Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 10:08 PM EST

PDB ID	:	6VVY
EMDB ID	:	EMD-21407
Title	:	Mycobacterium tuberculosis WT RNAP transcription open promoter complex with Sorangicin
Authors	:	Lilic, M.; Boyaci, H.; Chen, J.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2020-02-18
Resolution	:	3.42 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

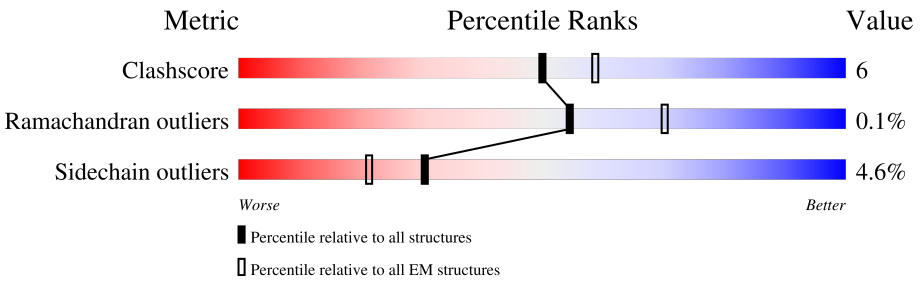
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	52% 13% • 35%
1	B	347	57% 10% • 32%
2	C	1179	77% 16% • 6%
3	D	1326	• 80% 14% • •
4	E	110	57% 16% • 25%
5	F	531	50% 10% 39%
6	J	111	• 77% 19% • •
7	O	90	• 61% 11% 28%

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Mol	Chain	Length	Quality of chain
8	P	90	62% 10% 28%
9	M	162	77% 18%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 30033 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	1716	1080	296	338	2	0	0
1	B	237	1765	1115	301	346	3	0	0

- 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	8602	5390	1511	1662	39	0	0

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	1270	9914	6208	1802	1862	42	0	0

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	322	2540	1583	459	489	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	109	880	543	166	168	3	0	0

- Molecule 7 is a DNA chain called DNA (65-MER).

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

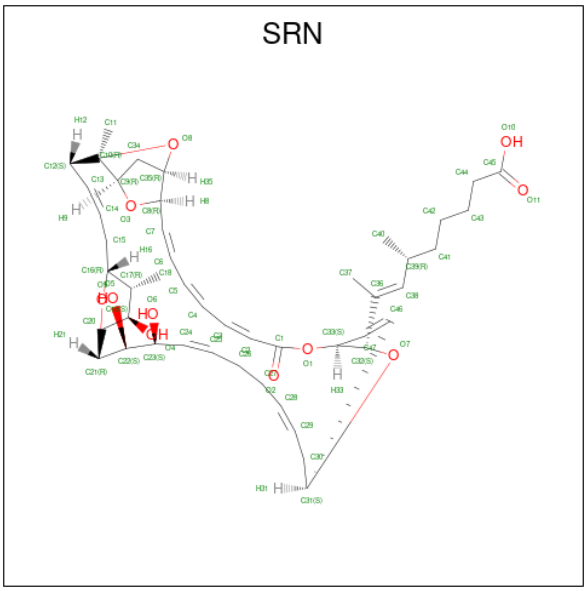
- Molecule 8 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	65	1329	629	250	385	65	0	0

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	159	1241	777	224	239	1	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).

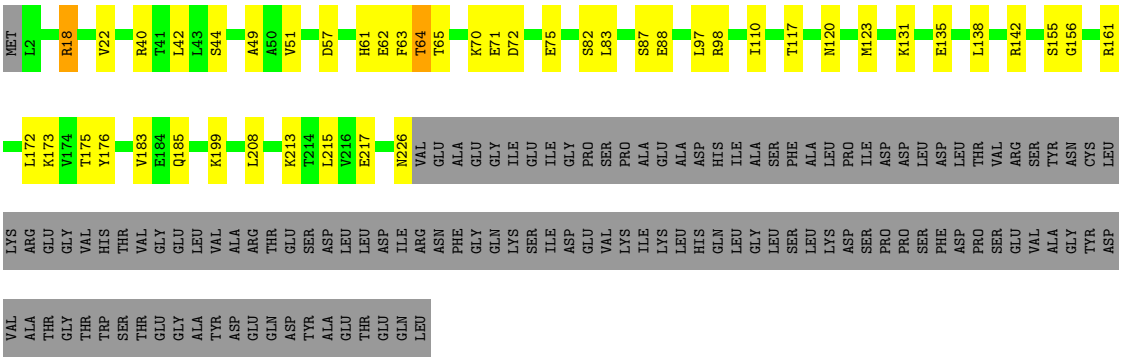
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	D	1	1	1	0

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.

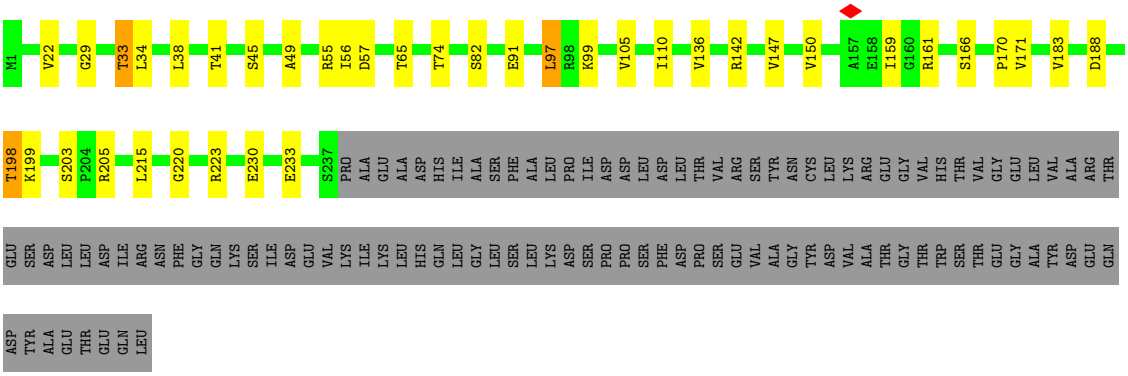
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



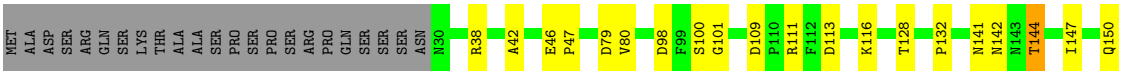
• Molecule 1: DNA-directed RNA polymerase subunit alpha

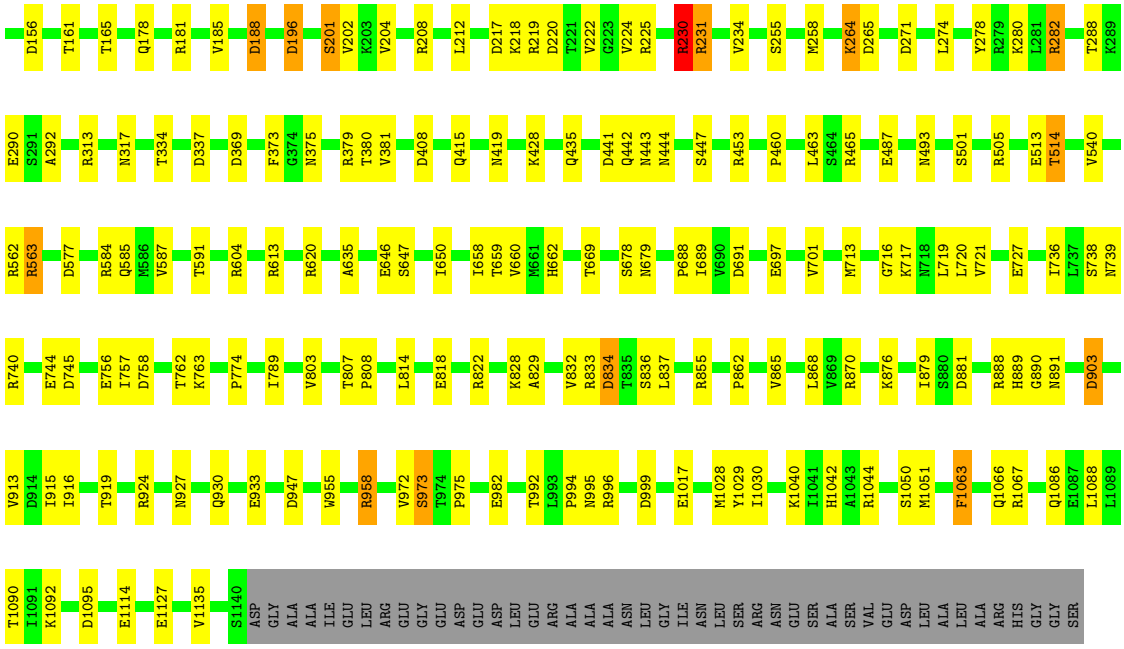
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

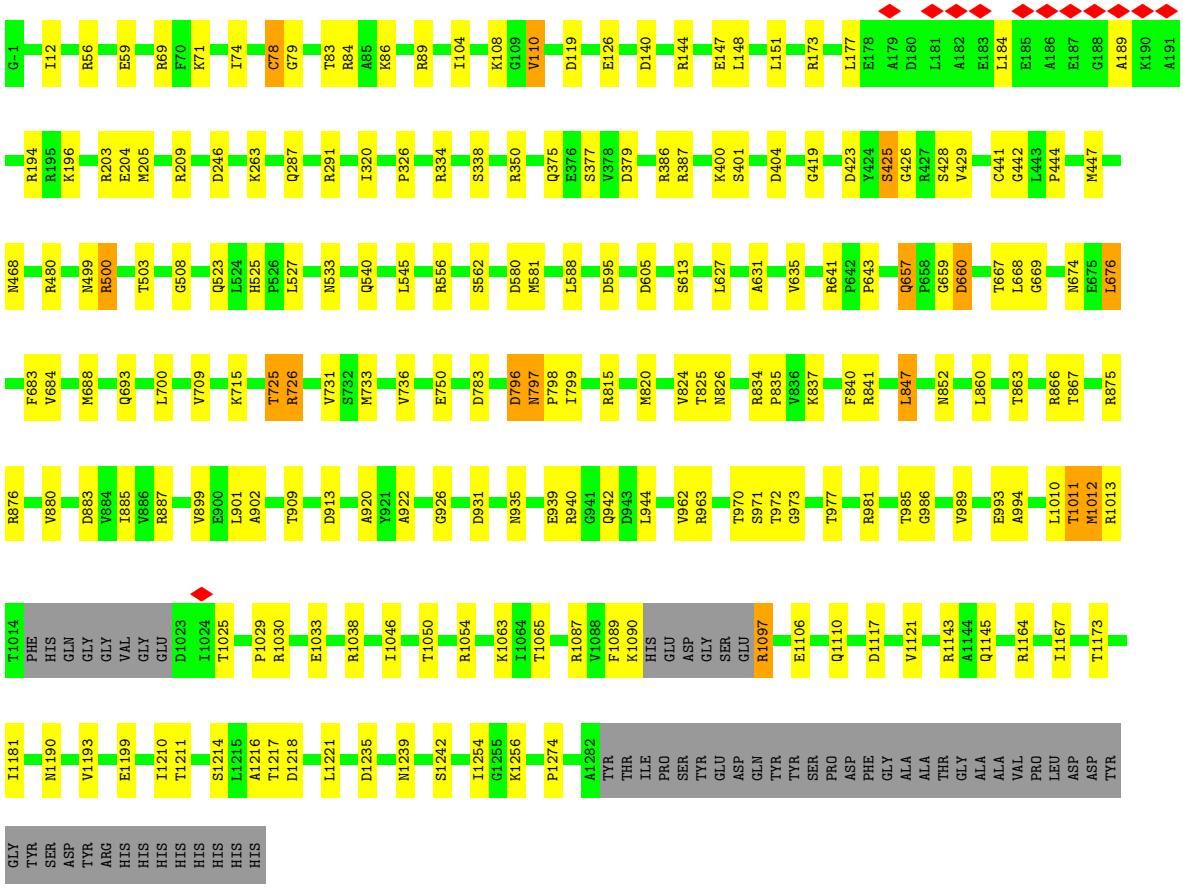
Chain C:





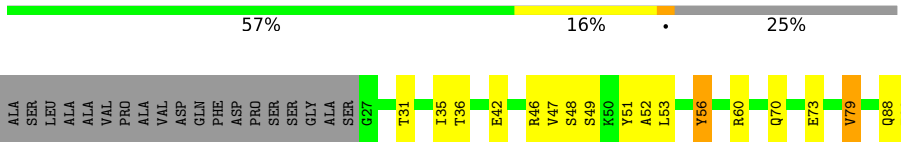
• Molecule 3: DNA-directed RNA polymerase subunit beta'

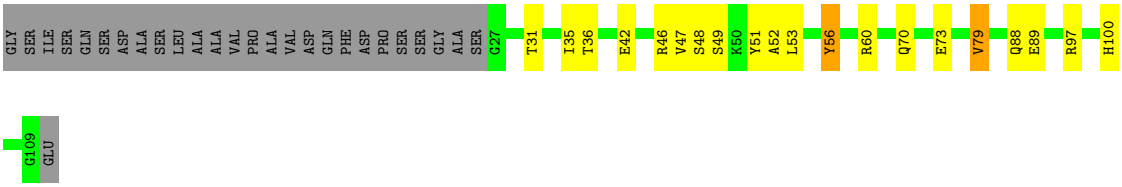
Chain D:



• Molecule 4: DNA-directed RNA polymerase subunit omega

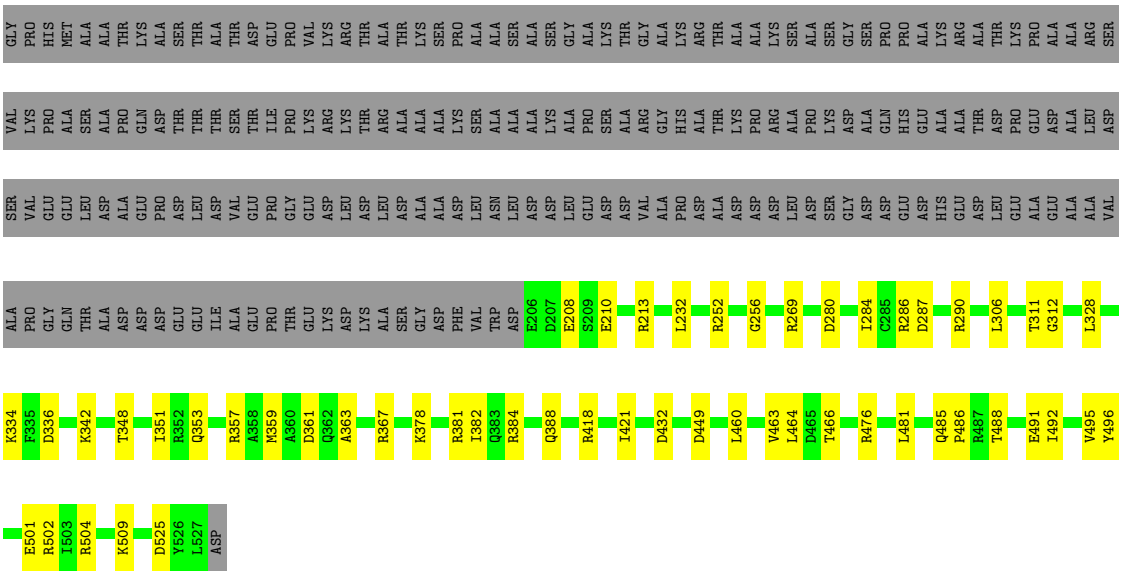
Chain E:





- Molecule 5: RNA polymerase sigma factor SigA

Chain F:

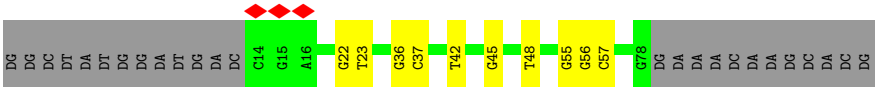


- Molecule 6: RNA polymerase-binding protein RbpA

Chain J:

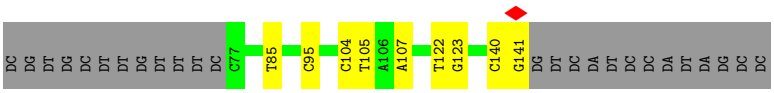
- Molecule 7: DNA (65-MER)

Chain O:



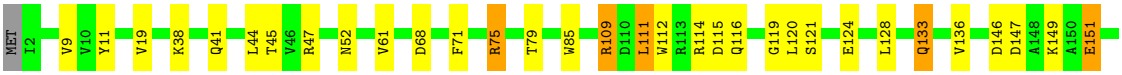
- Molecule 8: DNA (65-MER)

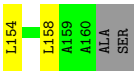
Chain P:



• Molecule 9: RNA polymerase-binding transcription factor CarD

Chain M:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98323	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	2.695	Depositor
Minimum map value	-0.795	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.433	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 (i)

5.1 Standard geometry (i)

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

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	0.52	0/2370
1	B	0.36	0/1792	0.53	0/2442
2	C	0.41	0/8761	0.54	0/11880
3	D	0.39	0/10078	0.54	2/13624 (0.0%)
4	E	0.39	0/662	0.53	0/901
5	F	0.32	0/2571	0.47	0/3468
6	J	0.29	0/896	0.50	0/1210
7	O	0.70	0/1497	0.99	1/2310 (0.0%)
8	P	0.73	1/1491 (0.1%)	0.98	1/2297 (0.0%)
9	M	0.30	0/1257	0.55	0/1700
All	All	0.43	1/30747 (0.0%)	0.60	4/42202 (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	2
3	D	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	95	DC	C1'-N1	5.48	1.56	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	140	ASP	CB-CG-OD2	5.24	123.01	118.30
7	O	42	DT	P-O3'-C3'	5.07	125.78	119.70
3	D	588	LEU	CA-CB-CG	5.02	126.85	115.30
8	P	105	DT	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	230	ARG	Peptide
2	C	282	ARG	Peptide
3	D	110	VAL	Peptide
3	D	657	GLN	Peptide
3	D	834	ARG	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	30	0
1	B	1765	0	1794	24	0
2	C	8602	0	8540	122	0
3	D	9914	0	9986	121	0
4	E	649	0	645	11	0
5	F	2540	0	2552	30	0
6	J	880	0	852	16	0
7	O	1336	0	732	7	0
8	P	1329	0	727	5	0
9	M	1241	0	1259	18	0
10	C	58	0	63	10	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	30033	0	28906	354	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 6.

All (354) 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	1.63
3:D:866:ARG:HD3	3:D:1012:MET:CE	1.41	1.49
10:C:1201:SRN:O3	10:C:1201:SRN:C8	1.79	1.30
10:C:1201:SRN:O3	10:C:1201:SRN:C9	1.81	1.28
3:D:1011:THR:HG23	3:D:1145:GLN:NE2	1.58	1.14
3:D:866:ARG:CD	3:D:1012:MET:CE	2.30	1.10
3:D:866:ARG:CD	3:D:1012:MET:HE1	1.86	1.05
3:D:866:ARG:HH11	3:D:1012:MET:HE3	1.30	0.96
3:D:866:ARG:HD3	3:D:1012:MET:HE1	0.95	0.92
3:D:1011:THR:CG2	3:D:1145:GLN:NE2	2.34	0.90
3:D:866:ARG:HH11	3:D:1012:MET:CE	1.87	0.88
3:D:866:ARG:HD3	3:D:1012:MET:HE2	1.56	0.87
3:D:1011:THR:CG2	3:D:1145:GLN:HE22	1.86	0.87
10:C:1201:SRN:C10	10:C:1201:SRN:C13	2.51	0.86
10:C:1201:SRN:C12	10:C:1201:SRN:C11	2.61	0.78
3:D:866:ARG:CD	3:D:1012:MET:HE2	2.10	0.78
3:D:866:ARG:NH1	3:D:1012:MET:HE3	2.00	0.76
1:A:40:ARG:HE	1:B:33:THR:HG22	1.53	0.74
2:C:225:ARG:HE	2:C:230:ARG:HB3	1.53	0.73
10:C:1201:SRN:C12	10:C:1201:SRN:C9	2.55	0.72
2:C:278:TYR:O	2:C:282:ARG:HB2	1.91	0.71
5:F:384:ARG:HG2	5:F:388:GLN:HE22	1.56	0.70
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.79	0.64
3:D:1011:THR:HG21	3:D:1145:GLN:HE22	1.60	0.64
3:D:880:VAL:HG21	3:D:1210:ILE:HB	1.81	0.62
2:C:147:ILE:HG12	9:M:47:ARG:HB2	1.80	0.62
1:A:183:VAL:HG13	1:A:185:GLN:H	1.65	0.62
2:C:453:ARG:NH2	2:C:501:SER:O	2.33	0.61
3:D:688:MET:HB3	3:D:693:GLN:HE21	1.66	0.60
5:F:306:LEU:HD11	5:F:348:THR:HG23	1.82	0.60
3:D:78:CYS:SG	3:D:79:GLY:N	2.76	0.59
2:C:408:ASP:OD1	2:C:408:ASP:N	2.36	0.59
2:C:659:THR:HG22	2:C:669:THR:HG22	1.85	0.59
2:C:1042:HIS:NE2	2:C:1063:PHE:O	2.28	0.59
1:A:64:THR:OG1	1:A:65:THR:N	2.37	0.58
2:C:903:ASP:OD1	2:C:903:ASP:N	2.35	0.58
2:C:369:ASP:O	2:C:375:ASN:ND2	2.36	0.58
2:C:188:ASP:OD1	2:C:188:ASP:N	2.36	0.58
3:D:676:LEU:HD12	3:D:715:LYS:HB3	1.84	0.58
1:A:142:ARG:NH2	1:B:230:GLU:OE1	2.37	0.58
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.84	0.58
2:C:891:ASN:ND2	2:C:930:GLN:OE1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:ASP:OD1	2:C:79:ASP:N	2.38	0.57
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.85	0.57
3:D:1010:LEU:O	3:D:1011:THR:O	2.22	0.57
3:D:83:THR:OG1	3:D:84:ARG:N	2.38	0.57
4:E:70:GLN:NE2	4:E:73:GLU:OE2	2.38	0.57
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.38	0.57
3:D:899:VAL:HG12	3:D:901:LEU:HB2	1.87	0.57
7:O:22:DG:H2"	7:O:23:DT:H5'	1.86	0.57
5:F:336:ASP:OD1	6:J:88:ARG:NH1	2.38	0.56
2:C:577:ASP:OD1	2:C:577:ASP:N	2.35	0.56
3:D:173:ARG:HG2	3:D:205:MET:HB2	1.86	0.56
3:D:876:ARG:HD3	3:D:1211:THR:HG23	1.86	0.56
3:D:885:ILE:HD11	3:D:887:ARG:HH21	1.68	0.56
5:F:286:ARG:HH11	5:F:290:ARG:HH12	1.53	0.56
9:M:112:TRP:O	9:M:116:GLN:HB2	2.05	0.56
3:D:796:ASP:OD1	3:D:796:ASP:N	2.33	0.56
5:F:464:LEU:HD23	5:F:476:ARG:HE	1.71	0.56
2:C:271:ASP:OD1	2:C:271:ASP:N	2.39	0.56
1:B:57:ASP:OD1	1:B:57:ASP:N	2.39	0.56
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.86	0.56
2:C:144:THR:O	9:M:52:ASN:ND2	2.39	0.56
3:D:468:ASN:OD1	3:D:468:ASN:N	2.38	0.56
1:A:87:SER:OG	1:A:88:GLU:N	2.39	0.55
2:C:38:ARG:NH1	2:C:972:VAL:O	2.38	0.55
2:C:380:THR:OG1	2:C:381:VAL:N	2.40	0.55
3:D:425:SER:OG	3:D:426:GLY:N	2.39	0.55
9:M:75:ARG:NH2	9:M:158:LEU:O	2.39	0.55
2:C:758:ASP:N	2:C:758:ASP:OD1	2.37	0.55
2:C:201:SER:OG	2:C:202:VAL:N	2.39	0.55
2:C:678:SER:OG	2:C:679:ASN:N	2.40	0.55
2:C:740:ARG:NH1	2:C:744:GLU:OE1	2.39	0.55
3:D:880:VAL:HG22	3:D:1214:SER:HB3	1.88	0.55
2:C:757:ILE:HB	2:C:837:LEU:HD22	1.88	0.55
3:D:147:GLU:O	3:D:151:LEU:HB2	2.06	0.55
1:B:33:THR:OG1	1:B:34:LEU:N	2.39	0.54
2:C:113:ASP:HB2	2:C:132:PRO:HD2	1.89	0.54
2:C:982:GLU:OE1	3:D:841:ARG:NH2	2.40	0.54
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.89	0.54
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.89	0.54
3:D:500:ARG:NH1	3:D:533:ASN:O	2.40	0.54
3:D:866:ARG:HD2	3:D:1012:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:20:ARG:NH1	6:J:23:ASP:O	2.41	0.54
9:M:121:SER:HB3	9:M:124:GLU:HB2	1.90	0.54
2:C:147:ILE:HD11	9:M:47:ARG:HH11	1.71	0.54
2:C:719:LEU:HD22	2:C:1030:ILE:HD11	1.90	0.54
1:A:217:GLU:HG2	1:B:233:GLU:HA	1.88	0.54
3:D:926:GLY:O	3:D:940:ARG:NH2	2.41	0.54
3:D:350:ARG:HH11	3:D:377:SER:HB3	1.73	0.53
2:C:150:GLN:HG3	9:M:44:LEU:HB3	1.91	0.53
2:C:334:THR:HG23	2:C:337:ASP:H	1.74	0.53
5:F:210:GLU:HA	5:F:213:ARG:HB3	1.90	0.53
8:P:107:DA:OP1	9:M:121:SER:OG	2.24	0.53
2:C:736:ILE:HD11	2:C:916:ILE:HD12	1.91	0.53
2:C:101:GLY:O	2:C:142:ASN:ND2	2.41	0.53
3:D:1087:ARG:NH1	3:D:1110:GLN:OE1	2.42	0.53
2:C:756:GLU:OE2	2:C:870:ARG:NH1	2.40	0.52
2:C:995:ASN:N	2:C:995:ASN:OD1	2.39	0.52
1:A:62:GLU:OE2	2:C:876:LYS:NZ	2.41	0.52
2:C:230:ARG:O	2:C:230:ARG:NH1	2.42	0.52
2:C:828:LYS:HE2	2:C:829:ALA:H	1.75	0.52
2:C:444:ASN:N	2:C:444:ASN:OD1	2.42	0.52
1:B:198:THR:OG1	1:B:199:LYS:O	2.28	0.52
2:C:808:PRO:HA	2:C:832:VAL:HG12	1.92	0.52
2:C:955:TRP:O	2:C:958:ARG:NH1	2.43	0.52
3:D:931:ASP:N	3:D:931:ASP:OD1	2.41	0.52
2:C:218:LYS:NZ	8:P:85:DT:OP1	2.39	0.52
2:C:855:ARG:NH1	2:C:865:VAL:O	2.43	0.52
10:C:1201:SRN:O3	10:C:1201:SRN:H6	2.10	0.52
3:D:144:ARG:O	3:D:148:LEU:HB2	2.11	0.52
2:C:789:ILE:HG22	2:C:803:VAL:HG22	1.92	0.51
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.92	0.51
5:F:232:LEU:HD22	7:O:55:DG:H2"	1.90	0.51
2:C:178:GLN:OE1	2:C:379:ARG:NH2	2.43	0.51
2:C:881:ASP:N	2:C:881:ASP:OD1	2.42	0.51
5:F:488:THR:OG1	5:F:491:GLU:OE1	2.25	0.51
5:F:336:ASP:OD1	6:J:89:ARG:NH2	2.43	0.51
1:A:71:GLU:HB3	1:A:75:GLU:HB3	1.93	0.51
3:D:1025:THR:HG21	3:D:1029:PRO:HB2	1.92	0.51
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.40	0.51
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.93	0.50
7:O:56:DG:H2'	7:O:57:DC:C2	2.45	0.50
1:B:171:VAL:HA	1:B:198:THR:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:381:ARG:HH21	8:P:104:DC:H1'	1.74	0.50
2:C:822:ARG:NH1	2:C:828:LYS:O	2.43	0.50
5:F:311:THR:OG1	5:F:312:GLY:N	2.45	0.50
5:F:463:VAL:O	5:F:466:THR:OG1	2.29	0.50
9:M:147:ASP:OD1	9:M:147:ASP:N	2.44	0.50
2:C:435:GLN:HE21	2:C:460:PRO:HG3	1.77	0.50
2:C:443:ASN:OD1	2:C:443:ASN:N	2.44	0.50
3:D:126:GLU:OE2	3:D:387:ARG:NE	2.43	0.50
1:B:56:ILE:HB	1:B:136:VAL:HG22	1.93	0.50
2:C:442:GLN:NE2	2:C:679:ASN:OD1	2.41	0.50
3:D:184:LEU:O	3:D:194:ARG:NH1	2.44	0.50
2:C:1092:LYS:NZ	3:D:545:LEU:O	2.44	0.50
3:D:750:GLU:OE1	3:D:837:LYS:NZ	2.43	0.50
3:D:922:ALA:HB1	3:D:981:ARG:HB3	1.94	0.50
1:A:82:SER:O	1:A:82:SER:OG	2.27	0.50
2:C:947:ASP:OD1	2:C:947:ASP:N	2.39	0.50
3:D:700:LEU:HD23	3:D:709:VAL:HG22	1.94	0.50
9:M:79:THR:OG1	9:M:109:ARG:NH2	2.45	0.50
5:F:485:GLN:NE2	5:F:486:PRO:O	2.44	0.50
6:J:20:ARG:NH1	6:J:23:ASP:OD1	2.45	0.49
10:C:1201:SRN:O3	10:C:1201:SRN:C6	2.60	0.49
3:D:74:ILE:HD12	6:J:42:VAL:HG13	1.94	0.49
3:D:334:ARG:HD3	5:F:418:ARG:HE	1.77	0.49
9:M:115:ASP:HA	9:M:119:GLY:H	1.75	0.49
1:A:70:LYS:NZ	2:C:691:ASP:OD1	2.45	0.49
5:F:256:GLY:HA2	5:F:284:ILE:HG22	1.94	0.49
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.77	0.49
1:B:45:SER:O	1:B:45:SER:OG	2.31	0.49
1:A:120:ASN:OD1	1:A:120:ASN:N	2.45	0.49
3:D:1089:PHE:O	3:D:1097:ARG:N	2.46	0.49
3:D:108:LYS:O	3:D:386:ARG:NH1	2.46	0.49
3:D:375:GLN:NE2	3:D:379:ASP:OD2	2.45	0.49
5:F:502:ARG:NH2	7:O:23:DT:OP2	2.44	0.49
2:C:231:ARG:HB2	2:C:280:LYS:HE2	1.94	0.49
10:C:1201:SRN:O3	10:C:1201:SRN:C35	2.53	0.49
3:D:444:PRO:HG2	3:D:447:MET:HB3	1.95	0.49
4:E:42:GLU:O	4:E:46:ARG:NH1	2.46	0.49
1:A:49:ALA:HB2	1:A:142:ARG:HD2	1.94	0.49
3:D:935:ASN:OD1	3:D:935:ASN:N	2.42	0.49
3:D:428:SER:OG	3:D:429:VAL:N	2.46	0.48
6:J:63:THR:OG1	6:J:64:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:64:LEU:HD23	6:J:66:GLU:H	1.78	0.48
1:B:183:VAL:HA	1:B:188:ASP:H	1.77	0.48
2:C:255:SER:HB2	2:C:258:MET:HB2	1.94	0.48
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.78	0.48
2:C:38:ARG:HG2	2:C:973:SER:HB3	1.95	0.48
2:C:1067:ARG:NH2	3:D:419:GLY:O	2.45	0.48
3:D:971:SER:OG	3:D:972:THR:N	2.45	0.48
3:D:985:THR:OG1	3:D:986:GLY:N	2.45	0.48
6:J:34:THR:OG1	6:J:36:ASN:OD1	2.31	0.48
3:D:641:ARG:HA	3:D:657:GLN:HG3	1.96	0.47
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	1.95	0.47
9:M:41:GLN:OE1	9:M:133:GLN:NE2	2.44	0.47
2:C:185:VAL:HG12	2:C:204:VAL:HG22	1.97	0.47
3:D:989:VAL:HG22	3:D:993:GLU:HG3	1.96	0.47
2:C:264:LYS:HD2	2:C:264:LYS:HA	1.74	0.47
2:C:836:SER:OG	2:C:837:LEU:N	2.47	0.47
4:E:48:SER:OG	4:E:49:SER:N	2.47	0.47
1:A:18:ARG:HH12	2:C:996:ARG:HH12	1.63	0.47
2:C:1135:VAL:HG22	3:D:12:ILE:HG13	1.97	0.47
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.95	0.47
3:D:605:ASP:OD1	3:D:605:ASP:N	2.45	0.47
3:D:1217:THR:OG1	3:D:1218:ASP:N	2.48	0.47
5:F:367:ARG:NH2	7:O:45:DG:OP1	2.42	0.47
5:F:464:LEU:HB3	5:F:476:ARG:HH21	1.80	0.47
9:M:111:LEU:HB3	9:M:128:LEU:HD12	1.96	0.47
2:C:915:ILE:HD13	2:C:1030:ILE:HD13	1.96	0.47
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.97	0.47
2:C:505:ARG:NH2	2:C:513:GLU:OE1	2.48	0.47
2:C:727:GLU:H	3:D:725:THR:HG22	1.80	0.47
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.97	0.47
3:D:643:PRO:HD3	3:D:683:PHE:HB3	1.96	0.47
6:J:79:ARG:NH1	7:O:48:DT:OP1	2.45	0.47
2:C:994:PRO:HB3	2:C:999:ASP:H	1.80	0.47
3:D:1254:ILE:HD11	3:D:1256:LYS:HD2	1.96	0.46
1:A:40:ARG:NH2	1:B:29:GLY:O	2.38	0.46
1:B:97:LEU:HB3	1:B:110:ILE:HG13	1.96	0.46
2:C:647:SER:HB2	2:C:697:GLU:HA	1.97	0.46
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.97	0.46
1:A:57:ASP:OD1	1:A:57:ASP:N	2.42	0.46
2:C:1088:LEU:HD23	2:C:1092:LYS:HD2	1.97	0.46
3:D:825:THR:OG1	3:D:826:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.48	0.46
3:D:1030:ARG:NH1	3:D:1033:GLU:OE2	2.42	0.46
2:C:891:ASN:OD1	2:C:891:ASN:N	2.40	0.46
3:D:56:ARG:HB2	3:D:59:GLU:HB2	1.97	0.46
3:D:674:ASN:HD21	3:D:684:VAL:H	1.63	0.46
5:F:252:ARG:NE	5:F:287:ASP:OD2	2.47	0.46
9:M:136:VAL:HG21	9:M:151:GLU:HG2	1.97	0.46
3:D:963:ARG:NH1	3:D:977:THR:OG1	2.49	0.46
2:C:587:VAL:HG22	2:C:591:THR:HB	1.98	0.46
2:C:265:ASP:OD1	2:C:265:ASP:N	2.41	0.46
2:C:620:ARG:HB3	2:C:717:LYS:HZ1	1.81	0.46
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.98	0.46
3:D:69:ARG:HG3	6:J:20:ARG:HH22	1.81	0.46
3:D:660:ASP:OD1	3:D:660:ASP:N	2.49	0.46
2:C:441:ASP:OD2	2:C:447:SER:OG	2.32	0.46
2:C:1066:GLN:NE2	3:D:425:SER:OG	2.40	0.46
5:F:501:GLU:OE2	5:F:504:ARG:NH2	2.45	0.46
5:F:359:MET:O	5:F:363:ALA:HB2	2.16	0.45
2:C:888:ARG:NH2	2:C:933:GLU:OE2	2.45	0.45
3:D:525:HIS:CE1	3:D:527:LEU:HD12	2.51	0.45
5:F:334:LYS:HG3	6:J:84:MET:HG2	1.98	0.45
2:C:879:ILE:HD12	2:C:879:ILE:HA	1.83	0.45
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.40	0.45
6:J:89:ARG:HD3	6:J:89:ARG:HA	1.77	0.45
3:D:196:LYS:HD2	3:D:196:LYS:HA	1.77	0.45
3:D:657:GLN:O	3:D:659:GLY:N	2.50	0.45
2:C:927:ASN:OD1	2:C:927:ASN:N	2.49	0.45
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.99	0.45
1:B:159:ILE:H	1:B:159:ILE:HG13	1.51	0.45
2:C:465:ARG:NH1	2:C:493:ASN:OD1	2.37	0.45
2:C:762:THR:OG1	2:C:763:LYS:N	2.50	0.45
3:D:939:GLU:OE2	3:D:942:GLN:NE2	2.48	0.45
1:B:55:ARG:HB3	1:B:161:ARG:HA	1.98	0.45
2:C:109:ASP:OD2	2:C:111:ARG:NH1	2.50	0.45
2:C:514:THR:HG22	2:C:585:GLN:HE21	1.80	0.45
3:D:334:ARG:HD2	3:D:334:ARG:HA	1.73	0.45
9:M:114:ARG:HD3	9:M:120:LEU:HD21	1.98	0.45
9:M:146:ASP:O	9:M:149:LYS:N	2.49	0.45
1:B:41:THR:HG21	1:B:215:LEU:HG	1.99	0.45
3:D:173:ARG:O	3:D:177:LEU:HB2	2.16	0.45
5:F:492:ILE:O	5:F:496:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:LEU:HD22	2:C:292:ALA:HB1	1.99	0.44
2:C:774:PRO:HD2	2:C:834:ASP:HB2	1.99	0.44
3:D:173:ARG:NH1	3:D:204:GLU:OE1	2.50	0.44
8:P:140:DC:H2"	8:P:141:DG:C8	2.52	0.44
3:D:1235:ASP:N	3:D:1235:ASP:OD1	2.45	0.44
5:F:449:ASP:OD1	5:F:449:ASP:N	2.47	0.44
6:J:77:PRO:HA	6:J:78:PRO:HD3	1.90	0.44
1:A:175:THR:OG1	1:A:176:TYR:N	2.51	0.44
2:C:288:THR:OG1	2:C:290:GLU:OE1	2.31	0.44
5:F:382:ILE:HD13	5:F:382:ILE:HA	1.88	0.44
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.99	0.44
3:D:1274:PRO:HG2	4:E:79:VAL:HG21	1.99	0.44
5:F:502:ARG:HA	5:F:502:ARG:HD2	1.81	0.44
2:C:814:LEU:HD12	2:C:818:GLU:HG2	1.99	0.44
3:D:84:ARG:HD2	3:D:86:LYS:HG2	2.00	0.44
3:D:736:VAL:HG22	3:D:799:ILE:HD11	2.00	0.44
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.00	0.44
3:D:863:THR:O	3:D:867:THR:OG1	2.34	0.44
5:F:328:LEU:HD23	5:F:351:ILE:HD11	2.00	0.44
1:A:213:LYS:NZ	1:B:233:GLU:OE2	2.51	0.43
1:B:34:LEU:O	1:B:38:LEU:HB2	2.18	0.43
2:C:1086:GLN:O	2:C:1090:THR:OG1	2.25	0.43
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.99	0.43
10:C:1201:SRN:H152	10:C:1201:SRN:H181	1.78	0.43
2:C:973:SER:O	2:C:973:SER:OG	2.32	0.43
1:A:161:ARG:HE	1:A:161:ARG:HB2	1.65	0.43
2:C:1040:LYS:HD2	3:D:540:GLN:HE22	1.82	0.43
3:D:1054:ARG:N	3:D:1065:THR:O	2.44	0.43
1:A:155:SER:OG	1:A:156:GLY:N	2.52	0.43
2:C:435:GLN:H	2:C:435:GLN:HG2	1.52	0.43
3:D:627:LEU:HD13	3:D:668:LEU:HD12	2.00	0.43
5:F:432:ASP:OD1	5:F:432:ASP:N	2.51	0.43
2:C:604:ARG:NH2	2:C:890:GLY:O	2.44	0.43
3:D:326:PRO:O	3:D:338:SER:OG	2.36	0.43
1:A:97:LEU:HB2	1:A:110:ILE:HG12	2.00	0.43
2:C:716:GLY:N	2:C:1029:TYR:OH	2.43	0.43
2:C:1050:SER:OG	2:C:1051:MET:N	2.52	0.43
7:O:36:DG:H2"	7:O:37:DC:H5"	2.01	0.43
3:D:847:LEU:HD12	3:D:847:LEU:HA	1.88	0.43
3:D:866:ARG:HH11	3:D:1012:MET:HE2	1.79	0.43
1:A:98:ARG:HG2	1:A:135:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:H	1:A:199:LYS:HG2	1.70	0.43
2:C:646:GLU:HB3	2:C:662:HIS:CE1	2.53	0.43
1:A:83:LEU:HA	1:A:123:MET:HE1	2.01	0.42
3:D:119:ASP:OD1	3:D:291:ARG:NH2	2.53	0.42
1:A:51:VAL:HG21	1:A:138:LEU:HD23	2.02	0.42
1:A:61:HIS:HD2	1:A:63:PHE:H	1.66	0.42
4:E:52:ALA:O	4:E:56:TYR:HB2	2.19	0.42
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.86	0.42
3:D:580:ASP:OD1	3:D:580:ASP:N	2.52	0.42
2:C:98:ASP:OD1	2:C:98:ASP:N	2.53	0.42
3:D:902:ALA:H	3:D:913:ASP:HB2	1.83	0.42
2:C:161:THR:OG1	2:C:165:THR:O	2.31	0.42
2:C:738:SER:OG	2:C:739:ASN:N	2.53	0.42
3:D:556:ARG:NH2	4:E:35:ILE:O	2.53	0.42
3:D:815:ARG:NH1	3:D:820:MET:O	2.53	0.42
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.91	0.42
6:J:101:ARG:HA	6:J:101:ARG:HD3	1.82	0.42
3:D:203:ARG:HA	3:D:203:ARG:HD2	1.85	0.42
2:C:562:ARG:HD3	3:D:847:LEU:HD11	2.01	0.42
2:C:1017:GLU:H	2:C:1017:GLU:HG2	1.65	0.42
2:C:217:ASP:OD1	2:C:217:ASP:N	2.40	0.41
2:C:689:ILE:HD11	2:C:701:VAL:HG12	2.02	0.41
3:D:641:ARG:O	3:D:683:PHE:N	2.53	0.41
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.46	0.41
2:C:428:LYS:HE2	2:C:428:LYS:HB3	1.95	0.41
2:C:563:ARG:HD3	2:C:563:ARG:HA	1.68	0.41
3:D:189:ALA:O	3:D:194:ARG:NH2	2.53	0.41
3:D:993:GLU:OE2	4:E:51:TYR:OH	2.37	0.41
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.93	0.41
3:D:725:THR:OG1	3:D:726:ARG:NH1	2.53	0.41
5:F:378:LYS:HE2	5:F:378:LYS:HB3	1.84	0.41
1:B:220:GLY:HA2	1:B:223:ARG:HB3	2.02	0.41
2:C:224:VAL:HG21	2:C:234:VAL:HA	2.03	0.41
2:C:862:PRO:HG2	2:C:865:VAL:HG21	2.01	0.41
3:D:1190:ASN:HA	3:D:1193:VAL:HG12	2.02	0.41
6:J:15:SER:OG	6:J:16:TYR:N	2.53	0.41
1:B:49:ALA:HA	1:B:142:ARG:HA	2.03	0.41
3:D:401:SER:OG	3:D:404:ASP:OD2	2.39	0.41
3:D:503:THR:HG23	3:D:508:GLY:HA3	2.03	0.41
3:D:970:THR:OG1	3:D:973:GLY:O	2.31	0.41
1:A:215:LEU:HD13	1:A:215:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:ARG:NH1	2:C:317:ASN:OD1	2.54	0.41
2:C:435:GLN:HG3	2:C:460:PRO:HD3	2.03	0.41
3:D:1050:THR:HG22	3:D:1106:GLU:HA	2.02	0.41
3:D:1221:LEU:HD12	3:D:1221:LEU:HA	1.92	0.41
4:E:60:ARG:HA	4:E:60:ARG:HD2	1.92	0.41
6:J:93:GLU:H	6:J:93:GLU:HG3	1.74	0.41
2:C:46:GLU:HA	2:C:47:PRO:HD3	1.94	0.41
2:C:807:THR:O	2:C:833:ARG:N	2.53	0.41
8:P:122:DT:H2'	8:P:123:DG:C8	2.55	0.41
9:M:38:LYS:HE2	9:M:38:LYS:HB2	1.92	0.41
1:B:82:SER:O	1:B:82:SER:OG	2.36	0.40
2:C:150:GLN:HE22	2:C:415:GLN:HB2	1.86	0.40
3:D:797:ASN:HD22	3:D:798:PRO:HD2	1.86	0.40
5:F:492:ILE:HA	5:F:495:VAL:HG12	2.03	0.40
1:B:147:VAL:HG12	1:B:166:SER:HB2	2.03	0.40
2:C:1127:GLU:HG2	3:D:320:ILE:HD11	2.03	0.40
2:C:442:GLN:O	2:C:678:SER:OG	2.29	0.40
2:C:650:ILE:HD13	2:C:660:VAL:HG12	2.04	0.40
2:C:721:VAL:HG11	2:C:1028:MET:HB2	2.03	0.40
2:C:757:ILE:HD12	2:C:757:ILE:HA	1.87	0.40
3:D:667:THR:OG1	3:D:669:GLY:N	2.54	0.40
9:M:38:LYS:HA	9:M:45:THR:HA	2.03	0.40
2:C:1044:ARG:NE	3:D:423:ASP:OD1	2.55	0.40
1:B:203:SER:OG	1:B:205:ARG:NH2	2.54	0.40
2:C:196:ASP:OD1	2:C:196:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	223/347 (64%)	204 (92%)	19 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	235/347 (68%)	211 (90%)	24 (10%)	0	100	100
2	C	1109/1179 (94%)	1018 (92%)	90 (8%)	1 (0%)	51	83
3	D	1264/1326 (95%)	1167 (92%)	95 (8%)	2 (0%)	47	80
4	E	81/110 (74%)	74 (91%)	7 (9%)	0	100	100
5	F	320/531 (60%)	307 (96%)	13 (4%)	0	100	100
6	J	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
9	M	157/162 (97%)	147 (94%)	10 (6%)	0	100	100
All	All	3496/4113 (85%)	3226 (92%)	267 (8%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1011	THR
2	C	231	ARG
3	D	835	PRO

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%)	185 (95%)	9 (5%)	27	60
1	B	195/297 (66%)	187 (96%)	8 (4%)	30	62
2	C	936/997 (94%)	901 (96%)	35 (4%)	34	65
3	D	1048/1103 (95%)	1001 (96%)	47 (4%)	27	61
4	E	69/89 (78%)	64 (93%)	5 (7%)	14	46
5	F	266/429 (62%)	254 (96%)	12 (4%)	27	61
6	J	92/97 (95%)	85 (92%)	7 (8%)	13	43
9	M	129/131 (98%)	116 (90%)	13 (10%)	7	31
All	All	2929/3440 (85%)	2793 (95%)	136 (5%)	31	60

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	22	VAL
1	A	44	SER
1	A	64	THR
1	A	72	ASP
1	A	117	THR
1	A	131	LYS
1	A	172	LEU
1	A	226	ASN
1	B	22	VAL
1	B	33	THR
1	B	65	THR
1	B	74	THR
1	B	91	GLU
1	B	97	LEU
1	B	150	VAL
1	B	198	THR
2	C	80	VAL
2	C	100	SER
2	C	116	LYS
2	C	128	THR
2	C	141	ASN
2	C	144	THR
2	C	156	ASP
2	C	181	ARG
2	C	188	ASP
2	C	196	ASP
2	C	201	SER
2	C	208	ARG
2	C	212	LEU
2	C	219	ARG
2	C	220	ASP
2	C	222	VAL
2	C	230	ARG
2	C	264	LYS
2	C	373	PHE
2	C	419	ASN
2	C	463	LEU
2	C	514	THR
2	C	540	VAL
2	C	563	ARG
2	C	584	ARG

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Mol	Chain	Res	Type
2	C	745	ASP
2	C	834	ASP
2	C	903	ASP
2	C	924	ARG
2	C	958	ARG
2	C	973	SER
2	C	992	THR
2	C	1063	PHE
2	C	1095	ASP
2	C	1114	GLU
3	D	71	LYS
3	D	78	CYS
3	D	89	ARG
3	D	110	VAL
3	D	209	ARG
3	D	246	ASP
3	D	263	LYS
3	D	287	GLN
3	D	400	LYS
3	D	425	SER
3	D	441	CYS
3	D	480	ARG
3	D	499	ASN
3	D	500	ARG
3	D	562	SER
3	D	581	MET
3	D	613	SER
3	D	635	VAL
3	D	660	ASP
3	D	676	LEU
3	D	725	THR
3	D	726	ARG
3	D	733	MET
3	D	783	ASP
3	D	796	ASP
3	D	797	ASN
3	D	840	PHE
3	D	847	LEU
3	D	860	LEU
3	D	875	ARG
3	D	883	ASP
3	D	909	THR

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Mol	Chain	Res	Type
3	D	944	LEU
3	D	962	VAL
3	D	1012	MET
3	D	1013	ARG
3	D	1038	ARG
3	D	1063	LYS
3	D	1090	LYS
3	D	1097	ARG
3	D	1117	ASP
3	D	1121	VAL
3	D	1143	ARG
3	D	1173	THR
3	D	1199	GLU
3	D	1239	ASN
3	D	1242	SER
4	E	31	THR
4	E	36	THR
4	E	56	TYR
4	E	79	VAL
4	E	88	GLN
5	F	208	GLU
5	F	269	ARG
5	F	280	ASP
5	F	342	LYS
5	F	353	GLN
5	F	357	ARG
5	F	361	ASP
5	F	421	ILE
5	F	460	LEU
5	F	481	LEU
5	F	509	LYS
5	F	525	ASP
6	J	5	VAL
6	J	15	SER
6	J	27	ARG
6	J	55	LEU
6	J	63	THR
6	J	76	LYS
6	J	110	ARG
9	M	9	VAL
9	M	11	TYR
9	M	19	VAL

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Mol	Chain	Res	Type
9	M	61	VAL
9	M	68	ASP
9	M	71	PHE
9	M	75	ARG
9	M	85	TRP
9	M	109	ARG
9	M	111	LEU
9	M	133	GLN
9	M	151	GLU
9	M	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	226	ASN
1	B	124	HIS
1	B	226	ASN
2	C	141	ASN
2	C	419	ASN
2	C	585	GLN
2	C	662	HIS
2	C	920	HIS
2	C	1062	GLN
3	D	287	GLN
3	D	341	ASN
3	D	368	ASN
3	D	525	HIS
3	D	639	GLN
3	D	653	HIS
3	D	657	GLN
3	D	693	GLN
3	D	797	ASN
3	D	1145	GLN
5	F	299	ASN
5	F	353	GLN
5	F	377	ASN
5	F	388	GLN
6	J	22	HIS

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	5.00	33 (55%)	62,84,84	1.79	13 (20%)

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	-	-	12/52/105/105	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	19.40	1.79	1.44
10	C	1201	SRN	O3-C9	16.17	1.81	1.45
10	C	1201	SRN	C34-C9	-10.85	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1201	SRN	C3-C2	9.14	1.58	1.34
10	C	1201	SRN	C34-C35	-8.74	1.33	1.52
10	C	1201	SRN	C4-C5	7.87	1.56	1.36
10	C	1201	SRN	C13-C14	6.74	1.60	1.31
10	C	1201	SRN	C8-C7	-6.04	1.29	1.50
10	C	1201	SRN	C24-C25	6.01	1.57	1.31
10	C	1201	SRN	C6-C7	5.86	1.56	1.33
10	C	1201	SRN	C12-C13	-5.71	1.30	1.50
10	C	1201	SRN	C10-C9	-5.11	1.43	1.53
10	C	1201	SRN	C28-C29	5.08	1.61	1.31
10	C	1201	SRN	O7-C32	5.05	1.51	1.43
10	C	1201	SRN	C35-C8	-4.94	1.45	1.53
10	C	1201	SRN	O8-C12	4.87	1.51	1.43
10	C	1201	SRN	C3-C4	4.47	1.57	1.44
10	C	1201	SRN	C5-C6	4.40	1.56	1.44
10	C	1201	SRN	C11-C10	-4.31	1.44	1.53
10	C	1201	SRN	C33-C47	-3.79	1.43	1.49
10	C	1201	SRN	C46-C47	3.67	1.44	1.33
10	C	1201	SRN	O1-C1	3.57	1.42	1.34
10	C	1201	SRN	C30-C29	3.51	1.61	1.50
10	C	1201	SRN	O7-C31	3.42	1.53	1.44
10	C	1201	SRN	C2-C1	3.15	1.55	1.48
10	C	1201	SRN	C23-C24	2.82	1.54	1.50
10	C	1201	SRN	O1-C33	2.79	1.50	1.46
10	C	1201	SRN	C15-C14	2.62	1.58	1.50
10	C	1201	SRN	C22-C21	2.44	1.56	1.52
10	C	1201	SRN	O8-C35	2.39	1.50	1.44
10	C	1201	SRN	C17-C16	2.26	1.57	1.53
10	C	1201	SRN	C31-C46	2.22	1.53	1.50
10	C	1201	SRN	O6-C23	-2.05	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1201	SRN	C8-C7-C6	-5.39	115.06	125.61
10	C	1201	SRN	C6-C5-C4	-4.60	114.58	124.81
10	C	1201	SRN	C32-C33-C47	3.91	114.61	110.64
10	C	1201	SRN	C18-C17-C19	-3.26	107.37	111.36
10	C	1201	SRN	C35-O8-C12	3.09	118.31	112.81
10	C	1201	SRN	C3-C4-C5	-3.01	118.11	124.81
10	C	1201	SRN	C20-C19-C17	2.97	114.81	111.02
10	C	1201	SRN	C23-C24-C25	-2.95	118.20	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1201	SRN	C9-C34-C35	2.48	110.88	103.73
10	C	1201	SRN	C43-C44-C45	-2.34	108.58	114.47
10	C	1201	SRN	O9-C21-C20	2.29	112.32	109.94
10	C	1201	SRN	C30-C31-C46	-2.07	109.36	113.00
10	C	1201	SRN	C16-C15-C14	-2.01	107.97	113.26

There are no chirality outliers.

All (12) torsion outliers are listed below:

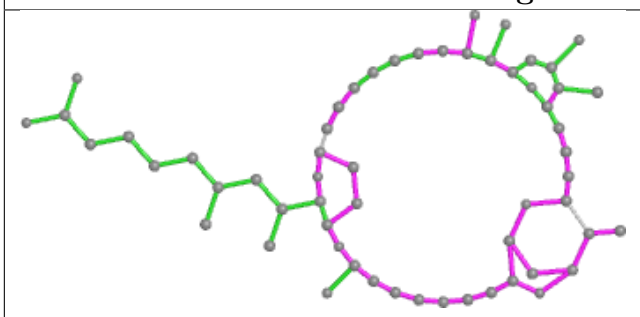
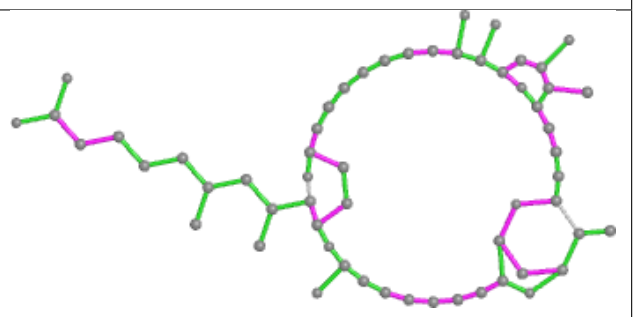
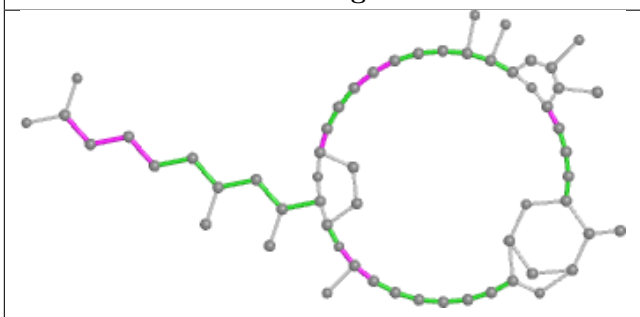
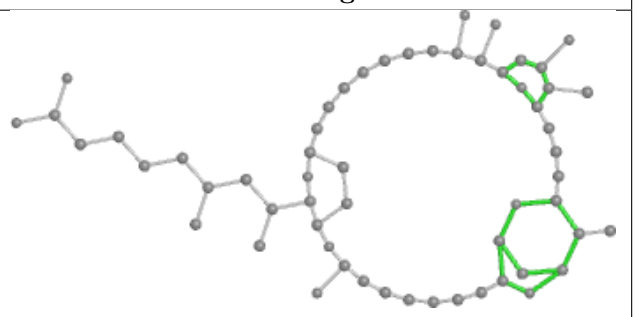
Mol	Chain	Res	Type	Atoms
10	C	1201	SRN	C29-C30-C31-O7
10	C	1201	SRN	C25-C26-C27-C28
10	C	1201	SRN	O1-C1-C2-C3
10	C	1201	SRN	O2-C1-C2-C3
10	C	1201	SRN	C42-C43-C44-C45
10	C	1201	SRN	O2-C1-O1-C33
10	C	1201	SRN	C2-C1-O1-C33
10	C	1201	SRN	C26-C27-C28-C29
10	C	1201	SRN	C43-C44-C45-O10
10	C	1201	SRN	C43-C44-C45-O11
10	C	1201	SRN	C41-C42-C43-C44
10	C	1201	SRN	C14-C15-C16-O9

There are no ring outliers.

1 monomer is involved in 10 short contacts:

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

Ligand SRN C 1201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

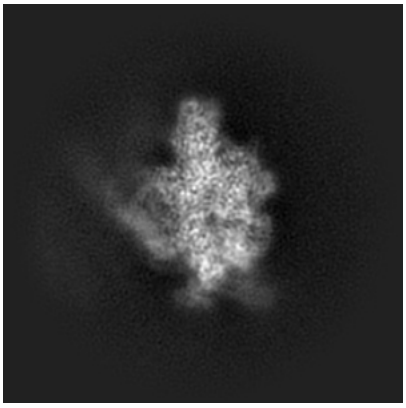
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21407. These allow visual inspection of the internal detail of the map and identification of artifacts.

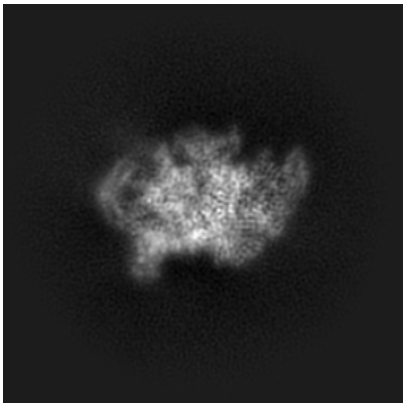
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

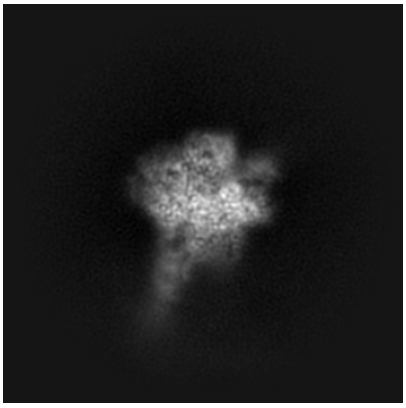
6.1.1 Primary map



X



Y

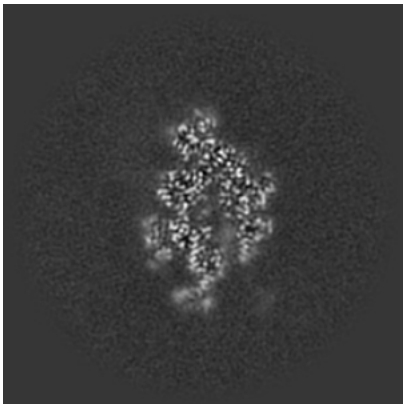


Z

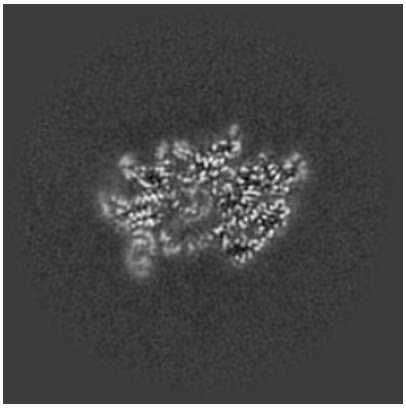
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

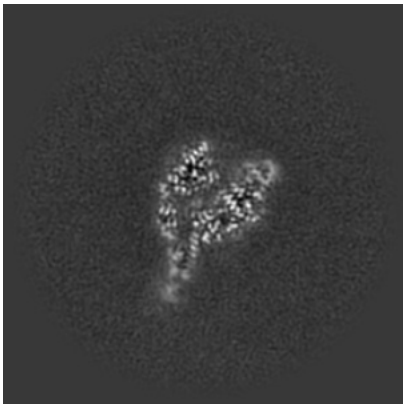
6.2.1 Primary map



X Index: 150



Y Index: 150

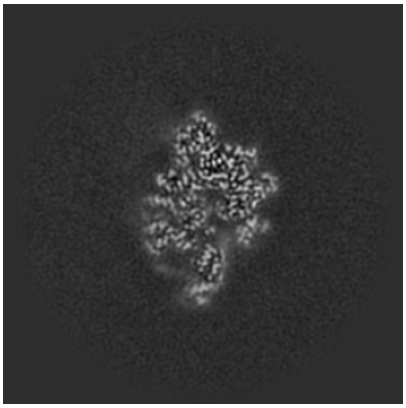


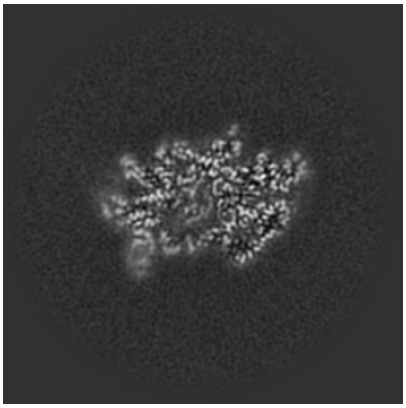
Z Index: 150

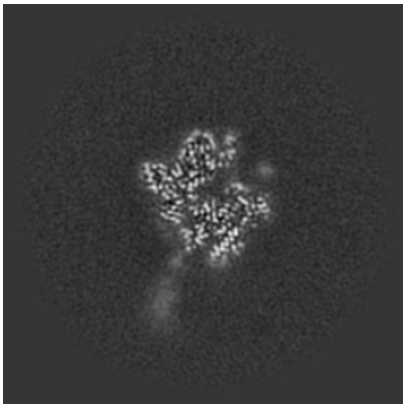
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 144

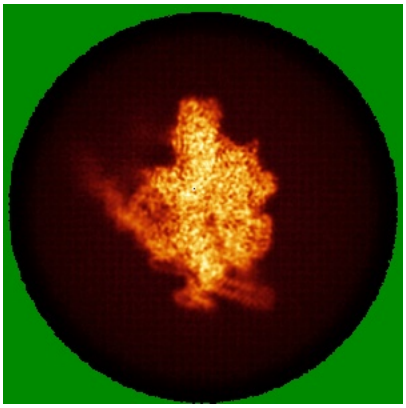

Y Index: 149

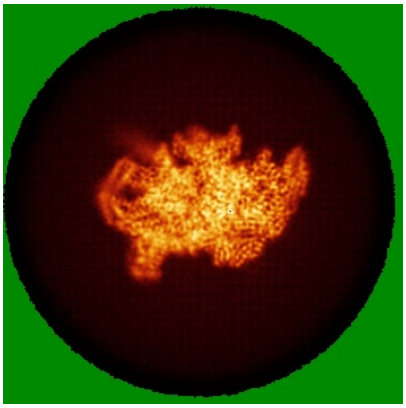

Z Index: 163

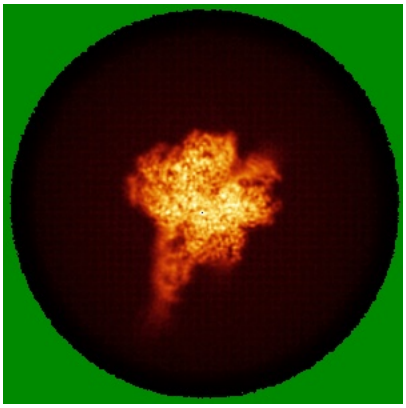
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.433. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

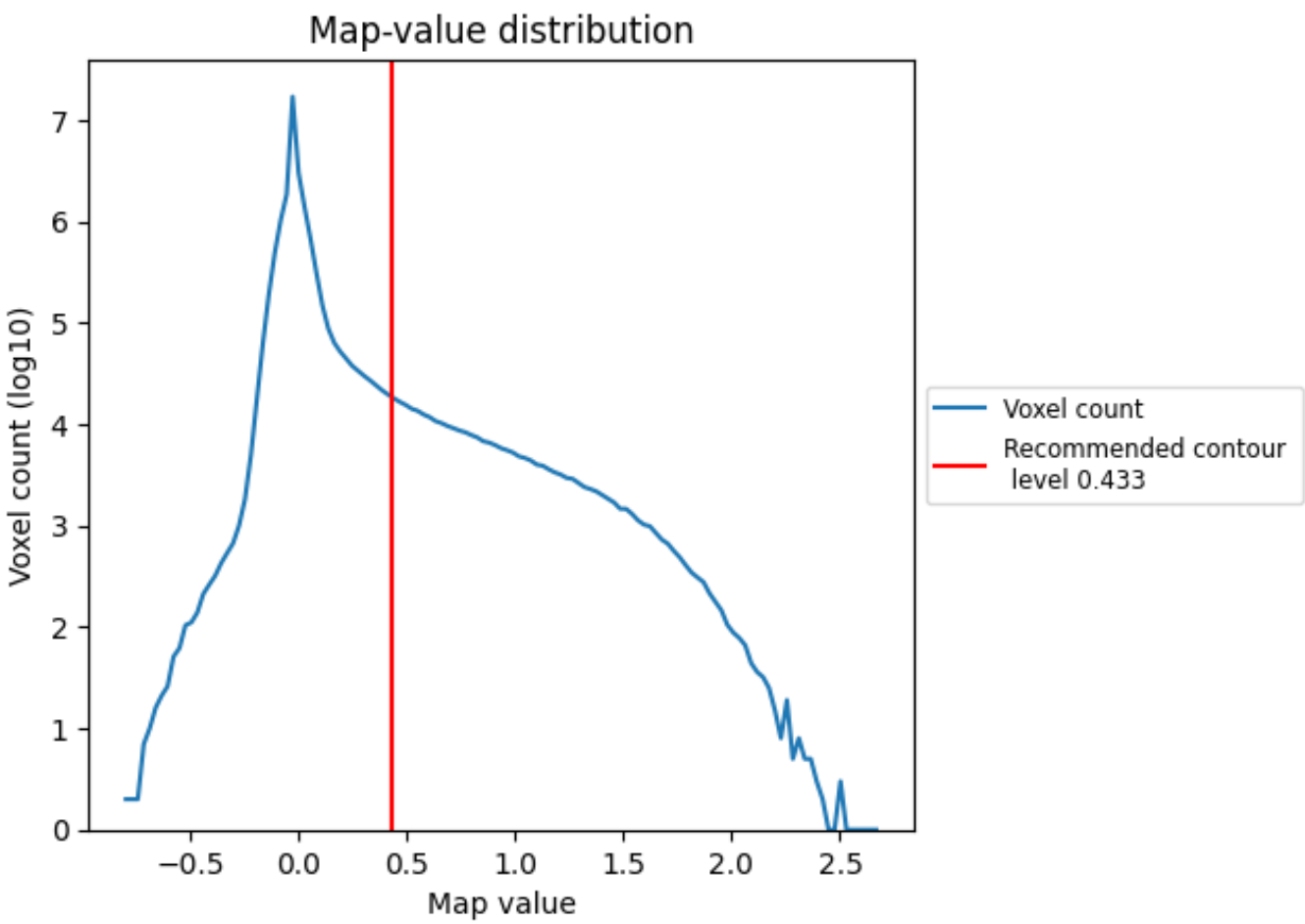
6.6 Mask visualisation (i)

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

7 Map analysis (i)

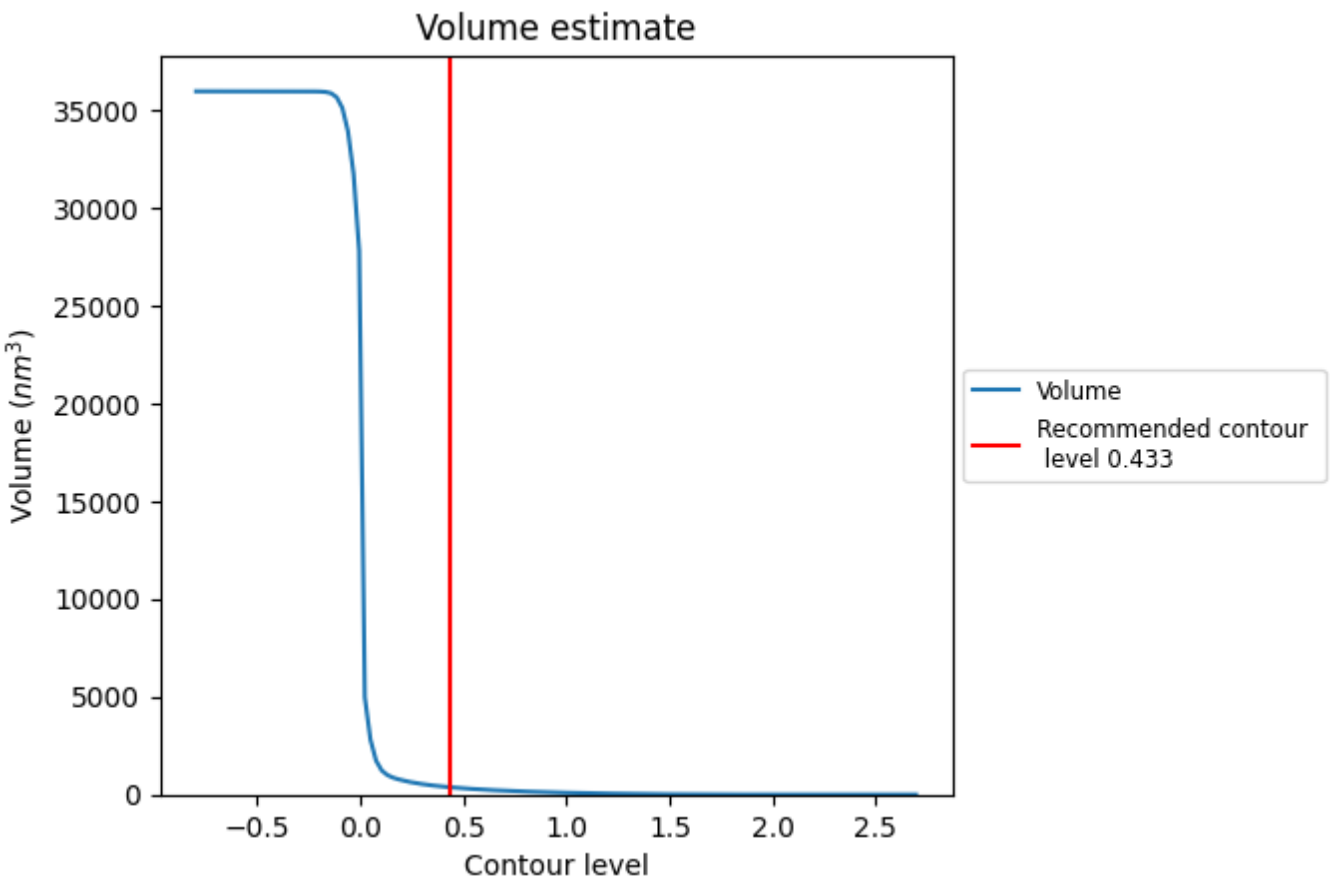
This section contains the results of statistical analysis of the map.

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.

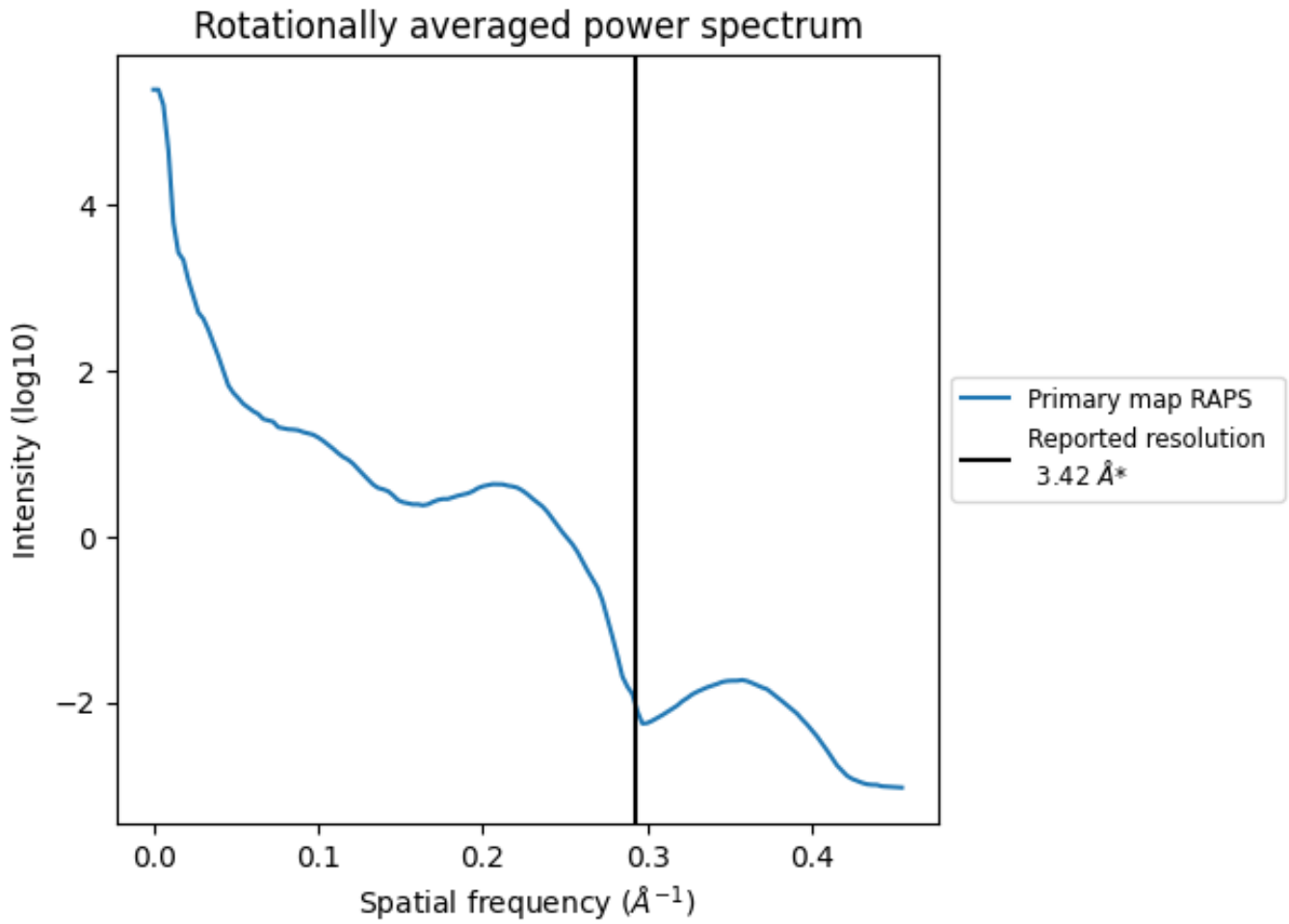
7.2 Volume estimate (i)



The volume at the recommended contour level is 376 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 0.292 Å^{-1}

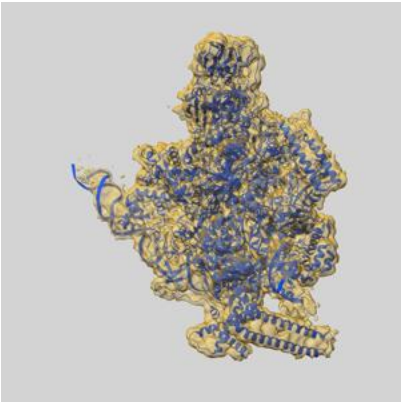
8 Fourier-Shell correlation (i)

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

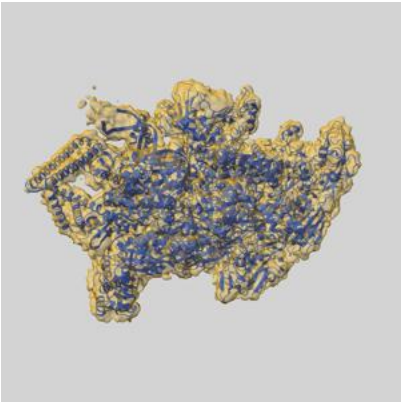
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21407 and PDB model 6VVY. Per-residue inclusion information can be found in section 3 on page 8.

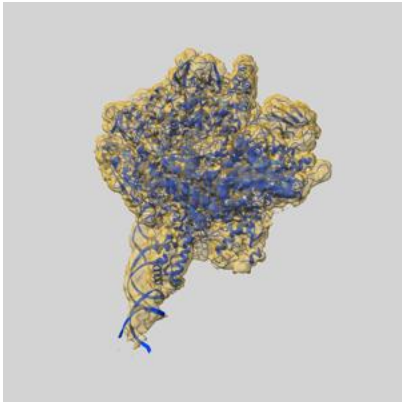
9.1 Map-model overlay (i)



X



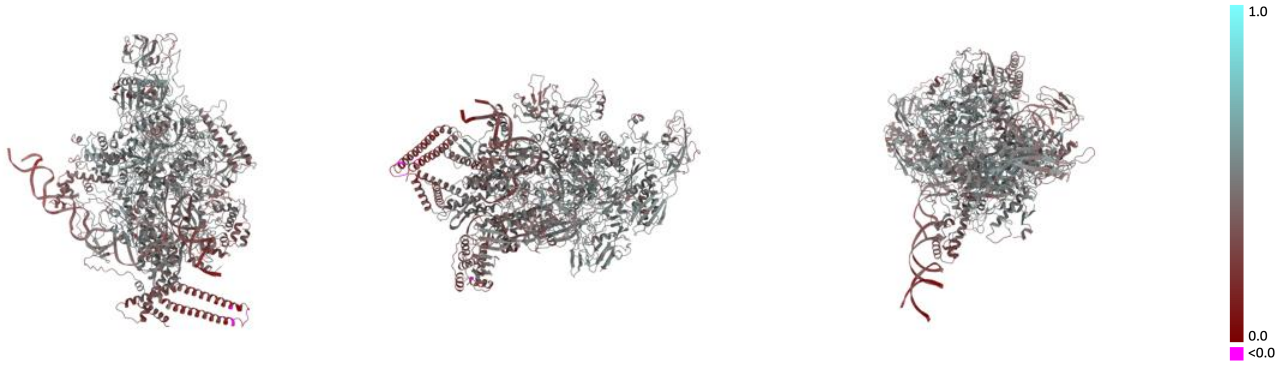
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.433 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

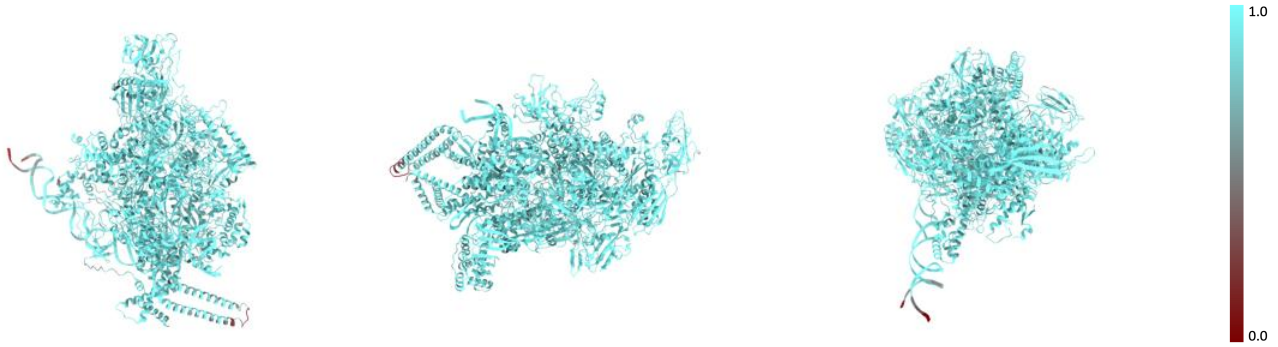
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

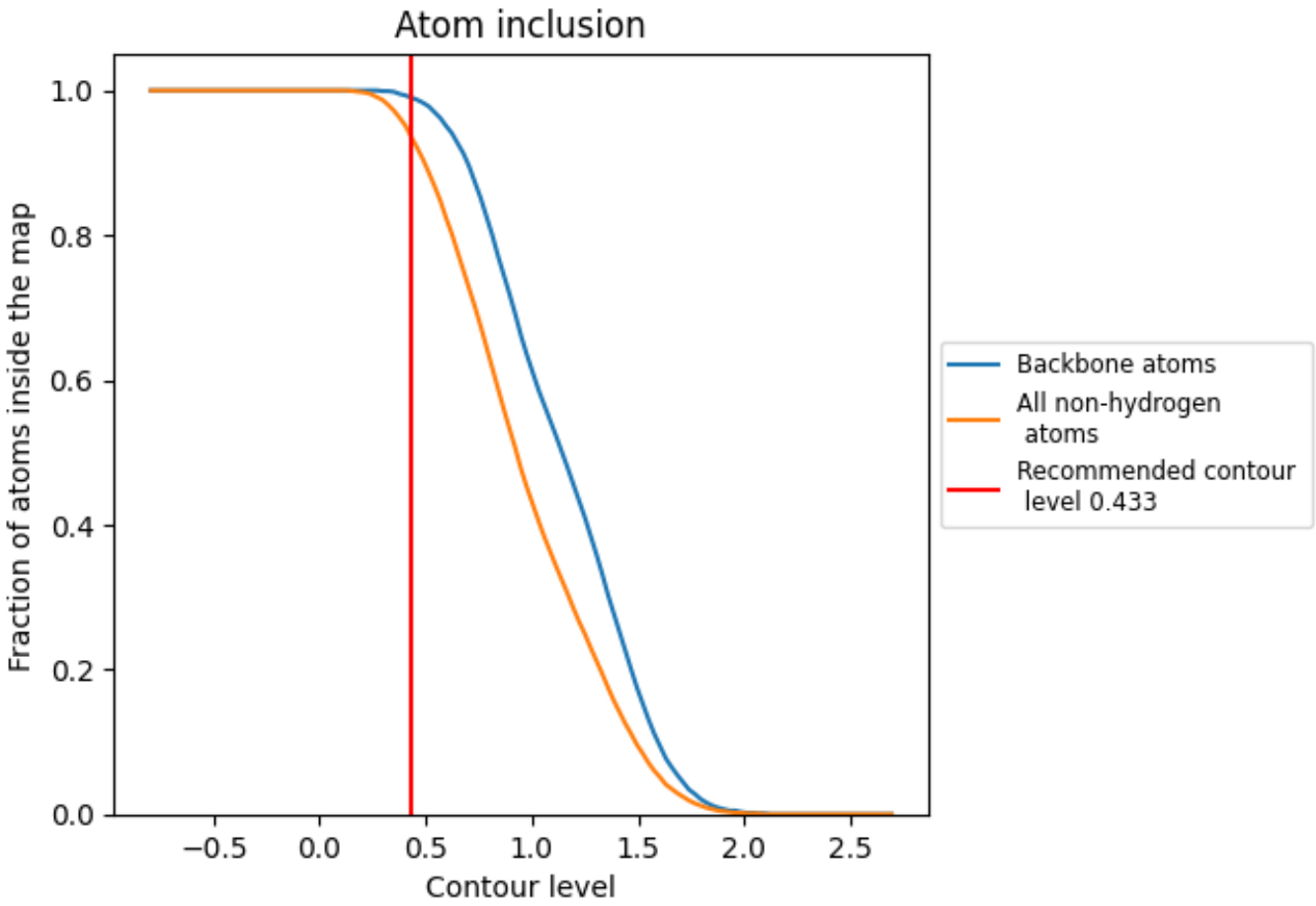
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.433).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.433) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9350	0.4360
A	0.9630	0.4850
B	0.9440	0.4540
C	0.9440	0.4710
D	0.9380	0.4540
E	0.9500	0.4740
F	0.9250	0.3900
J	0.8740	0.3920
M	0.9080	0.3480
O	0.9190	0.3050
P	0.9100	0.3090