:TYR:HE2	6:J:95:GLU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:284:TYR:OH	7:O:49:DT:OP2	2.30	0.42
9:Y:251:MET:HE2	9:Y:257:LEU:HD21	2.01	0.42
2:C:156:THR:HG22	2:C:165:VAL:HG22	2.02	0.41
3:D:1091:THR:OG1	3:D:1092:HIS:N	2.53	0.41
3:D:1190:GLU:OE2	3:D:1193:ARG:NH2	2.45	0.41
5:F:383:VAL:HG12	5:F:385:ALA:H	1.84	0.41
10:X:110:LEU:HD21	10:X:154:GLN:HB2	2.00	0.41
3:D:108:LYS:O	3:D:386:ARG:NH2	2.50	0.41
3:D:336:ALA:HB1	5:F:361:LEU:HG	2.02	0.41
3:D:556:ARG:HG2	4:E:32:ILE:HD11	2.03	0.41
10:X:291:THR:HG22	10:X:294:ARG:H	1.85	0.41
8:P:94:DC:H2'	8:P:95:DC:C6	2.55	0.41
2:C:595:ARG:NH2	2:C:881:GLY:O	2.52	0.41
3:D:963:SER:OG	3:D:1156:GLU:OE1	2.36	0.41
5:F:365:ILE:HD12	8:P:99:DC:H1'	2.01	0.41
9:Y:217:PRO:O	9:Y:220:PRO:HD2	2.19	0.41
10:X:107:SER:HB3	10:X:110:LEU:HD23	2.03	0.41
3:D:190:LYS:NZ	3:D:192:ASP:HB2	2.35	0.41
10:X:99:ALA:HB1	10:X:130:ALA:HB2	2.02	0.41
2:C:404:THR:O	2:C:407:THR:HG22	2.21	0.41
2:C:419:LYS:HD2	8:P:102:DG:C2	2.56	0.41
3:D:1255:ILE:HD11	3:D:1257:LYS:HE3	2.03	0.41
6:J:64:LEU:HD22	6:J:66:GLU:HG2	2.03	0.41
9:Y:5:SER:HB2	10:X:58:LEU:HD11	2.01	0.41
1:A:169:SER:HA	1:A:170:PRO:HD3	1.93	0.41
2:C:748:ILE:HD11	2:C:796:LYS:HE2	2.03	0.41
1:A:218:LEU:O	1:A:221:LEU:HG	2.20	0.41
3:D:1170:ASP:HB2	3:D:1203:ALA:HB3	2.03	0.41
5:F:461:LEU:HA	5:F:464:TYR:HD2	1.86	0.41
9:Y:154:ARG:HH21	9:Y:212:ASP:HA	1.84	0.41
2:C:788:ARG:HG2	2:C:789:ASP:H	1.86	0.41
3:D:73:ILE:HG22	6:J:27:ARG:HD3	2.02	0.41
5:F:192:GLU:OE1	6:J:89:ARG:NH1	2.53	0.41
2:C:289:ASN:HB3	2:C:296:ARG:HD2	2.03	0.40
2:C:1115:LEU:HD22	3:D:417:LEU:HD11	2.03	0.40
10:X:71:ASP:OD1	10:X:72:SER:N	2.53	0.40
3:D:831:ILE:HG22	3:D:833:ARG:H	1.85	0.40
5:F:179:LEU:HD21	5:F:232:HIS:HE1	1.85	0.40
9:Y:132:ILE:HD11	10:X:241:ARG:HB2	2.02	0.40
1:A:12:GLU:HG3	1:A:20:ARG:HB3	2.03	0.40
2:C:509:LYS:O	2:C:516:THR:OG1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:MET:SD	2:C:883:LYS:HD3	2.62	0.40
3:D:1062:PHE:CG	3:D:1080:LYS:HD2	2.56	0.40
1:B:83:LEU:HD13	1:B:123:MET:HE2	2.04	0.40
3:D:222:ILE:HD13	3:D:243:GLU:HG2	2.03	0.40
3:D:400:LYS:NZ	5:F:372:GLN:OE1	2.52	0.40
10:X:198:VAL:HG11	10:X:236:LEU:HD22	2.03	0.40
2:C:814:ALA:HB1	9:Y:58:GLY:HA3	2.03	0.40
3:D:442:GLY:HA3	3:D:523:GLN:HB2	2.04	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	223/350 (64%)	218 (98%)	5 (2%)	0	100	100
1	B	234/350 (67%)	227 (97%)	7 (3%)	0	100	100
2	C	1119/1169 (96%)	1087 (97%)	32 (3%)	0	100	100
3	D	1259/1317 (96%)	1230 (98%)	29 (2%)	0	100	100
4	E	87/107 (81%)	83 (95%)	4 (5%)	0	100	100
5	F	316/466 (68%)	306 (97%)	10 (3%)	0	100	100
6	J	87/114 (76%)	84 (97%)	3 (3%)	0	100	100
9	Y	315/318 (99%)	309 (98%)	6 (2%)	0	100	100
10	X	328/333 (98%)	326 (99%)	2 (1%)	0	100	100
All	All	3968/4524 (88%)	3870 (98%)	98 (2%)	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%)	191 (100%)	1 (0%)	86 89
1	B	201/297 (68%)	200 (100%)	1 (0%)	86 89
2	C	945/984 (96%)	936 (99%)	9 (1%)	73 81
3	D	1055/1095 (96%)	1049 (99%)	6 (1%)	84 88
4	E	73/86 (85%)	71 (97%)	2 (3%)	40 60
5	F	270/379 (71%)	268 (99%)	2 (1%)	81 86
6	J	78/98 (80%)	78 (100%)	0	100 100
9	Y	247/248 (100%)	246 (100%)	1 (0%)	89 91
10	X	260/262 (99%)	260 (100%)	0	100 100
All	All	3321/3746 (89%)	3299 (99%)	22 (1%)	80 86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	THR
1	B	183	VAL
2	C	210	ARG
2	C	364	PHE
2	C	510	VAL
2	C	531	VAL
2	C	572	VAL
2	C	767	VAL
2	C	976	LEU
2	C	1044	THR
2	C	1126	VAL
3	D	103	HIS
3	D	253	THR
3	D	320	ILE
3	D	644	THR
3	D	728	VAL
3	D	792	TYR
4	E	53	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	103	HIS
5	F	214	GLN
5	F	356	ARG
9	Y	45	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	369	ASN
3	D	1126	GLN
5	F	260	GLN
10	X	191	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

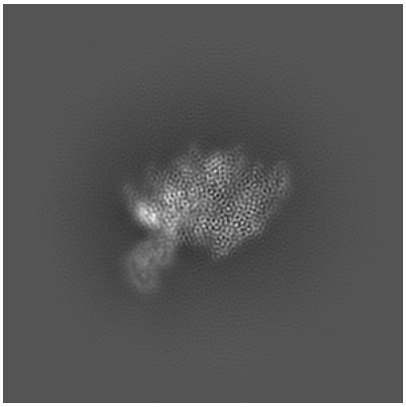
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50591. These allow visual inspection of the internal detail of the map and identification of artifacts.

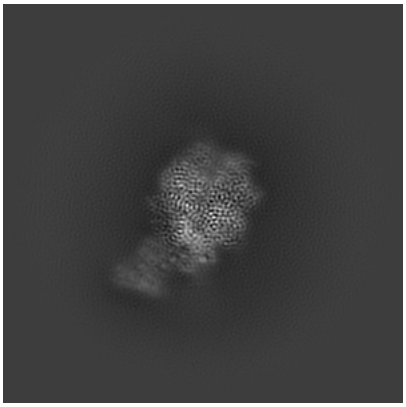
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

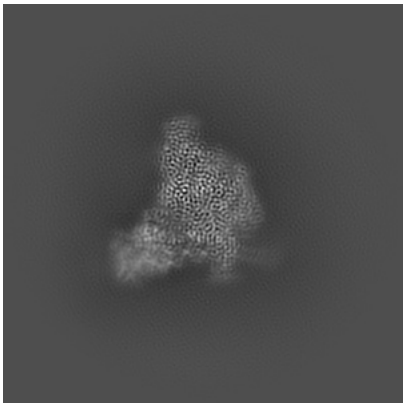
6.1.1 Primary map



X



Y

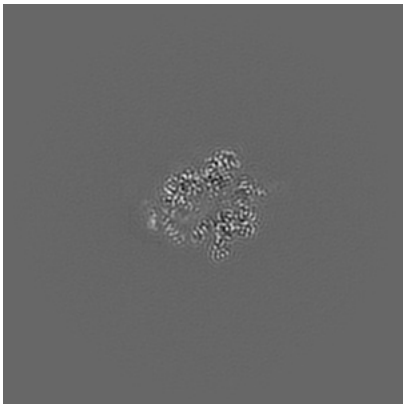


Z

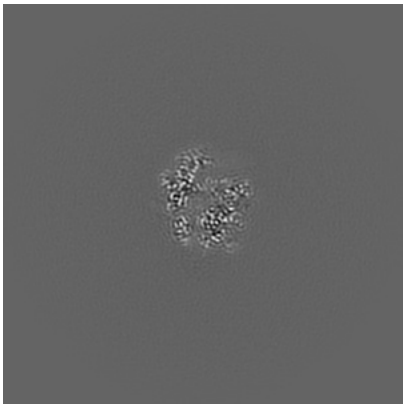
The images above show the map projected in three orthogonal directions.

6.2 Central slices

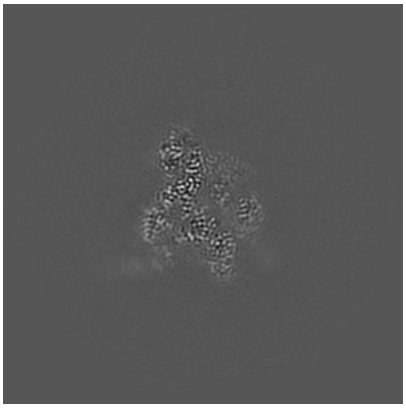
6.2.1 Primary map



X Index: 180



Y Index: 180

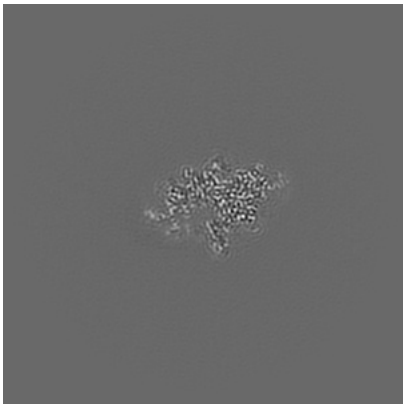


Z Index: 180

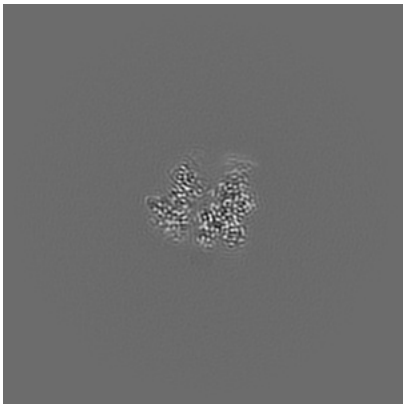
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

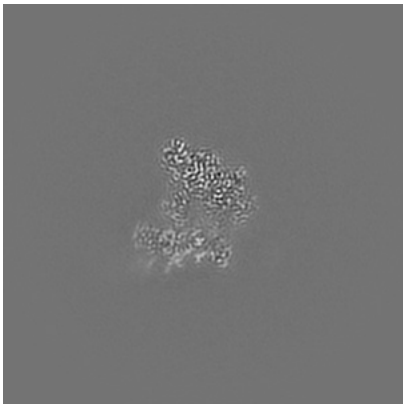
6.3.1 Primary map



X Index: 170



Y Index: 191

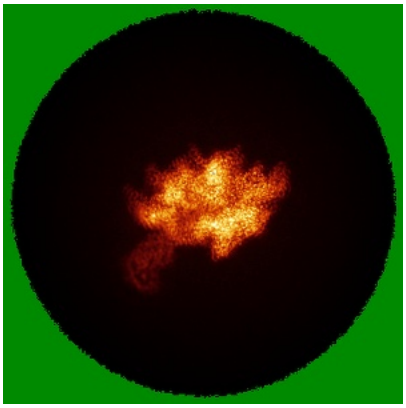


Z Index: 165

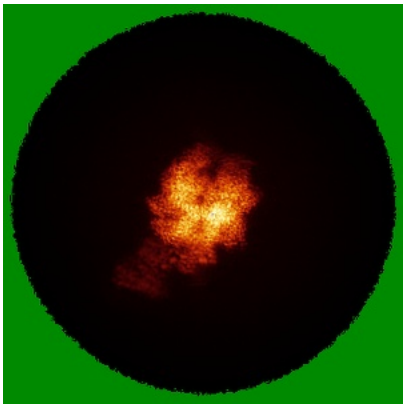
The images above show the largest variance slices of the map in three orthogonal directions.

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

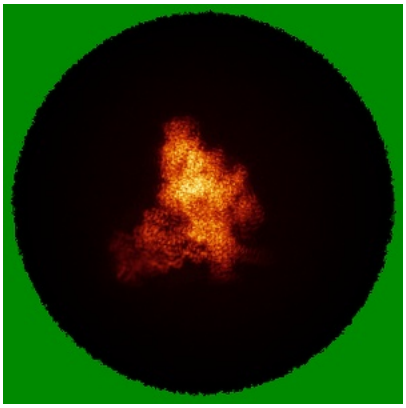
6.4.1 Primary map



X



Y

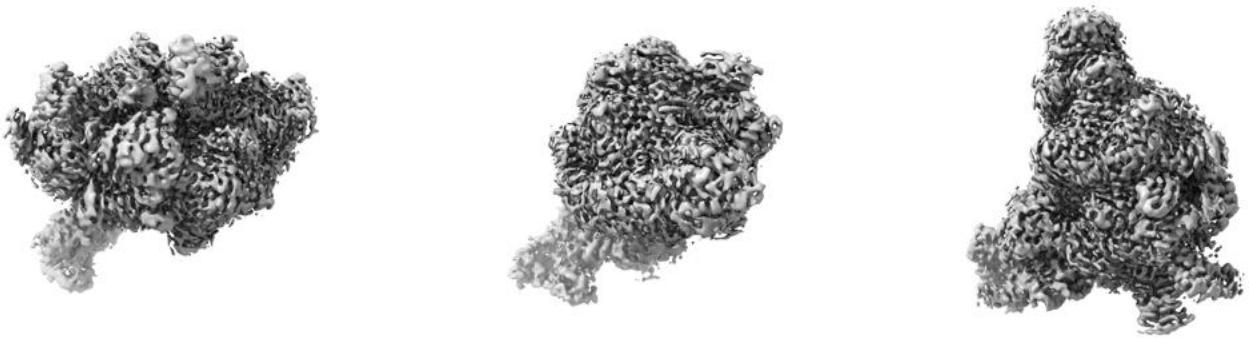


Z

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 3.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

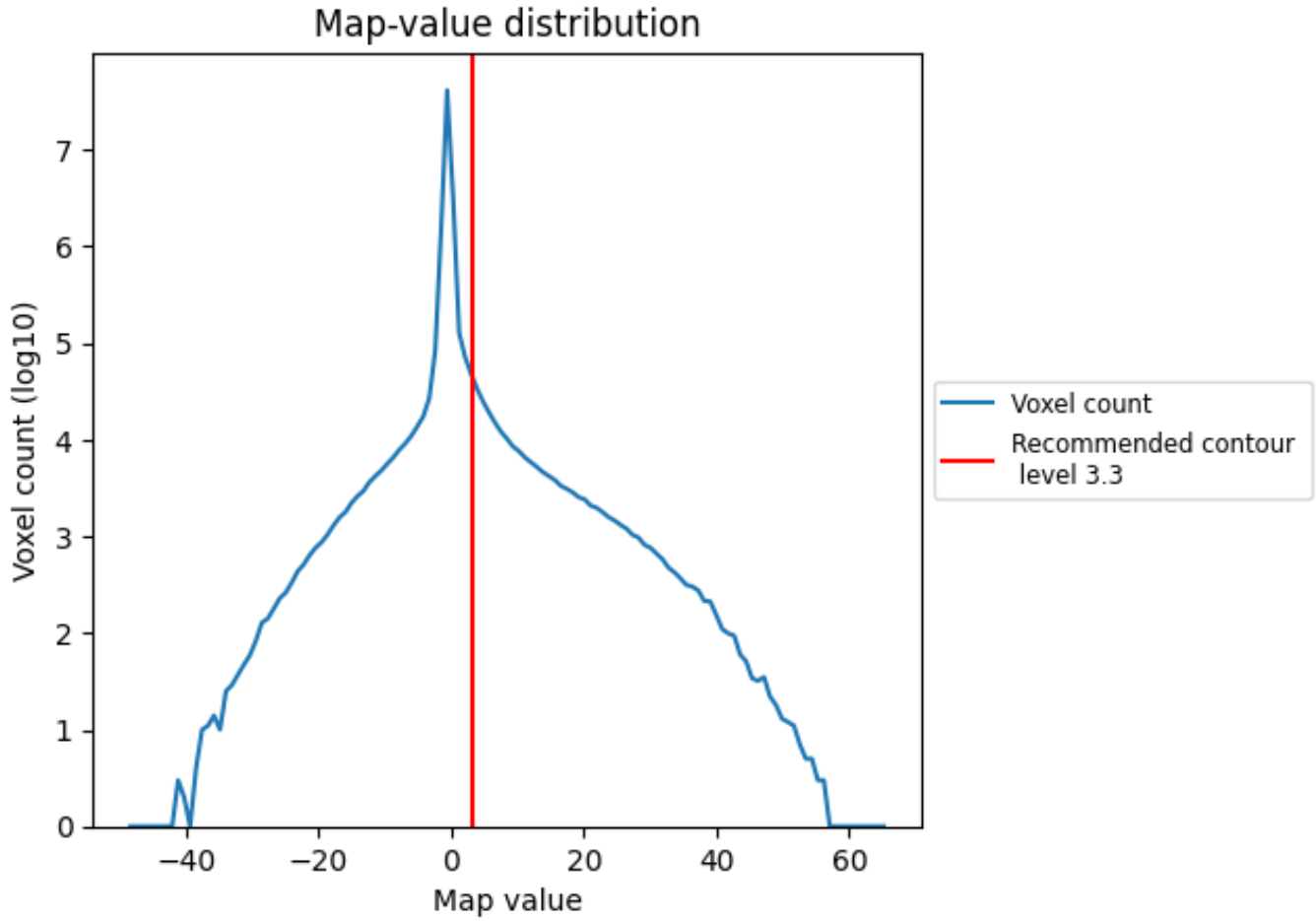
6.6 Mask visualisation (i)

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

7 Map analysis

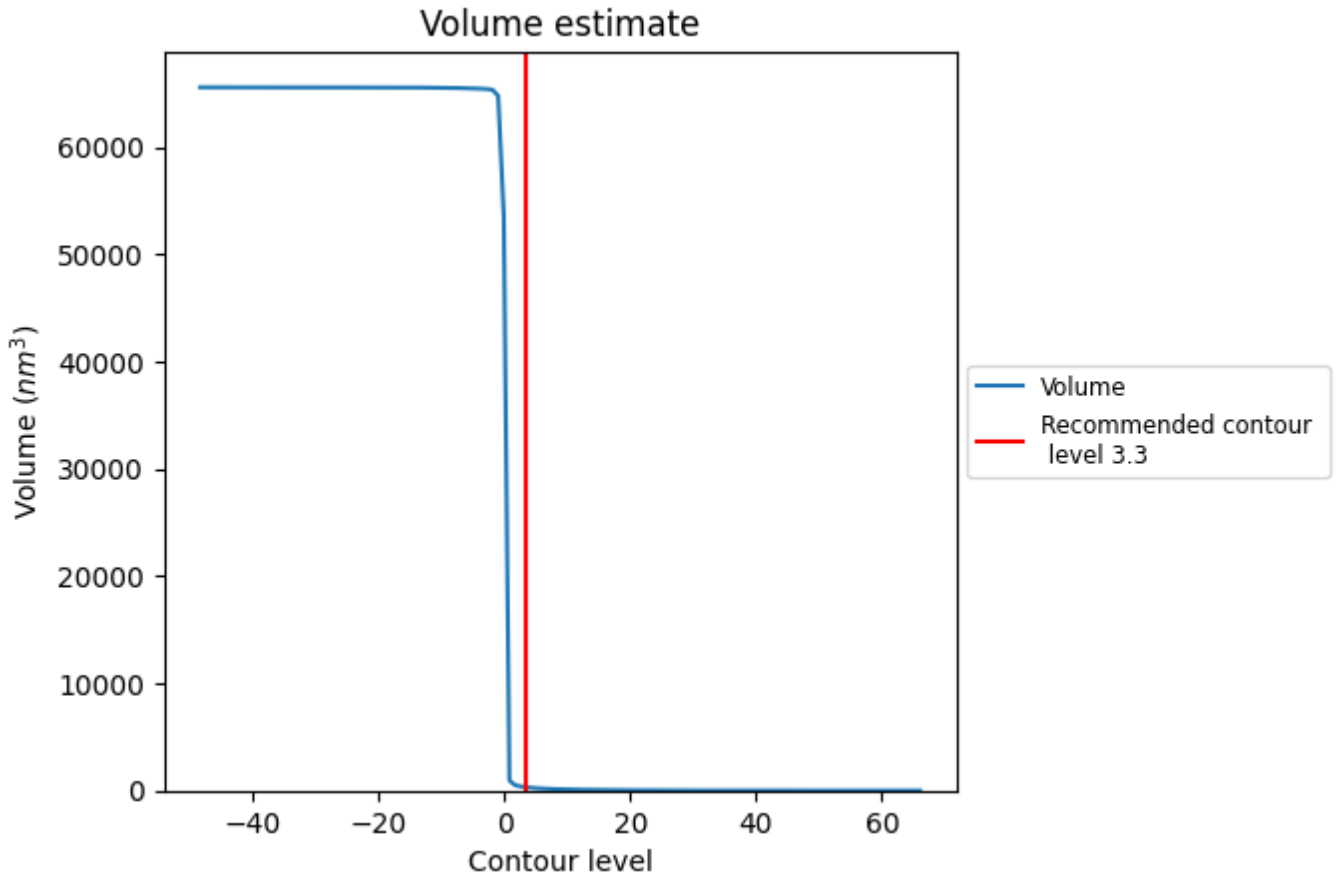
This section contains the results of statistical analysis of the map.

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.

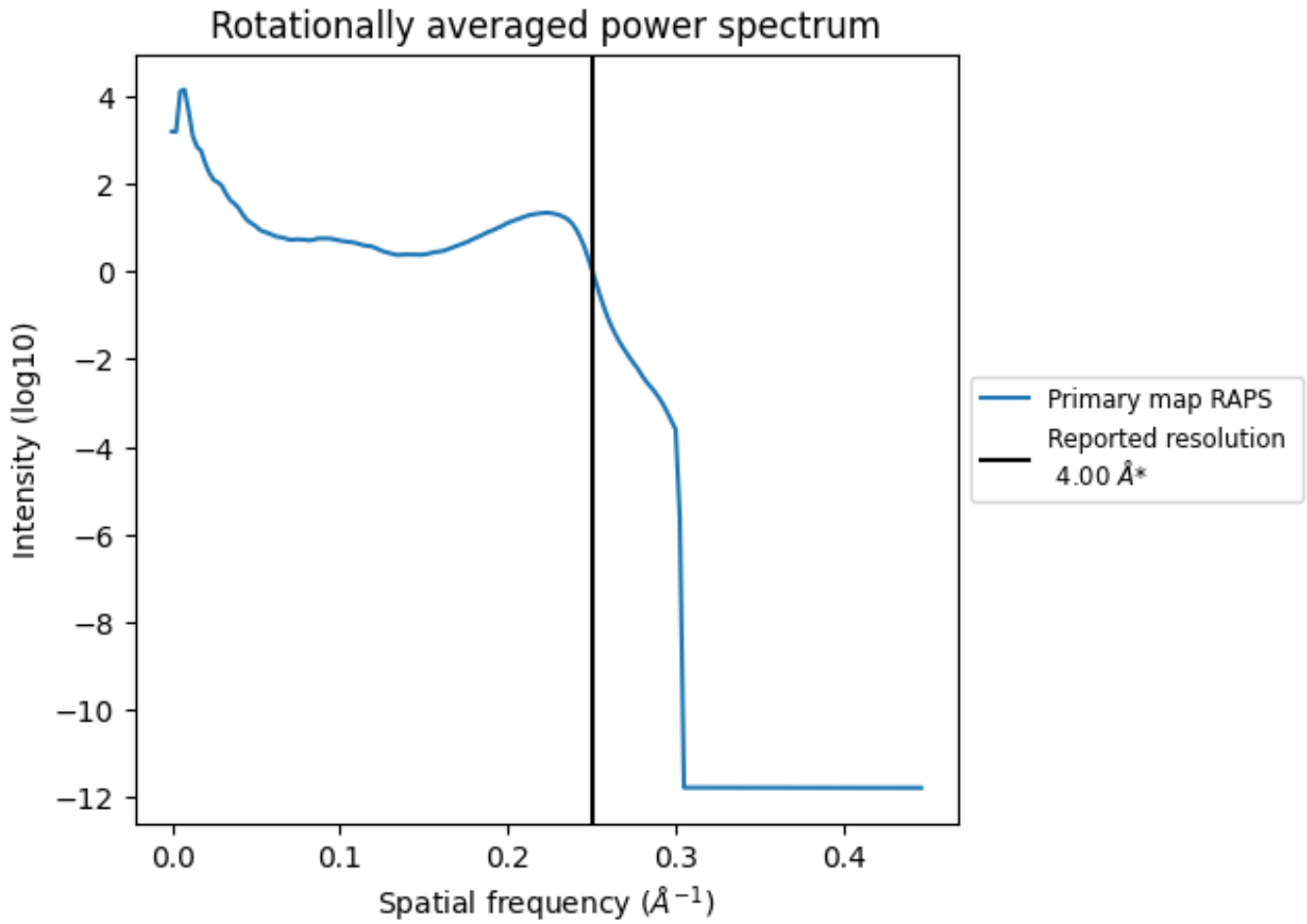
7.2 Volume estimate



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 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 0.250 Å^{-1}

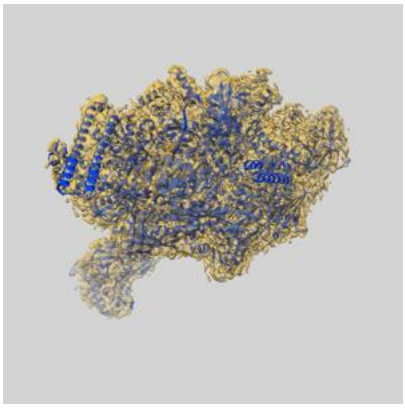
8 Fourier-Shell correlation

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

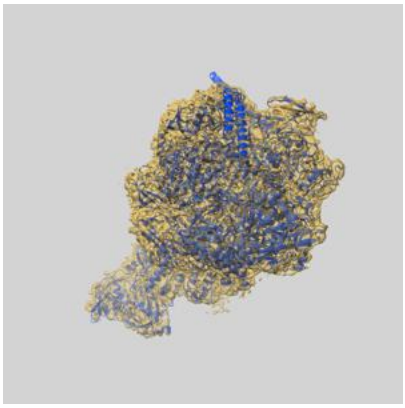
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50591 and PDB model 9FNE. Per-residue inclusion information can be found in section 3 on page 7.

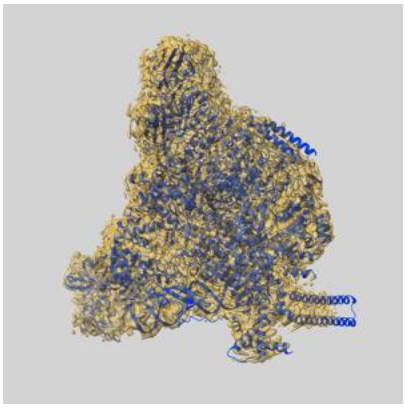
9.1 Map-model overlay



X



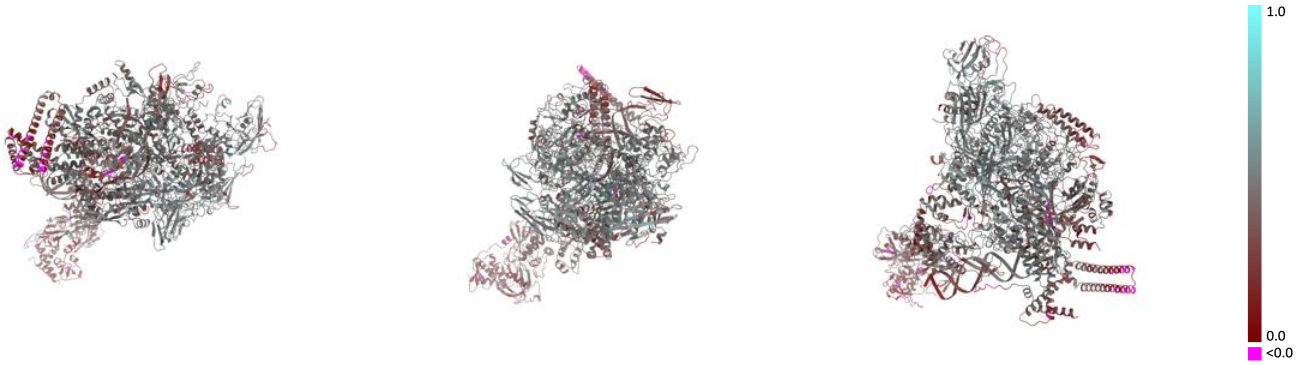
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.3 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.

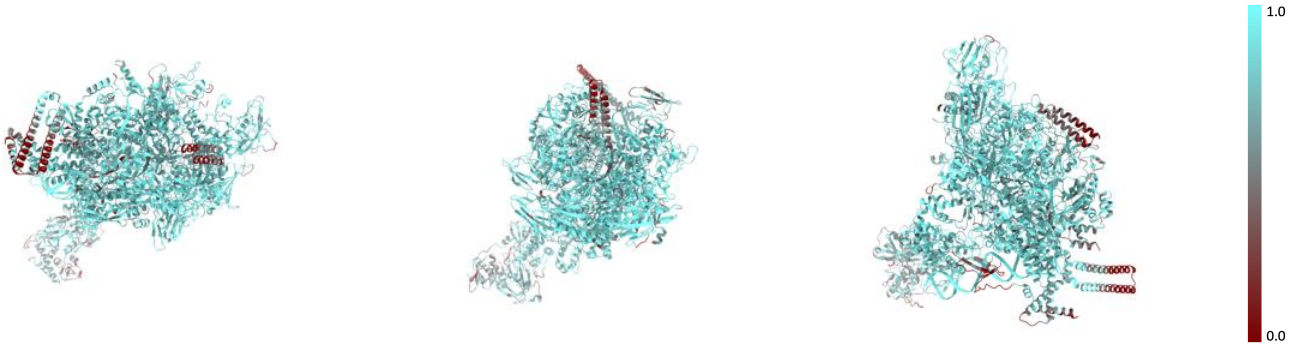
9.2 Q-score mapped to coordinate model (i)



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.

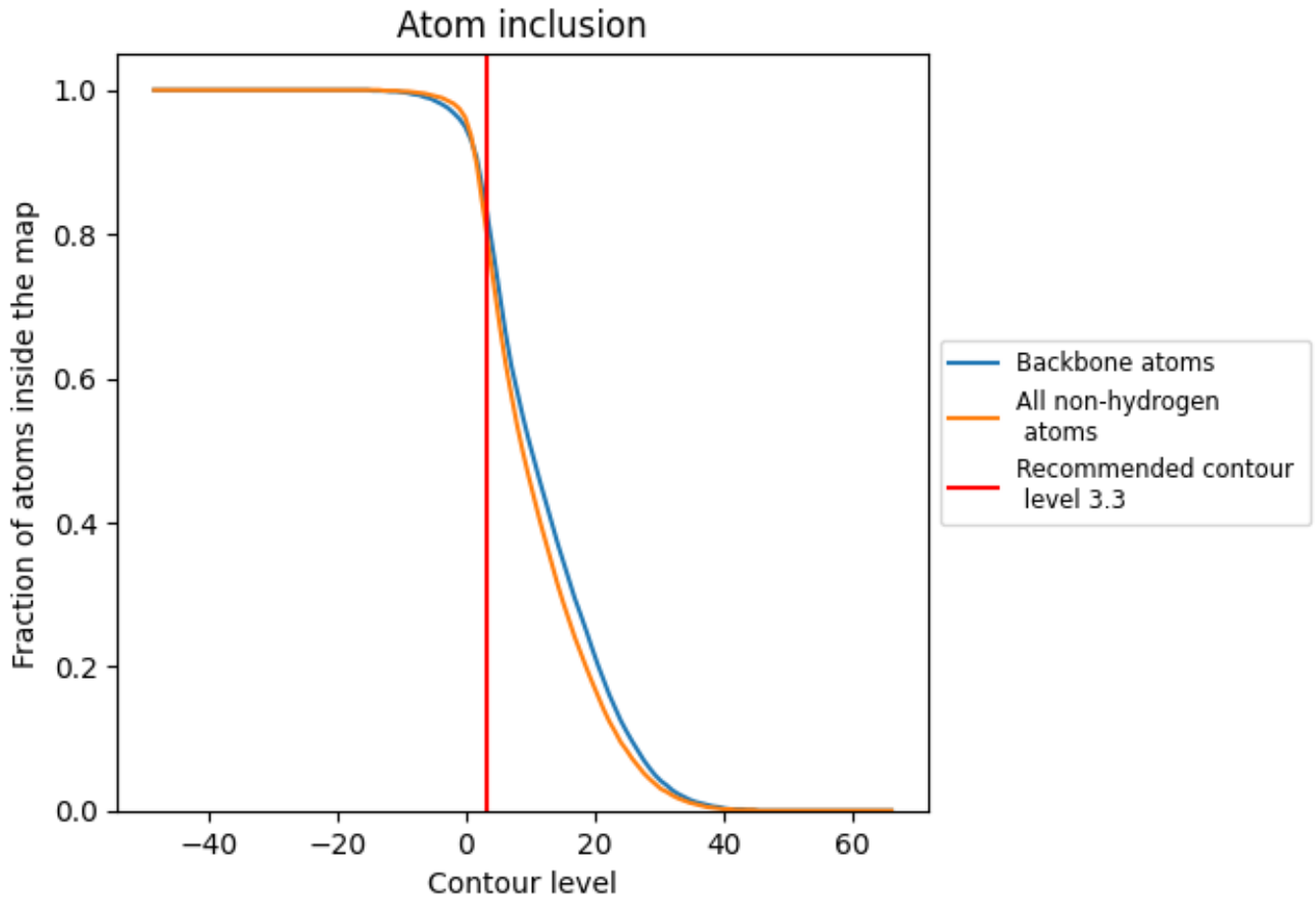
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.3).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (3.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.4150
A	0.8530	0.4690
B	0.8290	0.4570
C	0.8520	0.4570
D	0.7870	0.4370
E	0.8270	0.4400
F	0.8120	0.3970
J	0.4030	0.3100
O	0.8350	0.3390
P	0.8430	0.3340
X	0.7240	0.3130
Y	0.6990	0.3040