



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 11:32 am BST

PDB ID : 8B0G
EMDB ID : EMD-15780
Title : 2C9, C5b9-CD59 structure
Authors : Couves, E.C.; Gardner, S.; Bubeck, D.
Deposited on : 2022-09-07
Resolution : 3.30 Å(reported)
Based on initial models : 7NYD, 2J8B

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

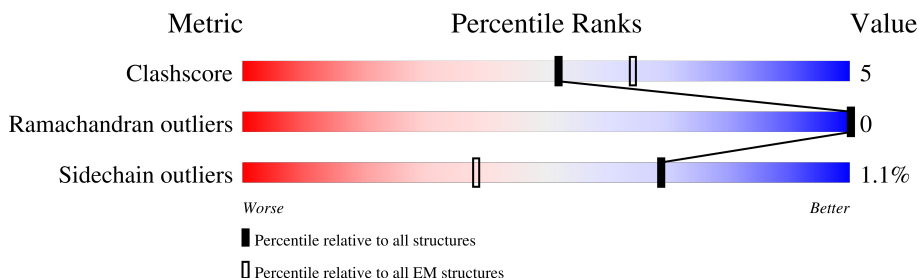
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.







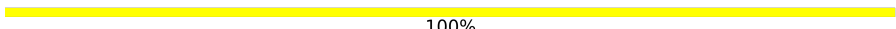


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	1676	
2	C	843	
3	D	591	
4	E	584	
5	F	202	
6	H	559	
6	I	559	
6	J	559	

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Mol	Chain	Length	Quality of chain
7	B	934	
8	G	78	
9	K	2	
9	L	2	
9	M	2	
9	N	2	
9	O	2	

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
9	NAG	N	2	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 79405 atoms, of which 38924 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 Complement C5.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1245	Total	C	H	N	O	S	0	0
			19687	6332	9834	1618	1875	28		

- Molecule 2 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	646	Total	C	H	N	O	S	0	0
			9762	3133	4727	876	986	40		

- Molecule 3 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	518	Total	C	H	N	O	S	0	0
			8096	2577	3958	738	786	37		

- Molecule 4 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	513	Total	C	H	N	O	S	0	0
			7865	2503	3813	716	794	39		

- Molecule 5 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	168	Total	C	H	N	O	S	0	0
			2603	841	1284	230	244	4		

- Molecule 6 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	407	Total	C	H	N	O	S	0	0
			6301	2008	3084	558	622	29		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	399	Total	C	H	N	O	S	0	0
			6135	1958	2989	547	611	30		
6	I	402	Total	C	H	N	O	S	0	0
			6203	1981	3027	550	616	29		

- Molecule 7 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	737	Total	C	H	N	O	S	0	0
			11267	3570	5491	1021	1135	50		

- Molecule 8 is a protein called CD59 glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	78	Total	C	H	N	O	S	0	0
			1211	389	582	106	123	11		

There is a discrepancy between the modelled and reference sequences:

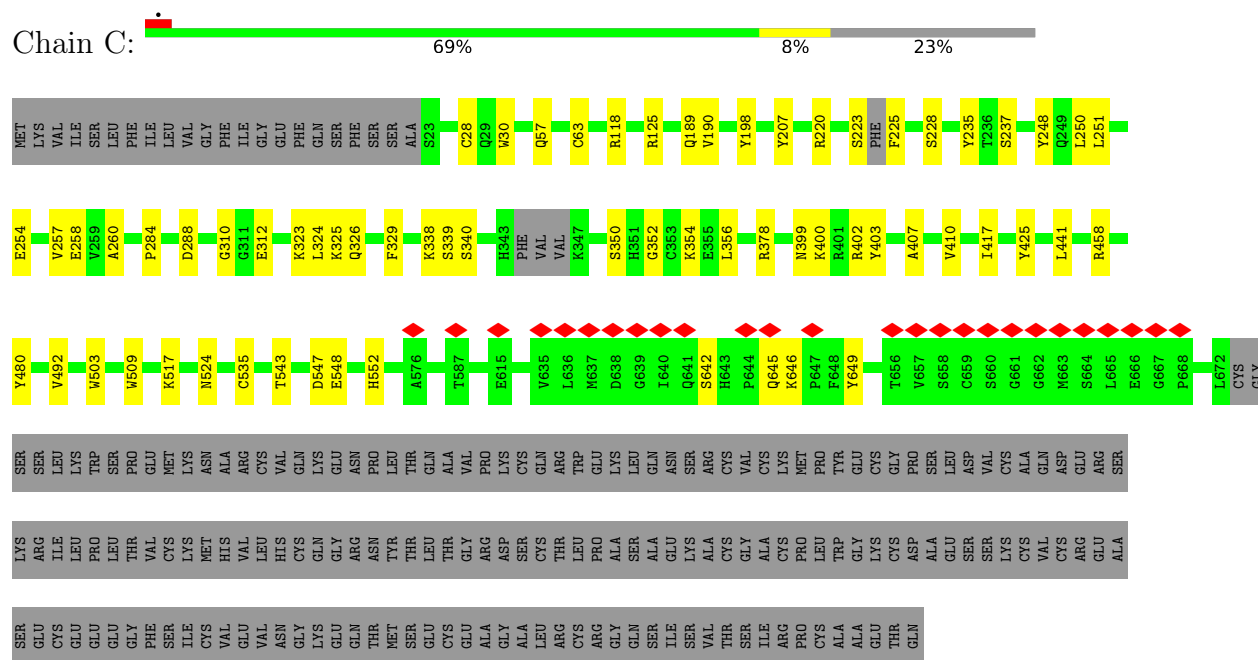
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	MET	-	initiating methionine	UNP P13987

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

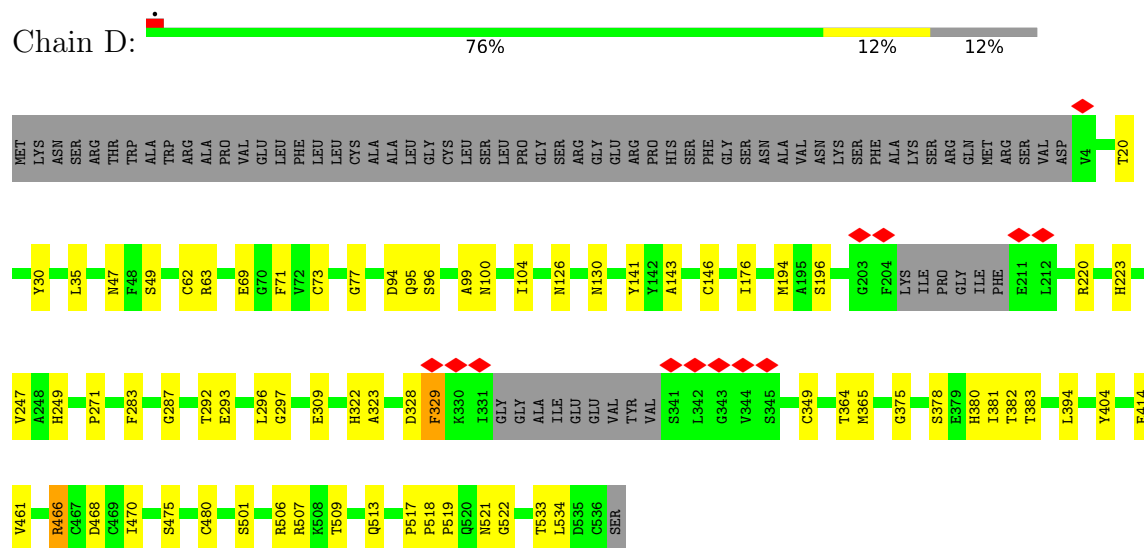


Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
9	L	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
9	M	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
9	N	2	Total	C	H	N	O		0	0
			55	16	27	2	10			
9	O	2	Total	C	H	N	O		0	0
			55	16	27	2	10			

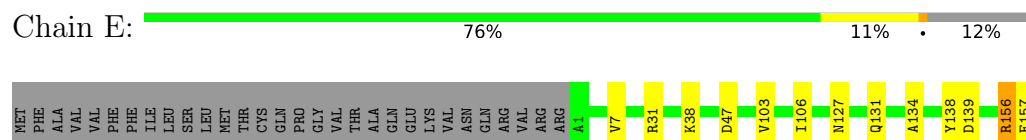
- Molecule 2: Complement component C7

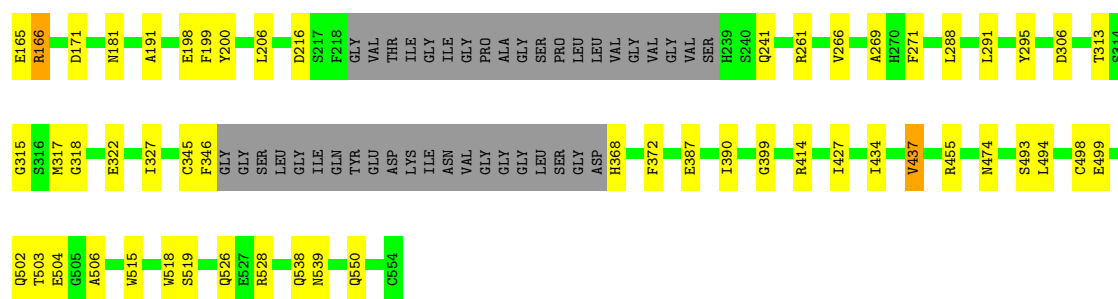


- Molecule 3: Complement component C8 beta chain



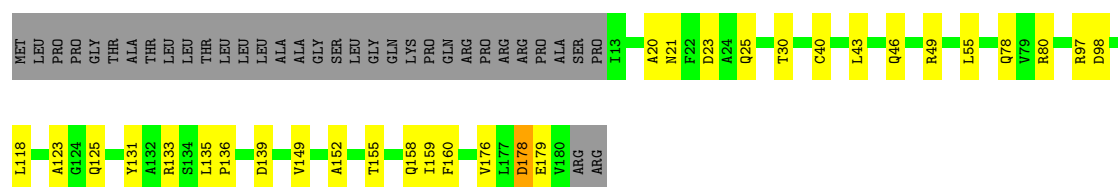
- Molecule 4: Complement component C8 alpha chain





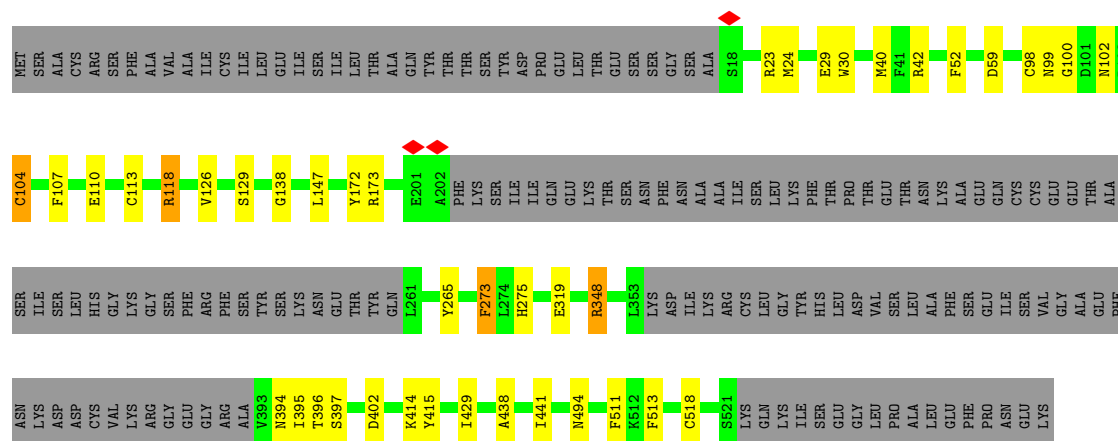
- Molecule 5: Complement component C8 gamma chain

Chain F: 68% 15% 17%



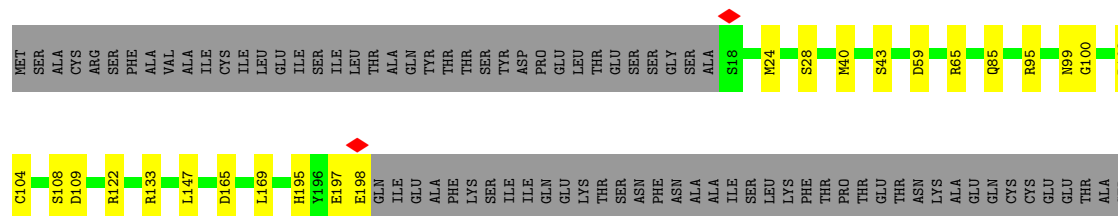
- Molecule 6: Complement component C9

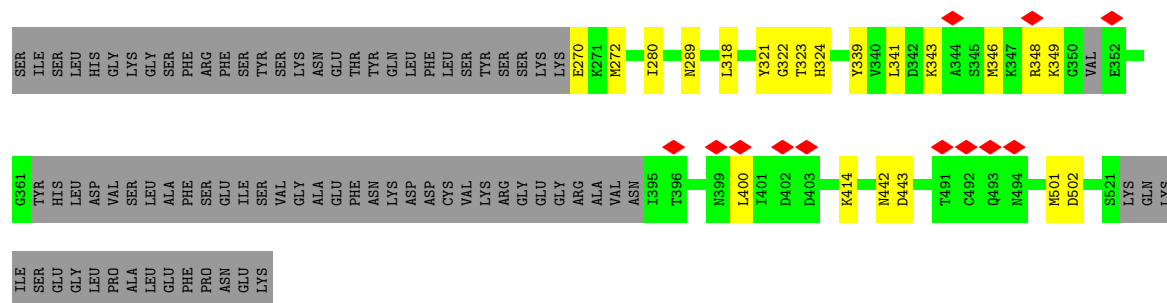
Chain H: 65% 7% 27%



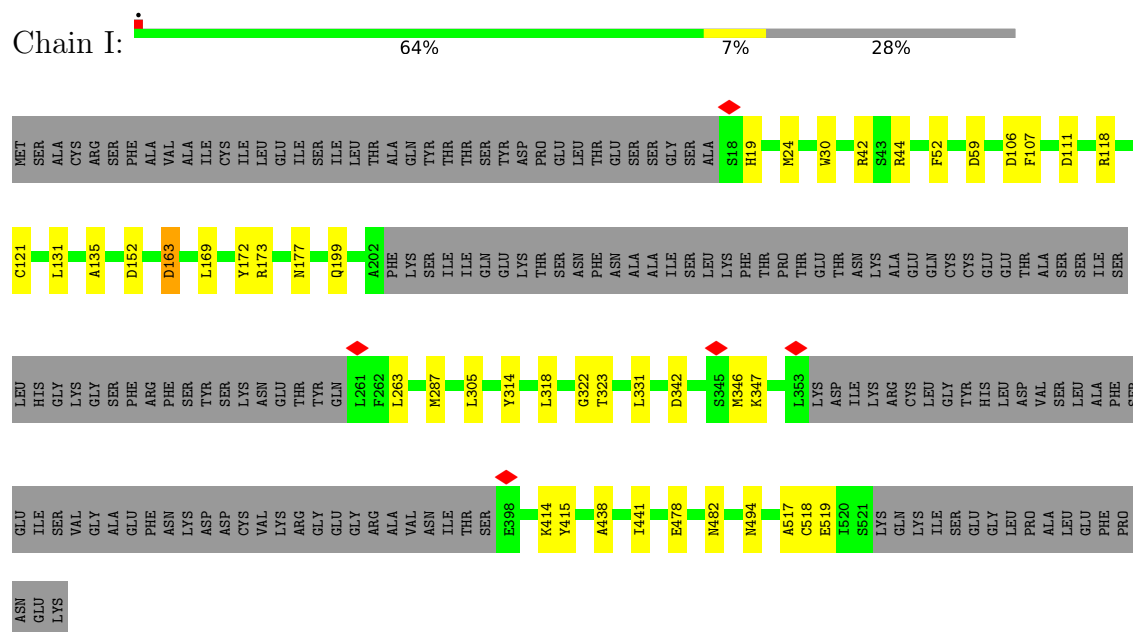
- Molecule 6: Complement component C9

Chain J: 64% 8% 29%

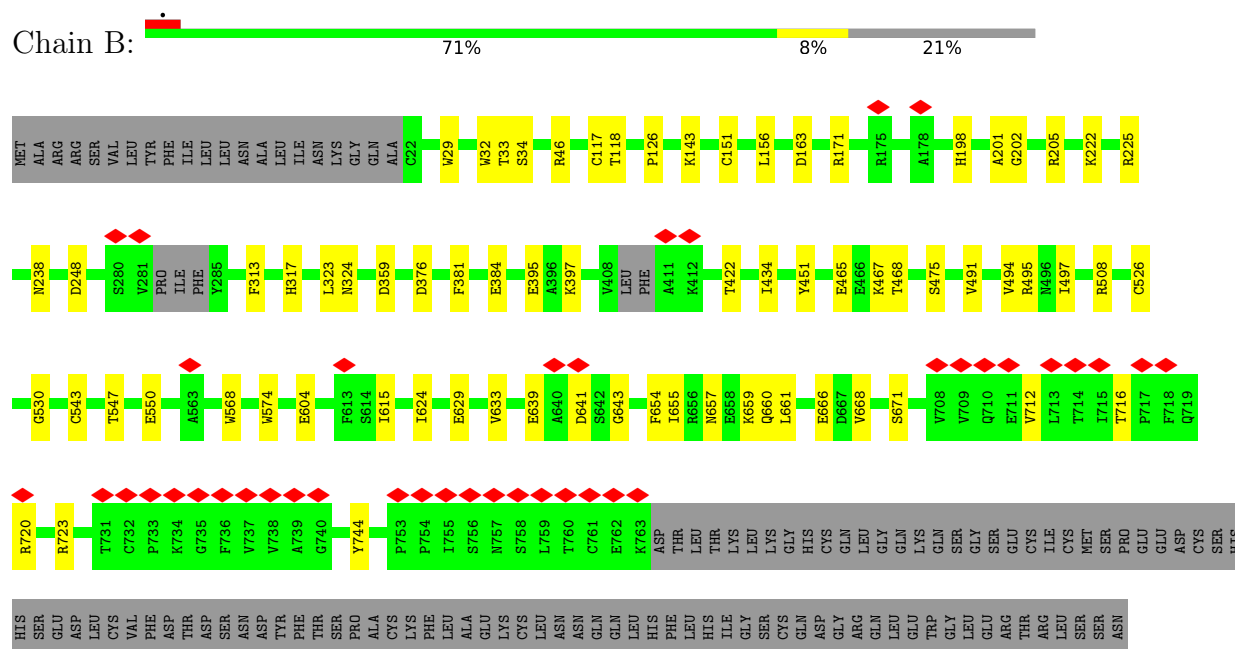


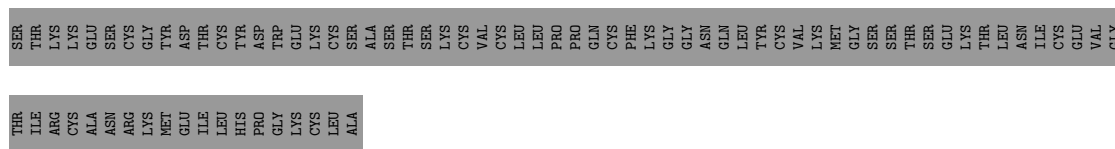


• Molecule 6: Complement component C9

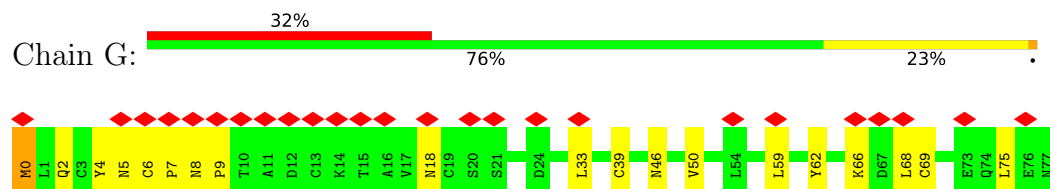


• Molecule 7: Complement component C6

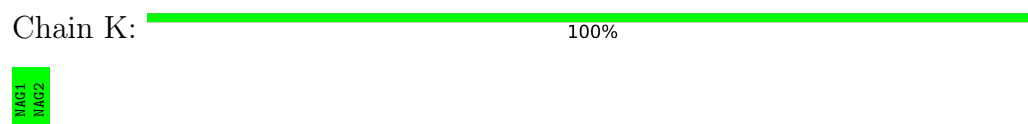




- Molecule 8: CD59 glycoprotein



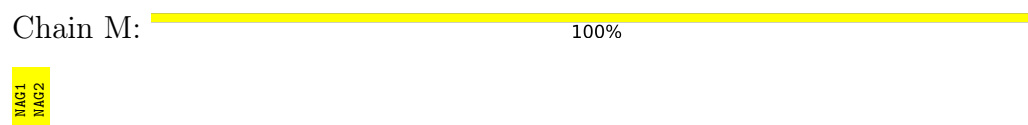
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47244	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0164	Depositor
Map size (Å)	448.74, 448.74, 448.74	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.29	2/10076 (0.0%)	0.52	0/13690
2	C	0.29	0/5160	0.54	0/6982
3	D	0.30	0/4232	0.58	0/5712
4	E	0.29	0/4135	0.59	2/5568 (0.0%)
5	F	0.28	0/1348	0.58	0/1829
6	H	0.27	0/3278	0.57	0/4422
6	I	0.26	0/3237	0.56	0/4368
6	J	0.25	0/3205	0.54	0/4322
7	B	0.26	0/5897	0.54	0/7962
8	G	0.30	0/641	0.68	3/867 (0.3%)
All	All	0.28	2/41209 (0.0%)	0.55	5/55722 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
4	E	0	1
6	J	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	671	GLU	CD-OE2	8.26	1.34	1.25
1	A	667	GLU	CD-OE2	8.19	1.34	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	7	PRO	CA-N-CD	-7.81	100.56	111.50
4	E	206	LEU	CB-CG-CD2	6.94	122.80	111.00
4	E	437	VAL	CG1-CB-CG2	6.88	121.91	110.90
8	G	6	CYS	C-N-CD	-5.57	108.35	120.60
8	G	0	MET	CG-SD-CE	5.36	108.78	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	466	ARG	Sidechain
4	E	156	ARG	Sidechain
6	J	133	ARG	Sidechain

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	9853	9834	9831	134	0
2	C	5035	4727	4724	39	0
3	D	4138	3958	3955	53	0
4	E	4052	3813	3813	45	0
5	F	1319	1284	1282	23	0
6	H	3217	3084	3081	32	0
6	I	3176	3027	3024	25	0
6	J	3146	2989	2985	25	0
7	B	5776	5491	5487	46	0
8	G	629	582	582	11	0
9	K	28	27	25	0	0
9	L	28	27	25	0	0
9	M	28	27	25	0	0
9	N	28	27	25	0	0
9	O	28	27	25	1	0
All	All	40481	38924	38889	409	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 (409) 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:A:1276:GLU:OE1	1:A:1278:GLN:NE2	1.69	1.23
3:D:394:LEU:HD21	4:E:414:ARG:NH1	1.56	1.17
3:D:394:LEU:CD2	4:E:414:ARG:HH12	1.65	1.09
3:D:394:LEU:CD2	4:E:414:ARG:NH1	2.16	1.08
3:D:394:LEU:HD21	4:E:414:ARG:HH12	0.99	1.06
7:B:317:HIS:ND1	7:B:376:ASP:OD1	2.08	0.86
6:J:323:THR:HG1	6:J:324:HIS:HD1	1.18	0.84
7:B:550:GLU:N	7:B:550:GLU:OE1	2.11	0.83
1:A:99:VAL:HG23	1:A:119:ILE:HD11	1.61	0.82
6:H:24:MET:HE3	6:H:59:ASP:HB2	1.63	0.80
1:A:992:LEU:HD21	1:A:1294:ILE:HD13	1.64	0.79
8:G:0:MET:O	8:G:2:GLN:NE2	2.16	0.79
6:I:494:ASN:ND2	6:I:518:CYS:O	2.17	0.77
1:A:937:GLU:N	1:A:937:GLU:OE1	2.19	0.76
1:A:1032:ASN:O	1:A:1035:HIS:NE2	2.17	0.76
4:E:506:ALA:O	4:E:539:ASN:ND2	2.20	0.75
1:A:92:LEU:HD22	1:A:99:VAL:HG21	1.72	0.72
6:H:494:ASN:ND2	6:H:518:CYS:O	2.22	0.72
7:B:659:LYS:NZ	7:B:666:GLU:OE2	2.21	0.72
6:J:323:THR:HG1	6:J:324:HIS:CE1	2.07	0.71
7:B:629:GLU:OE1	7:B:629:GLU:N	2.23	0.71
3:D:382:THR:HG22	4:E:266:VAL:HG21	1.72	0.70
5:F:25:GLN:N	5:F:25:GLN:OE1	2.25	0.70
1:A:1276:GLU:OE1	1:A:1278:GLN:CD	2.30	0.69
3:D:394:LEU:HD22	4:E:414:ARG:NH1	2.04	0.69
5:F:20:ALA:O	5:F:21:ASN:OD1	2.11	0.69
4:E:269:ALA:HB3	4:E:317:MET:HB2	1.74	0.69
1:A:992:LEU:HD21	1:A:1294:ILE:CD1	2.23	0.68
1:A:1066:TYR:HB3	1:A:1078:LEU:HD22	1.76	0.66
6:J:501:MET:SD	6:J:502:ASP:N	2.68	0.66
7:B:117:CYS:O	7:B:118:THR:HG22	1.96	0.65
6:J:501:MET:SD	6:J:502:ASP:OD1	2.53	0.65
1:A:1251:THR:HG21	1:A:1273:TRP:CZ3	2.32	0.65
5:F:30:THR:O	5:F:133:ARG:NH1	2.30	0.65
2:C:223:SER:N	2:C:225:PHE:O	2.30	0.64
3:D:501:SER:OG	3:D:507:ARG:NH1	2.31	0.64
7:B:465:GLU:O	7:B:468:THR:OG1	2.16	0.64
6:H:98:CYS:N	6:H:113:CYS:SG	2.70	0.63
1:A:1050:LYS:HA	1:A:1053:MET:SD	2.38	0.63
3:D:507:ARG:HE	3:D:509:THR:HG23	1.62	0.63
1:A:1310:SER:O	1:A:1354:SER:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:160:TYR:OH	4:E:165:GLU:OE1	2.14	0.61
1:A:291:MET:HA	1:A:291:MET:HE2	1.82	0.60
5:F:98:ASP:OD1	5:F:98:ASP:O	2.19	0.60
3:D:375:GLY:O	3:D:381:ILE:HD11	2.02	0.60
1:A:1276:GLU:CD	1:A:1278:GLN:NE2	2.52	0.60
1:A:1276:GLU:CD	1:A:1278:GLN:HE21	2.05	0.59
6:J:40:MET:N	6:J:65:ARG:O	2.35	0.59
1:A:1278:GLN:CD	7:B:624:ILE:HD13	2.22	0.59
2:C:509:TRP:CE3	2:C:517:LYS:HB3	2.37	0.59
1:A:241:LYS:HD3	1:A:241:LYS:N	2.17	0.59
4:E:538:GLN:OE1	4:E:539:ASN:ND2	2.35	0.58
7:B:397:LYS:NZ	7:B:422:THR:OG1	2.32	0.58
4:E:198:GLU:OE1	4:E:200:TYR:OH	2.19	0.57
2:C:312:GLU:OE2	2:C:378:ARG:NH1	2.35	0.57
6:H:348:ARG:NH2	6:H:397:SER:OG	2.37	0.57
1:A:520:ASP:OD1	1:A:520:ASP:O	2.23	0.57
4:E:502:GLN:OE1	4:E:503:THR:HG23	2.03	0.57
1:A:865:ILE:HD12	1:A:901:LEU:O	2.05	0.57
1:A:1011:GLU:O	1:A:1015:VAL:HG13	2.05	0.57
1:A:1053:MET:O	1:A:1056:ILE:HG22	2.05	0.57
4:E:434:ILE:O	4:E:437:VAL:HG12	2.04	0.56
7:B:171:ARG:HG3	7:B:171:ARG:HH11	1.70	0.56
1:A:865:ILE:HD11	1:A:900:VAL:HB	1.88	0.56
1:A:1276:GLU:HB3	1:A:1278:GLN:HG3	1.87	0.56
1:A:905:ILE:HG22	1:A:906:GLY:N	2.21	0.56
2:C:642:SER:OG	2:C:645:GLN:OE1	2.14	0.56
1:A:1278:GLN:NE2	7:B:624:ILE:HD13	2.21	0.55
1:A:386:VAL:N	1:A:411:THR:OG1	2.38	0.55
4:E:519:SER:O	4:E:526:GLN:NE2	2.34	0.55
2:C:480:TYR:HD2	2:C:492:VAL:HG21	1.72	0.55
3:D:141:TYR:CZ	3:D:143:ALA:HB2	2.41	0.55
6:I:163:ASP:OD2	6:I:163:ASP:N	2.38	0.55
1:A:1086:LEU:HD22	1:A:1095:GLN:HG3	1.87	0.54
3:D:99:ALA:O	3:D:100:ASN:ND2	2.40	0.54
1:A:917:TRP:O	1:A:917:TRP:CE3	2.59	0.54
5:F:178:ASP:O	5:F:178:ASP:OD2	2.26	0.54
6:H:102:ASN:ND2	6:H:104:CYS:O	2.40	0.54
1:A:832:SER:HB3	1:A:930:VAL:HG13	1.90	0.54
7:B:397:LYS:HZ2	7:B:422:THR:HG1	1.51	0.54
1:A:1078:LEU:C	1:A:1078:LEU:HD23	2.28	0.54
2:C:118:ARG:NH1	2:C:118:ARG:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:97:ARG:NH2	5:F:179:GLU:O	2.41	0.54
3:D:73:CYS:O	3:D:77:GLY:N	2.39	0.54
1:A:1278:GLN:HG2	7:B:624:ILE:CD1	2.38	0.54
1:A:918:PHE:CG	1:A:918:PHE:O	2.61	0.54
1:A:1303:LEU:O	1:A:1307:LEU:HD23	2.09	0.53
1:A:1009:GLU:OE1	1:A:1059:TYR:CE2	2.61	0.53
1:A:575:LEU:HD22	1:A:588:VAL:HG11	1.90	0.53
1:A:992:LEU:HD12	7:B:615:ILE:HG22	1.90	0.53
4:E:261:ARG:NH2	4:E:322:GLU:OE2	2.41	0.53
1:A:24:VAL:CG2	1:A:545:ILE:HD11	2.38	0.53
1:A:1313:ILE:HD12	1:A:1328:MET:HG3	1.90	0.53
3:D:176:ILE:HG13	3:D:176:ILE:O	2.09	0.53
3:D:104:ILE:HD12	3:D:104:ILE:N	2.23	0.53
2:C:250:LEU:O	2:C:251:LEU:HD22	2.09	0.52
4:E:474:ASN:ND2	4:E:498:CYS:O	2.36	0.52
1:A:1086:LEU:HA	1:A:1089:VAL:HG22	1.89	0.52
6:H:29:GLU:OE1	6:H:29:GLU:N	2.42	0.52
1:A:1256:LEU:O	1:A:1260:ASN:ND2	2.42	0.52
2:C:189:GLN:HG2	2:C:260:ALA:HB2	1.92	0.52
7:B:604:GLU:OE2	7:B:604:GLU:N	2.38	0.52
6:J:99:ASN:OD1	6:J:100:GLY:N	2.42	0.52
1:A:1066:TYR:HB3	1:A:1078:LEU:CD2	2.40	0.52
3:D:513:GLN:HA	3:D:513:GLN:OE1	2.10	0.52
1:A:835:ARG:NH1	1:A:903:LEU:O	2.40	0.52
6:I:106:ASP:OD1	6:I:107:PHE:N	2.43	0.52
1:A:1278:GLN:HG2	7:B:624:ILE:HD11	1.91	0.52
6:I:478:GLU:O	6:I:482:ASN:ND2	2.39	0.52
1:A:1077:TRP:CZ2	1:A:1131:GLY:HA2	2.45	0.51
4:E:241:GLN:OE1	4:E:241:GLN:N	2.43	0.51
1:A:117:MET:HE3	1:A:652:THR:HG21	1.92	0.51
4:E:271:PHE:CE2	4:E:315:GLY:HA3	2.45	0.51
4:E:139:ASP:O	4:E:181:ASN:ND2	2.42	0.51
1:A:1029:ASN:O	1:A:1033:ILE:HD12	2.11	0.51
1:A:1055:SER:O	1:A:1059:TYR:CD1	2.64	0.51
3:D:521:ASN:O	3:D:521:ASN:OD1	2.28	0.51
5:F:139:ASP:OD1	5:F:139:ASP:N	2.44	0.51
2:C:399:ASN:OD1	2:C:402:ARG:NE	2.43	0.51
5:F:49:ARG:HG3	5:F:49:ARG:O	2.11	0.50
5:F:149:VAL:HG11	5:F:159:ILE:HD11	1.93	0.50
2:C:517:LYS:N	2:C:543:THR:O	2.44	0.50
6:H:30:TRP:HB3	6:H:40:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:323:LEU:HD23	7:B:324:ASN:N	2.26	0.50
6:I:24:MET:SD	6:I:44:ARG:NE	2.84	0.50
1:A:1320:LYS:HD3	1:A:1342:LEU:HD13	1.92	0.50
1:A:1049:LEU:O	1:A:1053:MET:HG3	2.11	0.50
1:A:1053:MET:O	1:A:1057:MET:HG2	2.11	0.50
6:J:104:CYS:SG	6:J:108:SER:OG	2.70	0.50
1:A:19:GLN:OE1	1:A:19:GLN:HA	2.12	0.50
3:D:309:GLU:OE1	3:D:309:GLU:N	2.44	0.50
6:J:339:TYR:CZ	6:J:341:LEU:HD21	2.47	0.50
7:B:660:GLN:O	7:B:661:LEU:HD22	2.11	0.50
2:C:400:LYS:HD2	2:C:400:LYS:N	2.27	0.50
6:H:273:PHE:CZ	6:H:275:HIS:HB2	2.47	0.50
2:C:189:GLN:CG	2:C:260:ALA:HB2	2.41	0.49
1:A:1278:GLN:NE2	7:B:624:ILE:CD1	2.75	0.49
3:D:323:ALA:O	3:D:349:CYS:SG	2.70	0.49
1:A:302:ASP:OD1	1:A:302:ASP:N	2.45	0.49
2:C:257:VAL:HG22	2:C:417:ILE:HD11	1.93	0.49
5:F:135:LEU:HD23	5:F:136:PRO:N	2.28	0.49
1:A:867:THR:OG1	1:A:900:VAL:HG12	2.12	0.49
7:B:716:THR:O	7:B:716:THR:HG23	2.13	0.49
6:I:135:ALA:HB1	6:I:287:MET:HE1	1.94	0.49
6:I:263:LEU:HD12	6:I:263:LEU:O	2.13	0.49
2:C:235:TYR:OH	2:C:237:SER:HB2	2.13	0.49
3:D:71:PHE:HE2	3:D:96:SER:HG	1.58	0.49
3:D:507:ARG:HA	3:D:533:THR:HA	1.95	0.49
1:A:1216:ALA:HB2	1:A:1228:TRP:CZ2	2.48	0.48
3:D:20:THR:HG22	3:D:30:TYR:H	1.78	0.48
3:D:126:ASN:O	3:D:130:ASN:N	2.47	0.48
7:B:205:ARG:NH1	7:B:359:ASP:O	2.44	0.48
1:A:992:LEU:HD23	1:A:1024:TYR:CZ	2.48	0.48
4:E:327:ILE:HG23	4:E:387:GLU:HB2	1.95	0.48
6:J:28:SER:N	6:J:43:SER:O	2.46	0.48
1:A:264:ASP:N	1:A:330:ILE:O	2.39	0.48
4:E:493:SER:O	4:E:494:LEU:HD13	2.13	0.48
6:J:442:ASN:OD1	6:J:443:ASP:N	2.46	0.48
1:A:1013:MET:HE2	1:A:1130:GLN:N	2.29	0.48
2:C:324:LEU:HD21	2:C:326:GLN:HG2	1.96	0.48
7:B:494:VAL:HG23	7:B:494:VAL:O	2.13	0.48
1:A:282:MET:SD	1:A:282:MET:N	2.87	0.48
6:H:438:ALA:HA	6:H:441:ILE:HD12	1.96	0.48
1:A:986:GLU:OE1	1:A:986:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:VAL:HG21	1:A:1095:GLN:HG2	1.95	0.47
1:A:135:TYR:CZ	1:A:141:VAL:HG12	2.49	0.47
1:A:1050:LYS:O	1:A:1054:LEU:HD13	2.15	0.47
3:D:63:ARG:HB3	3:D:63:ARG:CZ	2.44	0.47
6:I:135:ALA:CB	6:I:287:MET:HE1	2.44	0.47
1:A:1077:TRP:CD1	1:A:1147:PHE:CD1	3.02	0.47
3:D:196:SER:OG	3:D:220:ARG:HB3	2.14	0.47
6:J:270:GLU:OE1	6:J:343:LYS:N	2.47	0.47
2:C:198:TYR:CD1	2:C:250:LEU:HD22	2.49	0.47
6:I:438:ALA:HA	6:I:441:ILE:HD12	1.96	0.47
1:A:642:ASN:OD1	1:A:643:ALA:N	2.47	0.47
1:A:861:ALA:HB1	1:A:865:ILE:CG2	2.44	0.47
4:E:171:ASP:N	4:E:171:ASP:OD2	2.46	0.47
5:F:40:CYS:HB3	5:F:43:LEU:HD23	1.95	0.47
2:C:324:LEU:C	2:C:324:LEU:HD23	2.35	0.47
3:D:466:ARG:NH1	3:D:468:ASP:OD1	2.44	0.47
6:H:414:LYS:HG3	6:H:415:TYR:H	1.79	0.47
6:J:99:ASN:ND2	6:J:103:ASP:H	2.13	0.47
3:D:518:PRO:N	3:D:519:PRO:CD	2.78	0.47
6:H:138:GLY:O	6:H:147:LEU:N	2.47	0.47
3:D:35:LEU:C	3:D:35:LEU:HD23	2.35	0.47
1:A:665:ASN:HB2	1:A:667:GLU:HG3	1.96	0.47
1:A:918:PHE:O	1:A:918:PHE:CD1	2.67	0.46
3:D:283:PHE:O	3:D:287:GLY:N	2.44	0.46
7:B:395:GLU:N	7:B:395:GLU:OE1	2.48	0.46
1:A:843:GLY:O	1:A:895:LEU:HD12	2.15	0.46
6:H:102:ASN:OD1	6:H:107:PHE:N	2.45	0.46
6:H:319:GLU:OE2	6:H:319:GLU:HA	2.14	0.46
3:D:365:MET:HB3	4:E:199:PHE:HB3	1.97	0.46
7:B:491:VAL:HG21	7:B:508:ARG:HG3	1.96	0.46
7:B:639:GLU:OE2	7:B:643:GLY:N	2.49	0.46
1:A:20:GLU:OE1	1:A:20:GLU:N	2.48	0.46
1:A:329:VAL:C	1:A:330:ILE:HD12	2.35	0.46
1:A:1014:SER:O	1:A:1018:VAL:HG23	2.14	0.46
6:I:331:LEU:N	6:I:331:LEU:HD12	2.31	0.46
8:G:66:LYS:HB2	8:G:69:CYS:HB3	1.96	0.46
1:A:1216:ALA:HB1	1:A:1226:ARG:HG3	1.97	0.46
1:A:1287:THR:O	1:A:1291:ILE:HD12	2.15	0.46
2:C:30:TRP:CE2	2:C:63:CYS:HB3	2.50	0.46
8:G:18:ASN:OD1	8:G:18:ASN:O	2.33	0.46
2:C:258:GLU:OE1	2:C:310:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:126:VAL:HG11	6:H:173:ARG:HB2	1.98	0.46
1:A:997:ILE:HG12	1:A:1040:ILE:HD11	1.98	0.46
6:I:346:MET:HE1	6:I:347:LYS:O	2.15	0.46
2:C:28:CYS:HB3	2:C:63:CYS:N	2.30	0.46
2:C:190:VAL:HA	2:C:257:VAL:O	2.16	0.46
2:C:407:ALA:O	2:C:410:VAL:HG22	2.16	0.46
3:D:378:SER:O	3:D:382:THR:HG23	2.15	0.46
3:D:380:HIS:HA	3:D:383:THR:HG22	1.97	0.46
1:A:1179:THR:O	1:A:1179:THR:HG22	2.17	0.46
3:D:220:ARG:HD2	3:D:322:HIS:O	2.15	0.46
1:A:264:ASP:OD1	1:A:291:MET:HE1	2.17	0.45
1:A:494:ASP:N	1:A:494:ASP:OD1	2.49	0.45
6:H:129:SER:HB2	6:H:172:TYR:CG	2.52	0.45
8:G:33:LEU:HD23	8:G:33:LEU:H	1.81	0.45
3:D:309:GLU:HB2	3:D:364:THR:HG22	1.98	0.45
8:G:62:TYR:HB2	8:G:75:LEU:HD21	1.98	0.45
4:E:216:ASP:O	4:E:241:GLN:OE1	2.34	0.45
4:E:318:GLY:HA3	4:E:427:ILE:HG13	1.97	0.45
7:B:467:LYS:CG	7:B:468:THR:N	2.79	0.45
7:B:654:PHE:N	7:B:671:SER:O	2.45	0.45
3:D:517:PRO:N	3:D:518:PRO:CD	2.79	0.45
7:B:143:LYS:HB2	7:B:151:CYS:HB3	1.98	0.45
1:A:126:LEU:HD21	1:A:205:TYR:CE2	2.52	0.45
7:B:655:ILE:HG22	7:B:657:ASN:H	1.80	0.45
6:J:442:ASN:OD1	6:J:442:ASN:C	2.55	0.45
3:D:47:ASN:OD1	3:D:49:SER:OG	2.34	0.45
3:D:104:ILE:HD12	3:D:104:ILE:H	1.82	0.45
6:H:30:TRP:CE3	6:H:42:ARG:HG3	2.52	0.45
6:H:52:PHE:N	6:H:52:PHE:CD2	2.83	0.45
6:J:109:ASP:OD1	6:J:109:ASP:N	2.49	0.45
1:A:518:PHE:N	1:A:522:SER:O	2.50	0.45
6:H:394:ASN:C	6:H:395:ILE:HD12	2.37	0.45
1:A:1216:ALA:HB1	1:A:1226:ARG:CG	2.47	0.45
1:A:1019:PHE:O	1:A:1022:PHE:HB3	2.17	0.44
5:F:80:ARG:NH1	5:F:176:VAL:HG21	2.32	0.44
1:A:381:GLN:NE2	1:A:382:LEU:O	2.50	0.44
1:A:978:SER:N	1:A:1360:HIS:O	2.46	0.44
1:A:992:LEU:HD23	1:A:1024:TYR:CE2	2.52	0.44
1:A:1034:PHE:CE2	1:A:1037:ASP:HB2	2.52	0.44
3:D:247:VAL:HG22	3:D:297:GLY:HA2	2.00	0.44
7:B:712:VAL:O	7:B:712:VAL:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:GLY:N	1:A:896:VAL:O	2.47	0.44
2:C:646:LYS:N	2:C:649:TYR:OH	2.51	0.44
7:B:384:GLU:O	7:B:434:ILE:HA	2.18	0.44
3:D:475:SER:OG	3:D:480:CYS:HB3	2.18	0.44
1:A:1284:PHE:O	1:A:1284:PHE:CD2	2.71	0.44
4:E:138:TYR:OH	4:E:313:THR:HG22	2.17	0.44
4:E:504:GLU:OE1	4:E:504:GLU:N	2.49	0.44
6:J:280:ILE:O	6:J:280:ILE:HG22	2.18	0.44
1:A:347:TYR:O	1:A:348:VAL:CG1	2.65	0.44
1:A:1227:PHE:HZ	7:B:629:GLU:HG3	1.82	0.44
2:C:524:ASN:C	2:C:524:ASN:OD1	2.55	0.44
5:F:123:ALA:O	5:F:125:GLN:NE2	2.47	0.44
7:B:238:ASN:HB3	9:O:1:NAG:H81	2.00	0.44
7:B:641:ASP:N	7:B:641:ASP:OD1	2.50	0.44
6:I:121:CYS:SG	6:I:173:ARG:HD3	2.58	0.44
8:G:8:ASN:HB3	8:G:9:PRO:HD2	1.98	0.44
2:C:284:PRO:HG3	2:C:288:ASP:HB3	1.98	0.44
1:A:141:VAL:HG23	1:A:141:VAL:O	2.18	0.44
1:A:905:ILE:CG2	1:A:906:GLY:N	2.81	0.44
6:H:30:TRP:CE2	6:H:42:ARG:HD3	2.53	0.44
7:B:655:ILE:HG23	7:B:668:VAL:CG2	2.48	0.44
6:I:517:ALA:N	6:I:519:GLU:OE2	2.48	0.44
6:H:396:THR:N	6:I:199:GLN:O	2.48	0.43
6:I:163:ASP:OD2	6:I:172:TYR:CZ	2.71	0.43
1:A:330:ILE:HD12	1:A:330:ILE:N	2.33	0.43
1:A:1289:ASP:OD1	1:A:1290:THR:N	2.50	0.43
3:D:506:ARG:O	3:D:534:LEU:N	2.44	0.43
7:B:198:HIS:O	7:B:202:GLY:N	2.44	0.43
3:D:292:THR:HG21	3:D:414:GLU:HG3	2.00	0.43
6:H:99:ASN:OD1	6:H:118:ARG:NH1	2.51	0.43
1:A:837:GLU:OE1	1:A:837:GLU:HA	2.19	0.43
2:C:356:LEU:C	2:C:356:LEU:HD23	2.38	0.43
6:H:429:ILE:HD12	6:H:429:ILE:H	1.84	0.43
6:J:85:GLN:HA	6:J:85:GLN:OE1	2.18	0.43
1:A:117:MET:SD	1:A:652:THR:HG21	2.59	0.43
2:C:547:ASP:OD1	2:C:548:GLU:N	2.52	0.43
4:E:157:GLU:OE1	4:E:159:ARG:NE	2.43	0.43
1:A:569:ASN:OD1	1:A:807:THR:OG1	2.36	0.43
1:A:548:GLY:O	3:D:69:GLU:OE1	2.37	0.43
2:C:425:TYR:HA	2:C:441:LEU:HD23	1.99	0.43
6:J:318:LEU:O	6:J:322:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:349:LYS:HA	6:J:349:LYS:HE2	2.01	0.43
1:A:165:ASP:OD1	1:A:167:GLU:N	2.51	0.43
4:E:295:TYR:CE1	4:E:455:ARG:HD2	2.54	0.43
1:A:135:TYR:CE1	1:A:141:VAL:HG12	2.54	0.43
7:B:495:ARG:O	7:B:497:ILE:HG23	2.19	0.43
7:B:526:CYS:HB2	7:B:530:GLY:O	2.18	0.43
6:I:414:LYS:HG3	6:I:415:TYR:H	1.83	0.43
1:A:241:LYS:NZ	1:A:441:ASP:HB2	2.34	0.42
1:A:1065:SER:OG	1:A:1074:ALA:HB1	2.19	0.42
2:C:340:SER:O	2:C:350:SER:N	2.50	0.42
6:H:348:ARG:NH1	6:H:395:ILE:HG21	2.34	0.42
1:A:396:ASP:O	1:A:429:THR:OG1	2.28	0.42
5:F:118:LEU:HD13	5:F:131:TYR:HD2	1.84	0.42
7:B:32:TRP:CE2	7:B:46:ARG:HD3	2.54	0.42
6:I:305:LEU:HD21	6:I:314:TYR:CE2	2.54	0.42
6:I:318:LEU:O	6:I:322:GLY:N	2.52	0.42
3:D:94:ASP:OD1	3:D:95:GLN:N	2.52	0.42
4:E:31:ARG:NH2	4:E:47:ASP:O	2.43	0.42
8:G:50:VAL:HG21	8:G:59:LEU:HD11	2.01	0.42
1:A:518:PHE:CD2	1:A:522:SER:O	2.72	0.42
1:A:1365:VAL:HG22	1:A:1366:HIS:N	2.34	0.42
3:D:30:TYR:CE2	3:D:271:PRO:HB3	2.54	0.42
3:D:381:ILE:CG2	4:E:191:ALA:HB2	2.48	0.42
1:A:535:VAL:N	1:A:536:PRO:CD	2.82	0.42
1:A:1060:ARG:HG3	1:A:1066:TYR:CE1	2.54	0.42
1:A:1078:LEU:HD23	1:A:1078:LEU:O	2.19	0.42
2:C:125:ARG:HB3	2:C:125:ARG:CZ	2.49	0.42
4:E:390:ILE:O	4:E:390:ILE:HG13	2.18	0.42
3:D:404:TYR:CD2	4:E:156:ARG:HD2	2.55	0.42
4:E:103:VAL:O	4:E:106:ILE:HG23	2.20	0.42
6:H:118:ARG:O	6:H:118:ARG:HG2	2.20	0.42
6:J:272:MET:HG3	6:J:346:MET:SD	2.59	0.42
6:I:152:ASP:O	6:I:177:ASN:ND2	2.53	0.42
1:A:1012:LEU:HA	1:A:1015:VAL:HG22	2.01	0.42
1:A:537:SER:HB2	1:A:560:TRP:CZ2	2.55	0.42
2:C:57:GLN:HE22	2:C:458:ARG:N	2.17	0.42
4:E:127:ASN:O	4:E:131:GLN:N	2.48	0.42
4:E:346:PHE:O	4:E:368:HIS:NE2	2.53	0.42
5:F:178:ASP:O	5:F:178:ASP:CG	2.58	0.42
3:D:461:VAL:HG21	3:D:470:ILE:CD1	2.50	0.42
7:B:33:THR:HG22	7:B:34:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ASP:OD1	1:A:661:ASP:N	2.53	0.42
3:D:95:GLN:O	3:D:99:ALA:N	2.47	0.42
6:H:511:PHE:CB	6:H:513:PHE:CE2	3.03	0.42
8:G:4:TYR:N	8:G:68:LEU:HD13	2.35	0.42
1:A:165:ASP:OD1	1:A:165:ASP:C	2.59	0.41
1:A:208:ASP:OD1	1:A:209:PHE:CD2	2.73	0.41
1:A:979:VAL:HA	1:A:1359:VAL:HA	2.02	0.41
2:C:323:LYS:HE2	2:C:325:LYS:HD2	2.02	0.41
4:E:134:ALA:HB1	4:E:306:ASP:O	2.20	0.41
5:F:23:ASP:OD1	5:F:25:GLN:OE1	2.39	0.41
5:F:43:LEU:HB3	5:F:160:PHE:CE2	2.54	0.41
5:F:78:GLN:NE2	5:F:80:ARG:HH12	2.18	0.41
6:J:24:MET:SD	6:J:59:ASP:HB3	2.59	0.41
6:J:197:GLU:C	6:J:198:GLU:OE2	2.58	0.41
1:A:164:ILE:HD13	1:A:170:GLU:HA	2.02	0.41
1:A:339:GLU:N	1:A:339:GLU:OE2	2.53	0.41
1:A:1133:LEU:HG	1:A:1133:LEU:O	2.19	0.41
4:E:515:TRP:CH2	4:E:550:GLN:HB2	2.55	0.41
7:B:156:LEU:HB3	7:B:163:ASP:OD2	2.20	0.41
6:I:131:LEU:H	6:I:131:LEU:HD12	1.85	0.41
6:I:163:ASP:OD2	6:I:172:TYR:CE1	2.73	0.41
2:C:338:LYS:N	2:C:352:GLY:O	2.42	0.41
1:A:56:ILE:CG2	1:A:102:VAL:HG11	2.51	0.41
1:A:1019:PHE:CD1	1:A:1019:PHE:N	2.85	0.41
3:D:329:PHE:CD1	3:D:329:PHE:N	2.88	0.41
6:H:172:TYR:CD2	6:H:172:TYR:C	2.94	0.41
7:B:198:HIS:HB3	7:B:201:ALA:HB3	2.02	0.41
1:A:84:ILE:N	1:A:84:ILE:HD12	2.36	0.41
1:A:811:VAL:HG13	1:A:811:VAL:O	2.20	0.41
1:A:937:GLU:HA	1:A:1363:THR:O	2.20	0.41
5:F:149:VAL:O	5:F:152:ALA:HB3	2.20	0.41
6:J:122:ARG:NH1	6:I:111:ASP:OD1	2.53	0.41
8:G:5:ASN:OD1	8:G:39:CYS:N	2.45	0.41
3:D:249:HIS:NE2	3:D:293:GLU:OE2	2.50	0.41
6:H:265:TYR:CB	6:H:348:ARG:HG3	2.50	0.41
6:H:402:ASP:OD1	6:H:402:ASP:C	2.59	0.41
1:A:532:GLN:OE1	1:A:535:VAL:HG11	2.21	0.41
1:A:937:GLU:HB3	1:A:1364:VAL:HG22	2.01	0.41
3:D:247:VAL:HG22	3:D:296:LEU:O	2.21	0.41
6:J:165:ASP:O	6:J:169:LEU:N	2.53	0.41
1:A:347:TYR:O	1:A:348:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:SER:HB3	1:A:930:VAL:CG1	2.51	0.41
1:A:1024:TYR:CZ	1:A:1030:HIS:CE1	3.09	0.41
1:A:1041:GLU:HG3	1:A:1044:LYS:H	1.86	0.41
4:E:161:ASP:HB3	4:E:166:ARG:HG2	2.03	0.41
4:E:288:LEU:HD12	4:E:291:LEU:HD12	2.02	0.41
4:E:399:GLY:HA2	6:H:438:ALA:HB3	2.02	0.41
5:F:158:GLN:O	5:F:160:PHE:CE2	2.74	0.41
7:B:543:CYS:HB3	7:B:547:THR:OG1	2.21	0.41
1:A:1024:TYR:CZ	1:A:1030:HIS:NE2	2.89	0.41
1:A:1026:GLU:HA	1:A:1031:TRP:HZ3	1.86	0.41
2:C:329:PHE:CD1	2:C:329:PHE:C	2.95	0.41
2:C:503:TRP:CE2	2:C:535:CYS:HB2	2.57	0.41
5:F:46:GLN:CD	5:F:46:GLN:O	2.59	0.41
7:B:633:VAL:HG23	7:B:633:VAL:O	2.21	0.41
8:G:46:ASN:O	8:G:50:VAL:HG22	2.21	0.41
2:C:228:SER:O	2:C:339:SER:N	2.45	0.40
2:C:254:GLU:HG2	2:C:403:TYR:OH	2.21	0.40
2:C:552:HIS:NE2	7:B:126:PRO:O	2.42	0.40
4:E:372:PHE:CZ	8:G:62:TYR:CD1	3.10	0.40
5:F:155:THR:N	5:F:158:GLN:OE1	2.54	0.40
6:I:30:TRP:CE3	6:I:42:ARG:HG3	2.56	0.40
6:I:169:LEU:N	6:I:169:LEU:HD22	2.35	0.40
1:A:537:SER:HG	1:A:560:TRP:HH2	1.65	0.40
1:A:1000:LEU:HD13	1:A:1040:ILE:HD12	2.02	0.40
2:C:354:LYS:HE3	3:D:194:MET:SD	2.61	0.40
4:E:7:VAL:HG22	4:E:38:LYS:HB2	2.03	0.40
6:H:30:TRP:CE3	6:H:40:MET:HG3	2.56	0.40
7:B:222:LYS:O	7:B:225:ARG:NH2	2.54	0.40
6:J:349:LYS:HD2	6:J:400:LEU:HD12	2.03	0.40
5:F:30:THR:HA	5:F:55:LEU:O	2.21	0.40
6:H:100:GLY:N	6:H:110:GLU:OE1	2.46	0.40
6:J:147:LEU:HD23	6:J:321:TYR:HE1	1.86	0.40
1:A:492:TYR:HB2	1:A:546:VAL:HG21	2.03	0.40
3:D:382:THR:HG22	4:E:266:VAL:CG2	2.45	0.40
6:I:24:MET:HE3	6:I:59:ASP:HB2	2.03	0.40
1:A:236:ASN:HB2	1:A:379:LEU:HD23	2.03	0.40
3:D:517:PRO:O	3:D:522:GLY:HA3	2.22	0.40
4:E:518:TRP:CE3	4:E:528:ARG:HB2	2.57	0.40
6:H:265:TYR:HB2	6:H:348:ARG:HG3	2.03	0.40
7:B:451:TYR:CD2	7:B:475:SER:OG	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1239/1676 (74%)	1159 (94%)	80 (6%)	0	100	100
2	C	640/843 (76%)	617 (96%)	23 (4%)	0	100	100
3	D	512/591 (87%)	490 (96%)	22 (4%)	0	100	100
4	E	507/584 (87%)	481 (95%)	26 (5%)	0	100	100
5	F	166/202 (82%)	157 (95%)	9 (5%)	0	100	100
6	H	401/559 (72%)	385 (96%)	16 (4%)	0	100	100
6	I	396/559 (71%)	378 (96%)	18 (4%)	0	100	100
6	J	391/559 (70%)	368 (94%)	23 (6%)	0	100	100
7	B	731/934 (78%)	692 (95%)	39 (5%)	0	100	100
8	G	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
All	All	5059/6585 (77%)	4795 (95%)	264 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1102/1484 (74%)	1091 (99%)	11 (1%)	73	84
2	C	562/733 (77%)	559 (100%)	3 (0%)	86	91
3	D	458/517 (89%)	453 (99%)	5 (1%)	70	82
4	E	438/493 (89%)	435 (99%)	3 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	136/163 (83%)	135 (99%)	1 (1%)	81	88
6	H	356/494 (72%)	351 (99%)	5 (1%)	62	78
6	I	350/494 (71%)	344 (98%)	6 (2%)	56	74
6	J	346/494 (70%)	341 (99%)	5 (1%)	62	78
7	B	646/827 (78%)	637 (99%)	9 (1%)	62	78
8	G	73/73 (100%)	73 (100%)	0	100	100
All	All	4467/5772 (77%)	4419 (99%)	48 (1%)	69	82

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	169	SER
1	A	291	MET
1	A	317	ASP
1	A	381	GLN
1	A	468	ASP
1	A	621	GLU
1	A	827	MET
1	A	1022	PHE
1	A	1133	LEU
1	A	1238	SER
2	C	207	TYR
2	C	220	ARG
2	C	248	TYR
3	D	62	CYS
3	D	146	CYS
3	D	223	HIS
3	D	328	ASP
3	D	329	PHE
4	E	166	ARG
4	E	345	CYS
4	E	499	GLU
5	F	178	ASP
6	H	23	ARG
6	H	104	CYS
6	H	118	ARG
6	H	273	PHE
6	H	348	ARG
7	B	29	TRP

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Mol	Chain	Res	Type
7	B	248	ASP
7	B	313	PHE
7	B	381	PHE
7	B	568	TRP
7	B	574	TRP
7	B	720	ARG
7	B	723	ARG
7	B	744	TYR
6	J	95	ARG
6	J	195	HIS
6	J	289	ASN
6	J	348	ARG
6	J	414	LYS
6	I	19	HIS
6	I	52	PHE
6	I	118	ARG
6	I	163	ASP
6	I	323	THR
6	I	342	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	HIS
1	A	1278	GLN
2	C	472	HIS
3	D	100	ASN
7	B	263	HIS

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 ⓘ

10 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	$\# Z > 2$
9	NAG	K	1	1,9	14,14,15	0.24	0	17,19,21	0.59	0
9	NAG	K	2	9	14,14,15	0.24	0	17,19,21	0.57	0
9	NAG	L	1	9,3	14,14,15	0.20	0	17,19,21	0.62	1 (5%)
9	NAG	L	2	9	14,14,15	0.46	0	17,19,21	0.51	0
9	NAG	M	1	9,4	14,14,15	0.40	0	17,19,21	0.69	1 (5%)
9	NAG	M	2	9	14,14,15	0.67	1 (7%)	17,19,21	0.49	0
9	NAG	N	1	6,9	14,14,15	0.43	0	17,19,21	0.54	0
9	NAG	N	2	9	14,14,15	0.46	0	17,19,21	1.54	1 (5%)
9	NAG	O	1	7,9	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
9	NAG	O	2	9	14,14,15	0.31	0	17,19,21	0.60	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
9	NAG	K	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	NAG	L	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	L	2	9	-	0/6/23/26	0/1/1/1
9	NAG	M	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	NAG	N	1	6,9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	1/1/7/7	0/6/23/26	0/1/1/1
9	NAG	O	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	O	2	9	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	2	NAG	O5-C1	-2.15	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	2	NAG	C1-C2-N2	5.88	120.53	110.49
9	M	1	NAG	C1-O5-C5	2.32	115.33	112.19
9	L	1	NAG	C1-O5-C5	2.23	115.22	112.19
9	O	1	NAG	O4-C4-C5	2.16	114.67	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	N	2	NAG	C2

All (10) torsion outliers are listed below:

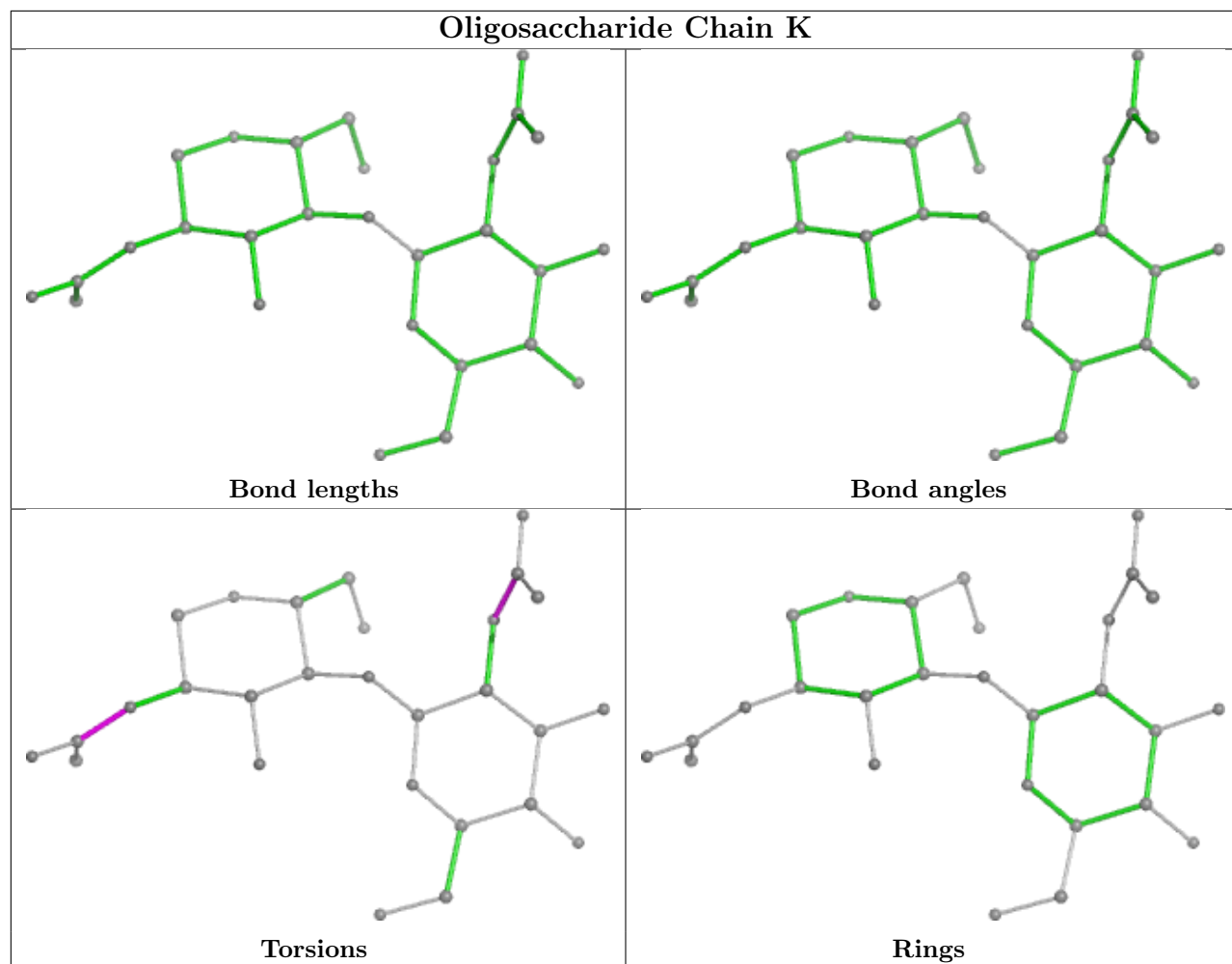
Mol	Chain	Res	Type	Atoms
9	K	1	NAG	C8-C7-N2-C2
9	K	1	NAG	O7-C7-N2-C2
9	K	2	NAG	C8-C7-N2-C2
9	K	2	NAG	O7-C7-N2-C2
9	N	1	NAG	O5-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
9	O	1	NAG	C3-C2-N2-C7
9	O	2	NAG	C3-C2-N2-C7

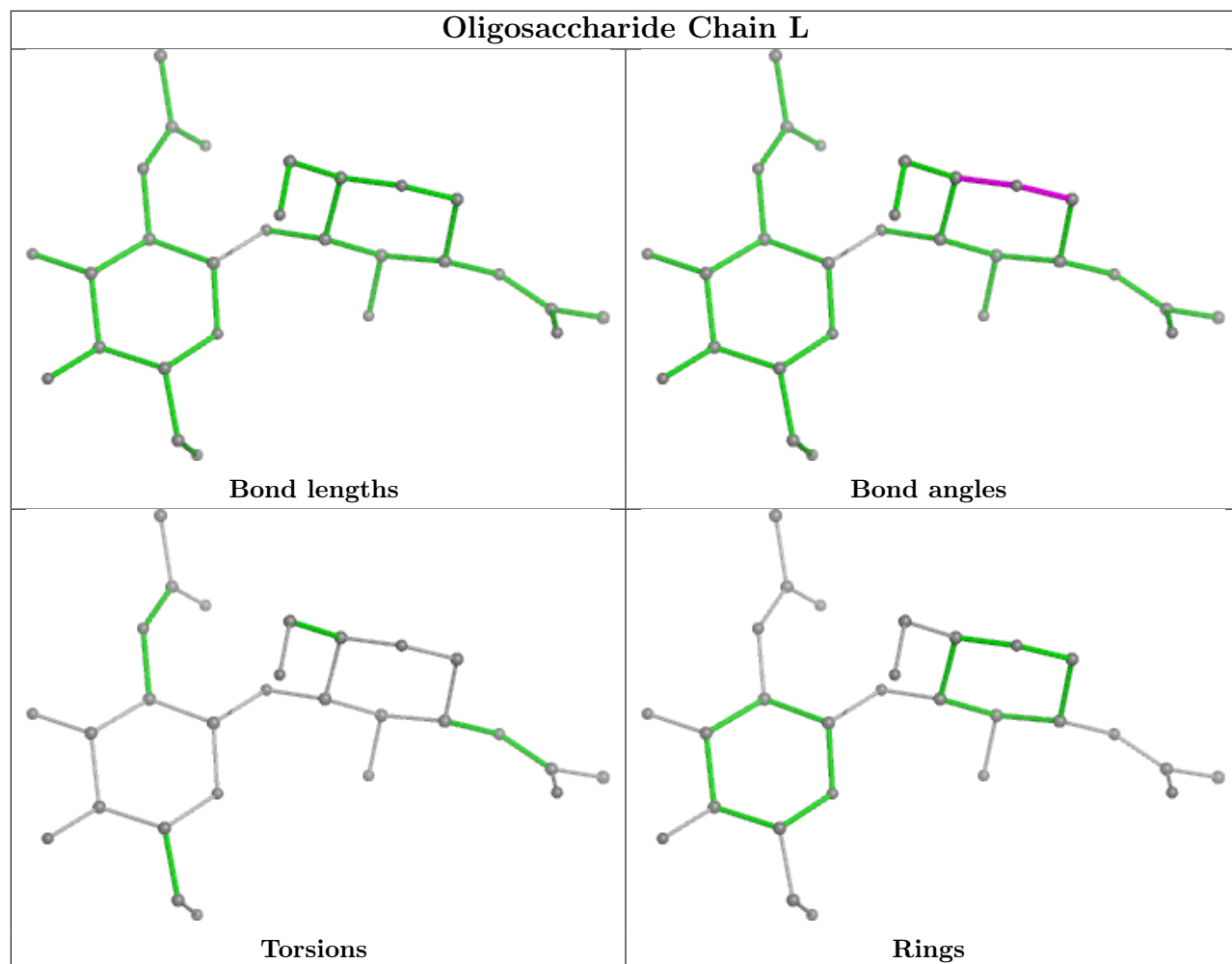
There are no ring outliers.

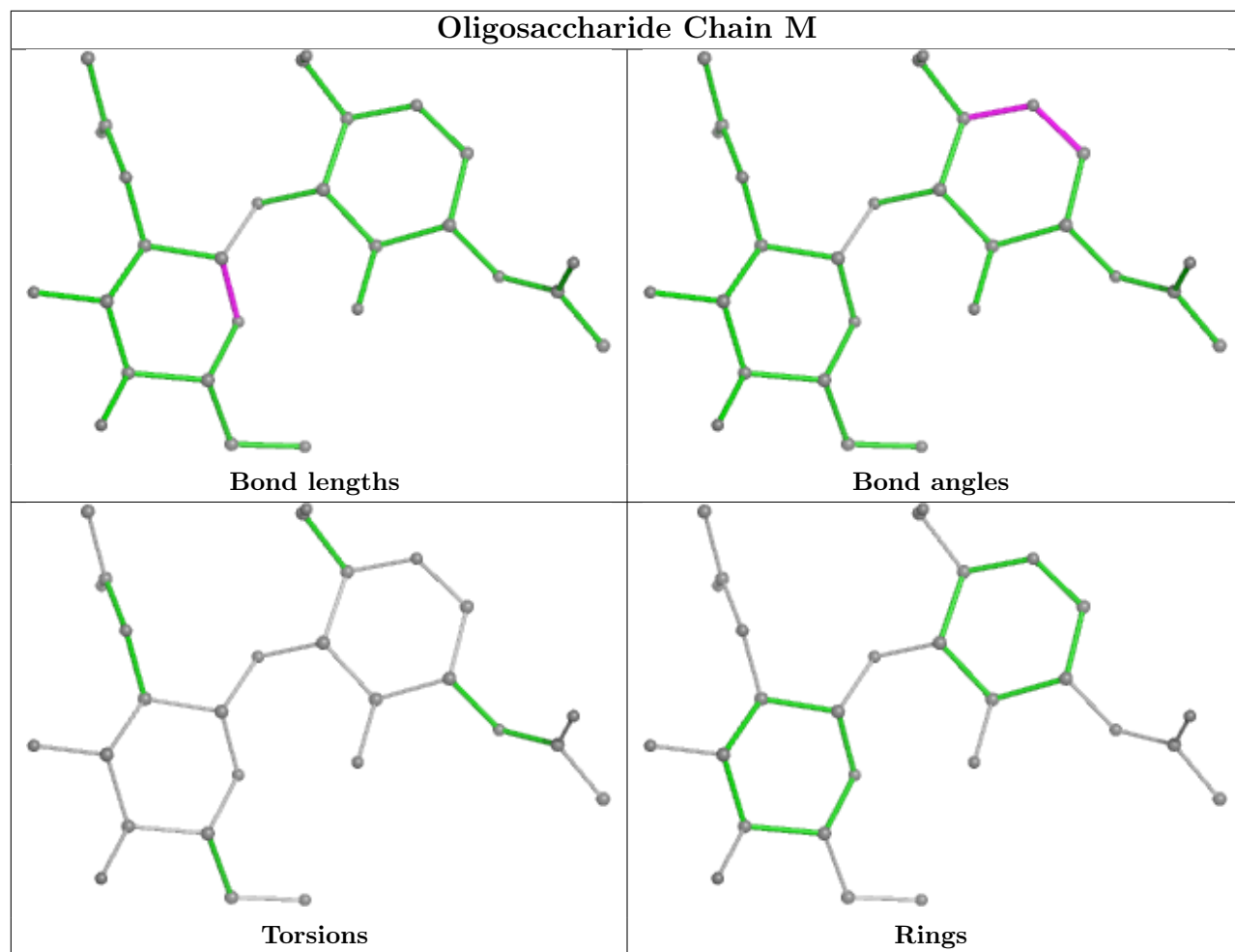
1 monomer is involved in 1 short contact:

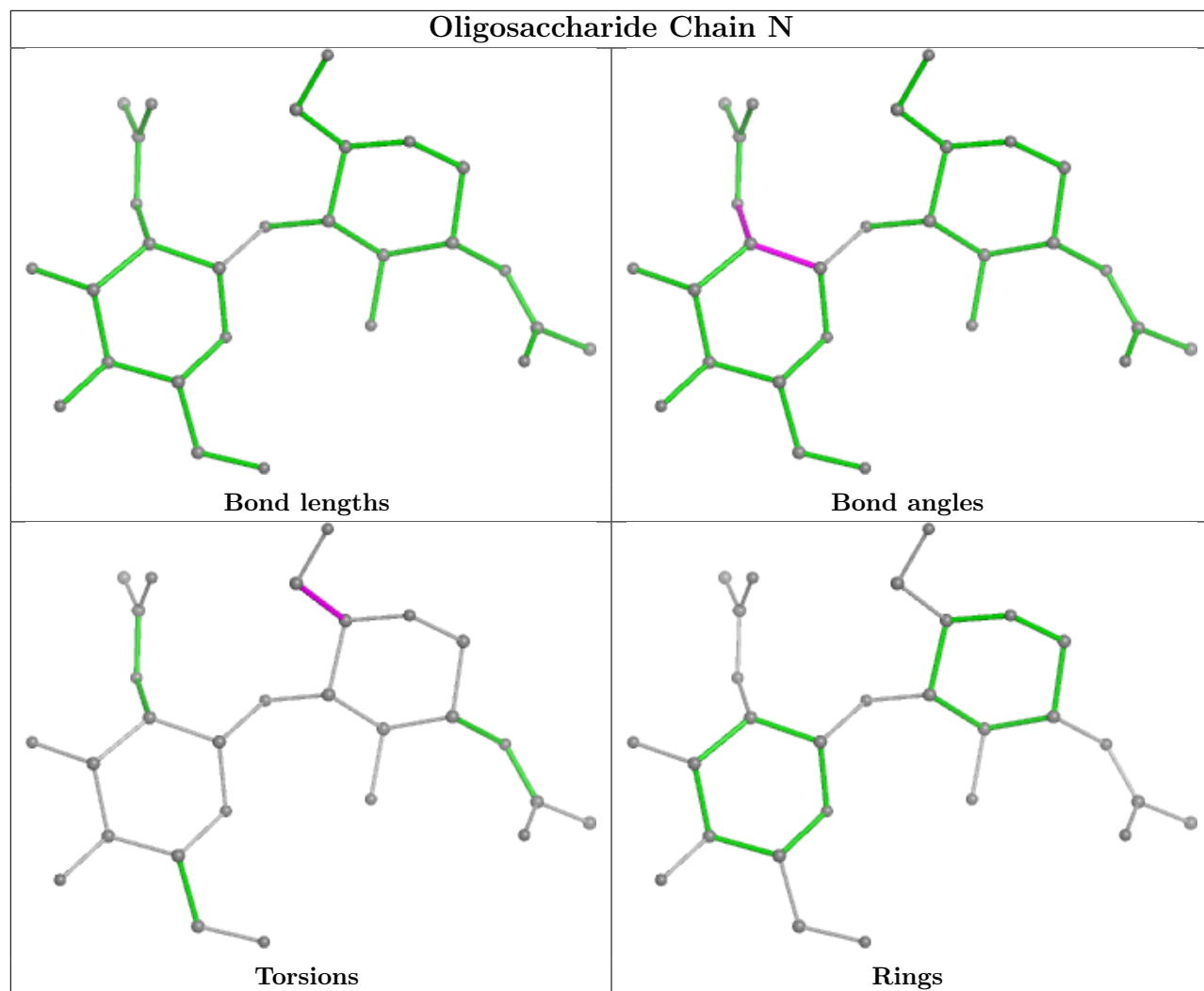
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	O	1	NAG	1	0

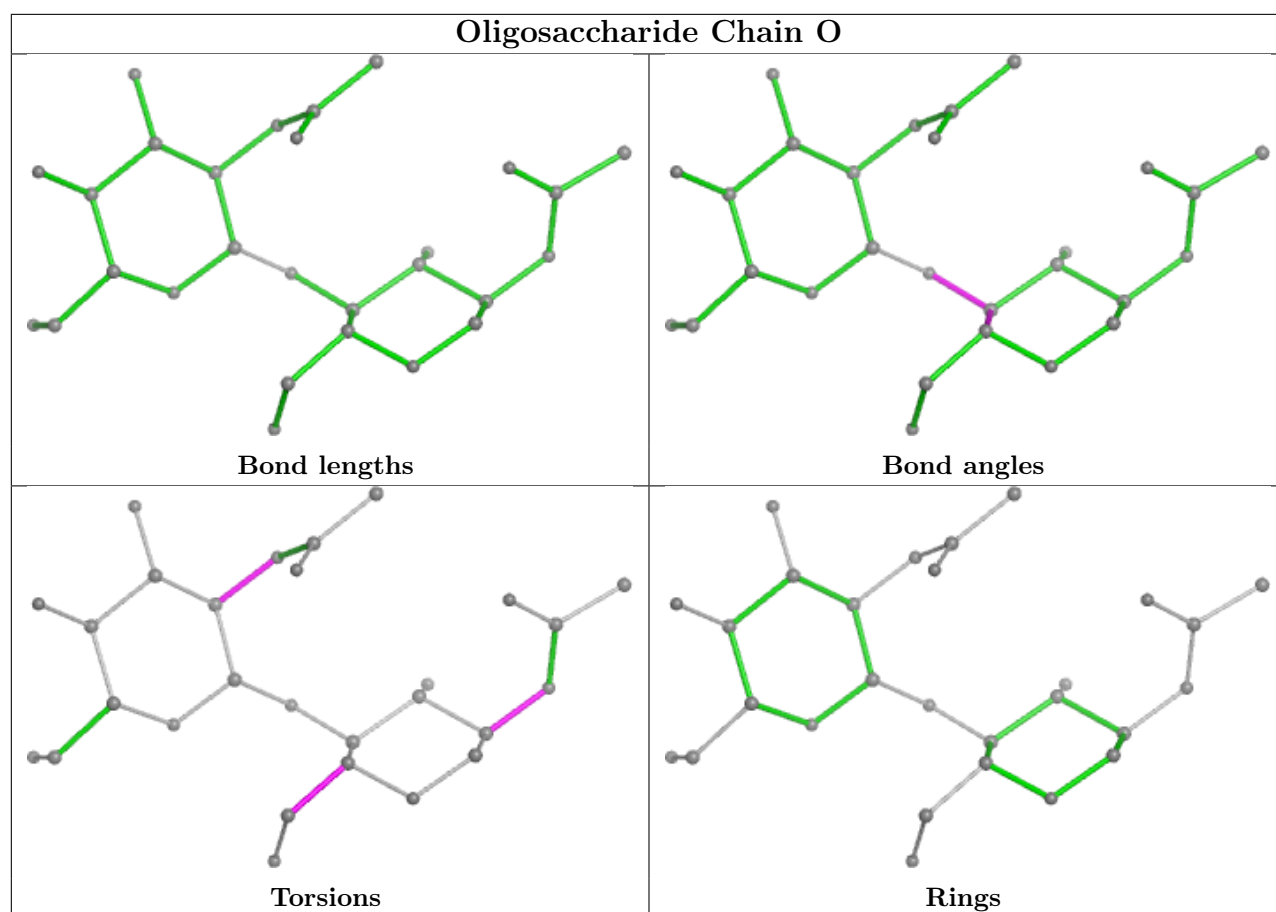
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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.

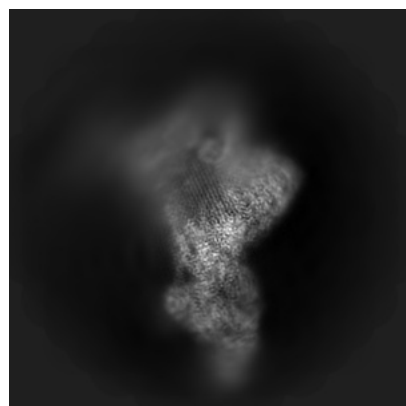
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15780. These allow visual inspection of the internal detail of the map and identification of artifacts.

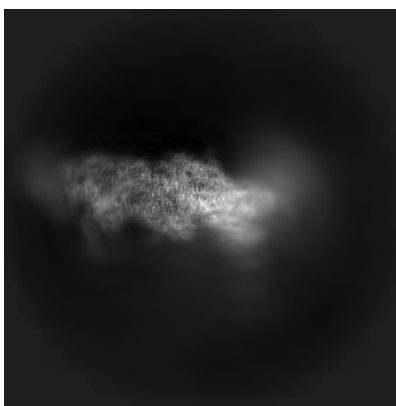
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

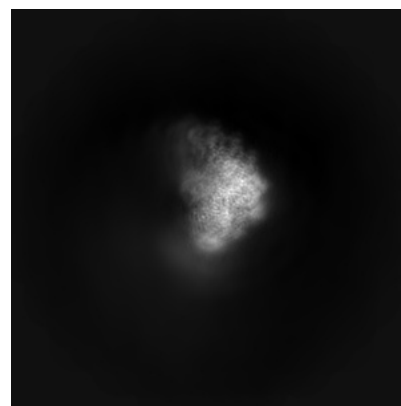
6.1.1 Primary map



X

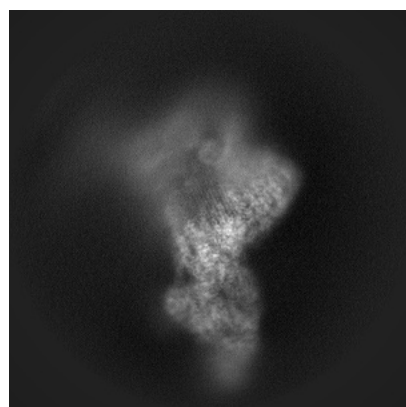


Y

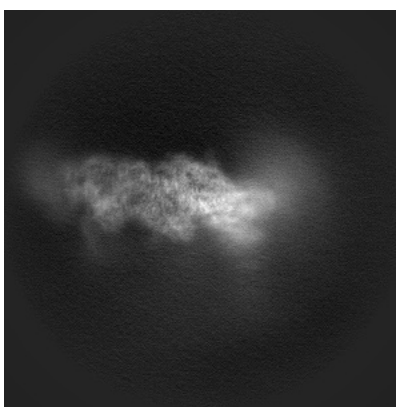


Z

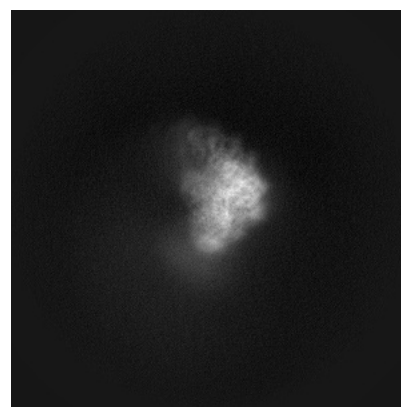
6.1.2 Raw map



X



Y

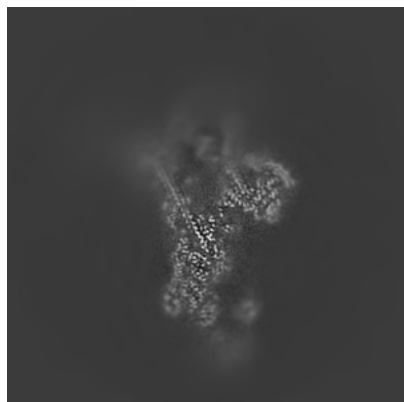


Z

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

6.2 Central slices [i](#)

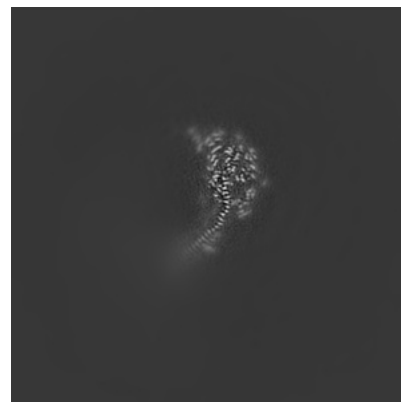
6.2.1 Primary map



X Index: 270

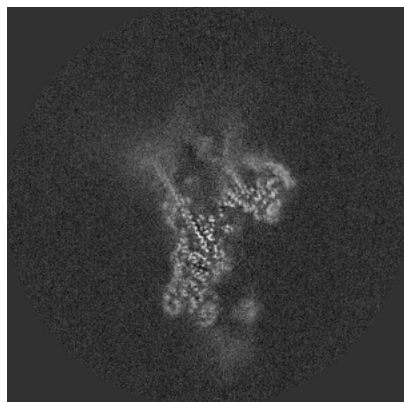


Y Index: 270

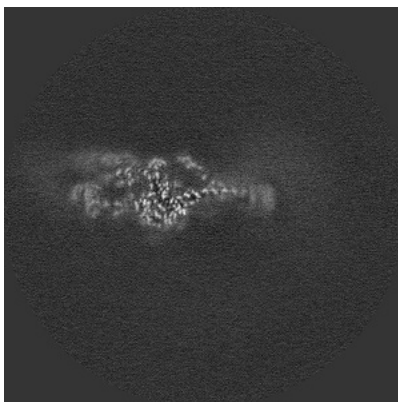


Z Index: 270

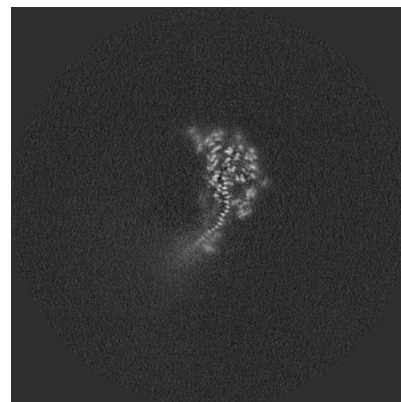
6.2.2 Raw map



X Index: 270



Y Index: 270

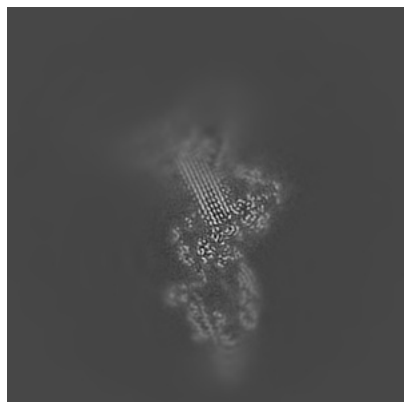


Z Index: 270

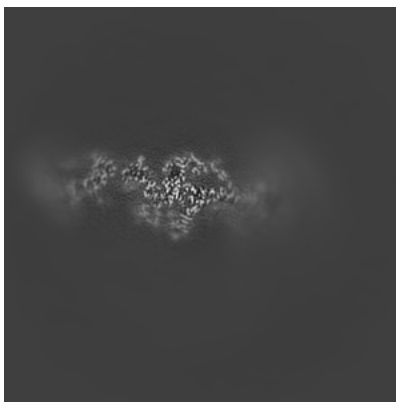
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

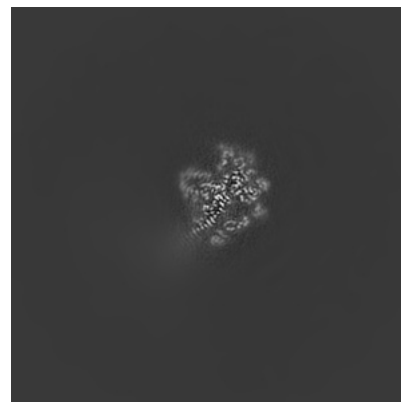
6.3.1 Primary map



X Index: 290

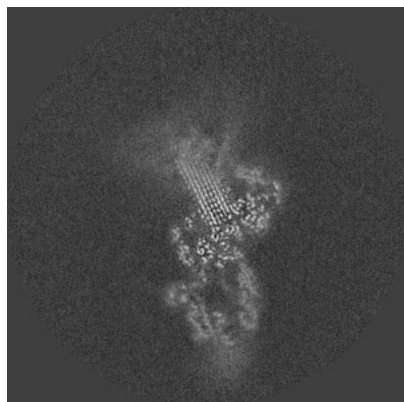


Y Index: 290

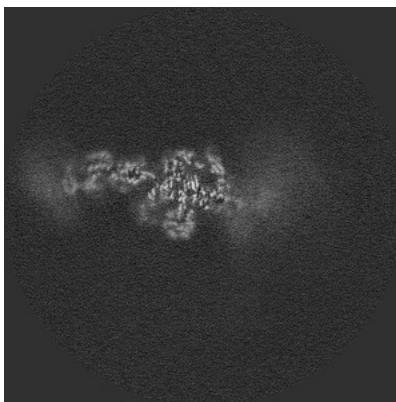


Z Index: 242

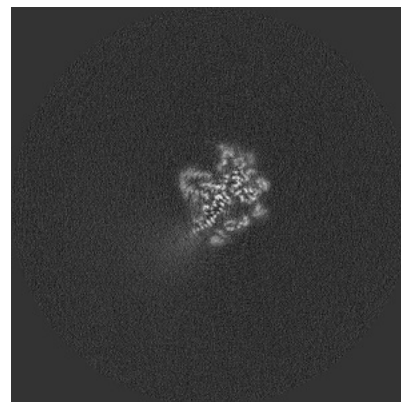
6.3.2 Raw map



X Index: 290



Y Index: 296

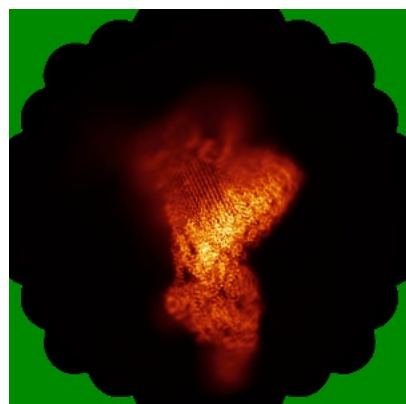


Z Index: 242

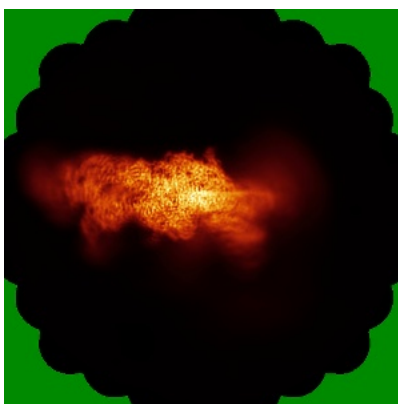
The images above show the largest variance slices of the map in three orthogonal directions.

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

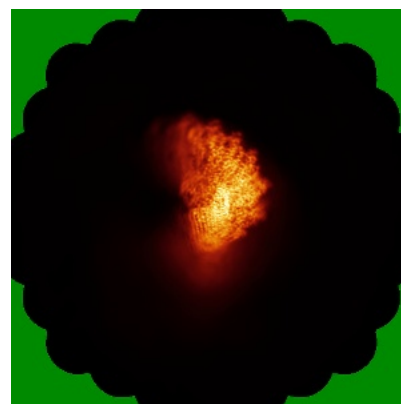
6.4.1 Primary map



X

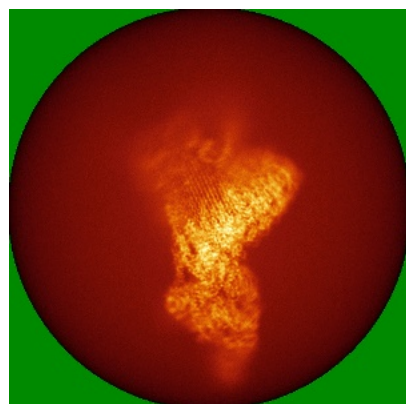


Y

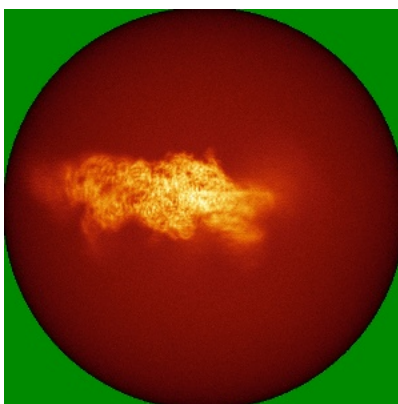


Z

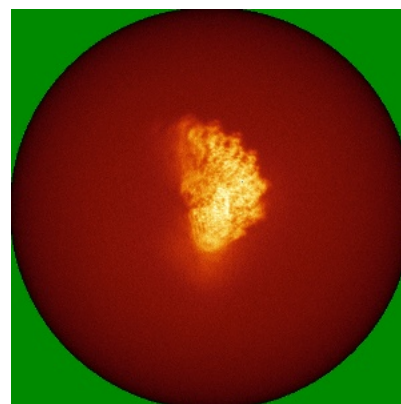
6.4.2 Raw map



X



Y

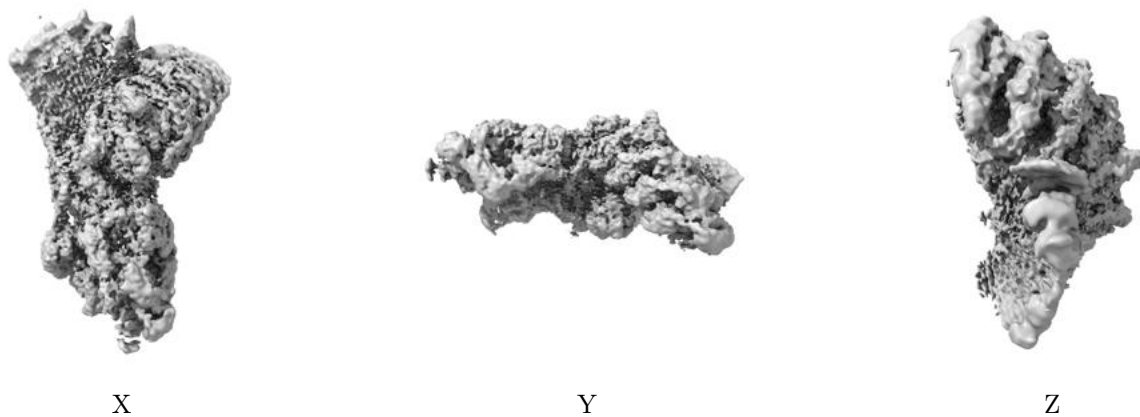


Z

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.

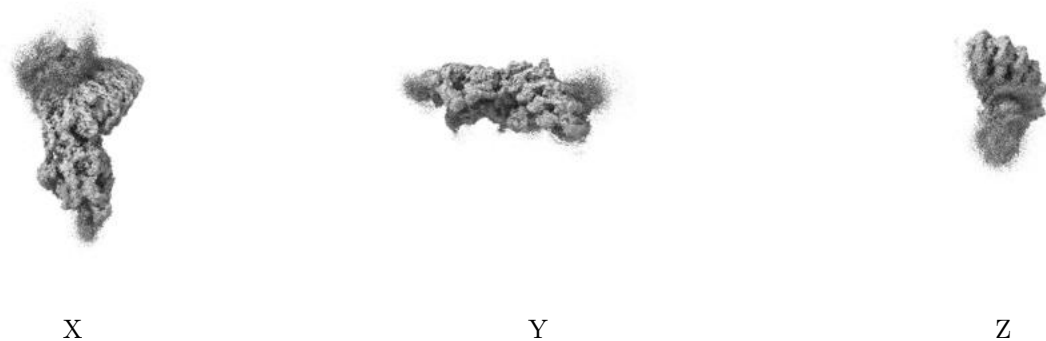
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0164. 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.

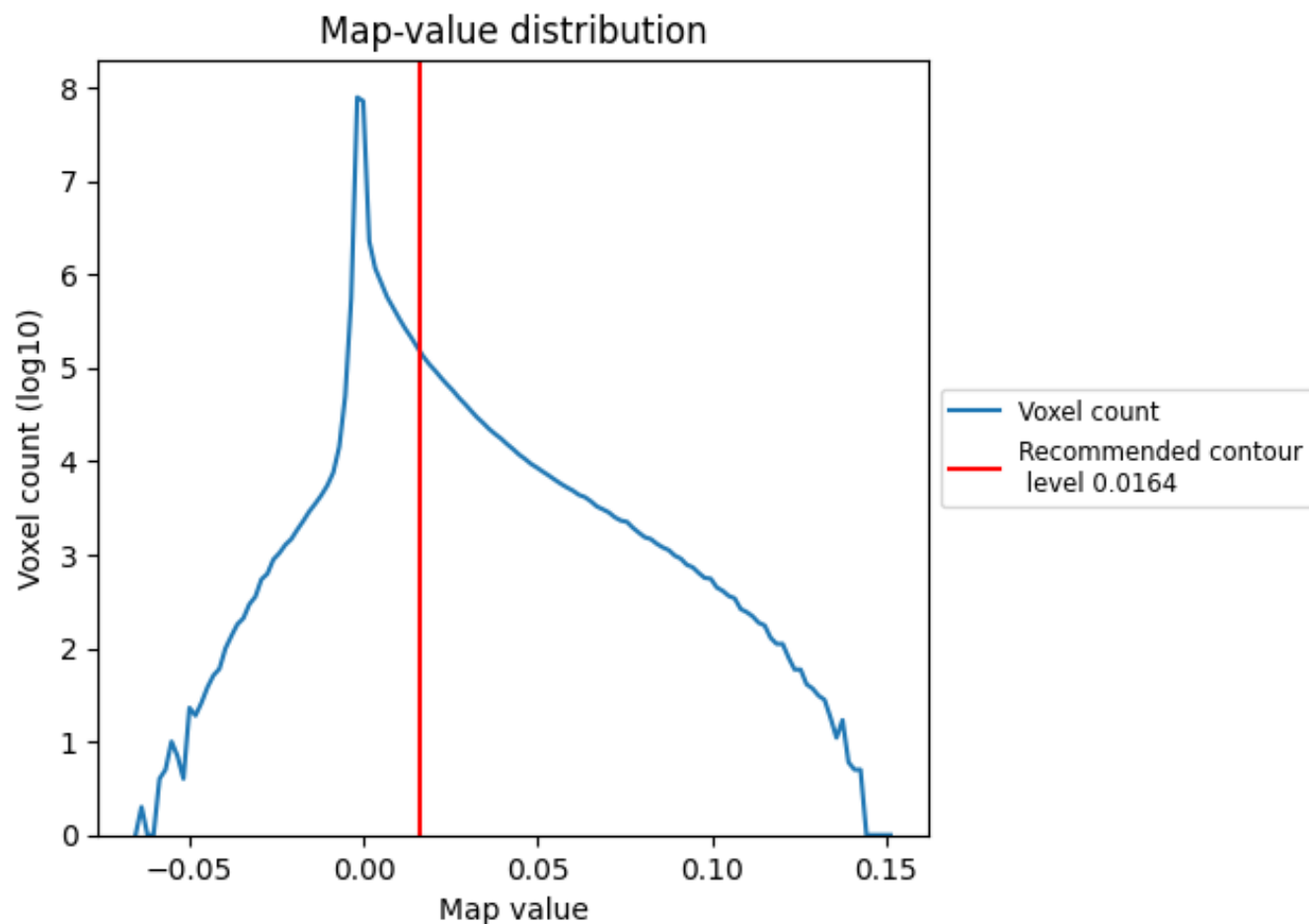
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

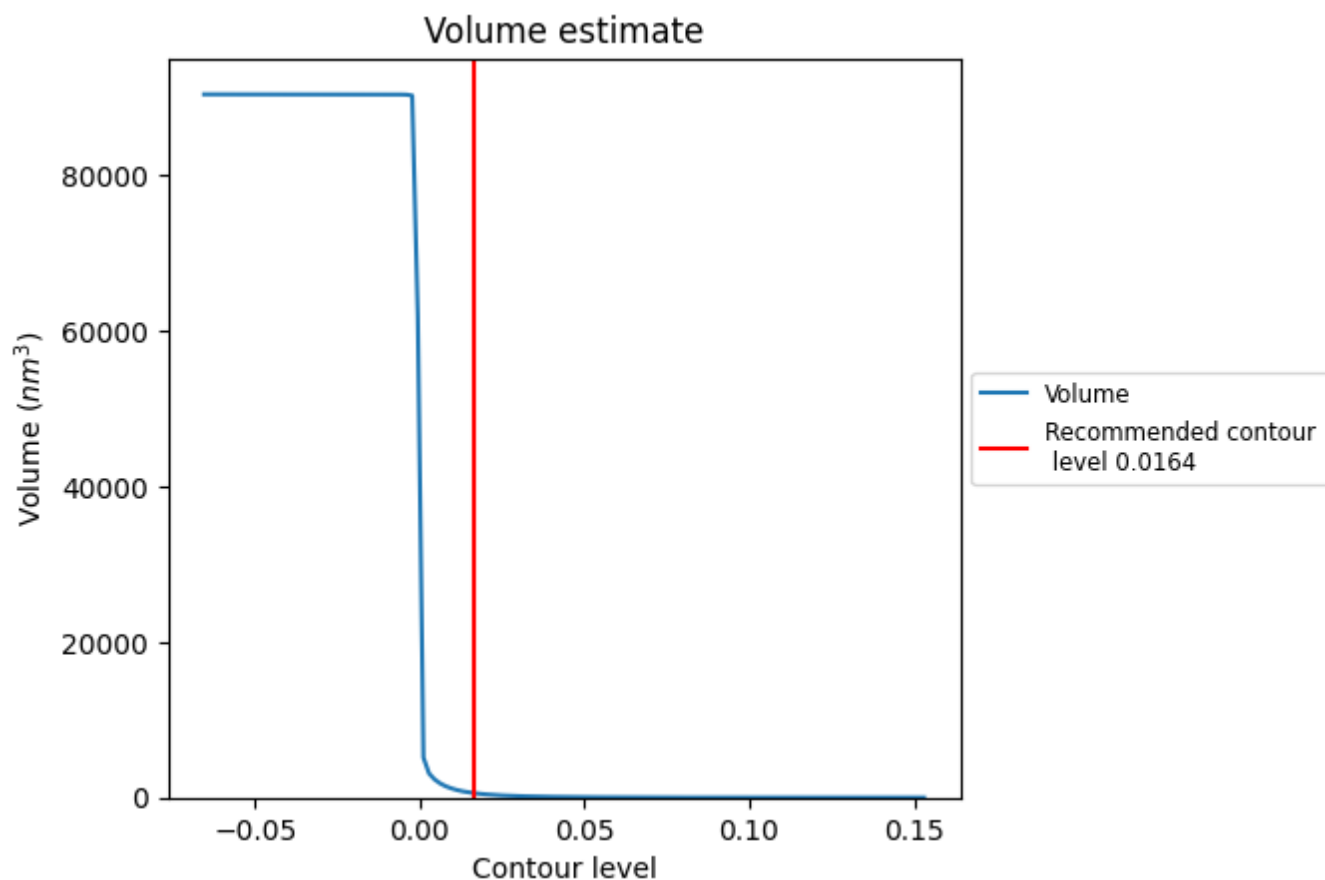
This section contains the results of statistical analysis of the map.

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.

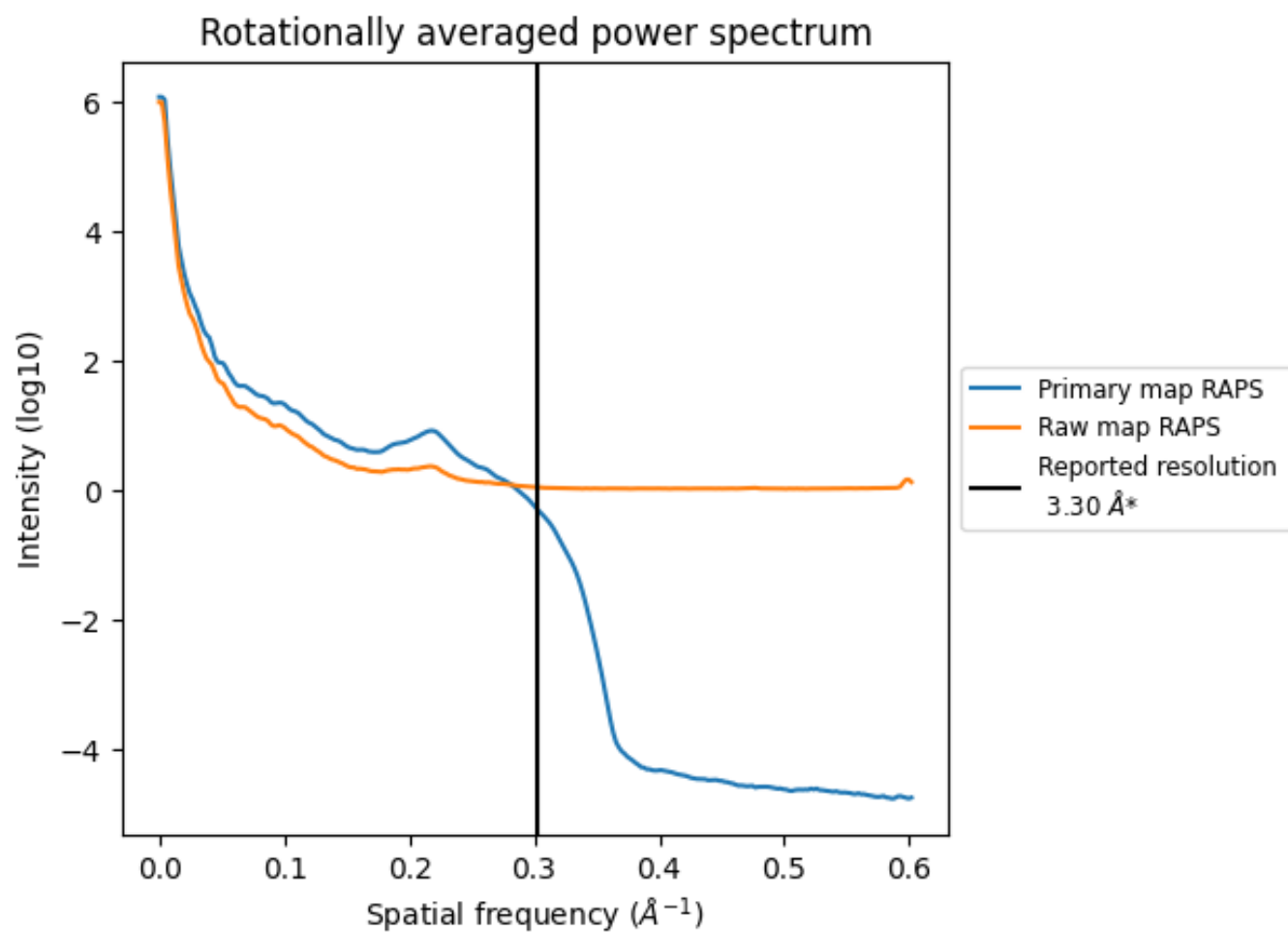
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm^3 ; this corresponds to an approximate mass of 516 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 ⓘ

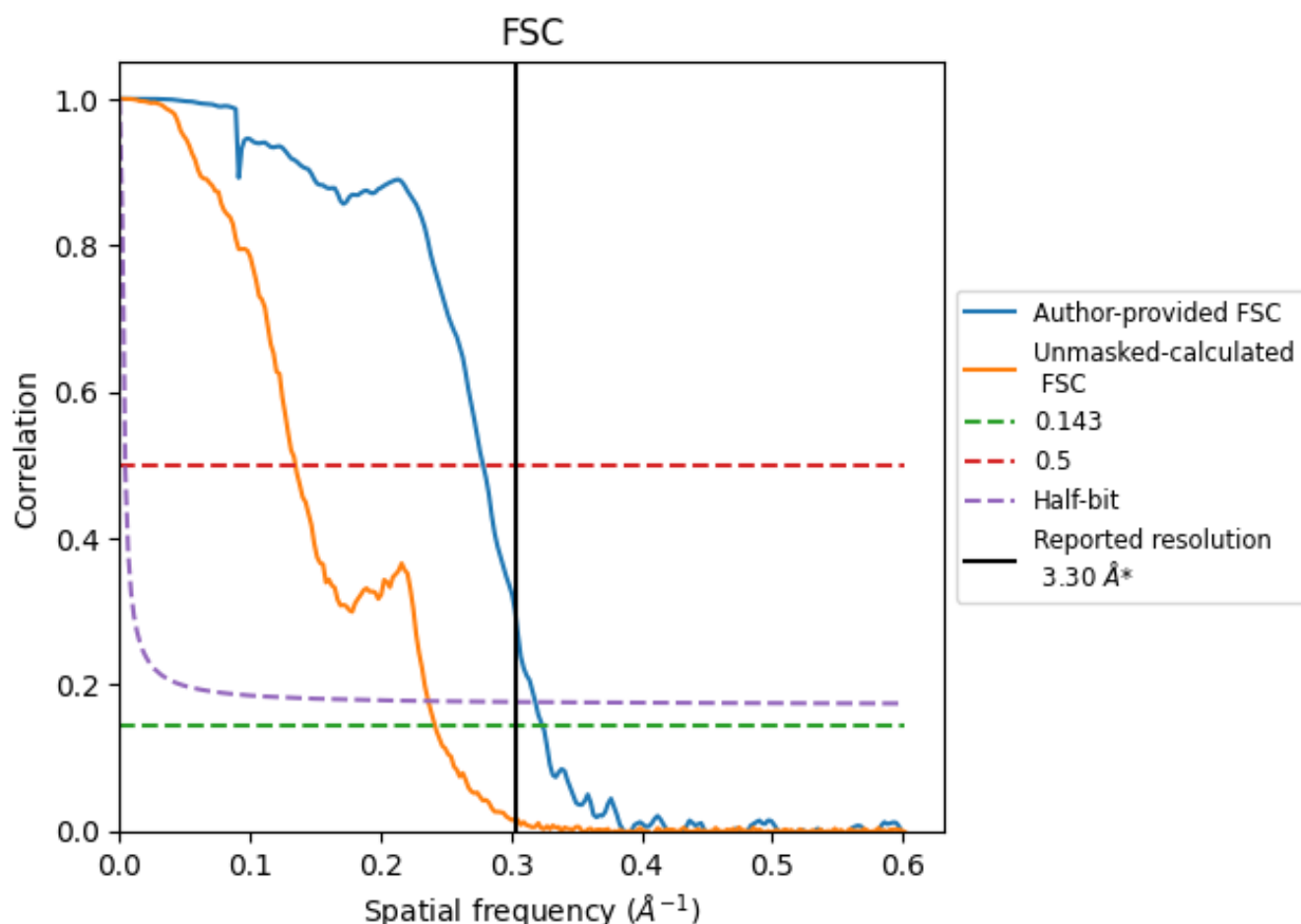


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

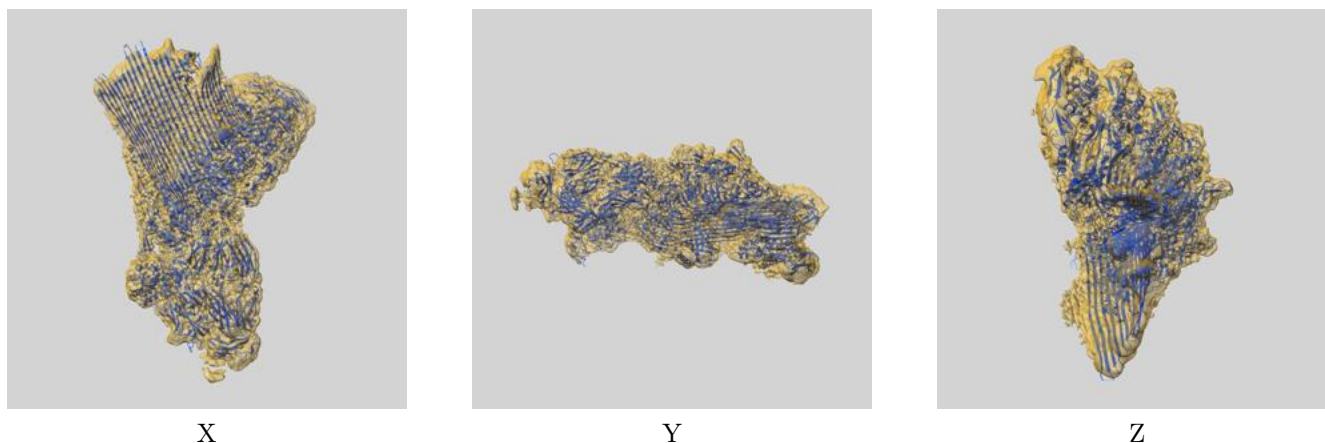
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.09	3.59	3.14
Unmasked-calculated*	4.14	7.42	4.22

*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 4.14 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

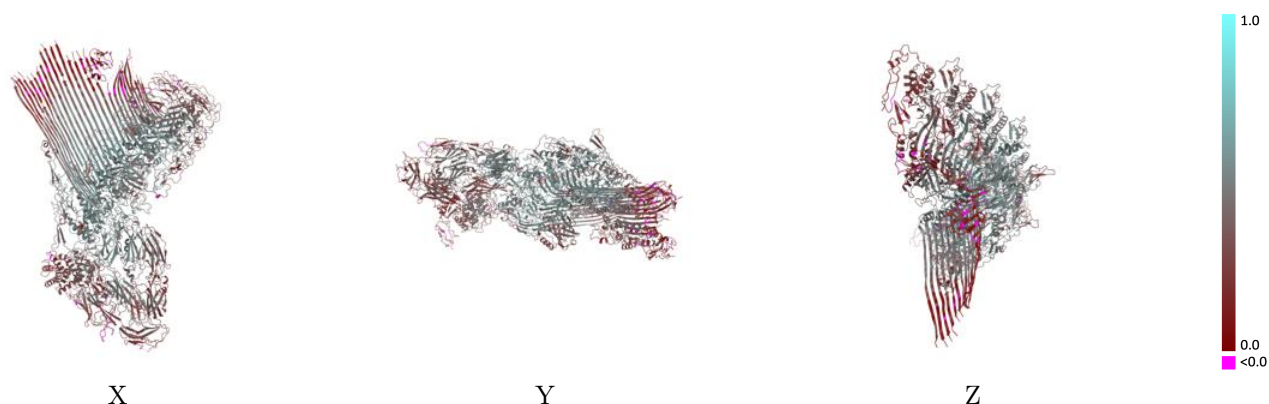
This section contains information regarding the fit between EMDB map EMD-15780 and PDB model 8B0G. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



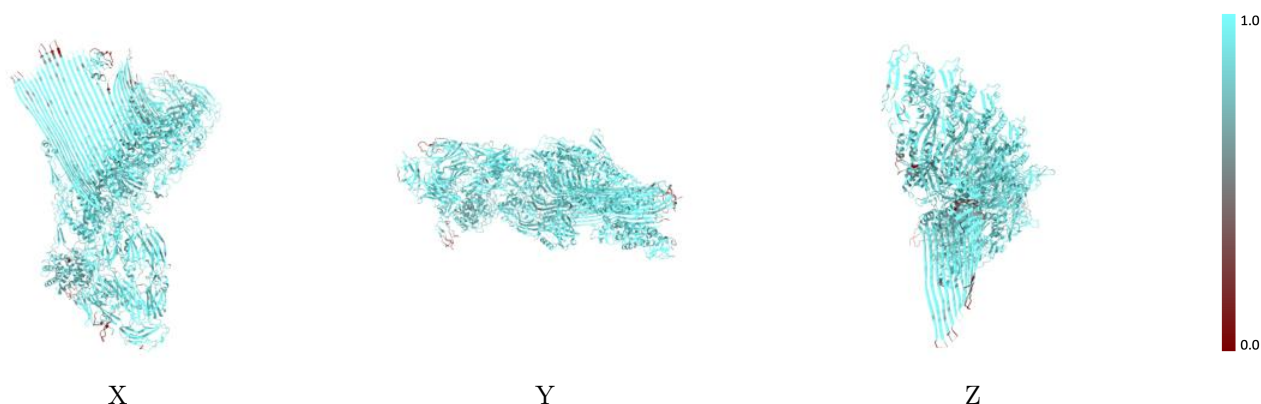
The images above show the 3D surface view of the map at the recommended contour level 0.0164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



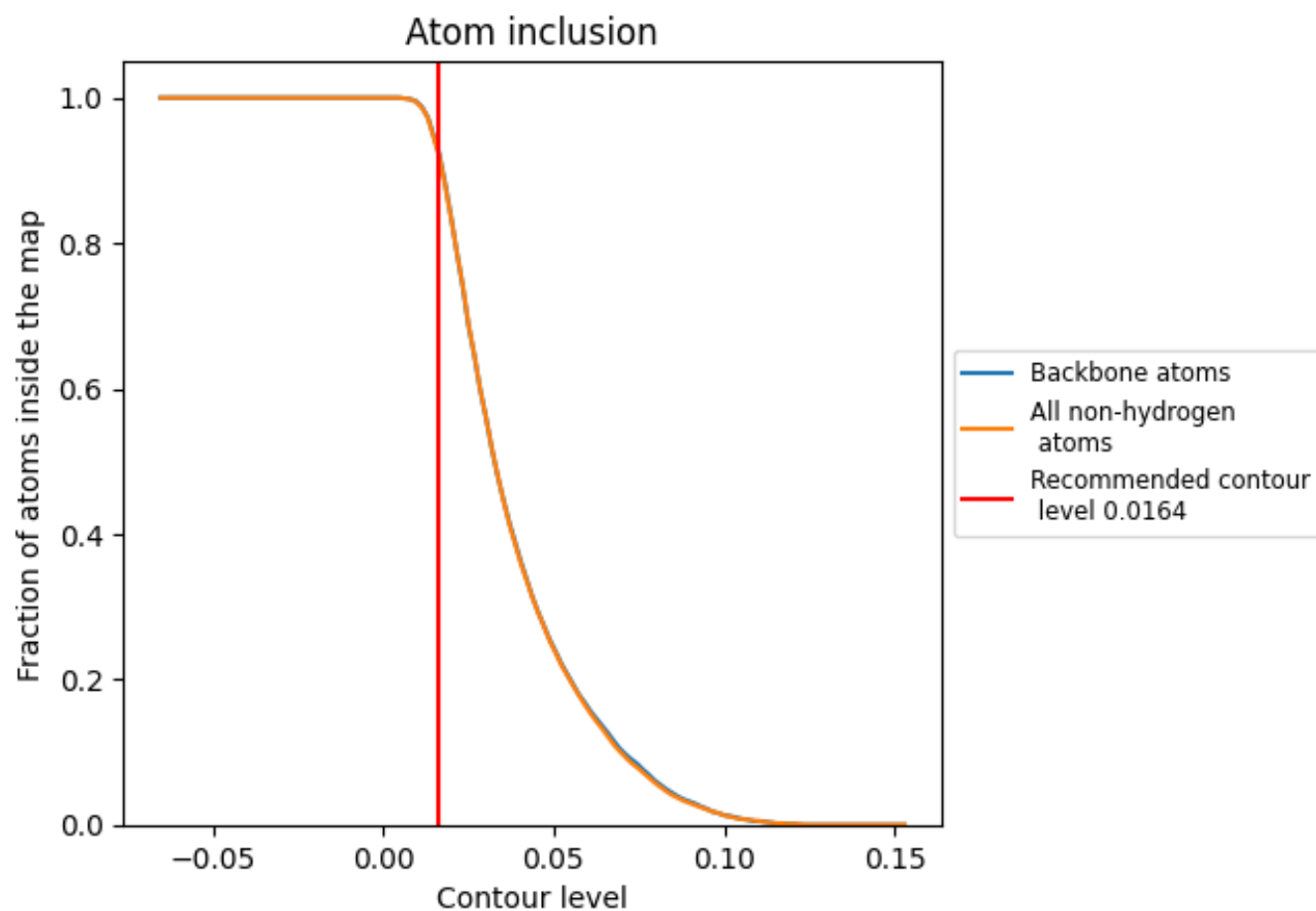
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0164).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9200	 0.3990
A	 0.9130	 0.3560
B	 0.9020	 0.4100
C	 0.9240	 0.4600
D	 0.9490	 0.4780
E	 0.9680	 0.4730
F	 0.9380	 0.3860
G	 0.6480	 0.1270
H	 0.9630	 0.4360
I	 0.9330	 0.3680
J	 0.8870	 0.2690
K	 0.8210	 0.3480
L	 0.8570	 0.3360
M	 0.9290	 0.4060
N	 0.6790	 0.2370
O	 0.9290	 0.2730

