



## Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 10:18 PM EST

PDB ID : 6VXX  
EMDB ID : EMD-21406  
Title : Mycobacterium tuberculosis WT RNAP transcription initiation intermediate structure with Sorangicin  
Authors : Lilic, M.; Boyaci, H.; Chen, J.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2020-02-18  
Resolution : 3.39 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:

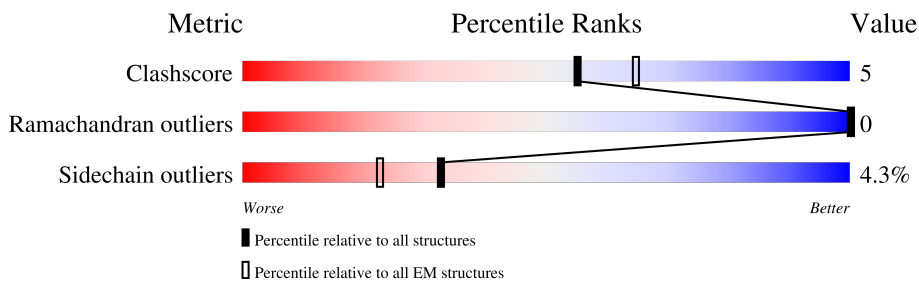
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.39 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	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	P	90	

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Mol	Chain	Length	Quality of chain
8	M	162	 75% 22% ..
9	O	90	 63% 7% • 28%

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 29858 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
			Total	C	N	O	S		
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
			1759	1112	298	346	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1111	Total	C	N	O	S	0	0
			8554	5357	1502	1656	39		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1266	Total	C	N	O	S	0	0
			9873	6184	1794	1853	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	319	2505	1564	456	476	9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	108	875	540	165	167	3	0	0

- Molecule 7 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	P	63	1289	610	242	374	63	0	0

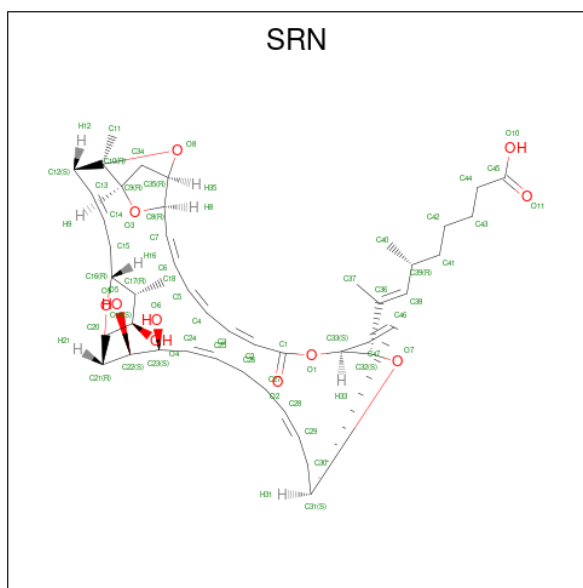
- Molecule 8 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	159	1241	777	224	239	1	0	0

- Molecule 9 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	O	65	1336	633	243	395	65	0	0

- Molecule 10 is SORANGICIN A (three-letter code: SRN) (formula:  $C_{47}H_{66}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	C	1	58	47	11	0

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

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

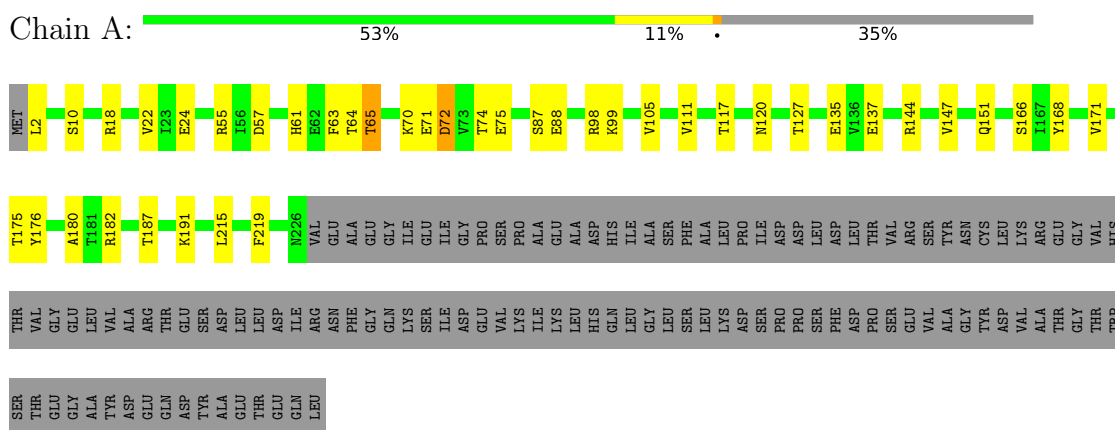
- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

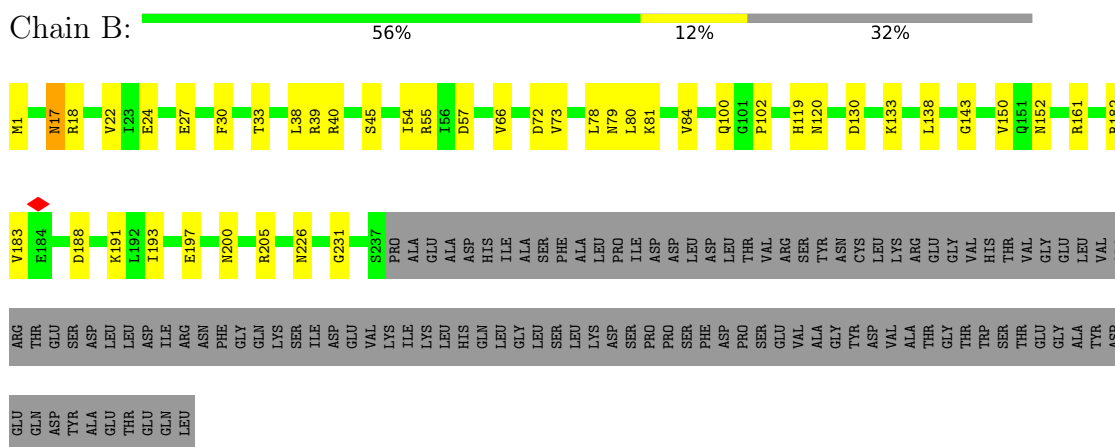
### 3 Residue-property plots [i](#)

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.

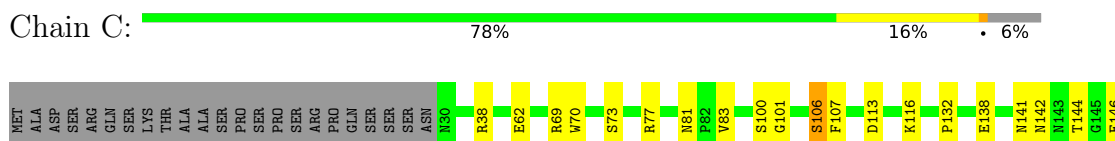
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta











• Molecule 9: DNA (65-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75398	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	3.045	Depositor
Minimum map value	-0.960	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.48	Depositor
Map size ( $\text{\AA}$ )	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: SRN, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/1742	0.53	0/2370
1	B	0.35	0/1786	0.53	0/2435
2	C	0.39	0/8712	0.54	2/11822 (0.0%)
3	D	0.37	0/10037	0.52	3/13570 (0.0%)
4	E	0.36	0/662	0.57	0/901
5	F	0.31	0/2536	0.47	0/3421
6	J	0.29	0/891	0.50	0/1203
7	P	0.73	1/1445 (0.1%)	0.99	2/2224 (0.1%)
8	M	0.29	0/1257	0.55	0/1700
9	O	0.72	0/1497	1.01	4/2310 (0.2%)
All	All	0.41	1/30565 (0.0%)	0.60	11/41956 (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
2	C	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	102	DG	C3'-O3'	6.74	1.52	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	131	DG	O4'-C1'-N9	7.05	112.94	108.00
3	D	834	ARG	C-N-CD	-6.05	107.29	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	59	DG	O4'-C1'-N9	5.89	112.12	108.00
2	C	1131	LEU	CA-CB-CG	5.83	128.72	115.30
2	C	584	ARG	CA-CB-CG	5.73	126.00	113.40
7	P	102	DG	P-O3'-C3'	5.61	126.43	119.70
9	O	59	DG	C1'-O4'-C4'	-5.45	104.65	110.10
9	O	58	DA	P-O3'-C3'	5.25	126.01	119.70
3	D	140	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	834	ARG	C-N-CA	5.17	143.70	122.00
9	O	42	DT	P-O3'-C3'	5.09	125.81	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	146	GLU	Peptide
2	C	226	ILE	Peptide
2	C	227	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	18	0
1	B	1759	0	1783	25	0
2	C	8554	0	8448	107	0
3	D	9873	0	9938	112	0
4	E	649	0	645	6	0
5	F	2505	0	2523	29	0
6	J	875	0	850	11	0
7	P	1289	0	706	7	0
8	M	1241	0	1259	22	0
9	O	1336	0	732	5	0
10	C	58	0	63	8	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	29858	0	28703	312	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 (312) 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)
10:C:1201:SRN:C10	10:C:1201:SRN:C12	1.76	1.57
10:C:1201:SRN:O3	10:C:1201:SRN:C8	1.79	1.30
10:C:1201:SRN:O3	10:C:1201:SRN:C9	1.80	1.29
10:C:1201:SRN:C10	10:C:1201:SRN:C13	2.49	0.90
10:C:1201:SRN:C12	10:C:1201:SRN:C11	2.62	0.76
6:J:64:LEU:HD23	6:J:66:GLU:H	1.59	0.68
8:M:112:TRP:O	8:M:116:GLN:HB2	1.94	0.67
10:C:1201:SRN:C12	10:C:1201:SRN:C9	2.55	0.67
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.78	0.65
7:P:102:DG:H21	7:P:103:DT:H2'	1.62	0.64
3:D:177:LEU:HD11	3:D:198:ARG:HA	1.81	0.63
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.33	0.62
1:A:72:ASP:OD1	1:A:72:ASP:N	2.32	0.62
1:A:2:LEU:HB3	1:B:143:GLY:HA2	1.83	0.60
3:D:144:ARG:O	3:D:148:LEU:HB2	2.02	0.60
2:C:947:ASP:OD1	2:C:947:ASP:N	2.36	0.59
2:C:881:ASP:N	2:C:881:ASP:OD1	2.36	0.59
2:C:1055:GLN:HE22	3:D:415:GLN:HE22	1.50	0.59
3:D:64:LYS:HE3	3:D:77:ARG:HH21	1.68	0.58
2:C:150:GLN:HG3	2:C:414:PRO:HG2	1.84	0.58
2:C:758:ASP:N	2:C:758:ASP:OD1	2.36	0.58
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.86	0.58
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.86	0.57
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.84	0.57
1:B:183:VAL:HA	1:B:188:ASP:H	1.68	0.57
2:C:38:ARG:NH1	2:C:972:VAL:O	2.38	0.57
3:D:119:ASP:OD2	3:D:295:ARG:NH1	2.38	0.57
3:D:239:ASN:HD21	3:D:242:ARG:HH21	1.53	0.57
8:M:81:GLU:HG2	8:M:88:ARG:HD3	1.87	0.57
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.88	0.56
3:D:108:LYS:O	3:D:386:ARG:NH1	2.38	0.56
2:C:748:THR:HG22	2:C:878:LYS:HA	1.88	0.56
3:D:144:ARG:NH1	3:D:226:PHE:O	2.37	0.56
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.69	0.56
1:B:152:ASN:OD1	1:B:152:ASN:N	2.39	0.56
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.38	0.56
2:C:678:SER:OG	2:C:679:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:952:LEU:HD22	3:D:957:ILE:HD11	1.87	0.55
2:C:1067:ARG:NH2	3:D:419:GLY:O	2.38	0.55
7:P:98:DG:H21	9:O:58:DA:H61	1.55	0.55
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.87	0.55
5:F:511:MET:HB3	5:F:515:ARG:HH22	1.71	0.55
2:C:101:GLY:O	2:C:142:ASN:ND2	2.40	0.55
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.71	0.55
3:D:796:ASP:OD1	3:D:796:ASP:N	2.33	0.55
2:C:772:ASP:OD2	2:C:830:ARG:NH2	2.41	0.54
5:F:254:GLU:OE1	6:J:89:ARG:NH1	2.40	0.54
3:D:83:THR:OG1	3:D:84:ARG:N	2.40	0.54
3:D:279:ASP:OD1	3:D:283:ASN:ND2	2.41	0.54
1:A:64:THR:OG1	1:A:65:THR:N	2.40	0.54
2:C:453:ARG:NH2	2:C:501:SER:O	2.41	0.54
2:C:822:ARG:NH1	2:C:828:LYS:O	2.41	0.54
3:D:577:PRO:HB3	3:D:581:MET:HG3	1.89	0.54
3:D:866:ARG:NH2	3:D:1008:THR:O	2.40	0.54
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.40	0.54
2:C:380:THR:OG1	2:C:381:VAL:N	2.41	0.54
1:B:22:VAL:HG12	1:B:193:ILE:HG12	1.90	0.54
5:F:516:HIS:O	5:F:520:SER:HB3	2.07	0.54
3:D:428:SER:OG	3:D:429:VAL:N	2.38	0.54
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.90	0.54
2:C:809:LYS:HD3	2:C:833:ARG:HB2	1.90	0.54
3:D:605:ASP:OD1	3:D:605:ASP:N	2.36	0.53
2:C:721:VAL:HG11	2:C:1028:MET:HB2	1.90	0.53
2:C:826:GLY:O	2:C:828:LYS:NZ	2.42	0.53
5:F:229:ARG:NH2	9:O:56:DG:O6	2.42	0.53
1:A:57:ASP:OD1	1:A:57:ASP:N	2.42	0.53
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.91	0.53
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.91	0.53
3:D:273:GLU:OE1	3:D:295:ARG:NH2	2.41	0.53
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.91	0.53
3:D:500:ARG:HB2	3:D:541:MET:HG2	1.90	0.53
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.41	0.53
3:D:71:LYS:O	6:J:27:ARG:NH1	2.42	0.53
3:D:293:LEU:HD22	3:D:1176:LEU:HD23	1.90	0.53
3:D:937:ILE:HG12	3:D:938:VAL:HG23	1.91	0.53
5:F:293:ASN:HA	5:F:296:LEU:HD12	1.90	0.53
5:F:449:ASP:OD1	5:F:449:ASP:N	2.41	0.53
3:D:757:GLU:OE1	3:D:770:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.89	0.52
2:C:577:ASP:OD1	2:C:577:ASP:N	2.37	0.52
3:D:810:ASN:OD1	3:D:810:ASN:N	2.42	0.52
2:C:1023:VAL:HA	3:D:730:THR:HG21	1.92	0.52
8:M:75:ARG:NH2	8:M:160:ALA:O	2.43	0.52
2:C:132:PRO:HB3	2:C:153:PHE:HE1	1.75	0.52
2:C:945:LYS:HG3	2:C:965:GLU:HB3	1.92	0.52
2:C:717:LYS:NZ	2:C:746:VAL:O	2.42	0.52
2:C:799:GLY:H	2:C:839:VAL:HG13	1.75	0.52
5:F:471:GLU:OE2	5:F:513:LYS:NZ	2.41	0.52
1:B:80:LEU:HD22	1:B:138:LEU:HD21	1.91	0.52
2:C:144:THR:O	8:M:52:ASN:ND2	2.43	0.52
2:C:604:ARG:NH1	2:C:607:MET:SD	2.83	0.52
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.92	0.52
3:D:475:MET:HG3	3:D:480:ARG:HG3	1.91	0.52
8:M:88:ARG:O	8:M:92:ASN:ND2	2.43	0.52
1:B:79:ASN:OD1	3:D:636:ARG:NH2	2.42	0.51
2:C:443:ASN:OD1	2:C:443:ASN:N	2.43	0.51
3:D:674:ASN:HD21	3:D:684:VAL:H	1.59	0.51
3:D:1089:PHE:O	3:D:1097:ARG:N	2.43	0.51
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.92	0.51
3:D:206:ARG:HE	3:D:209:ARG:HG2	1.76	0.51
3:D:360:LEU:HD21	5:F:329:ILE:HG21	1.92	0.51
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.38	0.51
5:F:381:ARG:NH2	7:P:104:DC:O3'	2.44	0.51
2:C:494:ILE:HD13	3:D:860:LEU:HB3	1.92	0.51
1:A:87:SER:OG	1:A:88:GLU:N	2.43	0.50
1:A:175:THR:OG1	1:A:176:TYR:N	2.44	0.50
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.92	0.50
9:O:72:DG:H1'	9:O:73:DC:H5'	1.93	0.50
1:A:180:ALA:HB1	1:A:182:ARG:HD3	1.93	0.50
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.93	0.50
2:C:222:VAL:HG21	2:C:234:VAL:HB	1.93	0.50
3:D:246:ASP:N	3:D:246:ASP:OD1	2.44	0.50
2:C:188:ASP:OD1	2:C:188:ASP:N	2.44	0.50
8:M:154:LEU:O	8:M:158:LEU:N	2.45	0.50
2:C:106:SER:OG	2:C:107:PHE:N	2.43	0.49
3:D:1036:GLU:HB3	3:D:1038:ARG:HG2	1.94	0.49
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.94	0.49
1:A:120:ASN:OD1	1:A:120:ASN:N	2.45	0.49
3:D:334:ARG:NH1	5:F:419:GLU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:84:ASN:N	8:M:84:ASN:OD1	2.46	0.49
3:D:893:THR:OG1	3:D:894:GLU:N	2.46	0.49
2:C:329:THR:OG1	2:C:330:SER:N	2.46	0.49
2:C:421:ARG:HA	2:C:424:VAL:HG12	1.94	0.49
2:C:587:VAL:HG22	2:C:591:THR:HB	1.95	0.49
2:C:760:ARG:HG2	2:C:865:VAL:HG22	1.95	0.48
3:D:262:GLN:HB2	3:D:313:VAL:HG21	1.94	0.48
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.78	0.48
1:A:55:ARG:NH2	1:A:137:GLU:OE2	2.45	0.48
2:C:445:PRO:HD2	2:C:707:CYS:HB2	1.94	0.48
3:D:567:SER:HB2	3:D:571:GLY:H	1.78	0.48
2:C:278:TYR:OH	2:C:282:ARG:NH1	2.47	0.48
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.95	0.48
3:D:396:ASN:ND2	7:P:99:DC:OP1	2.44	0.48
1:A:75:GLU:OE2	2:C:620:ARG:NH1	2.46	0.48
3:D:63:GLY:O	3:D:66:LYS:NZ	2.46	0.48
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.46	0.48
5:F:461:GLN:OE1	5:F:476:ARG:NH2	2.46	0.48
1:B:17:ASN:OD1	1:B:17:ASN:N	2.45	0.48
2:C:541:VAL:HG11	2:C:562:ARG:HH21	1.78	0.47
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.97	0.47
3:D:73:ILE:HD12	6:J:45:ALA:HB2	1.96	0.47
3:D:736:VAL:HG12	3:D:818:ALA:HB2	1.95	0.47
3:D:982:SER:HB2	3:D:989:VAL:HG23	1.95	0.47
5:F:500:ARG:NH2	7:P:126:DG:N7	2.62	0.47
2:C:891:ASN:OD1	2:C:891:ASN:N	2.41	0.47
3:D:641:ARG:HB3	3:D:682:PRO:HA	1.96	0.47
5:F:216:ARG:O	5:F:220:GLU:HB2	2.14	0.47
1:B:120:ASN:N	1:B:120:ASN:OD1	2.46	0.47
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.47	0.47
8:M:111:LEU:HB2	8:M:128:LEU:HD13	1.96	0.47
2:C:555:VAL:HG23	2:C:556:GLU:HG3	1.96	0.47
2:C:1050:SER:OG	2:C:1051:MET:N	2.48	0.47
5:F:289:ASP:O	5:F:293:ASN:ND2	2.48	0.47
5:F:335:PHE:O	6:J:88:ARG:NH1	2.48	0.47
2:C:803:VAL:O	2:C:836:SER:OG	2.31	0.47
3:D:332:GLY:O	5:F:418:ARG:NH1	2.48	0.47
3:D:566:LEU:HA	3:D:573:PRO:HA	1.96	0.47
1:A:24:GLU:HB3	1:A:191:LYS:HG3	1.97	0.46
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.97	0.46
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.48	0.46
8:M:4:LYS:HB2	8:M:4:LYS:HE2	1.70	0.46
3:D:28:VAL:HG21	3:D:46:LEU:HD23	1.98	0.46
4:E:40:ILE:HA	4:E:43:LEU:HB2	1.97	0.46
2:C:350:GLU:OE2	2:C:352:GLN:NE2	2.48	0.46
2:C:784:LEU:HA	2:C:790:VAL:HA	1.97	0.46
1:B:72:ASP:OD1	1:B:73:VAL:N	2.48	0.46
1:B:57:ASP:OD1	1:B:57:ASP:N	2.48	0.46
3:D:550:GLU:OE1	4:E:62:ARG:NH1	2.48	0.46
1:B:45:SER:O	1:B:45:SER:OG	2.34	0.46
3:D:331:ASP:OD1	3:D:331:ASP:N	2.40	0.46
2:C:215:ASP:N	2:C:223:GLY:O	2.47	0.46
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.97	0.46
3:D:108:LYS:HD2	3:D:108:LYS:HA	1.86	0.46
2:C:369:ASP:O	2:C:375:ASN:ND2	2.47	0.45
2:C:938:TRP:HB2	2:C:1026:GLY:HA2	1.98	0.45
5:F:242:ASN:ND2	5:F:244:GLU:OE2	2.49	0.45
3:D:281:ILE:HA	3:D:289:LYS:HG3	1.98	0.45
3:D:1173:THR:HB	3:D:1193:VAL:HG21	1.99	0.45
3:D:1262:THR:HB	4:E:55:ILE:HD11	1.97	0.45
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.98	0.45
2:C:835:THR:O	2:C:835:THR:OG1	2.32	0.45
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.81	0.45
7:P:134:DC:H2''	7:P:135:DA:C8	2.51	0.45
3:D:64:LYS:HB2	3:D:77:ARG:HH21	1.82	0.45
8:M:114:ARG:HA	8:M:114:ARG:HD3	1.73	0.45
3:D:500:ARG:NH1	3:D:533:ASN:O	2.50	0.45
3:D:1117:ASP:OD1	3:D:1117:ASP:N	2.49	0.45
1:B:78:LEU:HA	1:B:81:LYS:HB2	1.99	0.45
1:A:61:HIS:CD2	1:A:63:PHE:H	2.34	0.45
8:M:84:ASN:HD21	8:M:87:ARG:HH21	1.65	0.45
1:B:66:VAL:HG23	1:B:73:VAL:HG22	1.99	0.44
2:C:959:LEU:HD22	2:C:960:PRO:HD2	1.99	0.44
9:O:21:DG:H2'	9:O:22:DG:C8	2.52	0.44
2:C:1119:GLU:OE2	3:D:89:ARG:NH1	2.51	0.44
3:D:93:GLY:O	3:D:319:VAL:N	2.49	0.44
3:D:366:ILE:HG22	5:F:322:GLN:HE22	1.82	0.44
2:C:62:GLU:HG3	2:C:70:TRP:HB2	1.99	0.44
2:C:256:GLU:H	2:C:256:GLU:HG3	1.63	0.44
2:C:1051:MET:HE2	5:F:441:ASP:HA	1.99	0.44
1:B:119:HIS:O	1:B:200:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:828:LYS:HA	2:C:828:LYS:HD3	1.80	0.44
3:D:1163:ARG:HA	3:D:1163:ARG:HD2	1.87	0.44
2:C:234:VAL:HG22	2:C:238:LEU:HD23	2.00	0.44
3:D:641:ARG:O	3:D:683:PHE:N	2.50	0.44
3:D:362:ALA:HB1	3:D:366:ILE:HD12	1.99	0.44
2:C:622:GLU:HB3	2:C:717:LYS:HD3	2.00	0.44
10:C:1201:SRN:O3	10:C:1201:SRN:C35	2.55	0.44
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.99	0.44
3:D:248:TYR:HB3	3:D:251:TYR:HD2	1.82	0.44
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.98	0.44
1:B:39:ARG:NH1	3:D:623:ASP:OD2	2.45	0.44
3:D:739:PRO:HG2	3:D:742:LYS:HB2	2.00	0.44
3:D:1204:ARG:HE	3:D:1204:ARG:HB3	1.67	0.44
8:M:6:GLY:H	8:M:19:VAL:HG23	1.83	0.44
1:B:27:GLU:HB2	1:B:30:PHE:HD2	1.83	0.43
2:C:403:ARG:NH1	2:C:416:THR:O	2.51	0.43
3:D:170:LEU:HD23	3:D:205:MET:HB2	2.00	0.43
2:C:1131:LEU:HD23	3:D:402:LEU:HD22	1.99	0.43
3:D:263:LYS:HA	3:D:263:LYS:HD3	1.81	0.43
8:M:145:THR:OG1	8:M:146:ASP:N	2.50	0.43
2:C:760:ARG:N	2:C:767:GLU:OE1	2.50	0.43
3:D:74:ILE:HD12	6:J:42:VAL:HG13	2.00	0.43
3:D:205:MET:HA	3:D:208:ILE:HD12	2.00	0.43
2:C:789:ILE:H	2:C:789:ILE:HG13	1.62	0.43
3:D:397:ARG:NH1	5:F:424:ASP:O	2.51	0.43
3:D:468:ASN:OD1	3:D:468:ASN:N	2.49	0.43
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.54	0.43
3:D:638:THR:O	3:D:639:GLN:NE2	2.52	0.43
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.00	0.43
6:J:63:THR:OG1	6:J:64:LEU:N	2.51	0.43
2:C:995:ASN:OD1	2:C:995:ASN:N	2.41	0.43
1:B:55:ARG:HB3	1:B:161:ARG:HA	2.01	0.43
3:D:409:LYS:HB2	3:D:409:LYS:HE2	1.78	0.43
3:D:742:LYS:NZ	3:D:842:GLU:OE2	2.52	0.43
3:D:159:ARG:HG3	3:D:216:LEU:HD22	2.01	0.43
8:M:77:PRO:HB3	8:M:109:ARG:HH22	1.83	0.43
2:C:444:ASN:N	2:C:444:ASN:OD1	2.50	0.43
5:F:467:LEU:HD23	5:F:467:LEU:HA	1.87	0.43
1:B:1:MET:N	1:B:231:GLY:O	2.52	0.42
2:C:311:VAL:HG22	2:C:509:PHE:HD1	1.84	0.42
2:C:727:GLU:H	3:D:725:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:960:PRO:HG2	2:C:963:LEU:HD12	2.00	0.42
8:M:95:LYS:HZ3	8:M:104:VAL:HA	1.83	0.42
2:C:208:ARG:HH11	2:C:307:ASP:HB2	1.83	0.42
10:C:1201:SRN:H152	10:C:1201:SRN:H181	1.74	0.42
3:D:1257:LEU:HD12	3:D:1257:LEU:HA	1.88	0.42
8:M:38:LYS:HE2	8:M:38:LYS:HB2	1.92	0.42
1:B:40:ARG:HH12	3:D:623:ASP:HB3	1.84	0.42
2:C:323:HIS:ND1	2:C:326:GLU:OE2	2.41	0.42
5:F:463:VAL:O	5:F:466:THR:OG1	2.28	0.42
8:M:100:ASP:HB3	8:M:103:LYS:HD3	2.01	0.42
9:O:58:DA:H2''	9:O:59:DG:H2'	2.02	0.42
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.52	0.42
2:C:600:ASP:OD2	2:C:889:HIS:ND1	2.46	0.42
3:D:797:ASN:HD22	3:D:798:PRO:HD2	1.83	0.42
5:F:527:LEU:HD23	5:F:527:LEU:HA	1.87	0.42
8:M:95:LYS:HZ2	8:M:104:VAL:HG22	1.84	0.42
8:M:117:GLU:HG3	8:M:118:ARG:HG3	2.02	0.42
3:D:1040:PRO:HD3	3:D:1117:ASP:HB3	2.02	0.42
1:B:54:ILE:HG21	1:B:80:LEU:HD13	2.01	0.42
2:C:903:ASP:OD1	2:C:903:ASP:N	2.42	0.42
3:D:18:GLU:O	3:D:22:GLN:HB2	2.20	0.42
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.49	0.41
2:C:348:LEU:HD13	2:C:365:VAL:HG12	2.01	0.41
2:C:532:THR:OG1	2:C:533:ALA:N	2.53	0.41
3:D:580:ASP:N	3:D:580:ASP:OD1	2.53	0.41
2:C:927:ASN:OD1	2:C:927:ASN:N	2.53	0.41
3:D:10:LEU:HD12	3:D:10:LEU:HA	1.91	0.41
3:D:904:ARG:NH1	3:D:908:GLY:O	2.53	0.41
6:J:15:SER:OG	6:J:16:TYR:N	2.53	0.41
1:B:100:GLN:HA	1:B:133:LYS:HA	2.01	0.41
2:C:738:SER:OG	2:C:739:ASN:N	2.53	0.41
2:C:770:THR:OG1	2:C:771:ARG:N	2.53	0.41
4:E:43:LEU:HD23	4:E:43:LEU:HA	1.94	0.41
5:F:483:ASP:OD2	5:F:487:ARG:NH2	2.40	0.41
2:C:1109:GLY:O	4:E:69:ASN:ND2	2.42	0.41
2:C:518:LYS:HE3	2:C:518:LYS:HB2	1.79	0.41
3:D:741:ARG:H	3:D:741:ARG:HG3	1.68	0.41
2:C:69:ARG:O	2:C:73:SER:OG	2.30	0.41
7:P:137:DG:H2'	7:P:138:DT:H71	2.01	0.41
2:C:436:LEU:HD13	2:C:436:LEU:HA	1.89	0.41
2:C:635:ALA:HB2	2:C:713:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:771:ARG:NH2	2:C:781:LEU:O	2.54	0.41
3:D:326:PRO:O	3:D:338:SER:OG	2.39	0.41
3:D:442:GLY:HA3	3:D:523:GLN:HB2	2.02	0.41
3:D:937:ILE:HD11	3:D:951:ALA:HB1	2.03	0.41
5:F:326:LEU:HA	5:F:329:ILE:HD12	2.02	0.41
5:F:334:LYS:HG3	6:J:84:MET:HG2	2.03	0.41
1:A:98:ARG:HG3	1:A:135:GLU:HG2	2.02	0.41
2:C:830:ARG:HA	2:C:830:ARG:HD2	1.83	0.41
3:D:120:LEU:HD11	3:D:232:LYS:HB3	2.02	0.41
3:D:470:LYS:HD3	3:D:470:LYS:HA	1.93	0.41
8:M:10:VAL:HA	8:M:16:ALA:HA	2.03	0.41
1:B:38:LEU:HD12	1:B:38:LEU:HA	1.86	0.40
2:C:113:ASP:HB2	2:C:132:PRO:HD2	2.03	0.40
2:C:683:CYS:SG	2:C:684:ALA:N	2.94	0.40
2:C:885:LEU:HD13	2:C:895:ILE:HD11	2.03	0.40
2:C:907:LEU:HD13	2:C:908:ALA:H	1.85	0.40
3:D:911:ILE:H	3:D:911:ILE:HG13	1.73	0.40
2:C:150:GLN:HG2	8:M:44:LEU:HB3	2.03	0.40
2:C:444:ASN:HD22	2:C:715:LEU:HD22	1.87	0.40
1:A:147:VAL:HG13	1:A:166:SER:HB2	2.03	0.40
1:A:151:GLN:NE2	2:C:795:GLU:OE2	2.54	0.40
1:B:18:ARG:NH1	1:B:197:GLU:OE1	2.54	0.40
2:C:689:ILE:HD11	2:C:701:VAL:HG12	2.04	0.40
5:F:264:THR:O	5:F:267:SER:OG	2.39	0.40
8:M:153:ILE:HD13	8:M:153:ILE:HA	1.98	0.40
2:C:106:SER:HB3	2:C:138:GLU:HB3	2.04	0.40
3:D:832:ILE:HA	3:D:833:PRO:HD3	1.91	0.40
3:D:1050:THR:HG22	3:D:1106:GLU:HA	2.02	0.40
6:J:99:LYS:HA	6:J:99:LYS:HD3	1.87	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%)	211 (95%)	12 (5%)	0	100	100
1	B	235/347 (68%)	215 (92%)	20 (8%)	0	100	100
2	C	1109/1179 (94%)	1029 (93%)	80 (7%)	0	100	100
3	D	1260/1326 (95%)	1185 (94%)	75 (6%)	0	100	100
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	317/531 (60%)	309 (98%)	8 (2%)	0	100	100
6	J	106/111 (96%)	96 (91%)	10 (9%)	0	100	100
8	M	157/162 (97%)	150 (96%)	7 (4%)	0	100	100
All	All	3488/4113 (85%)	3271 (94%)	217 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/297 (65%)	179 (92%)	15 (8%)	13	40
1	B	194/297 (65%)	187 (96%)	7 (4%)	35	63
2	C	925/997 (93%)	886 (96%)	39 (4%)	30	59
3	D	1042/1103 (94%)	1004 (96%)	38 (4%)	35	63
4	E	69/89 (78%)	63 (91%)	6 (9%)	10	34
5	F	260/429 (61%)	253 (97%)	7 (3%)	44	70
6	J	92/97 (95%)	86 (94%)	6 (6%)	17	46
8	M	129/131 (98%)	121 (94%)	8 (6%)	18	48
All	All	2905/3440 (84%)	2779 (96%)	126 (4%)	33	59

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	18	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	22	VAL
1	A	65	THR
1	A	72	ASP
1	A	74	THR
1	A	111	VAL
1	A	117	THR
1	A	127	THR
1	A	144	ARG
1	A	168	TYR
1	A	171	VAL
1	A	187	THR
1	A	215	LEU
1	A	219	PHE
1	B	17	ASN
1	B	33	THR
1	B	84	VAL
1	B	150	VAL
1	B	182	ARG
1	B	205	ARG
1	B	226	ASN
2	C	77	ARG
2	C	81	ASN
2	C	83	VAL
2	C	100	SER
2	C	106	SER
2	C	116	LYS
2	C	141	ASN
2	C	193	LYS
2	C	219	ARG
2	C	254	PHE
2	C	258	MET
2	C	264	LYS
2	C	279	ARG
2	C	302	LYS
2	C	308	LEU
2	C	313	ARG
2	C	357	VAL
2	C	363	VAL
2	C	376	ARG
2	C	386	GLN
2	C	391	VAL
2	C	396	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	419	ASN
2	C	421	ARG
2	C	450	THR
2	C	453	ARG
2	C	518	LYS
2	C	584	ARG
2	C	626	VAL
2	C	777	SER
2	C	860	GLU
2	C	866	ASN
2	C	881	ASP
2	C	907	LEU
2	C	959	LEU
2	C	965	GLU
2	C	1011	PHE
2	C	1131	LEU
2	C	1137	VAL
3	D	22	GLN
3	D	107	PHE
3	D	135	VAL
3	D	137	THR
3	D	160	LYS
3	D	166	ARG
3	D	173	ARG
3	D	205	MET
3	D	209	ARG
3	D	239	ASN
3	D	244	LEU
3	D	403	SER
3	D	407	LYS
3	D	416	ASN
3	D	441	CYS
3	D	470	LYS
3	D	499	ASN
3	D	562	SER
3	D	623	ASP
3	D	624	ARG
3	D	627	LEU
3	D	636	ARG
3	D	727	SER
3	D	733	MET
3	D	741	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	793	TYR
3	D	797	ASN
3	D	887	ARG
3	D	940	ARG
3	D	975	CYS
3	D	1012	MET
3	D	1028	LEU
3	D	1030	ARG
3	D	1052	ARG
3	D	1097	ARG
3	D	1098	VAL
3	D	1186	PHE
3	D	1193	VAL
4	E	56	TYR
4	E	65	ASN
4	E	68	TYR
4	E	71	LEU
4	E	78	TYR
4	E	102	ASP
5	F	268	GLU
5	F	269	ARG
5	F	278	ARG
5	F	353	GLN
5	F	370	VAL
5	F	460	LEU
5	F	509	LYS
6	J	16	TYR
6	J	27	ARG
6	J	76	LYS
6	J	79	ARG
6	J	108	ARG
6	J	110	ARG
8	M	25	ARG
8	M	26	THR
8	M	44	LEU
8	M	74	LEU
8	M	95	LYS
8	M	114	ARG
8	M	143	GLU
8	M	156	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	B	151	GLN
1	B	226	ASN
2	C	81	ASN
2	C	141	ASN
2	C	266	ASN
2	C	298	ASN
2	C	352	GLN
2	C	415	GLN
2	C	419	ASN
2	C	662	HIS
2	C	775	ASN
2	C	1055	GLN
3	D	239	ASN
3	D	283	ASN
3	D	368	ASN
3	D	505	HIS
3	D	564	ASN
3	D	639	GLN
3	D	693	GLN
3	D	797	ASN
3	D	1190	ASN
4	E	65	ASN
5	F	388	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
10	SRN	C	1201	-	60,62,62	4.99	33 (55%)	62,84,84	1.40	7 (11%)

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
10	SRN	C	1201	-	-	22/52/105/105	0/4/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	O3-C8	19.20	1.79	1.44
10	C	1201	SRN	O3-C9	16.08	1.80	1.45
10	C	1201	SRN	C34-C9	-10.71	1.29	1.52
10	C	1201	SRN	C3-C2	9.32	1.58	1.34
10	C	1201	SRN	C34-C35	-8.76	1.33	1.52
10	C	1201	SRN	C4-C5	8.11	1.57	1.36
10	C	1201	SRN	C13-C14	6.62	1.60	1.31
10	C	1201	SRN	C24-C25	6.08	1.57	1.31
10	C	1201	SRN	C6-C7	6.05	1.57	1.33
10	C	1201	SRN	C8-C7	-5.95	1.30	1.50
10	C	1201	SRN	C12-C13	-5.87	1.30	1.50
10	C	1201	SRN	C28-C29	5.10	1.61	1.31
10	C	1201	SRN	C10-C9	-5.05	1.43	1.53
10	C	1201	SRN	O7-C32	4.89	1.51	1.43
10	C	1201	SRN	O8-C12	4.68	1.51	1.43
10	C	1201	SRN	C5-C6	4.63	1.57	1.44
10	C	1201	SRN	C35-C8	-4.47	1.46	1.53
10	C	1201	SRN	C3-C4	4.42	1.56	1.44
10	C	1201	SRN	C11-C10	-4.36	1.44	1.53
10	C	1201	SRN	C33-C47	-4.12	1.43	1.49
10	C	1201	SRN	C46-C47	3.64	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	O1-C1	3.62	1.42	1.34
10	C	1201	SRN	C30-C29	3.54	1.61	1.50
10	C	1201	SRN	C2-C1	3.38	1.56	1.48
10	C	1201	SRN	O7-C31	3.27	1.52	1.44
10	C	1201	SRN	O1-C33	3.00	1.51	1.46
10	C	1201	SRN	C23-C24	3.00	1.55	1.50
10	C	1201	SRN	C15-C14	2.45	1.57	1.50
10	C	1201	SRN	O8-C35	2.22	1.49	1.44
10	C	1201	SRN	C31-C46	2.16	1.53	1.50
10	C	1201	SRN	O6-C23	-2.14	1.39	1.43
10	C	1201	SRN	C22-C21	2.11	1.56	1.52
10	C	1201	SRN	C17-C16	2.07	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	SRN	C35-O8-C12	3.14	118.39	112.81
10	C	1201	SRN	C18-C17-C19	-2.73	108.01	111.36
10	C	1201	SRN	C30-C31-C46	-2.66	108.32	113.00
10	C	1201	SRN	C8-C7-C6	-2.62	120.48	125.61
10	C	1201	SRN	C20-C19-C17	2.54	114.25	111.02
10	C	1201	SRN	C9-C34-C35	2.53	111.03	103.73
10	C	1201	SRN	C43-C44-C45	-2.21	108.90	114.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	C25-C26-C27-C28
10	C	1201	SRN	C21-C22-C23-C24
10	C	1201	SRN	O9-C21-C22-C23
10	C	1201	SRN	C20-C21-C22-O5
10	C	1201	SRN	C14-C15-C16-O9
10	C	1201	SRN	O8-C12-C13-C14
10	C	1201	SRN	C10-C12-C13-C14
10	C	1201	SRN	O2-C1-O1-C33
10	C	1201	SRN	C2-C1-O1-C33
10	C	1201	SRN	C28-C29-C30-C31
10	C	1201	SRN	O1-C1-C2-C3
10	C	1201	SRN	O2-C1-C2-C3
10	C	1201	SRN	C42-C43-C44-C45
10	C	1201	SRN	C20-C21-C22-C23

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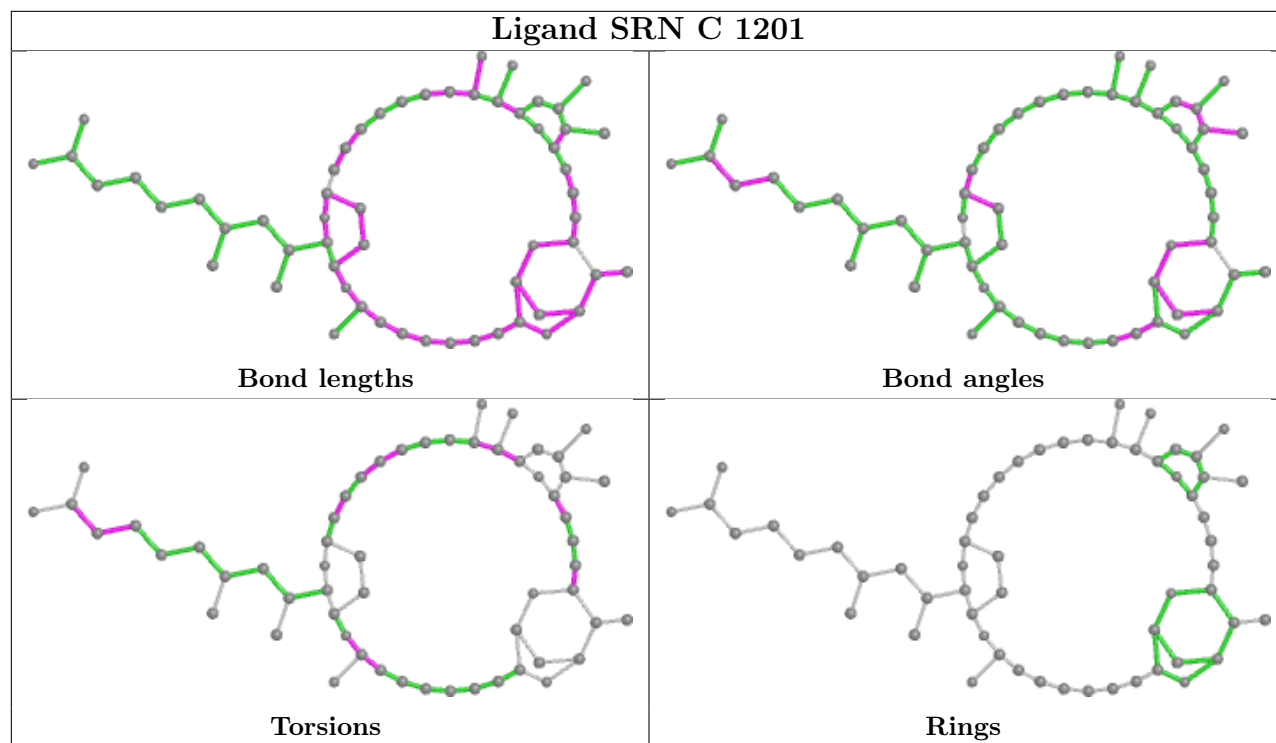
Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	O5-C22-C23-O6
10	C	1201	SRN	O9-C21-C22-O5
10	C	1201	SRN	O5-C22-C23-C24
10	C	1201	SRN	C26-C27-C28-C29
10	C	1201	SRN	C43-C44-C45-O11
10	C	1201	SRN	C43-C44-C45-O10
10	C	1201	SRN	C21-C22-C23-O6
10	C	1201	SRN	C14-C15-C16-C17

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	SRN	8	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.

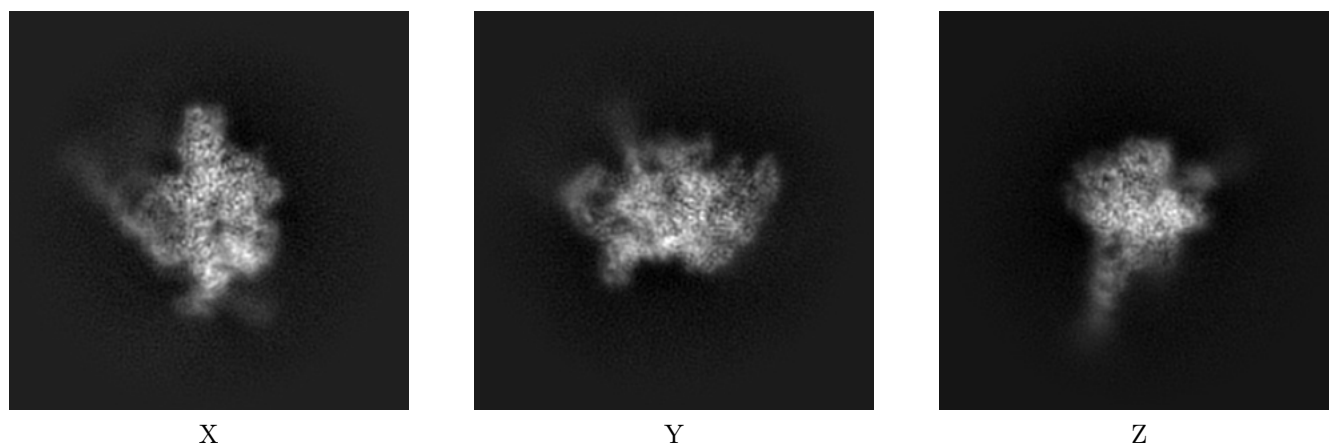
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21406. 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](#)

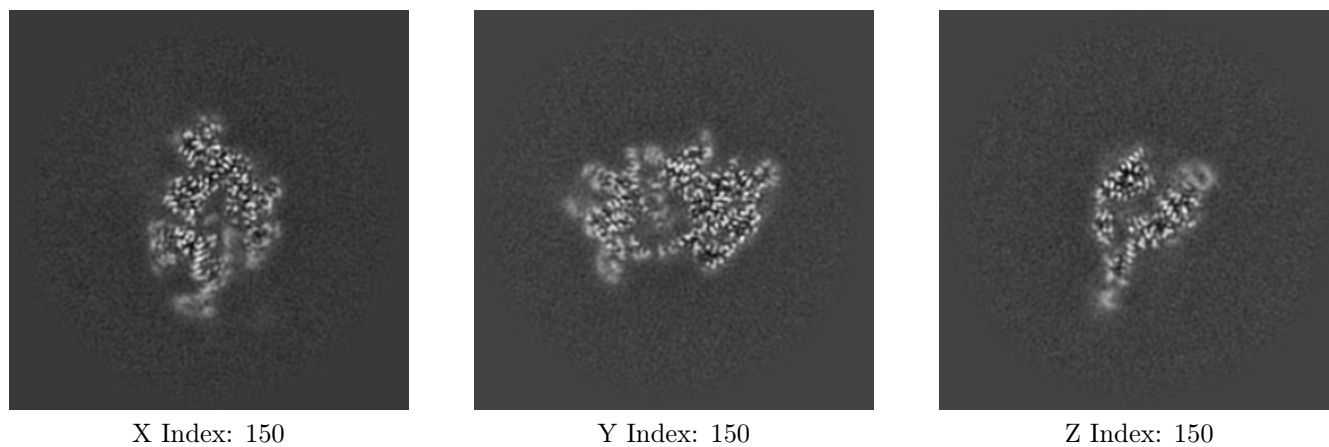
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map

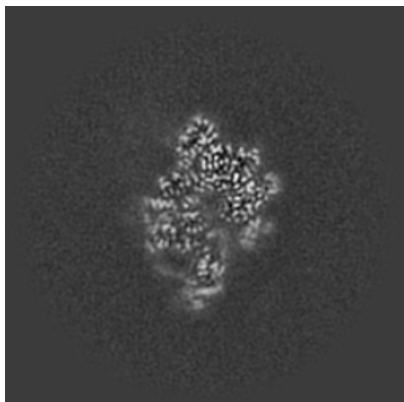




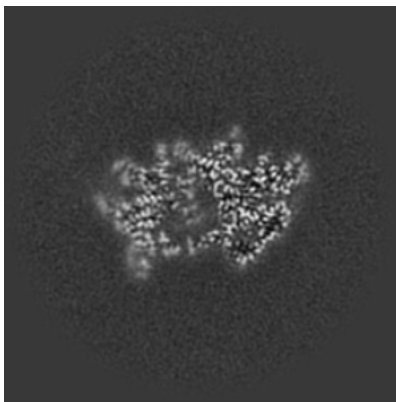
The images above show central slices of the map in three orthogonal directions.

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

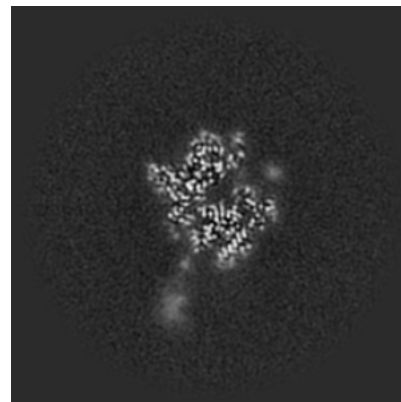
### 6.3.1 Primary map



X Index: 143



Y Index: 149

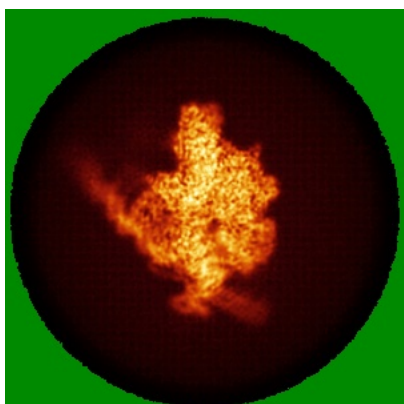


Z Index: 162

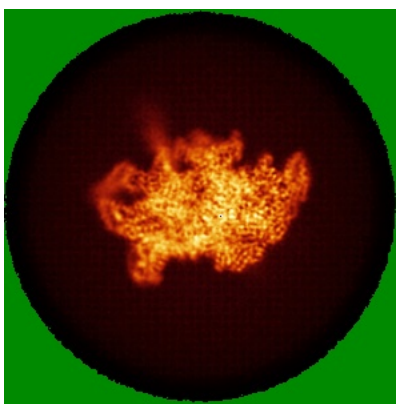
The images above show the largest variance slices of the map in three orthogonal directions.

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

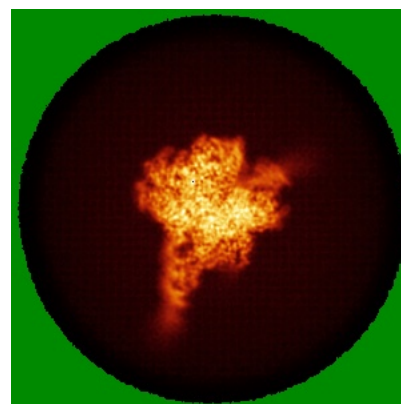
### 6.4.1 Primary map



X



Y

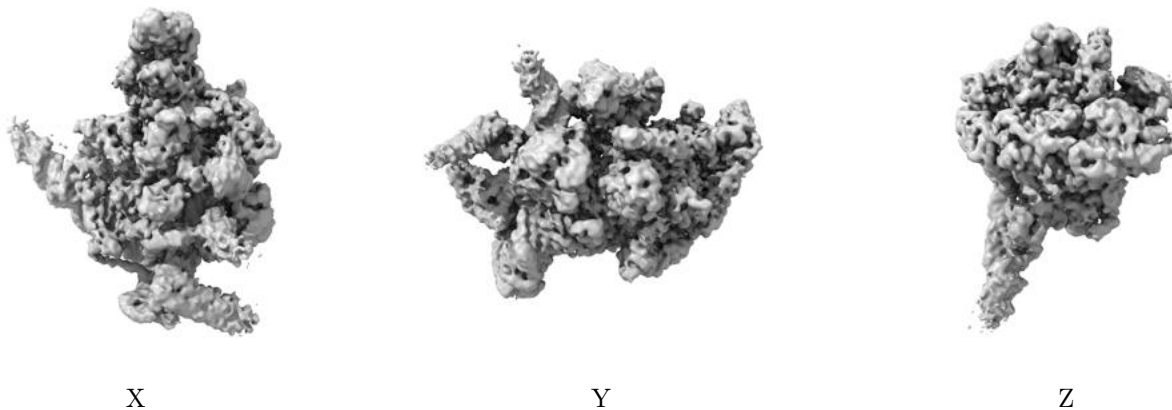


Z

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

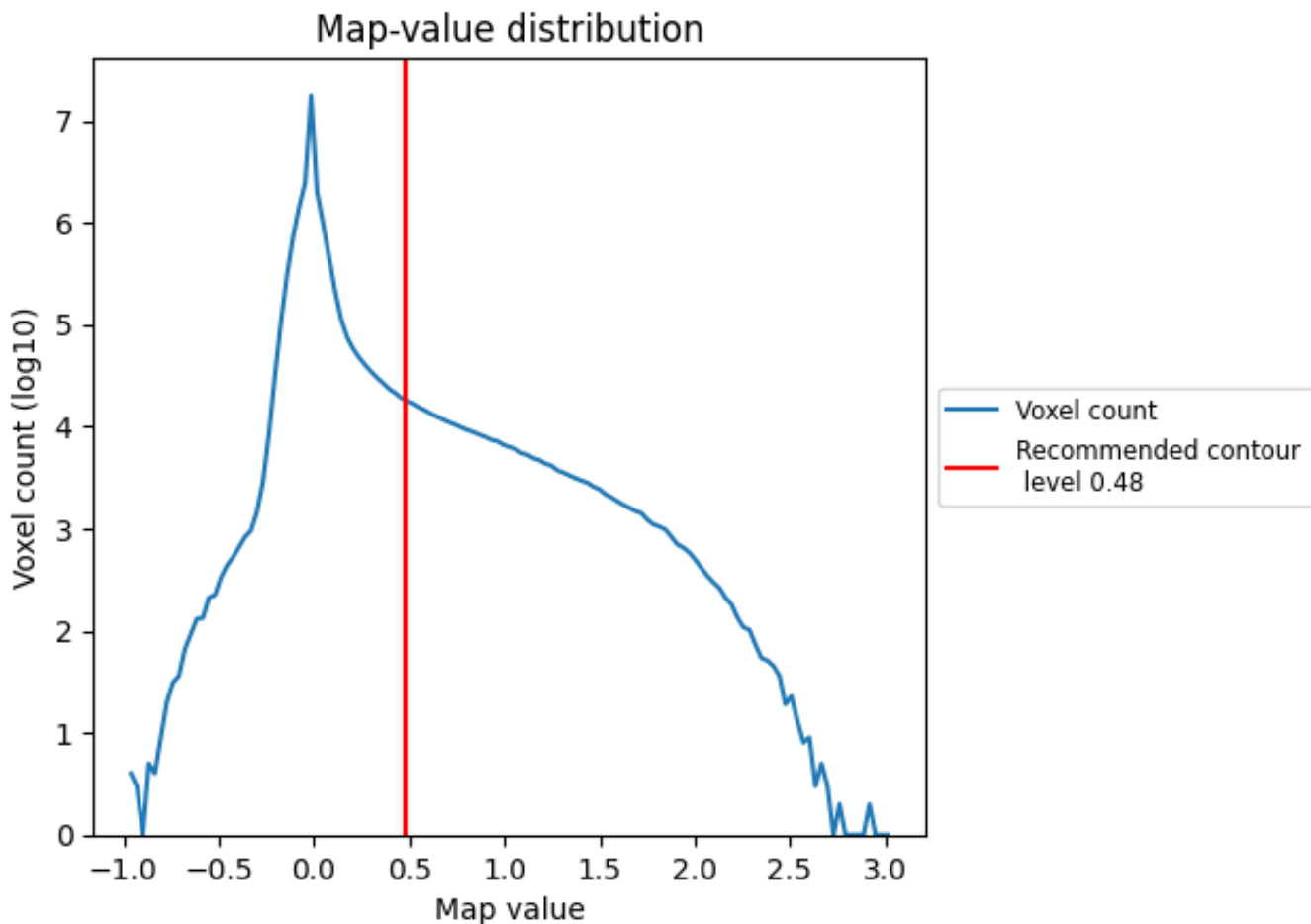
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

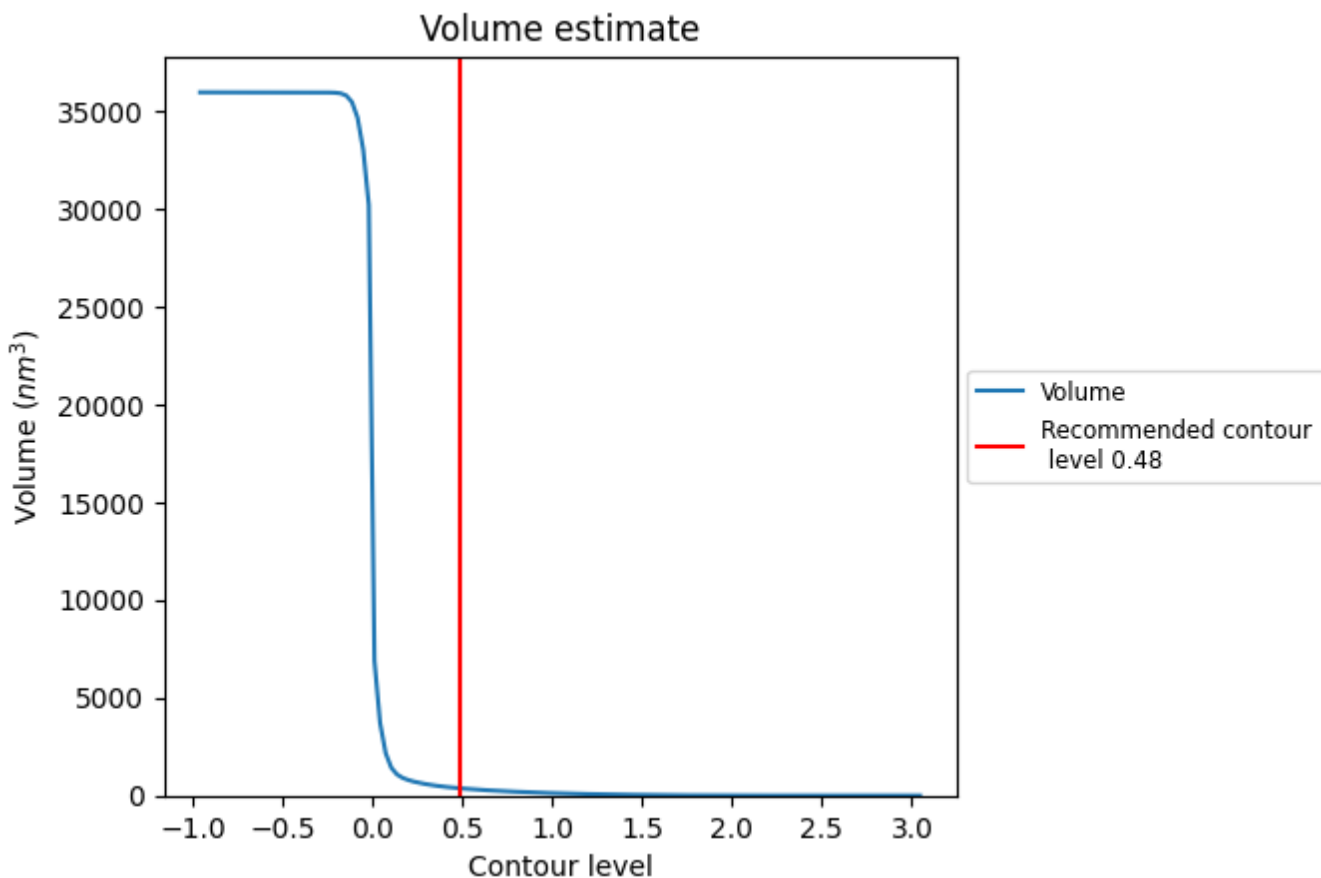
This section contains the results of statistical analysis of the map.

### 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.

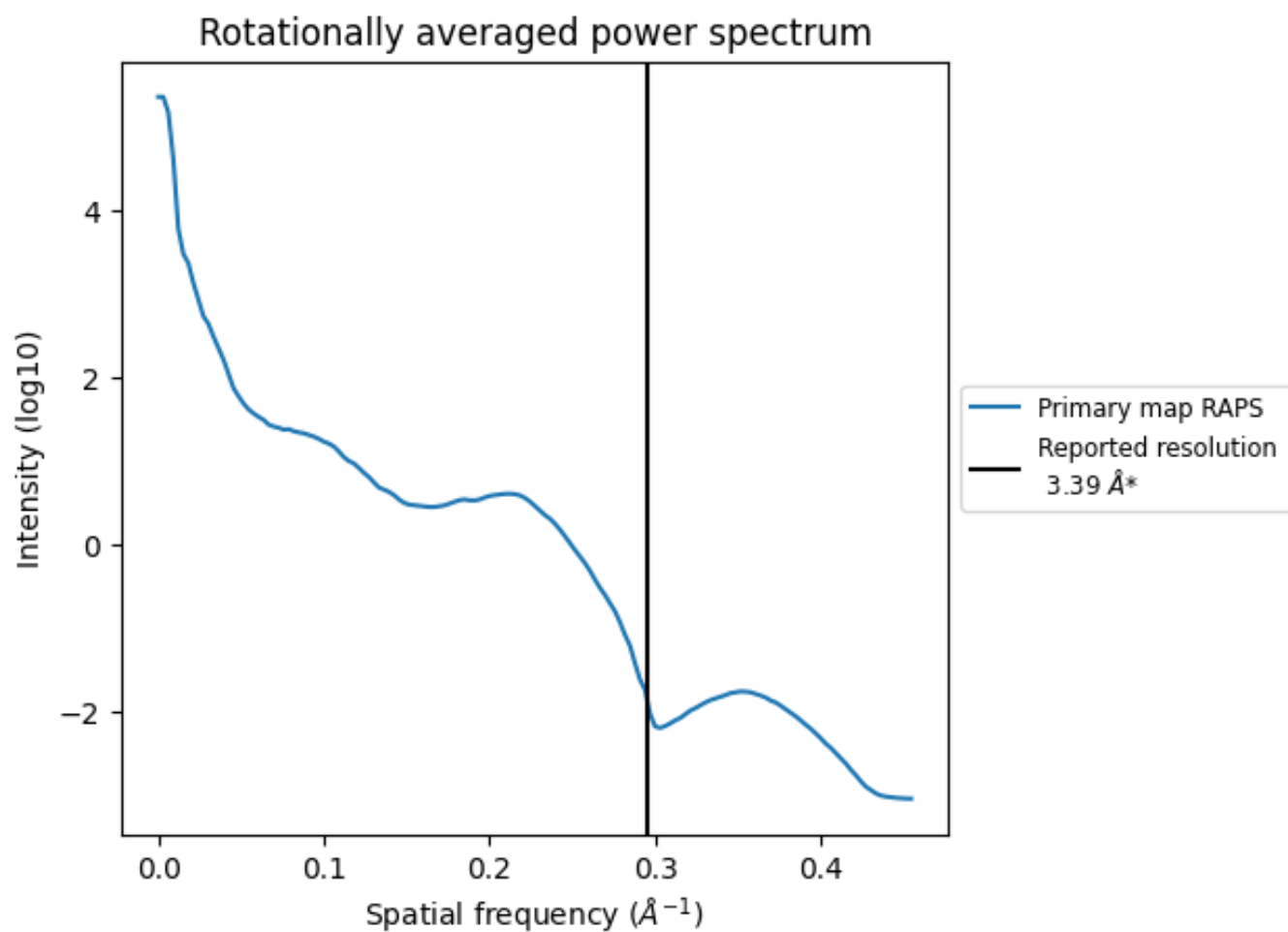
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 377  $\text{nm}^3$ ; this corresponds to an approximate mass of 340 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  $0.295 \text{\AA}^{-1}$

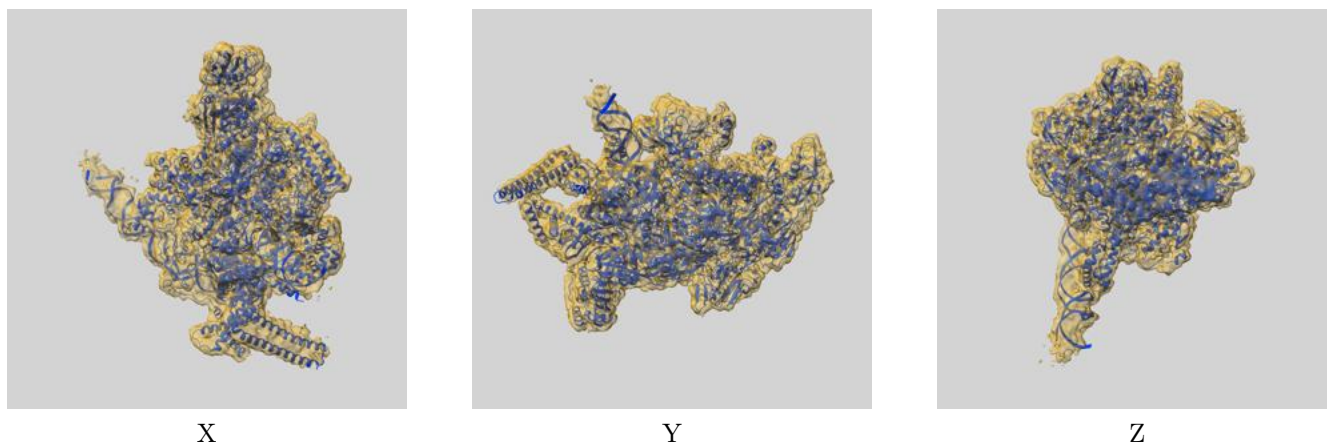
## 8 Fourier-Shell correlation

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

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

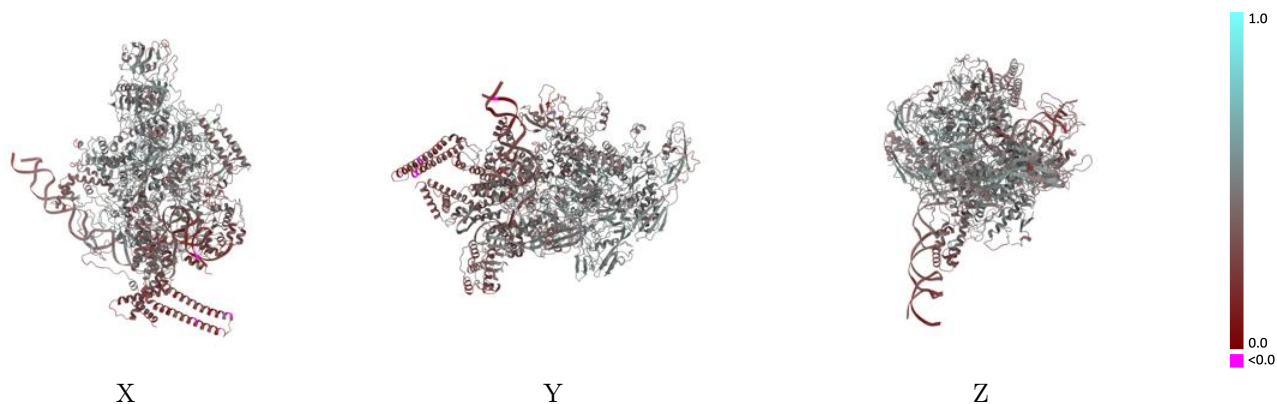
This section contains information regarding the fit between EMDB map EMD-21406 and PDB model 6VXX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



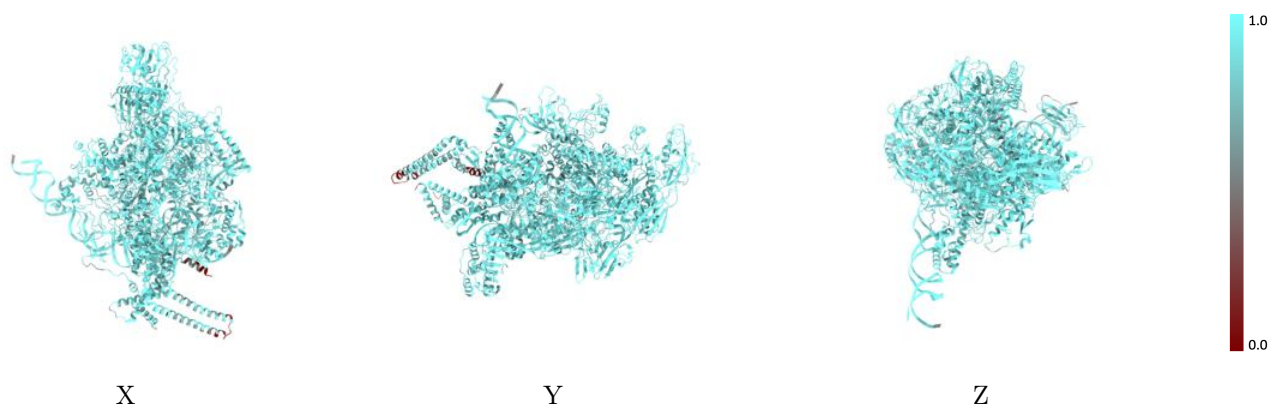
The images above show the 3D surface view of the map at the recommended contour level 0.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

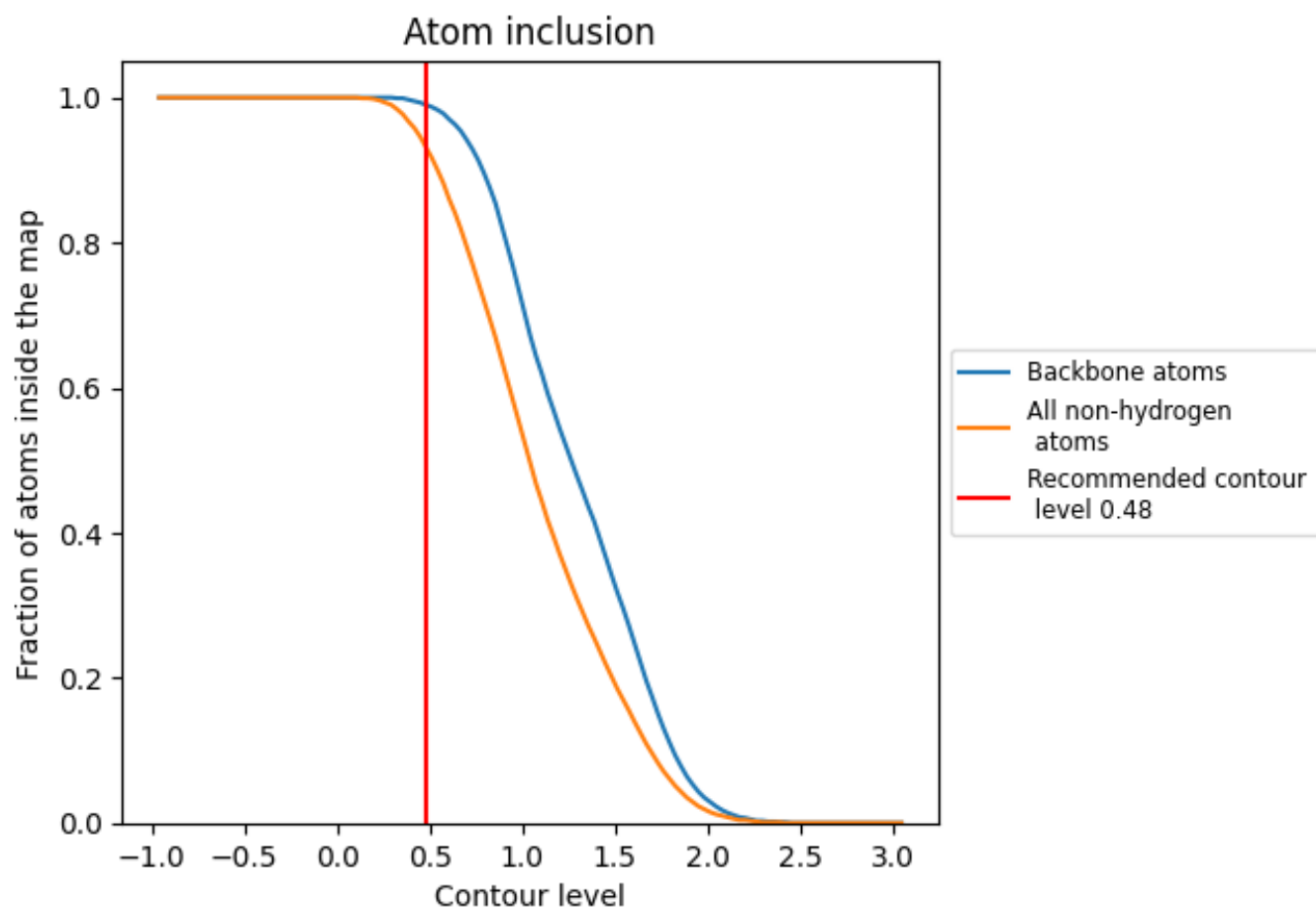
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.48).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.4250
A	 0.9540	 0.4820
B	 0.9420	 0.4570
C	 0.9410	 0.4670
D	 0.9240	 0.4330
E	 0.9450	 0.4620
F	 0.8960	 0.3750
J	 0.8850	 0.3850
M	 0.9010	 0.3420
O	 0.9600	 0.2970
P	 0.9550	 0.2900

