



## Full wwPDB EM Validation Report ⓘ

Aug 18, 2024 – 12:27 AM JST

PDB ID : 8Y8D  
EMDB ID : EMD-39042  
Title : Structure of HCoV-HKU1C spike in the inactive-1up conformation  
Authors : Lu, Y.C.; Zhang, X.; Wang, H.F.; Sun, L.; Yang, H.T.  
Deposited on : 2024-02-06  
Resolution : 3.41 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.37.1

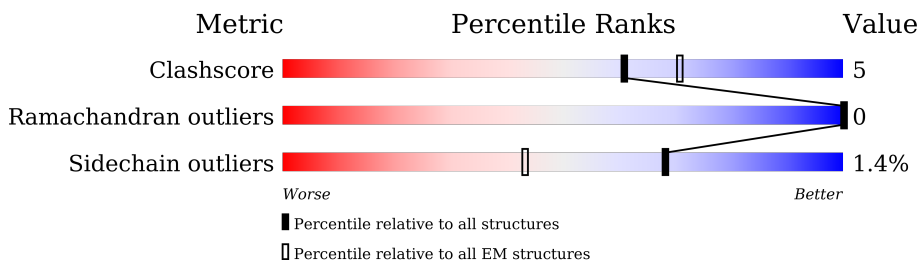
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.41 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	1263	 14% 79% 13% 7%
1	B	1263	 14% 81% 12% 6%
1	C	1263	 14% 80% 13% 7%
2	D	3	 100%
3	E	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27867 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1172	Total	C	N	O	S	0	0
			9117	5819	1491	1754	53		
1	A	1172	Total	C	N	O	S	0	0
			9100	5808	1485	1754	53		
1	B	1185	Total	C	N	O	S	0	0
			9219	5884	1513	1765	57		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	752	GLY	ARG	engineered mutation	UNP Q0ZME7
C	753	GLY	ARG	engineered mutation	UNP Q0ZME7
C	754	SER	LYS	engineered mutation	UNP Q0ZME7
C	755	GLY	ARG	engineered mutation	UNP Q0ZME7
C	756	SER	ARG	engineered mutation	UNP Q0ZME7
C	902	PRO	LEU	engineered mutation	UNP Q0ZME7
C	980	PRO	SER	engineered mutation	UNP Q0ZME7
C	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
C	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
C	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
A	752	GLY	ARG	engineered mutation	UNP Q0ZME7
A	753	GLY	ARG	engineered mutation	UNP Q0ZME7
A	754	SER	LYS	engineered mutation	UNP Q0ZME7
A	755	GLY	ARG	engineered mutation	UNP Q0ZME7
A	756	SER	ARG	engineered mutation	UNP Q0ZME7
A	902	PRO	LEU	engineered mutation	UNP Q0ZME7
A	980	PRO	SER	engineered mutation	UNP Q0ZME7
A	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
A	1068	PRO	LEU	engineered mutation	UNP Q0ZME7
B	752	GLY	ARG	engineered mutation	UNP Q0ZME7
B	753	GLY	ARG	engineered mutation	UNP Q0ZME7
B	754	SER	LYS	engineered mutation	UNP Q0ZME7
B	755	GLY	ARG	engineered mutation	UNP Q0ZME7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	756	SER	ARG	engineered mutation	UNP Q0ZME7
B	902	PRO	LEU	engineered mutation	UNP Q0ZME7
B	980	PRO	SER	engineered mutation	UNP Q0ZME7
B	1023	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1067	PRO	ASN	engineered mutation	UNP Q0ZME7
B	1068	PRO	LEU	engineered mutation	UNP Q0ZME7

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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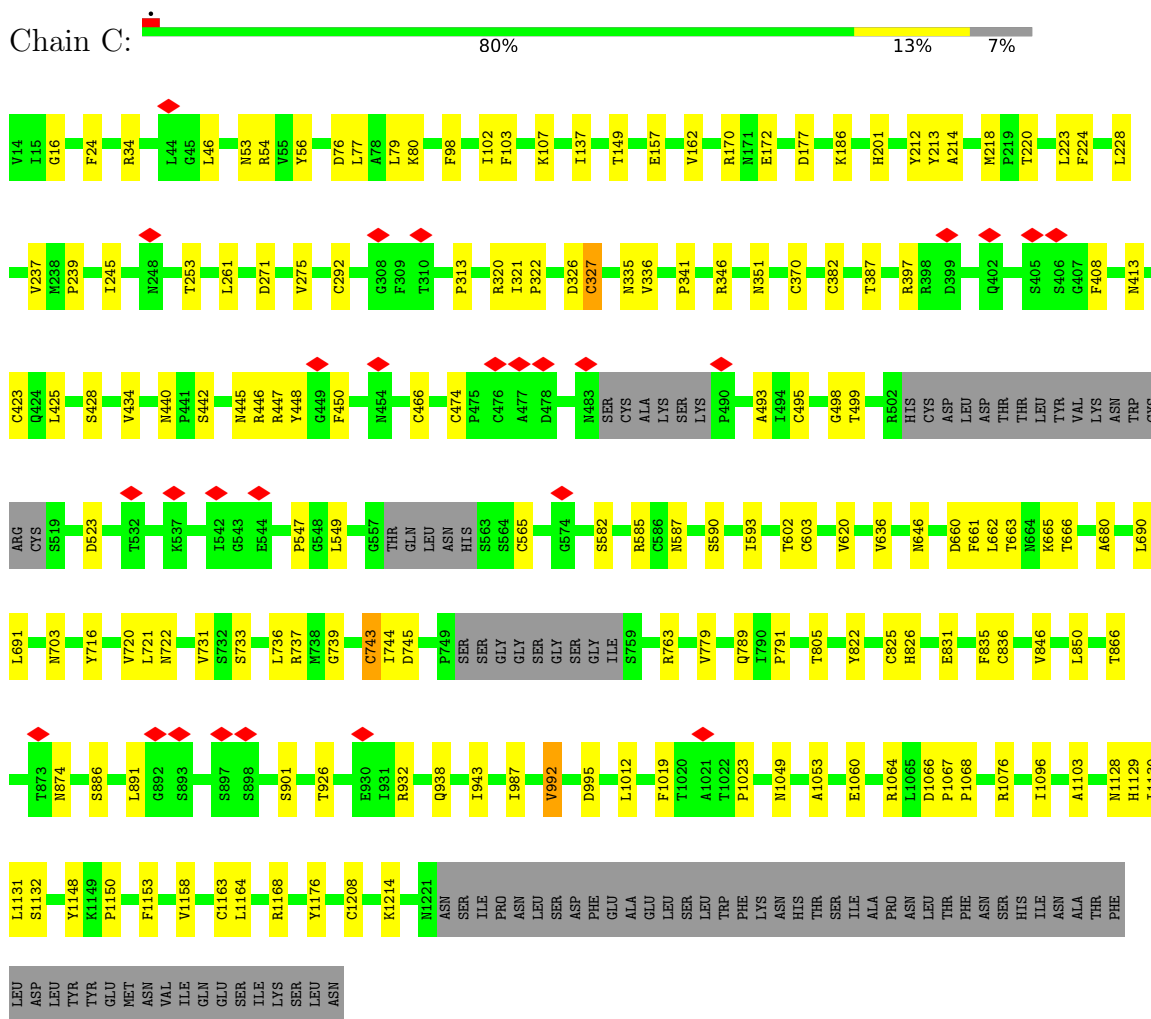
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

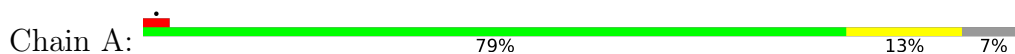
### 3 Residue-property plots

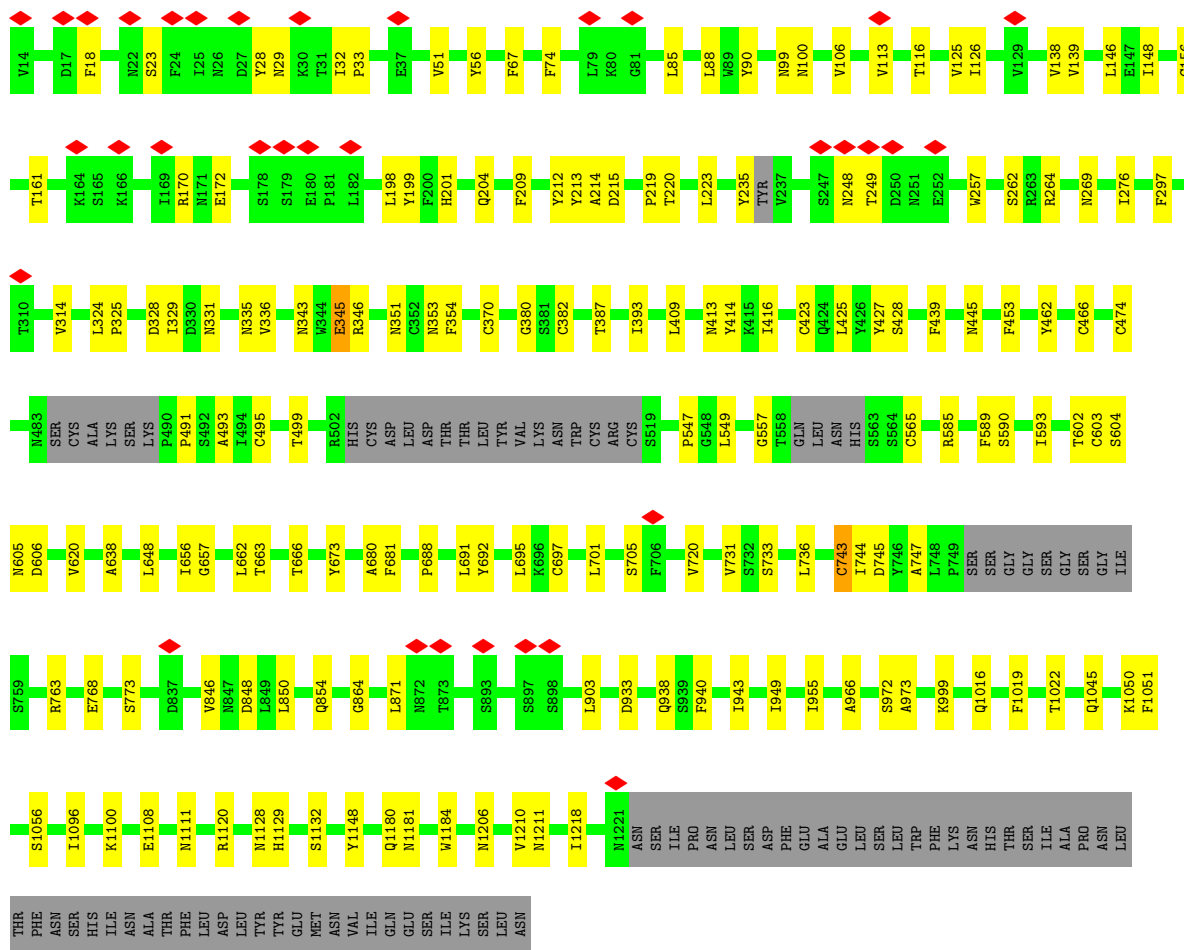
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein

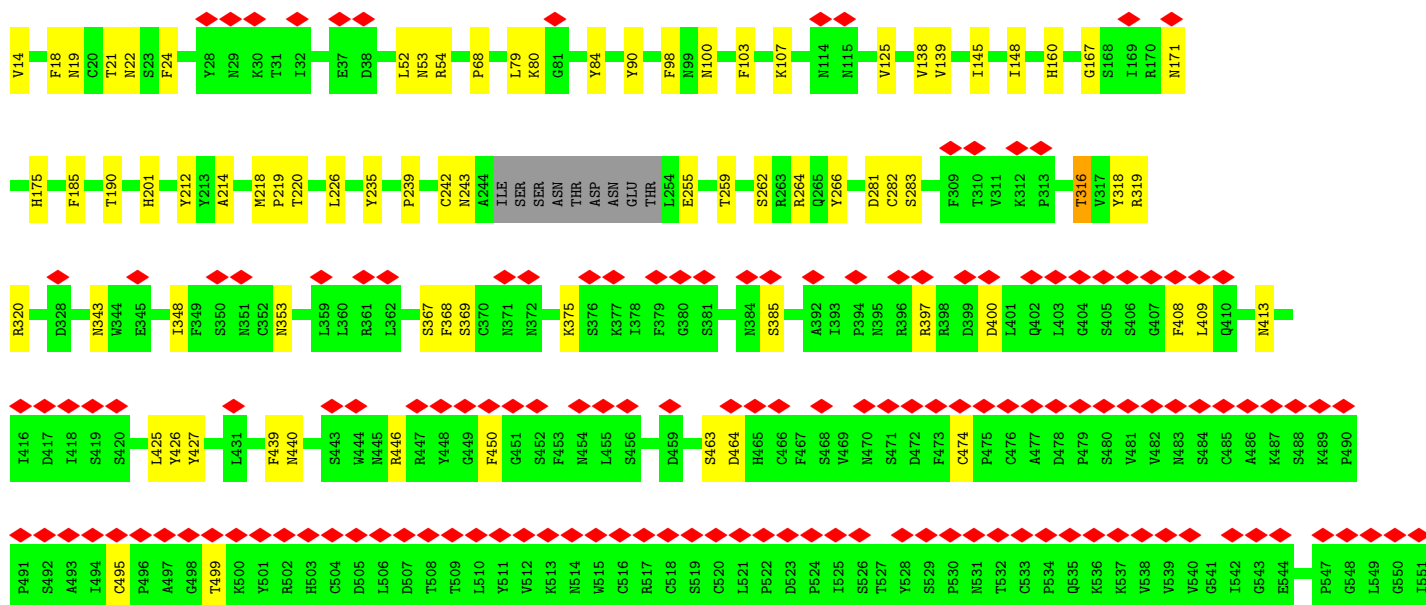
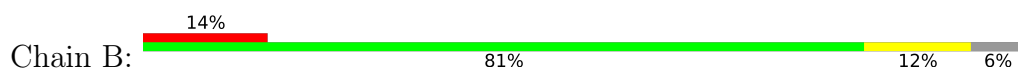


#### • Molecule 1: Spike glycoprotein

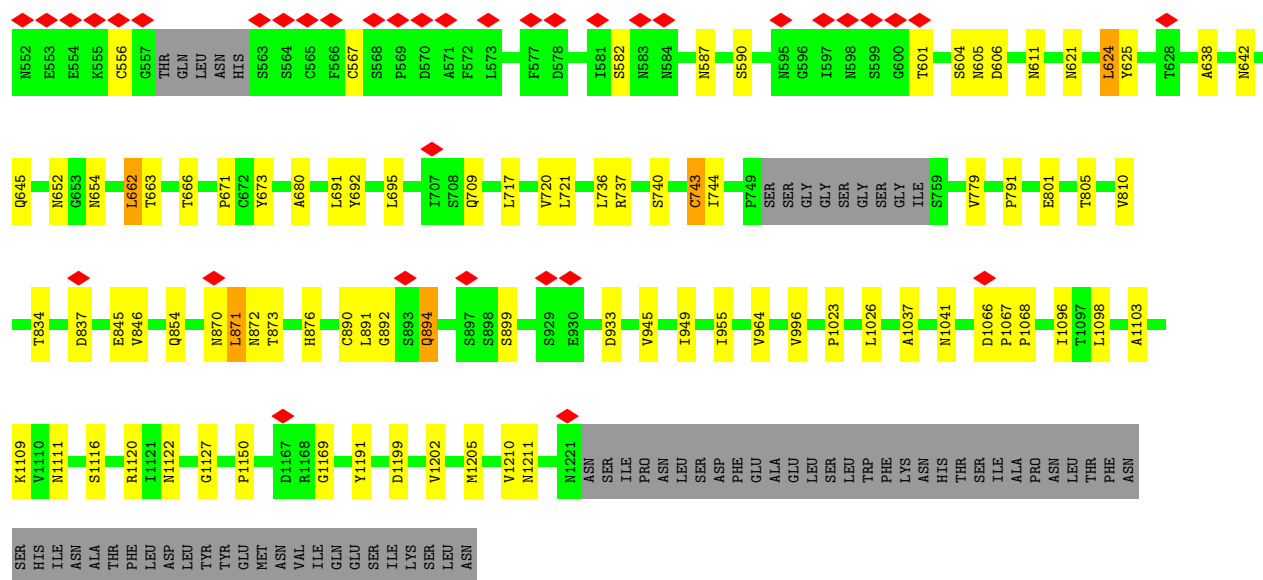




### • Molecule 1: Spike glycoprotein







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

Chain D:  100%

 NAG1  
NAG2  
EMA3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

 NAG1  
NAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27528	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.639	Depositor
Minimum map value	-0.894	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	A	0.24	0/9321	0.41	0/12701
1	B	0.24	0/9445	0.41	0/12868
1	C	0.24	0/9340	0.41	0/12726
All	All	0.24	0/28106	0.41	0/38295

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9100	0	8722	92	0
1	B	9219	0	8867	93	0
1	C	9117	0	8746	84	0
2	D	39	0	34	0	0
3	E	28	0	25	0	0
4	A	126	0	117	0	0
4	B	84	0	78	1	0
4	C	154	0	143	0	0
All	All	27867	0	26732	252	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 (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:CYS:HB3	1:C:547:PRO:HD2	1.65	0.78
1:B:871:LEU:HD23	1:B:892:GLY:HA2	1.70	0.73
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.72	0.71
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.72	0.71
1:A:1210:VAL:HG13	1:A:1211:ASN:HD22	1.55	0.70
1:A:445:ASN:HD21	1:A:549:LEU:H	1.39	0.69
1:A:106:VAL:HB	1:A:198:LEU:HB3	1.78	0.65
1:B:201:HIS:HB3	1:B:212:TYR:HB2	1.77	0.64
1:C:387:THR:HB	1:C:593:ILE:HB	1.79	0.64
1:B:214:ALA:HB2	1:B:220:THR:HA	1.78	0.64
1:B:691:LEU:HD13	1:B:720:VAL:HG22	1.79	0.64
1:A:409:LEU:HD12	1:A:413:ASN:HD22	1.62	0.63
1:C:440:ASN:HD21	1:C:442:SER:HB3	1.63	0.63
1:B:872:ASN:ND2	1:B:876:HIS:O	2.32	0.63
1:C:370:CYS:HA	1:C:423:CYS:HA	1.80	0.63
1:A:493:ALA:HB3	1:A:565:CYS:HB3	1.82	0.61
1:B:556:CYS:HA	1:B:567:CYS:HA	1.83	0.61
1:C:662:LEU:HD12	1:C:663:THR:HG23	1.83	0.61
1:B:1037:ALA:O	1:B:1041:ASN:ND2	2.32	0.61
1:A:199:TYR:HB2	1:A:214:ALA:HB3	1.83	0.60
1:C:162:VAL:HG22	1:C:172:GLU:HB2	1.83	0.60
1:B:167:GLY:O	1:B:243:ASN:ND2	2.35	0.60
1:A:262:SER:OG	1:A:264:ARG:NH1	2.35	0.60
1:C:1053:ALA:HA	1:C:1076:ARG:HH21	1.66	0.59
1:A:353:ASN:HB3	1:A:605:ASN:HD21	1.66	0.59
1:A:380:GLY:H	1:A:604:SER:HB3	1.67	0.59
1:B:348:ILE:HD11	1:B:385:SER:HB2	1.82	0.59
1:C:326:ASP:OD1	1:C:327:CYS:N	2.36	0.59
1:C:739:GLY:HA2	1:B:949:ILE:HA	1.85	0.58
1:A:204:GLN:HB3	1:A:209:PHE:HD1	1.68	0.58
1:B:1210:VAL:HG13	1:B:1211:ASN:HD22	1.69	0.58
1:B:680:ALA:HB1	1:B:736:LEU:HD13	1.86	0.58
1:A:335:ASN:OD1	1:A:336:VAL:N	2.37	0.57
1:A:387:THR:HB	1:A:593:ILE:HB	1.85	0.57
1:C:1060:GLU:O	1:C:1064:ARG:NH1	2.37	0.57
1:A:139:VAL:HB	1:A:146:LEU:HD11	1.87	0.57
1:A:1184:TRP:HB2	1:A:1218:ILE:HD11	1.86	0.57
1:B:319:ARG:HH12	1:B:611:ASN:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:CYS:SG	1:B:499:THR:OG1	2.63	0.57
1:A:495:CYS:SG	1:A:499:THR:OG1	2.63	0.57
1:C:866:THR:HG22	1:A:773:SER:HB2	1.85	0.56
1:C:320:ARG:NH2	1:C:382:CYS:SG	2.73	0.56
1:A:314:VAL:H	1:A:620:VAL:HG12	1.70	0.56
1:A:691:LEU:HD13	1:A:720:VAL:HG22	1.87	0.56
1:A:51:VAL:HG21	1:A:56:TYR:HE1	1.71	0.56
1:A:74:PHE:HB3	1:A:257:TRP:HB3	1.87	0.56
1:C:446:ARG:HA	1:C:450:PHE:HB3	1.87	0.56
1:A:850:LEU:HD21	1:A:1096:ILE:HD12	1.89	0.55
1:A:854:GLN:HE21	1:A:955:ILE:HD11	1.70	0.55
1:B:318:TYR:O	1:B:319:ARG:NH1	2.40	0.55
1:C:214:ALA:HB2	1:C:220:THR:HA	1.89	0.55
1:C:690:LEU:HB2	1:C:721:LEU:HB2	1.88	0.55
1:B:425:LEU:HB3	1:B:590:SER:HB3	1.88	0.55
1:B:264:ARG:NH2	1:B:283:SER:OG	2.40	0.55
1:C:743:CYS:SG	1:C:744:ILE:N	2.80	0.55
1:A:692:TYR:HB3	1:A:695:LEU:HD12	1.88	0.55
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	1.89	0.55
1:B:367:SER:HB3	1:B:426:TYR:HB2	1.89	0.55
1:C:493:ALA:HB3	1:C:565:CYS:HB3	1.88	0.55
1:A:99:ASN:ND2	1:A:100:ASN:OD1	2.39	0.55
1:A:864:GLY:O	1:A:972:SER:OG	2.25	0.54
1:A:903:LEU:HD12	1:A:1016:GLN:HE21	1.72	0.54
1:B:14:VAL:N	1:B:90:TYR:O	2.41	0.54
1:C:46:LEU:HB2	1:C:218:MET:HE1	1.90	0.54
1:B:873:THR:HG21	1:B:890:CYS:HA	1.89	0.54
1:B:139:VAL:HG12	1:B:148:ILE:HG13	1.89	0.54
1:A:32:ILE:HD12	1:A:33:PRO:HD2	1.89	0.54
1:B:353:ASN:HB3	1:B:605:ASN:HB2	1.90	0.54
1:C:886:SER:O	1:C:901:SER:OG	2.26	0.53
1:B:894:GLN:O	1:B:894:GLN:NE2	2.41	0.53
1:A:393:ILE:HD11	1:A:589:PHE:HB2	1.91	0.53
1:A:345:GLU:OE1	1:A:346:ARG:N	2.42	0.53
1:C:636:VAL:O	1:C:666:THR:OG1	2.26	0.53
1:C:79:LEU:HB2	1:C:239:PRO:HB3	1.91	0.53
1:C:680:ALA:HB1	1:C:736:LEU:HD13	1.92	0.52
1:A:1050:LYS:HG2	1:A:1056:SER:HB3	1.91	0.52
1:B:1169:GLY:O	1:B:1205:MET:N	2.40	0.52
1:C:16:GLY:H	1:C:157:GLU:HA	1.74	0.52
1:A:370:CYS:HA	1:A:423:CYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:SER:HB2	1:A:170:ARG:HH12	1.75	0.52
1:C:103:PHE:HB2	1:C:261:LEU:HD21	1.92	0.52
1:B:854:GLN:HE21	1:B:955:ILE:HD11	1.75	0.52
1:A:67:PHE:O	1:A:264:ARG:NH2	2.42	0.52
1:A:1108:GLU:OE2	1:A:1120:ARG:NH1	2.41	0.51
1:C:34:ARG:HB2	1:C:76:ASP:HB3	1.91	0.51
1:C:149:THR:HG22	1:C:186:LYS:HG3	1.93	0.51
1:A:248:ASN:HD22	1:A:249:THR:HG23	1.74	0.51
1:A:743:CYS:SG	1:A:744:ILE:N	2.83	0.51
1:C:495:CYS:SG	1:C:499:THR:OG1	2.69	0.51
1:A:113:VAL:O	1:A:116:THR:OG1	2.23	0.51
1:B:582:SER:OG	1:B:587:ASN:OD1	2.29	0.51
1:B:413:ASN:HD21	1:B:463:SER:H	1.58	0.51
1:A:126:ILE:HG12	1:A:235:TYR:HB2	1.92	0.51
1:B:52:LEU:O	1:B:54:ARG:N	2.43	0.51
1:B:80:LYS:NZ	1:B:242:CYS:O	2.37	0.51
1:C:1164:LEU:N	1:C:1168:ARG:O	2.43	0.50
1:A:747:ALA:HB2	1:A:763:ARG:HE	1.76	0.50
1:C:397:ARG:HH22	1:C:408:PHE:H	1.60	0.50
1:C:321:ILE:HD12	1:C:322:PRO:HD2	1.93	0.50
1:B:743:CYS:SG	1:B:744:ILE:N	2.85	0.50
1:A:745:ASP:OD2	1:A:763:ARG:NH2	2.45	0.50
1:B:692:TYR:HB3	1:B:695:LEU:HD12	1.92	0.50
1:A:680:ALA:HB1	1:A:736:LEU:HD13	1.94	0.49
1:C:1130:ILE:HG22	1:C:1131:LEU:HG	1.94	0.49
1:A:1045:GLN:NE2	1:B:652:ASN:OD1	2.45	0.49
1:C:223:LEU:HG	1:C:224:PHE:HD1	1.77	0.49
1:C:987:ILE:HG22	1:C:992:VAL:HG21	1.94	0.49
1:C:995:ASP:HB3	1:A:1206:ASN:HB3	1.94	0.48
1:B:79:LEU:HD12	1:B:239:PRO:HG3	1.93	0.48
1:B:125:VAL:HG12	1:B:138:VAL:HB	1.95	0.48
1:A:662:LEU:HD12	1:A:663:THR:HG23	1.95	0.48
1:A:324:LEU:HD12	1:A:325:PRO:HD2	1.93	0.48
1:A:938:GLN:HB3	1:A:943:ILE:HB	1.95	0.48
1:B:446:ARG:HA	1:B:450:PHE:HB3	1.95	0.48
1:B:791:PRO:HB3	1:B:1150:PRO:HB3	1.95	0.48
1:B:652:ASN:O	1:B:654:ASN:ND2	2.47	0.48
1:C:874:ASN:HA	1:C:891:LEU:HD22	1.96	0.48
1:A:466:CYS:HB3	1:A:547:PRO:HD2	1.94	0.48
1:A:351:ASN:N	1:A:602:THR:OG1	2.47	0.48
1:B:103:PHE:HB3	1:B:259:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:THR:HG22	1:B:1103:ALA:HA	1.96	0.48
1:C:425:LEU:HB3	1:C:590:SER:HB3	1.96	0.48
1:C:320:ARG:NE	1:C:603:CYS:SG	2.77	0.47
1:C:831:GLU:OE2	1:A:1051:PHE:N	2.45	0.47
1:C:54:ARG:NH1	1:C:56:TYR:OH	2.48	0.47
1:A:425:LEU:HB3	1:A:590:SER:HB3	1.96	0.47
1:A:427:TYR:HE1	1:A:590:SER:HB2	1.79	0.47
1:A:428:SER:O	1:A:585:ARG:NH2	2.47	0.47
1:A:1128:ASN:HB3	1:A:1148:TYR:HB3	1.95	0.47
1:C:177:ASP:OD1	1:C:177:ASP:N	2.47	0.47
1:B:145:ILE:HG13	1:B:190:THR:HG22	1.95	0.47
1:B:642:ASN:OD1	1:B:645:GLN:NE2	2.47	0.47
1:B:709:GLN:HG3	1:B:721:LEU:HD13	1.97	0.47
1:A:214:ALA:HB2	1:A:220:THR:HG23	1.95	0.47
1:A:949:ILE:HD13	1:B:737:ARG:HD3	1.97	0.46
1:C:938:GLN:HB3	1:C:943:ILE:HB	1.97	0.46
1:A:638:ALA:HB3	1:A:666:THR:HG21	1.96	0.46
1:B:440:ASN:H	1:B:446:ARG:HH21	1.64	0.46
1:B:624:LEU:HD13	1:B:625:TYR:H	1.79	0.46
1:B:427:TYR:HE1	1:B:590:SER:HB2	1.80	0.46
1:B:891:LEU:HD22	1:B:964:VAL:HG21	1.97	0.46
1:C:805:THR:HG22	1:C:1103:ALA:HA	1.98	0.46
1:C:850:LEU:HD21	1:C:1096:ILE:HD12	1.98	0.46
1:A:329:ILE:HD12	1:A:354:PHE:HB3	1.98	0.46
1:B:369:SER:HA	1:B:375:LYS:HD3	1.96	0.46
1:C:1158:VAL:HB	1:C:1176:TYR:HB3	1.98	0.46
1:B:662:LEU:H	1:B:662:LEU:HD23	1.81	0.46
1:C:646:ASN:OD1	1:B:53:ASN:ND2	2.48	0.46
1:C:346:ARG:HG3	1:C:387:THR:HG23	1.98	0.46
1:C:1128:ASN:HB3	1:C:1148:TYR:HB3	1.98	0.46
1:B:663:THR:HA	4:B:1302:NAG:H82	1.96	0.46
1:C:660:ASP:OD1	1:C:661:PHE:N	2.48	0.46
1:C:1066:ASP:OD1	1:C:1066:ASP:N	2.39	0.46
1:A:328:ASP:HB2	1:A:331:ASN:HB2	1.97	0.46
1:A:604:SER:OG	1:A:606:ASP:OD1	2.33	0.46
1:A:161:THR:HA	1:A:172:GLU:HG3	1.98	0.45
1:C:791:PRO:HB3	1:C:1150:PRO:HB3	1.98	0.45
1:C:313:PRO:HB3	1:C:620:VAL:HA	1.98	0.45
1:C:1019:PHE:HA	1:C:1023:PRO:HG3	1.99	0.45
1:B:343:ASN:ND2	1:B:439:PHE:O	2.44	0.45
1:B:1023:PRO:HD2	1:B:1026:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HB2	1:C:237:VAL:HG11	1.97	0.45
1:B:717:LEU:HD11	1:B:740:SER:HB3	1.97	0.45
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.98	0.45
1:A:85:LEU:HD21	1:A:90:TYR:HE2	1.80	0.45
1:A:1100:LYS:HG3	1:B:1098:LEU:HD11	1.99	0.45
1:B:810:VAL:HG12	1:B:945:VAL:HG22	1.99	0.45
1:C:745:ASP:OD2	1:C:763:ARG:NH2	2.42	0.45
1:A:29:ASN:HA	1:A:88:LEU:HD13	1.99	0.44
1:A:681:PHE:HB2	1:A:688:PRO:HB3	1.98	0.44
1:B:638:ALA:HB3	1:B:666:THR:HG21	1.99	0.44
1:C:428:SER:HB2	1:C:585:ARG:HB3	1.99	0.44
1:A:18:PHE:HB3	1:A:156:CYS:HA	1.98	0.44
1:B:1067:PRO:N	1:B:1068:PRO:HD2	2.32	0.44
1:C:107:LYS:NZ	1:C:253:THR:OG1	2.50	0.44
1:A:413:ASN:HD21	1:A:462:TYR:HB2	1.82	0.44
1:A:731:VAL:HG22	1:A:733:SER:H	1.83	0.44
1:C:789:GLN:HB3	1:C:1153:PHE:HB3	1.99	0.44
1:C:1067:PRO:N	1:C:1068:PRO:HD2	2.33	0.44
1:C:341:PRO:HB2	1:C:413:ASN:HD22	1.82	0.44
1:C:1163:CYS:HB3	1:C:1214:LYS:HD3	1.99	0.44
1:A:139:VAL:HG12	1:A:148:ILE:HG12	1.98	0.44
1:A:382:CYS:HA	1:A:603:CYS:HA	1.99	0.44
1:C:737:ARG:HD3	1:B:949:ILE:HD13	2.00	0.44
1:A:1111:ASN:HB3	1:B:1122:ASN:HB2	2.00	0.44
1:A:1050:LYS:HA	1:A:1056:SER:HA	1.99	0.43
1:A:1108:GLU:OE2	1:B:1120:ARG:NH2	2.51	0.43
1:A:1129:HIS:NE2	1:A:1132:SER:OG	2.35	0.43
1:A:219:PRO:HG3	1:A:276:ILE:HB	2.00	0.43
1:B:1122:ASN:HD22	1:B:1127:GLY:H	1.66	0.43
1:A:701:LEU:HA	1:A:705:SER:HB3	2.00	0.43
1:A:940:PHE:HD2	1:B:671:PRO:HB2	1.83	0.43
1:B:1111:ASN:O	1:B:1116:SER:OG	2.33	0.43
1:C:351:ASN:N	1:C:602:THR:OG1	2.51	0.43
1:B:68:PRO:O	1:B:266:TYR:OH	2.25	0.43
1:C:335:ASN:OD1	1:C:336:VAL:N	2.51	0.43
1:B:408:PHE:HB3	1:B:464:ASP:HA	2.01	0.43
1:B:604:SER:OG	1:B:606:ASP:OD1	2.37	0.43
1:B:890:CYS:HB3	1:B:899:SER:HB2	2.01	0.43
1:C:447:ARG:NH2	1:C:448:TYR:OH	2.52	0.43
1:A:1180:GLN:HG2	1:A:1181:ASN:HD22	1.83	0.43
1:B:801:GLU:OE1	1:B:1109:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:VAL:HG13	1:B:1096:ILE:HD12	2.00	0.43
1:C:137:ILE:HD11	1:C:228:LEU:HD11	2.01	0.43
1:C:271:ASP:OD1	1:C:275:VAL:N	2.39	0.43
1:B:368:PHE:HD1	1:B:425:LEU:HD13	1.84	0.43
1:A:1016:GLN:HA	1:A:1019:PHE:HD1	1.83	0.42
1:B:400:ASP:HB2	1:B:409:LEU:HD12	2.01	0.42
1:A:871:LEU:HD13	1:B:779:VAL:HG21	2.01	0.42
1:B:185:PHE:HB2	1:B:226:LEU:HD13	2.00	0.42
1:A:999:LYS:HE3	1:A:999:LYS:HB3	1.91	0.42
1:B:19:ASN:HD21	1:B:22:ASN:HB3	1.84	0.42
1:C:663:THR:HB	1:C:665:LYS:HE2	2.01	0.42
1:B:24:PHE:HB3	1:B:84:TYR:HD1	1.85	0.42
1:B:98:PHE:HB2	1:B:235:TYR:HD1	1.84	0.42
1:B:281:ASP:OD1	1:B:282:CYS:N	2.42	0.42
1:C:445:ASN:HD21	1:C:549:LEU:H	1.68	0.42
1:C:779:VAL:HB	1:B:870:ASN:HB2	2.02	0.42
1:C:822:TYR:O	1:C:826:HIS:ND1	2.41	0.42
1:A:673:TYR:CZ	1:A:695:LEU:HD11	2.54	0.42
1:B:100:ASN:HD21	1:B:262:SER:HA	1.83	0.42
1:B:673:TYR:CZ	1:B:695:LEU:HD11	2.54	0.42
1:B:933:ASP:OD1	1:B:933:ASP:N	2.53	0.42
1:C:98:PHE:HE1	1:C:102:ILE:HG12	1.85	0.41
1:C:731:VAL:HG22	1:C:733:SER:H	1.85	0.41
1:B:160:HIS:NE2	1:B:171:ASN:O	2.40	0.41
1:B:397:ARG:HH12	1:B:408:PHE:HD2	1.68	0.41
1:B:1066:ASP:HB3	1:B:1068:PRO:HD2	2.01	0.41
1:B:1199:ASP:HA	1:B:1202:VAL:HG12	2.02	0.41
1:C:24:PHE:HB2	1:C:170:ARG:HH21	1.85	0.41
1:B:218:MET:HB2	1:B:219:PRO:HD3	2.02	0.41
1:C:582:SER:HB3	1:C:587:ASN:HD21	1.86	0.41
1:A:343:ASN:HD22	1:A:439:PHE:HB3	1.85	0.41
1:B:996:VAL:HG21	1:B:1191:TYR:CZ	2.55	0.41
1:C:498:GLY:HA2	1:B:14:VAL:HG11	2.01	0.41
1:A:269:ASN:HB2	1:A:297:PHE:CE1	2.56	0.41
1:A:414:TYR:HE2	1:A:416:ILE:HG13	1.86	0.41
1:A:933:ASP:OD1	1:A:933:ASP:N	2.53	0.41
1:A:648:LEU:HD23	1:A:657:GLY:HA3	2.02	0.41
1:C:53:ASN:OD1	1:C:53:ASN:N	2.52	0.41
1:C:245:ILE:HD12	1:C:245:ILE:HA	1.93	0.41
1:C:691:LEU:HD13	1:C:720:VAL:HG22	2.03	0.41
1:C:932:ARG:HH12	1:A:656:ILE:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PRO:HB2	1:A:557:GLY:HA3	2.02	0.41
1:B:53:ASN:OD1	1:B:53:ASN:N	2.54	0.41
1:B:107:LYS:HD2	1:B:255:GLU:HG2	2.02	0.41
1:A:125:VAL:HG13	1:A:138:VAL:HG22	2.03	0.40
1:B:316:THR:HB	1:B:621:ASN:OD1	2.21	0.40
1:C:1049:ASN:HD21	1:B:834:THR:HB	1.85	0.40
1:A:966:ALA:HB2	1:A:973:ALA:HB3	2.03	0.40
1:C:1129:HIS:NE2	1:C:1132:SER:OG	2.42	0.40
1:C:53:ASN:O	1:C:54:ARG:HG3	2.21	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	1160/1263 (92%)	1123 (97%)	37 (3%)	0	100	100
1	B	1177/1263 (93%)	1121 (95%)	56 (5%)	0	100	100
1	C	1162/1263 (92%)	1129 (97%)	33 (3%)	0	100	100
All	All	3499/3789 (92%)	3373 (96%)	126 (4%)	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	1038/1132 (92%)	1026 (99%)	12 (1%)	71	87
1	B	1051/1132 (93%)	1037 (99%)	14 (1%)	69	86
1	C	1040/1132 (92%)	1022 (98%)	18 (2%)	60	82
All	All	3129/3396 (92%)	3085 (99%)	44 (1%)	68	85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	80	LYS
1	C	213	TYR
1	C	292	CYS
1	C	327	CYS
1	C	434	VAL
1	C	474	CYS
1	C	523	ASP
1	C	703	ASN
1	C	716	TYR
1	C	722	ASN
1	C	743	CYS
1	C	825	CYS
1	C	835	PHE
1	C	836	CYS
1	C	926	THR
1	C	992	VAL
1	C	1012	LEU
1	C	1208	CYS
1	A	28	TYR
1	A	213	TYR
1	A	215	ASP
1	A	223	LEU
1	A	345	GLU
1	A	453	PHE
1	A	474	CYS
1	A	697	CYS
1	A	743	CYS
1	A	768	GLU
1	A	848	ASP
1	A	1022	THR
1	B	18	PHE
1	B	21	THR
1	B	175	HIS
1	B	316	THR

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Mol	Chain	Res	Type
1	B	320	ARG
1	B	474	CYS
1	B	601	THR
1	B	624	LEU
1	B	662	LEU
1	B	743	CYS
1	B	837	ASP
1	B	845	GLU
1	B	871	LEU
1	B	894	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	440	ASN
1	C	587	ASN
1	C	847	ASN
1	C	1128	ASN
1	A	99	ASN
1	A	248	ASN
1	A	265	GLN
1	A	291	GLN
1	A	372	ASN
1	A	413	ASN
1	A	445	ASN
1	A	587	ASN
1	A	605	ASN
1	A	709	GLN
1	A	847	ASN
1	A	870	ASN
1	A	1016	GLN
1	A	1046	GLN
1	A	1071	GLN
1	A	1128	ASN
1	A	1174	GLN
1	A	1180	GLN
1	A	1181	ASN
1	B	19	ASN
1	B	645	GLN
1	B	654	ASN
1	B	683	GLN
1	B	804	GLN

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Mol	Chain	Res	Type
1	B	894	GLN
1	B	1128	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

5 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	$\# Z  > 2$
2	NAG	D	1	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	BMA	D	3	2	11,11,12	0.58	0	15,15,17	0.75	0
3	NAG	E	1	3,1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.41	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
2	NAG	D	1	2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

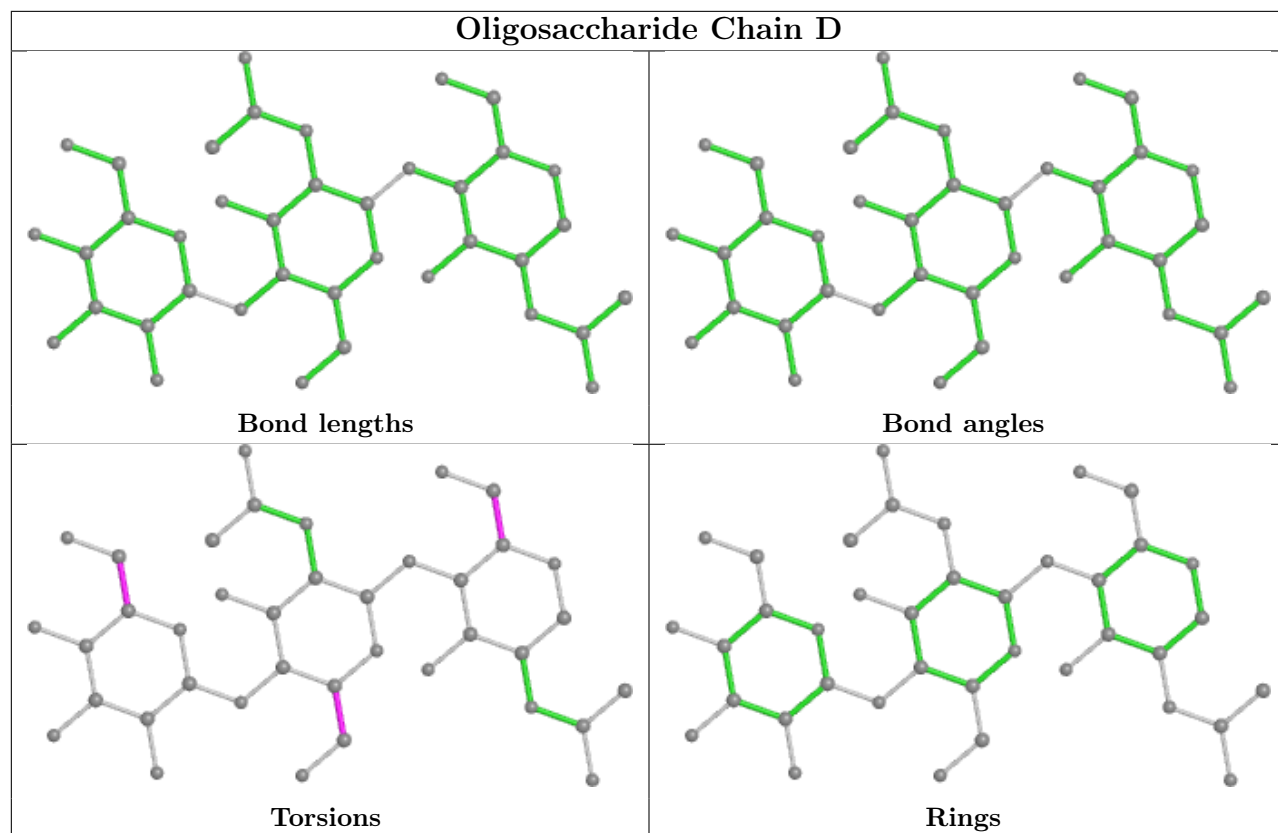
All (8) torsion outliers are listed below:

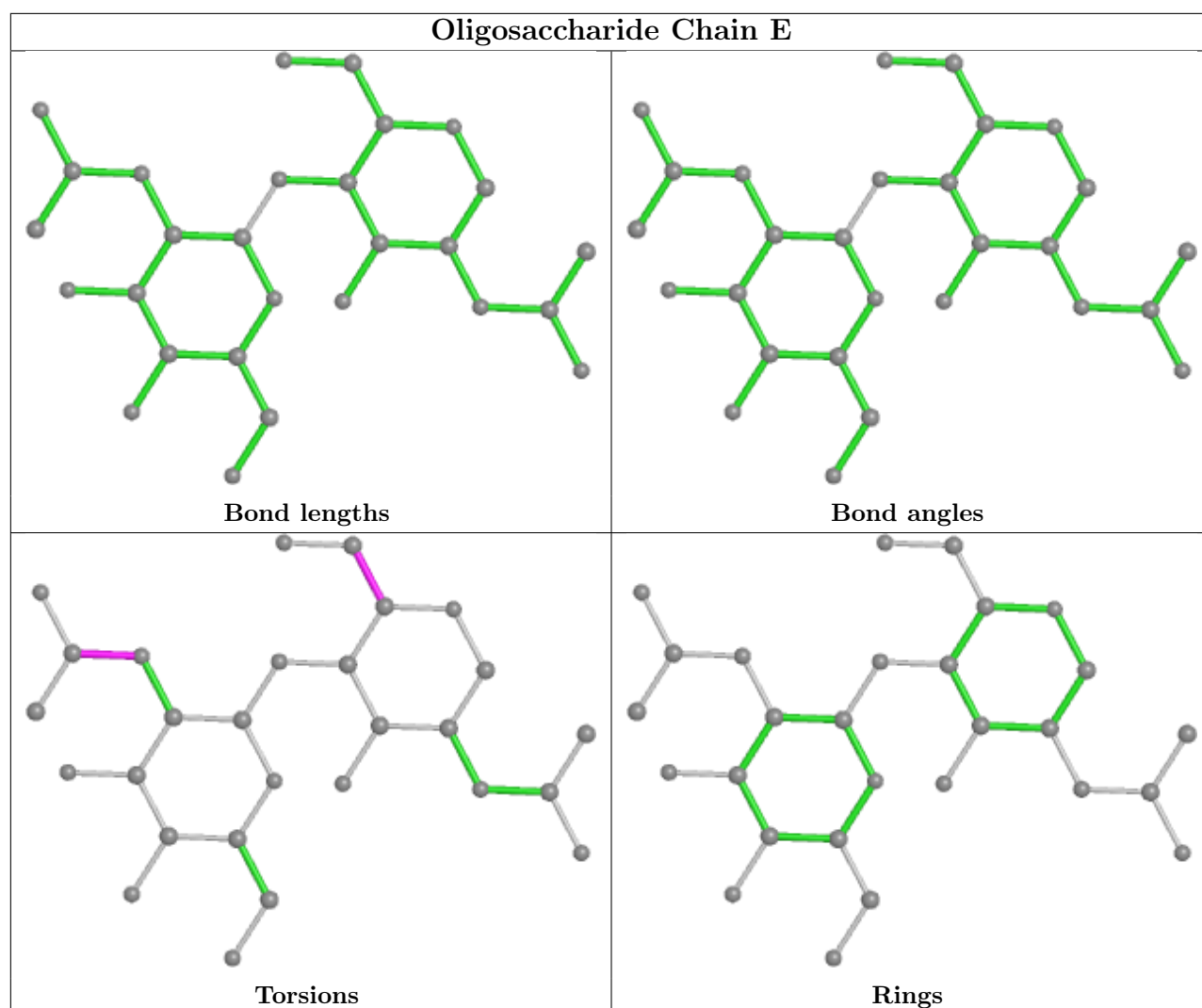
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

26 ligands 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	$\# Z  > 2$
4	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.42	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1308	1	14,14,15	0.92	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.53	0
4	NAG	A	1305	1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	B	1306	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	C	1311	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	1308	1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	A	1309	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.43	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
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1308	NAG	O5-C1	3.09	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1308	NAG	C1-O5-C5	4.05	117.68	112.19

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1303	NAG	C4-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	C	1309	NAG	C8-C7-N2-C2
4	C	1309	NAG	O7-C7-N2-C2
4	C	1311	NAG	C8-C7-N2-C2
4	C	1311	NAG	O7-C7-N2-C2
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	C	1310	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1306	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1309	NAG	C3-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7
4	B	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0

## 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.

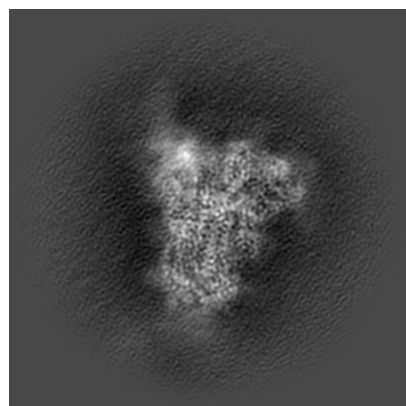
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39042. These allow visual inspection of the internal detail of the map and identification of artifacts.

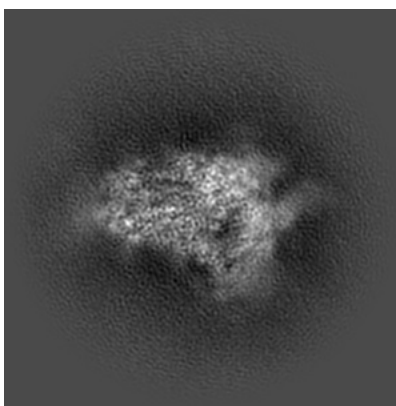
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

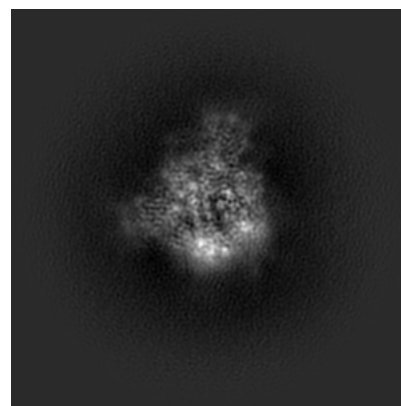
#### 6.1.1 Primary map



X

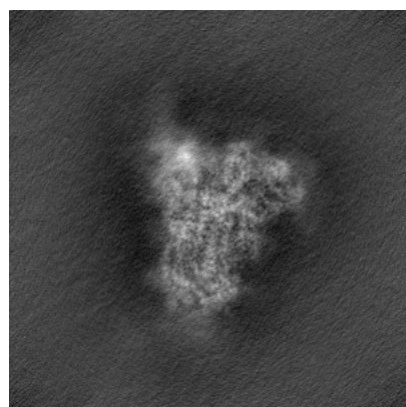


Y

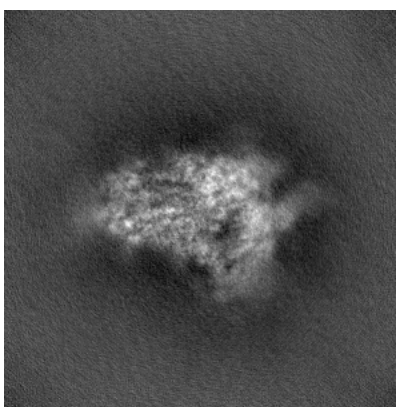


Z

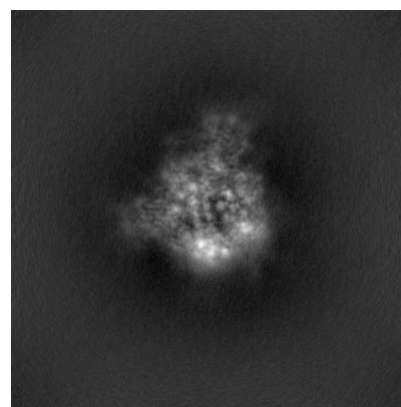
#### 6.1.2 Raw map



X



Y

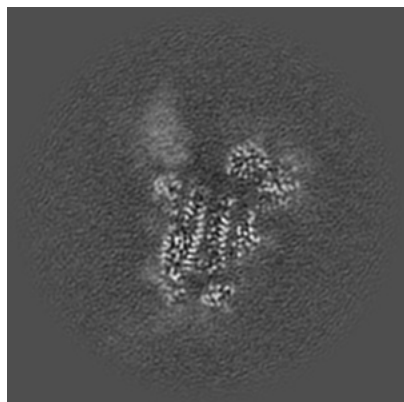


Z

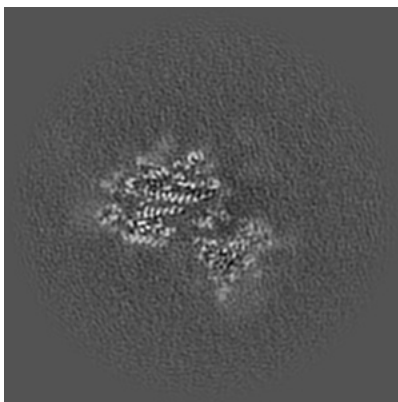
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

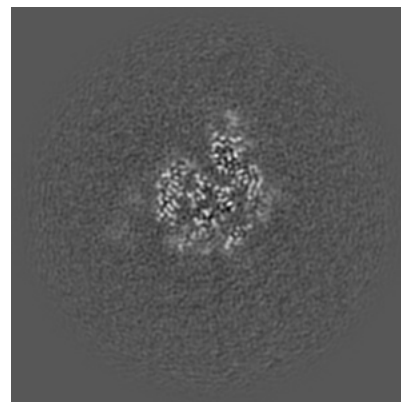
### 6.2.1 Primary map



X Index: 200

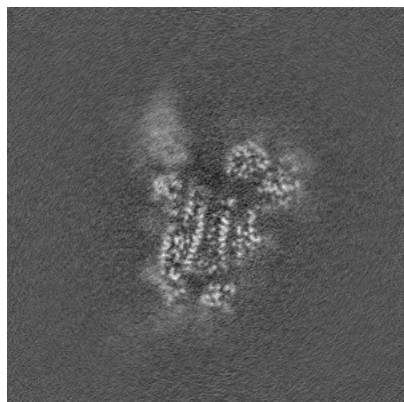


Y Index: 200

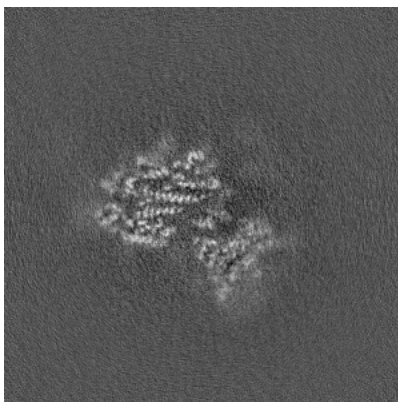


Z Index: 200

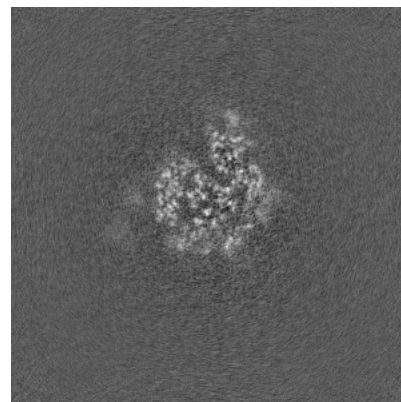
### 6.2.2 Raw map



X Index: 200



Y Index: 200



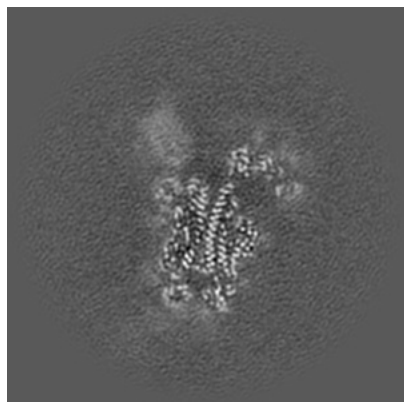
Z Index: 200

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

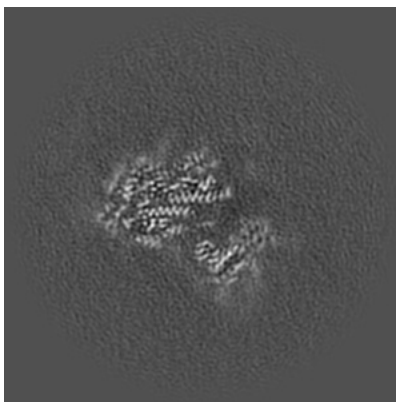


## 6.3 Largest variance slices [i](#)

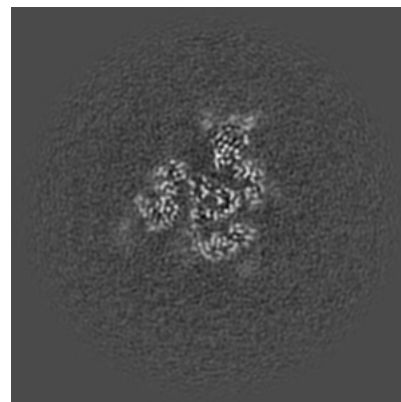
### 6.3.1 Primary map



X Index: 195

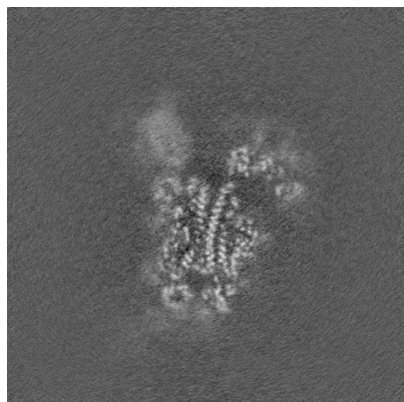


Y Index: 203

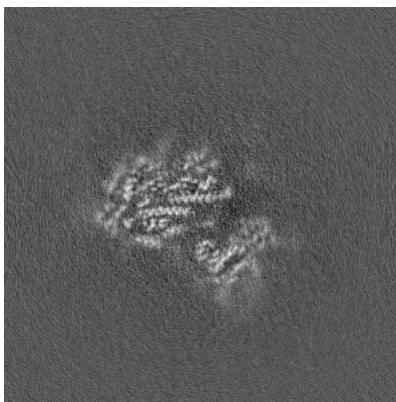


Z Index: 209

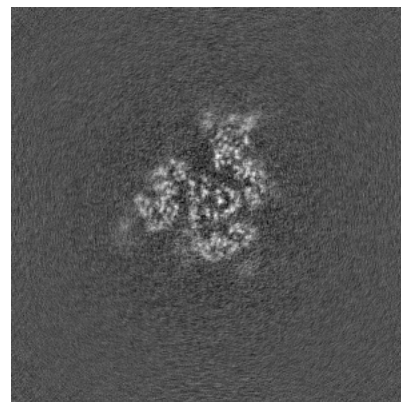
### 6.3.2 Raw map



X Index: 195



Y Index: 203

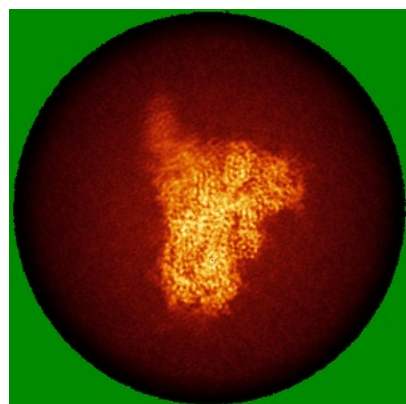


Z Index: 209

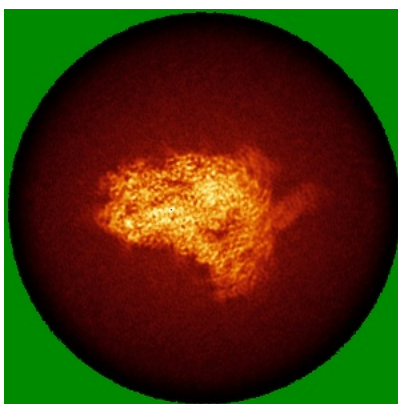
The images above show the largest variance slices of the map in three orthogonal directions.

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

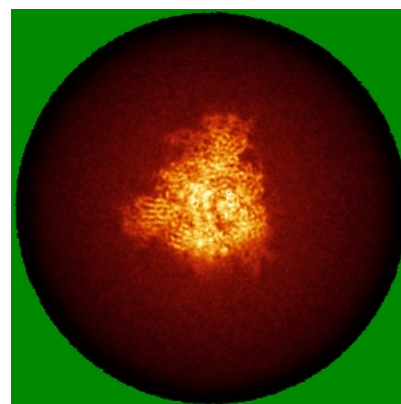
### 6.4.1 Primary map



X

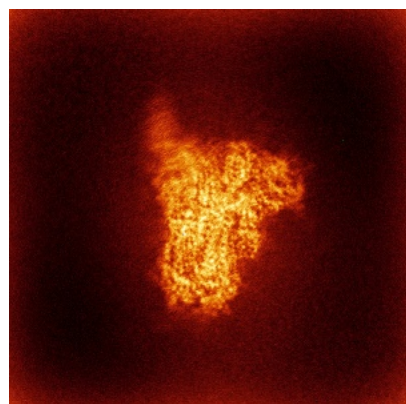


Y

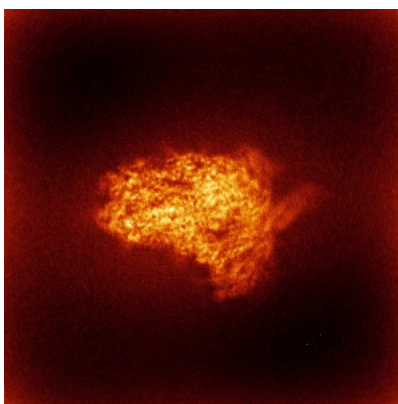


Z

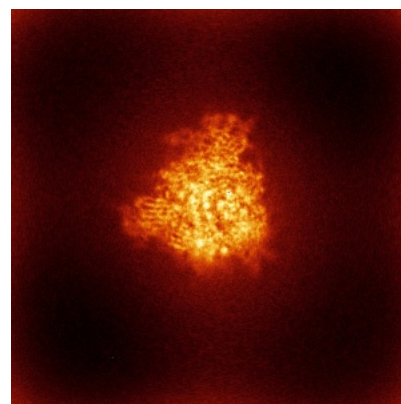
### 6.4.2 Raw map



X



Y



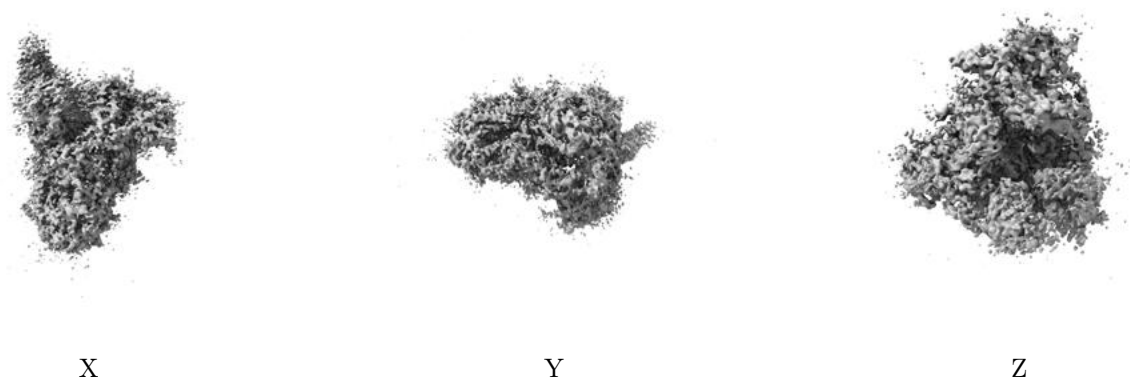
Z

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.



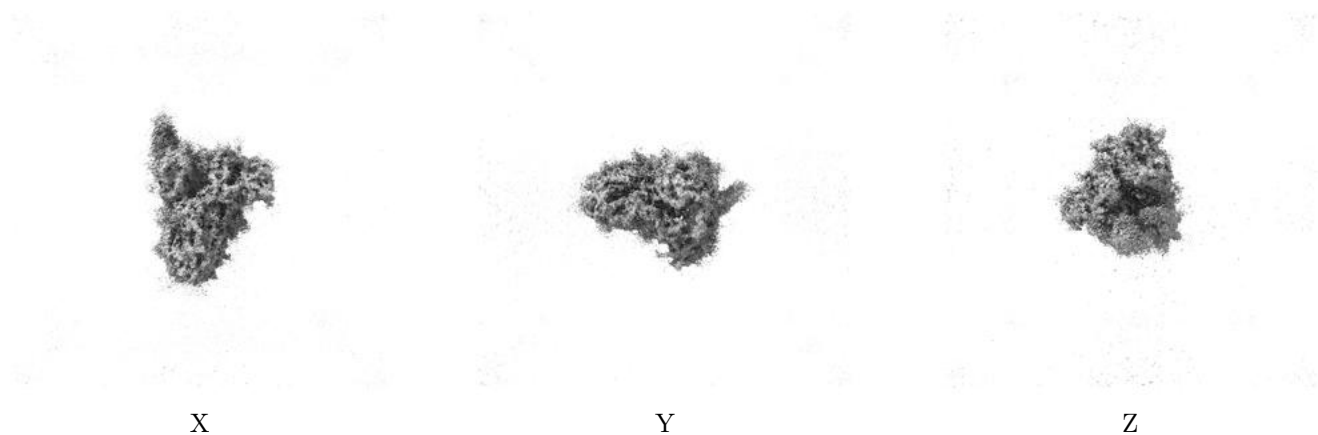
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

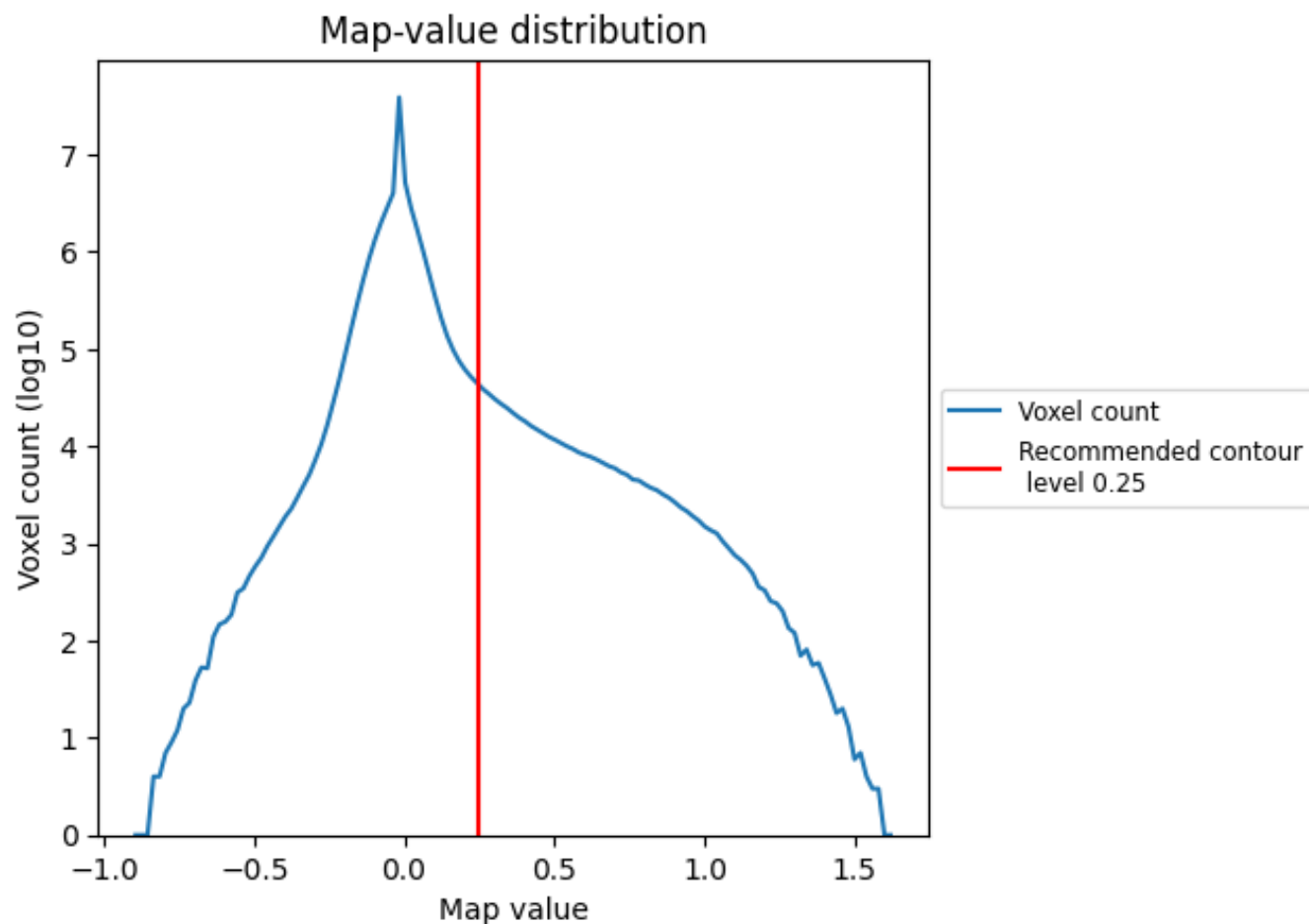
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

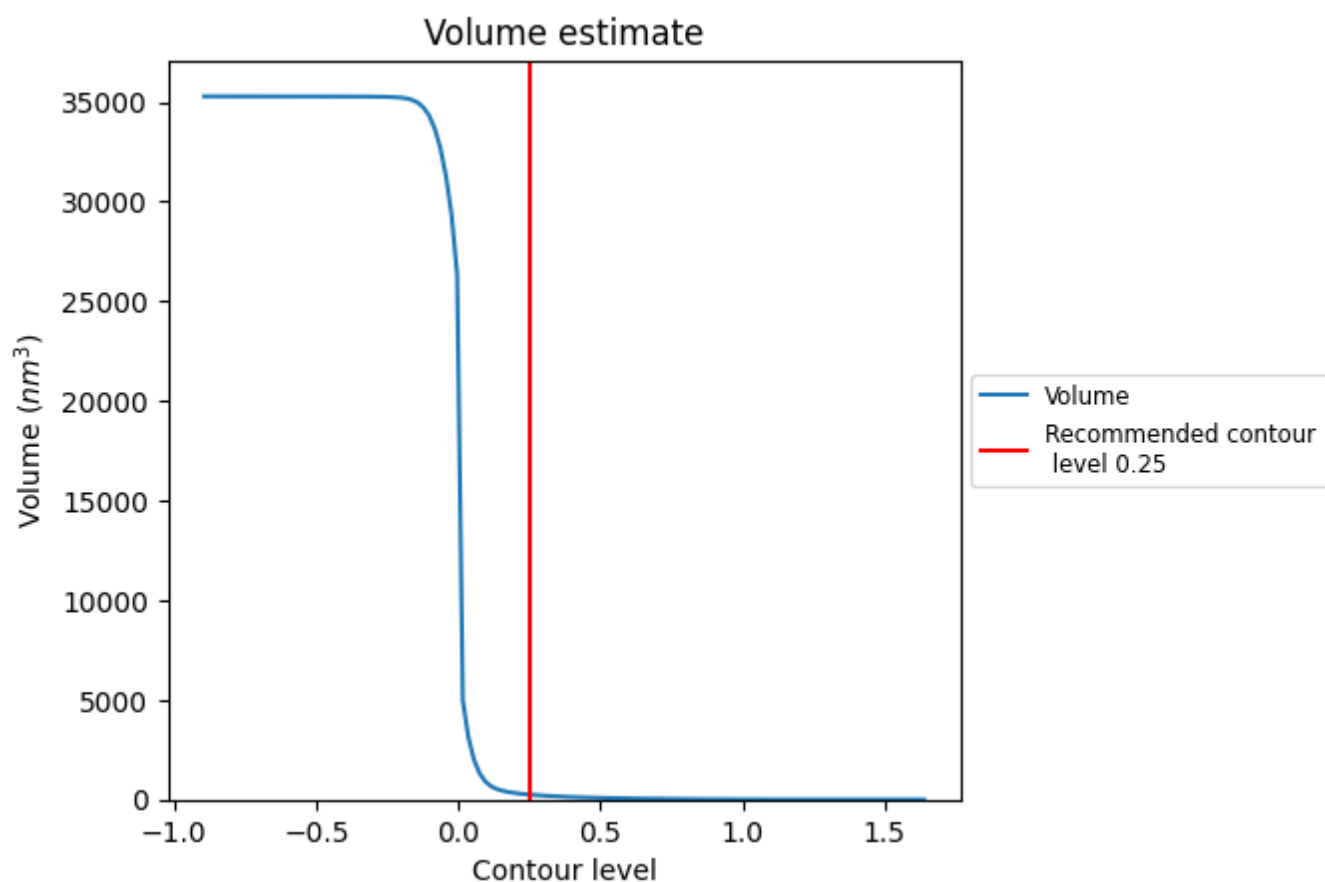
This section contains the results of statistical analysis of the map.

### 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.

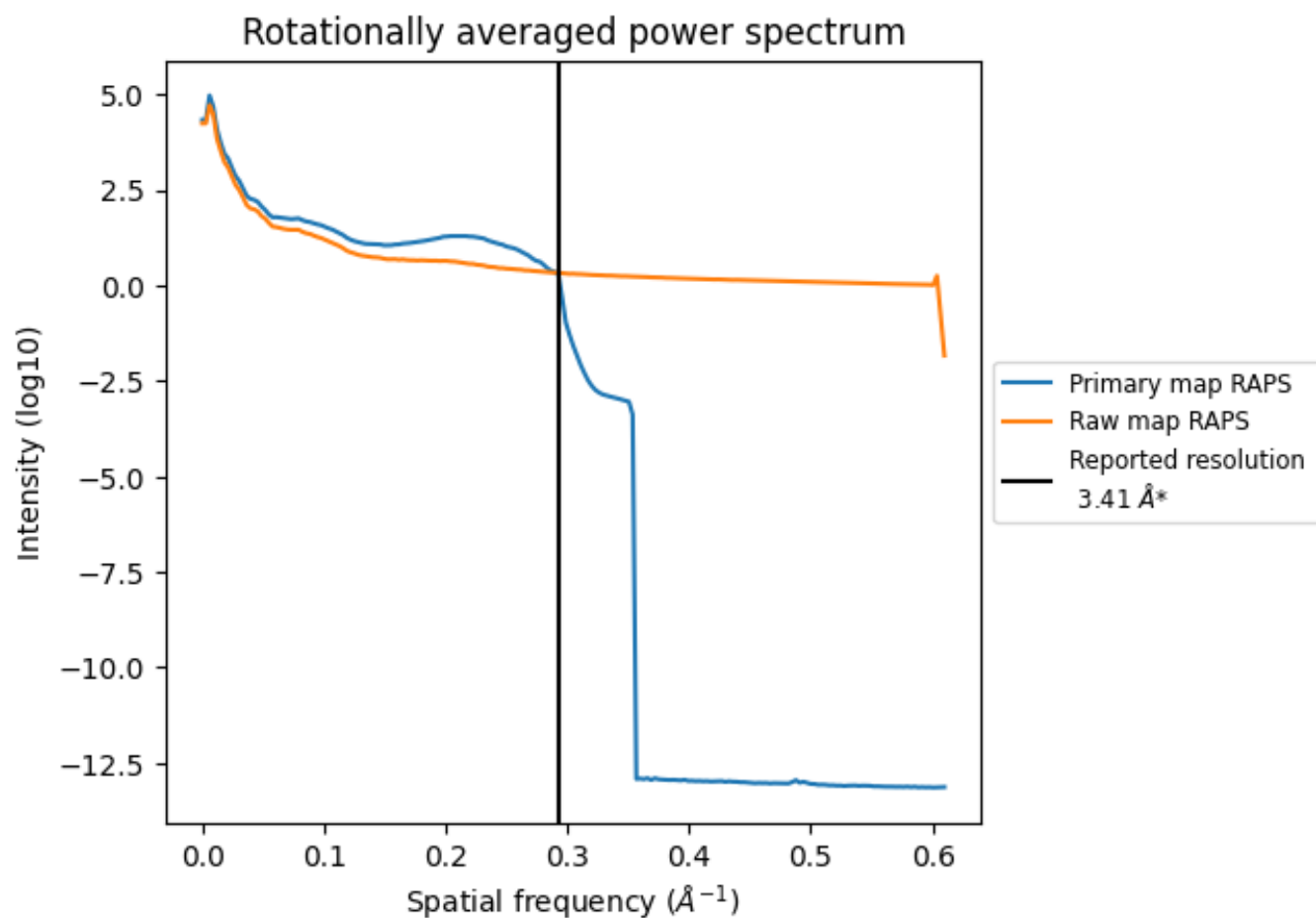
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm<sup>3</sup>; this corresponds to an approximate mass of 225 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

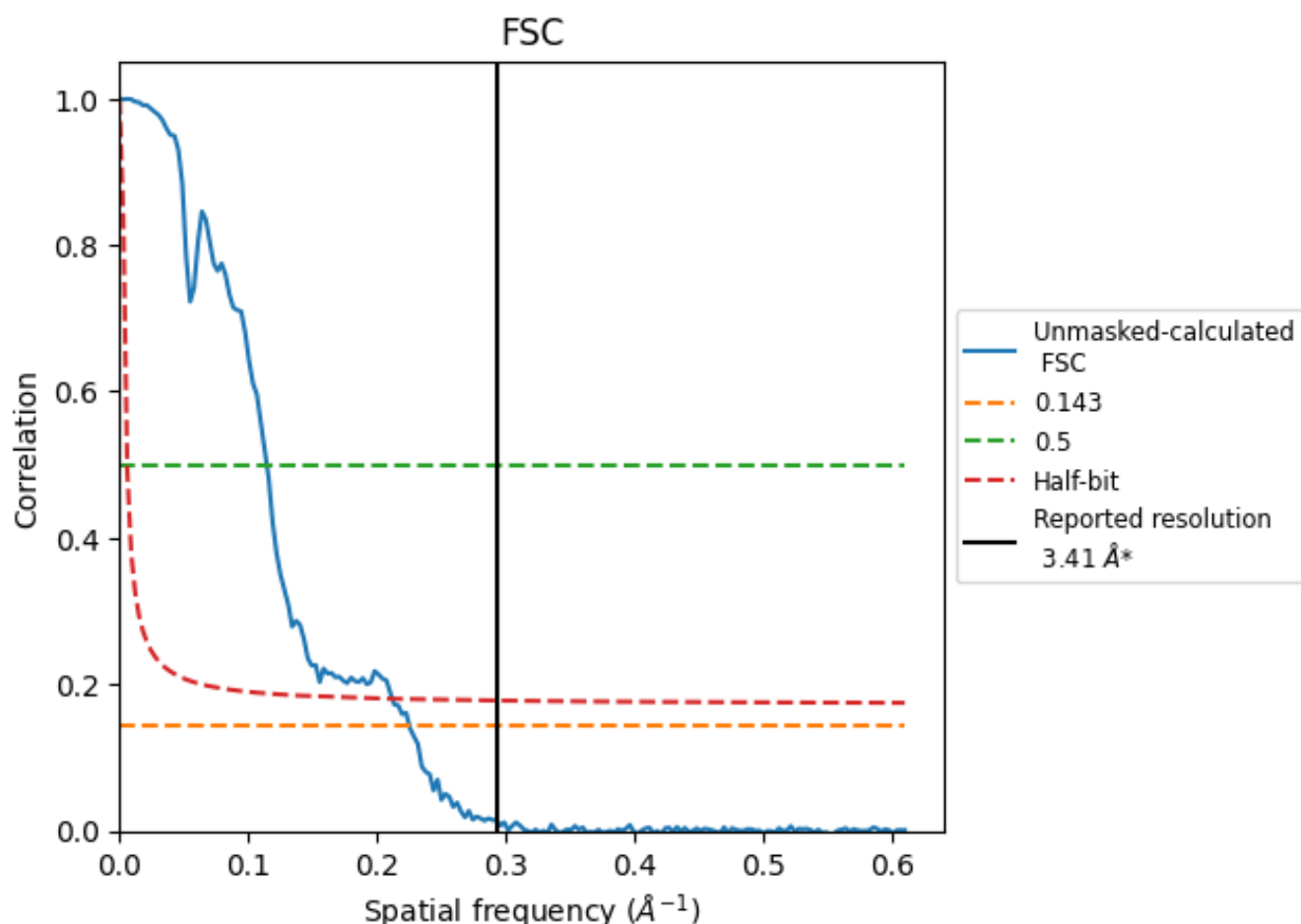


\*Reported resolution corresponds to spatial frequency of 0.293 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.293  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

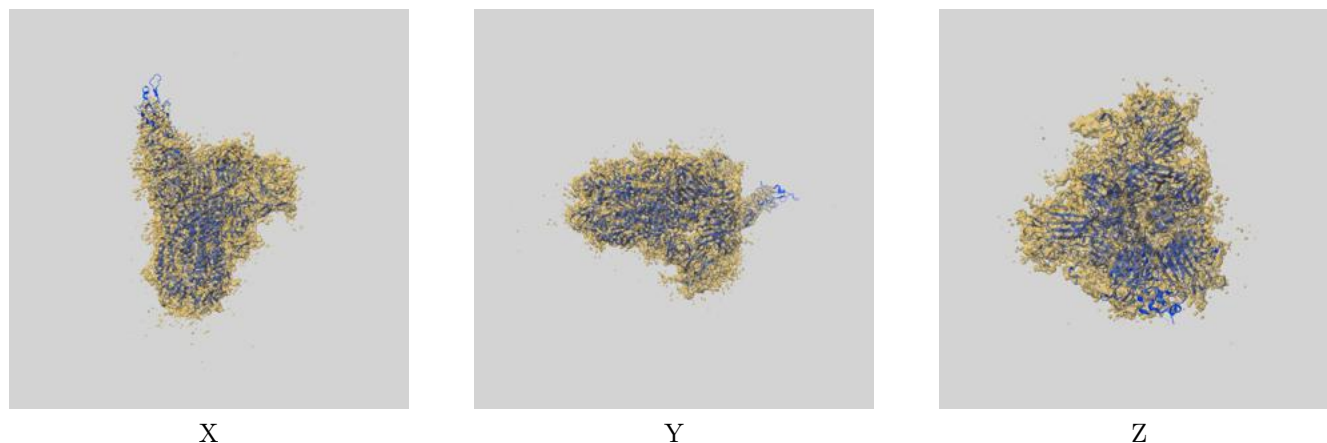
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	8.74	4.72

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.41 by more than 10 %

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

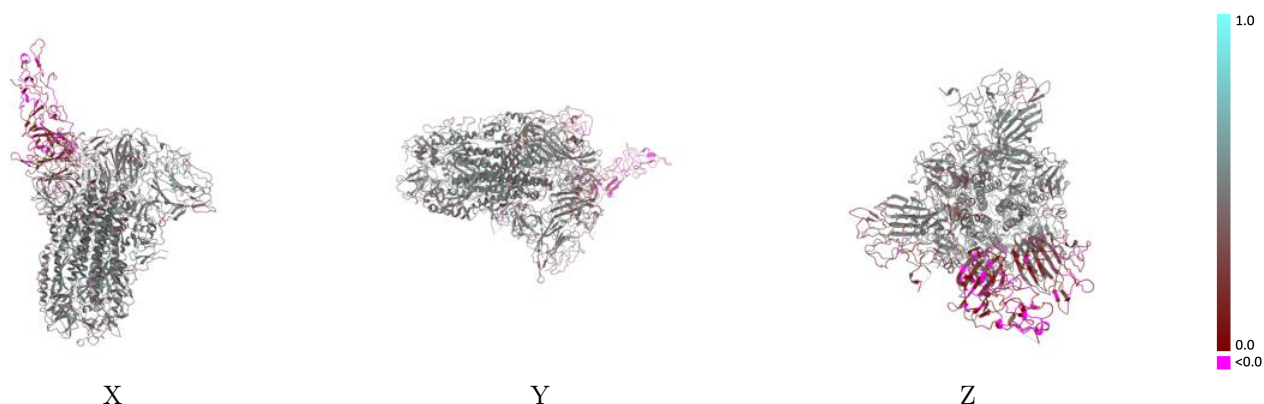
This section contains information regarding the fit between EMDB map EMD-39042 and PDB model 8Y8D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



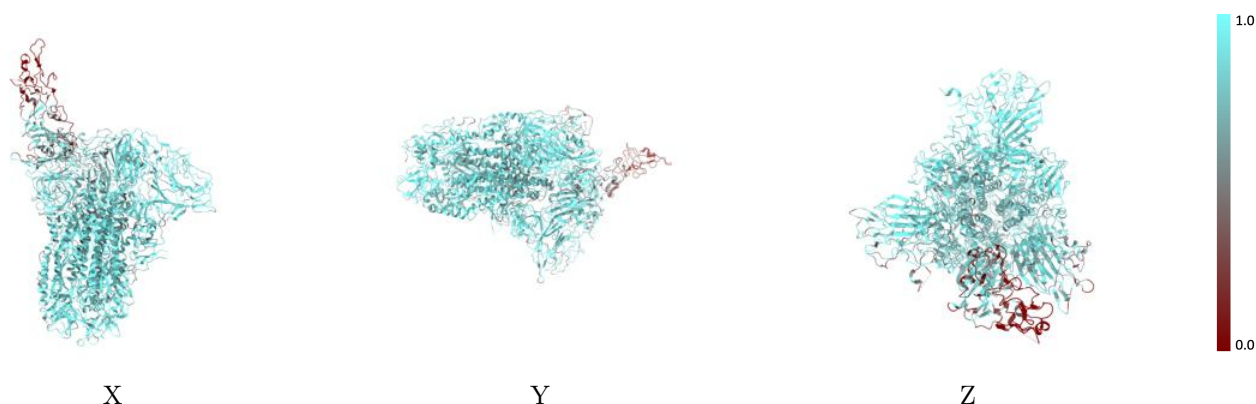
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

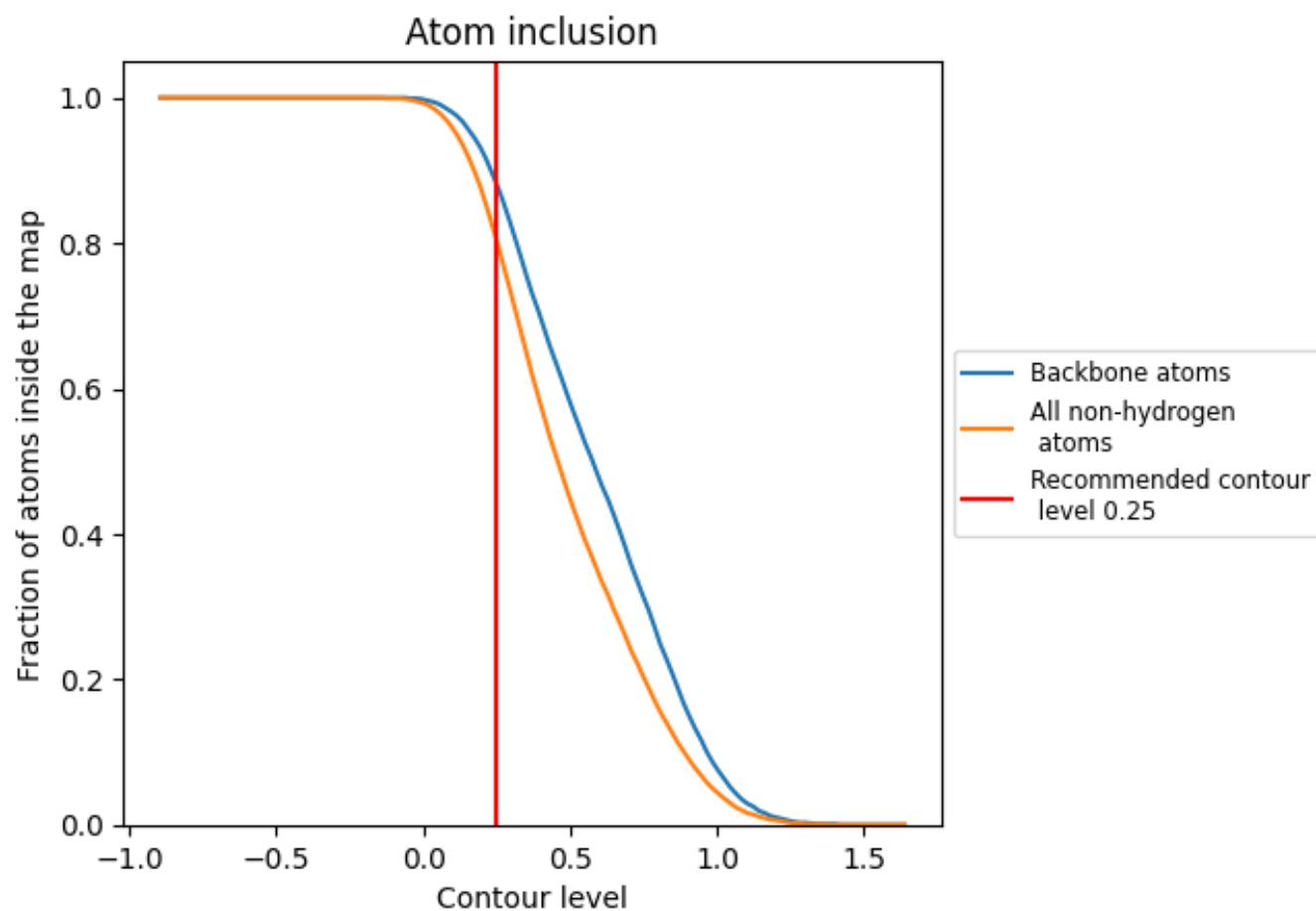
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.25).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8040	<div></div> 0.4090
A	<div></div> 0.8310	<div></div> 0.4160
B	<div></div> 0.7340	<div></div> 0.3630
C	<div></div> 0.8460	<div></div> 0.4490
D	<div></div> 0.8460	<div></div> 0.4330
E	<div></div> 0.8930	<div></div> 0.4100

