



Full wwPDB EM Validation Report ⓘ

Jul 20, 2023 – 12:41 PM JST

PDB ID : 7YFI
EMDB ID : EMD-33791
Title : Structure of the Rat tri-heteromeric GluN1-GluN2A-GluN2C NMDA receptor
in complex with glycine and glutamate
Authors : Zhang, M.; Zhang, J.; Guo, F.; Li, Y.; Zhu, S.
Deposited on : 2022-07-08
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

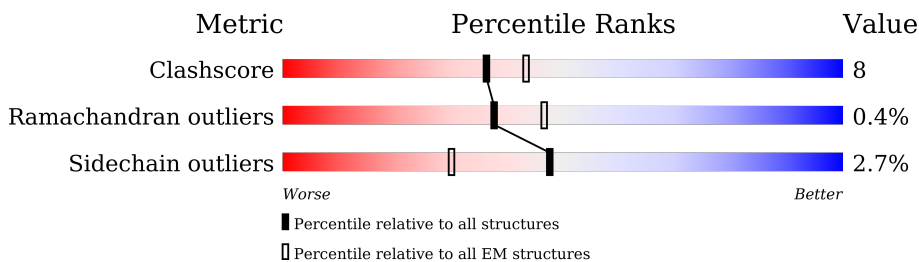
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	798	
1	C	798	
2	B	838	
3	D	835	
4	E	2	
4	F	2	
4	G	2	
4	H	2	

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Mol	Chain	Length	Quality of chain
4	I	2	<p>50% 50%</p>
4	K	2	<p>50% 50%</p>
4	L	2	<p>50% 50%</p>
4	M	2	<p>100% 100%</p>
4	N	2	<p>50% 50%</p>
5	J	3	<p>67% 33% 67%</p>
5	O	3	<p>67% 67% 33%</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 24135 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	748	Total	C	N	O	S	0	0
			5941	3778	1032	1097	34		
1	C	745	Total	C	N	O	S	0	0
			5920	3765	1029	1092	34		

- Molecule 2 is a protein called Glutamate receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	734	Total	C	N	O	S	0	0
			5805	3732	957	1083	33		

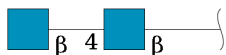
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PRO	-	expression tag	UNP G3V9C5

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	749	Total	C	N	O	S	0	0
			5815	3729	1001	1058	27		

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



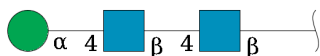
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-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
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



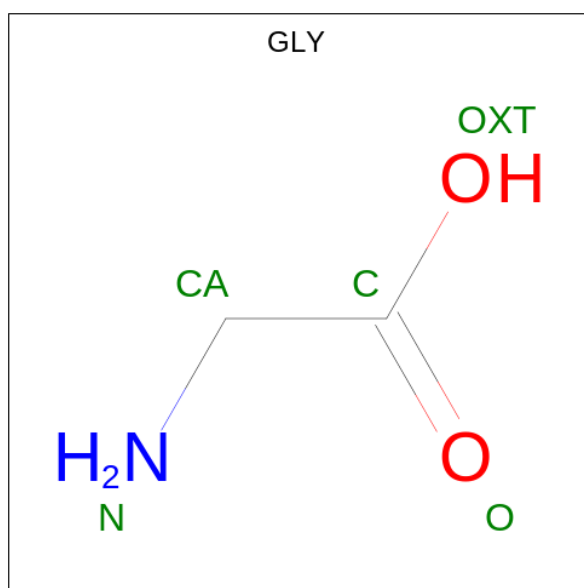
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	C	1	14	8	1	5	0
6	C	1	14	8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

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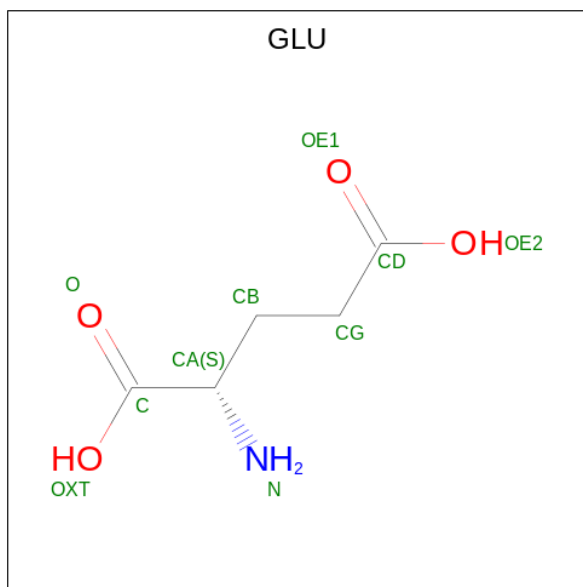
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	D	1	Total 14	C 8	N 1	O 5	0
6	D	1	Total 14	C 8	N 1	O 5	0

- Molecule 7 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 5	C 2	N 1	O 2	0
7	C	1	Total 5	C 2	N 1	O 2	0

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

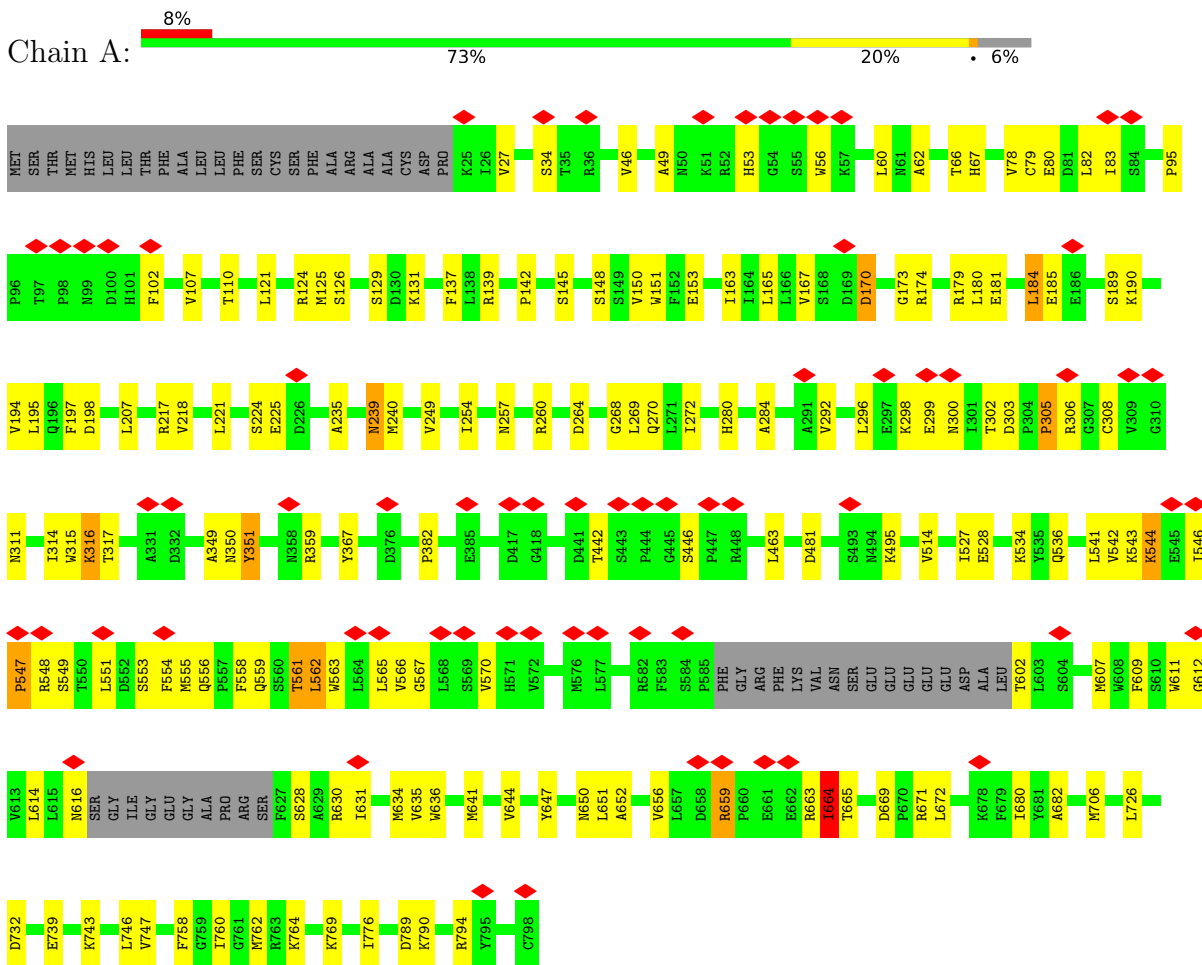


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	B	1	10	5	1	4	0
8	D	1	10	5	1	4	0

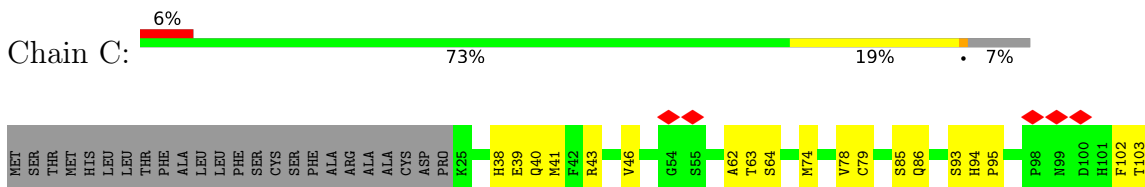
3 Residue-property plots [i](#)

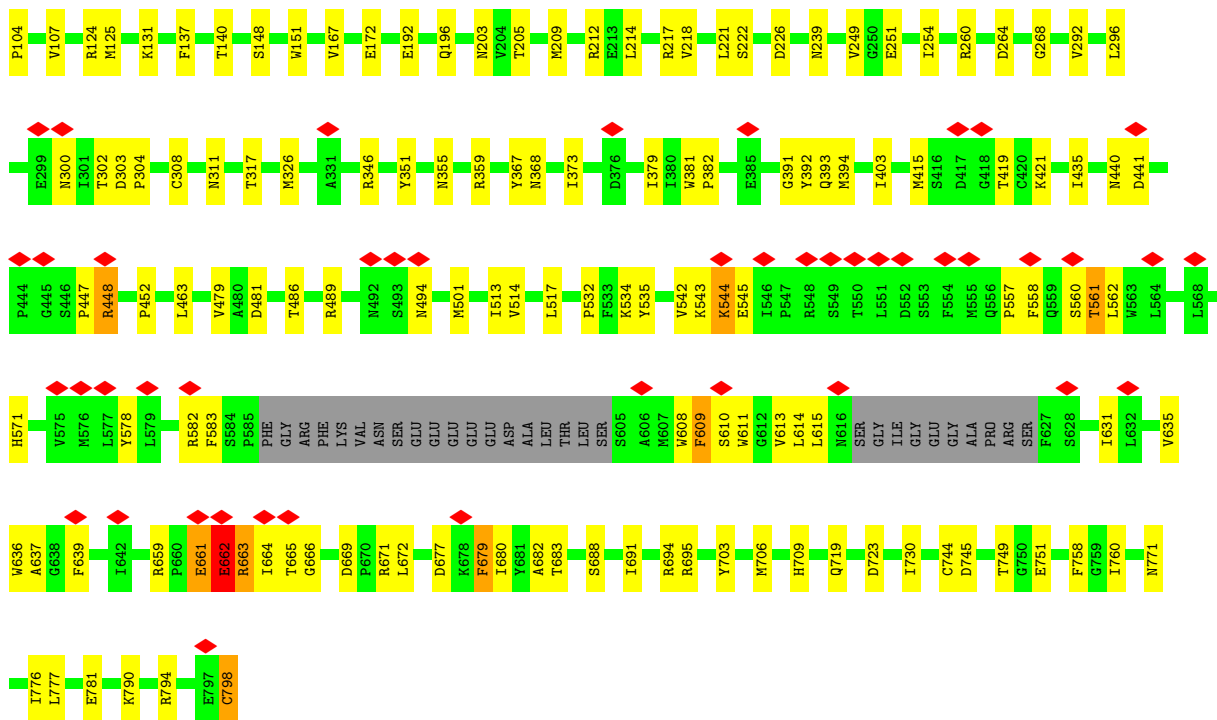
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Glutamate receptor ionotropic, NMDA 1

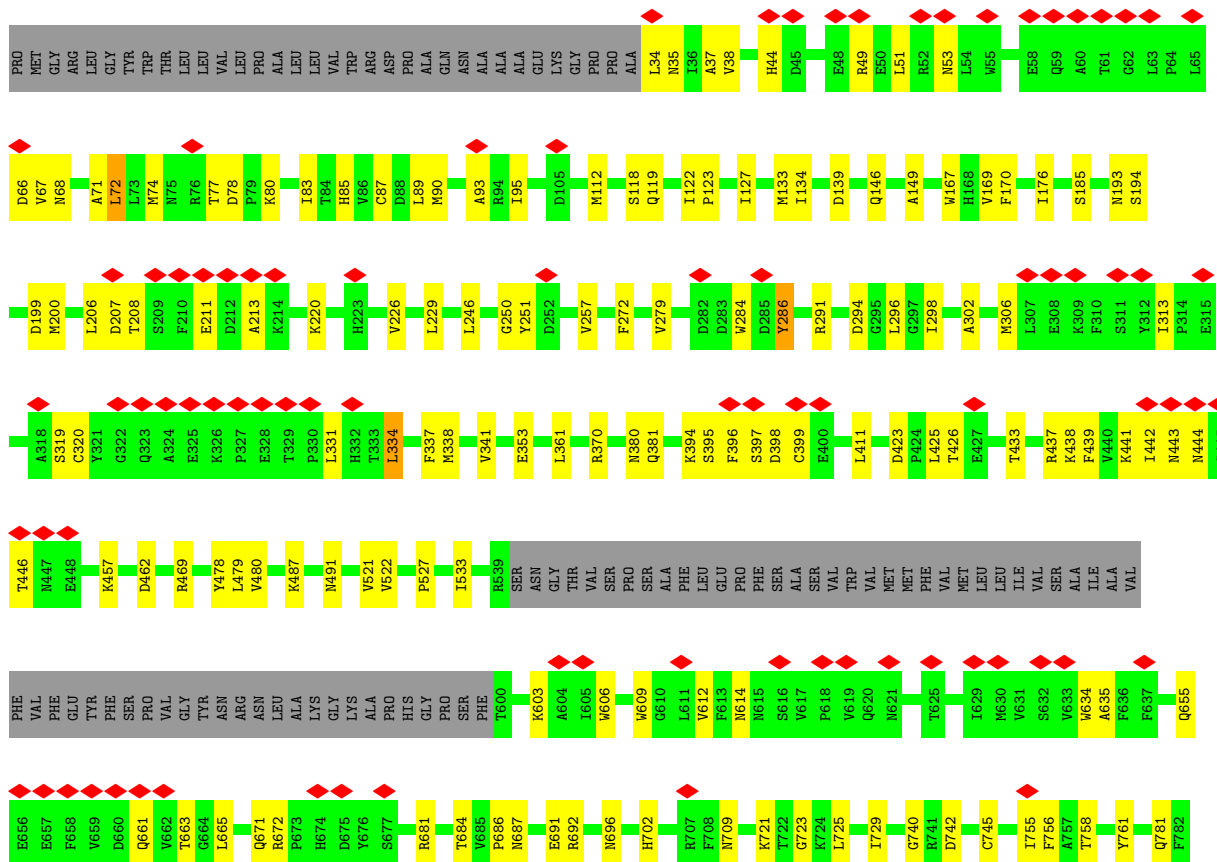


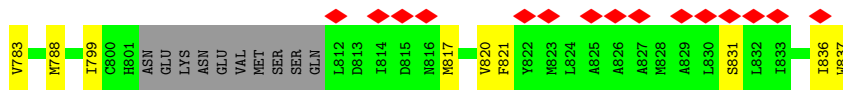
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



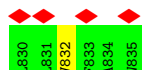
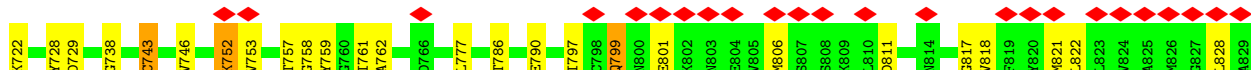
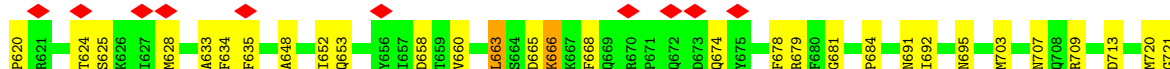
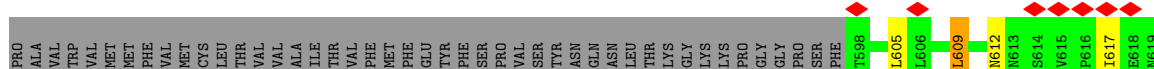
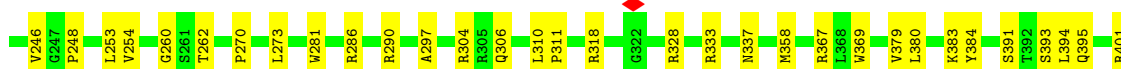


● Molecule 2: Glutamate receptor





• Molecule 3: Glutamate receptor ionotropic, NMDA 2C



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



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





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



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



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



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



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



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





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



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



- Molecule 5: alpha-D-mannopyranose-(1-4)-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, C1	Depositor
Number of particles used	278030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-10 (5k x 4k)	Depositor
Maximum map value	0.090	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	310.59, 310.59, 310.59	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.071, 1.071, 1.071	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: MAN, 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	0.27	0/6075	0.51	1/8230 (0.0%)
1	C	0.27	0/6054	0.50	0/8201
2	B	0.25	0/5940	0.48	0/8066
3	D	0.26	0/5953	0.51	0/8102
All	All	0.26	0/24022	0.50	1/32599 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	184	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	449	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5941	0	5901	110	0
1	C	5920	0	5880	117	0
2	B	5805	0	5735	96	0
3	D	5815	0	5833	92	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	1	0
4	K	28	0	25	2	0
4	L	28	0	25	2	0
4	M	28	0	25	0	0
4	N	28	0	25	1	0
5	J	39	0	34	1	0
5	O	39	0	34	0	0
6	A	98	0	91	0	0
6	B	70	0	65	2	0
6	C	98	0	91	5	0
6	D	28	0	26	1	0
7	A	5	0	2	1	0
7	C	5	0	2	2	0
8	B	10	0	5	0	0
8	D	10	0	5	2	0
All	All	24135	0	23929	404	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 8.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:HIS:CD2	1:C:611:TRP:CZ2	2.42	1.06
1:C:300:ASN:OD1	6:C:802:NAG:H2	1.56	1.02
1:C:543:LYS:HE3	1:C:745:ASP:HB2	1.04	1.02
1:C:571:HIS:NE2	1:C:611:TRP:CH2	2.29	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:LYS:CE	1:C:745:ASP:HB2	1.92	0.98
1:A:548:ARG:HE	1:A:549:SER:H	1.02	0.95
1:C:571:HIS:CD2	1:C:611:TRP:CH2	2.57	0.93
1:C:543:LYS:HE3	1:C:745:ASP:CB	1.98	0.92
2:B:635:ALA:HB1	1:C:615:LEU:HD22	1.52	0.91
1:A:83:ILE:HG13	1:A:306:ARG:HD2	1.56	0.88
1:C:543:LYS:HD2	1:C:745:ASP:O	1.75	0.86
1:C:571:HIS:NE2	1:C:611:TRP:CZ2	2.43	0.86
1:A:548:ARG:NE	1:A:549:SER:H	1.74	0.85
1:C:664:ILE:HB	1:C:669:ASP:OD2	1.76	0.85
1:A:546:ILE:HB	1:A:547:PRO:HD3	1.56	0.85
1:C:571:HIS:NE2	1:C:611:TRP:HH2	1.69	0.83
1:C:440:ASN:OD1	1:C:441:ASP:N	2.15	0.80
1:C:571:HIS:HD2	1:C:611:TRP:CZ2	2.00	0.79
3:D:752:LYS:HD2	3:D:753:VAL:HG13	1.65	0.79
1:C:571:HIS:CD2	1:C:611:TRP:HZ2	2.00	0.78
1:A:83:ILE:O	1:A:306:ARG:NH1	2.19	0.76
3:D:47:ARG:O	3:D:47:ARG:NE	2.19	0.73
1:A:80:GLU:O	1:A:83:ILE:HG22	1.88	0.72
1:C:664:ILE:HG22	1:C:666:GLY:H	1.54	0.72
1:A:272:ILE:HD12	1:A:350:ASN:HB3	1.72	0.71
2:B:298:ILE:HD11	2:B:338:MET:HB2	1.73	0.71
1:C:38:HIS:HA	1:C:41:MET:HG2	1.75	0.69
3:D:57:ASP:OD2	3:D:290:ARG:NH2	2.26	0.69
2:B:176:ILE:HG23	2:B:207:ASP:HA	1.74	0.68
1:C:662:GLU:C	1:C:671:ARG:HH12	1.97	0.68
3:D:383:LYS:HG2	3:D:384:TYR:CD1	2.29	0.67
3:D:98:ASN:O	3:D:99:VAL:HG13	1.94	0.67
1:A:78:VAL:HG21	1:A:107:VAL:HG22	1.78	0.66
1:C:665:THR:O	1:C:749:THR:OG1	2.10	0.66
2:B:433:THR:HG22	2:B:457:LYS:HB3	1.78	0.66
2:B:661:GLN:HG2	2:B:663:THR:HG23	1.79	0.65
3:D:761:ILE:HD12	3:D:777:LEU:HD11	1.78	0.65
1:C:682:ALA:HA	1:C:706:MET:HG2	1.79	0.65
1:A:663:ARG:NH2	1:A:747:VAL:HG11	2.12	0.64
2:B:279:VAL:HG12	2:B:361:LEU:HD12	1.79	0.64
1:C:663:ARG:HH12	1:C:672:LEU:HG	1.62	0.64
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.78	0.64
1:C:351:TYR:HB2	1:C:367:TYR:HB3	1.80	0.64
3:D:679:ARG:NH1	3:D:721:GLY:O	2.31	0.64
1:A:543:LYS:HG3	1:A:746:LEU:HD23	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:248:PRO:HD3	3:D:391:SER:HA	1.80	0.63
2:B:755:ILE:HG13	2:B:756:PHE:H	1.64	0.63
1:C:614:LEU:HB2	1:C:615:LEU:HD12	1.80	0.63
1:A:528:GLU:HG2	1:A:769:LYS:HD3	1.81	0.63
1:A:534:LYS:HB3	1:A:758:PHE:HB2	1.80	0.63
3:D:230:ARG:HH11	3:D:260:GLY:HA3	1.64	0.63
2:B:533:ILE:HG12	2:B:756:PHE:HB2	1.79	0.62
1:C:613:VAL:CG2	1:C:637:ALA:HB2	2.29	0.62
1:C:534:LYS:HB3	1:C:758:PHE:HB2	1.81	0.62
3:D:212:THR:OG1	3:D:239:GLU:OE2	2.17	0.62
1:C:613:VAL:HG21	1:C:637:ALA:HB2	1.82	0.62
1:A:647:TYR:CZ	1:A:651:LEU:HD11	2.35	0.62
2:B:49:ARG:O	2:B:53:ASN:ND2	2.30	0.61
3:D:304:ARG:HH21	3:D:310:LEU:HG	1.66	0.61
2:B:72:LEU:HG	2:B:89:LEU:HD21	1.82	0.60
1:A:760:ILE:HD12	1:A:776:ILE:HD11	1.83	0.60
3:D:128:VAL:O	3:D:141:GLN:NE2	2.33	0.60
3:D:818:VAL:O	3:D:822:LEU:HG	2.00	0.60
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.83	0.60
1:C:688:SER:HB3	7:C:808:GLY:O	2.00	0.60
1:C:78:VAL:HG21	1:C:107:VAL:HG22	1.84	0.60
1:A:167:VAL:HG13	1:A:173:GLY:HA3	1.83	0.60
2:B:133:MET:O	2:B:146:GLN:NE2	2.34	0.59
1:C:694:ARG:HD3	1:C:703:TYR:HE2	1.66	0.59
1:A:49:ALA:O	1:A:53:HIS:ND1	2.35	0.59
1:A:570:VAL:HG12	1:A:636:TRP:HH2	1.66	0.59
1:A:181:GLU:O	1:A:185:GLU:HG2	2.03	0.59
1:C:613:VAL:HG11	1:C:636:TRP:NE1	2.18	0.59
2:B:306:MET:HG3	2:B:337:PHE:HE2	1.66	0.58
1:A:34:SER:OG	1:A:67:HIS:N	2.36	0.58
2:B:220:LYS:HD3	2:B:246:LEU:HD22	1.86	0.58
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.85	0.58
1:C:308:CYS:O	3:D:75:SER:OG	2.19	0.58
2:B:614:ASN:OD1	1:C:615:LEU:HB3	2.04	0.57
3:D:310:LEU:HD22	3:D:311:PRO:HD2	1.86	0.57
1:C:93:SER:OG	1:C:94:HIS:N	2.38	0.57
2:B:272:PHE:O	2:B:370:ARG:NH1	2.37	0.57
2:B:286:TYR:OH	2:B:294:ASP:OD2	2.18	0.57
2:B:211:GLU:HG3	2:B:213:ALA:H	1.69	0.57
1:C:239:ASN:HB3	6:C:801:NAG:H83	1.86	0.57
2:B:394:LYS:HG3	2:B:397:SER:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:660:VAL:HG21	3:D:668:PHE:HE2	1.70	0.57
2:B:444:ASN:HB2	6:B:905:NAG:H4	1.87	0.56
3:D:246:VAL:HG13	3:D:270:PRO:HB3	1.87	0.56
1:A:129:SER:OG	1:A:139:ARG:NH2	2.38	0.56
2:B:35:ASN:ND2	2:B:93:ALA:O	2.39	0.56
2:B:139:ASP:N	2:B:139:ASP:OD1	2.39	0.56
2:B:487:LYS:HD2	2:B:687:ASN:HA	1.87	0.56
3:D:379:VAL:HG13	3:D:424:GLY:HA3	1.88	0.56
3:D:438:ASN:HB3	6:D:902:NAG:H2	1.88	0.56
3:D:811:ASP:N	3:D:811:ASP:OD1	2.39	0.56
1:C:212:ARG:HH21	6:C:801:NAG:H81	1.71	0.55
1:C:463:LEU:HB2	1:C:514:VAL:HG11	1.88	0.55
1:C:543:LYS:O	1:C:543:LYS:HG3	2.07	0.55
1:A:612:GLY:O	1:A:616:ASN:N	2.31	0.55
1:C:205:THR:HG21	4:L:1:NAG:H4	1.89	0.55
2:B:755:ILE:HG13	2:B:756:PHE:N	2.22	0.55
1:A:566:VAL:O	1:A:570:VAL:HG13	2.06	0.55
1:A:46:VAL:HG21	1:A:62:ALA:HB2	1.88	0.54
3:D:220:ASP:OD1	3:D:220:ASP:N	2.39	0.54
1:A:124:ARG:NH2	1:A:351:TYR:OH	2.40	0.54
1:A:650:ASN:OD1	1:A:651:LEU:N	2.40	0.54
3:D:430:THR:HG22	3:D:455:LYS:HB3	1.89	0.54
1:A:131:LYS:NZ	1:A:137:PHE:O	2.41	0.54
3:D:393:SER:HG	3:D:394:LEU:H	1.55	0.54
2:B:37:ALA:HB2	2:B:95:ILE:HG21	1.90	0.54
3:D:47:ARG:HH22	3:D:64:PRO:HG2	1.72	0.54
1:A:544:LYS:HD2	1:A:747:VAL:HB	1.90	0.54
1:C:489:ARG:NH2	1:C:494:ASN:OD1	2.38	0.53
3:D:49:ARG:HD3	3:D:286:ARG:HD3	1.89	0.53
1:A:170:ASP:HB3	1:A:174:ARG:HH21	1.73	0.53
1:A:270:GLN:O	1:A:351:TYR:HA	2.07	0.53
2:B:437:ARG:HG2	2:B:478:TYR:HB2	1.91	0.53
2:B:671:GLN:O	2:B:672:ARG:HD2	2.08	0.53
1:C:777:LEU:O	1:C:781:GLU:HG2	2.09	0.53
1:A:680:ILE:HG22	1:A:726:LEU:HD23	1.91	0.53
3:D:395:GLN:N	3:D:395:GLN:OE1	2.41	0.53
1:A:79:CYS:SG	2:B:80:LYS:HB2	2.49	0.53
1:A:80:GLU:O	1:A:83:ILE:CG2	2.57	0.53
1:A:257:ASN:HA	1:A:260:ARG:HG3	1.91	0.53
2:B:66:ASP:O	2:B:68:ASN:N	2.42	0.53
1:C:665:THR:HB	1:C:749:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HE	1:A:549:SER:N	1.87	0.52
3:D:684:PRO:HB3	3:D:707:ASN:HD21	1.75	0.52
3:D:59:PRO:HB3	3:D:297:ALA:HB1	1.92	0.52
1:A:142:PRO:HG3	1:A:349:ALA:HB2	1.91	0.52
1:A:305:PRO:HB2	1:A:311:ASN:ND2	2.24	0.52
1:C:46:VAL:HG11	1:C:62:ALA:HB2	1.92	0.52
1:C:254:ILE:HD13	1:C:268:GLY:HA3	1.91	0.52
2:B:411:LEU:HD13	2:B:480:VAL:HG12	1.91	0.52
2:B:614:ASN:OD1	1:C:615:LEU:HD23	2.10	0.52
1:C:131:LYS:NZ	1:C:137:PHE:O	2.41	0.52
3:D:660:VAL:HG21	3:D:668:PHE:CE2	2.43	0.52
1:A:308:CYS:HA	2:B:78:ASP:OD2	2.10	0.52
2:B:521:VAL:HG23	2:B:522:VAL:HG13	1.91	0.52
2:B:123:PRO:HG2	2:B:334:LEU:HD13	1.92	0.52
1:A:150:VAL:HG11	1:A:269:LEU:HD11	1.92	0.52
2:B:353:GLU:N	2:B:353:GLU:OE1	2.43	0.52
1:A:669:ASP:HB3	1:A:672:LEU:HD12	1.91	0.51
3:D:93:ILE:HB	3:D:119:ILE:HG12	1.91	0.51
3:D:144:VAL:HG21	3:D:358:MET:HE1	1.91	0.51
2:B:206:LEU:O	2:B:208:THR:N	2.42	0.51
1:C:760:ILE:HD12	1:C:776:ILE:HD11	1.92	0.51
1:A:732:ASP:OD2	7:A:808:GLY:N	2.43	0.51
1:C:571:HIS:NE2	1:C:611:TRP:HZ2	2.03	0.51
3:D:39:SER:OG	3:D:96:GLU:OE2	2.22	0.51
1:A:78:VAL:O	1:A:82:LEU:HG	2.10	0.51
1:C:578:TYR:OH	1:C:582:ARG:NH2	2.43	0.51
3:D:162:TRP:HB3	3:D:223:VAL:HG21	1.92	0.51
1:C:167:VAL:HG12	1:C:222:SER:HB3	1.91	0.51
2:B:149:ALA:HB2	2:B:361:LEU:HD21	1.92	0.51
1:C:86:GLN:NE2	1:C:304:PRO:O	2.43	0.51
1:A:165:LEU:HB3	1:A:194:VAL:HG12	1.93	0.51
1:A:299:GLU:O	1:A:300:ASN:C	2.48	0.51
2:B:229:LEU:HB3	2:B:257:VAL:HG12	1.92	0.50
2:B:681:ARG:HG3	2:B:725:LEU:HD12	1.93	0.50
1:C:302:THR:H	1:C:317:THR:HG21	1.77	0.50
1:C:659:ARG:HG3	1:C:661:GLU:OE1	2.10	0.50
1:C:661:GLU:O	1:C:662:GLU:C	2.50	0.50
3:D:666:LYS:HG3	3:D:674:GLN:OE1	2.12	0.50
1:C:85:SER:OG	4:K:2:NAG:H5	2.12	0.50
3:D:46:ALA:HA	3:D:49:ARG:HD2	1.92	0.50
1:A:664:ILE:HG23	1:A:671:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:ARG:N	1:C:671:ARG:HH12	2.10	0.50
2:B:250:GLY:HA2	2:B:396:PHE:HE1	1.77	0.49
2:B:302:ALA:HB2	2:B:338:MET:HB3	1.93	0.49
1:C:613:VAL:HG11	1:C:636:TRP:HE1	1.77	0.49
1:A:121:LEU:HD21	1:A:284:ALA:HB2	1.94	0.49
2:B:423:ASP:HB3	2:B:425:LEU:HD23	1.95	0.49
1:C:688:SER:N	7:C:808:GLY:O	2.44	0.49
1:C:447:PRO:O	1:C:448:ARG:NE	2.45	0.49
1:A:558:PHE:HB3	1:A:561:THR:HG23	1.94	0.49
3:D:433:CYS:HB3	3:D:475:LEU:HD23	1.94	0.49
1:C:663:ARG:HH22	1:C:672:LEU:HD21	1.78	0.49
2:B:250:GLY:HA2	2:B:396:PHE:CE1	2.47	0.49
1:C:40:GLN:OE1	1:C:43:ARG:NH1	2.46	0.49
1:C:218:VAL:HG23	1:C:391:GLY:HA3	1.95	0.48
3:D:817:GLY:O	3:D:821:MET:HG2	2.13	0.48
1:A:121:LEU:HB3	1:A:280:HIS:HB3	1.94	0.48
3:D:605:LEU:HD12	3:D:617:ILE:HB	1.94	0.48
1:A:235:ALA:HB1	1:A:240:MET:HB3	1.94	0.48
1:A:546:ILE:HB	1:A:547:PRO:CD	2.38	0.48
1:A:551:LEU:HD23	1:A:551:LEU:H	1.78	0.48
1:C:680:ILE:HD11	1:C:709:HIS:CG	2.49	0.48
3:D:709:ARG:NH2	3:D:713:ASP:OD2	2.47	0.48
1:A:195:LEU:HB3	1:A:207:LEU:HD22	1.95	0.48
1:A:565:LEU:HD12	1:A:565:LEU:H	1.77	0.48
2:B:306:MET:HG3	2:B:337:PHE:CE2	2.47	0.48
1:C:557:PRO:HB2	1:C:558:PHE:CE2	2.48	0.48
3:D:681:GLY:HA2	3:D:703:MET:HG3	1.96	0.48
3:D:620:PRO:HB2	3:D:625:SER:HB3	1.96	0.48
3:D:81:ILE:HG21	3:D:111:VAL:HG11	1.94	0.47
2:B:90:MET:SD	2:B:122:ILE:HD11	2.53	0.47
2:B:169:VAL:HA	2:B:199:ASP:HB3	1.97	0.47
2:B:691:GLU:OE2	2:B:702:HIS:NE2	2.47	0.47
3:D:333:ARG:HG2	4:N:2:NAG:H82	1.95	0.47
2:B:394:LYS:HE3	2:B:397:SER:H	1.80	0.47
1:C:542:VAL:HG23	1:C:544:LYS:HB2	1.95	0.47
1:C:790:LYS:HB2	1:C:794:ARG:HH21	1.76	0.47
1:C:373:ILE:HG13	1:C:373:ILE:O	2.14	0.47
1:C:148:SER:HA	1:C:151:TRP:CE3	2.50	0.47
3:D:799:GLN:HE22	3:D:801:GLU:HA	1.80	0.47
1:A:682:ALA:HA	1:A:706:MET:HG2	1.96	0.47
2:B:394:LYS:NZ	2:B:399:CYS:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:LYS:NZ	2:B:742:ASP:OD1	2.41	0.47
1:C:63:THR:HG23	4:K:1:NAG:H62	1.96	0.47
1:C:74:MET:HE2	1:C:78:VAL:HG23	1.97	0.47
2:B:443:ASN:HB3	6:B:905:NAG:H2	1.97	0.47
3:D:189:SER:HG	3:D:193:TRP:HE1	1.62	0.46
3:D:786:THR:O	3:D:790:GLU:HG3	2.15	0.46
1:A:790:LYS:HG3	1:A:794:ARG:HH21	1.81	0.46
1:C:435:ILE:HD11	1:C:452:PRO:HB2	1.96	0.46
1:C:486:THR:HG22	1:C:691:ILE:HD11	1.97	0.46
1:A:180:LEU:O	1:A:184:LEU:HD22	2.15	0.46
1:A:239:ASN:N	1:A:239:ASN:OD1	2.48	0.46
2:B:127:ILE:HG23	2:B:291:ARG:HB3	1.98	0.46
2:B:380:ASN:HB3	2:B:381:GLN:H	1.54	0.46
2:B:38:VAL:HG22	2:B:296:LEU:HD21	1.96	0.46
3:D:720:MET:SD	3:D:722:LYS:HB2	2.55	0.46
1:A:179:ARG:HE	1:A:179:ARG:HB3	1.56	0.46
1:A:628:SER:OG	2:B:831:SER:HB2	2.16	0.46
3:D:337:ASN:OD1	3:D:337:ASN:N	2.44	0.46
3:D:728:TYR:CZ	8:D:903:GLU:HG3	2.50	0.46
2:B:118:SER:OG	2:B:119:GLN:NE2	2.49	0.46
2:B:783:VAL:HG22	2:B:788:MET:HG3	1.97	0.46
3:D:383:LYS:HG2	3:D:384:TYR:CE1	2.51	0.46
3:D:407:THR:HG22	3:D:507:ILE:HG22	1.98	0.46
1:A:163:ILE:HG22	1:A:218:VAL:HB	1.96	0.46
2:B:85:HIS:O	2:B:89:LEU:HD13	2.16	0.46
2:B:394:LYS:HA	2:B:394:LYS:HD2	1.69	0.46
1:C:217:ARG:NH2	1:C:393:GLN:OE1	2.48	0.46
1:C:292:VAL:O	1:C:296:LEU:HG	2.16	0.46
1:C:355:ASN:ND2	1:C:379:ILE:HG23	2.30	0.46
1:A:189:SER:OG	1:A:190:LYS:N	2.49	0.46
1:A:630:ARG:O	1:A:634:MET:HG3	2.15	0.46
1:A:663:ARG:HH22	1:A:747:VAL:HG11	1.80	0.46
2:B:603:LYS:HG3	2:B:606:TRP:HZ3	1.81	0.46
2:B:684:THR:HG22	2:B:729:ILE:O	2.16	0.46
1:C:260:ARG:O	1:C:359:ARG:NH2	2.49	0.46
3:D:691:ASN:OD1	3:D:695:ASN:ND2	2.49	0.46
2:B:398:ASP:OD1	2:B:399:CYS:N	2.48	0.46
3:D:663:LEU:C	3:D:665:ASP:H	2.20	0.46
1:A:27:VAL:HB	1:A:60:LEU:HD13	1.97	0.45
1:A:561:THR:O	1:A:562:LEU:C	2.54	0.45
1:A:56:TRP:HE1	1:A:296:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASP:O	1:A:382:PRO:HA	2.17	0.45
1:A:463:LEU:HB2	1:A:514:VAL:HG11	1.98	0.45
1:A:641:MET:O	1:A:644:VAL:HG12	2.16	0.45
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.49	0.45
3:D:262:THR:HG21	3:D:281:TRP:HE3	1.81	0.45
1:A:554:PHE:O	1:A:555:MET:C	2.54	0.45
3:D:226:ALA:HB3	3:D:254:VAL:HG12	1.99	0.45
3:D:520:ILE:HD12	3:D:762:ALA:HB1	1.96	0.45
1:A:254:ILE:HD13	1:A:268:GLY:HA3	1.97	0.45
1:C:95:PRO:HG3	1:C:103:THR:HG21	1.97	0.45
1:C:631:ILE:O	1:C:635:VAL:HG13	2.17	0.45
2:B:170:PHE:CE2	2:B:200:MET:HG3	2.51	0.45
2:B:603:LYS:HG3	2:B:606:TRP:CZ3	2.51	0.45
3:D:383:LYS:HG2	3:D:384:TYR:HD1	1.79	0.45
1:A:148:SER:HA	1:A:151:TRP:CE3	2.51	0.45
1:C:609:PHE:O	1:C:613:VAL:N	2.50	0.45
3:D:692:ILE:HD13	3:D:703:MET:HE3	1.98	0.45
1:A:82:LEU:HD11	1:A:110:THR:HG22	1.99	0.45
3:D:76:SER:O	3:D:80:GLN:HG2	2.17	0.45
3:D:743:CYS:O	3:D:743:CYS:SG	2.75	0.45
1:A:764:LYS:HD3	1:A:764:LYS:HA	1.89	0.45
1:C:683:THR:HG22	1:C:730:ILE:HB	1.99	0.45
5:J:1:NAG:H61	5:J:2:NAG:N2	2.32	0.45
2:B:34:LEU:HB3	2:B:35:ASN:H	1.61	0.45
1:C:560:SER:O	1:C:562:LEU:N	2.49	0.45
3:D:509:SER:O	8:D:903:GLU:N	2.49	0.45
1:C:381:TRP:HB3	1:C:382:PRO:HD2	1.99	0.44
1:C:744:CYS:SG	1:C:798:CYS:SG	3.06	0.44
3:D:738:GLY:O	3:D:797:ILE:N	2.44	0.44
1:A:790:LYS:HA	1:A:794:ARG:HB2	1.98	0.44
1:A:95:PRO:HA	1:A:102:PHE:HB2	1.99	0.44
1:A:481:ASP:OD1	1:A:481:ASP:N	2.45	0.44
2:B:167:TRP:HB3	2:B:226:VAL:HG21	2.00	0.44
2:B:614:ASN:HD21	1:C:615:LEU:HD23	1.82	0.44
2:B:781:GLN:HG3	1:C:695:ARG:HH21	1.81	0.44
2:B:686:PRO:HD3	2:B:709:ASN:HD21	1.83	0.44
1:A:527:ILE:HB	1:A:762:MET:O	2.17	0.44
1:C:677:ASP:OD1	1:C:677:ASP:N	2.50	0.44
1:A:125:MET:O	1:A:139:ARG:NH1	2.35	0.44
2:B:298:ILE:HD13	2:B:341:VAL:HG11	2.00	0.44
2:B:692:ARG:NH2	2:B:696:ASN:OD1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HG2	1:C:214:LEU:HD12	2.00	0.44
1:C:125:MET:HE3	1:C:172:GLU:OE2	2.18	0.43
2:B:134:ILE:HD12	2:B:134:ILE:HA	1.88	0.43
2:B:319:SER:OG	2:B:320:CYS:N	2.52	0.43
1:C:771:ASN:HD22	6:C:807:NAG:C7	2.31	0.43
3:D:306:GLN:HE21	3:D:306:GLN:HB2	1.64	0.43
3:D:525:PRO:HA	3:D:759:TYR:O	2.18	0.43
1:A:495:LYS:HE3	2:B:193:ASN:HD22	1.84	0.43
1:A:607:MET:HG2	1:A:611:TRP:HE1	1.83	0.43
1:C:300:ASN:OD1	6:C:802:NAG:C2	2.42	0.43
1:C:326:MET:HE3	1:C:326:MET:HB3	1.91	0.43
3:D:30:VAL:HG22	3:D:61:GLU:O	2.19	0.43
1:A:126:SER:OG	1:A:145:SER:OG	2.18	0.43
3:D:144:VAL:HG11	3:D:358:MET:HE3	2.01	0.43
1:A:170:ASP:O	1:A:174:ARG:HB2	2.17	0.43
1:A:554:PHE:O	1:A:554:PHE:CG	2.72	0.43
2:B:306:MET:SD	2:B:313:ILE:HG23	2.59	0.43
3:D:729:ASP:OD2	3:D:759:TYR:OH	2.22	0.43
1:A:316:LYS:H	1:A:316:LYS:HZ2	1.67	0.43
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.90	0.43
1:C:226:ASP:OD1	1:C:226:ASP:N	2.52	0.43
3:D:35:VAL:HG12	3:D:67:VAL:HG13	2.00	0.43
1:C:102:PHE:CE1	1:C:125:MET:HG3	2.54	0.43
1:C:403:ILE:HB	1:C:501:MET:SD	2.58	0.43
1:C:666:GLY:HA2	1:C:751:GLU:OE1	2.19	0.43
1:A:555:MET:SD	1:A:555:MET:N	2.92	0.42
1:A:602:THR:O	1:A:602:THR:OG1	2.32	0.42
1:C:662:GLU:HB2	1:C:663:ARG:H	1.57	0.42
3:D:757:THR:OG1	3:D:758:GLY:N	2.51	0.42
2:B:612:VAL:HG22	2:B:634:TRP:HE1	1.84	0.42
1:A:570:VAL:HG12	1:A:636:TRP:CH2	2.50	0.42
2:B:681:ARG:NH2	2:B:723:GLY:O	2.52	0.42
1:C:662:GLU:O	1:C:663:ARG:C	2.56	0.42
3:D:318:ARG:HD3	3:D:318:ARG:HA	1.87	0.42
2:B:83:ILE:HD11	2:B:112:MET:HE1	2.00	0.42
2:B:742:ASP:HB3	2:B:745:CYS:HA	2.01	0.42
1:C:639:PHE:CE1	3:D:818:VAL:HG22	2.55	0.42
3:D:153:LEU:HD22	3:D:253:LEU:HD23	2.01	0.42
2:B:836:ILE:HG22	2:B:837:TRP:CD1	2.54	0.42
3:D:383:LYS:HE3	3:D:383:LYS:HB2	1.82	0.42
1:A:315:TRP:NE1	1:A:317:THR:OG1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:HG21	3:D:652:ILE:HG13	2.02	0.42
3:D:49:ARG:HH11	3:D:286:ARG:HD3	1.85	0.42
2:B:686:PRO:HD2	4:I:1:NAG:H82	2.02	0.42
1:C:669:ASP:OD2	1:C:671:ARG:NH2	2.47	0.42
3:D:328:ARG:H	3:D:328:ARG:HG2	1.66	0.42
2:B:469:ARG:CZ	2:B:469:ARG:HB2	2.49	0.42
2:B:527:PRO:HA	2:B:761:TYR:O	2.20	0.42
3:D:166:ALA:HB3	3:D:224:LEU:HD23	2.01	0.42
3:D:393:SER:HG	3:D:394:LEU:N	2.17	0.42
3:D:624:THR:O	3:D:628:MET:HE2	2.20	0.42
3:D:828:LEU:O	3:D:832:VAL:HG23	2.19	0.42
1:A:153:GLU:HG3	1:A:367:TYR:HE1	1.84	0.42
2:B:817:MET:HE3	2:B:820:VAL:HB	2.01	0.42
1:C:421:LYS:HB2	1:C:421:LYS:HE2	1.72	0.42
3:D:439:HIS:CG	3:D:440:THR:H	2.38	0.42
1:A:260:ARG:O	1:A:359:ARG:NH2	2.53	0.42
1:A:292:VAL:O	1:A:296:LEU:HD13	2.19	0.42
1:C:167:VAL:O	1:C:196:GLN:HA	2.20	0.42
2:B:438:LYS:HD2	2:B:479:LEU:HD12	2.01	0.41
2:B:609:TRP:HA	2:B:612:VAL:HG23	2.02	0.41
1:C:264:ASP:O	1:C:382:PRO:HA	2.20	0.41
1:A:567:GLY:O	1:A:570:VAL:HG22	2.20	0.41
1:A:659:ARG:HD3	1:A:659:ARG:HA	1.87	0.41
2:B:74:MET:CE	2:B:77:THR:HA	2.50	0.41
2:B:395:SER:OG	2:B:396:PHE:N	2.53	0.41
1:C:125:MET:HE3	1:C:125:MET:HA	2.02	0.41
1:C:561:THR:OG1	1:C:562:LEU:N	2.52	0.41
1:A:614:LEU:HD12	1:A:614:LEU:H	1.86	0.41
1:A:647:TYR:CE2	1:A:651:LEU:HD11	2.55	0.41
1:A:652:ALA:O	1:A:656:VAL:HG12	2.20	0.41
1:A:739:GLU:OE1	1:A:743:LYS:NZ	2.48	0.41
2:B:294:ASP:O	2:B:298:ILE:HG22	2.20	0.41
2:B:756:PHE:O	2:B:758:THR:N	2.54	0.41
1:C:39:GLU:HG2	1:C:64:SER:HB3	2.02	0.41
1:C:479:VAL:HG13	1:C:481:ASP:O	2.20	0.41
1:C:513:ILE:HG21	1:C:517:LEU:HD22	2.01	0.41
2:B:425:LEU:HG	2:B:426:THR:HG23	2.01	0.41
2:B:740:GLY:O	2:B:799:ILE:HG22	2.20	0.41
2:B:442:ILE:HB	2:B:446:THR:HG21	2.01	0.41
1:C:103:THR:N	1:C:104:PRO:HD2	2.35	0.41
3:D:478:VAL:HG22	3:D:480:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:PRO:HG2	1:C:535:TYR:CZ	2.56	0.41
1:C:639:PHE:CZ	3:D:818:VAL:HG22	2.56	0.41
4:L:2:NAG:H83	4:L:2:NAG:H2	1.87	0.41
1:A:442:THR:O	1:A:446:SER:HB2	2.21	0.41
1:A:536:GLN:OE1	1:A:732:ASP:HB3	2.21	0.41
1:C:543:LYS:O	1:C:545:GLU:N	2.53	0.41
3:D:159:GLU:HG3	3:D:380:LEU:HD23	2.02	0.41
1:A:150:VAL:HG22	1:A:367:TYR:CD2	2.56	0.41
1:A:561:THR:C	1:A:563:TRP:N	2.73	0.41
1:A:790:LYS:HG3	1:A:794:ARG:NH2	2.36	0.41
3:D:609:LEU:HD21	3:D:633:ALA:HB2	2.03	0.41
1:A:34:SER:HA	1:A:66:THR:HG22	2.03	0.40
1:A:647:TYR:HA	1:A:650:ASN:ND2	2.36	0.40
2:B:51:LEU:HD12	2:B:71:ALA:HB1	2.03	0.40
1:C:543:LYS:CD	1:C:745:ASP:O	2.59	0.40
1:C:663:ARG:HG2	1:C:679:PHE:HZ	1.85	0.40
3:D:273:LEU:HD23	3:D:369:TRP:HH2	1.86	0.40
1:C:140:THR:O	1:C:346:ARG:NH1	2.51	0.40
3:D:408:LEU:HD12	3:D:408:LEU:HA	1.93	0.40
1:A:224:SER:OG	1:A:225:GLU:N	2.54	0.40
3:D:462:LEU:HB2	3:D:507:ILE:HG12	2.03	0.40
1:A:553:SER:O	1:A:554:PHE:C	2.59	0.40
1:A:631:ILE:O	1:A:635:VAL:HG12	2.21	0.40
1:C:415:MET:HB2	1:C:419:THR:HG23	2.02	0.40
1:C:719:GLN:O	1:C:723:ASP:N	2.49	0.40
3:D:97:ASP:OD2	3:D:101:THR:OG1	2.40	0.40
3:D:168:ILE:HD11	3:D:224:LEU:HD22	2.03	0.40
2:B:90:MET:HA	2:B:95:ILE:HG12	2.02	0.40
2:B:439:PHE:CZ	2:B:441:LYS:HG2	2.56	0.40
3:D:537:ARG:HB3	3:D:746:VAL:HG12	2.04	0.40
3:D:648:ALA:O	3:D:652:ILE:HG12	2.21	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	742/798 (93%)	691 (93%)	44 (6%)	7 (1%)	17	48
1	C	739/798 (93%)	701 (95%)	36 (5%)	2 (0%)	41	71
2	B	728/838 (87%)	684 (94%)	43 (6%)	1 (0%)	51	81
3	D	745/835 (89%)	686 (92%)	57 (8%)	2 (0%)	41	71
All	All	2954/3269 (90%)	2762 (94%)	180 (6%)	12 (0%)	38	66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	ARG
2	B	67	VAL
3	D	58	LEU
3	D	99	VAL
1	C	561	THR
1	A	351	TYR
1	A	547	PRO
1	C	662	GLU
1	A	556	GLN
1	A	665	THR
1	A	305	PRO
1	A	664	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	652/692 (94%)	634 (97%)	18 (3%)	43	70
1	C	649/692 (94%)	630 (97%)	19 (3%)	42	69
2	B	642/727 (88%)	628 (98%)	14 (2%)	52	74
3	D	631/698 (90%)	614 (97%)	17 (3%)	44	71
All	All	2574/2809 (92%)	2506 (97%)	68 (3%)	48	71

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ASP
1	A	197	PHE
1	A	198	ASP
1	A	217	ARG
1	A	239	ASN
1	A	298	LYS
1	A	302	THR
1	A	303	ASP
1	A	314	ILE
1	A	316	LYS
1	A	542	VAL
1	A	544	LYS
1	A	559	GLN
1	A	561	THR
1	A	562	LEU
1	A	609	PHE
1	A	664	ILE
1	A	789	ASP
2	B	44	HIS
2	B	72	LEU
2	B	87	CYS
2	B	185	SER
2	B	194	SER
2	B	251	TYR
2	B	284	TRP
2	B	286	TYR
2	B	334	LEU
2	B	462	ASP
2	B	491	ASN
2	B	655	GLN
2	B	665	LEU
2	B	821	PHE
1	C	79	CYS
1	C	203	ASN
1	C	209	MET
1	C	303	ASP
1	C	311	ASN
1	C	368	ASN
1	C	392	TYR
1	C	394	MET
1	C	448	ARG
1	C	544	LYS

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Mol	Chain	Res	Type
1	C	583	PHE
1	C	608	TRP
1	C	609	PHE
1	C	610	SER
1	C	661	GLU
1	C	662	GLU
1	C	663	ARG
1	C	679	PHE
1	C	798	CYS
3	D	190	TYR
3	D	367	ARG
3	D	401	ARG
3	D	434	ARG
3	D	609	LEU
3	D	612	ASN
3	D	634	PHE
3	D	635	PHE
3	D	653	GLN
3	D	658	ASP
3	D	663	LEU
3	D	666	LYS
3	D	678	PHE
3	D	743	CYS
3	D	752	LYS
3	D	799	GLN
3	D	806	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	ASN
1	C	371	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates i

24 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
4	NAG	E	1	1,4	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	F	1	1,4	14,14,15	0.39	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	G	1	1,4	14,14,15	0.54	0	17,19,21	1.44	1 (5%)
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.78	0
4	NAG	H	1	1,4	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	H	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	I	1	4,2	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	I	2	4	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	J	1	1,5	14,14,15	0.55	0	17,19,21	0.86	1 (5%)
5	NAG	J	2	5	14,14,15	0.68	0	17,19,21	1.87	3 (17%)
5	MAN	J	3	5	11,11,12	0.43	0	15,15,17	1.38	3 (20%)
4	NAG	K	1	1,4	14,14,15	0.31	0	17,19,21	1.13	1 (5%)
4	NAG	K	2	4	14,14,15	0.37	0	17,19,21	0.80	0
4	NAG	L	1	1,4	14,14,15	0.33	0	17,19,21	0.88	1 (5%)
4	NAG	L	2	4	14,14,15	0.29	0	17,19,21	0.82	0
4	NAG	M	1	1,4	14,14,15	0.40	0	17,19,21	0.93	0
4	NAG	M	2	4	14,14,15	0.34	0	17,19,21	0.80	0
4	NAG	N	1	3,4	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	N	2	4	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	O	1	3,5	14,14,15	0.19	0	17,19,21	0.43	0
5	NAG	O	2	5	14,14,15	0.23	0	17,19,21	0.48	0
5	MAN	O	3	5	11,11,12	0.67	0	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	MAN	J	3	5	-	0/2/19/22	1/1/1/1
4	NAG	K	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	O	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	MAN	O	3	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C2-N2-C7	-5.31	115.34	122.90
5	J	2	NAG	C1-O5-C5	5.13	119.14	112.19
5	J	2	NAG	O5-C1-C2	-3.97	105.02	111.29
4	K	1	NAG	C4-C3-C2	-2.98	106.65	111.02
5	J	3	MAN	O5-C1-C2	-2.78	106.48	110.77
5	J	3	MAN	C1-O5-C5	2.68	115.83	112.19
5	J	1	NAG	O5-C1-C2	-2.65	107.11	111.29
5	J	3	MAN	C3-C4-C5	-2.49	105.81	110.24
4	L	1	NAG	O5-C1-C2	-2.31	107.64	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	3	MAN	O2-C2-C3	-2.26	105.61	110.14
5	J	2	NAG	C2-N2-C7	-2.05	119.98	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	O	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	O	3	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

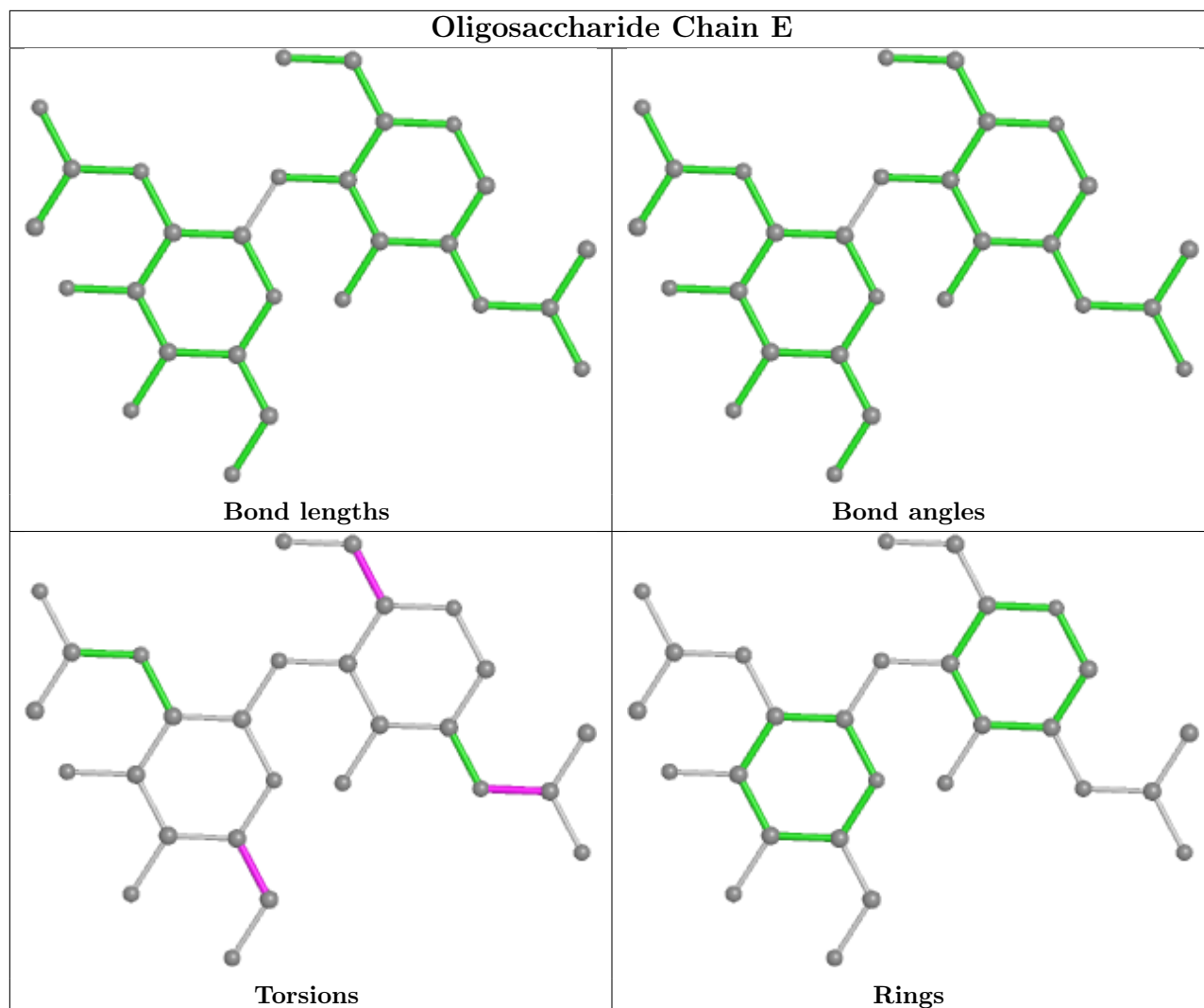
All (1) ring outliers are listed below:

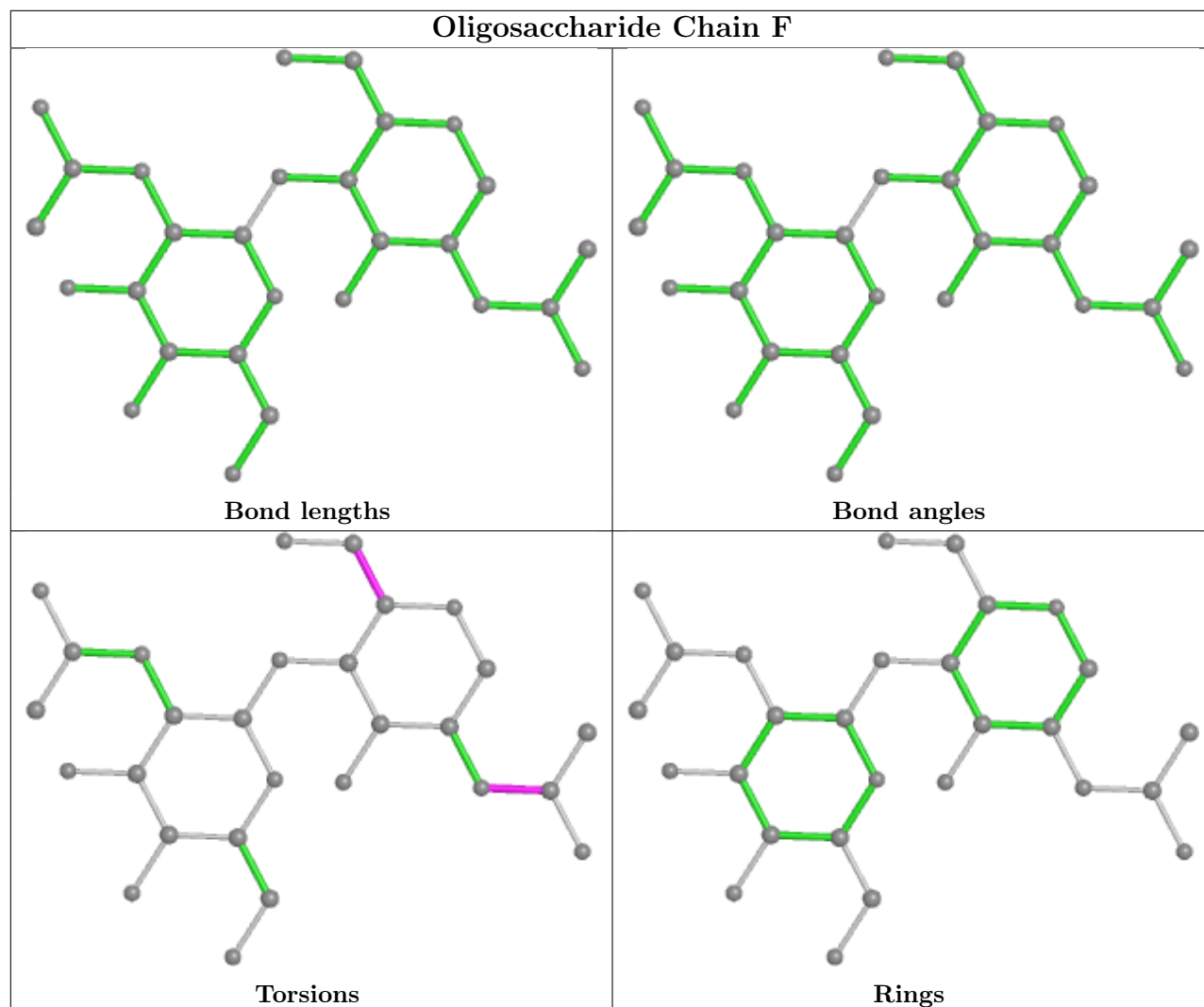
Mol	Chain	Res	Type	Atoms
5	J	3	MAN	C1-C2-C3-C4-C5-O5

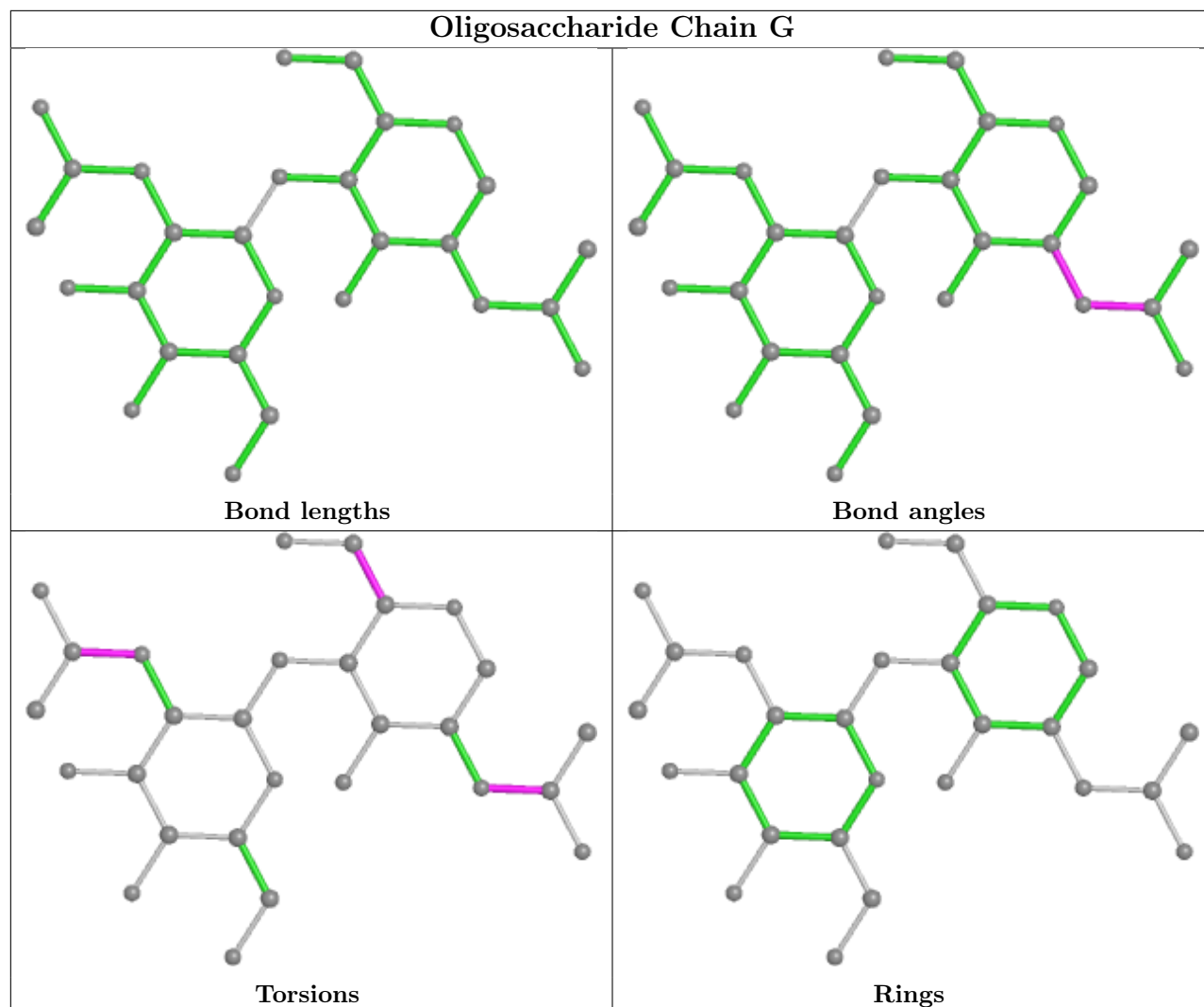
8 monomers are involved in 7 short contacts:

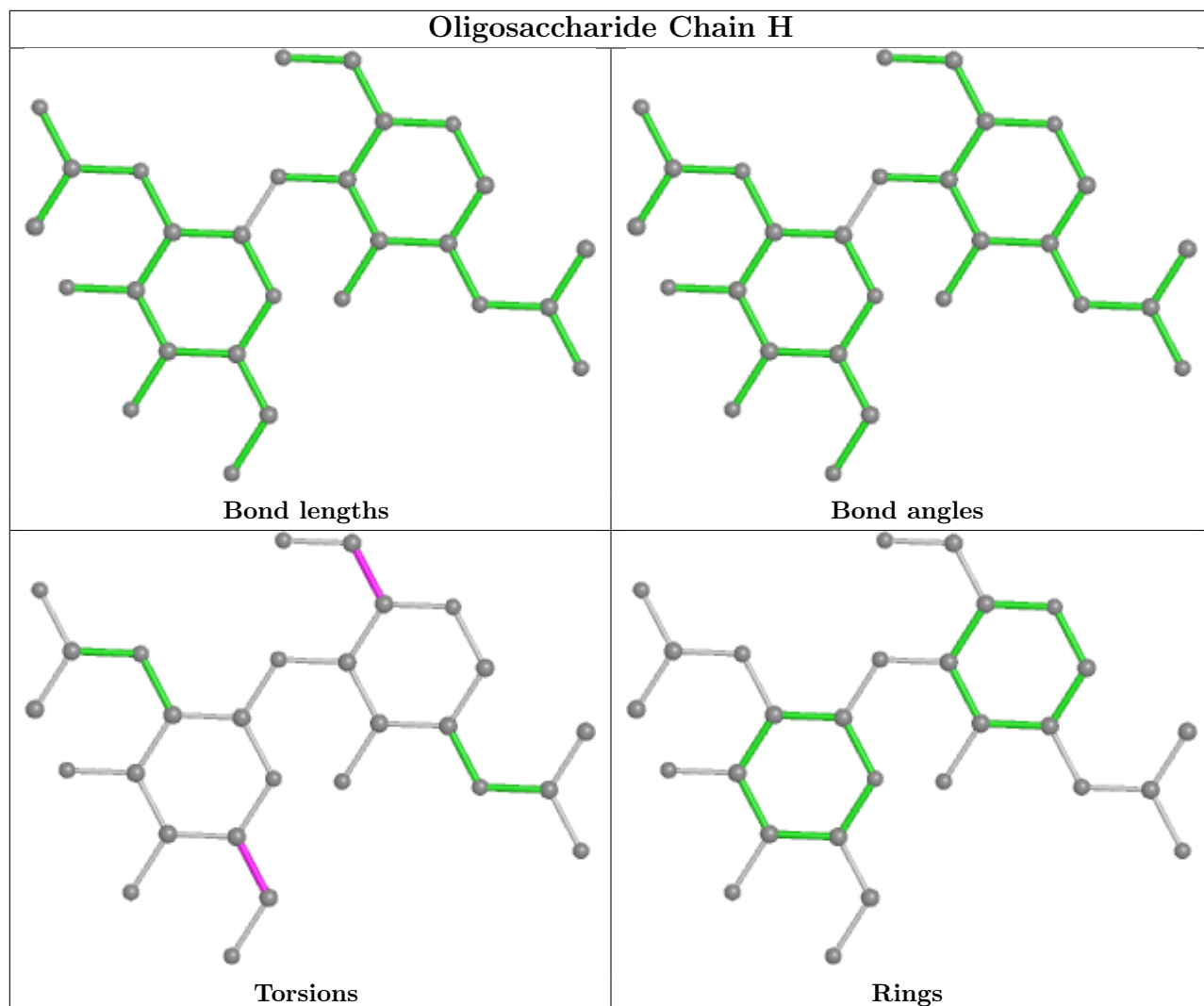
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	K	1	NAG	1	0
5	J	2	NAG	1	0
4	N	2	NAG	1	0
4	L	2	NAG	1	0
4	K	2	NAG	1	0
5	J	1	NAG	1	0
4	L	1	NAG	1	0

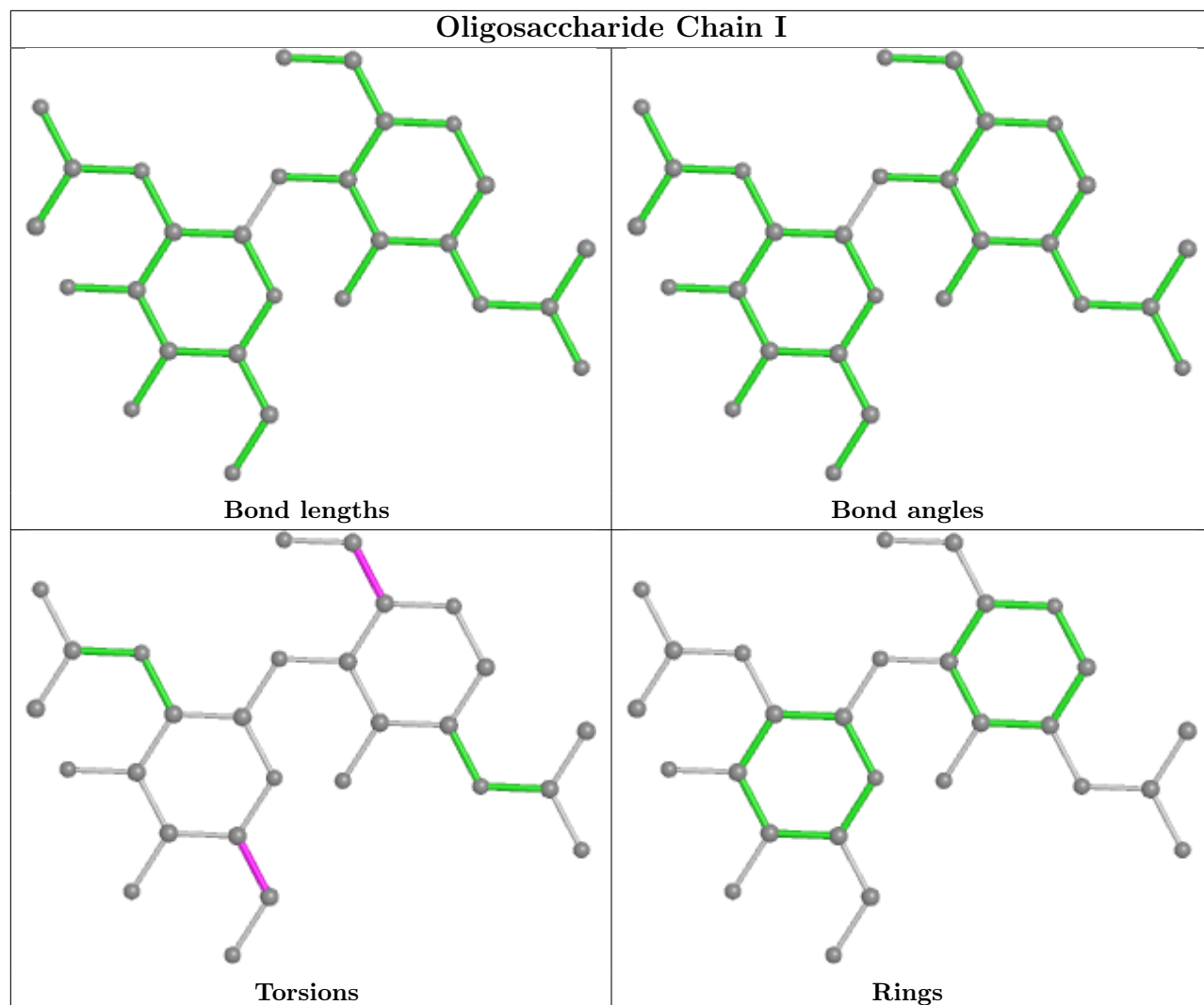
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

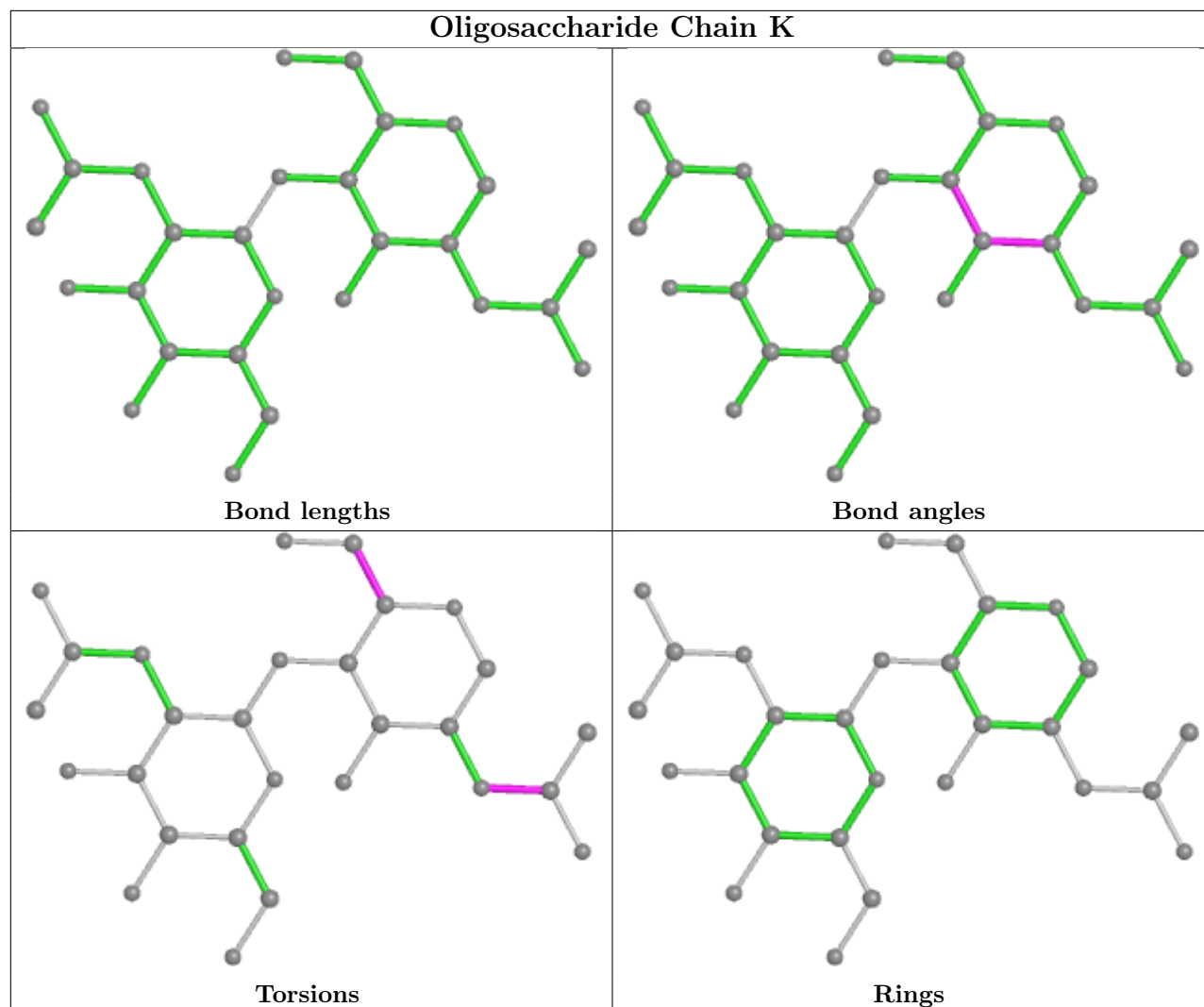


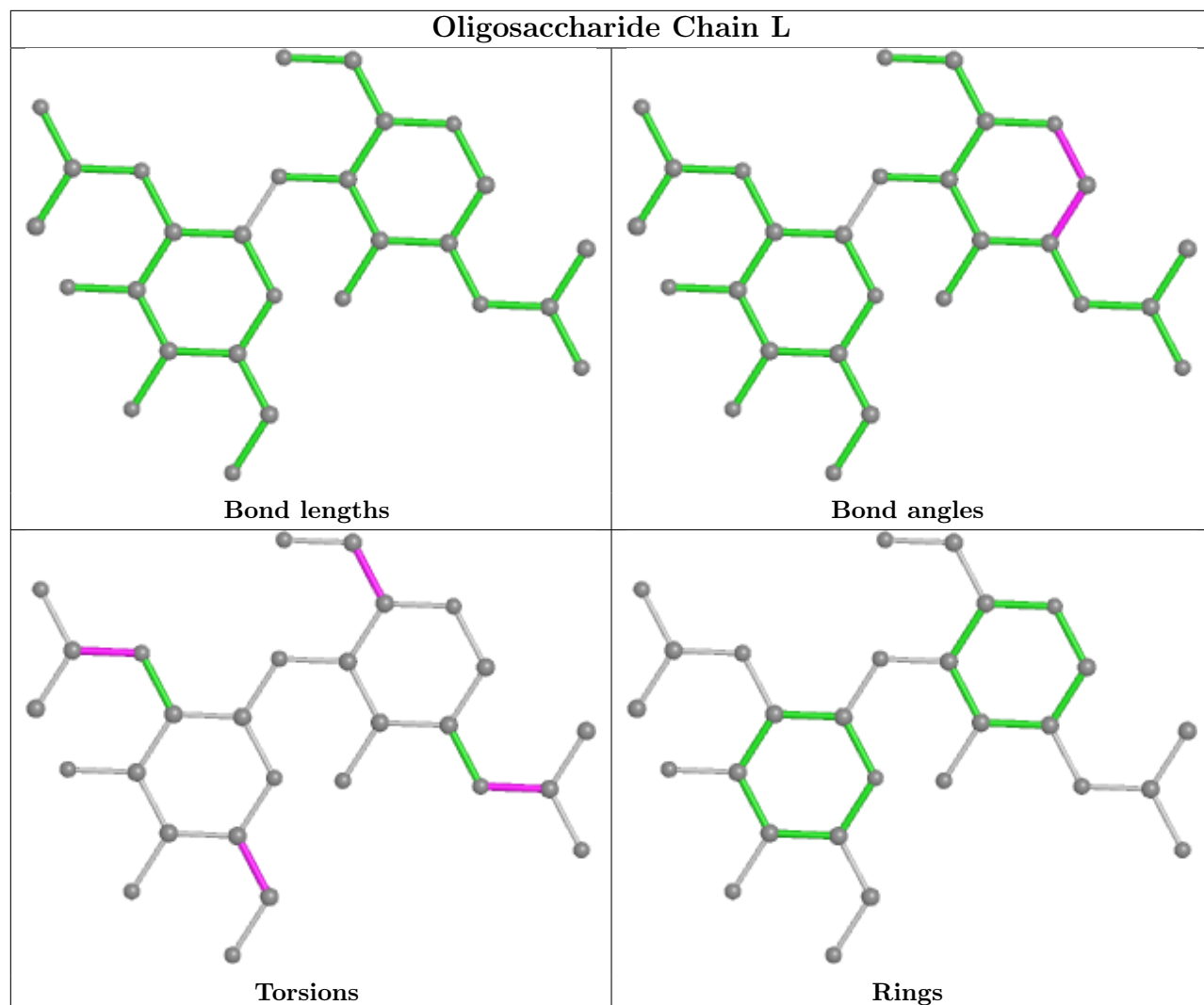


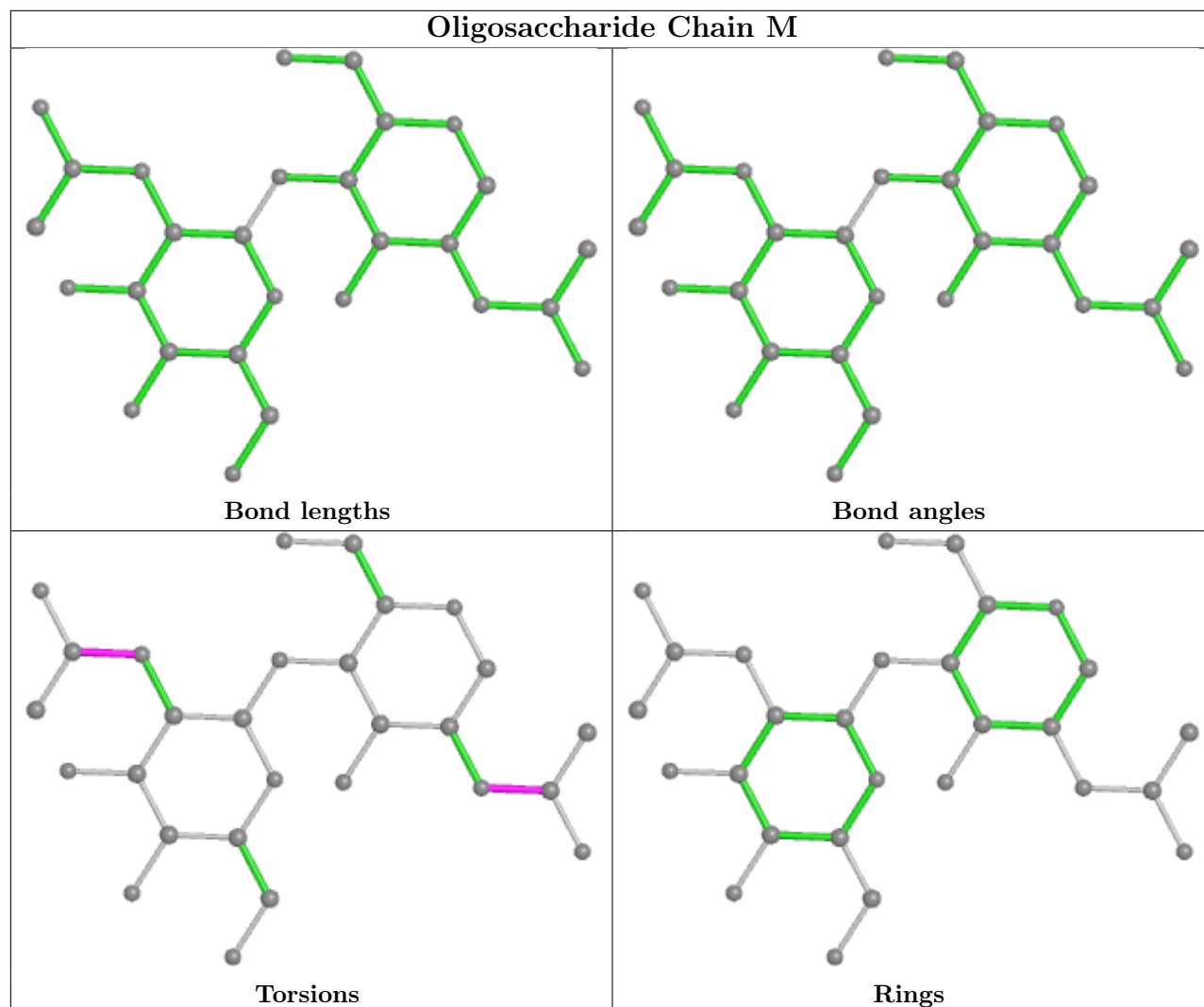


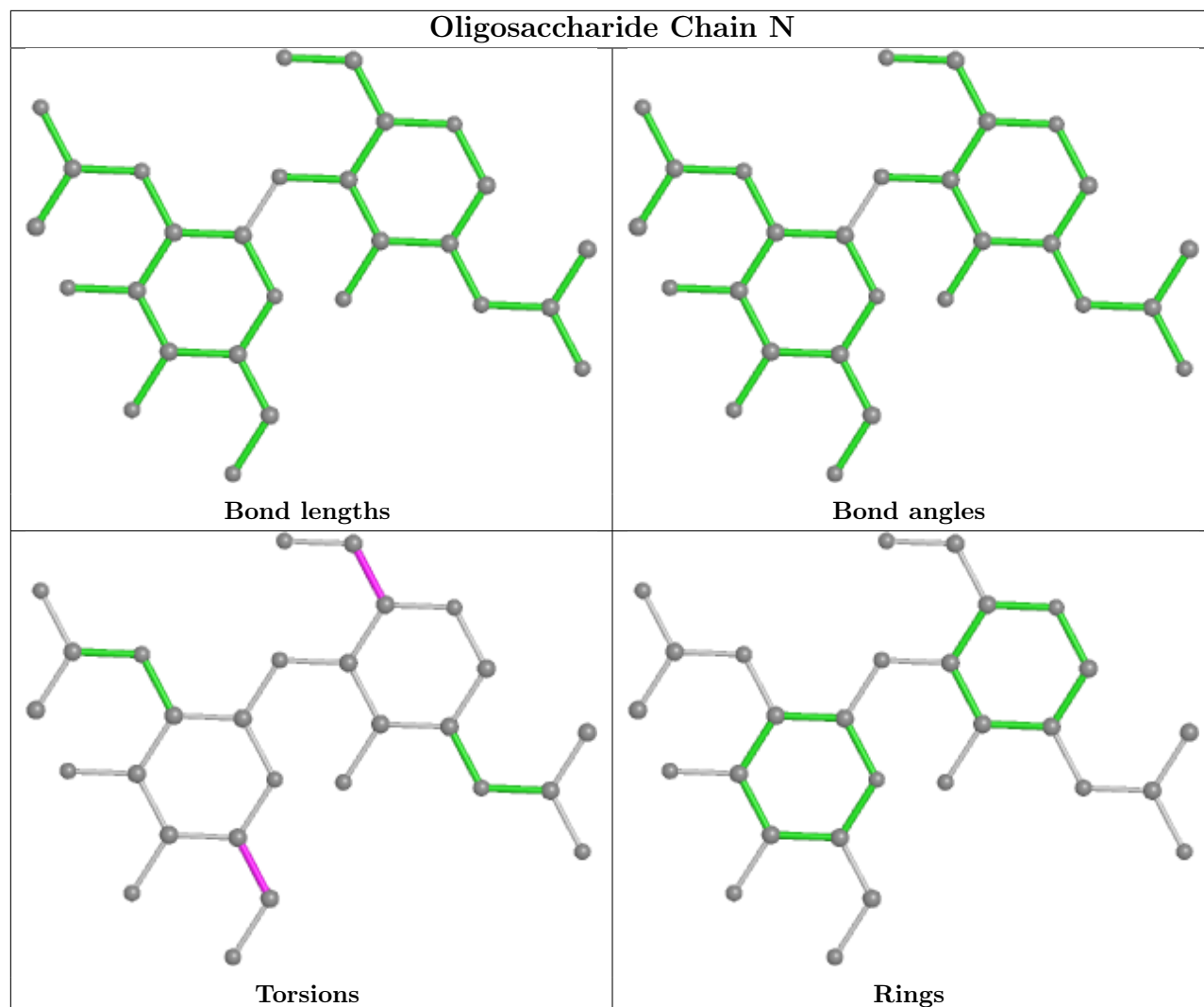


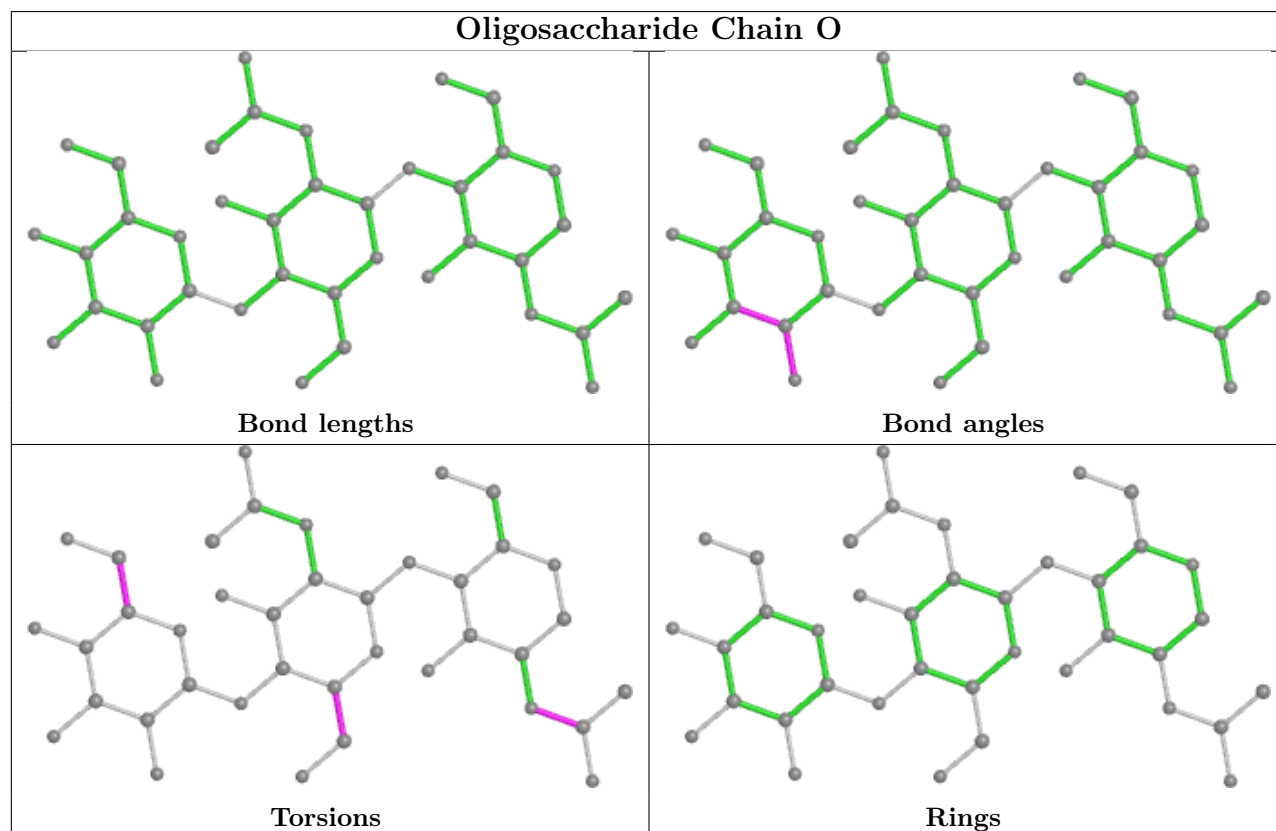
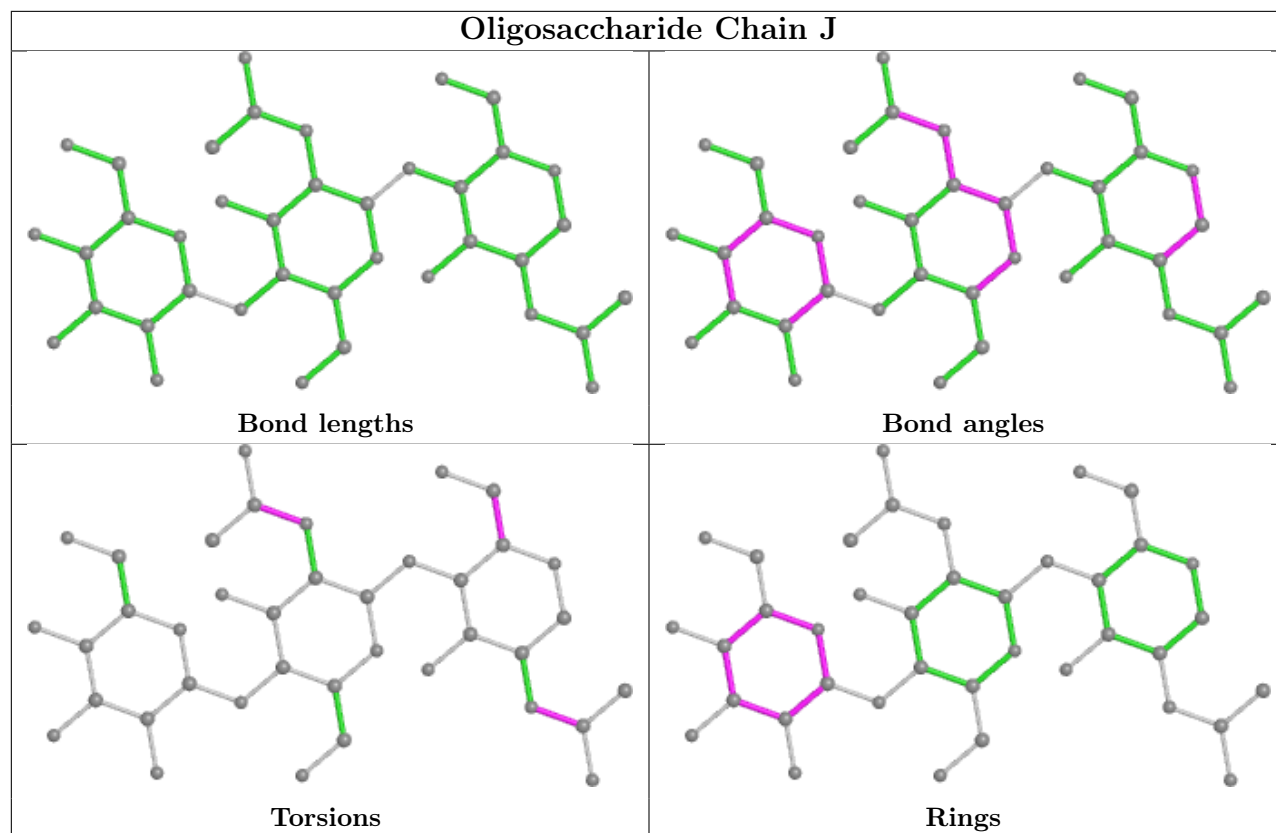












5.6 Ligand geometry

25 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
6	NAG	C	807	1	14,14,15	0.29	0	17,19,21	0.79	1 (5%)
6	NAG	D	901	3	14,14,15	0.92	1 (7%)	17,19,21	1.28	1 (5%)
7	GLY	A	808	-	4,4,4	1.15	1 (25%)	3,4,4	1.70	1 (33%)
6	NAG	B	904	2	14,14,15	0.42	0	17,19,21	0.72	0
8	GLU	B	906	-	8,9,9	1.06	1 (12%)	10,11,11	1.29	2 (20%)
6	NAG	C	803	1	14,14,15	0.32	0	17,19,21	1.10	1 (5%)
6	NAG	B	903	2	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	C	805	1	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
6	NAG	A	804	1	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	B	902	2	14,14,15	0.19	0	17,19,21	0.44	0
6	NAG	B	905	2	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	D	902	3	14,14,15	0.35	0	17,19,21	0.37	0
7	GLY	C	808	-	4,4,4	1.19	1 (25%)	3,4,4	1.70	2 (66%)
6	NAG	C	804	1	14,14,15	0.39	0	17,19,21	1.13	1 (5%)
8	GLU	D	903	-	8,9,9	1.07	1 (12%)	10,11,11	1.29	2 (20%)
6	NAG	A	805	1	14,14,15	0.34	0	17,19,21	0.49	0
6	NAG	C	806	1	14,14,15	0.35	0	17,19,21	0.81	0
6	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.37	0
6	NAG	C	802	-	14,14,15	0.33	0	17,19,21	1.10	2 (11%)
6	NAG	A	807	1	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	A	802	1	14,14,15	0.18	0	17,19,21	0.39	0
6	NAG	A	806	1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	A	803	1	14,14,15	0.26	0	17,19,21	0.37	0
6	NAG	B	901	2	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	C	801	1	14,14,15	0.25	0	17,19,21	0.98	2 (11%)

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
6	NAG	C	807	1	-	0/6/23/26	0/1/1/1
6	NAG	D	901	3	-	0/6/23/26	0/1/1/1
7	GLY	A	808	-	-	0/2/2/2	-
6	NAG	B	904	2	-	2/6/23/26	0/1/1/1
8	GLU	B	906	-	-	4/9/9/9	-
6	NAG	C	803	1	-	3/6/23/26	0/1/1/1
6	NAG	B	903	2	-	2/6/23/26	0/1/1/1
6	NAG	C	805	1	-	4/6/23/26	0/1/1/1
6	NAG	A	804	1	-	2/6/23/26	0/1/1/1
6	NAG	B	902	2	-	3/6/23/26	0/1/1/1
6	NAG	B	905	2	-	2/6/23/26	0/1/1/1
6	NAG	D	902	3	-	1/6/23/26	0/1/1/1
7	GLY	C	808	-	-	0/2/2/2	-
6	NAG	C	804	1	-	2/6/23/26	0/1/1/1
8	GLU	D	903	-	-	3/9/9/9	-
6	NAG	A	805	1	-	4/6/23/26	0/1/1/1
6	NAG	C	806	1	-	4/6/23/26	0/1/1/1
6	NAG	A	801	1	-	2/6/23/26	0/1/1/1
6	NAG	C	802	-	-	6/6/23/26	0/1/1/1
6	NAG	A	807	1	-	4/6/23/26	0/1/1/1
6	NAG	A	802	1	-	4/6/23/26	0/1/1/1
6	NAG	A	806	1	-	1/6/23/26	0/1/1/1
6	NAG	A	803	1	-	4/6/23/26	0/1/1/1
6	NAG	B	901	2	-	3/6/23/26	0/1/1/1
6	NAG	C	801	1	-	5/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	901	NAG	O5-C1	3.34	1.49	1.43
7	C	808	GLY	OXT-C	-2.24	1.23	1.30
8	D	903	GLU	OXT-C	-2.21	1.23	1.30
7	A	808	GLY	OXT-C	-2.17	1.23	1.30
8	B	906	GLU	OXT-C	-2.17	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	901	NAG	C1-O5-C5	5.04	119.02	112.19
6	C	803	NAG	C1-O5-C5	3.45	116.87	112.19
6	C	804	NAG	C1-O5-C5	-3.35	107.65	112.19
6	C	802	NAG	C1-O5-C5	3.34	116.72	112.19
8	D	903	GLU	OXT-C-O	-2.81	117.70	124.09
8	B	906	GLU	OXT-C-O	-2.70	117.97	124.09
6	C	801	NAG	C1-O5-C5	2.55	115.65	112.19
8	B	906	GLU	OXT-C-CA	2.27	121.13	113.38
6	C	801	NAG	O5-C5-C6	2.20	110.66	107.20
7	A	808	GLY	OXT-C-O	-2.18	117.86	123.30
8	D	903	GLU	OXT-C-CA	2.17	120.79	113.38
6	C	805	NAG	C1-O5-C5	2.17	115.13	112.19
6	C	802	NAG	O5-C5-C6	2.13	110.54	107.20
6	C	807	NAG	O5-C1-C2	-2.12	107.94	111.29
7	C	808	GLY	OXT-C-O	-2.06	118.16	123.30
7	C	808	GLY	OXT-C-CA	2.05	121.61	113.45

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	904	NAG	C8-C7-N2-C2
6	B	904	NAG	O7-C7-N2-C2
6	C	801	NAG	O7-C7-N2-C2
6	C	802	NAG	C8-C7-N2-C2
6	C	802	NAG	O7-C7-N2-C2
6	C	804	NAG	C8-C7-N2-C2
6	C	804	NAG	O7-C7-N2-C2
6	C	806	NAG	C8-C7-N2-C2
6	C	806	NAG	O7-C7-N2-C2
8	B	906	GLU	C-CA-CB-CG
8	D	903	GLU	N-CA-CB-CG
8	D	903	GLU	C-CA-CB-CG
6	C	801	NAG	C8-C7-N2-C2
6	A	802	NAG	O5-C5-C6-O6
6	A	804	NAG	C4-C5-C6-O6
6	A	802	NAG	C4-C5-C6-O6
6	B	903	NAG	O5-C5-C6-O6
6	A	803	NAG	O5-C5-C6-O6
6	A	804	NAG	O5-C5-C6-O6
6	C	802	NAG	O5-C5-C6-O6
6	C	801	NAG	C1-C2-N2-C7
6	C	802	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	A	807	NAG	O5-C5-C6-O6
6	A	803	NAG	C4-C5-C6-O6
6	C	803	NAG	O5-C5-C6-O6
6	A	802	NAG	C8-C7-N2-C2
6	A	802	NAG	O7-C7-N2-C2
6	A	803	NAG	C8-C7-N2-C2
6	A	803	NAG	O7-C7-N2-C2
6	A	805	NAG	C8-C7-N2-C2
6	A	805	NAG	O7-C7-N2-C2
6	A	807	NAG	C8-C7-N2-C2
6	A	807	NAG	O7-C7-N2-C2
6	B	901	NAG	C8-C7-N2-C2
6	B	901	NAG	O7-C7-N2-C2
6	B	902	NAG	C8-C7-N2-C2
6	B	902	NAG	O7-C7-N2-C2
6	B	905	NAG	C8-C7-N2-C2
6	B	905	NAG	O7-C7-N2-C2
6	C	803	NAG	C4-C5-C6-O6
6	A	807	NAG	C4-C5-C6-O6
6	C	805	NAG	C4-C5-C6-O6
6	C	802	NAG	C4-C5-C6-O6
6	D	902	NAG	O5-C5-C6-O6
6	C	801	NAG	O5-C5-C6-O6
6	A	801	NAG	C4-C5-C6-O6
6	C	805	NAG	C8-C7-N2-C2
6	C	806	NAG	O5-C5-C6-O6
6	C	805	NAG	O5-C5-C6-O6
6	B	903	NAG	C4-C5-C6-O6
6	C	805	NAG	O7-C7-N2-C2
6	A	801	NAG	O5-C5-C6-O6
6	A	805	NAG	C4-C5-C6-O6
6	B	901	NAG	O5-C5-C6-O6
6	B	902	NAG	O5-C5-C6-O6
6	A	805	NAG	O5-C5-C6-O6
6	C	802	NAG	C3-C2-N2-C7
6	A	806	NAG	C4-C5-C6-O6
8	B	906	GLU	OE1-CD-CG-CB
8	B	906	GLU	OE2-CD-CG-CB
6	C	806	NAG	C4-C5-C6-O6
6	C	801	NAG	C4-C5-C6-O6
6	C	803	NAG	C8-C7-N2-C2
8	D	903	GLU	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
8	B	906	GLU	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	807	NAG	1	0
7	A	808	GLY	1	0
6	B	905	NAG	2	0
6	D	902	NAG	1	0
7	C	808	GLY	2	0
8	D	903	GLU	2	0
6	C	802	NAG	2	0
6	C	801	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

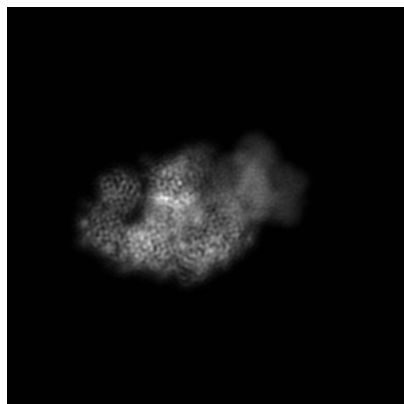
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33791. These allow visual inspection of the internal detail of the map and identification of artifacts.

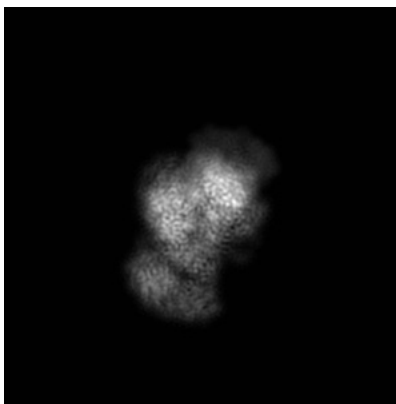
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

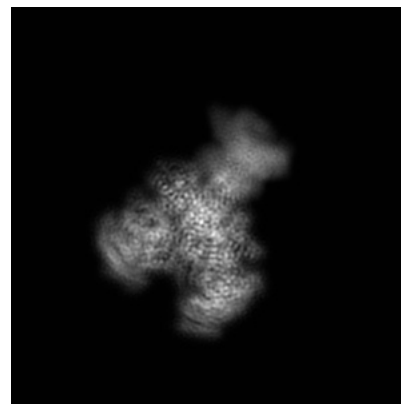
6.1.1 Primary map



X

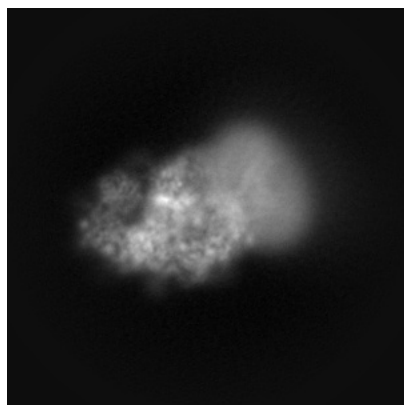


Y

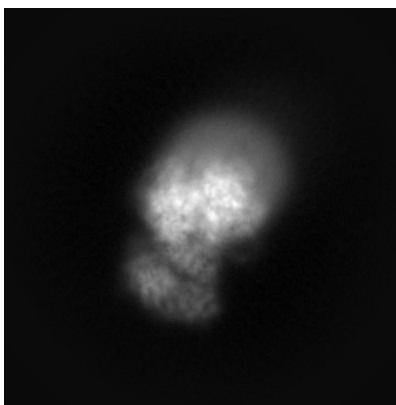


Z

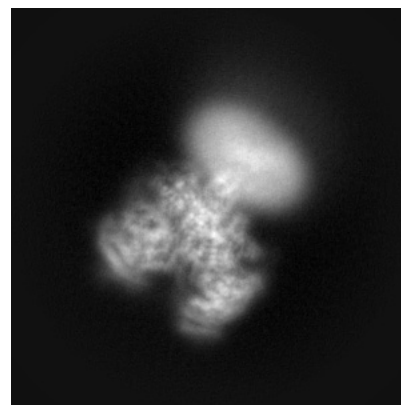
6.1.2 Raw map



X



Y

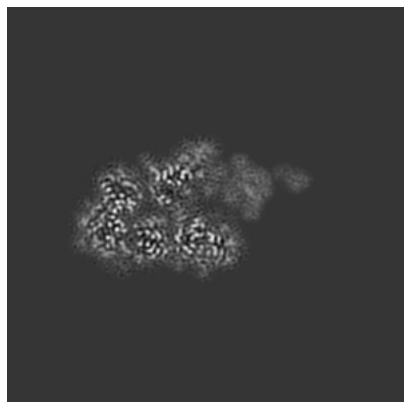


Z

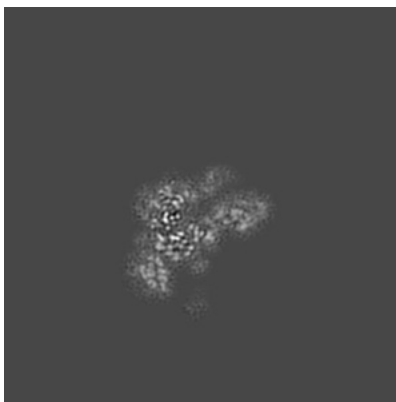
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

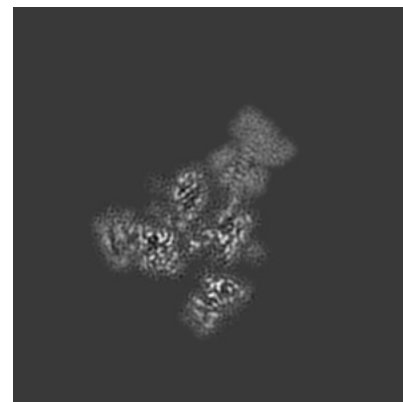
6.2.1 Primary map



X Index: 145

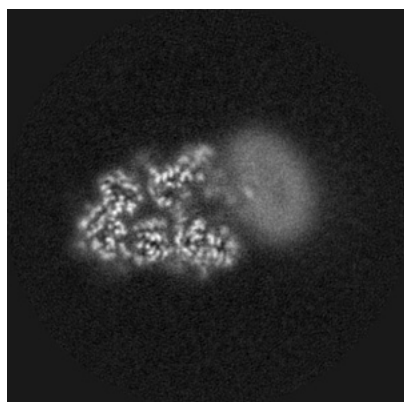


Y Index: 145

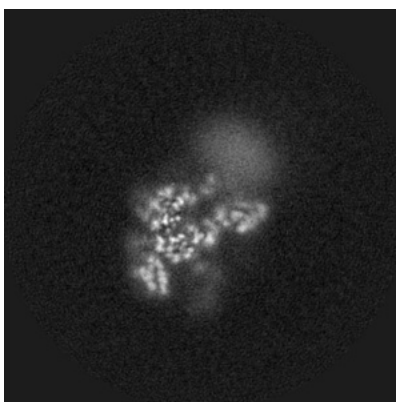


Z Index: 145

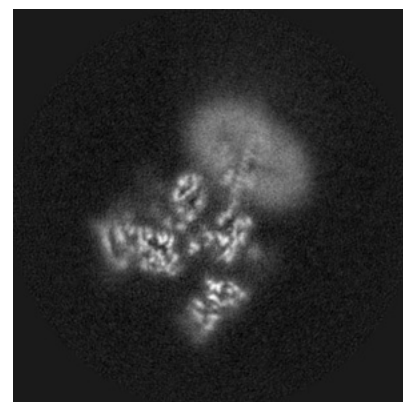
6.2.2 Raw map



X Index: 145



Y Index: 145

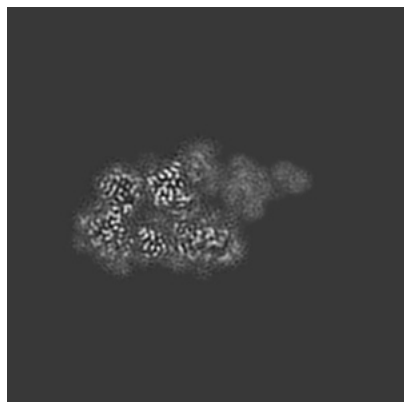


Z Index: 145

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

6.3 Largest variance slices [i](#)

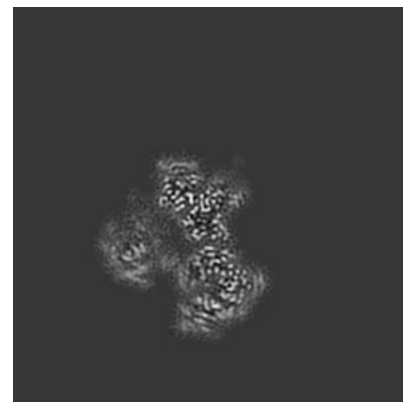
6.3.1 Primary map



X Index: 148

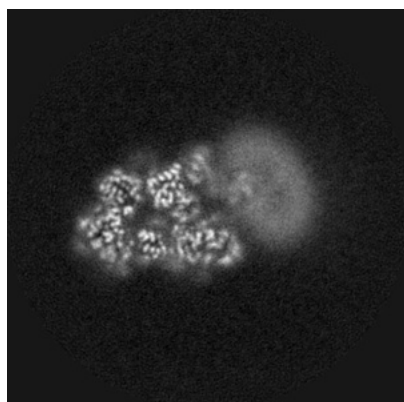


Y Index: 114

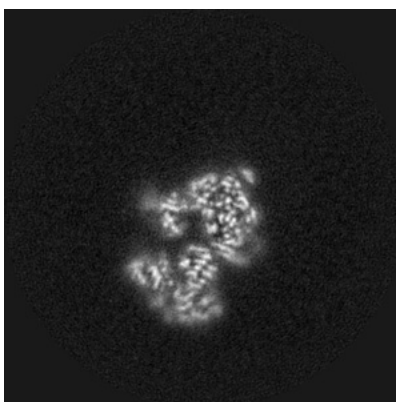


Z Index: 122

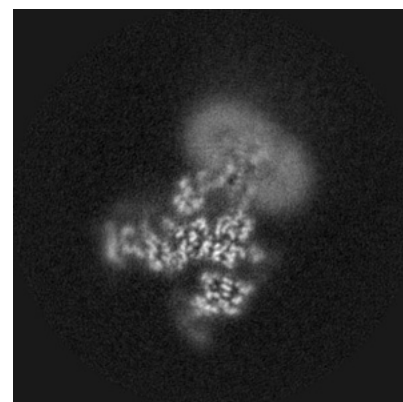
6.3.2 Raw map



X Index: 148



Y Index: 124

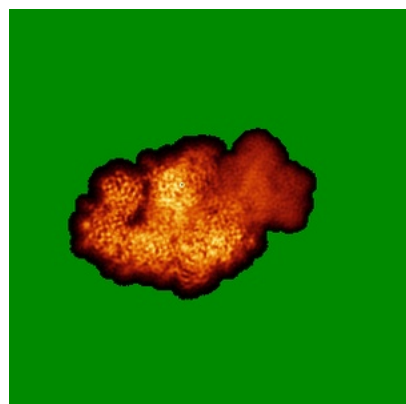


Z Index: 151

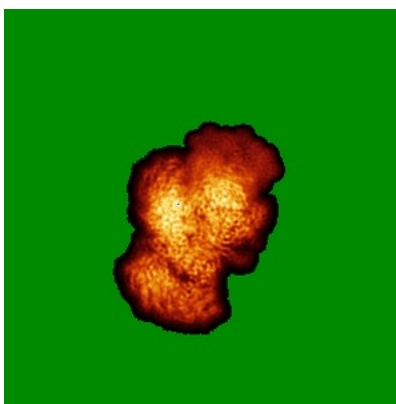
The images above show the largest variance slices of the map in three orthogonal directions.

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

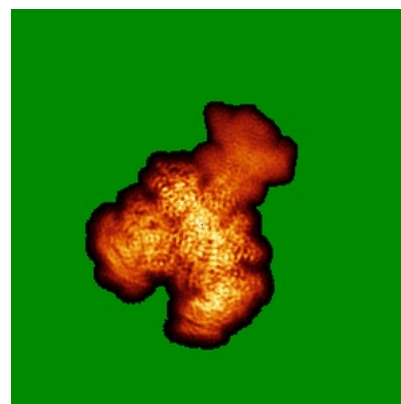
6.4.1 Primary map



X

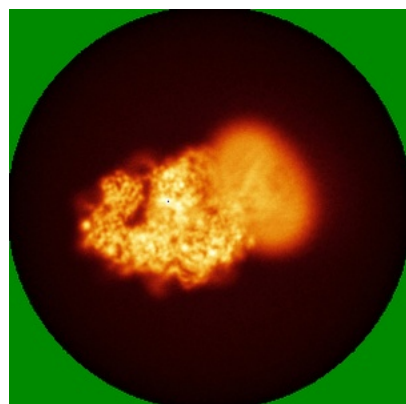


Y



Z

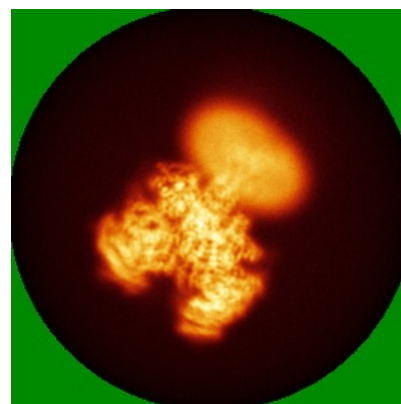
6.4.2 Raw map



X



Y

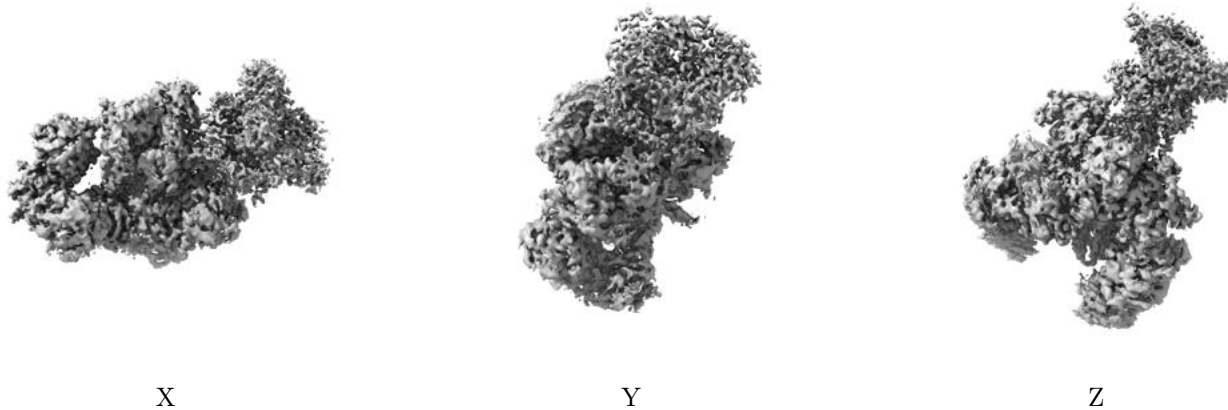


Z

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.

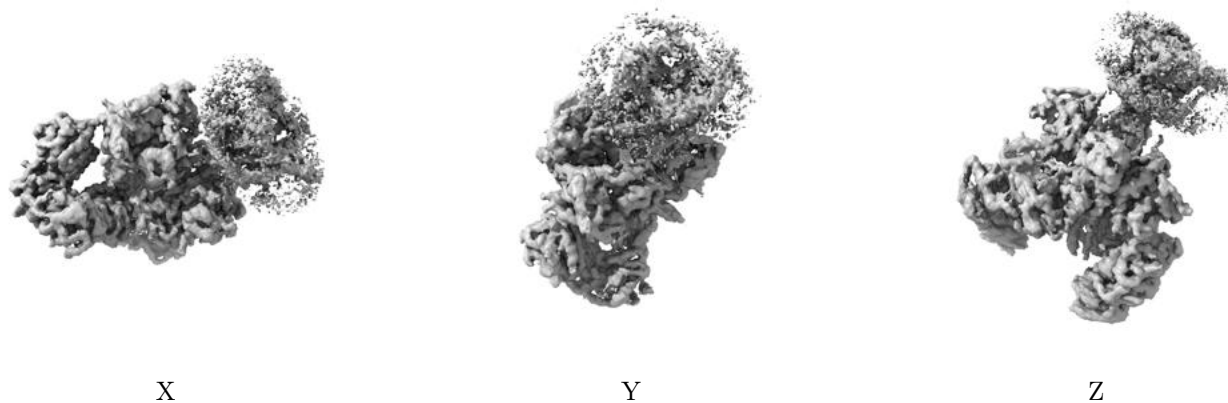
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

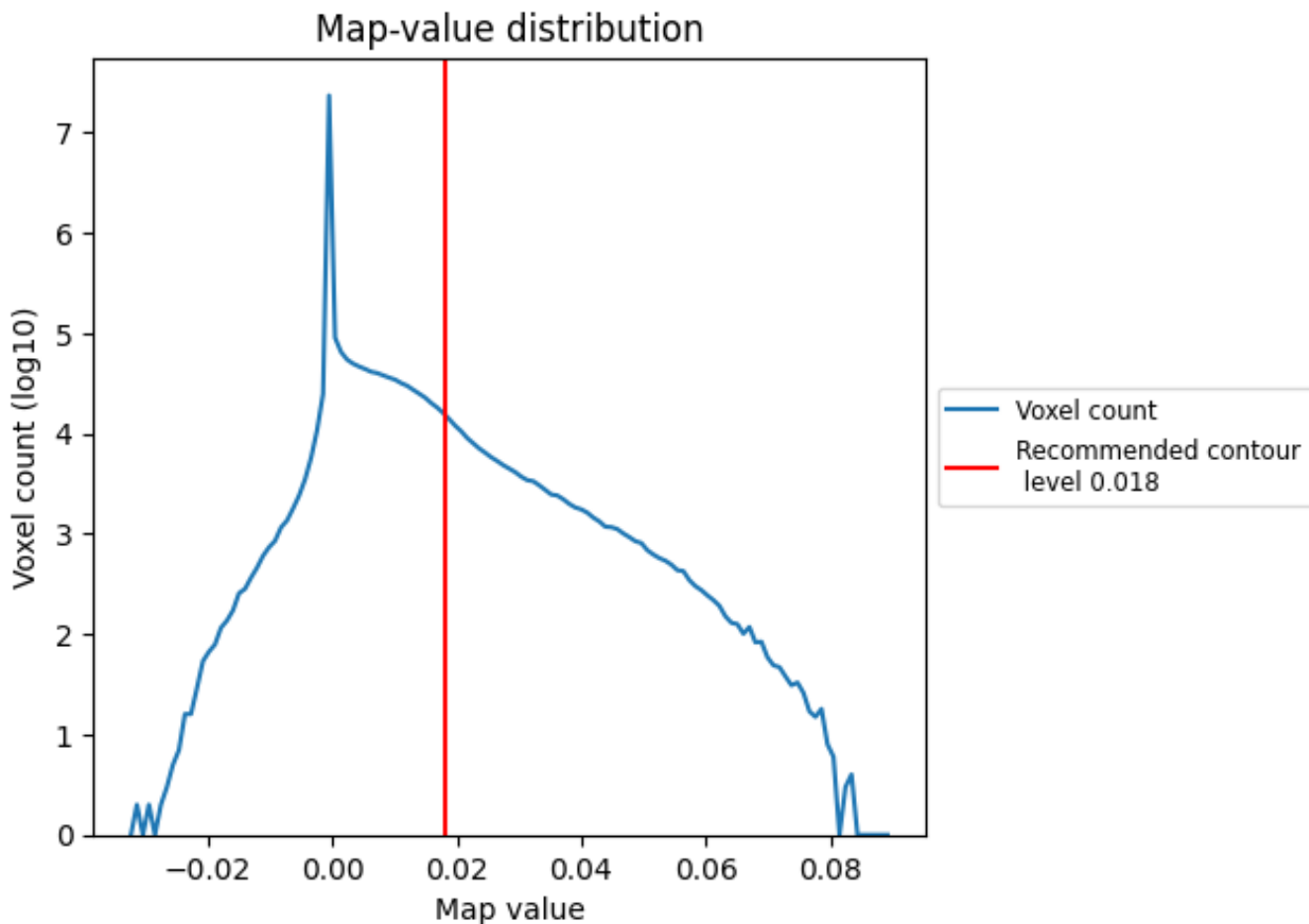
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

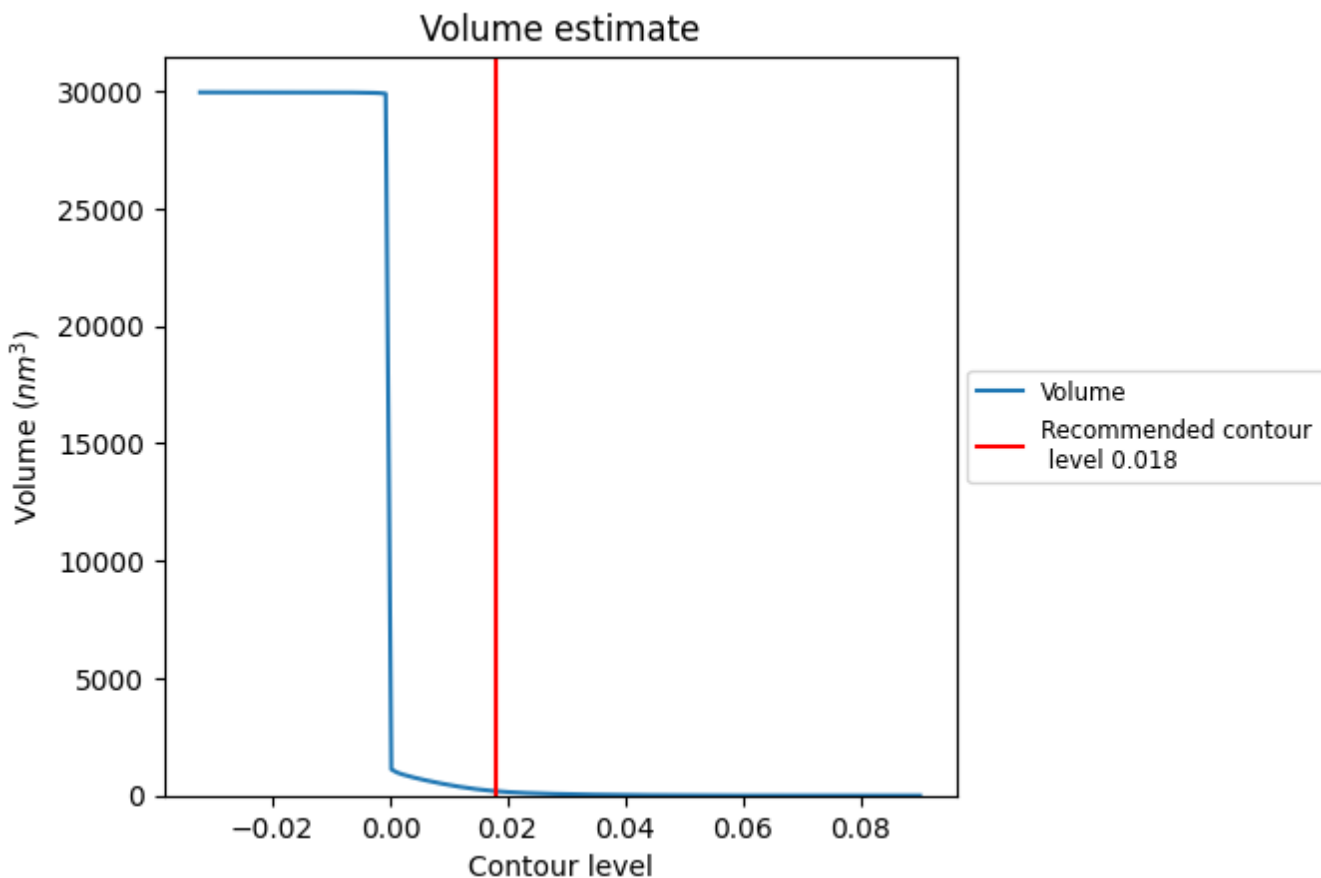
This section contains the results of statistical analysis of the map.

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.

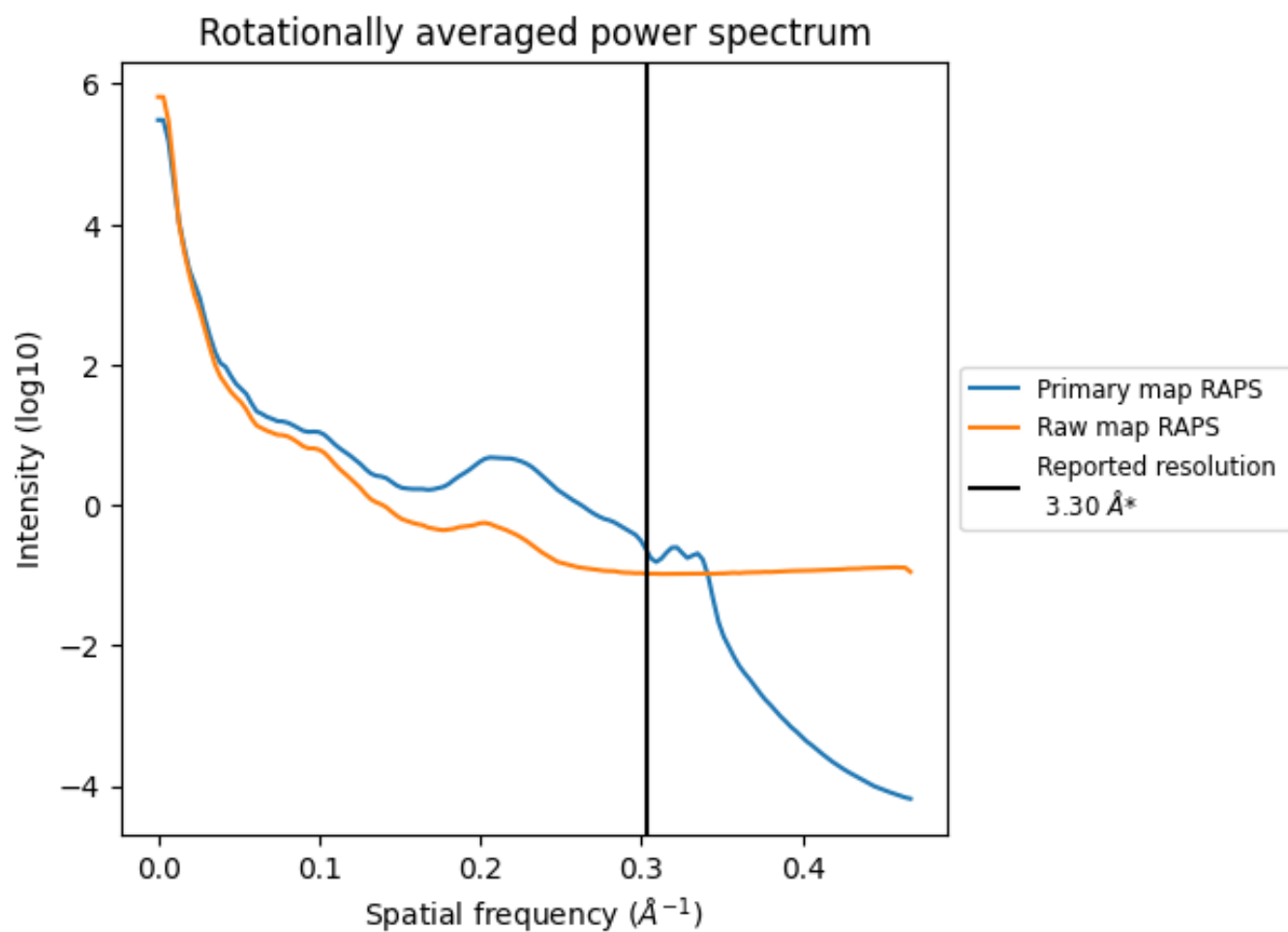
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 168 kDa.

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

7.3 Rotationally averaged power spectrum i

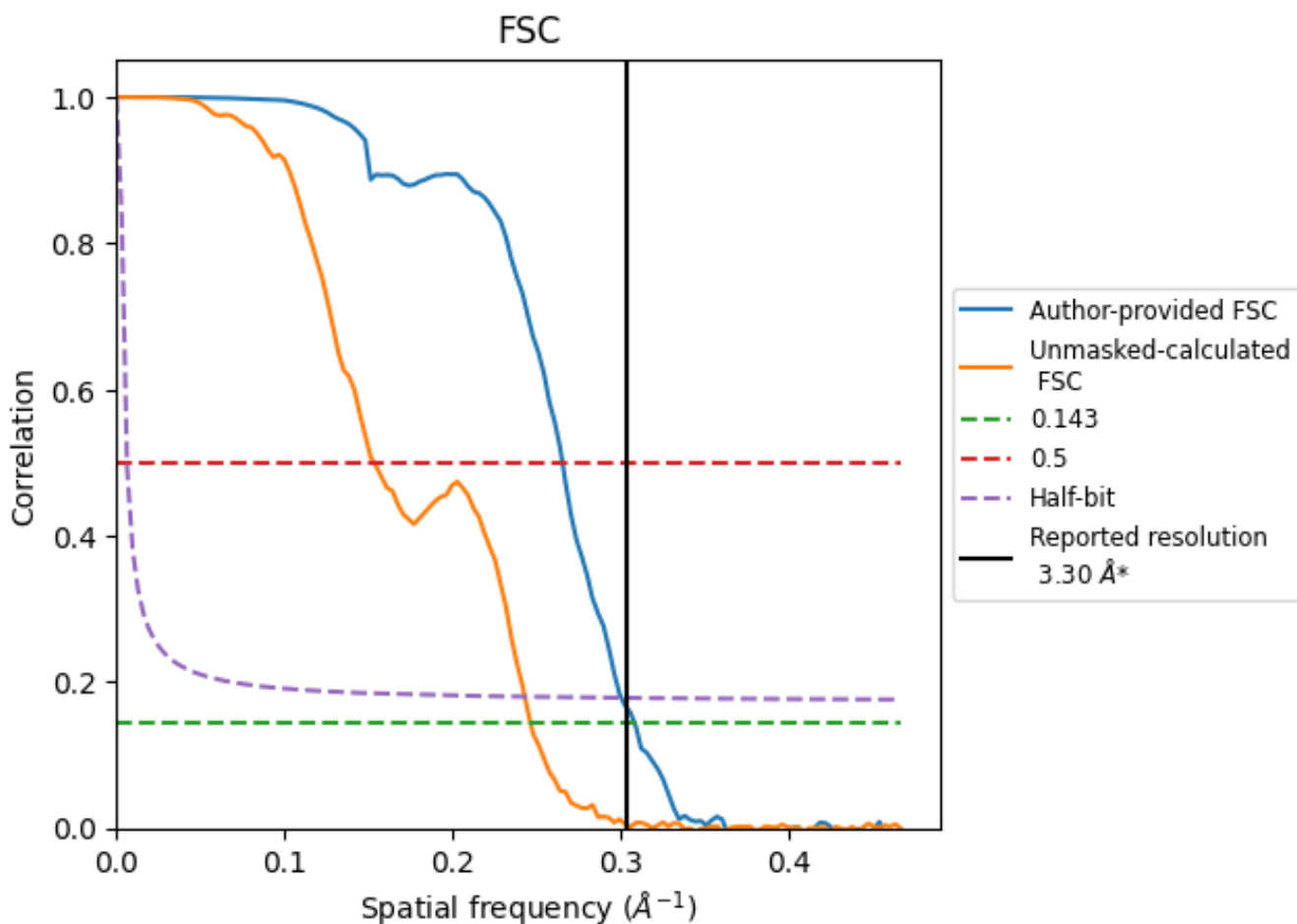


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

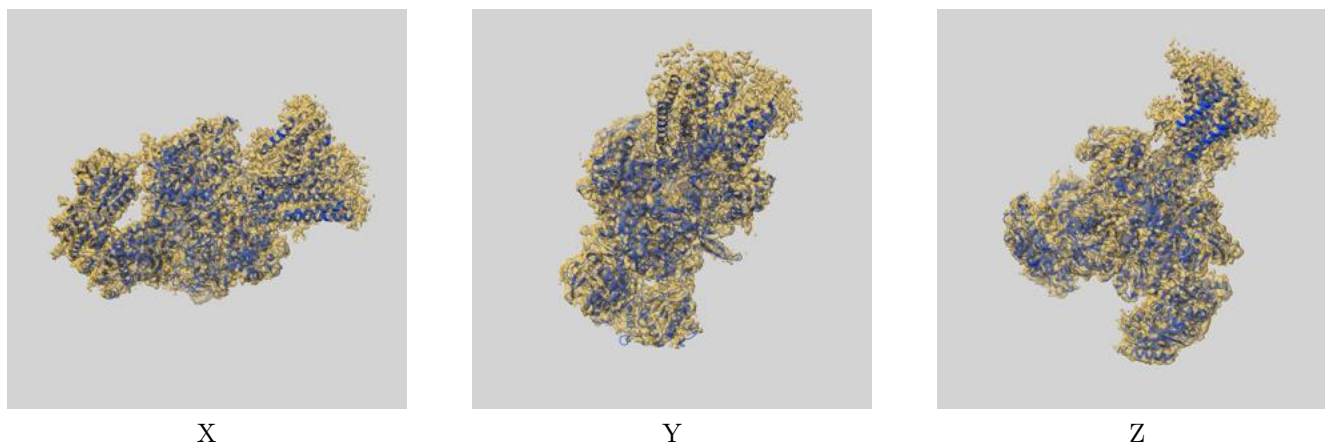
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.24	3.77	3.33
Unmasked-calculated*	4.06	6.52	4.12

*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 4.06 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-33791 and PDB model 7YFI. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



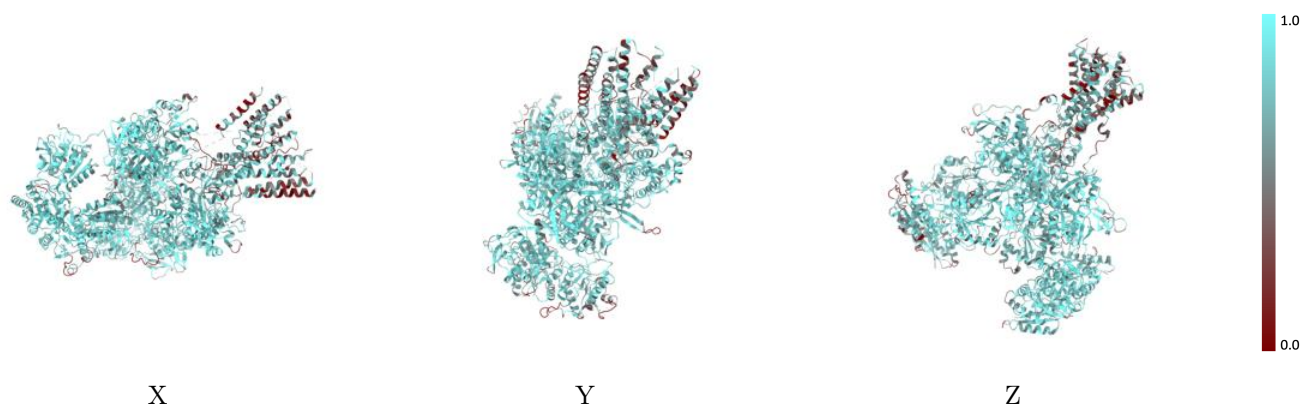
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



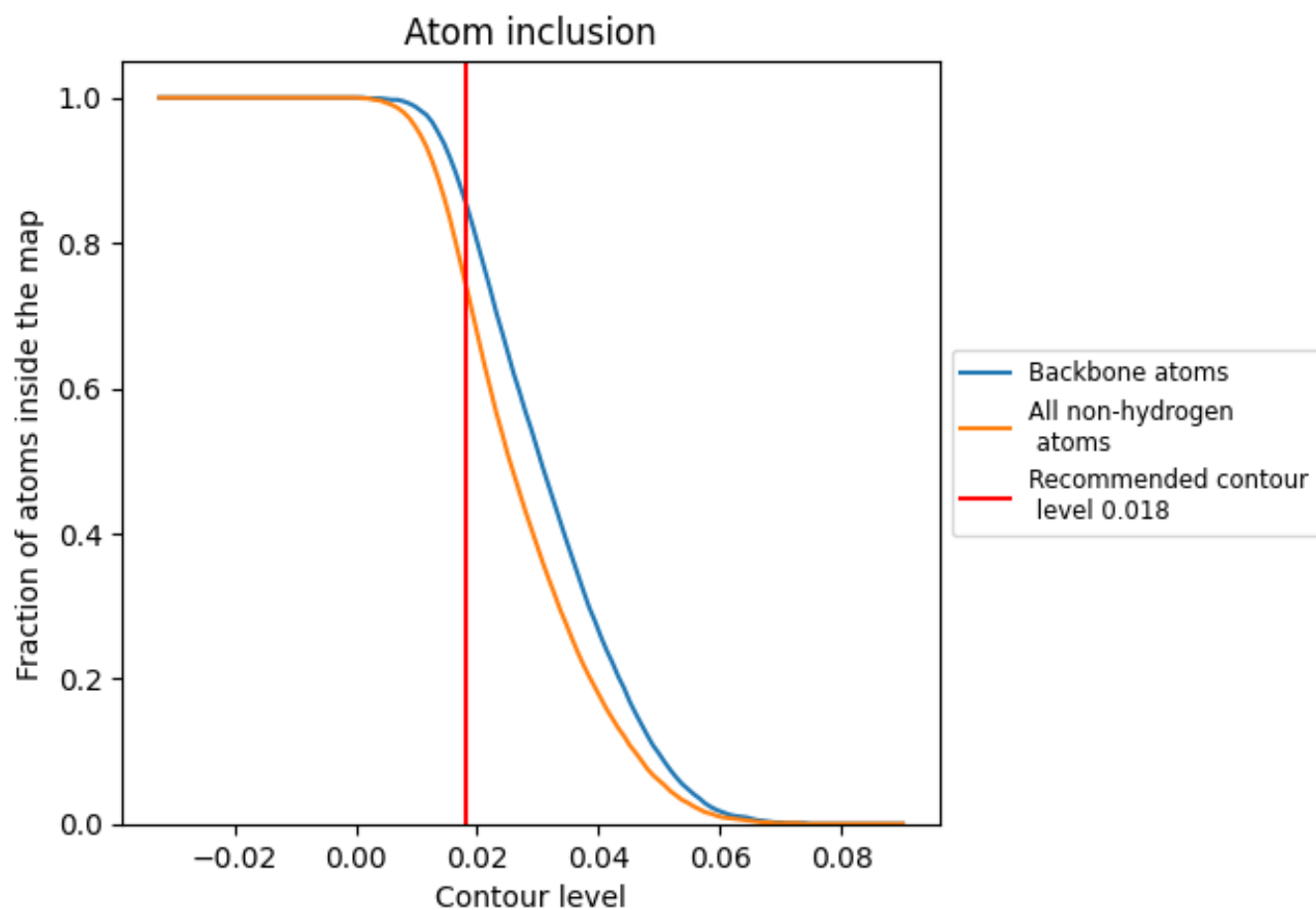
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.4010
A	 0.7520	 0.3900
B	 0.7210	 0.3890
C	 0.7800	 0.4220
D	 0.7520	 0.4080
E	 0.6070	 0.4010
F	 0.4290	 0.3080
G	 0.1430	 0.2550
H	 0.6070	 0.3880
I	 0.5360	 0.2700
J	 0.3080	 0.2080
K	 0.5360	 0.2690
L	 0.3210	 0.1750
M	 0.1430	 0.1650
N	 0.5360	 0.3840
O	 0.4100	 0.3200

