



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:05 PM JST

PDB ID : 7CBP  
EMDB ID : EMD-30337  
Title : CryoEM structure of Zika virus with Fab at 4.1 Angstrom  
Authors : Tyagi, A.; Ahmed, T.; Shi, J.; Bhushan, S.  
Deposited on : 2020-06-13  
Resolution : 4.10 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:

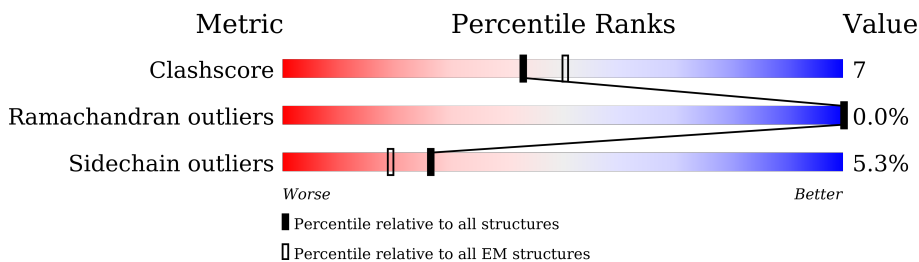
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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	T	75	
1	U	75	
1	V	75	
2	K	501	
2	N	501	
2	Q	501	
3	D	222	
3	R	222	

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Mol	Chain	Length	Quality of chain
4	E	215	<p>92% 80% 19%</p>
4	S	215	<p>72% 80% 19%</p>
5	A	2	<p>50% 50%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19739 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 Small envelope protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	75	Total	C	N	O	S	0	0
			599	391	104	103	1		
1	U	75	Total	C	N	O	S	0	0
			599	391	104	103	1		
1	V	75	Total	C	N	O	S	0	0
			599	391	104	103	1		

- Molecule 2 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	501	Total	C	N	O	S	0	0
			3748	2362	651	704	31		
2	N	501	Total	C	N	O	S	0	0
			3748	2360	651	707	30		
2	K	501	Total	C	N	O	S	0	0
			3784	2379	657	718	30		

- Molecule 3 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	222	Total	C	N	O	S	0	0
			1641	1036	271	327	7		
3	R	222	Total	C	N	O	S	0	0
			1660	1049	273	330	8		

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	215	Total	C	N	O	S	0	0
			1665	1044	286	329	6		
4	S	215	Total	C	N	O	S	0	0
			1668	1048	285	329	6		

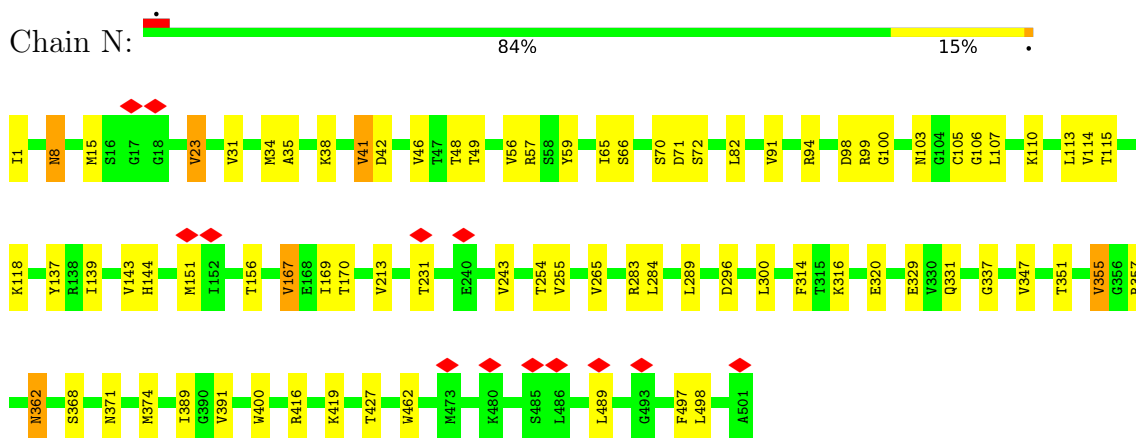
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



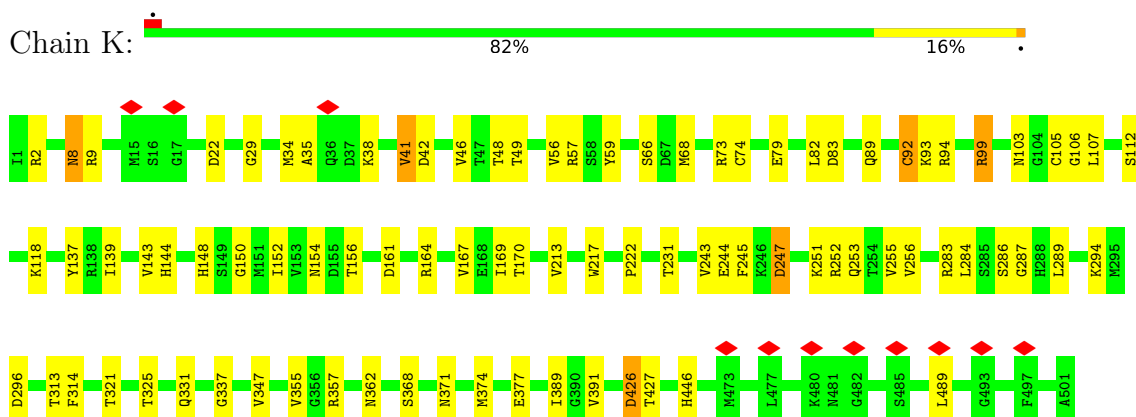
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	A	2	28	16	2	10	0	0



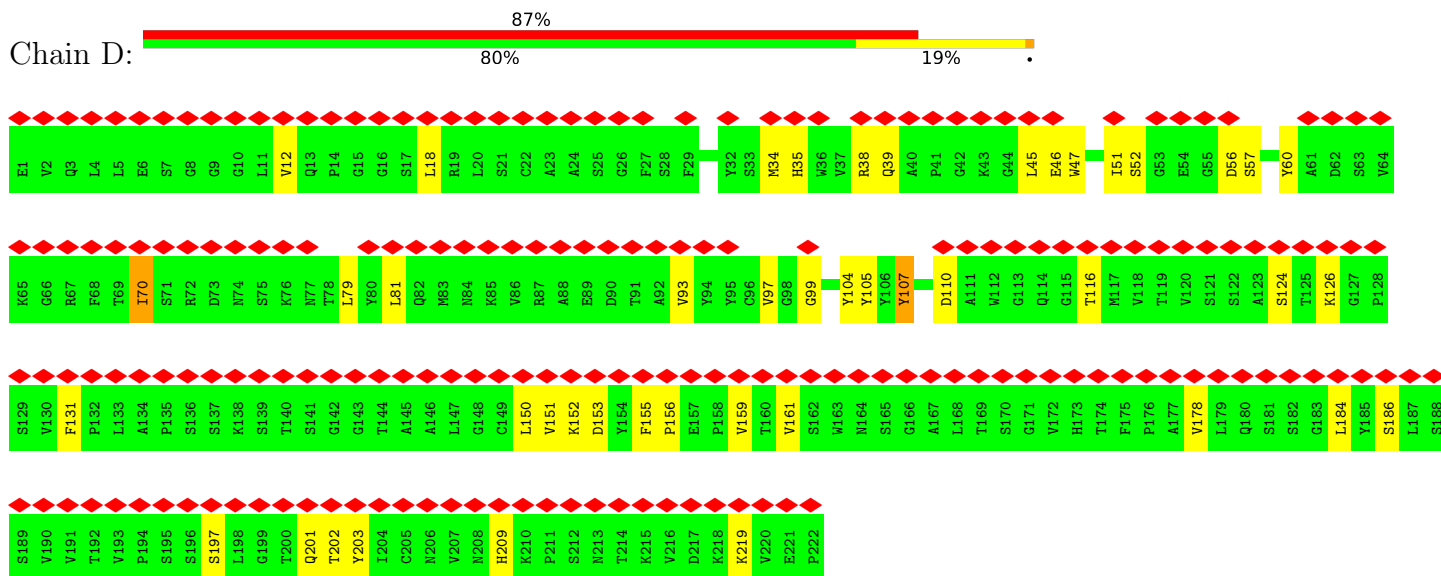
• Molecule 2: Envelope protein E



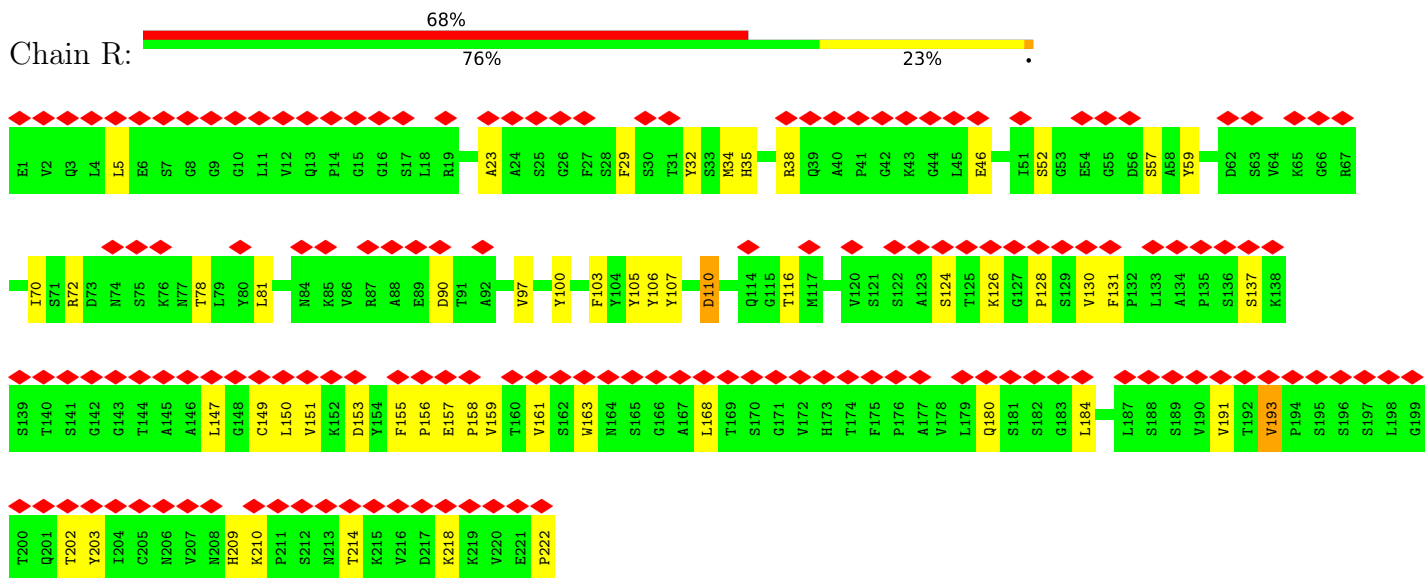
• Molecule 2: Envelope protein E



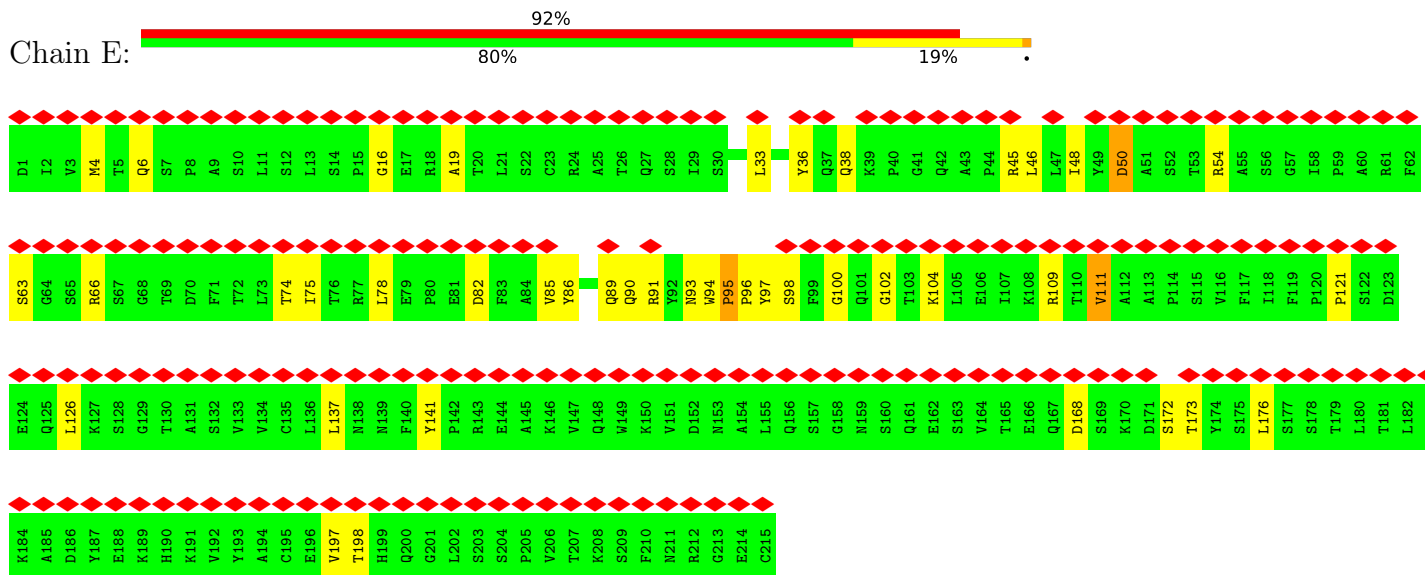
• Molecule 3: Fab Heavy chain



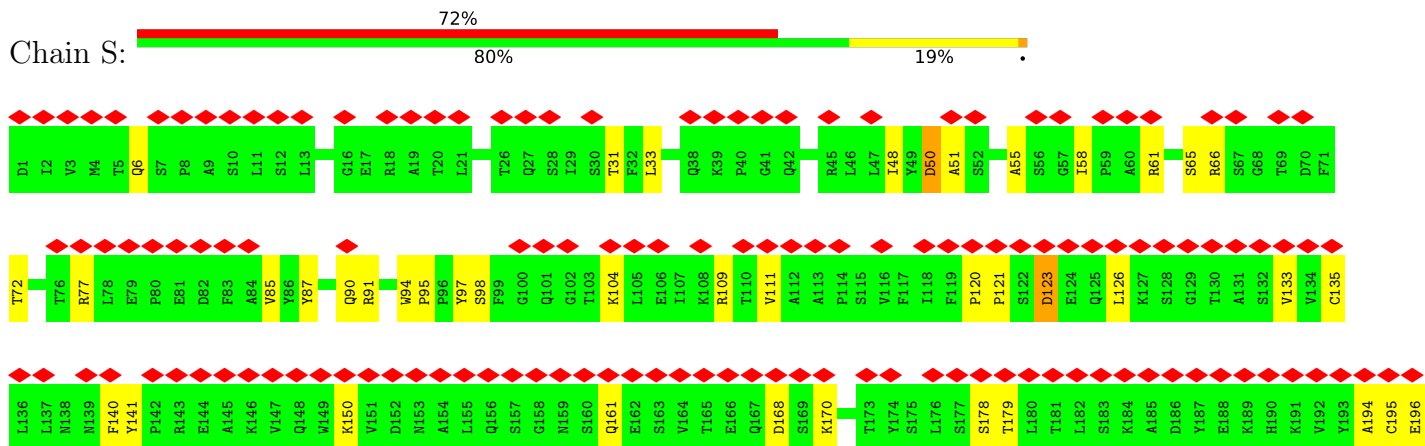
• Molecule 3: Fab Heavy chain



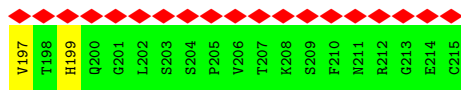
• Molecule 4: Fab light chain



• Molecule 4: Fab light chain







- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  50% 50%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ( $\text{\AA}$ )	833.91, 833.91, 833.91	wwPDB
Map dimensions	798, 798, 798	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.045, 1.045, 1.045	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: NAG

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	T	0.31	0/614	0.58	0/836
1	U	0.29	0/614	0.46	0/836
1	V	0.28	0/614	0.46	0/836
2	K	0.28	0/3863	0.49	0/5229
2	N	0.30	0/3825	0.54	1/5179 (0.0%)
2	Q	0.28	0/3825	0.49	0/5178
3	D	0.27	0/1682	0.50	0/2292
3	R	0.28	0/1702	0.52	0/2317
4	E	0.26	0/1703	0.48	0/2314
4	S	0.27	0/1707	0.51	0/2320
All	All	0.28	0/20149	0.51	1/27337 (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
4	E	0	1
4	S	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	82	LEU	CB-CG-CD2	-6.37	100.18	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	95	PRO	Peptide
4	S	120	PRO	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	T	599	0	617	3	0
1	U	599	0	617	10	0
1	V	599	0	617	9	0
2	K	3784	0	3735	70	0
2	N	3748	0	3682	35	0
2	Q	3748	0	3689	31	0
3	D	1641	0	1569	60	0
3	R	1660	0	1603	31	0
4	E	1665	0	1619	65	0
4	S	1668	0	1622	31	0
5	A	28	0	21	14	0
All	All	19739	0	19391	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:68:MET:SD	3:D:56:ASP:HB3	1.59	1.42
2:K:154:ASN:ND2	5:A:1:NAG:H5	1.32	1.37
4:E:90:GLN:O	4:E:97:TYR:CD1	1.76	1.35
4:E:90:GLN:O	4:E:97:TYR:HD1	0.96	1.27
2:K:154:ASN:ND2	5:A:1:NAG:C5	2.07	1.17
3:D:51:ILE:HD11	3:D:70:ILE:HB	1.16	1.13
2:K:68:MET:SD	3:D:56:ASP:CB	2.36	1.12
2:K:154:ASN:HD21	5:A:1:NAG:C5	1.60	1.11
4:E:91:ARG:HA	4:E:97:TYR:CE1	1.98	0.98
4:S:90:GLN:O	4:S:97:TYR:HD1	1.51	0.93
3:D:105:TYR:CE2	4:E:94:TRP:CZ2	2.57	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:TYR:CD2	4:E:91:ARG:NH2	2.37	0.93
3:D:104:TYR:HB2	4:E:94:TRP:CH2	2.05	0.91
3:D:104:TYR:HB2	4:E:94:TRP:HH2	1.35	0.88
3:D:51:ILE:HD11	3:D:70:ILE:CB	2.03	0.85
3:D:104:TYR:HD2	4:E:94:TRP:CH2	1.95	0.84
3:D:105:TYR:HE2	4:E:94:TRP:CZ2	1.92	0.83
3:D:51:ILE:CD1	3:D:70:ILE:HB	2.07	0.83
3:D:104:TYR:CB	4:E:94:TRP:HH2	1.93	0.82
2:K:73:ARG:HD3	4:E:93:ASN:HD21	1.44	0.81
3:D:107:TYR:HD2	4:E:91:ARG:NH2	1.79	0.81
4:E:91:ARG:HA	4:E:97:TYR:CD1	2.17	0.79
3:D:107:TYR:CD2	4:E:91:ARG:CZ	2.66	0.79
3:R:105:TYR:CD2	4:S:94:TRP:HZ3	2.01	0.79
4:S:90:GLN:O	4:S:97:TYR:CD1	2.36	0.78
4:E:90:GLN:C	4:E:97:TYR:HD1	1.84	0.78
3:D:104:TYR:CD2	4:E:94:TRP:HH2	2.02	0.77
3:D:105:TYR:HE2	4:E:94:TRP:HZ2	1.32	0.77
4:E:91:ARG:HA	4:E:97:TYR:HE1	1.45	0.77
2:K:68:MET:CG	3:D:56:ASP:HB3	2.14	0.77
2:K:154:ASN:HD22	5:A:1:NAG:C1	1.97	0.76
3:D:104:TYR:CD2	4:E:94:TRP:CH2	2.73	0.76
2:K:154:ASN:ND2	5:A:1:NAG:C1	2.47	0.76
3:D:52:SER:HG	3:D:57:SER:HG	1.26	0.76
3:D:107:TYR:CE2	4:E:91:ARG:NE	2.54	0.74
3:D:107:TYR:CE2	4:E:91:ARG:NH2	2.55	0.74
3:D:47:TRP:CZ3	4:E:96:PRO:HB3	2.23	0.74
3:D:107:TYR:HE2	4:E:91:ARG:HE	1.34	0.73
4:E:90:GLN:O	4:E:97:TYR:CG	2.42	0.72
3:D:105:TYR:CD2	4:E:94:TRP:CZ2	2.79	0.71
4:E:90:GLN:O	4:E:97:TYR:HB3	1.91	0.70
2:N:105:CYS:SG	2:N:106:GLY:N	2.66	0.69
3:D:51:ILE:HG13	3:D:70:ILE:HD12	1.75	0.68
2:K:156:THR:HG22	5:A:2:NAG:O7	1.95	0.67
3:D:107:TYR:CE2	4:E:91:ARG:CZ	2.78	0.67
3:D:107:TYR:HD2	4:E:91:ARG:CZ	2.06	0.67
2:K:68:MET:CE	3:D:56:ASP:HB3	2.25	0.66
2:K:156:THR:CG2	5:A:2:NAG:O7	2.44	0.65
3:D:104:TYR:CB	4:E:94:TRP:CH2	2.75	0.64
3:R:105:TYR:CD2	4:S:94:TRP:CZ3	2.86	0.64
2:Q:105:CYS:SG	2:Q:106:GLY:N	2.71	0.62
3:D:107:TYR:HE2	4:E:91:ARG:NE	1.93	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:105:TYR:HD2	4:S:94:TRP:HZ3	1.46	0.62
2:K:74:CYS:N	4:E:93:ASN:OD1	2.33	0.62
3:D:47:TRP:CE3	4:E:96:PRO:HB3	2.36	0.60
2:N:94:ARG:HG2	2:N:114:VAL:HG22	1.83	0.59
2:K:347:VAL:HG23	2:K:355:VAL:HG11	1.84	0.59
4:E:94:TRP:CG	4:E:95:PRO:HD2	2.38	0.58
2:K:154:ASN:HD21	5:A:1:NAG:H5	0.65	0.58
2:K:154:ASN:ND2	5:A:1:NAG:O5	2.35	0.58
4:E:90:GLN:O	4:E:97:TYR:CB	2.52	0.57
2:K:156:THR:O	5:A:1:NAG:H61	2.03	0.57
3:R:105:TYR:HD2	4:S:94:TRP:CZ3	2.22	0.57
2:K:105:CYS:SG	2:K:106:GLY:N	2.78	0.57
3:D:52:SER:OG	3:D:57:SER:OG	2.07	0.57
1:U:38:ARG:HD2	2:Q:216:GLU:HB3	1.87	0.56
2:Q:189:ASP:HB3	2:Q:292:ARG:HB3	1.87	0.56
2:K:156:THR:O	5:A:1:NAG:C6	2.52	0.56
2:K:156:THR:C	5:A:1:NAG:H61	2.23	0.56
3:D:110:ASP:OD2	4:E:91:ARG:NH2	2.38	0.56
2:K:68:MET:CE	3:D:56:ASP:CG	2.74	0.56
2:N:66:SER:HB3	2:N:118:LYS:HB3	1.85	0.56
2:K:68:MET:SD	3:D:56:ASP:CG	2.84	0.56
3:D:39:GLN:HB3	3:D:93:VAL:HB	1.87	0.56
3:D:104:TYR:CG	4:E:94:TRP:HH2	2.23	0.56
4:E:111:VAL:HG13	4:E:141:TYR:HB3	1.86	0.56
2:N:49:THR:HG22	2:N:283:ARG:HG2	1.86	0.56
2:Q:49:THR:HG22	2:Q:283:ARG:HG2	1.87	0.55
3:D:12:VAL:HG22	3:D:18:LEU:HD12	1.88	0.55
3:R:147:LEU:H	3:R:191:VAL:HG12	1.70	0.55
3:R:52:SER:OG	3:R:57:SER:OG	2.06	0.55
2:K:313:THR:HB	2:K:331:GLN:HB3	1.89	0.55
3:D:105:TYR:CE2	4:E:94:TRP:HZ2	2.12	0.55
2:N:70:SER:HB2	2:N:115:THR:HG23	1.89	0.54
3:D:151:VAL:HG21	3:D:161:VAL:HG21	1.89	0.54
2:N:34:MET:SD	2:N:357:ARG:NH1	2.75	0.54
2:N:100:GLY:H	2:N:103:ASN:HB2	1.70	0.54
3:R:180:GLN:HA	4:S:161:GLN:HE22	1.72	0.54
2:K:34:MET:SD	2:K:357:ARG:NH1	2.80	0.54
3:R:59:TYR:CG	4:S:95:PRO:HG2	2.43	0.54
4:E:16:GLY:H	4:E:78:LEU:HB2	1.73	0.54
4:E:19:ALA:HB3	4:E:75:ILE:HD12	1.89	0.53
2:K:73:ARG:HA	4:E:93:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:57:ARG:NH2	2:N:59:TYR:OH	2.40	0.53
2:N:1:ILE:HD12	2:N:144:HIS:HA	1.91	0.53
1:T:24:GLU:OE1	1:T:27:LYS:NZ	2.41	0.52
1:V:23:ARG:NH1	2:K:244:GLU:OE1	2.41	0.52
2:K:247:ASP:OD1	2:K:247:ASP:N	2.40	0.52
1:U:23:ARG:NH2	2:Q:243:VAL:O	2.41	0.52
2:K:41:VAL:HA	2:K:143:VAL:HA	1.91	0.52
2:K:42:ASP:OD2	2:K:144:HIS:NE2	2.42	0.52
1:U:10:ARG:NH2	1:V:38:ARG:O	2.43	0.52
4:E:63:SER:HG	4:E:74:THR:HG1	1.57	0.52
3:R:29:PHE:HA	3:R:32:TYR:HB2	1.92	0.52
3:R:105:TYR:CE2	4:S:94:TRP:CZ3	2.97	0.52
3:D:197:SER:HB2	3:D:201:GLN:HB3	1.92	0.52
2:N:462:TRP:NE1	2:N:498:LEU:O	2.42	0.52
3:R:105:TYR:CE2	4:S:94:TRP:HZ3	2.28	0.52
2:K:57:ARG:NH2	2:K:59:TYR:OH	2.44	0.51
2:Q:66:SER:HB3	2:Q:118:LYS:HB3	1.92	0.51
3:R:153:ASP:HA	3:R:184:LEU:HB3	1.91	0.51
1:T:15:ARG:HH12	2:N:419:LYS:HB3	1.75	0.51
3:D:131:PHE:HB2	3:D:150:LEU:HB2	1.91	0.51
2:K:161:ASP:OD2	2:K:164:ARG:NH2	2.42	0.51
4:E:90:GLN:HB2	4:E:98:SER:H	1.75	0.51
3:R:59:TYR:CD1	4:S:95:PRO:HG2	2.46	0.51
2:Q:8:ASN:HB3	2:Q:29:GLY:HA2	1.93	0.51
2:N:331:GLN:HE21	2:N:371:ASN:HB3	1.76	0.50
4:S:135:CYS:HB3	4:S:178:SER:HB3	1.93	0.50
4:E:85:VAL:HG22	4:E:104:LYS:HG2	1.93	0.50
3:D:153:ASP:HA	3:D:184:LEU:HB3	1.92	0.50
2:N:320:GLU:HB2	2:N:400:TRP:HZ2	1.76	0.50
1:U:23:ARG:NH1	2:Q:244:GLU:OE1	2.45	0.50
3:D:178:VAL:HB	3:D:186:SER:HB2	1.94	0.50
2:K:8:ASN:HB3	2:K:29:GLY:HA2	1.93	0.50
2:Q:34:MET:SD	2:Q:357:ARG:NH1	2.85	0.49
2:K:137:TYR:HB2	2:K:169:ILE:HB	1.93	0.49
2:Q:237:ASN:OD1	2:Q:237:ASN:N	2.45	0.49
2:K:2:ARG:H	2:K:152:ILE:HG23	1.77	0.49
2:K:337:GLY:HA2	2:K:368:SER:HA	1.95	0.49
2:K:66:SER:HB3	2:K:118:LYS:HB3	1.94	0.49
2:K:331:GLN:HE21	2:K:371:ASN:HB3	1.78	0.49
4:E:137:LEU:HD12	4:E:176:LEU:HD22	1.94	0.49
1:U:24:GLU:OE1	1:U:27:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:121:PRO:HG3	4:S:133:VAL:HG22	1.93	0.49
2:Q:196:LEU:HD22	2:Q:287:GLY:HA2	1.94	0.49
2:N:48:THR:HB	2:N:284:LEU:HB2	1.94	0.49
3:D:124:SER:OG	3:D:126:LYS:NZ	2.46	0.49
2:K:74:CYS:SG	4:E:93:ASN:CG	2.91	0.49
2:Q:57:ARG:NH2	2:Q:59:TYR:OH	2.46	0.49
2:N:296:ASP:OD1	2:N:296:ASP:N	2.45	0.49
2:K:73:ARG:HB3	2:K:112:SER:HB3	1.93	0.49
2:Q:58:SER:OG	2:Q:226:HIS:NE2	2.45	0.49
2:Q:323:HIS:HE1	2:Q:416:ARG:HH22	1.60	0.49
3:D:107:TYR:OH	4:E:89:GLN:NE2	2.46	0.49
3:R:124:SER:OG	3:R:126:LYS:NZ	2.46	0.49
3:D:35:HIS:HB2	3:D:97:VAL:HB	1.95	0.49
3:D:47:TRP:CE3	4:E:96:PRO:CB	2.96	0.49
2:N:99:ARG:HE	2:N:103:ASN:HB3	1.79	0.48
1:U:5:PRO:O	2:K:217:TRP:NE1	2.44	0.48
3:R:35:HIS:HB2	3:R:97:VAL:HB	1.94	0.48
2:K:247:ASP:HA	2:K:253:GLN:HA	1.95	0.48
4:S:85:VAL:HG22	4:S:104:LYS:HG2	1.95	0.48
4:S:48:ILE:HD12	4:S:51:ALA:HA	1.95	0.48
2:K:426:ASP:OD1	2:K:426:ASP:N	2.46	0.48
4:S:195:CYS:SG	4:S:196:GLU:N	2.87	0.48
2:K:68:MET:CE	3:D:56:ASP:CB	2.89	0.48
4:S:31:THR:O	4:S:66:ARG:NH2	2.47	0.48
2:K:48:THR:HB	2:K:284:LEU:HB2	1.95	0.47
2:K:49:THR:HG22	2:K:283:ARG:HG2	1.96	0.47
3:D:159:VAL:HG13	3:D:209:HIS:HB2	1.96	0.47
4:S:91:ARG:HA	4:S:97:TYR:CE1	2.49	0.47
4:S:90:GLN:NE2	4:S:98:SER:OG	2.42	0.47
2:K:139:ILE:HB	2:K:167:VAL:HB	1.95	0.47
4:E:168:ASP:H	4:E:172:SER:HA	1.80	0.47
2:K:79:GLU:HB3	2:K:94:ARG:HH22	1.79	0.47
4:E:36:TYR:HA	4:E:46:LEU:HA	1.96	0.47
3:R:151:VAL:HG21	3:R:161:VAL:HG21	1.97	0.47
2:K:35:ALA:HB3	2:K:38:LYS:HB2	1.97	0.47
3:R:38:ARG:NH2	3:R:90:ASP:OD1	2.47	0.47
2:K:9:ARG:NH1	2:K:377:GLU:OE2	2.48	0.46
3:R:110:ASP:N	3:R:110:ASP:OD1	2.47	0.46
3:D:34:MET:HG3	3:D:79:LEU:HD21	1.97	0.46
3:D:45:LEU:HD21	4:E:38:GLN:HE22	1.80	0.46
1:V:32:VAL:HG23	1:V:72:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:41:VAL:HA	2:Q:143:VAL:HA	1.97	0.46
2:Q:137:TYR:HB2	2:Q:169:ILE:HB	1.98	0.46
2:K:154:ASN:OD1	2:K:156:THR:OG1	2.33	0.46
3:R:168:LEU:HD11	3:R:193:VAL:HG12	1.98	0.46
3:R:131:PHE:HB2	3:R:150:LEU:HB2	1.97	0.46
1:U:3:THR:HA	1:V:31:ARG:HH21	1.79	0.46
2:K:148:HIS:HD1	2:K:150:GLY:H	1.64	0.46
2:K:286:SER:OG	2:K:287:GLY:N	2.49	0.46
4:S:91:ARG:HA	4:S:97:TYR:CD1	2.51	0.46
4:S:123:ASP:HA	4:S:126:LEU:HD12	1.98	0.46
4:E:94:TRP:CD2	4:E:95:PRO:HD2	2.51	0.46
4:S:55:ALA:H	4:S:58:ILE:HD12	1.80	0.46
4:S:109:ARG:HD3	4:S:141:TYR:HB2	1.98	0.45
2:K:99:ARG:HA	2:K:103:ASN:HD22	1.81	0.45
3:R:59:TYR:CG	4:S:95:PRO:CG	2.99	0.45
3:R:163:TRP:HZ3	3:R:203:TYR:HB3	1.82	0.45
1:T:64:LEU:O	1:T:68:LEU:HB2	2.17	0.45
2:N:23:VAL:HG21	2:N:31:VAL:HG11	1.98	0.45
2:N:316:LYS:HG2	4:S:31:THR:HB	1.99	0.45
2:N:151:MET:O	2:N:156:THR:OG1	2.33	0.44
1:V:10:ARG:HD3	1:V:10:ARG:HA	1.83	0.44
2:Q:83:ASP:OD1	2:Q:83:ASP:N	2.49	0.44
3:D:203:TYR:H	3:D:219:LYS:HE2	1.81	0.44
4:E:50:ASP:OD1	4:E:50:ASP:N	2.50	0.44
2:K:156:THR:O	5:A:1:NAG:H62	2.16	0.44
3:R:38:ARG:HB2	3:R:46:GLU:HB2	2.00	0.44
2:Q:212:LEU:HD23	2:Q:212:LEU:HA	1.91	0.44
2:Q:247:ASP:OD1	2:Q:247:ASP:N	2.43	0.44
1:U:75:SER:HB3	1:V:73:ALA:HB3	2.00	0.44
2:Q:495:LEU:O	2:Q:499:SER:CB	2.66	0.44
2:K:296:ASP:OD1	2:K:296:ASP:N	2.51	0.44
1:V:5:PRO:O	2:Q:217:TRP:NE1	2.45	0.44
2:Q:42:ASP:OD2	2:Q:144:HIS:NE2	2.51	0.44
4:S:65:SER:OG	4:S:72:THR:OG1	2.36	0.44
4:S:150:LYS:HB2	4:S:194:ALA:HB3	1.99	0.44
2:Q:156:THR:O	2:Q:164:ARG:NH2	2.51	0.44
2:N:35:ALA:HB3	2:N:38:LYS:HB2	2.00	0.44
2:K:74:CYS:SG	4:E:93:ASN:OD1	2.76	0.44
2:K:41:VAL:HB	2:K:143:VAL:HG12	1.99	0.44
4:S:50:ASP:OD1	4:S:50:ASP:N	2.51	0.44
2:Q:313:THR:HB	2:Q:331:GLN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:ASP:N	2:K:83:ASP:OD1	2.43	0.43
2:K:321:THR:OG1	2:K:325:THR:OG1	2.36	0.43
3:R:5:LEU:HB2	3:R:23:ALA:HB3	1.99	0.43
3:R:128:PRO:HD2	3:R:214:THR:HB	1.99	0.43
2:N:8:ASN:HA	2:N:416:ARG:HH21	1.84	0.43
2:Q:103:ASN:OD1	2:Q:103:ASN:N	2.51	0.43
2:Q:296:ASP:N	2:Q:296:ASP:OD1	2.52	0.43
4:S:6:GLN:HE22	4:S:87:TYR:HA	1.83	0.43
3:R:130:VAL:HG11	3:R:218:LYS:HB2	2.00	0.43
2:N:72:SER:OG	2:N:99:ARG:NH1	2.51	0.43
2:N:316:LYS:HD3	2:N:329:GLU:HG2	2.00	0.43
2:K:156:THR:HG21	5:A:2:NAG:O7	2.18	0.43
3:D:155:PHE:HA	3:D:156:PRO:HA	1.91	0.43
2:N:41:VAL:HA	2:N:143:VAL:HA	2.00	0.43
3:R:34:MET:HG2	3:R:72:ARG:HH21	1.84	0.42
2:Q:55:GLU:HA	2:Q:128:LYS:HA	2.01	0.42
2:N:98:ASP:OD1	2:N:110:LYS:NZ	2.40	0.42
2:K:73:ARG:HD3	4:E:93:ASN:ND2	2.22	0.42
2:N:65:ILE:HD11	2:N:243:VAL:HG12	2.01	0.42
2:K:92:CYS:SG	2:K:93:LYS:N	2.93	0.42
4:E:6:GLN:OE1	4:E:102:GLY:N	2.51	0.42
4:S:61:ARG:NH1	4:S:77:ARG:O	2.52	0.42
2:Q:239:LYS:HE2	2:Q:239:LYS:HB2	1.91	0.42
2:K:289:LEU:HD23	2:K:289:LEU:HA	1.90	0.42
4:E:168:ASP:HB2	4:E:173:THR:H	1.85	0.42
1:V:23:ARG:NH2	2:K:243:VAL:O	2.43	0.42
2:Q:379:ASP:OD1	2:Q:402:ARG:NH1	2.52	0.42
2:N:91:VAL:HG11	2:N:243:VAL:HG21	2.02	0.42
3:D:110:ASP:HB2	4:E:46:LEU:HD11	2.02	0.42
4:E:4:MET:HB2	4:E:100:GLY:HA2	2.00	0.42
2:Q:41:VAL:HB	2:Q:143:VAL:HG12	2.02	0.42
3:R:155:PHE:HA	3:R:156:PRO:HA	1.83	0.42
2:N:42:ASP:OD2	2:N:144:HIS:NE2	2.53	0.41
2:Q:39:PRO:HD3	2:Q:300:LEU:HA	2.02	0.41
4:E:109:ARG:HD3	4:E:141:TYR:HB2	2.01	0.41
1:U:4:LEU:HD13	2:K:222:PRO:HD2	2.01	0.41
2:N:72:SER:HB3	2:N:113:LEU:HD13	2.02	0.41
3:D:152:LYS:HA	3:D:186:SER:HA	2.01	0.41
2:K:68:MET:SD	3:D:56:ASP:OD2	2.78	0.41
2:K:89:GLN:OE1	2:K:118:LYS:NZ	2.53	0.41
1:U:4:LEU:HD13	1:U:4:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:137:TYR:HB2	2:N:169:ILE:HB	2.02	0.41
3:D:99:GLY:HA3	3:D:107:TYR:HB3	2.02	0.41
4:E:91:ARG:HG2	4:E:97:TYR:CE1	2.56	0.41
1:V:51:TRP:HA	1:V:60:LYS:HD3	2.03	0.41
2:N:289:LEU:HD23	2:N:289:LEU:HA	1.93	0.41
2:K:93:LYS:HD3	2:K:245:PHE:HB2	2.02	0.41
3:R:157:GLU:HA	3:R:158:PRO:HA	1.92	0.41
2:N:347:VAL:HG23	2:N:355:VAL:HG11	2.03	0.41
2:K:139:ILE:HD11	2:K:289:LEU:HD12	2.03	0.41
4:E:82:ASP:O	4:E:86:TYR:OH	2.36	0.41
4:E:109:ARG:HD2	4:E:172:SER:HB2	2.03	0.41
4:E:121:PRO:HB2	4:E:126:LEU:HD11	2.01	0.41
2:K:426:ASP:HA	2:K:446:HIS:HD2	1.86	0.41
3:D:38:ARG:HB2	3:D:46:GLU:HB2	2.03	0.41
3:R:137:SER:OG	3:R:222:PRO:O	2.38	0.41
3:R:159:VAL:HG13	3:R:209:HIS:HB2	2.03	0.40
2:N:337:GLY:HA2	2:N:368:SER:HA	2.02	0.40
2:N:139:ILE:HB	2:N:167:VAL:HG23	2.03	0.40
2:N:300:LEU:HD21	2:N:362:ASN:HB2	2.04	0.40
3:D:110:ASP:OD1	4:E:91:ARG:NH2	2.54	0.40
4:S:140:PHE:HB2	4:S:199:HIS:CD2	2.56	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	T	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
1	U	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
1	V	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
2	K	499/501 (100%)	463 (93%)	36 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	499/501 (100%)	465 (93%)	34 (7%)	0	100	100
2	Q	499/501 (100%)	454 (91%)	45 (9%)	0	100	100
3	D	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
3	R	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
4	E	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
4	S	213/215 (99%)	192 (90%)	20 (9%)	1 (0%)	29	67
All	All	2582/2602 (99%)	2397 (93%)	184 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	S	123	ASP

### 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	T	64/64 (100%)	61 (95%)	3 (5%)	26	53
1	U	64/64 (100%)	62 (97%)	2 (3%)	40	63
1	V	64/64 (100%)	62 (97%)	2 (3%)	40	63
2	K	406/408 (100%)	380 (94%)	26 (6%)	17	45
2	N	394/408 (97%)	369 (94%)	25 (6%)	18	46
2	Q	394/408 (97%)	374 (95%)	20 (5%)	24	52
3	D	179/184 (97%)	173 (97%)	6 (3%)	37	61
3	R	184/184 (100%)	171 (93%)	13 (7%)	14	42
4	E	186/188 (99%)	177 (95%)	9 (5%)	25	53
4	S	186/188 (99%)	179 (96%)	7 (4%)	33	59
All	All	2121/2160 (98%)	2008 (95%)	113 (5%)	26	51

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	3	THR
1	T	13	GLN
1	T	64	LEU
1	U	3	THR
1	U	13	GLN
1	V	3	THR
1	V	13	GLN
2	Q	8	ASN
2	Q	21	VAL
2	Q	23	VAL
2	Q	41	VAL
2	Q	46	VAL
2	Q	55	GLU
2	Q	56	VAL
2	Q	92	CYS
2	Q	103	ASN
2	Q	107	LEU
2	Q	152	ILE
2	Q	213	VAL
2	Q	237	ASN
2	Q	255	VAL
2	Q	314	PHE
2	Q	347	VAL
2	Q	349	MET
2	Q	374	MET
2	Q	389	ILE
2	Q	427	THR
2	N	8	ASN
2	N	15	MET
2	N	23	VAL
2	N	41	VAL
2	N	46	VAL
2	N	56	VAL
2	N	71	ASP
2	N	107	LEU
2	N	167	VAL
2	N	170	THR
2	N	213	VAL
2	N	231	THR
2	N	254	THR
2	N	255	VAL
2	N	265	VAL
2	N	314	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	N	351	THR
2	N	355	VAL
2	N	362	ASN
2	N	374	MET
2	N	389	ILE
2	N	391	VAL
2	N	427	THR
2	N	489	LEU
2	N	497	PHE
2	K	8	ASN
2	K	22	ASP
2	K	41	VAL
2	K	46	VAL
2	K	56	VAL
2	K	82	LEU
2	K	92	CYS
2	K	99	ARG
2	K	107	LEU
2	K	170	THR
2	K	213	VAL
2	K	231	THR
2	K	247	ASP
2	K	251	LYS
2	K	252	ARG
2	K	255	VAL
2	K	256	VAL
2	K	294	LYS
2	K	314	PHE
2	K	362	ASN
2	K	374	MET
2	K	389	ILE
2	K	391	VAL
2	K	426	ASP
2	K	427	THR
2	K	489	LEU
3	D	60	TYR
3	D	70	ILE
3	D	81	LEU
3	D	107	TYR
3	D	116	THR
3	D	202	THR
4	E	33	LEU

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Mol	Chain	Res	Type
4	E	45	ARG
4	E	48	ILE
4	E	50	ASP
4	E	54	ARG
4	E	66	ARG
4	E	111	VAL
4	E	197	VAL
4	E	198	THR
3	R	70	ILE
3	R	78	THR
3	R	81	LEU
3	R	100	TYR
3	R	103	PHE
3	R	106	TYR
3	R	107	TYR
3	R	110	ASP
3	R	116	THR
3	R	149	CYS
3	R	193	VAL
3	R	202	THR
3	R	210	LYS
4	S	33	LEU
4	S	50	ASP
4	S	111	VAL
4	S	168	ASP
4	S	170	LYS
4	S	179	THR
4	S	197	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	39	ASN
2	N	249	HIS
2	N	331	GLN
2	N	446	HIS
2	K	85	GLN
2	K	103	ASN
2	K	154	ASN
2	K	163	ASN
2	K	235	HIS
2	K	237	ASN

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Mol	Chain	Res	Type
2	K	331	GLN
2	K	446	HIS
4	E	38	GLN
4	E	89	GLN
3	R	102	ASN
3	R	180	GLN
3	R	209	HIS
4	S	38	GLN
4	S	161	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](#)

2 monosaccharides are modelled in this entry.

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	$\# Z  > 2$
5	NAG	A	1	2,5	14,14,15	0.59	1 (7%)	17,19,21	1.00	2 (11%)
5	NAG	A	2	5	14,14,15	0.33	0	17,19,21	0.52	0

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
5	NAG	A	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	A	2	5	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	NAG	O5-C1	-2.07	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	NAG	O4-C4-C5	-2.71	102.57	109.30
5	A	1	NAG	O3-C3-C2	-2.32	104.66	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

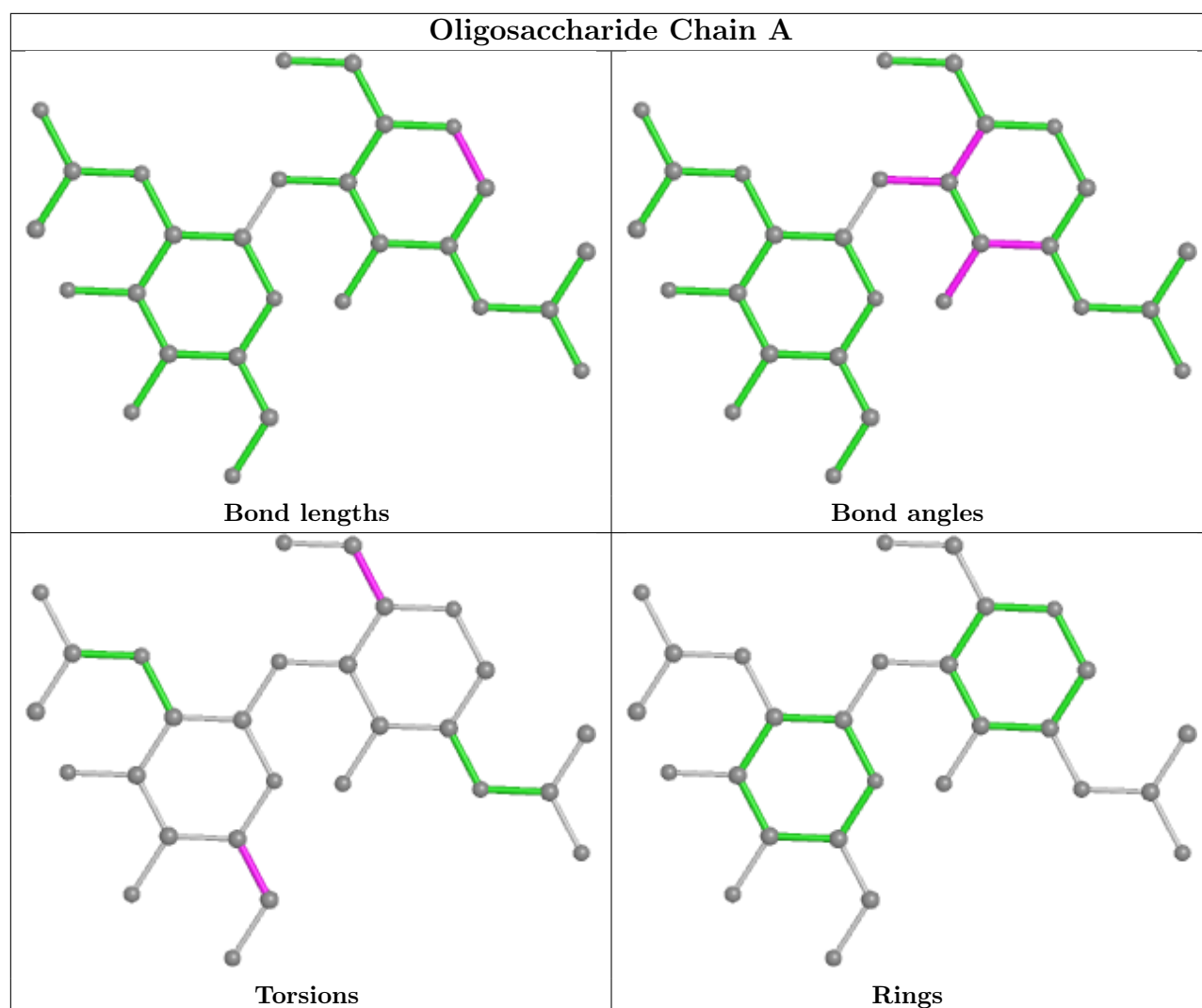
Mol	Chain	Res	Type	Atoms
5	A	1	NAG	O5-C5-C6-O6
5	A	1	NAG	C4-C5-C6-O6
5	A	2	NAG	O5-C5-C6-O6
5	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	NAG	3	0
5	A	1	NAG	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

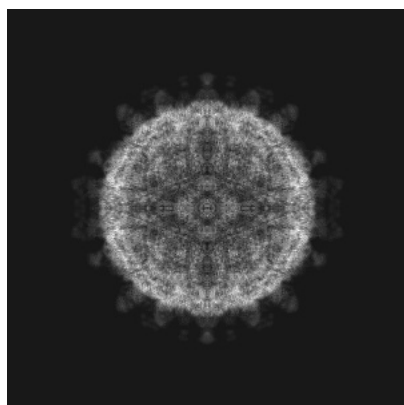
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30337. These allow visual inspection of the internal detail of the map and identification of artifacts.

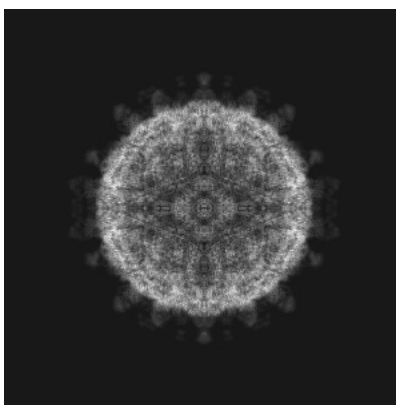
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

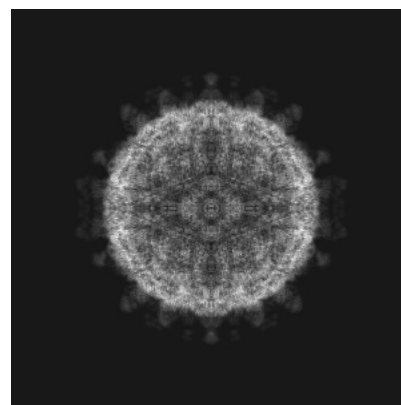
#### 6.1.1 Primary map



X



Y

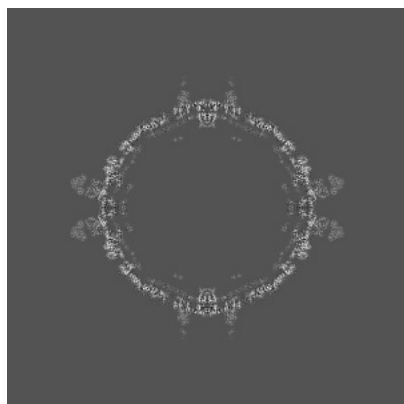


Z

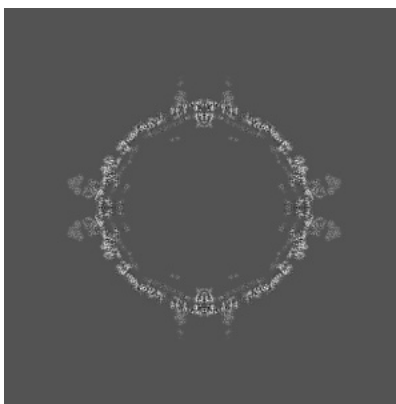
The images above show the map projected in three orthogonal directions.

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

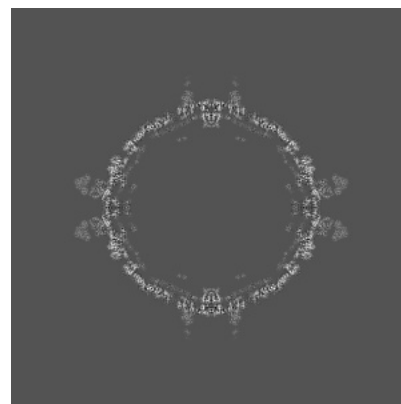
#### 6.2.1 Primary map



X Index: 399



Y Index: 399

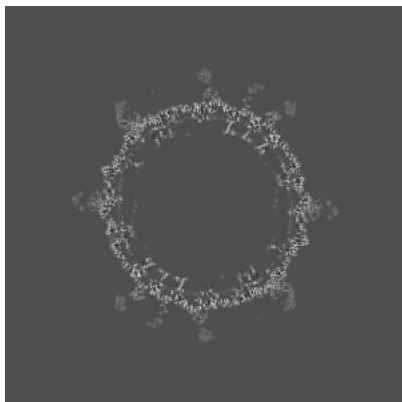


Z Index: 399

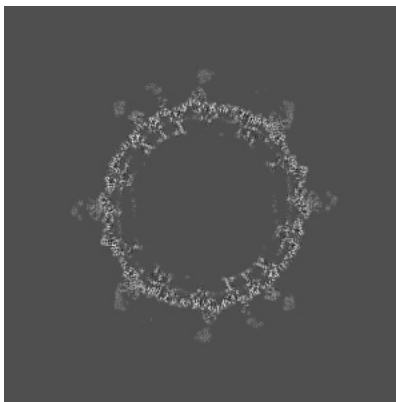
The images above show central slices of the map in three orthogonal directions.

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

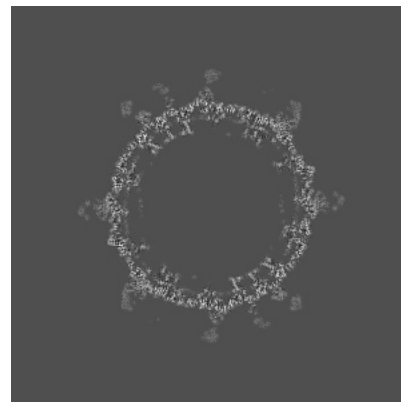
### 6.3.1 Primary map



X Index: 449



Y Index: 349

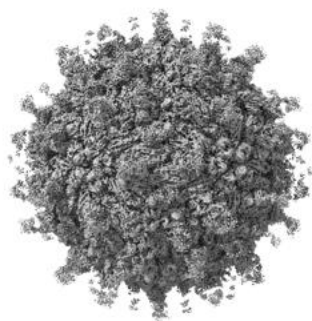


Z Index: 349

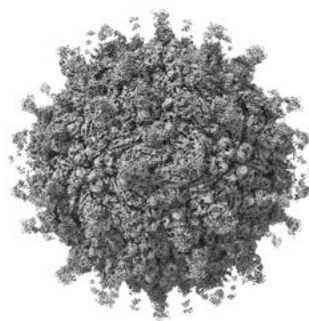
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

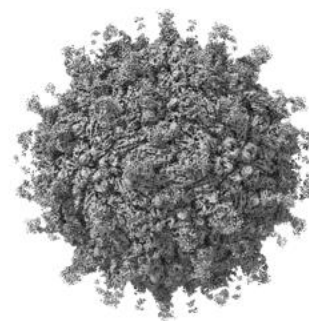
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

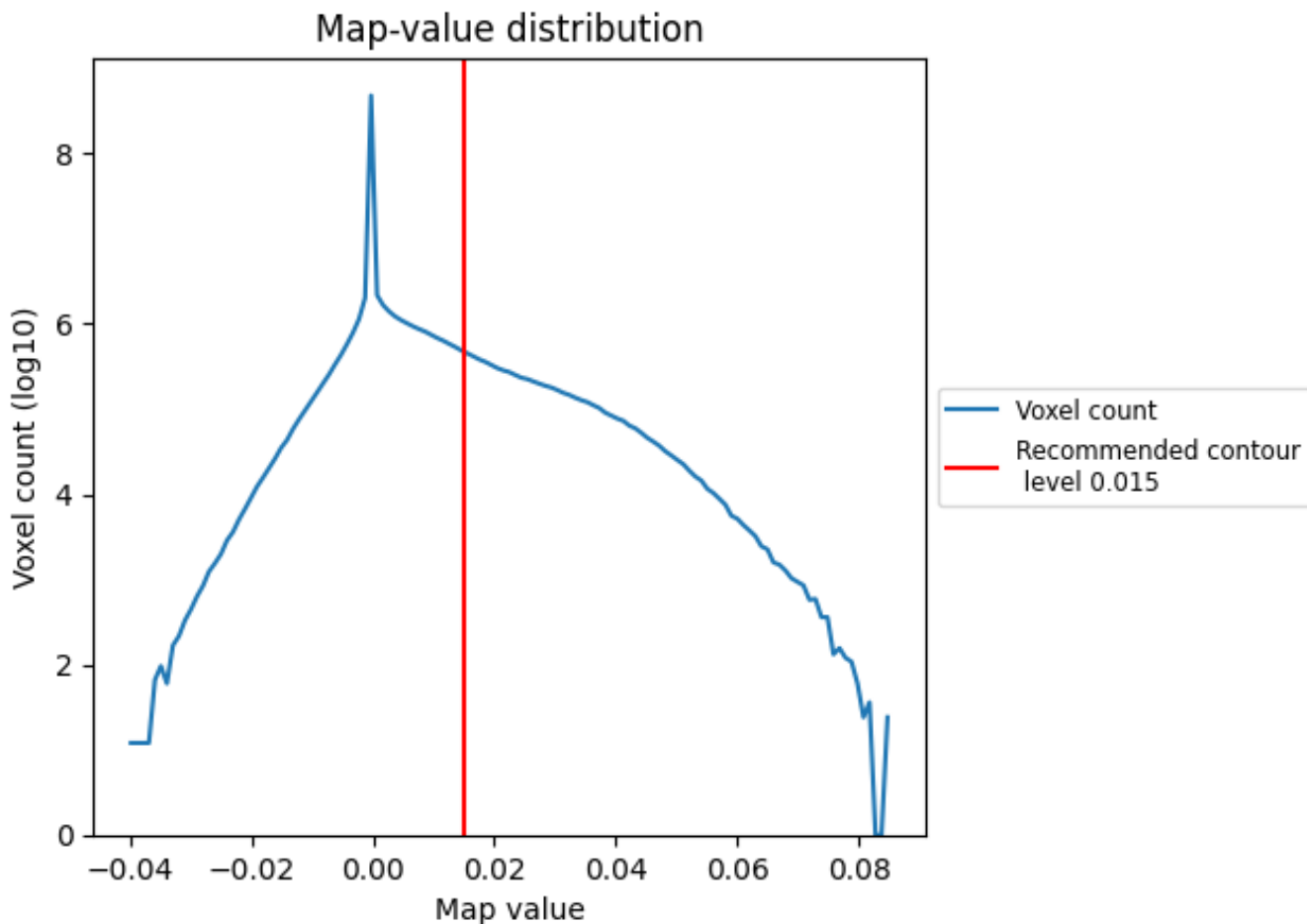
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

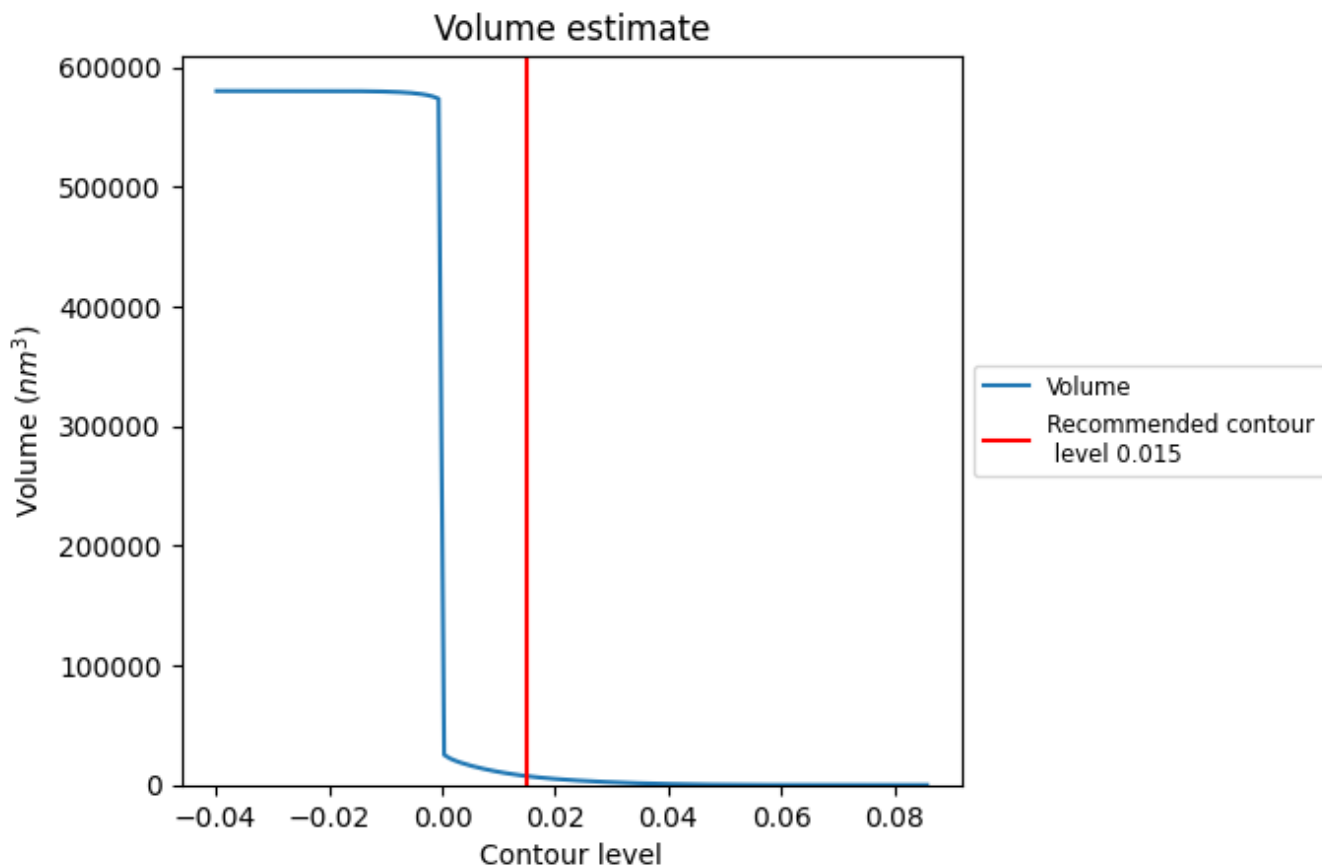
This section contains the results of statistical analysis of the map.

### 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.

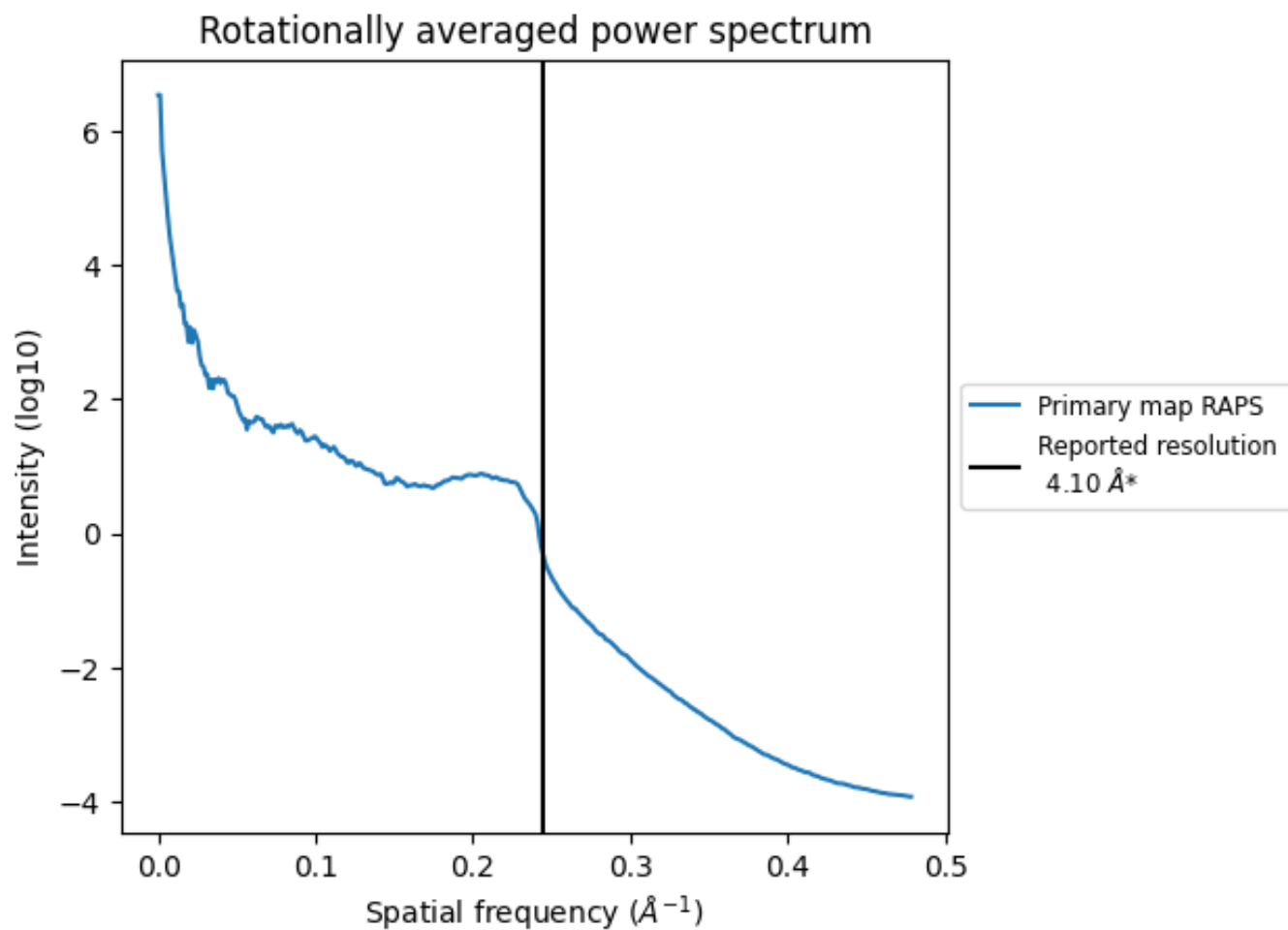
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 7381 nm<sup>3</sup>; this corresponds to an approximate mass of 6668 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  $0.244 \text{\AA}^{-1}$



## 8 Fourier-Shell correlation

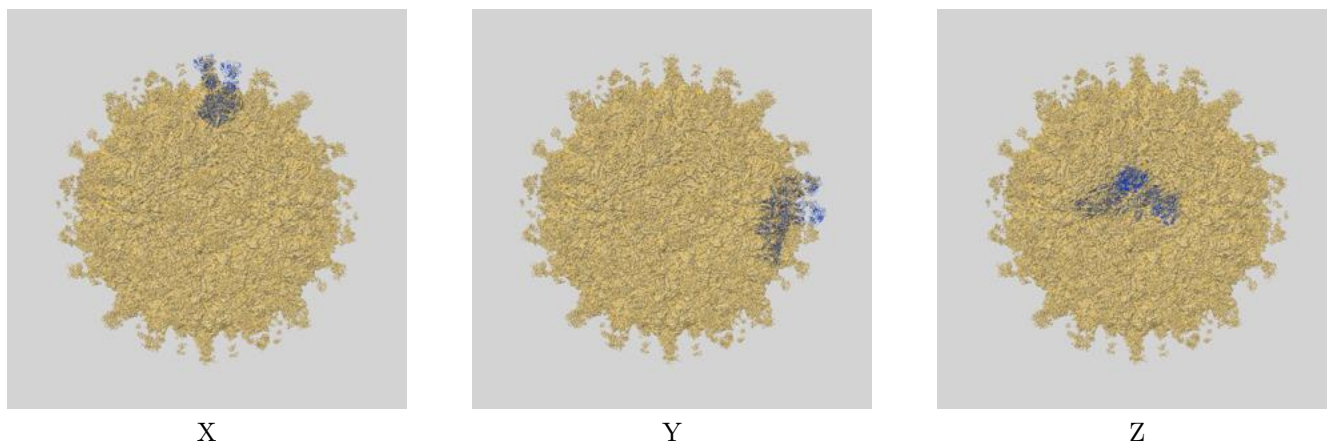
This section was not generated. No FSC curve or half-maps provided.

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

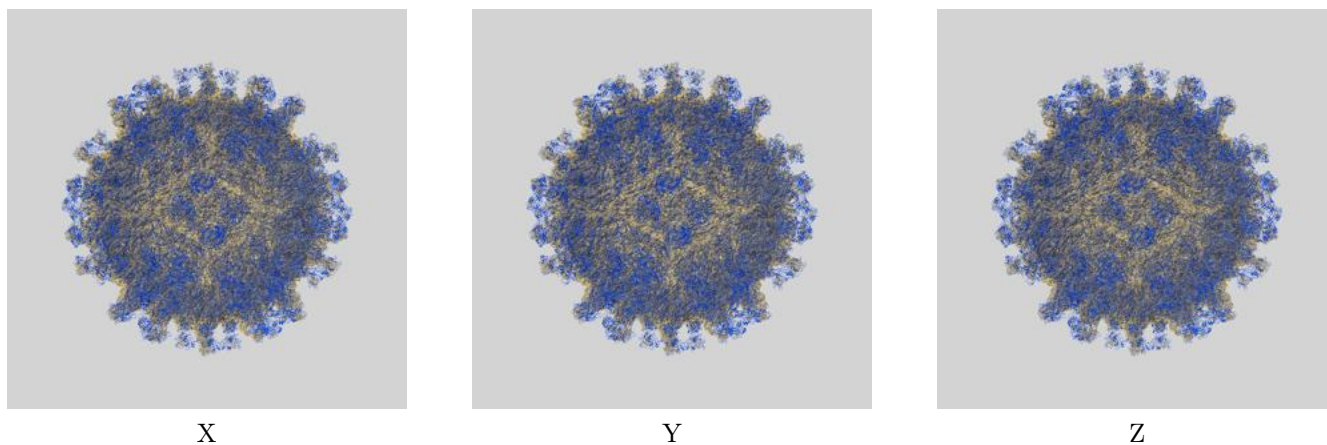
This section contains information regarding the fit between EMD map EMD-30337 and PDB model 7CBP. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

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



#### 9.1.2 Map-model assembly overlay [i](#)



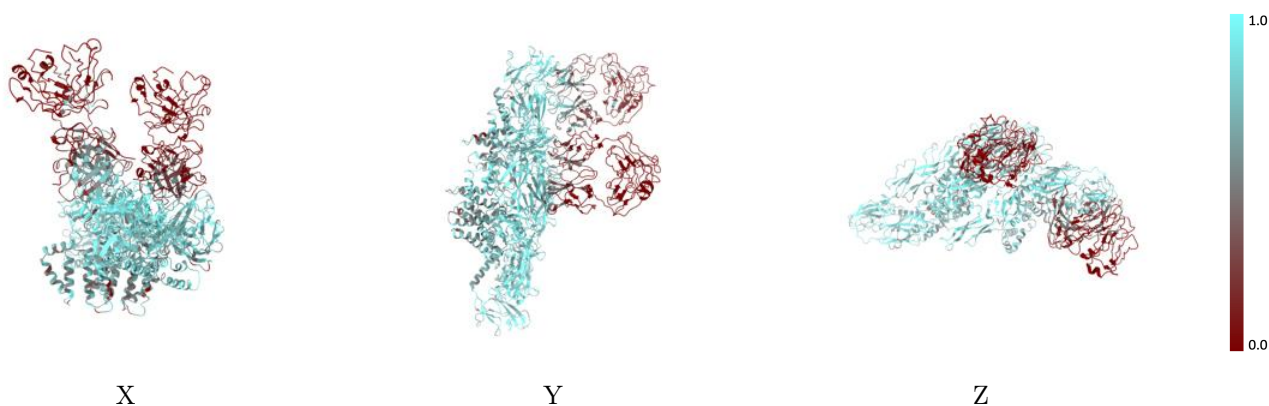
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



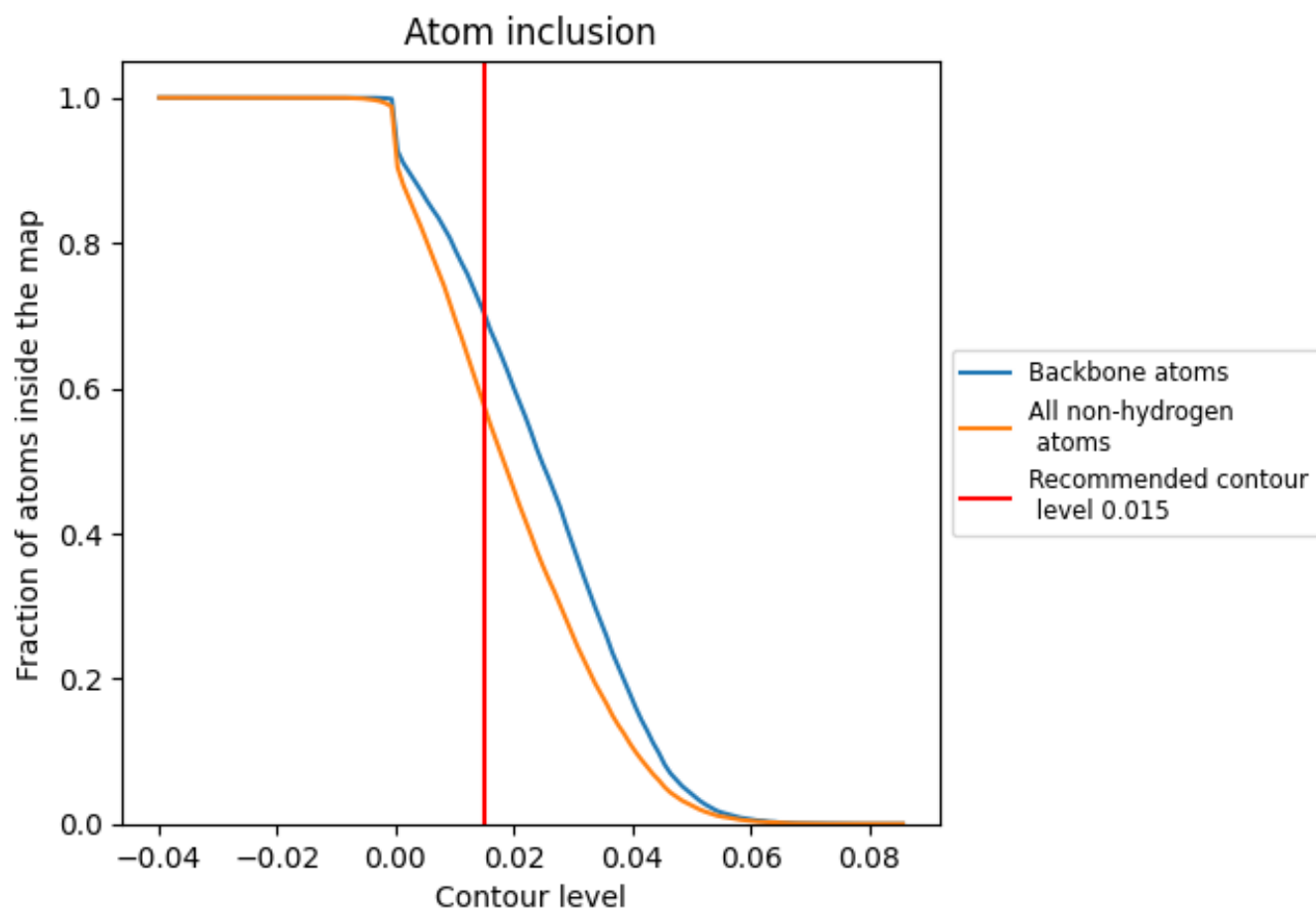
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 58% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5757	 0.3110
A	 0.8214	 0.3970
D	 0.1283	 0.1320
E	 0.1091	 0.0920
K	 0.7886	 0.3930
N	 0.7847	 0.3920
Q	 0.7649	 0.3870
R	 0.2788	 0.2190
S	 0.2664	 0.2140
T	 0.6981	 0.3470
U	 0.6690	 0.3350
V	 0.7067	 0.3580

