



## Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 08:11 AM EDT

PDB ID : 7KIM  
EMDB ID : EMD-22887  
Title : Mycobacterium tuberculosis WT RNAP transcription closed promoter complex with WhiB7 transcription factor  
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2020-10-23  
Resolution : 3.38 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.36.2

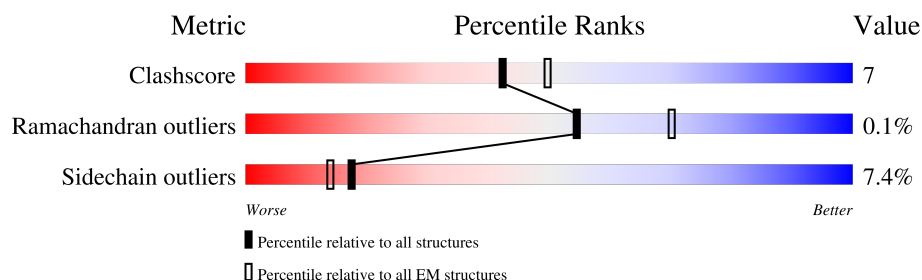
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.38 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1172	
3	D	1318	
4	E	110	
5	F	528	
6	J	111	
7	M	162	

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Mol	Chain	Length	Quality of chain
8	O	100	<div><div></div><div>34%10%•55%</div></div>
9	P	100	<div><div></div><div>38%6%•55%</div></div>
10	Z	92	<div><div></div><div>•59%25%••13%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29573 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
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1765	1115	301	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8606	5392	1511	1664	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1270	Total	C	N	O	S	0	0
			9914	6208	1802	1862	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	322	Total	C	N	O	S	0	0
			2544	1585	460	490	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	109	Total	C	N	O	S	0	0
			880	543	166	168	3		

- Molecule 7 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	135	Total	C	N	O	S	0	0
			1039	656	185	197	1		

- Molecule 8 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	45	Total	C	N	O	P	0	0
			920	438	168	270	44		

- Molecule 9 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	45	Total	C	N	O	P	0	0
			922	437	172	268	45		

- Molecule 10 is a protein called Probable transcriptional regulator WhiB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	80	Total	C	N	O	S	0	0
			607	384	117	102	4		

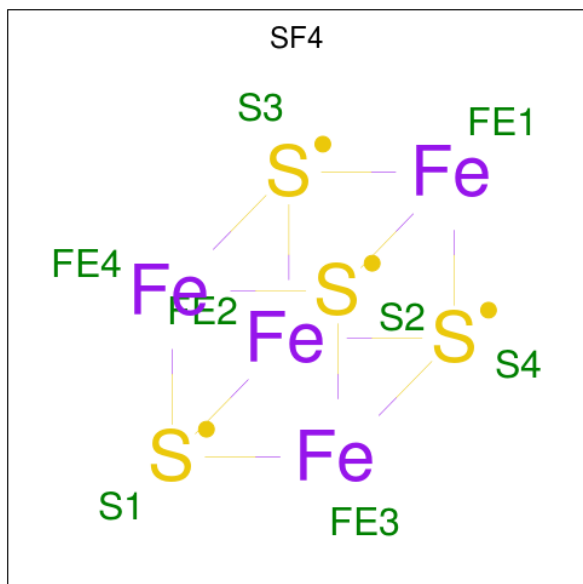
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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
12	D	1	Total	Mg	0
			1	1	

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).

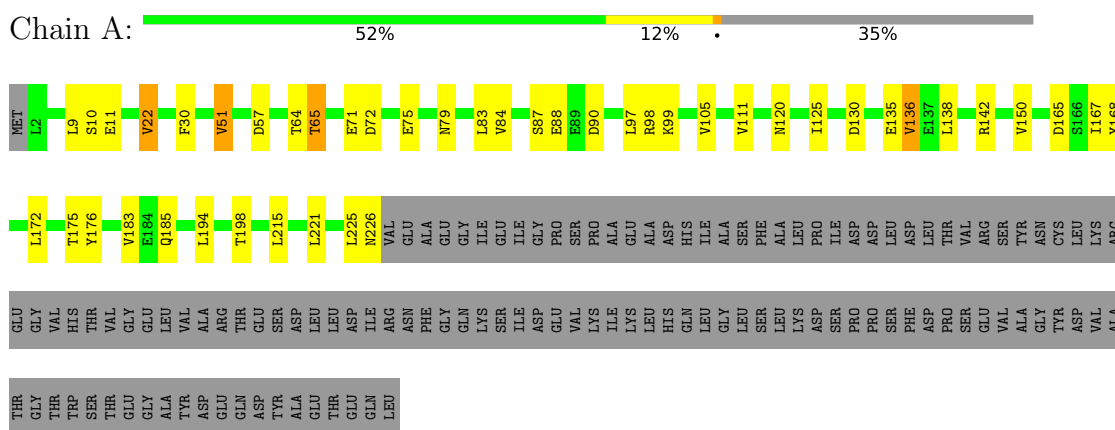


Mol	Chain	Residues	Atoms			AltConf
13	Z	1	Total	Fe	S	0
			8	4	4	

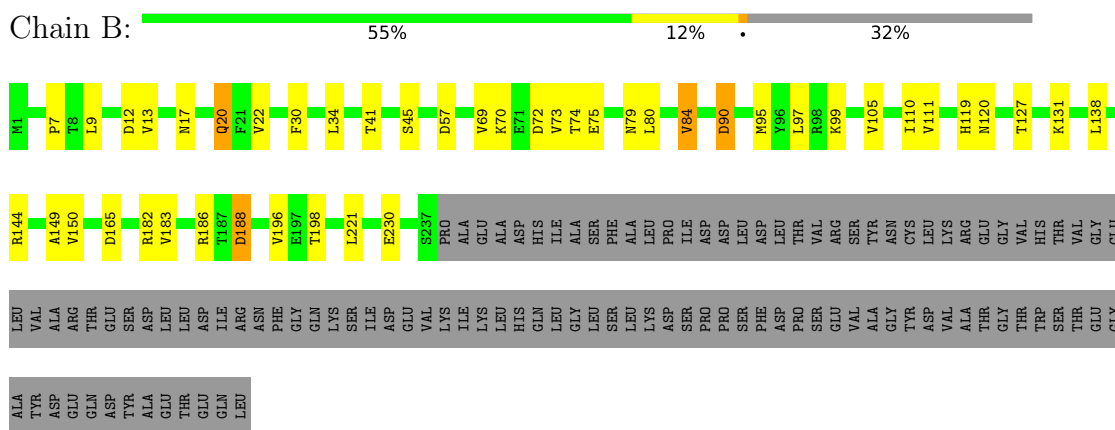
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

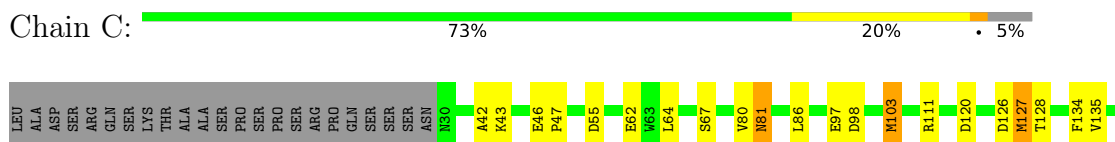
- Molecule 1: DNA-directed RNA polymerase subunit alpha

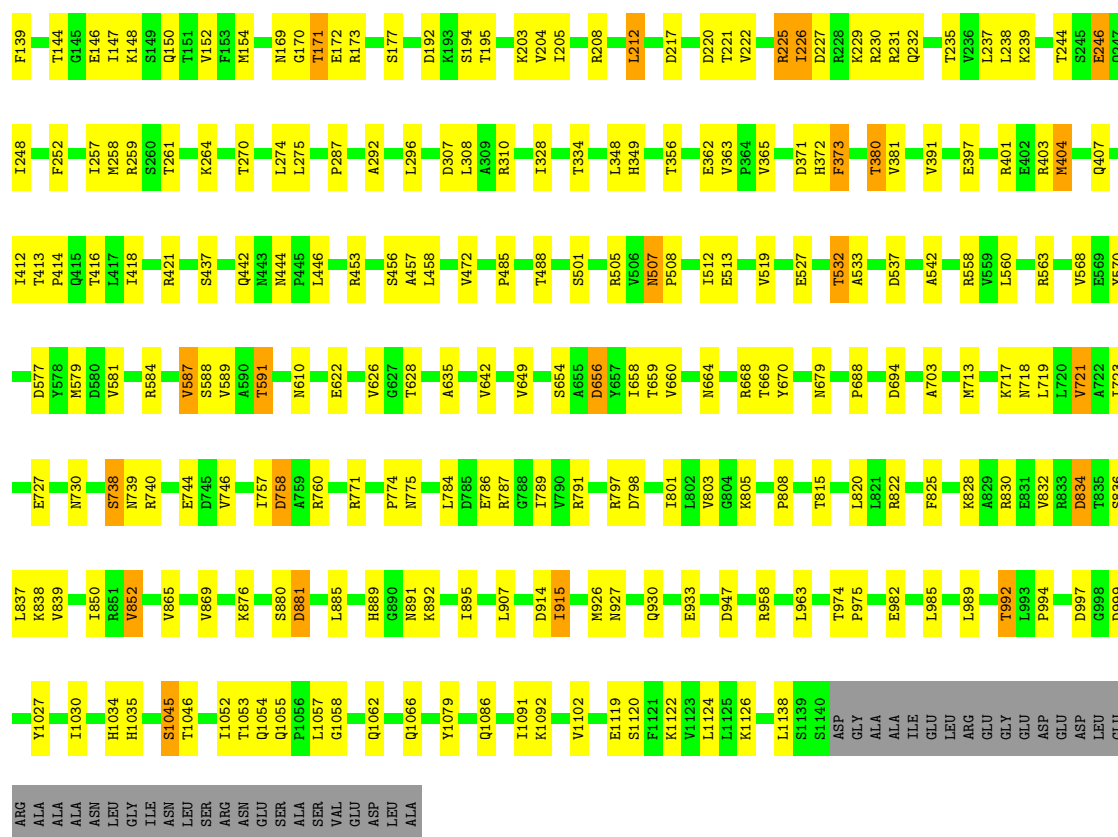


- Molecule 1: DNA-directed RNA polymerase subunit alpha

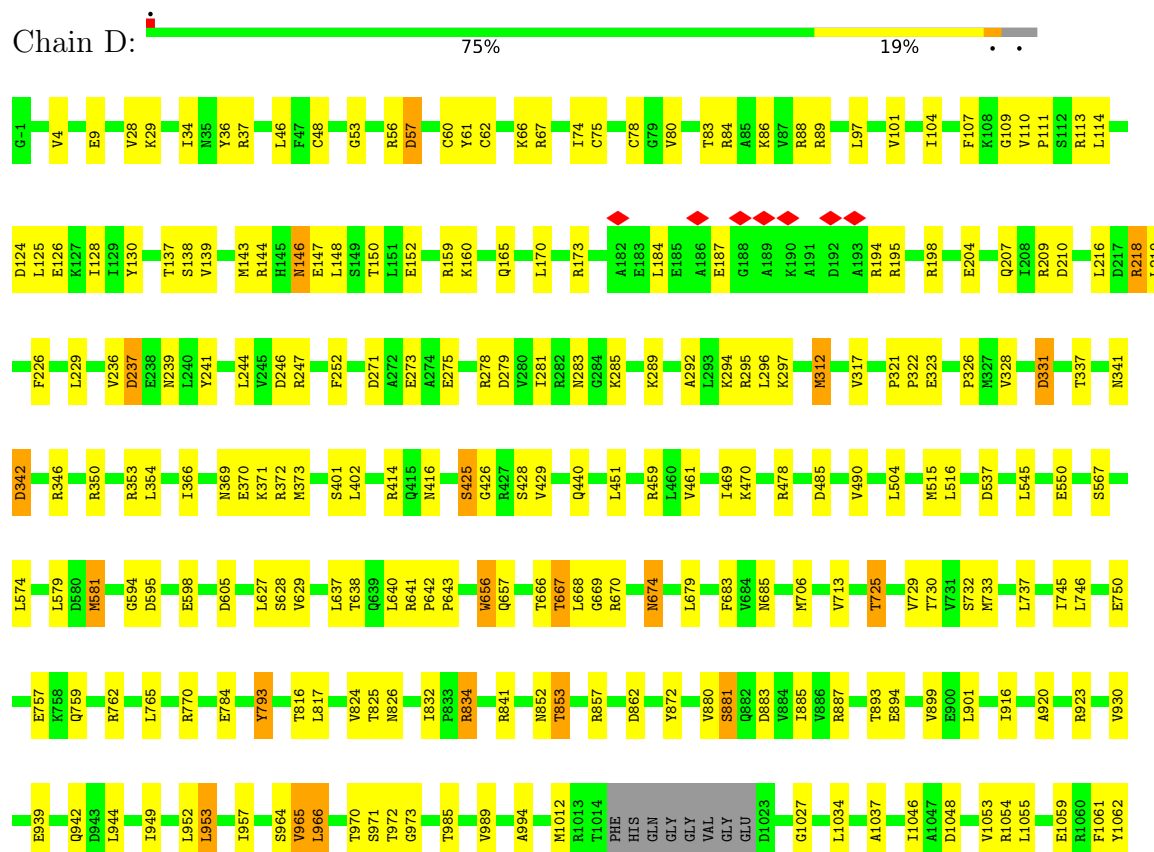


- Molecule 2: DNA-directed RNA polymerase subunit beta

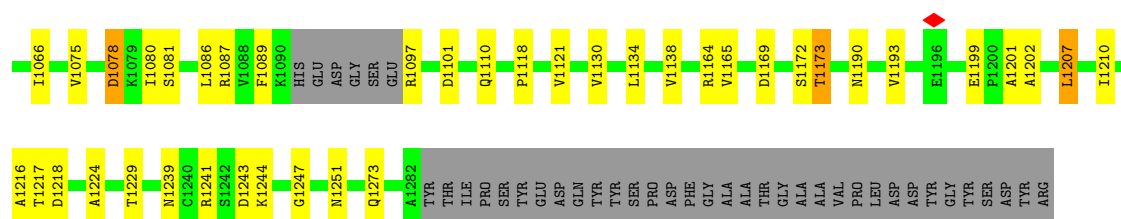




• Molecule 3: DNA-directed RNA polymerase subunit beta'

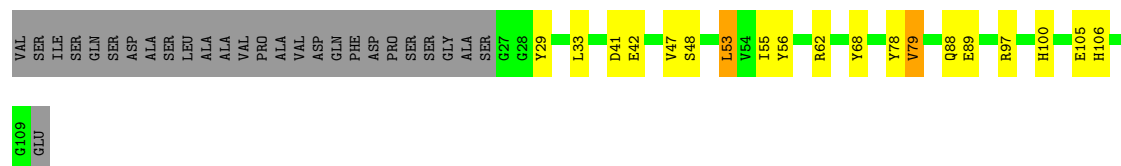






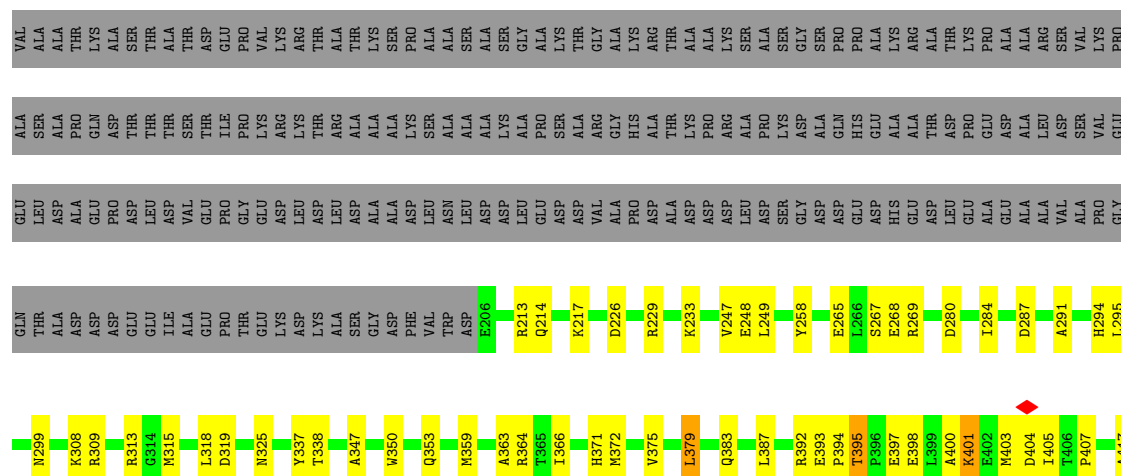
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 58% 15% 25%



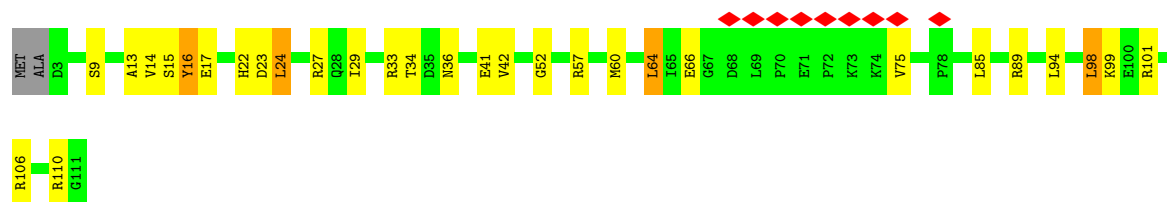
• Molecule 5: RNA polymerase sigma factor SigA

Chain F: 46% 14% 39%

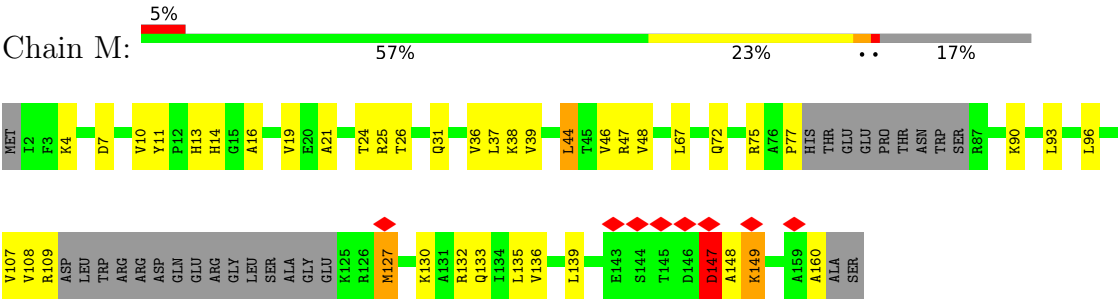


• Molecule 6: RNA polymerase-binding protein RbpA

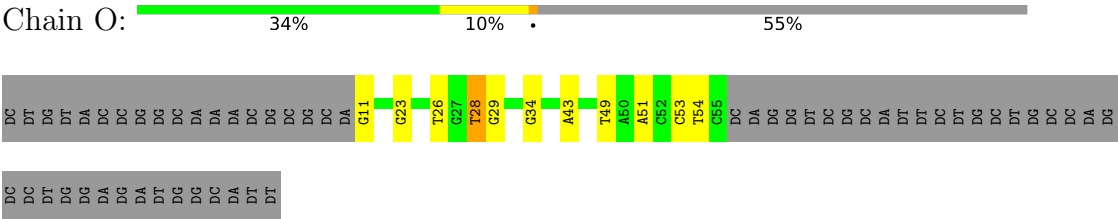
Chain J: 8% 71% 23%



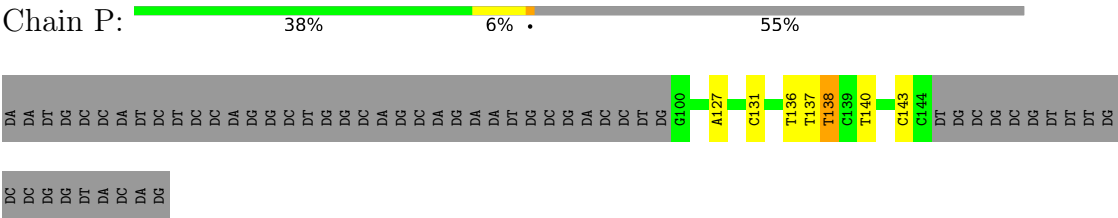
• Molecule 7: RNA polymerase-binding transcription factor CarD



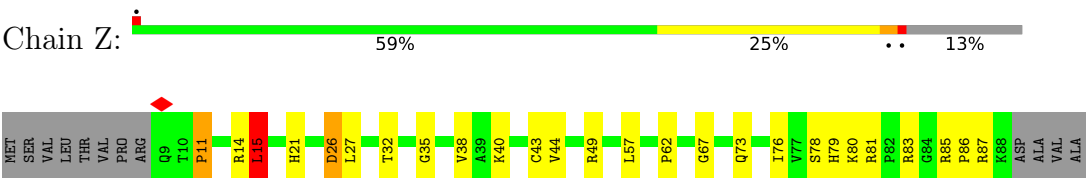
• Molecule 8: DNA (45-MER)



• Molecule 9: DNA (45-MER)



• Molecule 10: Probable transcriptional regulator WhiB7



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	35.858	Depositor
Minimum map value	-13.292	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.022	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	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, SF4

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	0.47	1/1742 (0.1%)	0.53	0/2370
1	B	0.41	0/1792	0.56	0/2442
2	C	0.46	0/8765	0.54	0/11885
3	D	0.44	0/10078	0.54	3/13624 (0.0%)
4	E	0.42	0/662	0.53	0/901
5	F	0.30	0/2575	0.46	0/3473
6	J	0.30	0/896	0.48	0/1210
7	M	0.26	0/1047	0.51	0/1411
8	O	0.92	0/1031	1.17	7/1590 (0.4%)
9	P	0.93	0/1034	1.12	4/1593 (0.3%)
10	Z	0.41	0/624	0.62	2/850 (0.2%)
All	All	0.48	1/30246 (0.0%)	0.60	16/41349 (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
3	D	0	1
4	E	0	1
7	M	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ASP	C-N	-5.61	1.21	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	131	DC	O4'-C1'-N1	7.36	113.15	108.00
8	O	28	DT	O4'-C1'-N1	7.29	113.10	108.00
10	Z	11	PRO	N-CA-CB	7.28	112.04	103.30
8	O	11	DG	O4'-C1'-N9	6.58	112.61	108.00
3	D	834	ARG	C-N-CD	-6.33	106.66	120.60
8	O	28	DT	C1'-O4'-C4'	-5.80	104.30	110.10
9	P	131	DC	C1'-O4'-C4'	-5.61	104.49	110.10
10	Z	15	LEU	CA-CB-CG	5.59	128.17	115.30
3	D	834	ARG	C-N-CA	5.22	143.94	122.00
8	O	34	DG	O4'-C1'-N9	5.22	111.66	108.00
3	D	965	VAL	C-N-CA	5.20	134.70	121.70
9	P	138	DT	O4'-C1'-N1	5.17	111.62	108.00
8	O	49	DT	C5-C4-O4	-5.13	121.31	124.90
8	O	49	DT	N3-C4-O4	5.13	122.98	119.90
9	P	143	DC	O4'-C4'-C3'	-5.12	102.45	104.50
8	O	26	DT	OP1-P-O3'	5.10	116.43	105.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1173	THR	Peptide
4	E	79	VAL	Peptide
7	M	147	ASP	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	1716	0	1756	23	0
1	B	1765	0	1794	24	0
2	C	8606	0	8544	132	0
3	D	9914	0	9986	154	0
4	E	649	0	645	8	0
5	F	2544	0	2558	48	0
6	J	880	0	852	20	0
7	M	1039	0	1081	25	0
8	O	920	0	508	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	922	0	505	4	0
10	Z	607	0	592	17	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
13	Z	8	0	0	1	0
All	All	29573	0	28821	415	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 7.

All (415) 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:183:VAL:HA	1:B:188:ASP:H	1.56	0.69
3:D:61:TYR:HB3	3:D:78:CYS:HB2	1.74	0.68
5:F:502:ARG:HD3	8:O:23:DG:H2'	1.74	0.68
2:C:656:ASP:OD1	2:C:656:ASP:N	2.28	0.66
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.79	0.63
3:D:670:ARG:O	3:D:674:ASN:HB2	1.98	0.62
2:C:225:ARG:HD2	2:C:231:ARG:HG2	1.81	0.62
5:F:265:GLU:HG3	5:F:269:ARG:HH22	1.63	0.62
10:Z:43:CYS:O	10:Z:49:ARG:NH1	2.33	0.62
2:C:719:LEU:HD12	2:C:1030:ILE:HD11	1.81	0.62
3:D:312:MET:SD	3:D:312:MET:N	2.74	0.61
7:M:75:ARG:HD3	7:M:160:ALA:HB1	1.82	0.60
3:D:241:TYR:HA	3:D:244:LEU:HD12	1.84	0.60
2:C:892:LYS:NZ	3:D:537:ASP:O	2.34	0.60
3:D:170:LEU:HD21	3:D:209:ARG:HB3	1.83	0.59
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.85	0.59
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.85	0.59
6:J:29:ILE:HD11	6:J:41:GLU:HB3	1.83	0.59
2:C:881:ASP:N	2:C:881:ASP:OD1	2.35	0.59
2:C:1055:GLN:NE2	3:D:416:ASN:OD1	2.35	0.59
3:D:1061:PHE:HB2	3:D:1081:SER:HA	1.85	0.59
2:C:822:ARG:NH1	2:C:828:LYS:O	2.36	0.58
2:C:380:THR:OG1	2:C:381:VAL:N	2.33	0.58
2:C:588:SER:OG	2:C:589:VAL:N	2.36	0.58
2:C:758:ASP:N	2:C:758:ASP:OD1	2.36	0.58
3:D:195:ARG:HD3	3:D:198:ARG:HD2	1.85	0.58
5:F:392:ARG:NH1	5:F:393:GLU:O	2.36	0.58
2:C:453:ARG:NH2	2:C:501:SER:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:401:SER:OG	3:D:402:LEU:N	2.36	0.58
2:C:798:ASP:O	3:D:478:ARG:NH2	2.36	0.58
3:D:125:LEU:HD12	3:D:128:ILE:HD12	1.85	0.58
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.86	0.57
5:F:359:MET:O	5:F:363:ALA:HB2	2.04	0.57
1:A:9:LEU:H	1:B:221:LEU:HD11	1.70	0.57
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.87	0.57
2:C:507:ASN:ND2	2:C:513:GLU:OE2	2.36	0.57
3:D:187:GLU:O	3:D:194:ARG:NH1	2.38	0.57
2:C:147:ILE:HD13	7:M:25:ARG:HH12	1.70	0.57
3:D:834:ARG:O	3:D:834:ARG:NH1	2.38	0.57
1:A:183:VAL:HG13	1:A:185:GLN:H	1.70	0.57
3:D:440:GLN:NE2	3:D:515:MET:SD	2.78	0.57
5:F:504:ARG:NH1	9:P:127:DA:OP2	2.37	0.57
1:A:72:ASP:OD1	1:A:72:ASP:N	2.36	0.57
1:B:95:MET:HB2	1:B:138:LEU:HB2	1.87	0.57
2:C:252:PHE:O	2:C:259:ARG:NH1	2.37	0.57
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.38	0.56
3:D:143:MET:SD	3:D:143:MET:N	2.78	0.56
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.38	0.56
2:C:147:ILE:HD11	7:M:47:ARG:HD3	1.87	0.56
6:J:64:LEU:HD22	6:J:66:GLU:HG2	1.86	0.56
2:C:128:THR:HG22	2:C:169:ASN:H	1.68	0.56
2:C:403:ARG:NH1	2:C:416:THR:O	2.39	0.56
2:C:532:THR:OG1	2:C:533:ALA:N	2.37	0.56
3:D:83:THR:OG1	3:D:84:ARG:N	2.38	0.56
2:C:208:ARG:NH2	2:C:307:ASP:OD2	2.38	0.56
3:D:825:THR:OG1	3:D:826:ASN:N	2.39	0.56
10:Z:67:GLY:N	13:Z:101:SF4:S2	2.77	0.56
2:C:622:GLU:OE2	2:C:718:ASN:ND2	2.36	0.56
1:A:98:ARG:NH1	1:A:135:GLU:OE1	2.39	0.56
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.87	0.56
5:F:315:MET:SD	5:F:315:MET:N	2.79	0.56
1:B:17:ASN:OD1	1:B:17:ASN:N	2.38	0.56
2:C:97:GLU:O	2:C:401:ARG:NH1	2.39	0.56
3:D:57:ASP:OD1	3:D:57:ASP:N	2.36	0.56
2:C:120:ASP:OD1	2:C:120:ASP:N	2.40	0.55
2:C:456:SER:OG	2:C:457:ALA:N	2.38	0.55
2:C:577:ASP:OD1	2:C:577:ASP:N	2.37	0.55
3:D:331:ASP:OD1	3:D:331:ASP:N	2.37	0.55
2:C:485:PRO:O	3:D:857:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:354:LEU:HD11	3:D:371:LYS:HG2	1.89	0.55
3:D:1062:TYR:N	3:D:1080:ILE:O	2.37	0.55
7:M:10:VAL:HA	7:M:16:ALA:HA	1.89	0.55
3:D:885:ILE:HD11	3:D:887:ARG:HH21	1.71	0.55
2:C:227:ASP:O	2:C:229:LYS:NZ	2.40	0.55
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.40	0.55
3:D:425:SER:OG	3:D:426:GLY:N	2.37	0.55
5:F:429:ASP:N	5:F:429:ASP:OD1	2.39	0.55
7:M:11:TYR:HD2	7:M:14:HIS:H	1.54	0.55
3:D:354:LEU:HD12	3:D:370:GLU:HG3	1.89	0.55
3:D:1218:ASP:O	3:D:1241:ARG:NH2	2.39	0.55
5:F:249:LEU:HD22	5:F:291:ALA:HB1	1.88	0.55
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.88	0.54
3:D:53:GLY:O	3:D:88:ARG:NH1	2.40	0.54
2:C:310:ARG:HB3	2:C:328:ILE:HD13	1.90	0.54
3:D:970:THR:OG1	3:D:973:GLY:O	2.25	0.54
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.36	0.54
10:Z:44:VAL:O	10:Z:49:ARG:NH2	2.40	0.54
2:C:373:PHE:HE2	2:C:512:ILE:HD12	1.72	0.54
3:D:279:ASP:OD1	3:D:283:ASN:ND2	2.41	0.54
6:J:60:MET:SD	6:J:60:MET:N	2.80	0.54
2:C:994:PRO:HB3	2:C:999:ASP:H	1.73	0.53
2:C:444:ASN:N	2:C:444:ASN:OD1	2.39	0.53
3:D:342:ASP:N	3:D:342:ASP:OD1	2.42	0.53
1:B:17:ASN:ND2	1:B:198:THR:O	2.41	0.53
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.38	0.53
7:M:67:LEU:HD22	7:M:139:LEU:HD23	1.89	0.53
3:D:1239:ASN:HB2	3:D:1241:ARG:HG3	1.90	0.53
5:F:521:GLN:OE1	10:Z:21:HIS:ND1	2.35	0.53
10:Z:15:LEU:O	10:Z:21:HIS:NE2	2.42	0.53
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.40	0.53
2:C:230:ARG:O	2:C:232:GLN:NE2	2.41	0.53
3:D:36:TYR:OH	3:D:37:ARG:NH2	2.41	0.53
3:D:952:LEU:HD22	3:D:957:ILE:HD11	1.90	0.53
5:F:502:ARG:NE	8:O:23:DG:OP2	2.38	0.53
2:C:173:ARG:NH1	2:C:437:SER:O	2.42	0.53
2:C:659:THR:HG22	2:C:669:THR:HG22	1.91	0.53
7:M:96:LEU:HG	7:M:107:VAL:HG21	1.90	0.53
2:C:171:THR:OG1	2:C:172:GLU:N	2.40	0.52
2:C:239:LYS:HG2	2:C:244:THR:HA	1.91	0.52
3:D:428:SER:OG	3:D:429:VAL:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:THR:O	1:B:45:SER:HB3	2.09	0.52
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.91	0.52
3:D:1218:ASP:OD1	3:D:1218:ASP:N	2.43	0.52
2:C:1045:SER:OG	2:C:1046:THR:N	2.41	0.52
1:B:45:SER:O	1:B:144:ARG:NH1	2.43	0.52
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.42	0.52
3:D:246:ASP:OD1	3:D:247:ARG:NH1	2.43	0.52
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.42	0.51
3:D:66:LYS:O	3:D:67:ARG:NH1	2.43	0.51
3:D:294:LYS:HA	3:D:297:LYS:HE3	1.92	0.51
5:F:247:VAL:HG13	5:F:337:TYR:HB2	1.91	0.51
5:F:465:ASP:OD1	5:F:476:ARG:NH2	2.43	0.51
3:D:148:LEU:O	3:D:152:GLU:HB3	2.10	0.51
7:M:108:VAL:HB	7:M:132:ARG:HE	1.75	0.51
2:C:775:ASN:N	2:C:775:ASN:OD1	2.42	0.51
2:C:836:SER:O	2:C:838:LYS:NZ	2.44	0.51
3:D:893:THR:OG1	3:D:894:GLU:N	2.43	0.51
5:F:517:PRO:HA	5:F:520:SER:HB3	1.92	0.51
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.92	0.51
2:C:758:ASP:O	2:C:805:LYS:NZ	2.41	0.51
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.39	0.51
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.93	0.51
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.91	0.51
3:D:184:LEU:O	3:D:194:ARG:NH1	2.43	0.51
3:D:459:ARG:NH2	4:E:88:GLN:OE1	2.43	0.51
5:F:309:ARG:O	5:F:313:ARG:NH2	2.43	0.51
10:Z:80:LYS:NZ	10:Z:81:ARG:O	2.41	0.51
3:D:56:ARG:HG2	6:J:13:ALA:H	1.76	0.51
3:D:1066:ILE:HB	3:D:1075:VAL:HB	1.93	0.51
2:C:146:GLU:O	2:C:148:LYS:NZ	2.41	0.51
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.43	0.51
2:C:217:ASP:OD1	2:C:221:THR:OG1	2.30	0.50
3:D:939:GLU:OE2	3:D:942:GLN:NE2	2.38	0.50
7:M:147:ASP:O	7:M:149:LYS:N	2.44	0.50
3:D:1046:ILE:HA	3:D:1110:GLN:HA	1.92	0.50
7:M:127:MET:SD	7:M:127:MET:N	2.75	0.50
3:D:1273:GLN:NE2	4:E:105:GLU:OE2	2.44	0.50
5:F:522:VAL:HG23	5:F:523:LEU:HG	1.93	0.50
3:D:759:GLN:HG2	3:D:762:ARG:HH21	1.76	0.50
6:J:52:GLY:HA2	6:J:64:LEU:HD12	1.93	0.50
10:Z:78:SER:OG	10:Z:79:HIS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:740:ARG:NH2	2:C:914:ASP:OD2	2.35	0.50
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.45	0.50
3:D:1169:ASP:HB2	3:D:1202:ALA:H	1.77	0.50
3:D:1034:LEU:HD13	3:D:1138:VAL:HG22	1.94	0.49
5:F:226:ASP:N	5:F:226:ASP:OD1	2.45	0.49
1:A:64:THR:OG1	1:A:65:THR:N	2.44	0.49
3:D:97:LEU:HD11	3:D:317:VAL:HG23	1.94	0.49
6:J:33:ARG:NH1	6:J:34:THR:O	2.45	0.49
9:P:136:DT:O2	10:Z:83:ARG:NH1	2.46	0.49
3:D:281:ILE:HA	3:D:289:LYS:HG3	1.95	0.49
1:A:57:ASP:OD1	1:A:57:ASP:N	2.37	0.49
5:F:518:SER:HA	10:Z:21:HIS:HB3	1.93	0.49
2:C:1052:ILE:HG22	3:D:326:PRO:HG3	1.93	0.49
1:B:149:ALA:N	1:B:165:ASP:OD1	2.45	0.49
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.43	0.49
3:D:832:ILE:HG22	3:D:834:ARG:H	1.77	0.49
3:D:916:ILE:HG23	3:D:920:ALA:HB3	1.94	0.49
5:F:248:GLU:OE2	6:J:101:ARG:NH1	2.46	0.49
5:F:397:GLU:HA	5:F:407:PRO:HG3	1.95	0.49
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.94	0.48
1:A:51:VAL:HG21	1:A:138:LEU:HD23	1.96	0.48
3:D:275:GLU:OE2	3:D:278:ARG:NH1	2.45	0.48
3:D:923:ARG:HD3	3:D:964:SER:HB2	1.96	0.48
5:F:519:ARG:NH2	10:Z:26:ASP:OD1	2.46	0.48
6:J:15:SER:OG	6:J:16:TYR:N	2.46	0.48
7:M:136:VAL:HA	7:M:139:LEU:HB2	1.95	0.48
9:P:140:DT:OP2	10:Z:87:ARG:NH2	2.47	0.48
3:D:237:ASP:OD1	3:D:239:ASN:ND2	2.42	0.48
3:D:883:ASP:OD1	3:D:883:ASP:N	2.46	0.48
7:M:90:LYS:HE2	8:O:51:DA:H2'	1.96	0.48
2:C:275:LEU:HB2	2:C:287:PRO:HB2	1.95	0.48
2:C:774:PRO:HD2	2:C:834:ASP:HB2	1.96	0.48
1:A:165:ASP:N	1:A:165:ASP:OD1	2.44	0.48
3:D:144:ARG:NH1	3:D:226:PHE:O	2.47	0.48
3:D:899:VAL:HG12	3:D:901:LEU:HB2	1.95	0.48
7:M:77:PRO:O	7:M:109:ARG:NH1	2.44	0.48
3:D:550:GLU:OE1	4:E:62:ARG:NH2	2.46	0.48
5:F:347:ALA:HA	5:F:350:TRP:HD1	1.79	0.48
10:Z:32:THR:HG22	10:Z:35:GLY:H	1.79	0.48
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.96	0.48
2:C:135:VAL:HG13	2:C:154:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1066:GLN:OE1	3:D:425:SER:OG	2.31	0.47
3:D:139:VAL:HA	3:D:252:PHE:HA	1.96	0.47
2:C:221:THR:O	2:C:231:ARG:NH2	2.47	0.47
5:F:442:SER:HB3	6:J:9:SER:HB3	1.95	0.47
1:A:10:SER:OG	1:A:11:GLU:N	2.47	0.47
1:A:10:SER:HB3	1:A:22:VAL:HG13	1.95	0.47
2:C:828:LYS:HZ2	2:C:830:ARG:HA	1.80	0.47
3:D:124:ASP:OD1	3:D:124:ASP:N	2.45	0.47
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.41	0.47
8:O:53:DC:H2''	8:O:54:DT:H5''	1.96	0.47
2:C:55:ASP:N	2:C:55:ASP:OD1	2.46	0.47
3:D:160:LYS:O	3:D:160:LYS:NZ	2.42	0.47
3:D:292:ALA:O	3:D:296:LEU:HB2	2.15	0.47
2:C:220:ASP:HB2	2:C:257:ILE:HG23	1.96	0.47
4:E:55:ILE:HD13	4:E:55:ILE:HA	1.77	0.47
5:F:371:HIS:CE1	8:O:43:DA:H3'	2.50	0.47
1:B:120:ASN:N	1:B:120:ASN:OD1	2.48	0.47
1:A:79:ASN:ND2	1:A:125:ILE:O	2.47	0.47
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.97	0.47
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.41	0.47
3:D:273:GLU:OE2	3:D:295:ARG:NH2	2.43	0.47
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.96	0.46
5:F:379:LEU:O	5:F:383:GLN:HB3	2.14	0.46
2:C:1057:LEU:HD23	2:C:1062:GLN:HG3	1.96	0.46
2:C:738:SER:OG	2:C:739:ASN:N	2.47	0.46
2:C:98:ASP:OD1	2:C:98:ASP:N	2.42	0.46
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.97	0.46
3:D:353:ARG:HH12	5:F:319:ASP:HA	1.80	0.46
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.49	0.46
2:C:507:ASN:HD22	2:C:508:PRO:HD2	1.80	0.46
6:J:36:ASN:OD1	6:J:36:ASN:N	2.41	0.46
3:D:218:ARG:HH21	3:D:219:LEU:HG	1.80	0.46
3:D:971:SER:OG	3:D:972:THR:N	2.49	0.46
10:Z:26:ASP:OD1	10:Z:26:ASP:N	2.48	0.46
2:C:152:VAL:HG21	2:C:418:ILE:HD12	1.98	0.46
6:J:24:LEU:HG	6:J:27:ARG:HH22	1.80	0.46
9:P:137:DT:H2''	9:P:138:DT:H2'	1.98	0.46
2:C:356:THR:HG22	2:C:362:GLU:HB3	1.97	0.46
3:D:139:VAL:HG21	3:D:229:LEU:HB3	1.97	0.46
5:F:258:TYR:HB3	6:J:98:LEU:HD13	1.98	0.46
3:D:86:LYS:HE3	3:D:86:LYS:HB3	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:605:ASP:OD1	3:D:605:ASP:N	2.44	0.45
2:C:1053:THR:OG1	2:C:1054:GLN:N	2.50	0.45
3:D:1224:ALA:HB1	3:D:1229:THR:HG23	1.97	0.45
2:C:239:LYS:HB3	2:C:270:THR:HA	1.97	0.45
2:C:717:LYS:NZ	2:C:746:VAL:O	2.42	0.45
3:D:537:ASP:OD1	3:D:537:ASP:N	2.46	0.45
7:M:135:LEU:O	7:M:139:LEU:N	2.49	0.45
2:C:111:ARG:N	2:C:134:PHE:O	2.50	0.45
2:C:926:MET:SD	3:D:816:THR:OG1	2.69	0.45
2:C:1126:LYS:HA	2:C:1126:LYS:HD3	1.69	0.45
1:A:225:LEU:HD12	1:B:9:LEU:HD21	1.98	0.45
3:D:173:ARG:NH1	3:D:204:GLU:OE1	2.50	0.45
5:F:525:ASP:OD1	5:F:525:ASP:N	2.47	0.45
2:C:127:MET:O	2:C:170:GLY:N	2.48	0.45
7:M:72:GLN:HA	7:M:75:ARG:HG2	1.98	0.45
2:C:192:ASP:OD2	2:C:194:SER:OG	2.34	0.45
3:D:29:LYS:HB3	3:D:29:LYS:HE2	1.77	0.45
3:D:642:PRO:HD2	3:D:657:GLN:HG3	1.99	0.45
6:J:85:LEU:HD11	6:J:94:LEU:HD21	1.98	0.45
8:O:28:DT:H4'	8:O:29:DG:H5'	1.98	0.45
2:C:372:HIS:NE2	2:C:537:ASP:OD2	2.48	0.44
3:D:1190:ASN:HD21	3:D:1201:ALA:HB3	1.81	0.44
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.50	0.44
1:A:87:SER:OG	1:A:88:GLU:N	2.50	0.44
3:D:28:VAL:HG21	3:D:46:LEU:HD23	1.99	0.44
3:D:757:GLU:OE1	3:D:770:ARG:NH1	2.43	0.44
5:F:383:GLN:NE2	5:F:393:GLU:OE2	2.51	0.44
2:C:139:PHE:HB3	2:C:414:PRO:HD3	1.98	0.44
1:A:97:LEU:HB3	1:A:136:VAL:HG13	1.99	0.44
2:C:1119:GLU:HA	2:C:1122:LYS:HE3	1.99	0.44
3:D:746:LEU:O	3:D:750:GLU:HB2	2.17	0.44
1:B:70:LYS:HD3	1:B:127:THR:HB	1.99	0.44
3:D:369:ASN:OD1	3:D:372:ARG:NH2	2.51	0.44
3:D:746:LEU:HD23	3:D:746:LEU:HA	1.82	0.44
10:Z:62:PRO:HA	10:Z:73:GLN:HA	2.00	0.44
2:C:235:THR:HA	2:C:238:LEU:HB2	2.00	0.44
2:C:820:LEU:HD13	5:F:481:LEU:HD11	1.99	0.44
3:D:641:ARG:HA	3:D:657:GLN:HG3	2.00	0.44
2:C:542:ALA:HB3	2:C:579:MET:HA	1.98	0.44
2:C:885:LEU:HD13	2:C:895:ILE:HD11	2.00	0.44
2:C:927:ASN:OD1	2:C:930:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:504:LEU:HD13	3:D:504:LEU:HA	1.87	0.44
3:D:1053:VAL:HG23	3:D:1066:ILE:HG23	1.99	0.44
2:C:668:ARG:NH1	2:C:670:TYR:OH	2.50	0.44
3:D:111:PRO:O	3:D:113:ARG:NH1	2.51	0.44
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.92	0.44
5:F:338:THR:H	6:J:89:ARG:HH22	1.66	0.44
5:F:503:ILE:HD13	5:F:503:ILE:HA	1.85	0.44
2:C:348:LEU:HD13	2:C:365:VAL:HG12	2.00	0.44
2:C:771:ARG:NH1	2:C:784:LEU:O	2.49	0.44
3:D:567:SER:HB3	3:D:574:LEU:HG	1.99	0.44
3:D:581:MET:H	3:D:581:MET:HG2	1.41	0.44
2:C:760:ARG:HA	2:C:865:VAL:HA	2.00	0.43
2:C:947:ASP:OD1	2:C:947:ASP:N	2.44	0.43
3:D:595:ASP:N	3:D:598:GLU:OE2	2.44	0.43
2:C:203:LYS:HE2	2:C:205:ILE:HD11	1.99	0.43
2:C:274:LEU:HG	2:C:292:ALA:HB1	1.99	0.43
3:D:1089:PHE:O	3:D:1097:ARG:N	2.51	0.43
10:Z:15:LEU:HB2	10:Z:21:HIS:CE1	2.53	0.43
2:C:587:VAL:HG22	2:C:591:THR:HB	1.99	0.43
3:D:1012:MET:HG2	3:D:1027:GLY:HA3	2.00	0.43
5:F:463:VAL:O	5:F:466:THR:OG1	2.25	0.43
6:J:23:ASP:OD1	6:J:23:ASP:N	2.40	0.43
2:C:801:ILE:HD13	2:C:838:LYS:HG2	2.00	0.43
3:D:881:SER:O	3:D:881:SER:OG	2.30	0.43
3:D:1055:LEU:N	3:D:1101:ASP:OD1	2.50	0.43
5:F:422:SER:O	5:F:425:GLN:NE2	2.49	0.43
5:F:422:SER:OG	5:F:423:LEU:N	2.51	0.43
2:C:150:GLN:HE21	7:M:44:LEU:HB3	1.84	0.43
2:C:238:LEU:HD13	2:C:248:ILE:HG12	1.99	0.43
2:C:985:LEU:HD23	2:C:985:LEU:HA	1.84	0.43
3:D:516:LEU:HD13	3:D:516:LEU:HA	1.83	0.43
2:C:992:THR:O	2:C:992:THR:OG1	2.36	0.43
3:D:147:GLU:OE1	3:D:150:THR:OG1	2.30	0.43
3:D:159:ARG:HH11	3:D:216:LEU:HB3	1.84	0.43
5:F:372:MET:HA	5:F:375:VAL:HG22	2.01	0.43
1:A:71:GLU:HB3	1:A:75:GLU:HB3	2.00	0.43
3:D:229:LEU:HD12	3:D:229:LEU:HA	1.85	0.43
3:D:346:ARG:O	3:D:350:ARG:HG2	2.19	0.43
1:A:226:ASN:OD1	1:A:226:ASN:N	2.51	0.43
1:B:97:LEU:HD22	1:B:110:ILE:HD12	2.01	0.43
5:F:400:ALA:O	5:F:404:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:21:ALA:H	7:M:36:VAL:HG22	1.84	0.43
3:D:1086:LEU:HD12	3:D:1086:LEU:HA	1.91	0.43
3:D:1243:ASP:OD1	3:D:1244:LYS:N	2.51	0.43
2:C:264:LYS:HA	2:C:264:LYS:HD2	1.92	0.43
2:C:852:VAL:HB	2:C:869:VAL:HG23	1.99	0.43
6:J:106:ARG:O	6:J:110:ARG:HB3	2.19	0.43
1:A:120:ASN:OD1	1:A:120:ASN:N	2.52	0.42
1:B:57:ASP:OD1	1:B:57:ASP:N	2.52	0.42
2:C:963:LEU:HD23	2:C:963:LEU:HA	1.82	0.42
3:D:366:ILE:HG23	5:F:325:ASN:HD22	1.83	0.42
1:A:175:THR:OG1	1:A:176:TYR:N	2.52	0.42
3:D:793:TYR:HD1	3:D:793:TYR:HA	1.72	0.42
3:D:1172:SER:HB3	3:D:1199:GLU:HB3	2.02	0.42
7:M:24:THR:HB	7:M:31:GLN:HB3	2.01	0.42
2:C:244:THR:OG1	2:C:246:GLU:OE2	2.37	0.42
2:C:694:ASP:OD1	2:C:694:ASP:N	2.51	0.42
3:D:74:ILE:HD13	6:J:42:VAL:HG13	2.00	0.42
3:D:656:TRP:HE3	3:D:656:TRP:H	1.68	0.42
2:C:558:ARG:NH2	2:C:570:TYR:O	2.51	0.42
3:D:373:MET:HE2	5:F:318:LEU:HD13	2.00	0.42
1:B:12:ASP:OD1	1:B:13:VAL:N	2.53	0.42
3:D:114:LEU:HG	3:D:312:MET:HG2	2.02	0.42
2:C:560:LEU:HD13	2:C:560:LEU:HA	1.84	0.42
3:D:146:ASN:ND2	3:D:147:GLU:OE2	2.50	0.42
3:D:1173:THR:O	3:D:1173:THR:OG1	2.27	0.42
5:F:295:LEU:O	5:F:299:ASN:ND2	2.40	0.42
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.87	0.42
1:B:182:ARG:HB3	1:B:186:ARG:HB2	2.02	0.42
3:D:1037:ALA:HB1	3:D:1207:LEU:HD21	2.02	0.42
5:F:267:SER:OG	5:F:268:GLU:N	2.53	0.42
10:Z:85:ARG:HD2	10:Z:86:PRO:HD2	2.02	0.42
6:J:52:GLY:O	6:J:64:LEU:N	2.52	0.42
1:B:75:GLU:O	1:B:79:ASN:HB2	2.19	0.42
2:C:43:LYS:HE2	2:C:958:ARG:HB3	2.02	0.42
2:C:446:LEU:HB2	2:C:713:MET:HE1	2.00	0.42
7:M:7:ASP:OD1	7:M:7:ASP:N	2.51	0.42
7:M:37:LEU:HB2	7:M:46:VAL:HB	2.01	0.42
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.52	0.42
3:D:737:LEU:N	3:D:793:TYR:OH	2.52	0.42
5:F:308:LYS:HE3	5:F:308:LYS:HB2	1.86	0.42
2:C:147:ILE:HG12	7:M:47:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:387:LEU:HB3	5:F:394:PRO:HD3	2.01	0.41
1:A:221:LEU:HD22	1:B:7:PRO:HG2	2.01	0.41
1:B:72:ASP:OD1	1:B:73:VAL:N	2.53	0.41
2:C:46:GLU:HA	2:C:47:PRO:HD3	1.90	0.41
2:C:407:GLN:HB3	2:C:412:ILE:HG21	2.02	0.41
2:C:876:LYS:HB2	2:C:876:LYS:HE3	1.87	0.41
3:D:706:MET:N	4:E:41:ASP:OD2	2.45	0.41
6:J:15:SER:OG	6:J:17:GLU:OE2	2.37	0.41
7:M:75:ARG:HD3	7:M:75:ARG:HA	1.86	0.41
2:C:727:GLU:HG2	3:D:725:THR:HG21	2.01	0.41
2:C:212:LEU:HA	2:C:226:ILE:HA	2.02	0.41
2:C:1138:LEU:HB2	3:D:9:GLU:HB2	2.02	0.41
3:D:1054:ARG:HD3	3:D:1054:ARG:HA	1.83	0.41
5:F:364:ARG:NH1	5:F:417:ALA:O	2.51	0.41
6:J:99:LYS:HA	6:J:99:LYS:HD2	1.85	0.41
7:M:11:TYR:HD2	7:M:13:HIS:H	1.67	0.41
7:M:130:LYS:HG2	7:M:133:GLN:HE21	1.86	0.41
1:A:130:ASP:OD1	1:A:130:ASP:N	2.50	0.41
2:C:258:MET:O	2:C:261:THR:OG1	2.27	0.41
2:C:642:VAL:HB	2:C:703:ALA:HB3	2.02	0.41
3:D:1172:SER:O	3:D:1172:SER:OG	2.33	0.41
1:B:84:VAL:HG22	1:B:119:HIS:HB2	2.03	0.41
2:C:771:ARG:HD2	2:C:786:GLU:HA	2.03	0.41
3:D:1134:LEU:HD12	3:D:1134:LEU:HA	1.83	0.41
3:D:137:THR:OG1	3:D:138:SER:N	2.54	0.41
3:D:666:THR:OG1	3:D:667:THR:O	2.37	0.41
2:C:81:ASN:OD1	2:C:81:ASN:N	2.53	0.41
3:D:461:VAL:HG21	3:D:469:ILE:HD13	2.02	0.41
3:D:594:GLY:N	3:D:598:GLU:OE2	2.53	0.41
1:B:90:ASP:OD1	1:B:90:ASP:N	2.54	0.41
2:C:654:SER:HG	2:C:656:ASP:H	1.65	0.41
2:C:880:SER:OG	2:C:881:ASP:N	2.53	0.41
3:D:294:LYS:HE2	3:D:294:LYS:HB3	1.91	0.41
3:D:628:SER:OG	3:D:629:VAL:N	2.53	0.41
3:D:745:ILE:HD13	3:D:784:GLU:HG3	2.02	0.41
5:F:214:GLN:HA	5:F:217:LYS:HE2	2.02	0.41
2:C:926:MET:HG2	3:D:817:LEU:HD12	2.02	0.41
5:F:395:THR:OG1	5:F:398:GLU:N	2.48	0.41
7:M:93:LEU:HA	7:M:96:LEU:HD12	2.02	0.41
1:B:20:GLN:O	1:B:20:GLN:NE2	2.52	0.40
2:C:568:VAL:HB	3:D:834:ARG:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:HIS:O	2:C:1035:HIS:ND1	2.54	0.40
3:D:667:THR:OG1	3:D:669:GLY:N	2.54	0.40
3:D:964:SER:OG	3:D:965:VAL:N	2.53	0.40
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	2.03	0.40
5:F:233:LYS:HA	5:F:233:LYS:HD3	1.94	0.40
10:Z:40:LYS:HB3	10:Z:40:LYS:HE2	1.89	0.40
1:B:80:LEU:HA	1:B:80:LEU:HD23	1.89	0.40
2:C:98:ASP:HB3	2:C:404:MET:HE1	2.04	0.40
2:C:103:MET:HB2	2:C:139:PHE:HE1	1.86	0.40
3:D:89:ARG:HA	3:D:323:GLU:HB2	2.03	0.40
3:D:109:GLY:O	3:D:113:ARG:NH1	2.54	0.40
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.90	0.40
5:F:398:GLU:O	5:F:401:LYS:NZ	2.48	0.40
2:C:1058:GLY:O	2:C:1062:GLN:NE2	2.55	0.40
3:D:126:GLU:HG2	3:D:130:TYR:HD2	1.87	0.40
3:D:637:LEU:HD13	3:D:640:LEU:HD12	2.04	0.40
3:D:953:LEU:HD13	3:D:953:LEU:HA	1.84	0.40
5:F:284:ILE:HD13	5:F:284:ILE:HA	1.99	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	223/347 (64%)	205 (92%)	18 (8%)	0	100	100
1	B	235/347 (68%)	211 (90%)	24 (10%)	0	100	100
2	C	1109/1172 (95%)	1012 (91%)	97 (9%)	0	100	100
3	D	1264/1318 (96%)	1185 (94%)	78 (6%)	1 (0%)	51	82
4	E	81/110 (74%)	77 (95%)	4 (5%)	0	100	100
5	F	320/528 (61%)	312 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	107/111 (96%)	102 (95%)	5 (5%)	0	100	100
7	M	129/162 (80%)	117 (91%)	10 (8%)	2 (2%)	9	37
10	Z	78/92 (85%)	63 (81%)	14 (18%)	1 (1%)	12	42
All	All	3546/4187 (85%)	3284 (93%)	258 (7%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	M	148	ALA
10	Z	11	PRO
3	D	966	LEU
7	M	147	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/297 (65%)	180 (93%)	14 (7%)	14	44
1	B	195/297 (66%)	182 (93%)	13 (7%)	16	47
2	C	937/993 (94%)	859 (92%)	78 (8%)	11	37
3	D	1048/1095 (96%)	981 (94%)	67 (6%)	17	48
4	E	69/90 (77%)	60 (87%)	9 (13%)	4	17
5	F	267/427 (62%)	253 (95%)	14 (5%)	23	54
6	J	92/97 (95%)	84 (91%)	8 (9%)	10	35
7	M	108/131 (82%)	99 (92%)	9 (8%)	11	37
10	Z	61/76 (80%)	54 (88%)	7 (12%)	5	22
All	All	2971/3503 (85%)	2752 (93%)	219 (7%)	17	42

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	30	PHE
1	A	51	VAL
1	A	65	THR
1	A	84	VAL
1	A	111	VAL
1	A	136	VAL
1	A	150	VAL
1	A	167	ILE
1	A	168	TYR
1	A	172	LEU
1	A	194	LEU
1	A	198	THR
1	A	215	LEU
1	B	20	GLN
1	B	22	VAL
1	B	30	PHE
1	B	34	LEU
1	B	69	VAL
1	B	74	THR
1	B	84	VAL
1	B	90	ASP
1	B	111	VAL
1	B	131	LYS
1	B	150	VAL
1	B	188	ASP
1	B	196	VAL
2	C	62	GLU
2	C	64	LEU
2	C	67	SER
2	C	80	VAL
2	C	81	ASN
2	C	86	LEU
2	C	103	MET
2	C	126	ASP
2	C	127	MET
2	C	144	THR
2	C	171	THR
2	C	177	SER
2	C	195	THR
2	C	204	VAL
2	C	212	LEU
2	C	222	VAL

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Mol	Chain	Res	Type
2	C	225	ARG
2	C	226	ILE
2	C	237	LEU
2	C	246	GLU
2	C	296	LEU
2	C	308	LEU
2	C	334	THR
2	C	349	HIS
2	C	363	VAL
2	C	371	ASP
2	C	373	PHE
2	C	380	THR
2	C	391	VAL
2	C	397	GLU
2	C	404	MET
2	C	421	ARG
2	C	458	LEU
2	C	472	VAL
2	C	488	THR
2	C	507	ASN
2	C	519	VAL
2	C	527	GLU
2	C	532	THR
2	C	563	ARG
2	C	581	VAL
2	C	584	ARG
2	C	587	VAL
2	C	591	THR
2	C	610	ASN
2	C	626	VAL
2	C	628	THR
2	C	649	VAL
2	C	656	ASP
2	C	660	VAL
2	C	664	ASN
2	C	721	VAL
2	C	723	ILE
2	C	730	ASN
2	C	738	SER
2	C	758	ASP
2	C	787	ARG
2	C	791	ARG

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Mol	Chain	Res	Type
2	C	797	ARG
2	C	815	THR
2	C	825	PHE
2	C	834	ASP
2	C	839	VAL
2	C	850	ILE
2	C	852	VAL
2	C	881	ASP
2	C	907	LEU
2	C	915	ILE
2	C	974	THR
2	C	989	LEU
2	C	992	THR
2	C	997	ASP
2	C	1027	TYR
2	C	1045	SER
2	C	1079	TYR
2	C	1086	GLN
2	C	1120	SER
2	C	1124	LEU
3	D	4	VAL
3	D	34	ILE
3	D	48	CYS
3	D	57	ASP
3	D	60	CYS
3	D	62	CYS
3	D	75	CYS
3	D	80	VAL
3	D	101	VAL
3	D	104	ILE
3	D	107	PHE
3	D	110	VAL
3	D	146	ASN
3	D	165	GLN
3	D	207	GLN
3	D	210	ASP
3	D	218	ARG
3	D	236	VAL
3	D	237	ASP
3	D	271	ASP
3	D	285	LYS
3	D	312	MET

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Mol	Chain	Res	Type
3	D	328	VAL
3	D	331	ASP
3	D	337	THR
3	D	341	ASN
3	D	342	ASP
3	D	414	ARG
3	D	425	SER
3	D	451	LEU
3	D	470	LYS
3	D	485	ASP
3	D	490	VAL
3	D	579	LEU
3	D	581	MET
3	D	627	LEU
3	D	638	THR
3	D	656	TRP
3	D	667	THR
3	D	668	LEU
3	D	674	ASN
3	D	679	LEU
3	D	713	VAL
3	D	725	THR
3	D	729	VAL
3	D	730	THR
3	D	732	SER
3	D	733	MET
3	D	765	LEU
3	D	793	TYR
3	D	853	THR
3	D	862	ASP
3	D	872	TYR
3	D	881	SER
3	D	930	VAL
3	D	944	LEU
3	D	953	LEU
3	D	966	LEU
3	D	985	THR
3	D	989	VAL
3	D	1048	ASP
3	D	1059	GLU
3	D	1078	ASP
3	D	1130	VAL

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Mol	Chain	Res	Type
3	D	1165	VAL
3	D	1193	VAL
3	D	1207	LEU
4	E	29	TYR
4	E	33	LEU
4	E	48	SER
4	E	53	LEU
4	E	56	TYR
4	E	68	TYR
4	E	78	TYR
4	E	79	VAL
4	E	106	HIS
5	F	213	ARG
5	F	229	ARG
5	F	280	ASP
5	F	287	ASP
5	F	294	HIS
5	F	353	GLN
5	F	366	ILE
5	F	379	LEU
5	F	395	THR
5	F	401	LYS
5	F	403	MET
5	F	405	ILE
5	F	446	VAL
5	F	488	THR
6	J	14	VAL
6	J	16	TYR
6	J	22	HIS
6	J	24	LEU
6	J	57	ARG
6	J	64	LEU
6	J	75	VAL
6	J	98	LEU
7	M	4	LYS
7	M	19	VAL
7	M	26	THR
7	M	38	LYS
7	M	39	VAL
7	M	44	LEU
7	M	48	VAL
7	M	127	MET

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Mol	Chain	Res	Type
7	M	149	LYS
10	Z	14	ARG
10	Z	15	LEU
10	Z	26	ASP
10	Z	27	LEU
10	Z	38	VAL
10	Z	57	LEU
10	Z	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	150	GLN
2	C	1055	GLN
2	C	1066	GLN
3	D	207	GLN
3	D	416	ASN
3	D	440	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	SF4	Z	101	10	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	Z	101	10	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

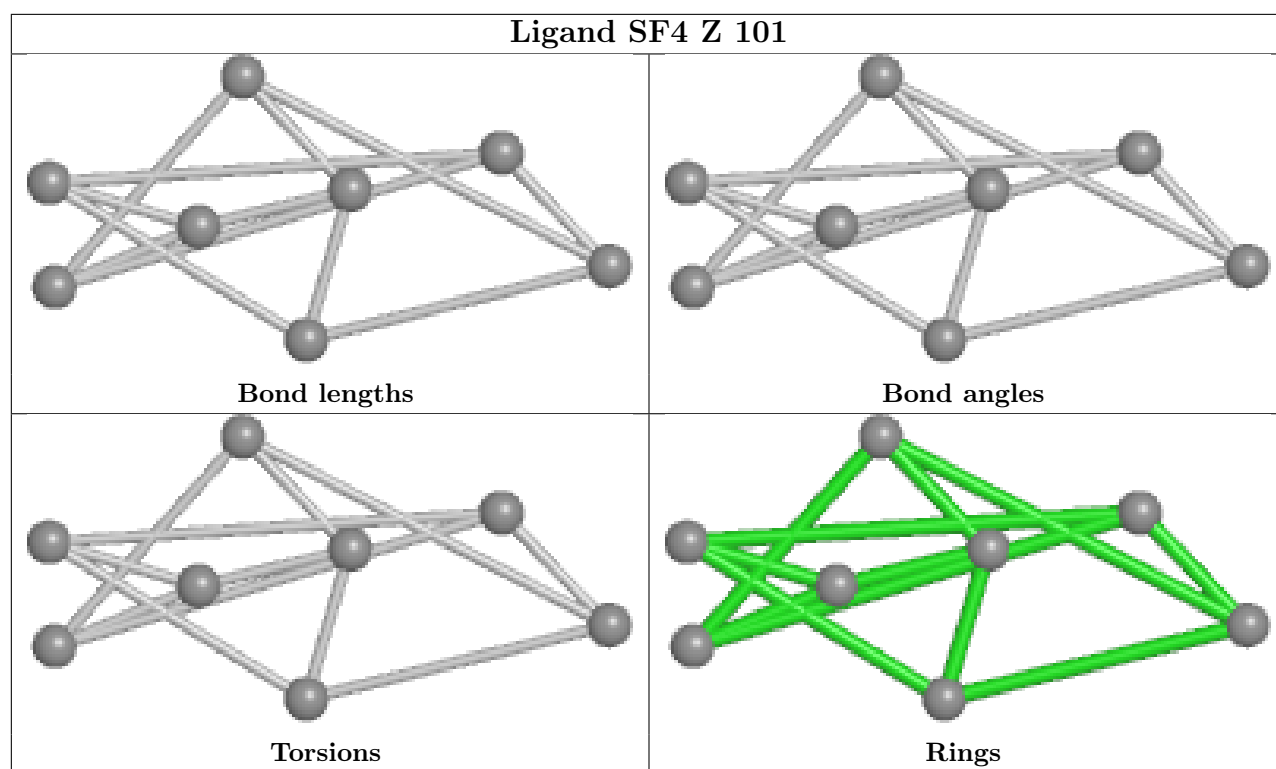
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Z	101	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

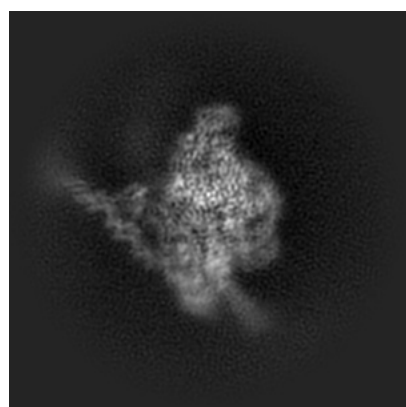
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22887. These allow visual inspection of the internal detail of the map and identification of artifacts.

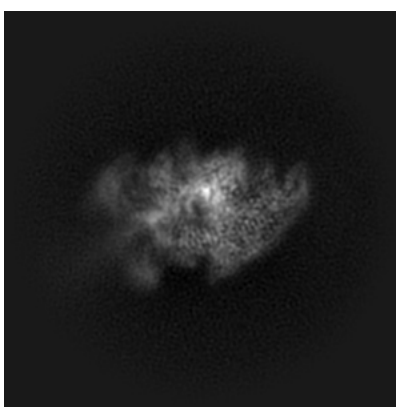
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

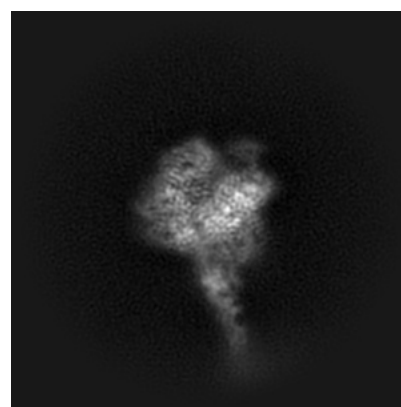
#### 6.1.1 Primary map



X



Y

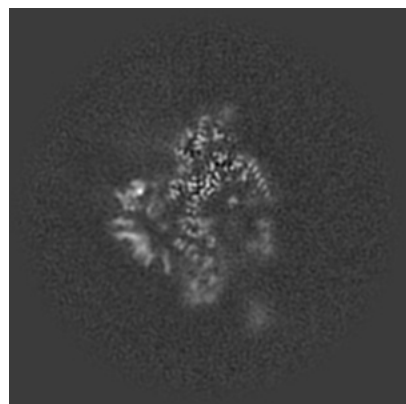


Z

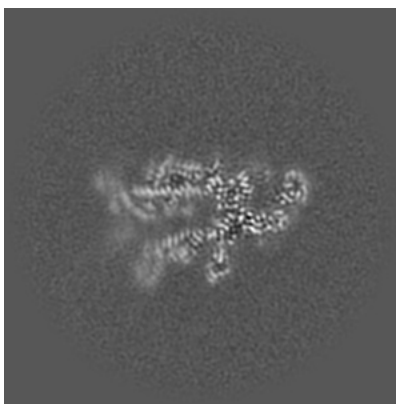
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

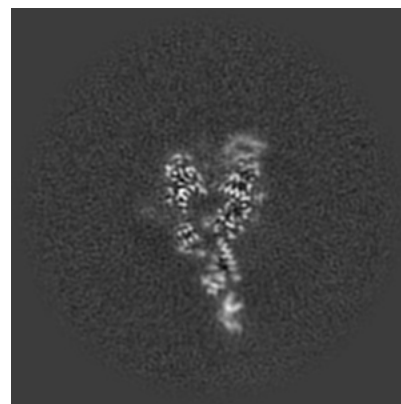
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

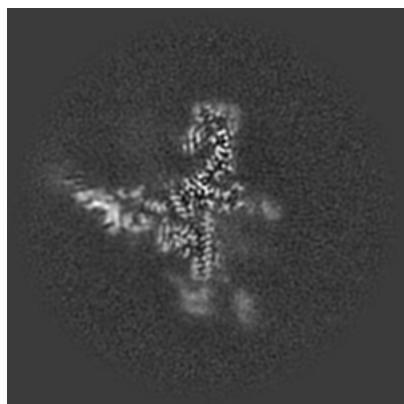


Z Index: 150

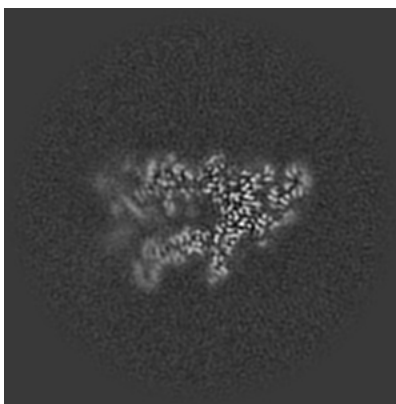
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

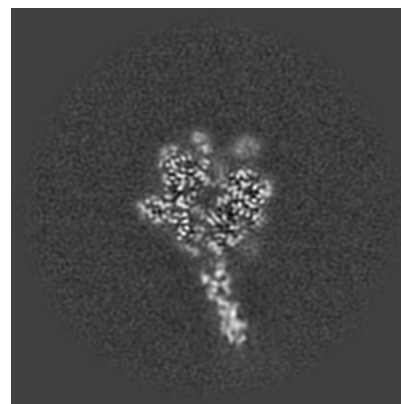
### 6.3.1 Primary map



X Index: 163



Y Index: 153

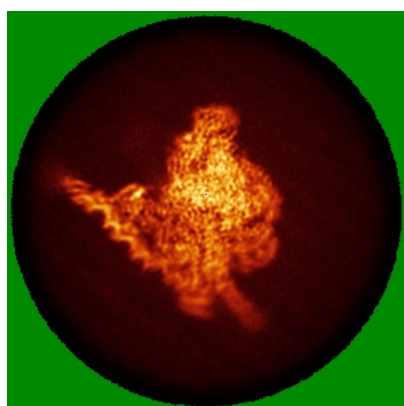


Z Index: 158

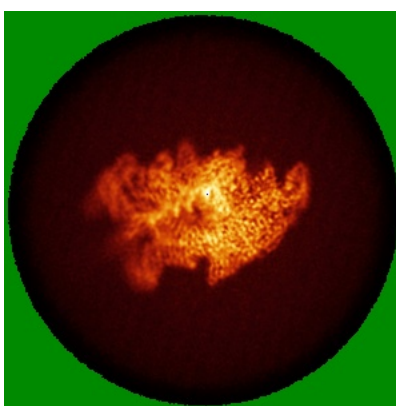
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

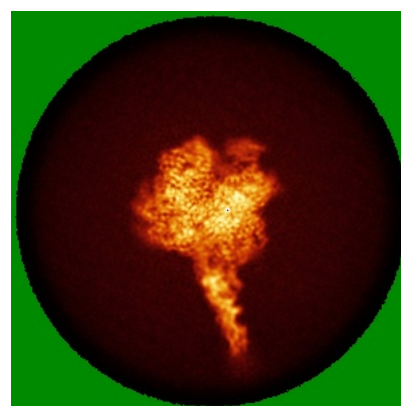
### 6.4.1 Primary map



X



Y

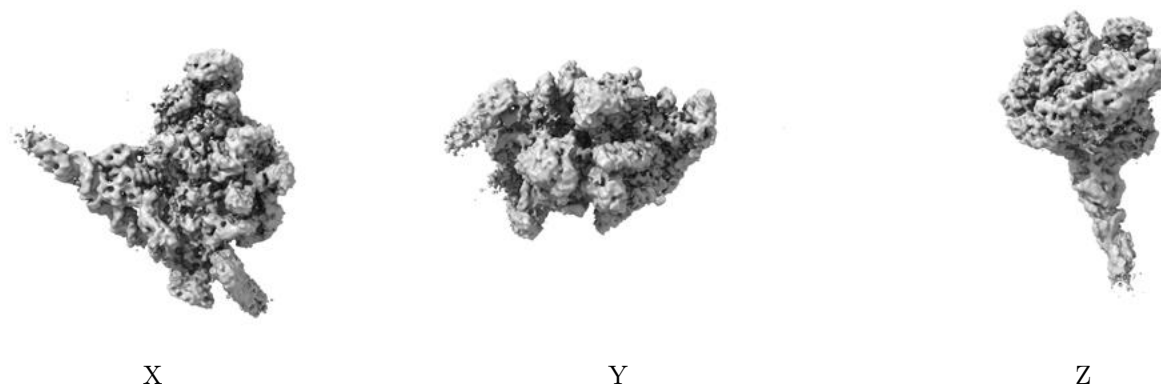


Z

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



The images above show the 3D surface view of the map at the recommended contour level 3.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

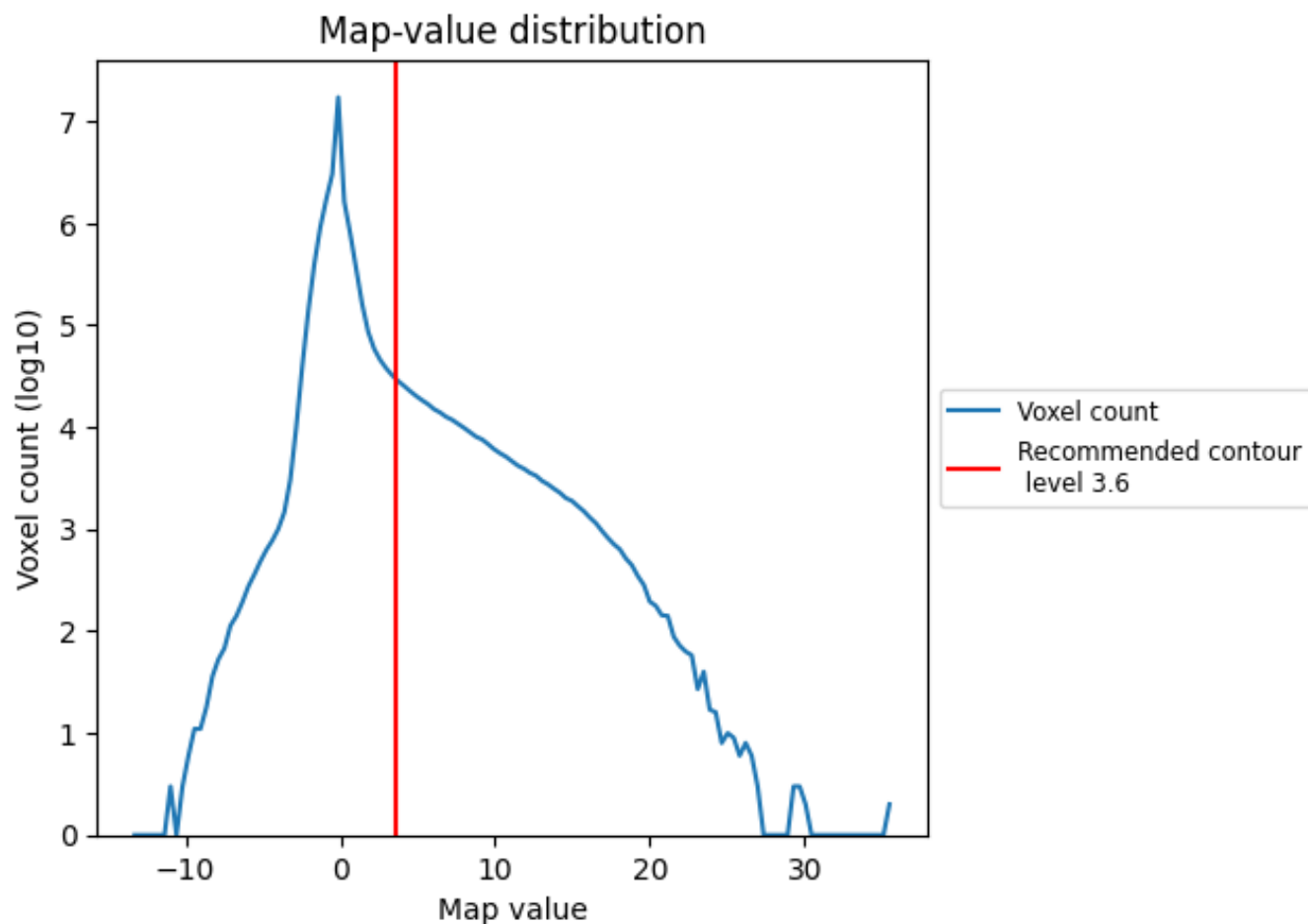
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

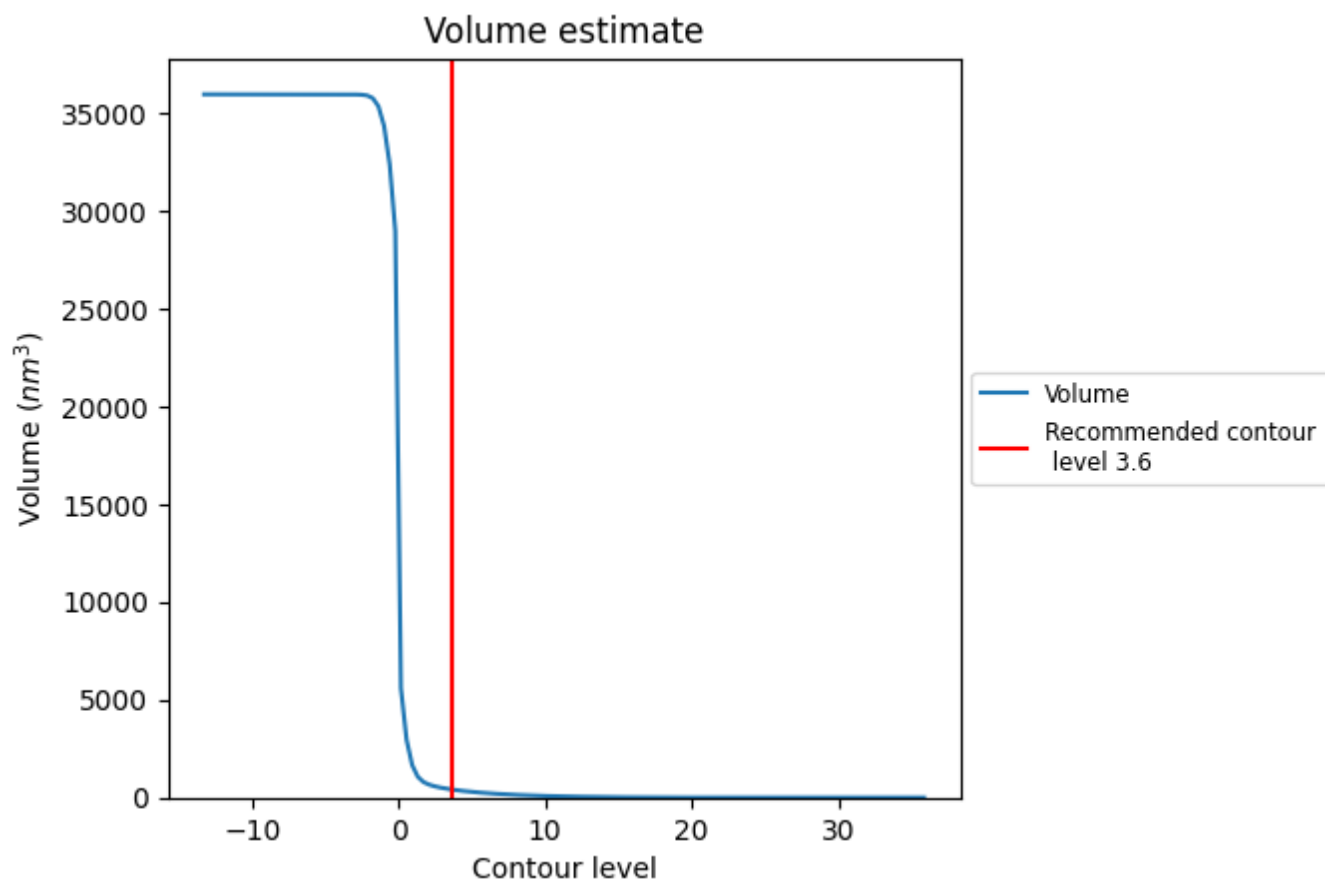
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

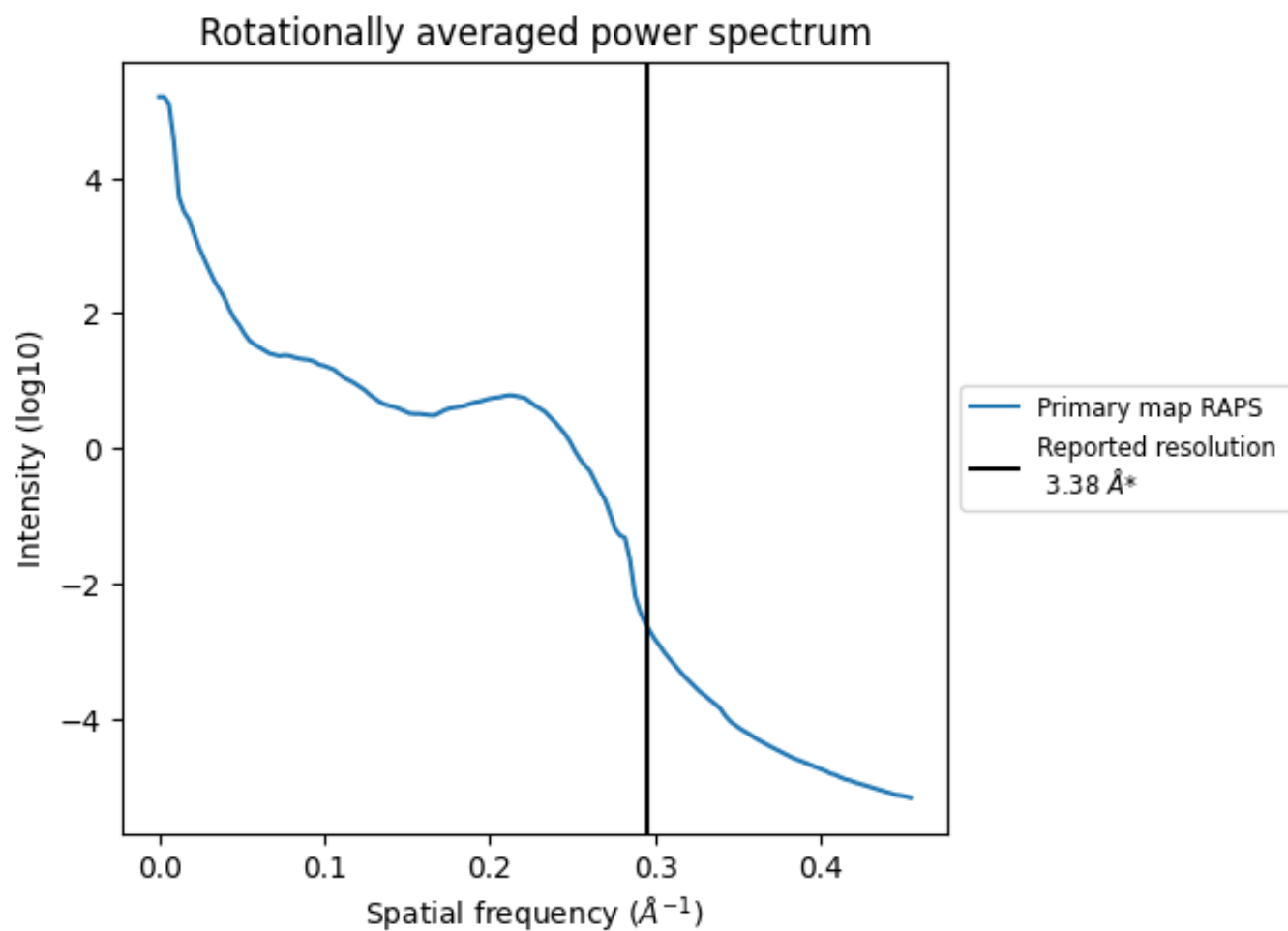
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 413 nm<sup>3</sup>; this corresponds to an approximate mass of 373 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.296 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

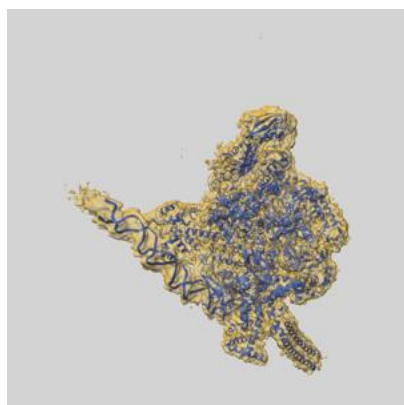
This section was not generated. No FSC curve or half-maps provided.



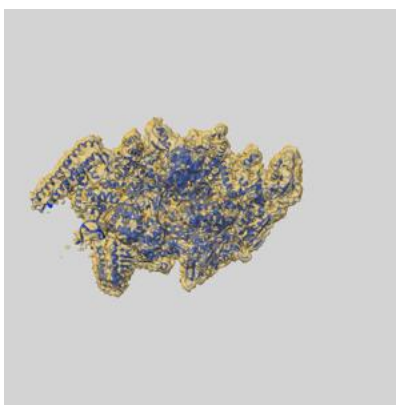
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22887 and PDB model 7KIM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

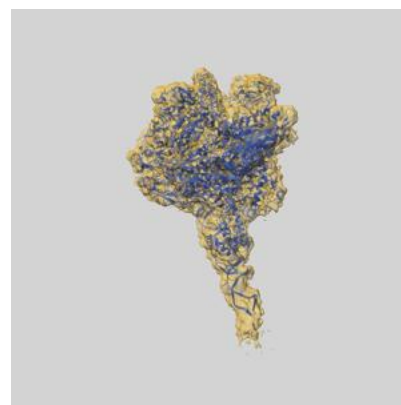
### 9.1 Map-model overlay [i](#)



X



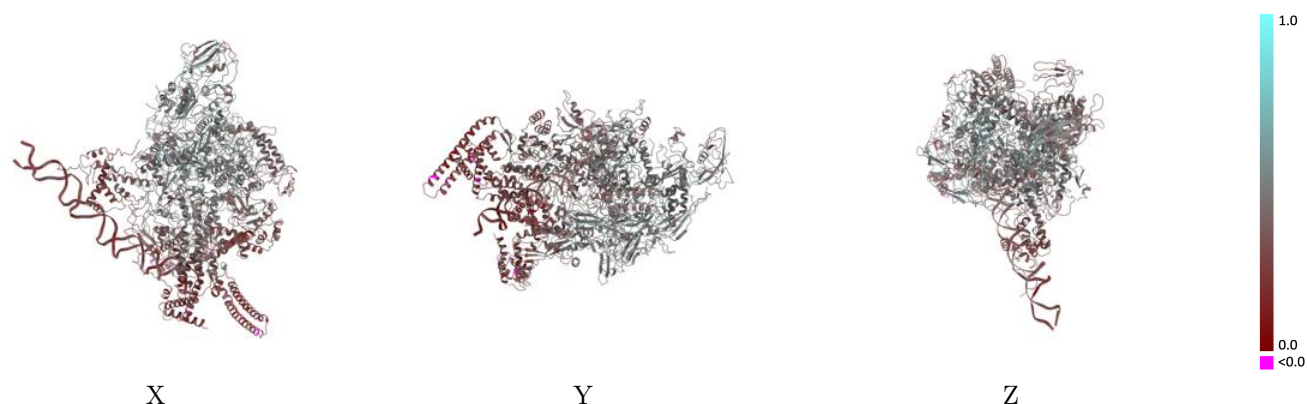
Y



Z

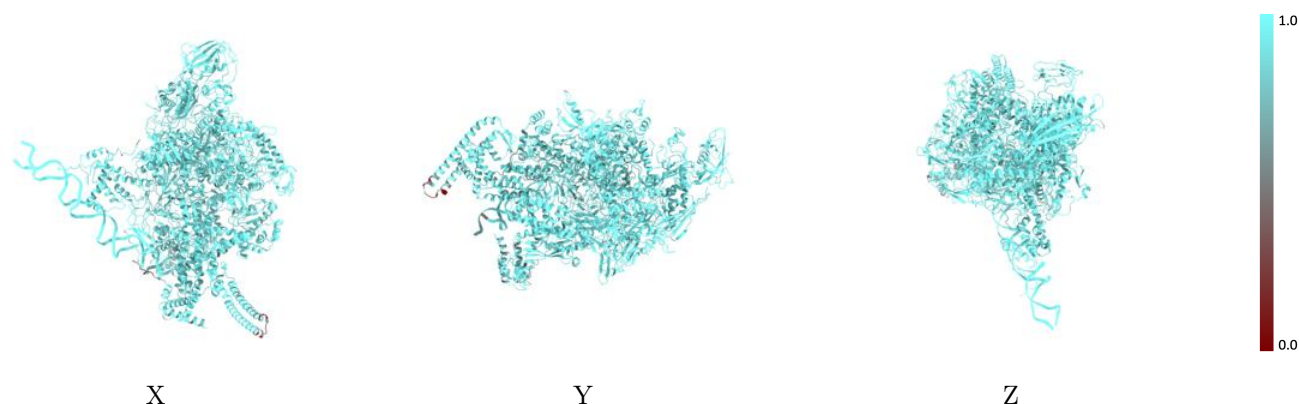
The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



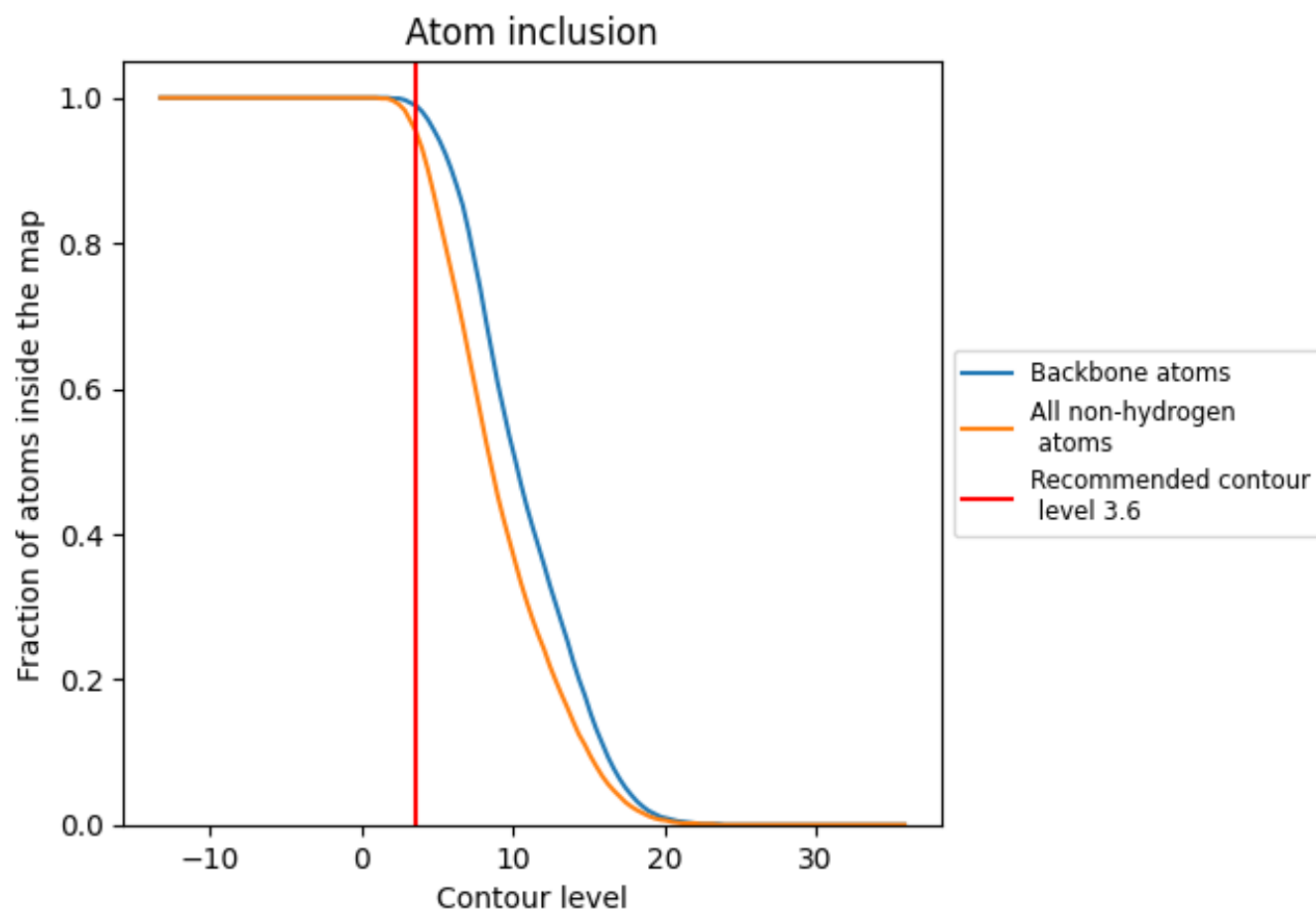
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (3.6).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4090
A	 0.9750	 0.4790
B	 0.9720	 0.4550
C	 0.9640	 0.4530
D	 0.9590	 0.4280
E	 0.9720	 0.4640
F	 0.9160	 0.3030
J	 0.8750	 0.3350
M	 0.8440	 0.2840
O	 0.9710	 0.2720
P	 0.9560	 0.2460
Z	 0.9750	 0.3180

