



Full wwPDB EM Validation Report i

Dec 2, 2025 – 05:03 PM JST

PDB ID : 9XW6 / pdb_00009xw6
EMDB ID : EMD-67326
Title : EriCoV RU15-1 RBD - E.amu APN monomer complex
Deposited on : 2025-11-27
Resolution : 3.38 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the i symbol.

The types of validation reports are described at

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

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

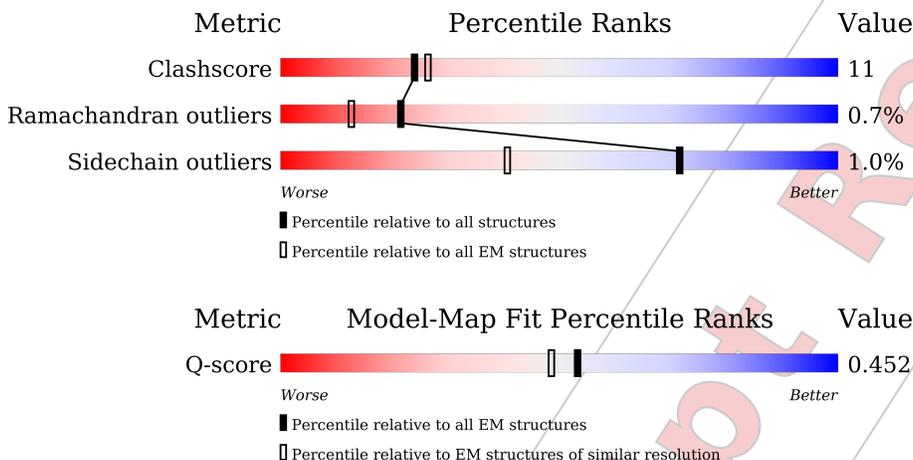
EMDB validation analysis	: 0.0.1.dev129
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4-5-2 with Phenix2.0
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	: 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	: 1.9.13
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.38 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.



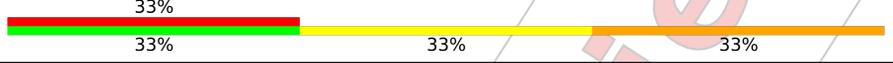
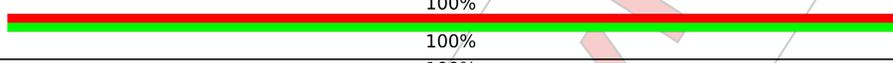
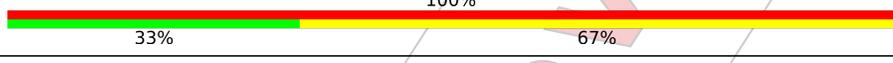
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14261 (2.88 - 3.88)

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	B	938	
2	C	247	
3	A	2	
3	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	 50% 100%
4	D	3	 33% 33% 33%
4	G	3	 100%
4	H	3	 33% 67%

For Manuscript Review

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9153 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 Aminopeptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	901	7263	4633	1235	1373	22	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	MET	-	initiating methionine	UNP A0A1S2ZAK1
B	37	PRO	-	expression tag	UNP A0A1S2ZAK1
B	38	MET	-	expression tag	UNP A0A1S2ZAK1
B	39	GLY	-	expression tag	UNP A0A1S2ZAK1
B	40	SER	-	expression tag	UNP A0A1S2ZAK1
B	41	LEU	-	expression tag	UNP A0A1S2ZAK1
B	42	GLN	-	expression tag	UNP A0A1S2ZAK1
B	43	PRO	-	expression tag	UNP A0A1S2ZAK1
B	44	LEU	-	expression tag	UNP A0A1S2ZAK1
B	45	ALA	-	expression tag	UNP A0A1S2ZAK1
B	46	THR	-	expression tag	UNP A0A1S2ZAK1
B	47	LEU	-	expression tag	UNP A0A1S2ZAK1
B	48	TYR	-	expression tag	UNP A0A1S2ZAK1
B	49	LEU	-	expression tag	UNP A0A1S2ZAK1
B	50	LEU	-	expression tag	UNP A0A1S2ZAK1
B	51	GLY	-	expression tag	UNP A0A1S2ZAK1
B	52	MET	-	expression tag	UNP A0A1S2ZAK1
B	53	LEU	-	expression tag	UNP A0A1S2ZAK1
B	54	VAL	-	expression tag	UNP A0A1S2ZAK1
B	55	ALA	-	expression tag	UNP A0A1S2ZAK1
B	56	SER	-	expression tag	UNP A0A1S2ZAK1
B	57	VAL	-	expression tag	UNP A0A1S2ZAK1
B	58	LEU	-	expression tag	UNP A0A1S2ZAK1
B	59	ALA	-	expression tag	UNP A0A1S2ZAK1
B	961	GLY	-	expression tag	UNP A0A1S2ZAK1
B	962	GLY	-	expression tag	UNP A0A1S2ZAK1
B	963	GLY	-	expression tag	UNP A0A1S2ZAK1
B	964	GLY	-	expression tag	UNP A0A1S2ZAK1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	965	SER	-	expression tag	UNP A0A1S2ZAK1
B	966	HIS	-	expression tag	UNP A0A1S2ZAK1
B	967	HIS	-	expression tag	UNP A0A1S2ZAK1
B	968	HIS	-	expression tag	UNP A0A1S2ZAK1
B	969	HIS	-	expression tag	UNP A0A1S2ZAK1
B	970	HIS	-	expression tag	UNP A0A1S2ZAK1
B	971	HIS	-	expression tag	UNP A0A1S2ZAK1
B	972	HIS	-	expression tag	UNP A0A1S2ZAK1
B	973	HIS	-	expression tag	UNP A0A1S2ZAK1

- Molecule 2 is a protein called RU15-1 RBD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	208	1619	1026	265	315	13	0	0

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

- Molecule 4 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.



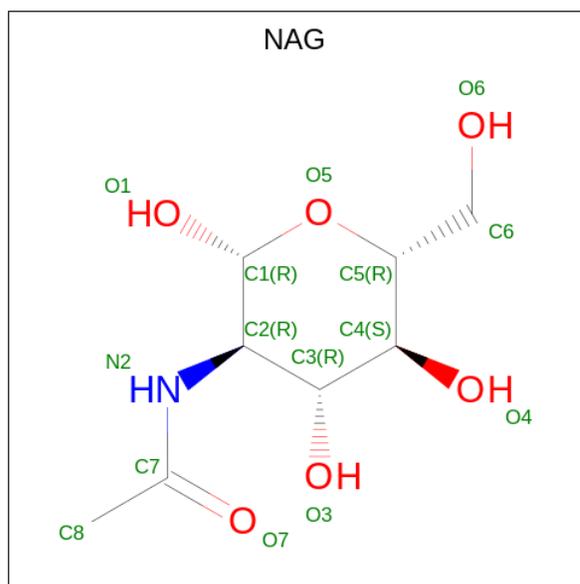
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	3	39	22	2	15	0	0

Continued on next page...

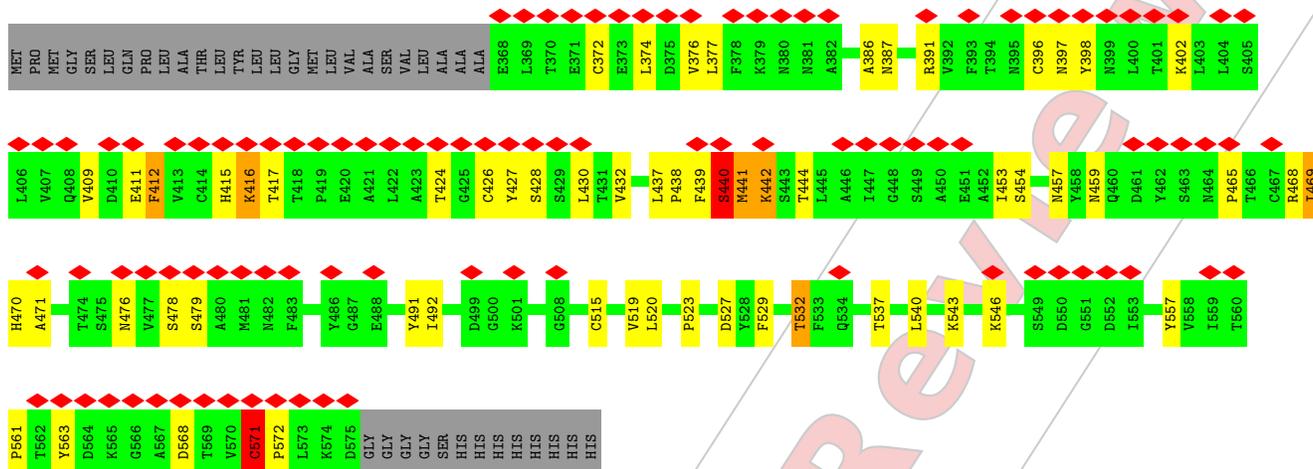
Continued from previous page...

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

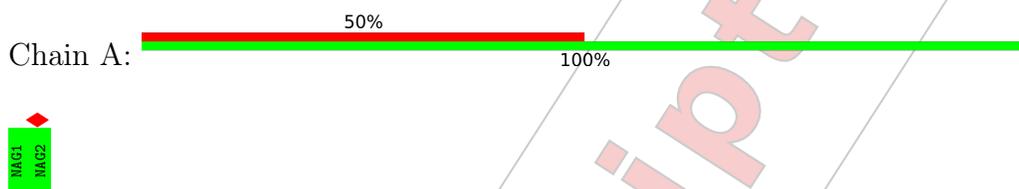
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



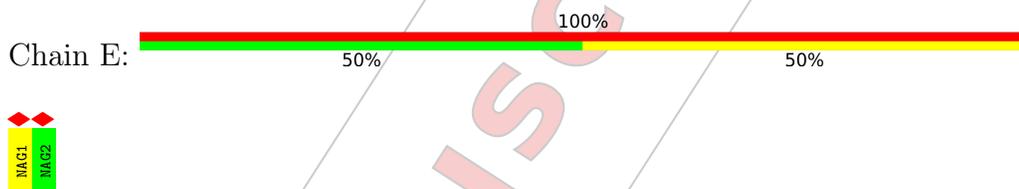
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	



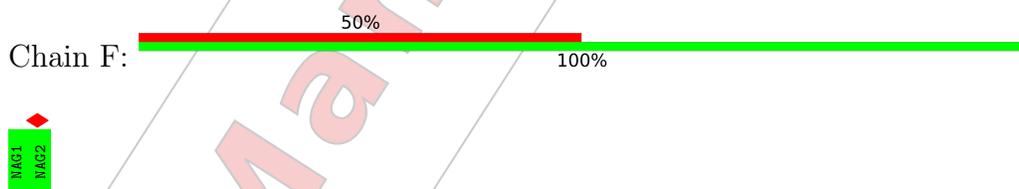
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



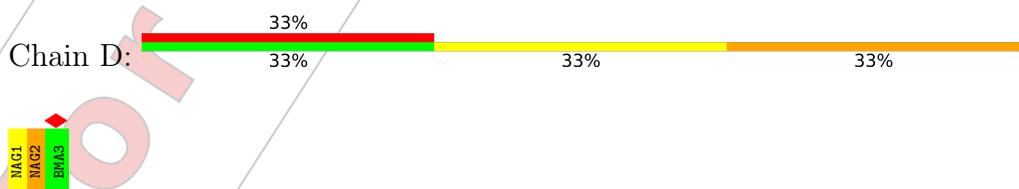
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



For Manuscript Review

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1178055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.113	Depositor
Minimum map value	-2.050	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.374	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	B	0.22	0/7449	0.47	1/10151 (0.0%)
2	C	0.34	0/1657	0.62	1/2255 (0.0%)
All	All	0.24	0/9106	0.50	2/12406 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	PRO	CA-N-CD	-10.21	97.70	112.00
2	C	571	CYS	CA-CB-SG	5.25	126.48	114.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	468	ARG	Sidechain
2	C	571	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7263	0	7053	143	0
2	C	1619	0	1559	46	0
3	A	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	D	39	0	34	2	0
4	G	39	0	34	0	0
4	H	39	0	34	2	0
5	B	42	0	39	0	0
5	C	28	0	26	1	0
All	All	9153	0	8854	190	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 11.

All (190) 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:B:944:VAL:O	1:B:948:LYS:HB3	1.78	0.84
1:B:583:MET:HG2	1:B:617:ILE:HD11	1.63	0.80
1:B:384:GLN:HA	1:B:388:ASN:HD22	1.47	0.77
1:B:87:LEU:HD21	1:B:199:ALA:HB2	1.72	0.72
2:C:426:CYS:HA	2:C:571:CYS:HB2	1.74	0.69
2:C:457:ASN:HD21	2:C:492:ILE:H	1.41	0.68
1:B:877:TRP:CD1	1:B:918:ASN:HD21	2.11	0.68
2:C:415:HIS:O	2:C:416:LYS:HB2	1.94	0.66
1:B:249:LEU:HD12	1:B:250:PRO:HD2	1.78	0.66
1:B:239:ASN:ND2	1:B:348:TRP:O	2.27	0.66
1:B:944:VAL:O	1:B:948:LYS:CB	2.43	0.66
1:B:395:TRP:CD1	1:B:459:ILE:HD11	2.30	0.66
1:B:188:GLU:HG2	1:B:197:VAL:HG22	1.77	0.66
1:B:92:GLN:OE1	1:B:92:GLN:N	2.29	0.66
2:C:426:CYS:HA	2:C:571:CYS:CB	2.26	0.66
1:B:545:THR:OG1	1:B:554:ASN:OD1	2.12	0.65
1:B:117:HIS:HB3	1:B:209:ARG:HD3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:SER:O	1:B:901:ARG:NH2	2.30	0.64
1:B:720:THR:O	1:B:724:THR:HG23	1.98	0.64
1:B:206:ALA:HB1	1:B:209:ARG:HH12	1.63	0.64
1:B:834:LEU:HD11	1:B:862:ASN:HD21	1.63	0.64
2:C:442:LYS:HD3	2:C:470:HIS:CE1	2.34	0.63
1:B:379:HIS:HA	1:B:409:GLU:HB2	1.80	0.63
1:B:434:VAL:O	1:B:438:ASP:N	2.30	0.61
1:B:139:PRO:HG2	1:B:157:LEU:HD23	1.82	0.61
1:B:937:THR:O	1:B:941:ILE:HG12	2.00	0.61
1:B:186:ARG:NH1	1:B:188:GLU:OE2	2.32	0.61
1:B:80:SER:OG	1:B:102:THR:OG1	2.13	0.61
1:B:710:PRO:HB2	1:B:955:PHE:HB3	1.83	0.61
1:B:435:MET:HB3	1:B:624:ARG:HH22	1.66	0.60
1:B:701:MET:HG3	1:B:903:ASN:HD22	1.66	0.60
2:C:439:PHE:O	2:C:440:SER:C	2.44	0.60
2:C:471:ALA:HB2	2:C:557:TYR:HE2	1.67	0.60
2:C:527:ASP:OD2	2:C:543:LYS:NZ	2.35	0.60
1:B:816:ASN:OD1	1:B:817:GLU:N	2.35	0.59
1:B:344:ALA:HB1	1:B:353:TYR:HD1	1.66	0.59
1:B:653:GLN:NE2	1:B:657:ASP:OD2	2.33	0.58
1:B:842:LEU:HD22	1:B:872:PHE:HZ	1.69	0.58
2:C:377:LEU:HD21	2:C:432:VAL:HG11	1.85	0.58
1:B:779:ASN:HD21	1:B:786:ARG:CZ	2.17	0.57
1:B:786:ARG:HH11	1:B:786:ARG:HG3	1.69	0.57
2:C:424:THR:HA	2:C:572:PRO:HG3	1.87	0.57
1:B:428:LEU:HD22	1:B:686:MET:SD	2.44	0.57
1:B:543:VAL:HG23	1:B:624:ARG:HB3	1.87	0.57
1:B:455:THR:HG22	1:B:458:GLN:HG3	1.87	0.57
1:B:94:LEU:HD12	1:B:176:GLU:HG3	1.87	0.56
1:B:644:LYS:O	1:B:646:ILE:N	2.38	0.56
1:B:651:ARG:HB2	1:B:687:PRO:HG3	1.88	0.56
1:B:754:CYS:N	1:B:761:CYS:SG	2.78	0.56
1:B:866:GLN:HG3	1:B:901:ARG:HE	1.71	0.56
1:B:703:ASP:OD2	1:B:901:ARG:NH1	2.39	0.56
1:B:116:ILE:HG23	1:B:153:LEU:HB3	1.87	0.56
2:C:457:ASN:HD21	2:C:492:ILE:N	2.04	0.55
1:B:420:TRP:CG	1:B:740:LEU:HD13	2.42	0.55
1:B:221:LYS:HB3	1:B:265:LYS:HG2	1.89	0.55
1:B:404:PHE:CD1	1:B:475:LEU:HD21	2.41	0.55
1:B:441:VAL:HG22	1:B:559:LEU:HD22	1.88	0.55
4:D:2:NAG:H83	4:D:2:NAG:H3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TYR:HE1	1:B:380:GLU:HG3	1.70	0.55
2:C:546:LYS:HE3	2:C:546:LYS:HA	1.90	0.54
1:B:339:ASP:OD2	1:B:848:ARG:NH1	2.41	0.53
2:C:428:SER:OG	2:C:568:ASP:OD1	2.24	0.53
2:C:396:CYS:SG	2:C:397:ASN:N	2.81	0.53
1:B:402:GLU:HG2	1:B:468:TYR:CE1	2.44	0.53
2:C:438:PRO:O	2:C:439:PHE:C	2.52	0.53
1:B:420:TRP:O	1:B:421:ASN:C	2.52	0.52
2:C:515:CYS:HA	2:C:540:LEU:HD21	1.91	0.52
2:C:398:TYR:HE1	2:C:571:CYS:HA	1.74	0.52
1:B:663:SER:HA	1:B:943:TRP:NE1	2.25	0.52
1:B:615:LEU:HB2	1:B:625:VAL:HG21	1.90	0.52
1:B:312:THR:HG23	1:B:381:LEU:HD11	1.91	0.52
1:B:660:THR:O	1:B:663:SER:OG	2.28	0.51
1:B:875:ASP:OD1	1:B:876:ASN:N	2.43	0.51
2:C:454:SER:O	2:C:459:ASN:ND2	2.41	0.51
1:B:673:LEU:HD11	1:B:951:VAL:HG22	1.92	0.51
1:B:698:PHE:O	1:B:702:PHE:HB2	2.10	0.51
1:B:445:PRO:HA	1:B:539:MET:HB3	1.93	0.51
1:B:717:LYS:O	1:B:720:THR:HG22	2.10	0.51
1:B:216:ASP:HA	1:B:268:THR:HG21	1.92	0.51
1:B:314:PRO:HG3	2:C:529:PHE:HA	1.92	0.51
1:B:340:PHE:HZ	1:B:345:MET:HB2	1.76	0.50
1:B:241:PRO:HG3	1:B:331:LYS:HD2	1.93	0.50
1:B:427:VAL:O	1:B:431:VAL:HB	2.12	0.50
1:B:394:TRP:HD1	1:B:396:ASN:HD22	1.59	0.50
1:B:453:VAL:HG21	1:B:462:GLN:HE22	1.77	0.50
1:B:663:SER:HA	1:B:943:TRP:CD1	2.46	0.50
1:B:477:MET:HE1	1:B:535:TRP:CE2	2.47	0.50
2:C:409:VAL:HG13	2:C:411:GLU:O	2.11	0.50
1:B:782:HIS:ND1	1:B:783:PRO:HD2	2.26	0.50
2:C:491:TYR:CE2	2:C:543:LYS:HB2	2.47	0.49
1:B:400:LEU:O	1:B:402:GLU:N	2.44	0.49
1:B:559:LEU:HD11	1:B:566:VAL:HG22	1.95	0.49
1:B:361:ASP:O	1:B:362:ASN:C	2.55	0.48
1:B:534:ARG:HD3	1:B:577:ILE:HG13	1.94	0.48
1:B:779:ASN:OD1	1:B:786:ARG:NH2	2.45	0.48
1:B:200:THR:HA	1:B:274:ILE:HG12	1.95	0.48
1:B:270:LEU:HD11	1:B:388:ASN:OD1	2.14	0.48
2:C:376:VAL:HG21	2:C:391:ARG:HH12	1.79	0.48
1:B:370:GLN:HG2	1:B:420:TRP:HH2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:PHE:CE2	2:C:469:ILE:HD12	2.49	0.48
1:B:316:LEU:HD13	1:B:381:LEU:HD22	1.95	0.47
1:B:913:GLN:NE2	1:B:917:ASP:OD2	2.44	0.47
1:B:750:ILE:HD12	1:B:785:LEU:HD21	1.96	0.47
1:B:323:TYR:OH	1:B:408:VAL:HG11	2.15	0.47
1:B:206:ALA:HB1	1:B:209:ARG:NH1	2.29	0.47
1:B:794:ILE:HD12	1:B:824:ALA:HB1	1.96	0.47
1:B:431:VAL:O	1:B:435:MET:HG2	2.15	0.47
1:B:681:GLN:O	1:B:682:GLU:HG2	2.15	0.46
2:C:402:LYS:NZ	4:H:1:NAG:O6	2.36	0.46
2:C:430:LEU:HD12	2:C:561:PRO:HB3	1.98	0.46
1:B:192:ASP:O	1:B:194:VAL:HG23	2.15	0.46
1:B:544:ILE:O	1:B:626:ASN:N	2.46	0.46
1:B:398:LEU:O	1:B:400:LEU:O	2.33	0.46
1:B:941:ILE:O	1:B:944:VAL:HG12	2.16	0.46
1:B:295:ALA:HB3	1:B:300:ILE:HD11	1.97	0.46
1:B:673:LEU:O	1:B:676:THR:HG22	2.16	0.46
2:C:441:MET:O	2:C:444:THR:OG1	2.34	0.46
1:B:731:GLN:O	1:B:734:THR:HG23	2.17	0.45
1:B:781:ILE:O	1:B:786:ARG:NH1	2.49	0.45
1:B:444:HIS:ND1	1:B:445:PRO:O	2.48	0.45
1:B:420:TRP:CD1	1:B:740:LEU:HD13	2.52	0.45
1:B:545:THR:HA	1:B:626:ASN:O	2.16	0.45
2:C:478:SER:OG	2:C:479:SER:N	2.49	0.45
1:B:504:VAL:HG23	1:B:506:SER:H	1.81	0.45
2:C:372:CYS:HB3	2:C:396:CYS:HB2	1.61	0.45
1:B:226:ILE:HD11	1:B:271:LEU:HD11	1.97	0.45
1:B:353:TYR:CD2	1:B:358:LEU:HD13	2.52	0.45
1:B:410:TYR:CD1	1:B:426:ILE:HB	2.52	0.45
1:B:821:LEU:O	1:B:825:LEU:HG	2.16	0.44
1:B:434:VAL:HG13	1:B:438:ASP:HB2	1.99	0.44
1:B:80:SER:HA	1:B:225:ASN:HB2	1.99	0.44
1:B:357:ALA:HB1	1:B:376:VAL:HG11	2.00	0.44
1:B:478:LEU:HA	1:B:481:PHE:CE2	2.52	0.44
2:C:374:LEU:O	2:C:374:LEU:HD23	2.17	0.44
2:C:444:THR:HG21	2:C:453:ILE:HD12	1.99	0.44
2:C:492:ILE:HG12	2:C:519:VAL:HG21	1.99	0.44
1:B:442:SER:OG	1:B:932:GLN:HA	2.17	0.44
1:B:540:GLY:HA3	1:B:557:HIS:HE1	1.82	0.44
1:B:419:HIS:NE2	2:C:523:PRO:HD3	2.33	0.44
1:B:772:TRP:CD1	1:B:779:ASN:HB3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:VAL:HG21	2:C:391:ARG:NH1	2.33	0.44
2:C:426:CYS:HA	2:C:571:CYS:HB3	1.99	0.43
1:B:902:PHE:HB2	1:B:907:ASP:OD2	2.18	0.43
4:H:1:NAG:H61	4:H:2:NAG:N2	2.34	0.43
1:B:136:ALA:HB2	1:B:165:LYS:HD2	2.01	0.43
1:B:753:ALA:HB1	1:B:758:LEU:HD12	2.00	0.43
1:B:802:TRP:CZ2	1:B:837:TYR:HB2	2.54	0.43
1:B:340:PHE:O	1:B:354:ARG:NE	2.51	0.43
1:B:210:LYS:HE2	1:B:210:LYS:HB3	1.79	0.43
2:C:387:ASN:HB2	2:C:520:LEU:HD11	1.99	0.43
2:C:417:THR:HB	2:C:465:PRO:HB3	2.01	0.43
2:C:427:TYR:HE1	2:C:563:TYR:CZ	2.37	0.43
1:B:655:ILE:HD11	1:B:678:PHE:CE2	2.54	0.42
1:B:778:ASN:OD1	1:B:778:ASN:N	2.53	0.42
2:C:386:ALA:HB2	2:C:491:TYR:HA	2.01	0.42
2:C:465:PRO:HG2	2:C:563:TYR:CE1	2.54	0.42
4:D:1:NAG:H61	4:D:2:NAG:H82	2.01	0.42
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.83	0.42
1:B:708:TYR:O	1:B:712:LYS:HB2	2.20	0.42
2:C:519:VAL:HG13	2:C:540:LEU:HD23	2.00	0.42
1:B:271:LEU:HD13	1:B:273:TYR:HE1	1.84	0.42
1:B:629:GLN:NE2	1:B:633:ARG:HE	2.18	0.42
1:B:455:THR:HG23	1:B:458:GLN:H	1.85	0.42
1:B:853:THR:HG23	1:B:894:LEU:HB2	2.02	0.42
1:B:786:ARG:HG3	1:B:786:ARG:NH1	2.34	0.42
1:B:204:GLN:HA	1:B:204:GLN:OE1	2.18	0.41
1:B:219:ALA:HA	1:B:502:ASN:ND2	2.35	0.41
1:B:903:ASN:ND2	1:B:944:VAL:HG21	2.35	0.41
1:B:940:ASN:O	1:B:944:VAL:HB	2.20	0.41
2:C:476:ASN:OD1	5:C:601:NAG:N2	2.53	0.41
1:B:902:PHE:HZ	1:B:911:LEU:HD22	1.86	0.41
1:B:726:PHE:CE1	1:B:746:GLU:HB3	2.55	0.41
2:C:412:PHE:HE2	2:C:469:ILE:HD12	1.84	0.41
2:C:532:THR:HG23	2:C:537:THR:HG22	2.02	0.41
1:B:145:GLU:HG2	1:B:154:VAL:HB	2.02	0.41
1:B:200:THR:OG1	1:B:201:THR:N	2.52	0.41
1:B:271:LEU:HA	1:B:271:LEU:HD23	1.74	0.41
1:B:842:LEU:HD12	1:B:842:LEU:HA	1.88	0.41
1:B:428:LEU:HD12	1:B:432:TYR:HD2	1.86	0.41
2:C:439:PHE:O	2:C:442:LYS:N	2.53	0.41
1:B:307:TYR:O	1:B:311:VAL:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:937:THR:HA	1:B:940:ASN:HB2	2.02	0.41
2:C:442:LYS:HA	2:C:442:LYS:HD2	1.76	0.41
1:B:769:PHE:CG	1:B:793:ALA:HB1	2.57	0.40
2:C:402:LYS:HE2	2:C:402:LYS:HB2	1.96	0.40
1:B:94:LEU:HD23	1:B:94:LEU:H	1.85	0.40
1:B:435:MET:HB3	1:B:624:ARG:NH2	2.33	0.40
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.83	0.40
1:B:217:GLU:HG2	1:B:219:ALA:H	1.86	0.40
1:B:624:ARG:CZ	1:B:660:THR:HG21	2.52	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	B	899/938 (96%)	837 (93%)	56 (6%)	6 (1%)	19	47
2	C	206/247 (83%)	186 (90%)	18 (9%)	2 (1%)	13	39
All	All	1105/1185 (93%)	1023 (93%)	74 (7%)	8 (1%)	21	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	ALA
1	B	362	ASN
2	C	416	LYS
1	B	483	THR
1	B	539	MET
2	C	440	SER
1	B	364	THR
1	B	645	VAL

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	B	798/826 (97%)	795 (100%)	3 (0%)	89	93
2	C	180/208 (86%)	173 (96%)	7 (4%)	27	54
All	All	978/1034 (95%)	968 (99%)	10 (1%)	71	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	363	LEU
1	B	364	THR
1	B	591	HIS
2	C	412	PHE
2	C	437	LEU
2	C	440	SER
2	C	441	MET
2	C	442	LYS
2	C	469	ILE
2	C	532	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	B	421	ASN
1	B	626	ASN
1	B	743	GLN
1	B	775	ASN
1	B	862	ASN
1	B	903	ASN
2	C	457	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

15 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
3	NAG	A	1	1,3	14,14,15	0.24	0	17,19,21	0.35	0
3	NAG	A	2	3	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	D	1	1,4	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	1.28	2 (11%)
4	BMA	D	3	4	11,11,12	0.60	0	15,15,17	0.78	0
3	NAG	E	1	1,3	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
3	NAG	E	2	3	14,14,15	0.43	0	17,19,21	0.48	0
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.48	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	G	1	2,4	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.22	0	17,19,21	0.45	0
4	BMA	G	3	4	11,11,12	0.59	0	15,15,17	0.72	0
4	NAG	H	1	2,4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	H	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	BMA	H	3	4	11,11,12	0.61	0	15,15,17	0.88	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
3	NAG	A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C2-N2-C7	4.38	129.14	122.90
3	E	1	NAG	C1-O5-C5	3.41	116.81	112.19
4	D	2	NAG	C1-C2-N2	2.05	113.98	110.49

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	A	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	A	2	NAG	C8-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C4-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

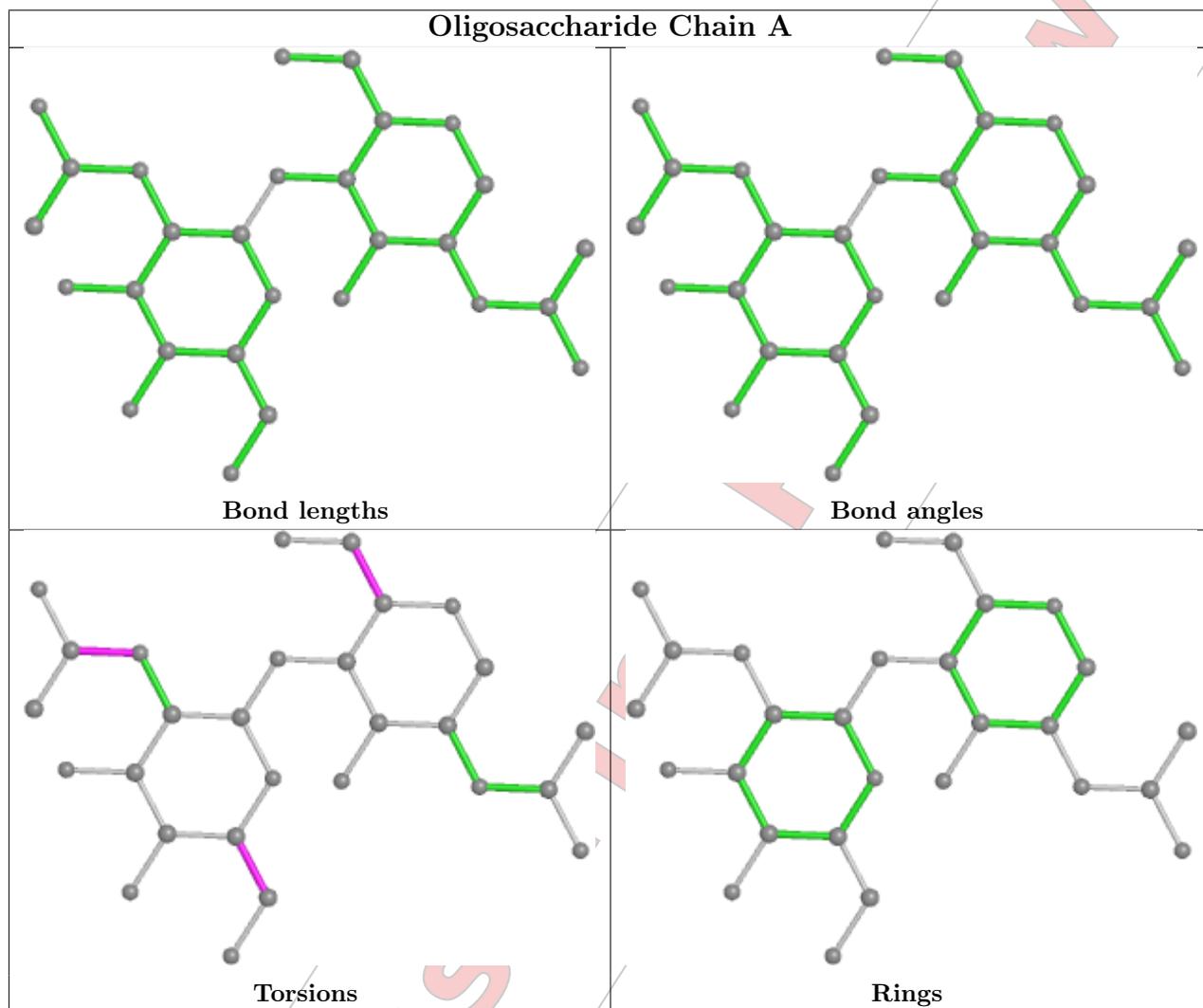
Mol	Chain	Res	Type	Atoms
4	H	3	BMA	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7

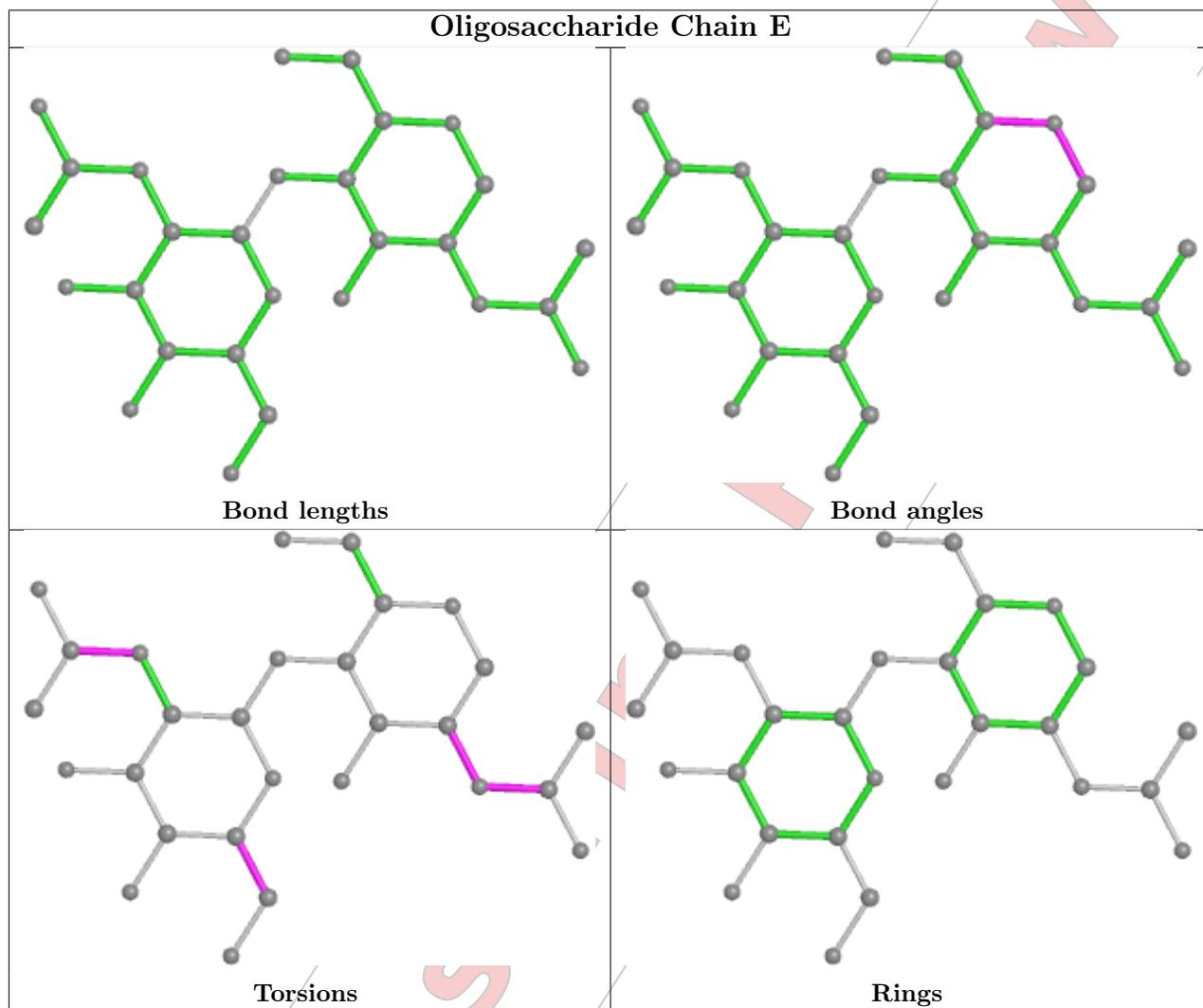
There are no ring outliers.

4 monomers are involved in 4 short contacts:

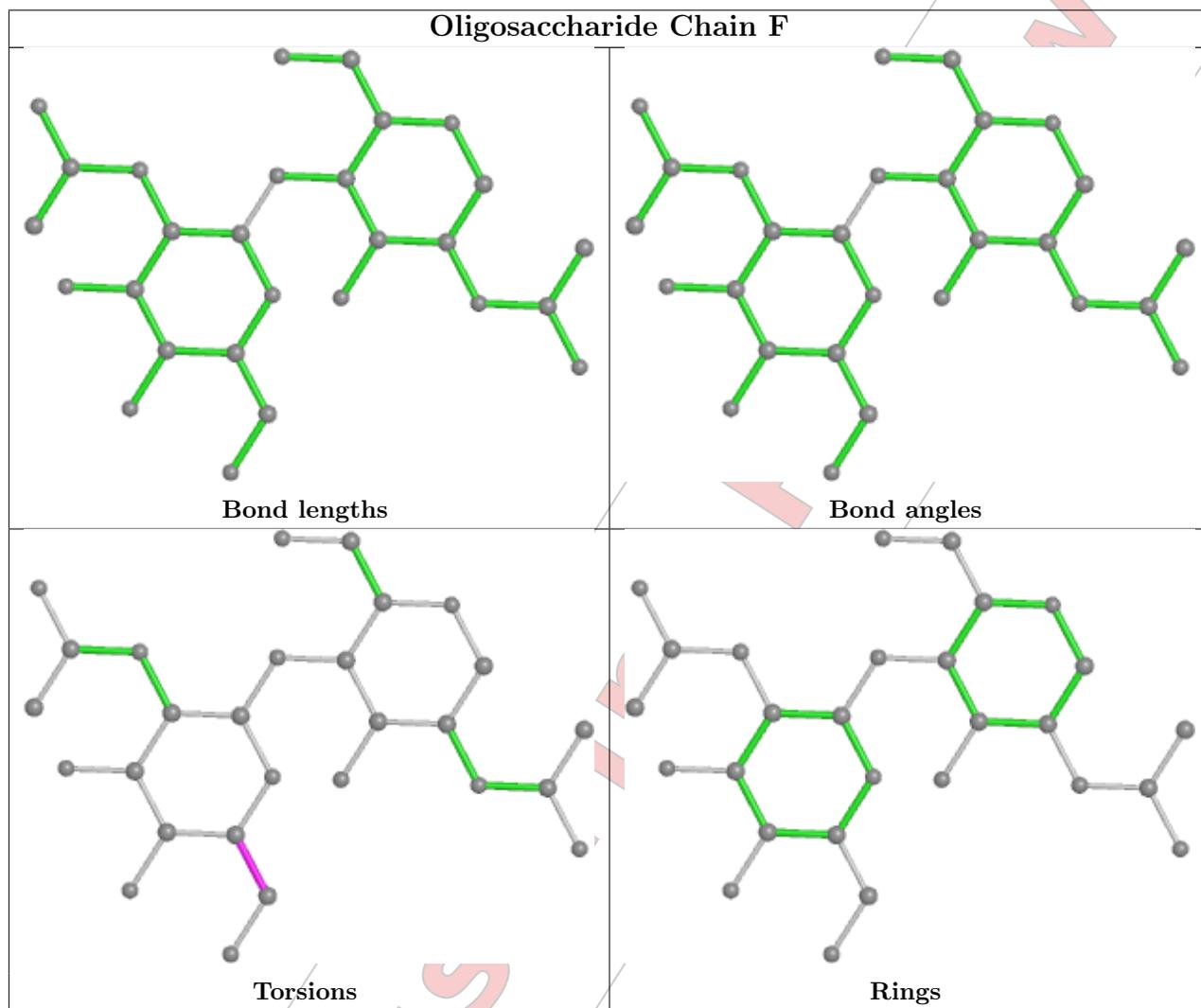
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	2	0
4	H	2	NAG	1	0
4	H	1	NAG	2	0
4	D	1	NAG	1	0

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

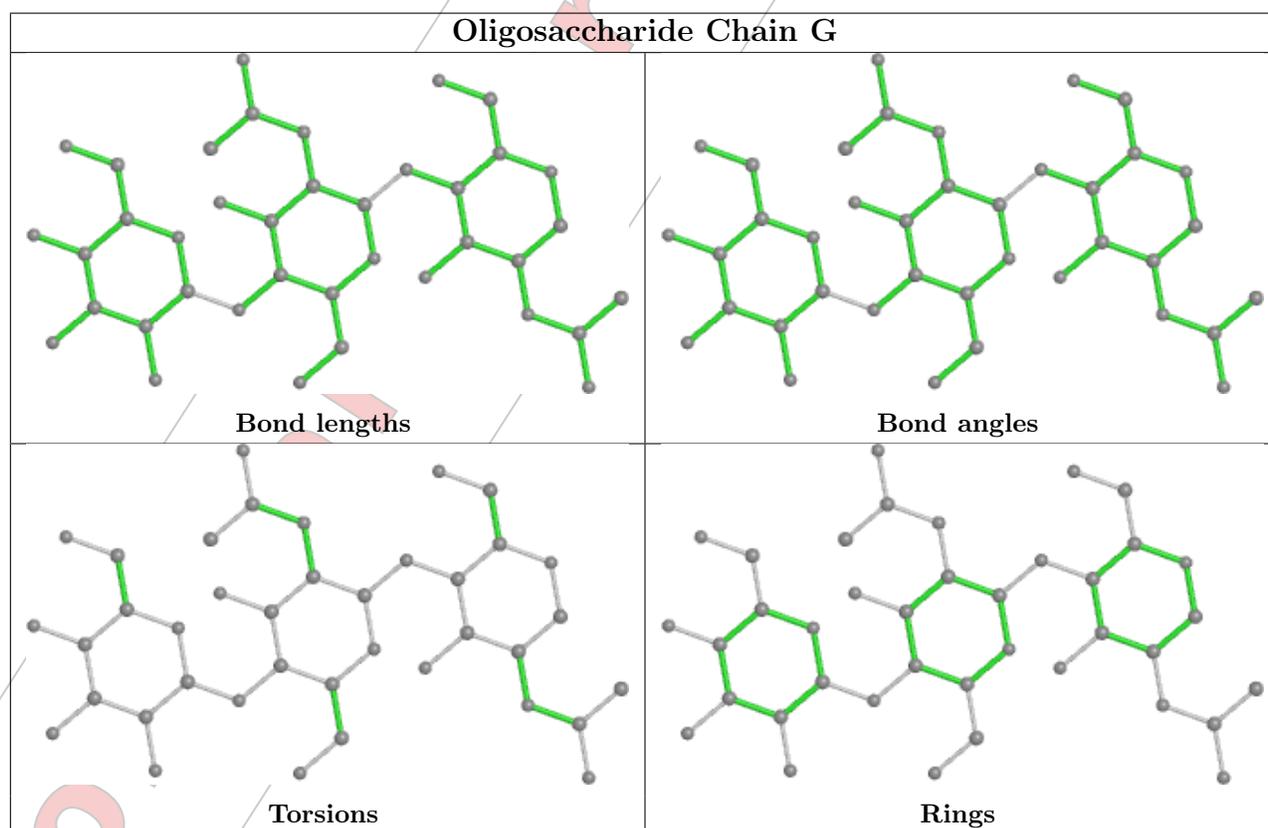
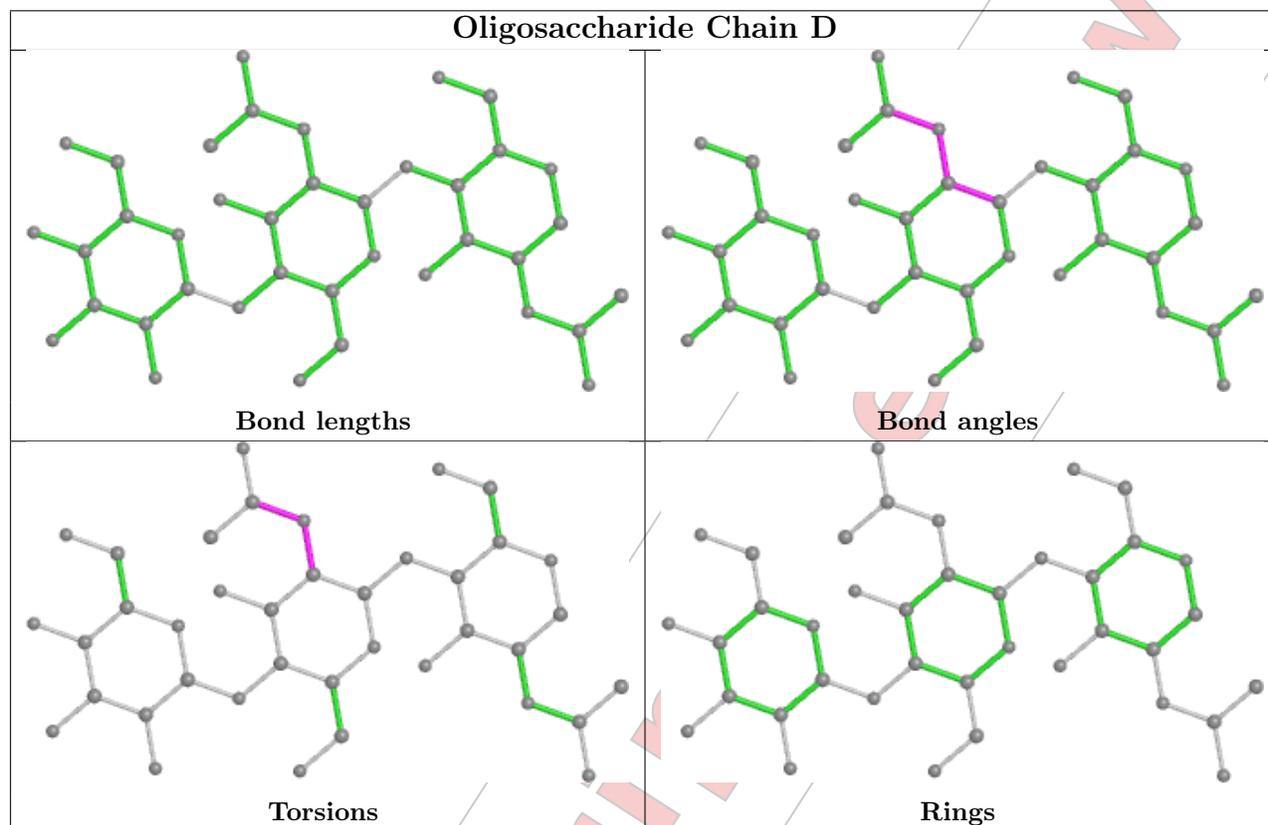


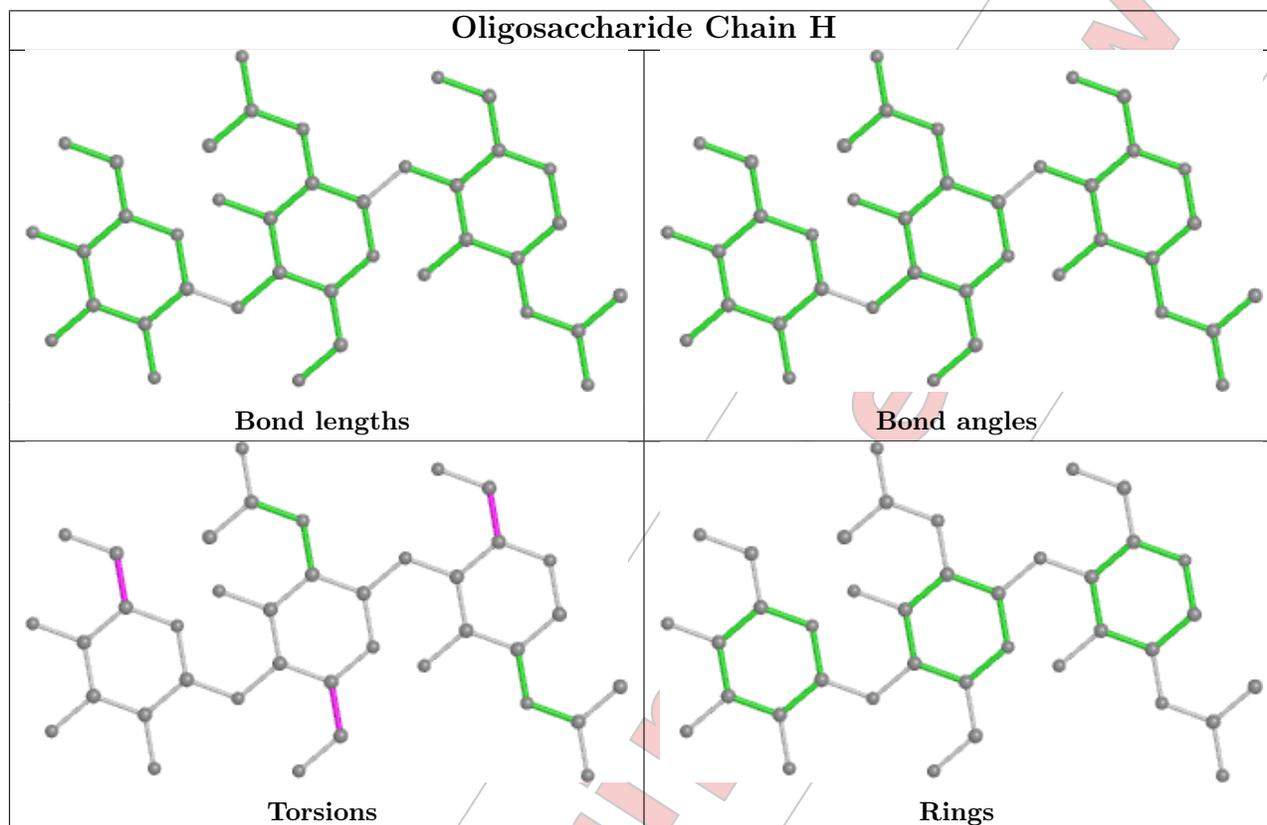


For Manuscript



For Manuscript





5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
5	NAG	C	601	2	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	B	1001	1	14,14,15	0.89	1 (7%)	17,19,21	0.82	1 (5%)
5	NAG	C	602	2	14,14,15	0.18	0	17,19,21	0.39	0
5	NAG	B	1003	1	14,14,15	0.18	0	17,19,21	0.46	0
5	NAG	B	1002	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	601	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
5	NAG	C	602	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1002	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	NAG	O5-C1	2.65	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1002	NAG	O5-C1-C2	-3.79	105.31	111.29
5	B	1001	NAG	C1-O5-C5	3.16	116.48	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1002	NAG	C8-C7-N2-C2
5	B	1002	NAG	O7-C7-N2-C2
5	B	1002	NAG	O5-C5-C6-O6
5	B	1001	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	B	1002	NAG	C4-C5-C6-O6
5	B	1001	NAG	O5-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	B	1003	NAG	O5-C5-C6-O6
5	B	1003	NAG	C4-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6
5	C	602	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
5	C	601	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.

For Manuscript Review

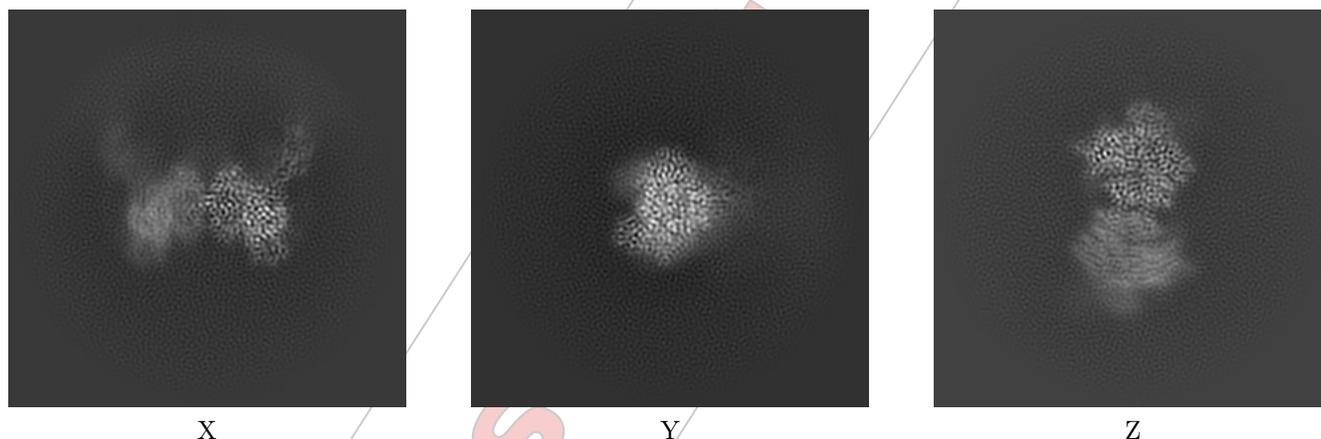
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67326. These allow visual inspection of the internal detail of the map and identification of artifacts.

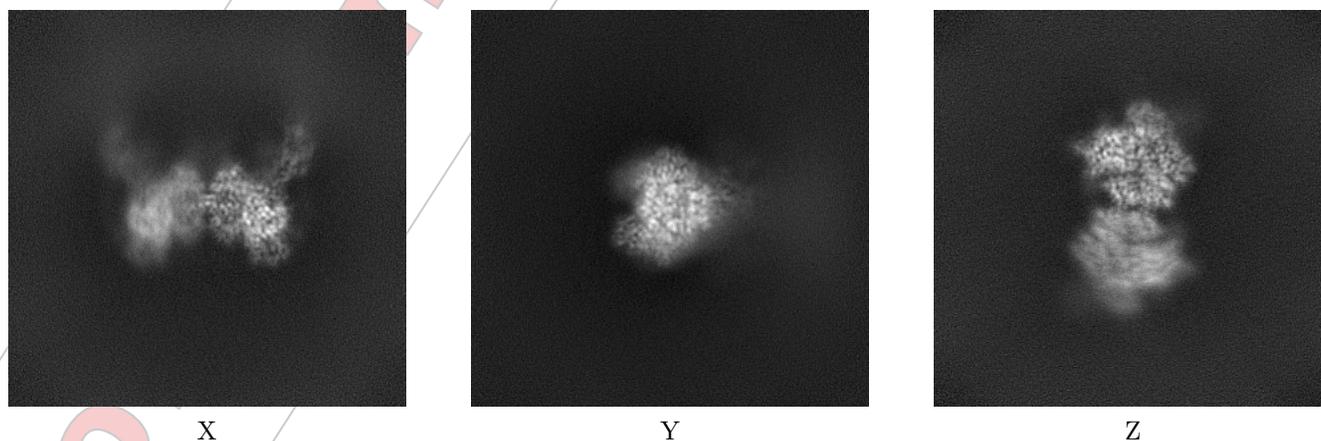
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



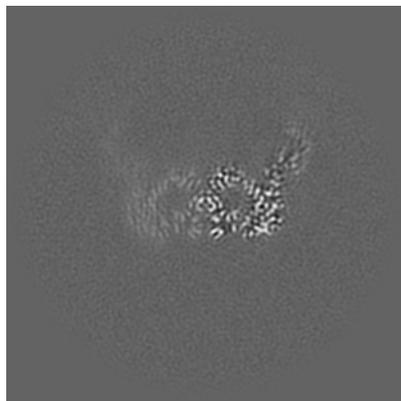
6.1.2 Raw map



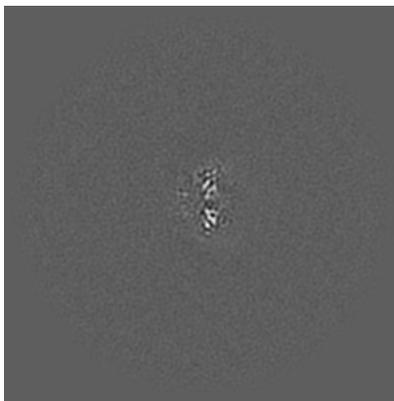
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

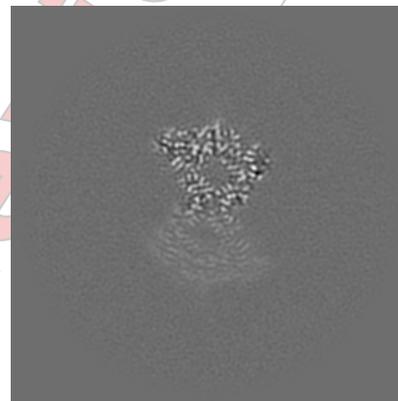
6.2.1 Primary map



X Index: 180

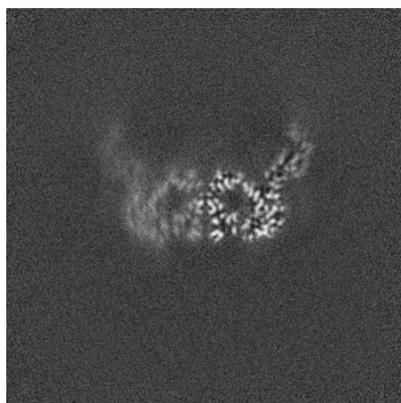


Y Index: 180



Z Index: 180

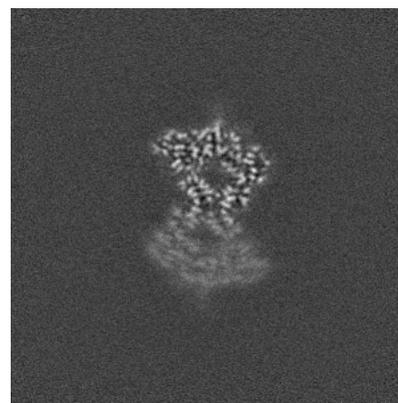
6.2.2 Raw map



X Index: 180



Y Index: 180

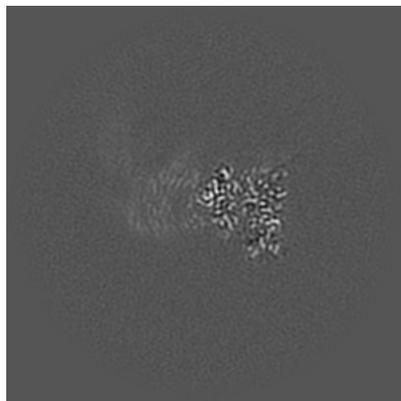


Z Index: 180

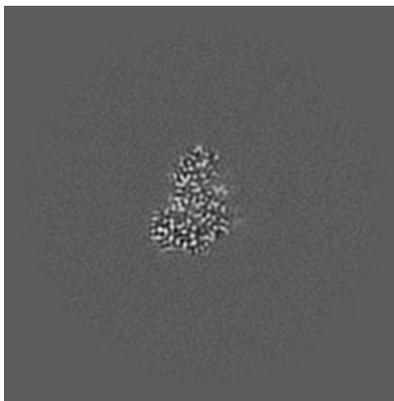
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

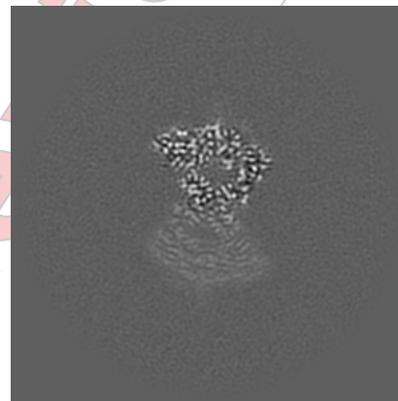
6.3.1 Primary map



X Index: 168

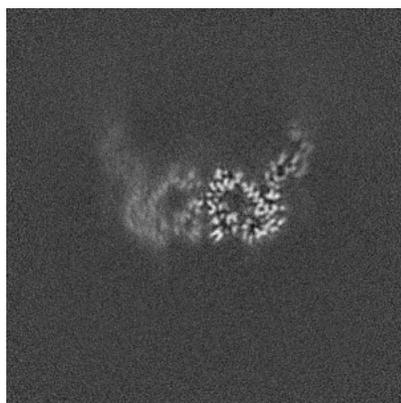


Y Index: 226

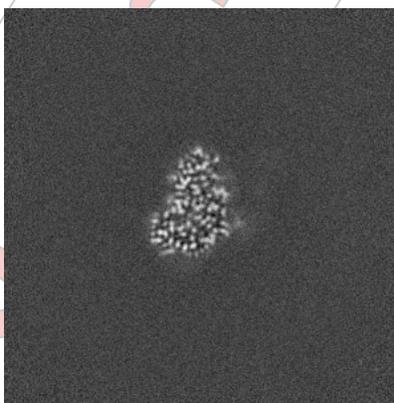


Z Index: 179

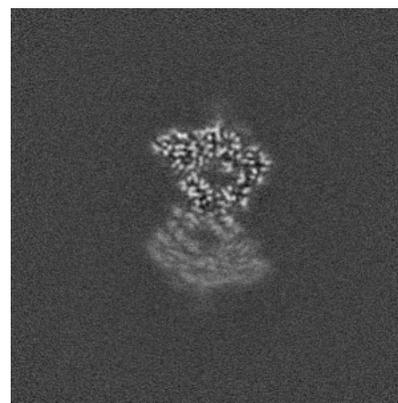
6.3.2 Raw map



X Index: 179



Y Index: 226

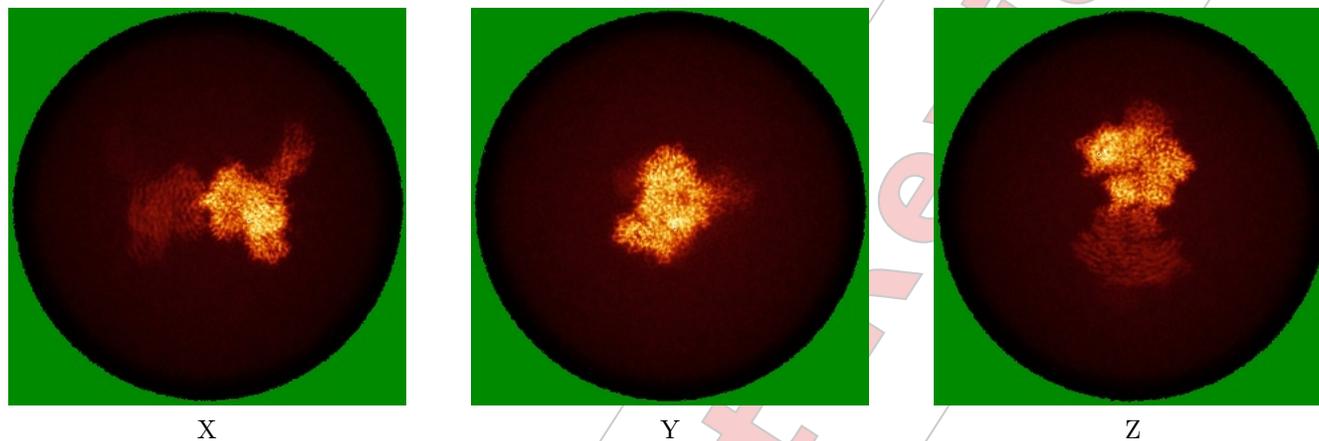


Z Index: 179

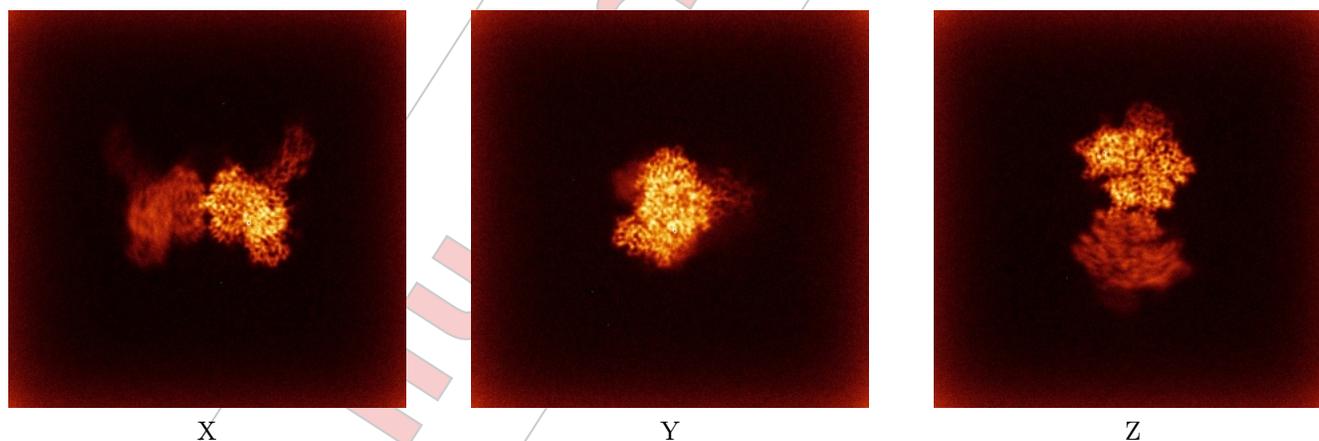
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



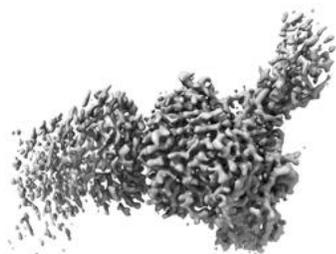
6.4.2 Raw map



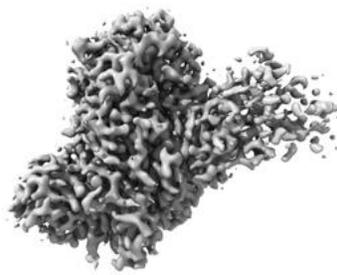
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.374. 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



X



Y



Z

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.

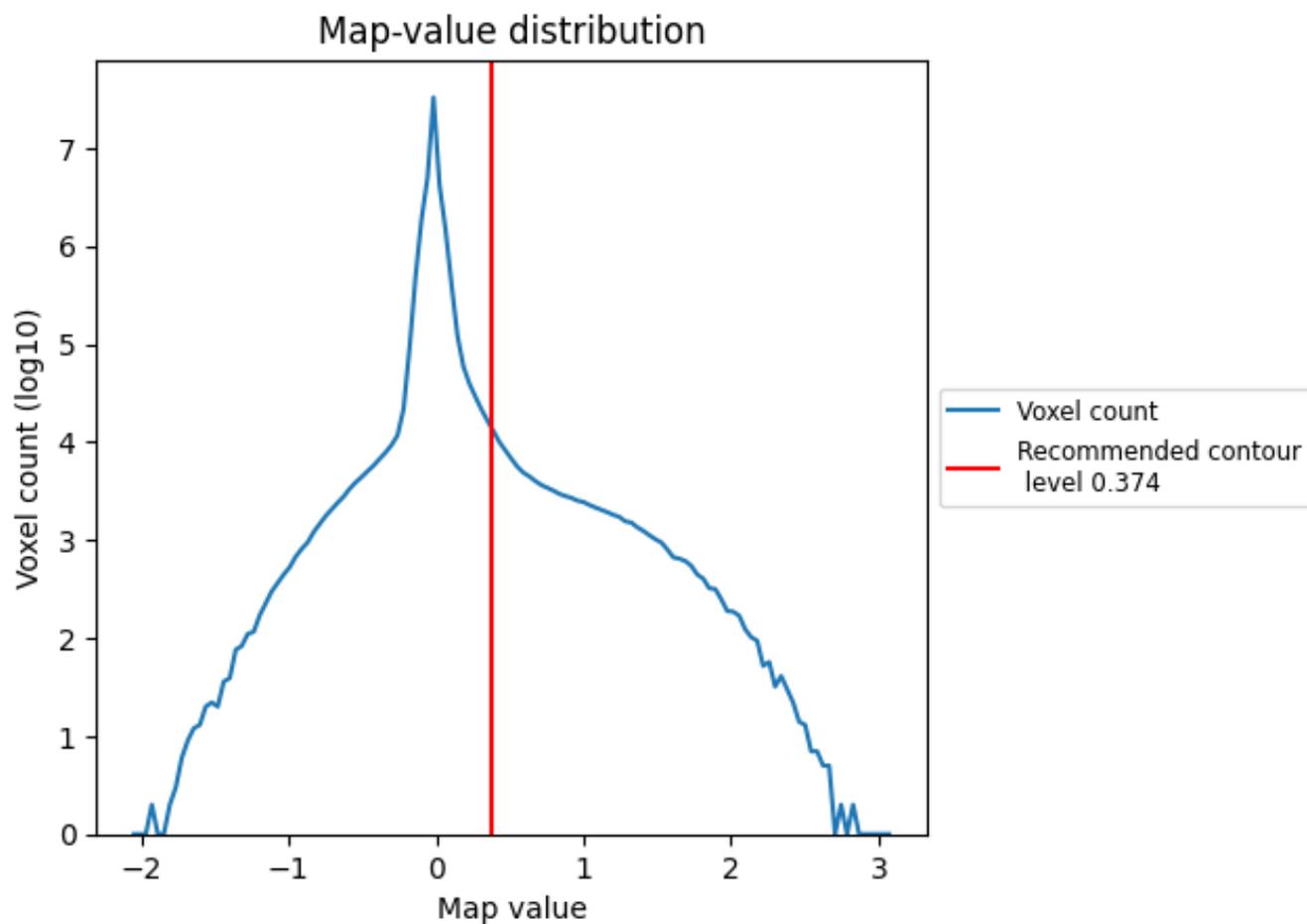
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

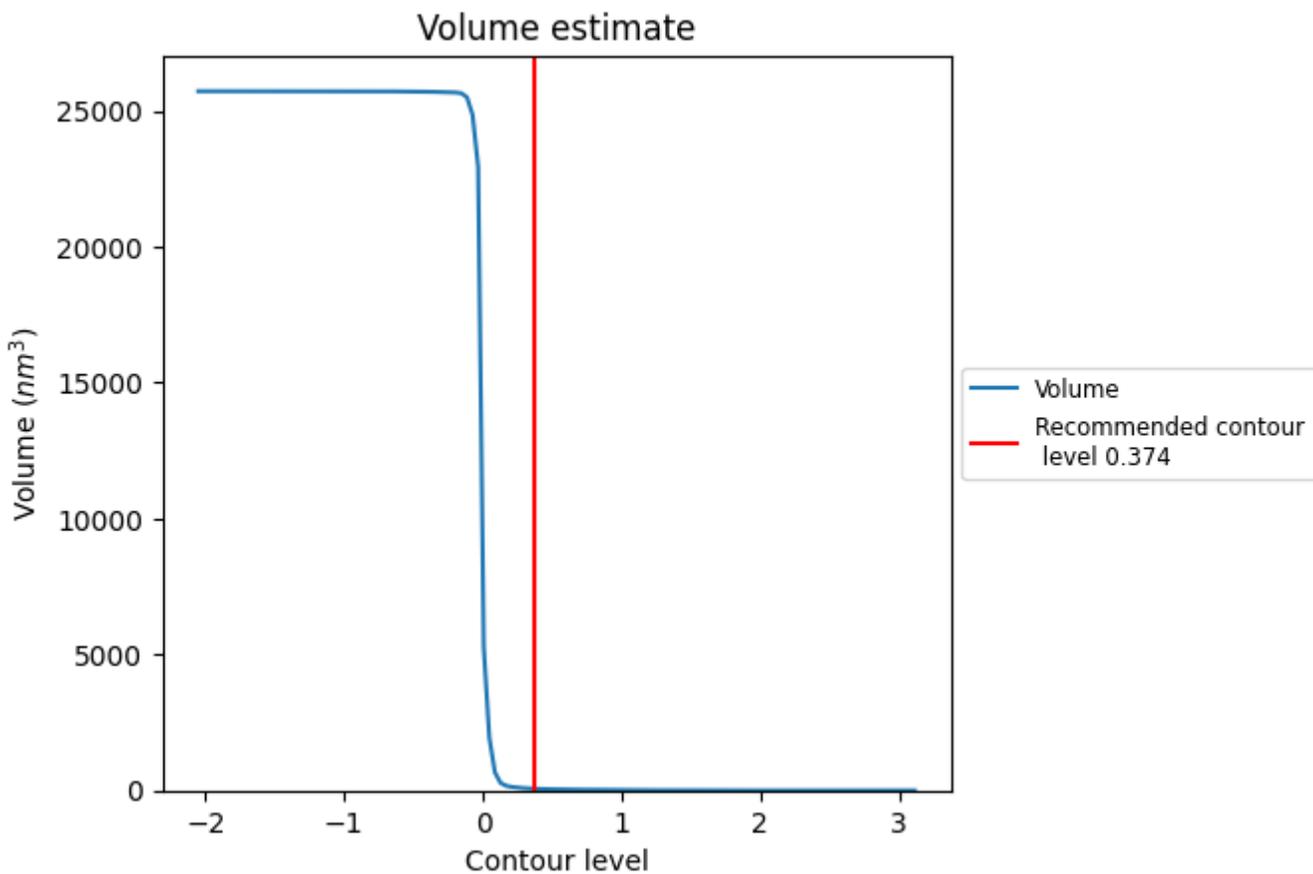
This section contains the results of statistical analysis of the map.

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.

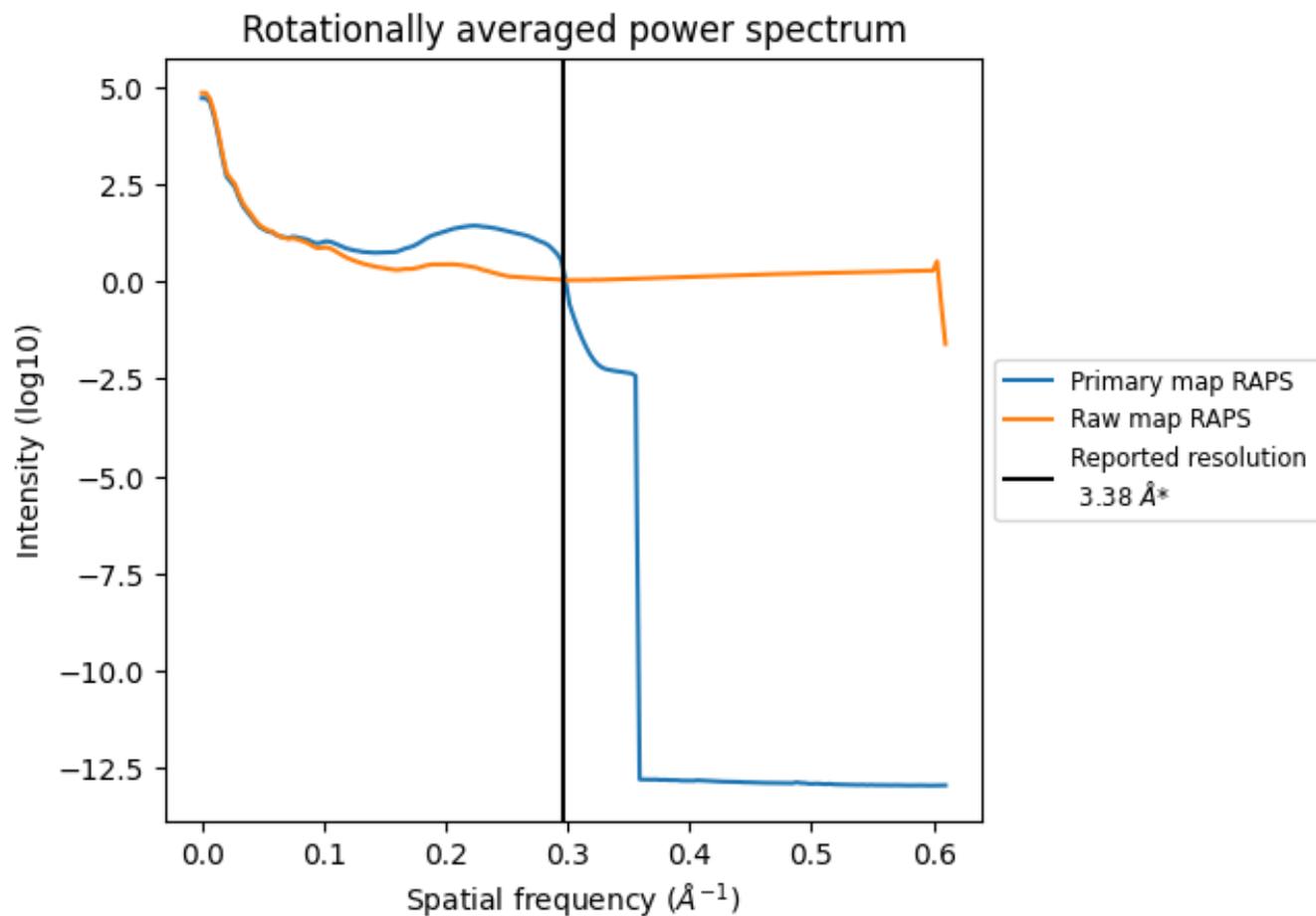
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 ⓘ

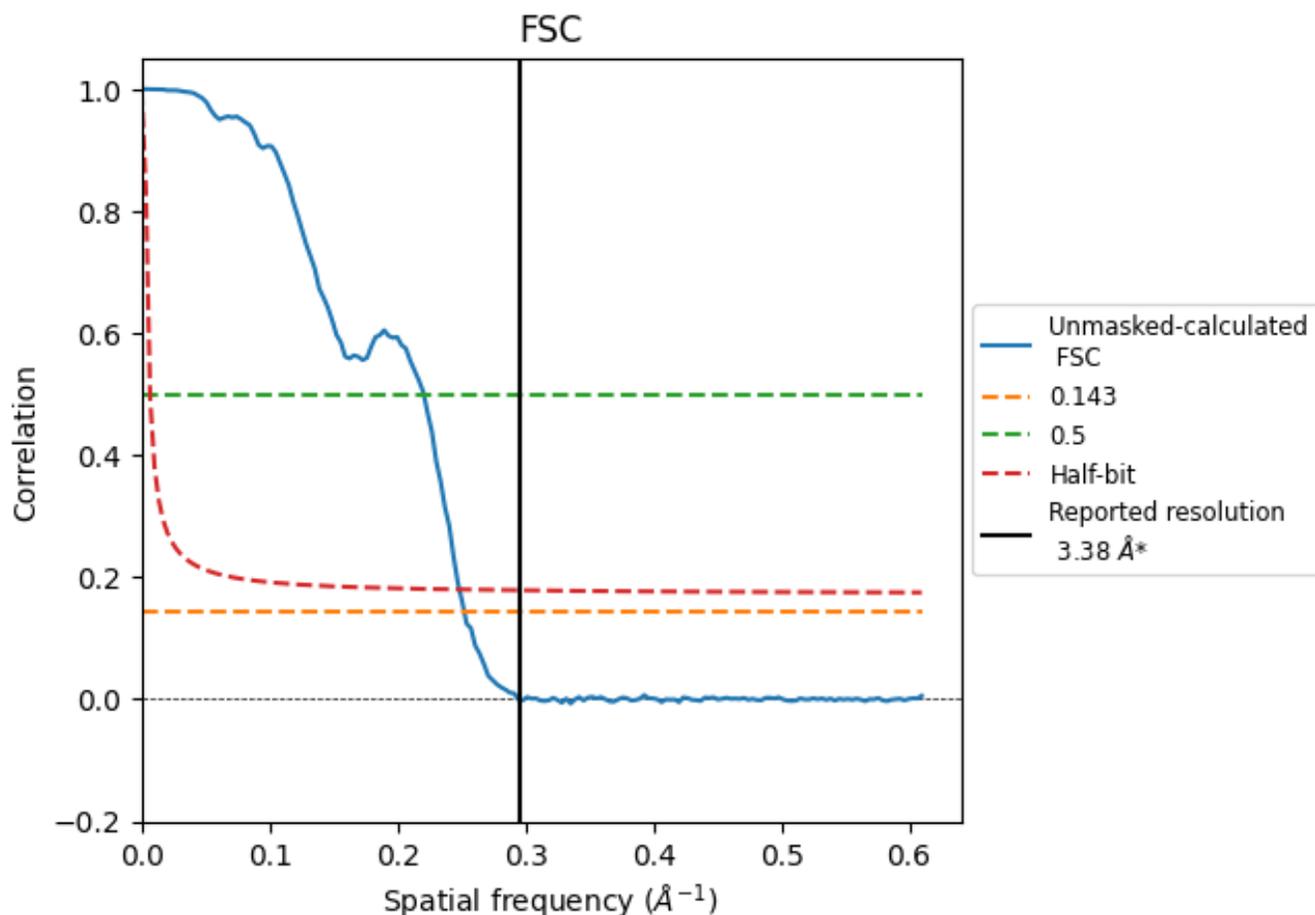


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

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 0.296 Å⁻¹

8.2 Resolution estimates [\(i\)](#)

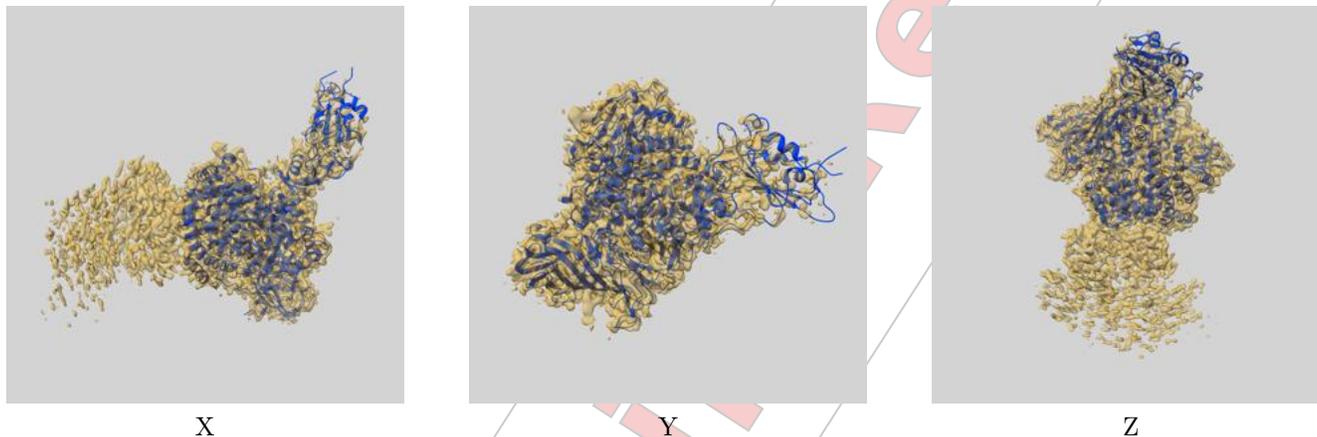
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	4.54	4.02

*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 3.97 differs from the reported value 3.38 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67326 and PDB model 9XW6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



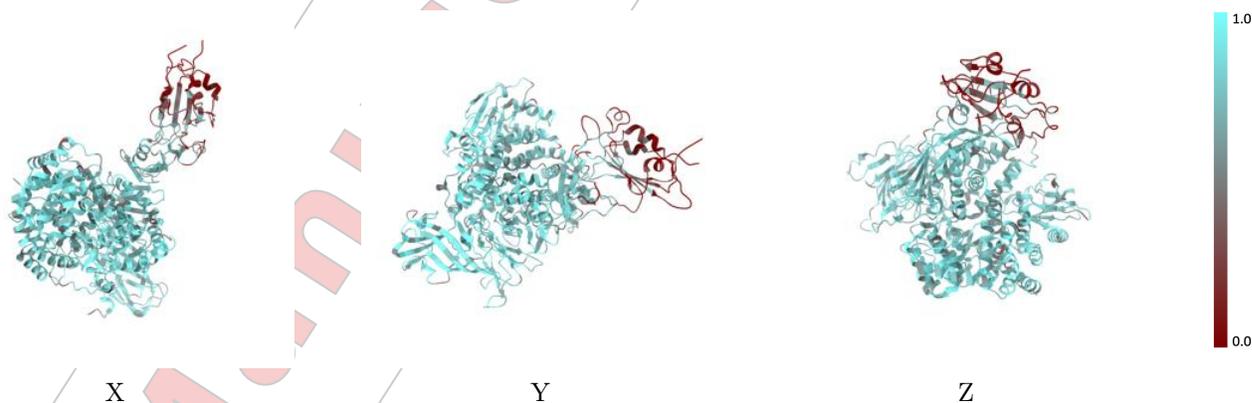
The images above show the 3D surface view of the map at the recommended contour level 0.374 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



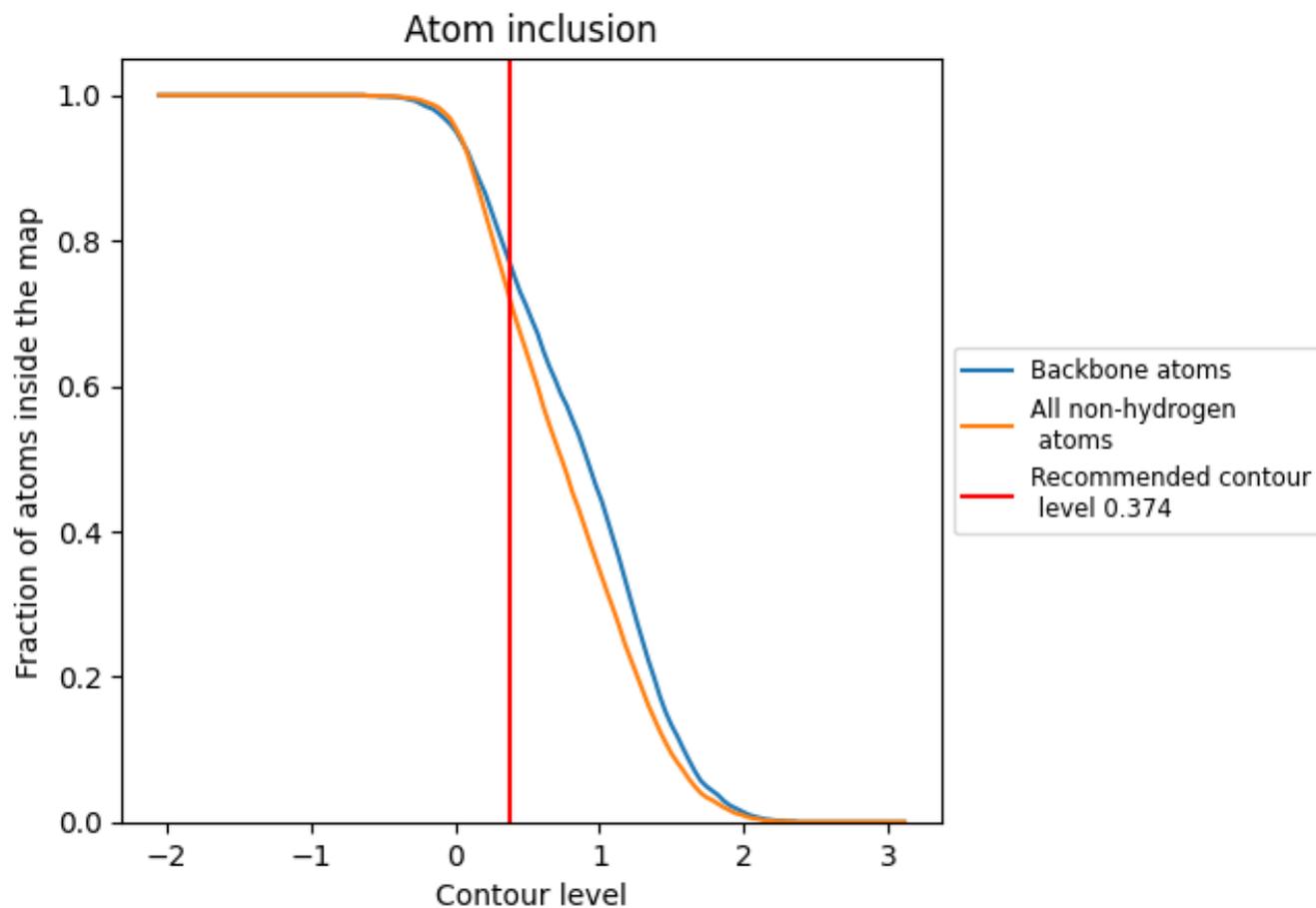
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.374).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 72% 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 (0.374) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.4520
A	 0.3570	 0.2290
B	 0.8080	 0.4830
C	 0.4090	 0.3360
D	 0.5380	 0.4050
E	 0.2140	 0.3340
F	 0.4640	 0.2490
G	 0.1030	 0.3490
H	 0.0000	 0.0480

