



Full wwPDB EM Validation Report ⓘ

May 9, 2026 – 01:00 PM EDT

PDB ID : 9OVU / pdb_00009ovu
EMDB ID : EMD-70919
Title : Composite map of GluA1/A2 in the activated state, in complex with positive allosteric modulator (R,R)-2b and agonist glutamate (ATD-LBD-TMD)
Authors : Yen, L.Y.; Sobolevsky, A.I.; Newton, T.P.; Gangwar, S.P.
Deposited on : 2025-05-31
Resolution : 3.20 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:

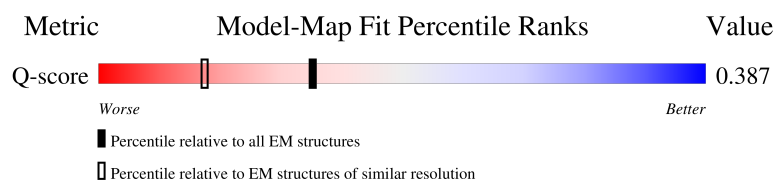
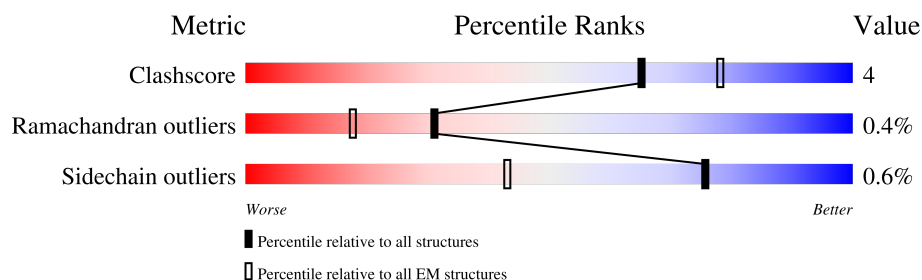
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	835	
1	C	835	
2	B	842	
2	D	842	

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%
3	G	2	50% 50%
3	H	2	50% 100%
3	I	2	50% 100%
3	K	2	50% 50%
3	L	2	100% 100%
4	F	3	100%
4	J	3	67% 33% 67%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25011 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 Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	775	Total	C	N	O	S	0	0
			6175	3964	1046	1134	31		
1	C	775	Total	C	N	O	S	0	0
			6175	3964	1046	1134	31		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P19490
A	?	-	THR	deletion	UNP P19490
A	?	-	ASP	deletion	UNP P19490
A	?	-	ALA	deletion	UNP P19490
A	?	-	GLN	deletion	UNP P19490
A	?	-	ALA	deletion	UNP P19490
C	?	-	ALA	deletion	UNP P19490
C	?	-	THR	deletion	UNP P19490
C	?	-	ASP	deletion	UNP P19490
C	?	-	ALA	deletion	UNP P19490
C	?	-	GLN	deletion	UNP P19490
C	?	-	ALA	deletion	UNP P19490

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	780	Total	C	N	O	S	0	0
			6153	3952	1022	1149	30		
2	D	780	Total	C	N	O	S	0	0
			6153	3952	1022	1149	30		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	GLY	GLN	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	586	ARG	GLN	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
D	-13	GLY	GLN	conflict	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



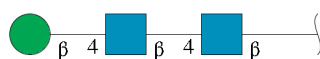
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

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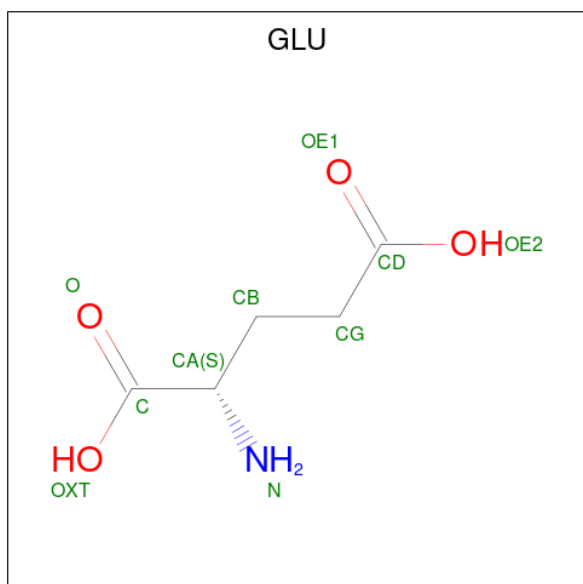
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
4	F	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			10	5	1	4	

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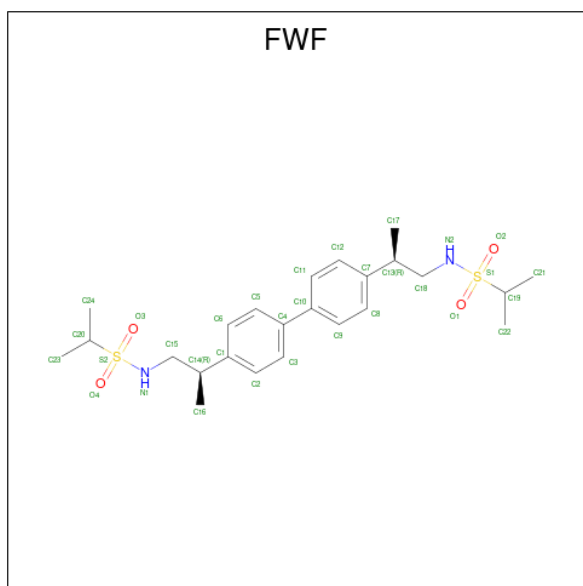
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			10	5	1	4	
5	C	1	Total	C	N	O	0
			10	5	1	4	
5	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Na	0
			1	1	

- Molecule 7 is N,N'-[biphenyl-4,4'-diyl-di(2R)propane-2,1-diyl]dipropane-2-sulfonamide (CCD ID: FWF) (formula: C₂₄H₃₆N₂O₄S₂).



Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	S	0
			32	24	2	4	2	
7	D	1	Total	C	N	O	S	0
			32	24	2	4	2	

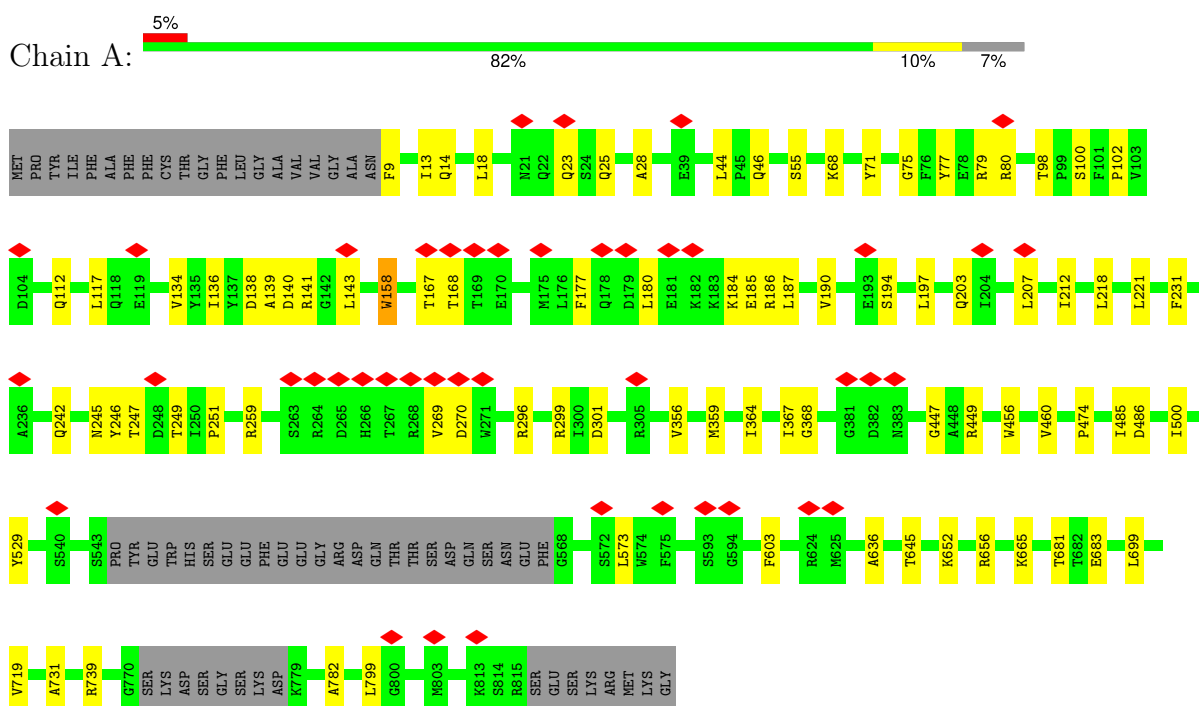
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total 1	O 1	0
8	B	1	Total 1	O 1	0
8	C	1	Total 1	O 1	0
8	D	1	Total 1	O 1	0

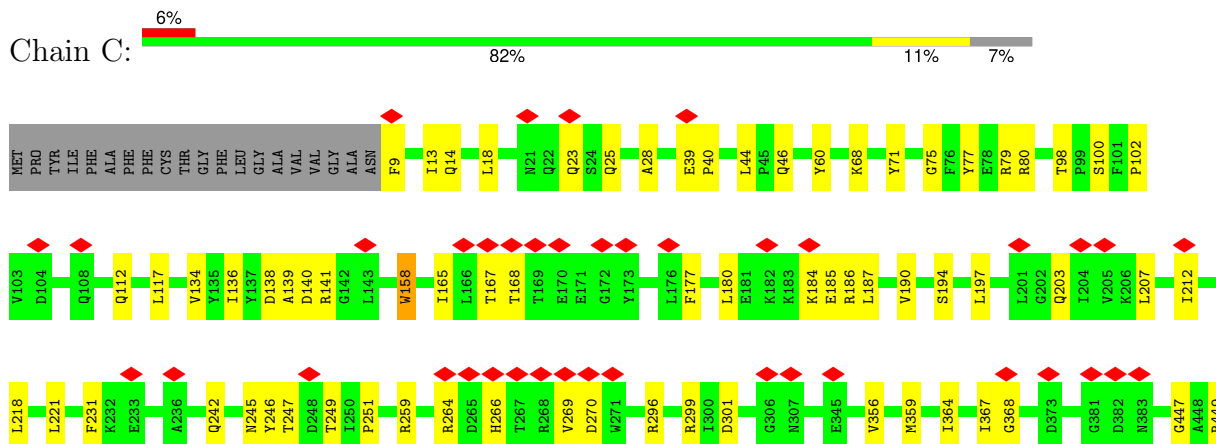
3 Residue-property plots

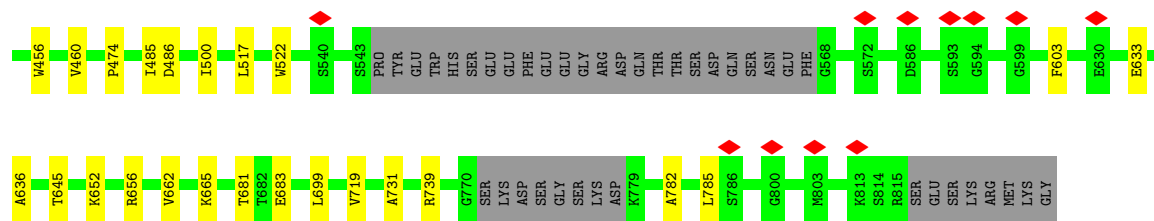
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Isoform Flip of Glutamate receptor 1



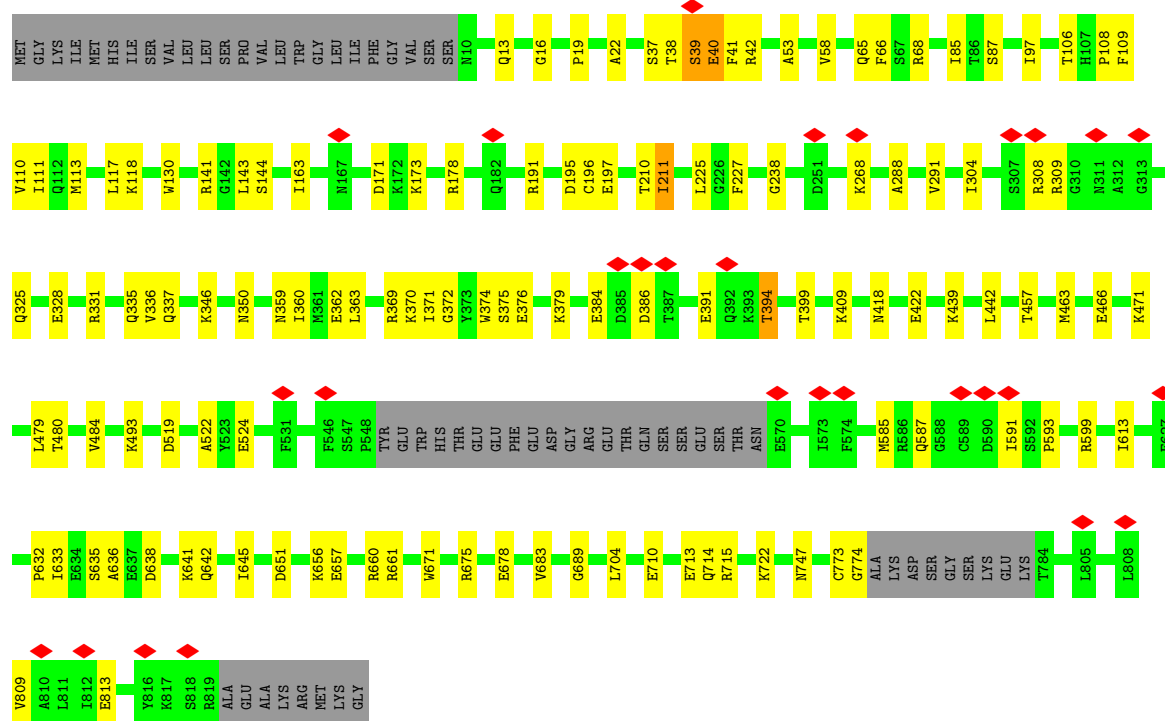
- Molecule 1: Isoform Flip of Glutamate receptor 1





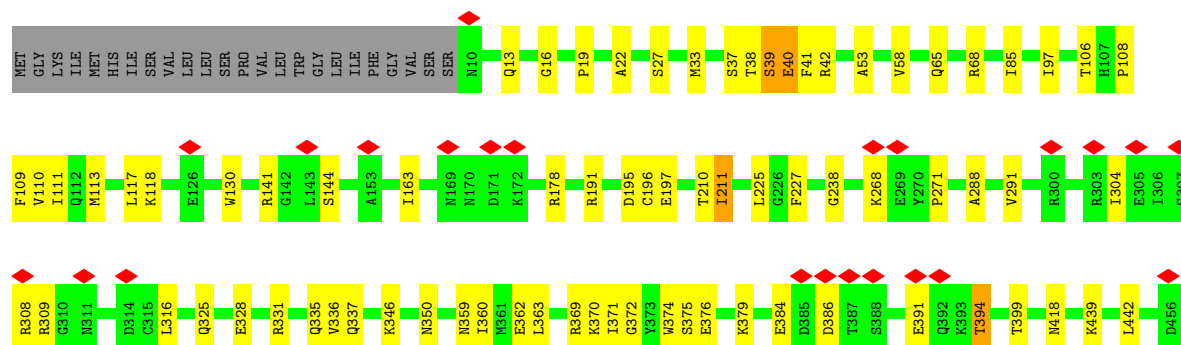
• Molecule 2: Isoform Flip of Glutamate receptor 2

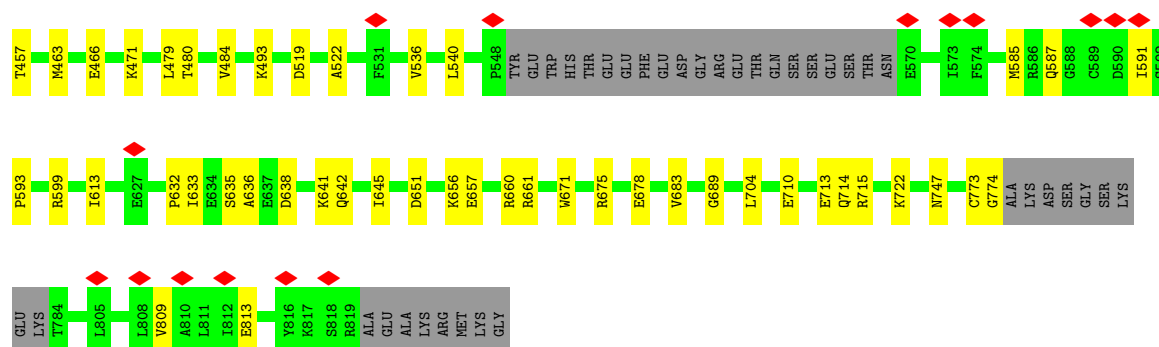
Chain B: 78% 14% 7%



• Molecule 2: Isoform Flip of Glutamate receptor 2

Chain D: 5% 78% 14% 7%





- 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 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	74183	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.03	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.735	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FWF, NAG, NA, 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	A	0.27	0/6310	0.75	7/8529 (0.1%)
1	C	0.27	0/6310	0.75	7/8529 (0.1%)
2	B	0.27	0/6283	0.79	8/8488 (0.1%)
2	D	0.27	0/6283	0.79	8/8488 (0.1%)
All	All	0.27	0/25186	0.77	30/34034 (0.1%)

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
1	A	0	6
1	C	0	6
2	B	0	6
2	D	0	6
All	All	0	24

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	ILE	N-CA-C	-7.46	106.62	113.71
2	B	457	THR	N-CA-C	-7.43	105.38	114.75
2	D	457	THR	N-CA-C	-7.40	105.42	114.75
1	A	212	ILE	N-CA-C	-7.39	106.69	113.71
2	B	591	ILE	CA-C-N	6.87	138.55	121.80
2	B	591	ILE	C-N-CA	6.87	138.55	121.80
2	D	591	ILE	CA-C-N	6.84	138.49	121.80
2	D	591	ILE	C-N-CA	6.84	138.49	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	SER	CA-C-N	6.33	129.26	120.65
1	C	100	SER	C-N-CA	6.33	129.26	120.65
1	A	100	SER	CA-C-N	6.32	129.24	120.65
1	A	100	SER	C-N-CA	6.32	129.24	120.65
1	A	167	THR	CA-C-N	5.87	132.75	121.54
1	A	167	THR	C-N-CA	5.87	132.75	121.54
1	C	167	THR	CA-C-N	5.83	132.67	121.54
1	C	167	THR	C-N-CA	5.83	132.67	121.54
2	B	38	THR	N-CA-C	-5.50	101.07	109.65
2	D	38	THR	N-CA-C	-5.48	101.10	109.65
2	D	53	ALA	N-CA-C	-5.46	106.08	114.16
2	B	53	ALA	N-CA-C	-5.46	106.09	114.16
1	C	158	TRP	CA-C-N	5.37	131.79	121.54
1	C	158	TRP	C-N-CA	5.37	131.79	121.54
1	A	158	TRP	CA-C-N	5.37	131.79	121.54
1	A	158	TRP	C-N-CA	5.37	131.79	121.54
2	B	384	GLU	CA-C-N	5.35	131.77	121.54
2	B	384	GLU	C-N-CA	5.35	131.77	121.54
2	D	384	GLU	CA-C-N	5.34	131.74	121.54
2	D	384	GLU	C-N-CA	5.34	131.74	121.54
2	B	40	GLU	N-CA-C	5.01	121.46	110.80
2	D	40	GLU	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	THR	Peptide
1	A	184	LYS	Peptide
1	A	185	GLU	Peptide
1	A	207	LEU	Peptide
1	A	246	TYR	Peptide
1	A	247	THR	Peptide
2	B	110	VAL	Peptide
2	B	39	SER	Peptide
2	B	394	THR	Peptide
2	B	519	ASP	Peptide
2	B	632	PRO	Peptide
2	B	678	GLU	Peptide
1	C	168	THR	Peptide
1	C	184	LYS	Peptide
1	C	185	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	207	LEU	Peptide
1	C	246	TYR	Peptide
1	C	247	THR	Peptide
2	D	110	VAL	Peptide
2	D	39	SER	Peptide
2	D	394	THR	Peptide
2	D	519	ASP	Peptide
2	D	632	PRO	Peptide
2	D	678	GLU	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	6175	0	6163	42	0
1	C	6175	0	6163	45	0
2	B	6153	0	6147	63	0
2	D	6153	0	6147	62	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	F	39	0	34	0	0
4	J	39	0	34	0	0
5	A	10	0	5	1	0
5	B	10	0	5	1	0
5	C	10	0	5	1	0
5	D	10	0	5	1	0
6	B	1	0	0	0	0
7	C	32	0	36	0	0
7	D	32	0	36	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
All	All	25011	0	24930	201	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 4.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG23	1:A:251:PRO:HD2	1.73	0.70
1:C:249:THR:HG23	1:C:251:PRO:HD2	1.73	0.69
1:A:356:VAL:H	1:A:368:GLY:HA3	1.60	0.67
1:C:356:VAL:H	1:C:368:GLY:HA3	1.60	0.67
2:B:773:CYS:SG	2:B:774:GLY:N	2.73	0.61
2:D:773:CYS:SG	2:D:774:GLY:N	2.73	0.61
2:B:238:GLY:HA2	2:D:211:ILE:HG22	1.83	0.60
2:B:480:THR:HG1	5:B:901:GLU:N	1.99	0.60
2:D:480:THR:HG1	5:D:901:GLU:N	1.99	0.59
2:B:638:ASP:OD1	2:B:641:LYS:NZ	2.36	0.58
2:D:638:ASP:OD1	2:D:641:LYS:NZ	2.36	0.58
2:B:522:ALA:HB2	1:C:782:ALA:HB1	1.87	0.57
1:C:474:PRO:O	5:C:901:GLU:N	2.39	0.56
1:C:636:ALA:HB1	1:C:665:LYS:HD2	1.87	0.56
1:A:474:PRO:O	5:A:901:GLU:N	2.39	0.55
1:C:186:ARG:HG2	1:C:187:LEU:HD23	1.88	0.55
1:A:636:ALA:HB1	1:A:665:LYS:HD2	1.87	0.55
2:B:141:ARG:NH1	2:B:195:ASP:OD2	2.40	0.55
1:C:138:ASP:HB3	1:C:141:ARG:HE	1.72	0.55
2:D:196:CYS:SG	2:D:197:GLU:N	2.80	0.55
1:C:296:ARG:O	1:C:299:ARG:NH1	2.40	0.55
1:A:138:ASP:HB3	1:A:141:ARG:HE	1.72	0.55
2:B:369:ARG:NH2	2:B:386:ASP:OD2	2.40	0.54
2:D:369:ARG:NH2	2:D:386:ASP:OD2	2.41	0.54
2:D:585:MET:O	2:D:587:GLN:NE2	2.41	0.54
2:B:196:CYS:SG	2:B:197:GLU:N	2.80	0.54
1:A:186:ARG:HG2	1:A:187:LEU:HD23	1.89	0.54
2:D:141:ARG:NH1	2:D:195:ASP:OD2	2.40	0.54
2:B:331:ARG:HH12	2:B:335:GLN:HG3	1.73	0.53
2:B:585:MET:O	2:B:587:GLN:NE2	2.41	0.53
2:B:374:TRP:HE1	2:B:379:LYS:HG2	1.73	0.53
1:A:9:PHE:N	1:A:301:ASP:OD1	2.41	0.53
1:C:9:PHE:N	1:C:301:ASP:OD1	2.41	0.53
2:D:374:TRP:HE1	2:D:379:LYS:HG2	1.73	0.53
2:D:493:LYS:HG2	2:D:747:ASN:HD21	1.73	0.53
2:D:331:ARG:HH12	2:D:335:GLN:HG3	1.73	0.52
2:D:359:ASN:ND2	2:D:372:GLY:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:LYS:HG2	2:B:747:ASN:HD21	1.73	0.52
1:C:102:PRO:HA	1:C:112:GLN:HG2	1.92	0.52
2:D:16:GLY:O	2:D:65:GLN:NE2	2.38	0.52
2:B:359:ASN:ND2	2:B:372:GLY:O	2.42	0.52
1:C:603:PHE:HA	2:D:585:MET:HE2	1.91	0.52
1:A:102:PRO:HA	1:A:112:GLN:HG2	1.92	0.52
2:B:16:GLY:O	2:B:65:GLN:NE2	2.38	0.52
1:A:296:ARG:O	1:A:299:ARG:NH1	2.40	0.51
1:A:177:PHE:HE2	1:A:203:GLN:HE22	1.59	0.51
1:A:603:PHE:HA	2:B:585:MET:HE2	1.93	0.51
1:A:500:ILE:HD12	1:A:719:VAL:HG21	1.92	0.51
1:C:177:PHE:HE2	1:C:203:GLN:HE22	1.59	0.51
2:D:651:ASP:OD1	2:D:656:LYS:NZ	2.42	0.51
1:C:79:ARG:HD2	1:C:80:ARG:HG3	1.93	0.50
2:B:211:ILE:HG22	2:D:238:GLY:HA2	1.94	0.50
1:A:190:VAL:HB	1:A:218:LEU:HD23	1.94	0.50
2:D:118:LYS:NZ	2:D:144:SER:OG	2.45	0.50
1:C:190:VAL:HB	1:C:218:LEU:HD23	1.94	0.50
2:B:130:TRP:CD2	2:B:191:ARG:HD3	2.46	0.49
1:C:14:GLN:HG3	1:C:44:LEU:HD11	1.93	0.49
1:C:500:ILE:HD12	1:C:719:VAL:HG21	1.92	0.49
2:D:130:TRP:CD2	2:D:191:ARG:HD3	2.46	0.49
2:D:39:SER:O	2:D:41:PHE:N	2.45	0.49
1:A:79:ARG:HD2	1:A:80:ARG:HG3	1.93	0.49
1:C:359:MET:HA	1:C:364:ILE:HG22	1.93	0.49
2:B:651:ASP:OD1	2:B:656:LYS:NZ	2.42	0.49
1:A:14:GLN:HG3	1:A:44:LEU:HD11	1.93	0.49
2:B:39:SER:O	2:B:41:PHE:N	2.45	0.49
2:D:304:ILE:HG21	2:D:328:GLU:HG2	1.95	0.49
1:A:359:MET:HA	1:A:364:ILE:HG22	1.93	0.49
2:B:13:GLN:HE22	2:B:68:ARG:HG2	1.78	0.49
2:B:642:GLN:HE22	2:B:645:ILE:HD12	1.78	0.48
2:D:484:VAL:HG11	2:D:661:ARG:HH12	1.78	0.48
2:D:657:GLU:OE2	2:D:660:ARG:NH1	2.46	0.48
2:B:118:LYS:NZ	2:B:144:SER:OG	2.45	0.48
2:B:710:GLU:OE2	2:B:722:LYS:NZ	2.47	0.48
2:D:642:GLN:HE22	2:D:645:ILE:HD12	1.78	0.48
2:B:657:GLU:OE2	2:B:660:ARG:NH1	2.46	0.48
2:D:27:SER:OG	2:D:271:PRO:O	2.29	0.48
2:B:304:ILE:HG21	2:B:328:GLU:HG2	1.95	0.48
2:D:37:SER:OG	2:D:42:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:HG3	2:B:309:ARG:H	1.79	0.48
1:C:485:ILE:HD12	1:C:731:ALA:HB1	1.96	0.48
2:D:13:GLN:HE22	2:D:68:ARG:HG2	1.78	0.48
1:C:60:TYR:HD1	2:D:316:LEU:HB2	1.79	0.48
2:B:484:VAL:HG11	2:B:661:ARG:HH12	1.78	0.47
1:A:782:ALA:HB1	2:D:522:ALA:HB2	1.97	0.47
2:B:37:SER:OG	2:B:42:ARG:NH2	2.46	0.47
2:D:291:VAL:HG13	2:D:336:VAL:HG21	1.97	0.47
1:A:18:LEU:HB2	1:A:75:GLY:HA3	1.96	0.47
1:A:231:PHE:HB2	1:A:359:MET:HE1	1.97	0.47
2:B:466:GLU:HG2	2:B:471:LYS:HE3	1.96	0.47
2:B:714:GLN:O	2:B:715:ARG:NE	2.48	0.47
1:A:46:GLN:HE22	1:A:68:LYS:HD2	1.80	0.47
1:A:485:ILE:HD12	1:A:731:ALA:HB1	1.96	0.47
2:B:391:GLU:HA	2:B:439:LYS:HD3	1.96	0.47
2:D:106:THR:HG23	2:D:350:ASN:HD22	1.80	0.47
1:A:55:SER:HB2	2:B:87:SER:HB2	1.96	0.47
1:A:652:LYS:HE2	1:A:656:ARG:HH12	1.80	0.47
2:B:633:ILE:HG23	2:B:638:ASP:HB2	1.97	0.47
1:C:18:LEU:HB2	1:C:75:GLY:HA3	1.96	0.47
2:B:106:THR:HG23	2:B:350:ASN:HD22	1.80	0.46
1:C:652:LYS:HE2	1:C:656:ARG:HH12	1.81	0.46
2:D:308:ARG:HG3	2:D:309:ARG:H	1.79	0.46
2:D:714:GLN:O	2:D:715:ARG:NE	2.48	0.46
2:B:713:GLU:OE2	2:B:722:LYS:N	2.46	0.46
2:B:391:GLU:O	2:B:394:THR:OG1	2.34	0.46
1:C:46:GLN:HE22	1:C:68:LYS:HD2	1.80	0.46
2:B:291:VAL:HG13	2:B:336:VAL:HG21	1.97	0.46
1:A:77:TYR:HE1	1:A:98:THR:HG21	1.81	0.46
1:A:242:GLN:OE1	1:A:245:ASN:N	2.46	0.46
1:C:231:PHE:HB2	1:C:359:MET:HE1	1.97	0.46
2:D:178:ARG:HH21	2:D:210:THR:HG23	1.81	0.46
2:D:391:GLU:HA	2:D:439:LYS:HD3	1.96	0.46
2:D:633:ILE:HG23	2:D:638:ASP:HB2	1.96	0.46
2:B:178:ARG:HH21	2:B:210:THR:HG23	1.81	0.46
2:D:710:GLU:OE2	2:D:722:LYS:NZ	2.47	0.46
1:C:13:ILE:HG23	1:C:71:TYR:HD2	1.81	0.46
2:D:466:GLU:HG2	2:D:471:LYS:HE3	1.97	0.46
2:D:713:GLU:OE2	2:D:722:LYS:N	2.46	0.46
1:A:13:ILE:HG23	1:A:71:TYR:HD2	1.81	0.46
1:C:77:TYR:HE1	1:C:98:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:THR:HG22	1:C:683:GLU:H	1.81	0.45
2:D:391:GLU:O	2:D:394:THR:OG1	2.34	0.45
2:D:19:PRO:HG2	2:D:22:ALA:HB2	1.98	0.45
1:A:645:THR:HG22	1:A:699:LEU:HB2	1.99	0.45
1:A:143:LEU:HD23	2:B:143:LEU:HD21	1.98	0.45
1:A:681:THR:HG22	1:A:683:GLU:H	1.81	0.45
2:B:337:GLN:HE22	2:B:346:LYS:HD2	1.82	0.45
2:B:19:PRO:HG2	2:B:22:ALA:HB2	1.98	0.45
1:C:242:GLN:OE1	1:C:245:ASN:N	2.46	0.45
1:C:645:THR:HG22	1:C:699:LEU:HB2	1.99	0.45
1:A:136:ILE:HB	1:A:190:VAL:HA	1.99	0.45
2:D:337:GLN:HE22	2:D:346:LYS:HD2	1.82	0.45
1:C:136:ILE:HB	1:C:190:VAL:HA	1.99	0.45
1:C:259:ARG:NH2	1:C:270:ASP:O	2.50	0.45
2:B:524:GLU:HB3	1:C:785:LEU:HD23	1.99	0.44
1:C:23:GLN:HE22	1:C:25:GLN:HB3	1.82	0.44
2:D:308:ARG:HG2	2:D:325:GLN:HE22	1.82	0.44
1:A:134:VAL:HG21	1:A:180:LEU:HD11	2.00	0.44
1:C:449:ARG:HH11	1:C:456:TRP:HE1	1.65	0.44
2:B:809:VAL:O	2:B:813:GLU:N	2.50	0.44
2:B:113:MET:HE1	2:B:288:ALA:HB2	2.00	0.44
1:A:449:ARG:HH11	1:A:456:TRP:HE1	1.65	0.44
2:D:113:MET:HE1	2:D:288:ALA:HB2	1.99	0.44
1:A:259:ARG:NH2	1:A:270:ASP:O	2.50	0.44
1:A:23:GLN:HE22	1:A:25:GLN:HB3	1.83	0.44
2:D:418:ASN:ND2	2:D:442:LEU:H	2.15	0.44
2:D:809:VAL:O	2:D:813:GLU:N	2.50	0.44
2:B:375:SER:OG	2:B:376:GLU:N	2.51	0.43
2:B:418:ASN:ND2	2:B:442:LEU:H	2.15	0.43
1:C:39:GLU:HA	1:C:40:PRO:HD3	1.84	0.43
1:A:799:LEU:HD11	2:D:536:VAL:HG12	2.01	0.43
2:B:66:PHE:O	2:B:309:ARG:NH1	2.48	0.43
2:B:308:ARG:HG2	2:B:325:GLN:HE22	1.82	0.43
2:B:359:ASN:HD21	2:B:370:LYS:HG3	1.83	0.43
2:D:97:ILE:HG22	2:D:111:ILE:HB	2.00	0.43
2:D:359:ASN:HD21	2:D:370:LYS:HG3	1.84	0.43
2:B:593:PRO:O	2:B:599:ARG:NH1	2.44	0.43
2:D:58:VAL:HG12	2:D:85:ILE:HD11	2.01	0.43
2:D:375:SER:OG	2:D:376:GLU:N	2.51	0.43
2:B:97:ILE:HG22	2:B:111:ILE:HB	2.01	0.43
1:C:134:VAL:HG21	1:C:180:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLY:HA3	1:C:460:VAL:HG12	2.01	0.43
1:A:529:TYR:OH	1:A:573:LEU:O	2.36	0.42
2:B:418:ASN:HD21	2:B:442:LEU:H	1.66	0.42
2:D:418:ASN:HD21	2:D:442:LEU:H	1.66	0.42
1:A:194:SER:HA	1:A:197:LEU:HD23	2.01	0.42
2:B:656:LYS:HE2	2:B:660:ARG:HH21	1.85	0.42
2:D:593:PRO:O	2:D:599:ARG:NH1	2.44	0.42
2:D:362:GLU:HG3	2:D:371:ILE:HD13	2.02	0.42
2:B:58:VAL:HG12	2:B:85:ILE:HD11	2.01	0.42
1:C:264:ARG:HG3	1:C:266:HIS:H	1.85	0.42
2:D:635:SER:OG	2:D:636:ALA:N	2.52	0.42
2:D:671:TRP:HE1	2:D:675:ARG:NH2	2.18	0.41
2:B:635:SER:OG	2:B:636:ALA:N	2.52	0.41
1:C:28:ALA:HB1	1:C:269:VAL:HB	2.02	0.41
1:C:165:ILE:H	1:C:165:ILE:HG13	1.74	0.41
1:C:138:ASP:O	1:C:140:ASP:N	2.53	0.41
1:C:194:SER:HA	1:C:197:LEU:HD23	2.01	0.41
2:B:360:ILE:HD11	2:B:374:TRP:HB2	2.02	0.41
2:B:463:MET:HE3	2:B:479:LEU:HD13	2.02	0.41
2:D:463:MET:HE3	2:D:479:LEU:HD13	2.02	0.41
2:D:656:LYS:HE2	2:D:660:ARG:HH21	1.85	0.41
1:A:447:GLY:HA3	1:A:460:VAL:HG12	2.02	0.41
2:D:33:MET:O	2:D:37:SER:OG	2.31	0.41
2:B:671:TRP:HE1	2:B:675:ARG:NH2	2.18	0.41
2:B:409:LYS:HZ1	2:B:422:GLU:HB3	1.85	0.41
1:C:486:ASP:HB3	1:C:739:ARG:HH11	1.85	0.41
1:A:28:ALA:HB1	1:A:269:VAL:HB	2.02	0.41
1:A:138:ASP:O	1:A:140:ASP:N	2.53	0.41
2:D:227:PHE:HZ	2:D:363:LEU:HD22	1.86	0.41
1:A:486:ASP:HB3	1:A:739:ARG:HH11	1.85	0.41
2:D:360:ILE:HD11	2:D:374:TRP:HB2	2.02	0.41
2:D:683:VAL:HG11	2:D:689:GLY:HA2	2.03	0.41
2:B:171:ASP:O	2:B:173:LYS:N	2.54	0.40
2:B:227:PHE:HZ	2:B:363:LEU:HD22	1.86	0.40
2:B:683:VAL:HG11	2:B:689:GLY:HA2	2.03	0.40
1:C:117:LEU:HD11	1:C:221:LEU:HD13	2.04	0.40
1:C:633:GLU:HG2	1:C:662:VAL:HG21	2.03	0.40
2:D:540:LEU:HD23	2:D:540:LEU:HA	1.96	0.40
1:A:117:LEU:HD11	1:A:221:LEU:HD13	2.04	0.40
2:B:362:GLU:HG3	2:B:371:ILE:HD13	2.02	0.40
1:C:517:LEU:HB2	1:C:522:TRP:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	769/835 (92%)	679 (88%)	88 (11%)	2 (0%)	36	68
1	C	769/835 (92%)	678 (88%)	89 (12%)	2 (0%)	36	68
2	B	774/842 (92%)	653 (84%)	117 (15%)	4 (0%)	24	59
2	D	774/842 (92%)	654 (84%)	116 (15%)	4 (0%)	24	59
All	All	3086/3354 (92%)	2664 (86%)	410 (13%)	12 (0%)	31	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	GLU
2	D	40	GLU
1	A	139	ALA
2	B	268	LYS
1	C	139	ALA
2	D	268	LYS
2	B	109	PHE
2	D	109	PHE
1	A	158	TRP
1	C	158	TRP
2	B	108	PRO
2	D	108	PRO

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	665/716 (93%)	664 (100%)	1 (0%)	87	89
1	C	665/716 (93%)	664 (100%)	1 (0%)	87	89
2	B	666/719 (93%)	659 (99%)	7 (1%)	65	79
2	D	666/719 (93%)	659 (99%)	7 (1%)	65	79
All	All	2662/2870 (93%)	2646 (99%)	16 (1%)	76	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
2	B	117	LEU
2	B	163	ILE
2	B	211	ILE
2	B	225	LEU
2	B	399	THR
2	B	613	ILE
2	B	704	LEU
1	C	367	ILE
2	D	117	LEU
2	D	163	ILE
2	D	211	ILE
2	D	225	LEU
2	D	399	THR
2	D	613	ILE
2	D	704	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	23	GLN
1	A	36	GLN
1	A	46	GLN
1	A	220	ASN
1	A	326	GLN
1	A	409	ASN
1	A	615	ASN
1	A	787	ASN
2	B	13	GLN

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Mol	Chain	Res	Type
2	B	60	ASN
2	B	170	ASN
2	B	236	GLN
2	B	318	ASN
2	B	335	GLN
2	B	337	GLN
2	B	344	ASN
2	B	359	ASN
2	B	418	ASN
2	B	747	ASN
1	C	14	GLN
1	C	23	GLN
1	C	36	GLN
1	C	46	GLN
1	C	220	ASN
1	C	321	GLN
1	C	326	GLN
1	C	409	ASN
1	C	615	ASN
2	D	13	GLN
2	D	60	ASN
2	D	170	ASN
2	D	236	GLN
2	D	318	ASN
2	D	335	GLN
2	D	337	GLN
2	D	359	ASN
2	D	418	ASN
2	D	747	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	E	1	3,1	14,14,15	0.53	0	17,19,21	0.65	0
3	NAG	E	2	3	14,14,15	1.32	1 (7%)	17,19,21	1.47	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.47	0	17,19,21	1.06	1 (5%)
4	NAG	F	2	4	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
4	BMA	F	3	4	11,11,12	1.29	2 (18%)	15,15,17	1.45	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.39	0	17,19,21	0.74	1 (5%)
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	H	1	3,2	14,14,15	1.17	1 (7%)	17,19,21	1.94	2 (11%)
3	NAG	H	2	3	14,14,15	1.81	2 (14%)	17,19,21	1.38	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.61	0	17,19,21	0.68	0
3	NAG	I	2	3	14,14,15	1.34	1 (7%)	17,19,21	1.50	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
4	NAG	J	2	4	14,14,15	0.38	0	17,19,21	0.76	0
4	BMA	J	3	4	11,11,12	1.59	2 (18%)	15,15,17	1.86	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.47	0	17,19,21	0.73	1 (5%)
3	NAG	K	2	3	14,14,15	0.39	0	17,19,21	0.48	0
3	NAG	L	1	3,2	14,14,15	1.34	1 (7%)	17,19,21	1.90	2 (11%)
3	NAG	L	2	3	14,14,15	1.65	2 (14%)	17,19,21	1.38	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	1/1/1/1
3	NAG	G	1	3,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	O5-C1	5.32	1.52	1.43
3	L	2	NAG	O5-C1	4.89	1.51	1.43
3	I	2	NAG	O5-C1	4.76	1.51	1.43
3	L	1	NAG	O5-C1	4.63	1.51	1.43
3	E	2	NAG	O5-C1	4.63	1.51	1.43
3	H	2	NAG	C1-C2	4.02	1.57	1.52
3	H	1	NAG	O5-C1	3.97	1.50	1.43
3	L	2	NAG	C1-C2	3.51	1.57	1.52
4	F	3	BMA	O5-C5	3.22	1.49	1.43
4	J	3	BMA	C1-C2	3.22	1.59	1.52
4	J	3	BMA	O5-C5	3.13	1.49	1.43
4	F	3	BMA	C1-C2	2.12	1.57	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	6.66	121.12	112.19
3	L	1	NAG	C1-O5-C5	6.59	121.02	112.19
3	I	2	NAG	C1-O5-C5	5.98	120.19	112.19
3	E	2	NAG	C1-O5-C5	5.88	120.07	112.19
4	J	3	BMA	C1-O5-C5	5.82	119.99	112.19
3	L	2	NAG	C1-O5-C5	5.30	119.29	112.19
3	H	2	NAG	C1-O5-C5	5.27	119.25	112.19
4	F	3	BMA	C1-O5-C5	4.62	118.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C2-N2-C7	3.36	127.40	122.90
3	H	1	NAG	C2-N2-C7	3.33	127.36	122.90
4	J	3	BMA	C1-C2-C3	2.77	113.68	109.64
4	J	1	NAG	O4-C4-C3	-2.35	104.84	110.38
4	F	1	NAG	O4-C4-C3	-2.34	104.86	110.38
3	G	1	NAG	C1-O5-C5	2.23	115.18	112.19
4	F	2	NAG	C1-O5-C5	2.21	115.14	112.19
3	K	1	NAG	C1-O5-C5	2.17	115.10	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

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

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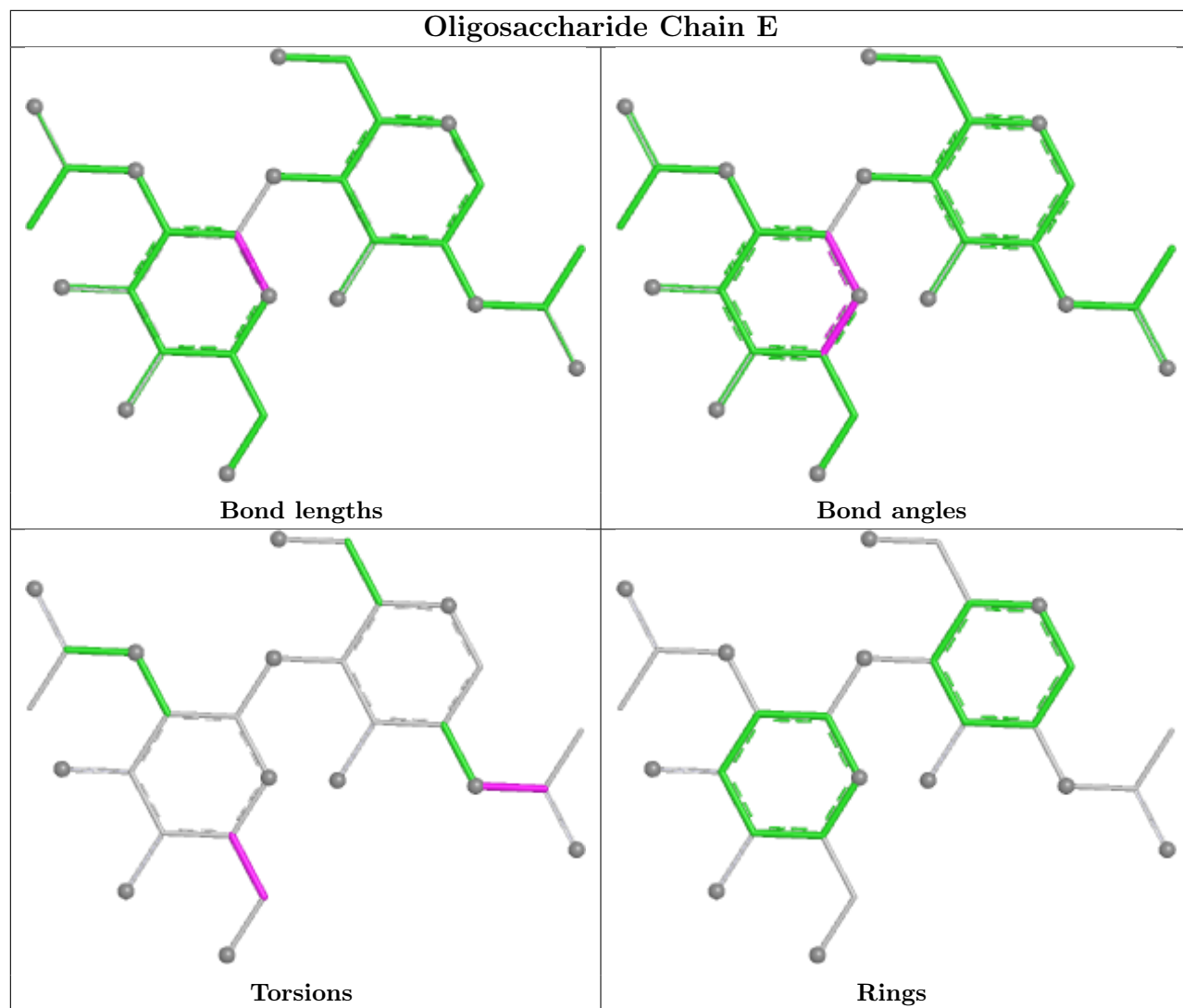
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C3-C2-N2-C7
3	L	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	L	1	NAG	C1-C2-N2-C7
3	L	2	NAG	C1-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
3	G	1	NAG	C4-C5-C6-O6

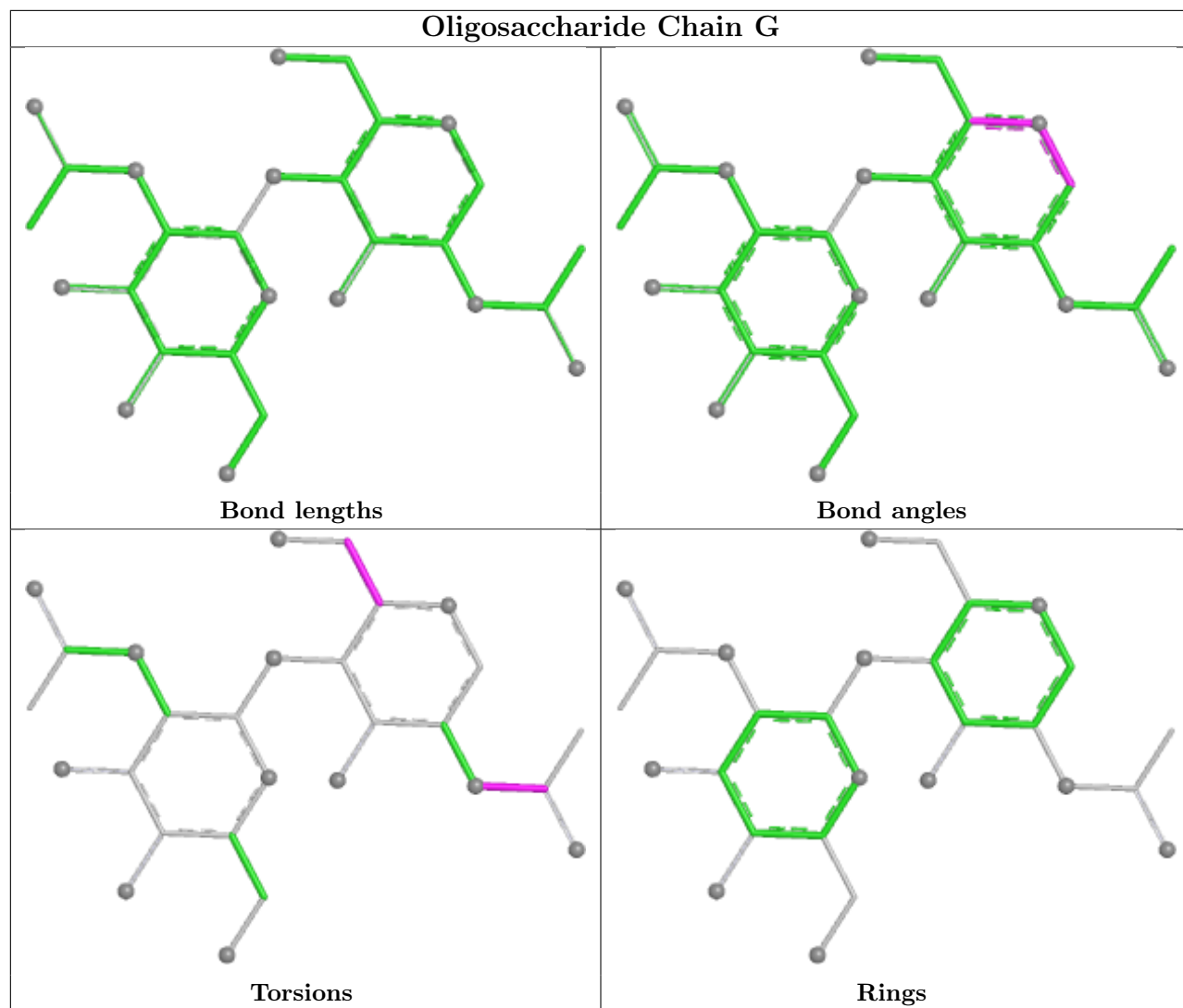
All (1) ring outliers are listed below:

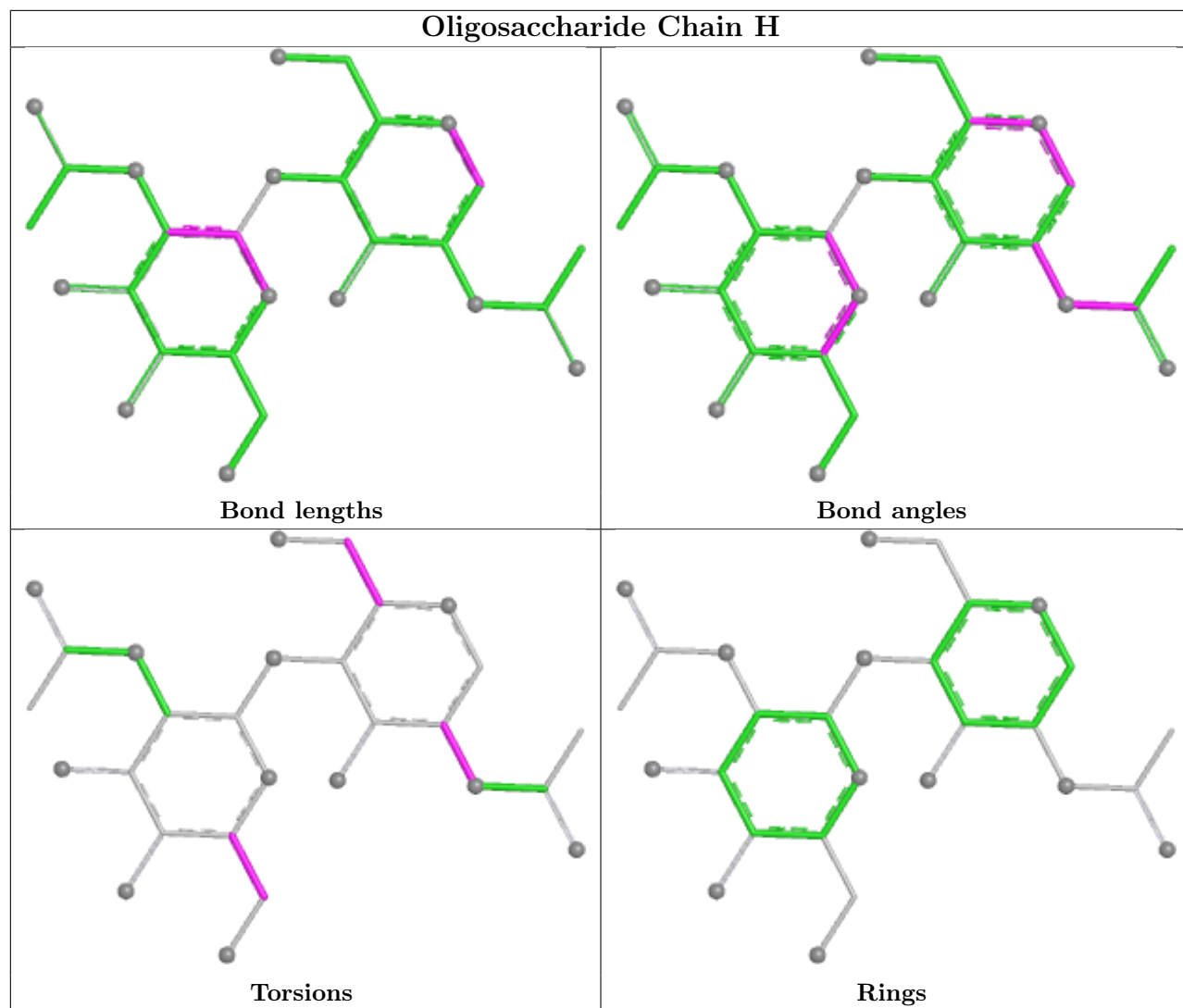
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C1-C2-C3-C4-C5-O5

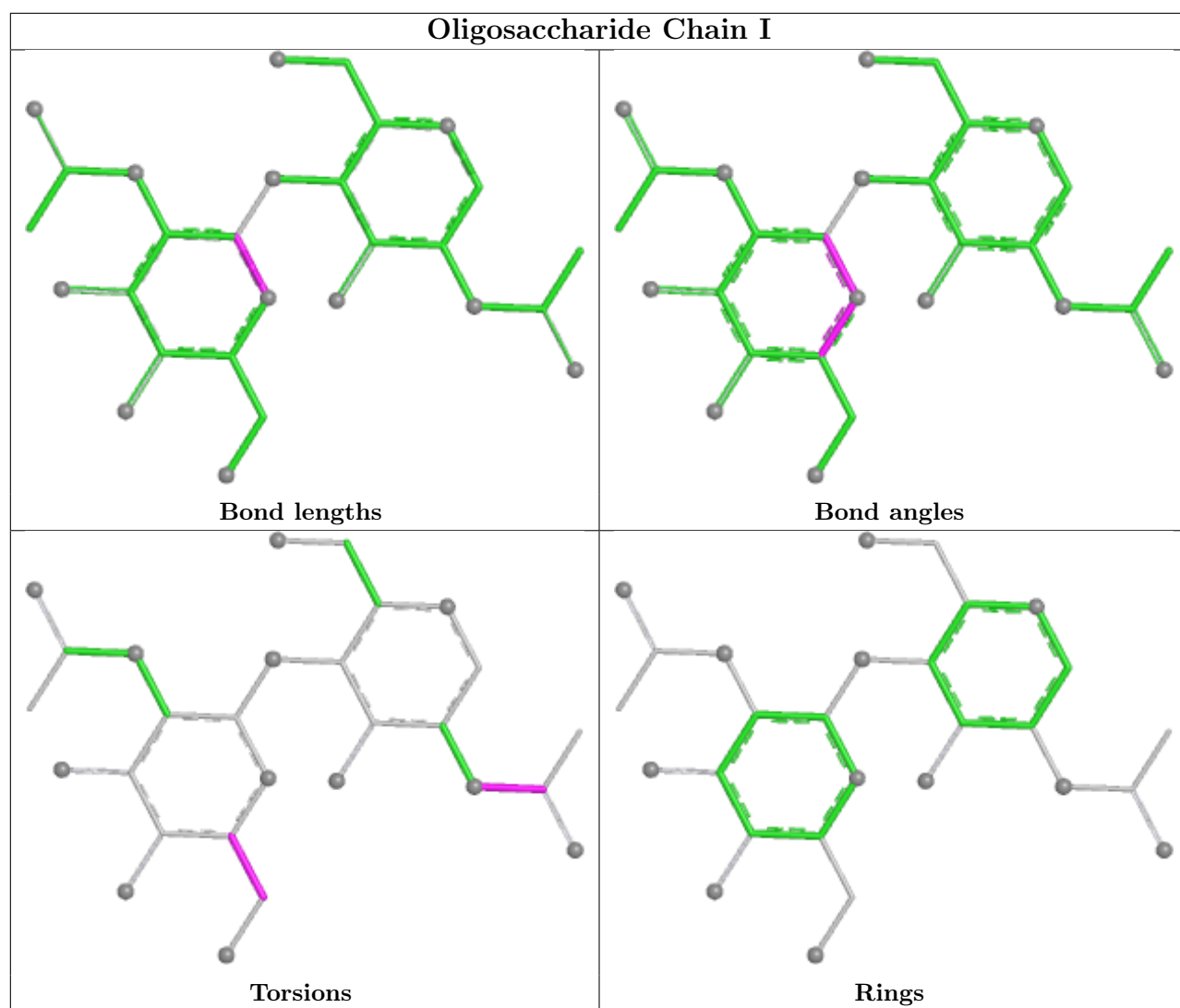
No monomer is involved in short contacts.

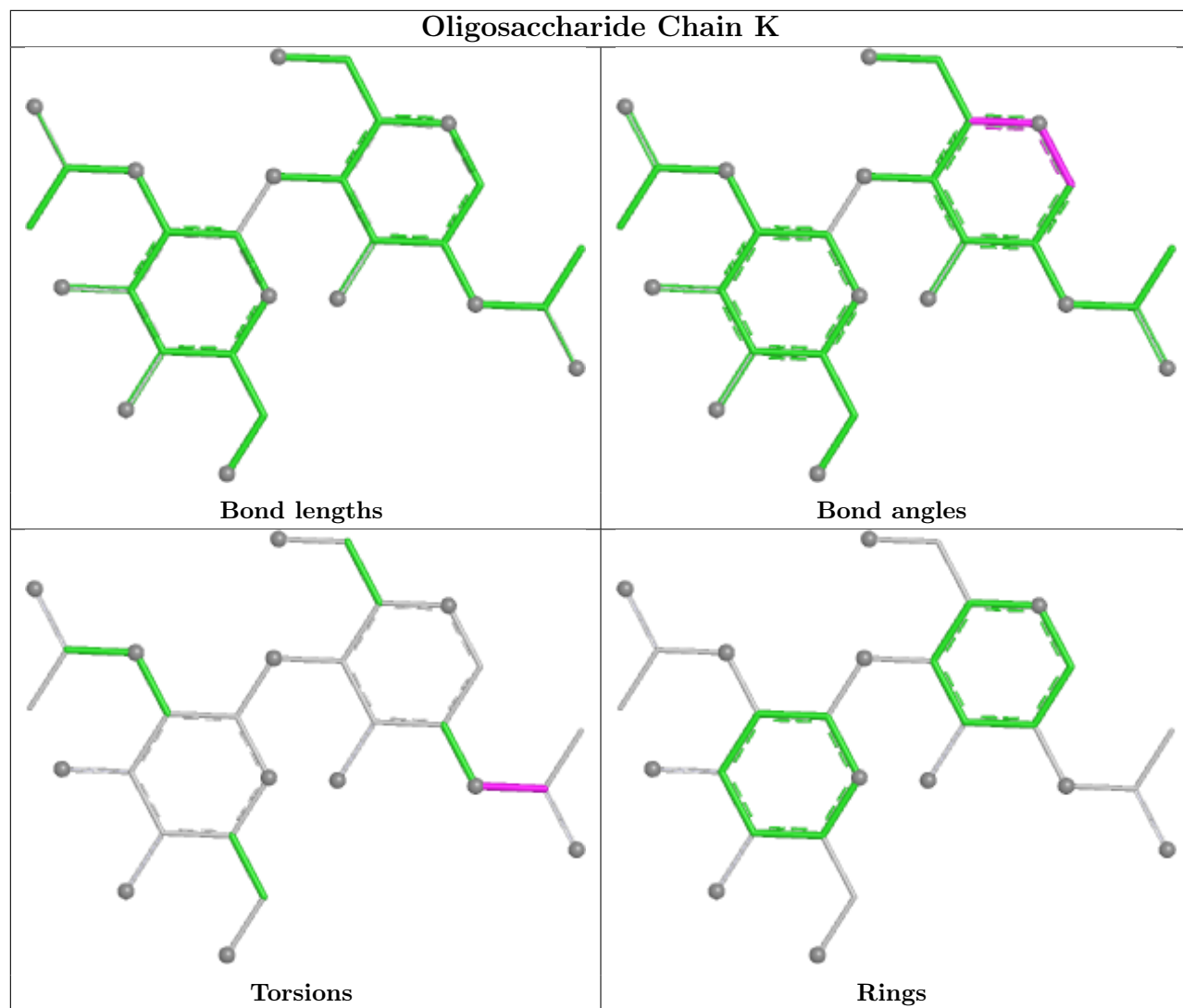
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

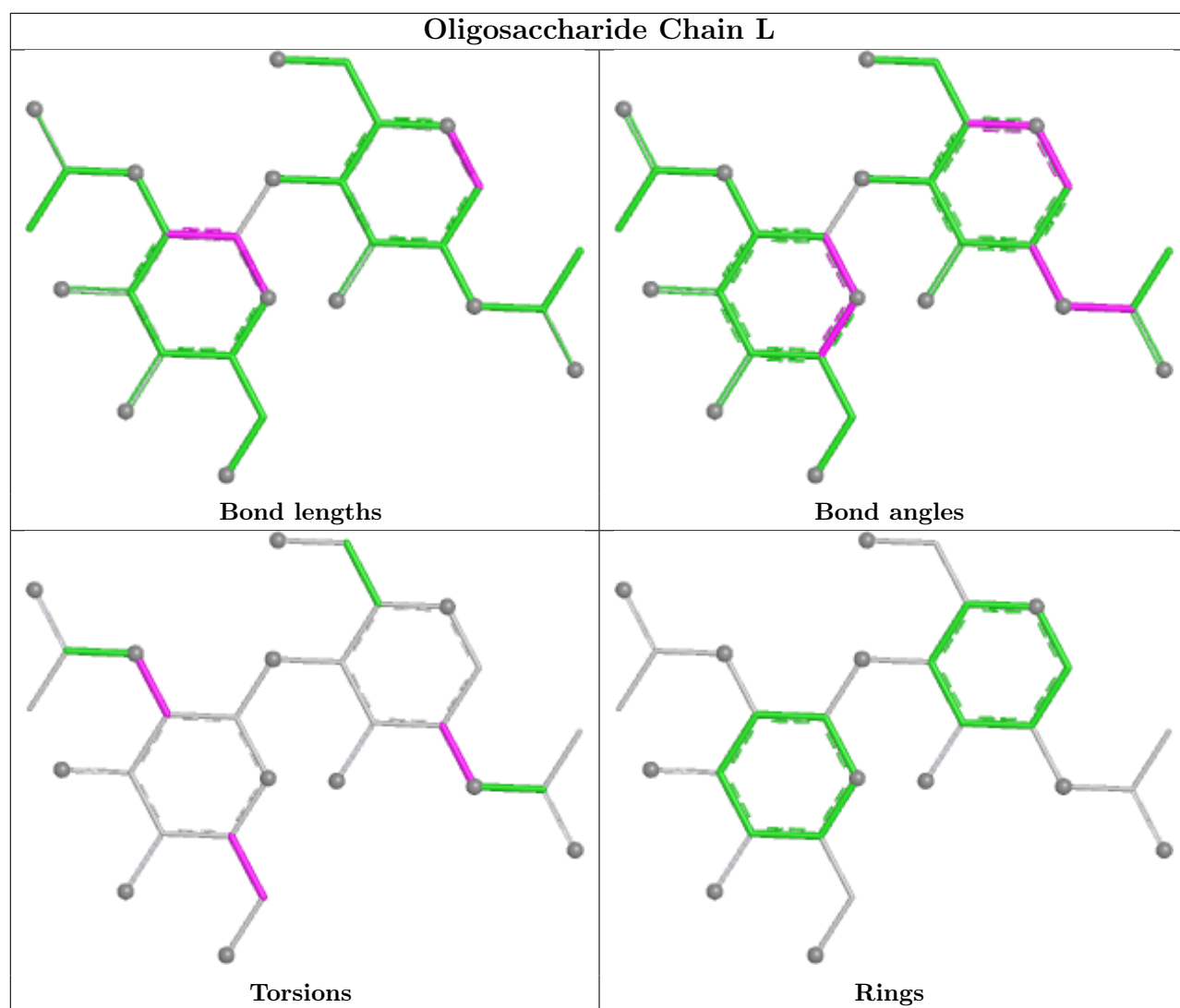


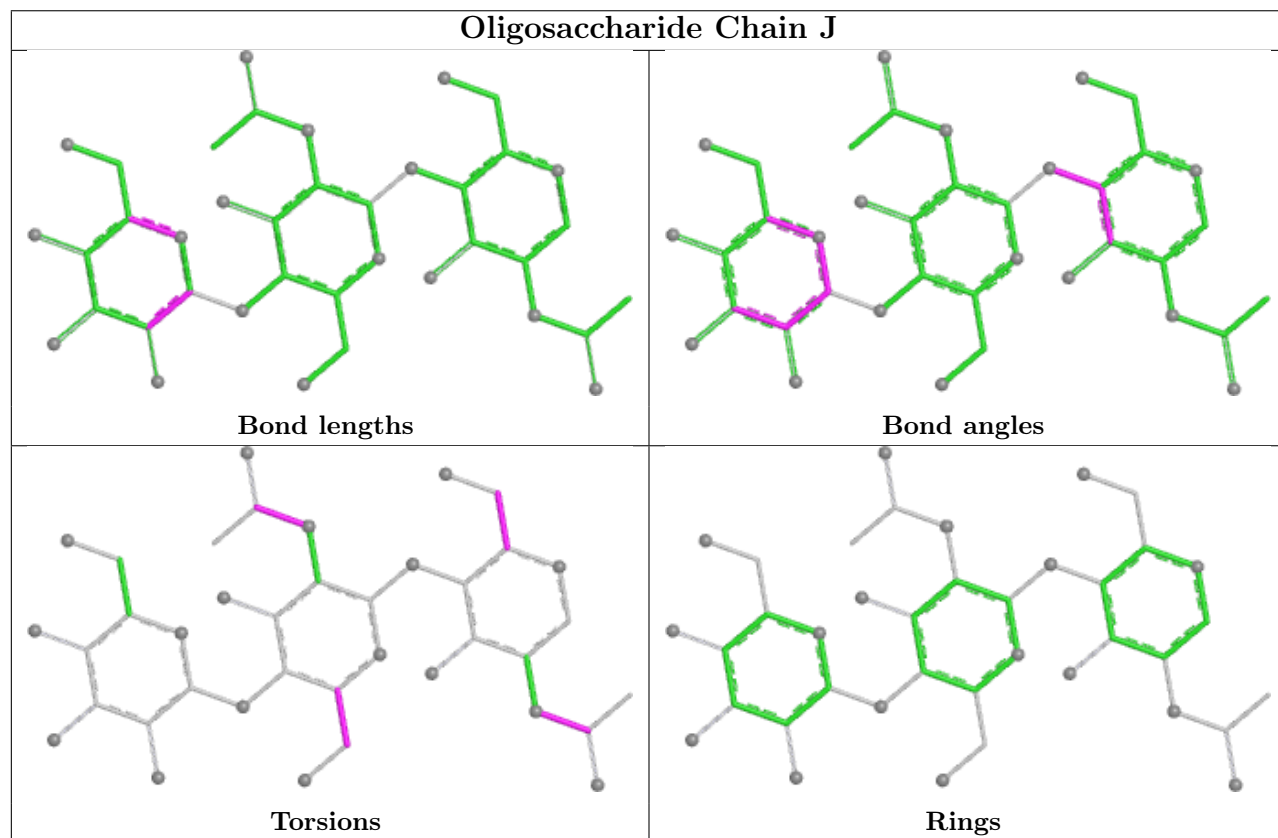
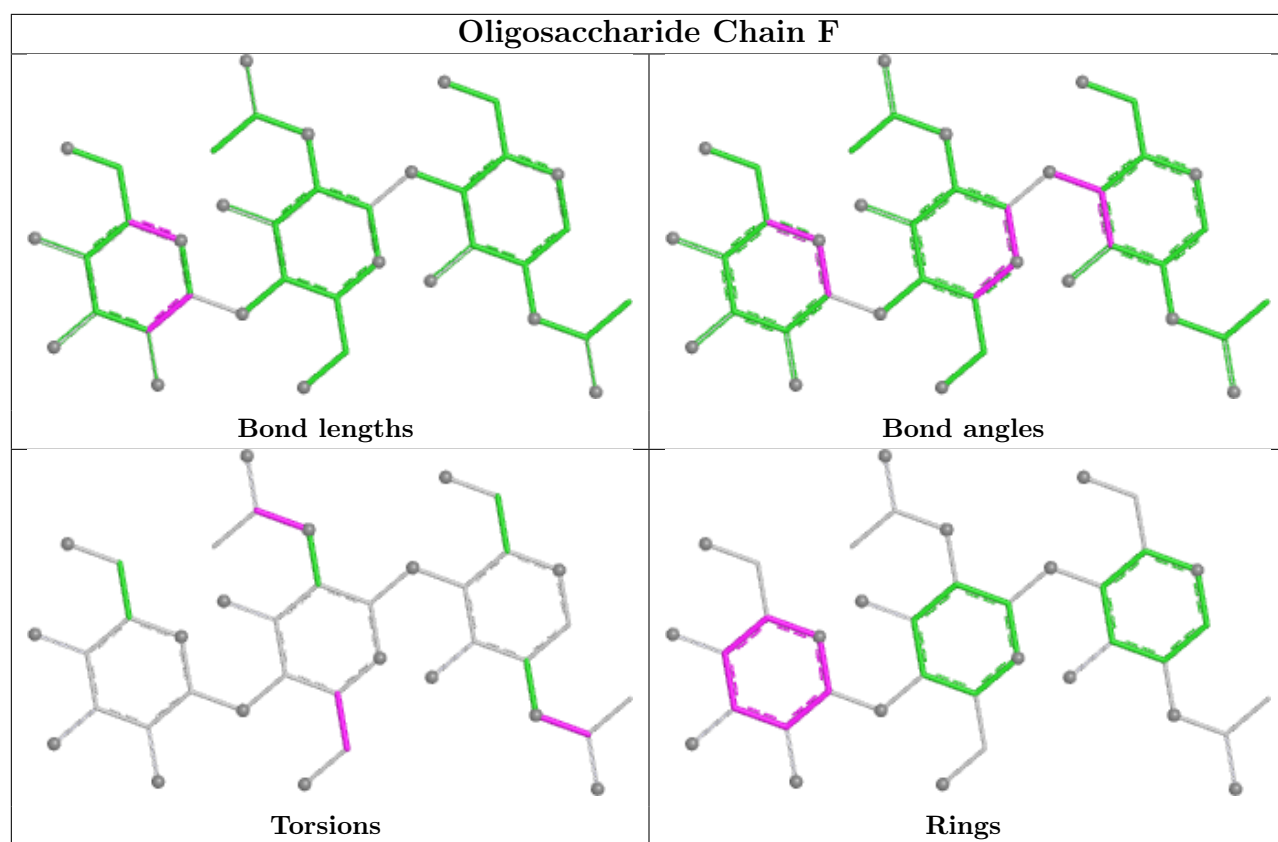












5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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
7	FWF	C	902	-	31,33,33	0.25	0	40,48,48	0.25	0
7	FWF	D	902	-	31,33,33	0.21	0	40,48,48	0.21	0
5	GLU	A	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.35	1 (12%)
5	GLU	B	901	-	8,9,9	1.15	1 (12%)	8,11,11	1.31	1 (12%)
5	GLU	C	901	-	8,9,9	1.10	1 (12%)	8,11,11	1.35	1 (12%)
5	GLU	D	901	-	8,9,9	1.15	1 (12%)	8,11,11	1.31	1 (12%)

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
7	FWF	C	902	-	-	8/32/36/36	0/2/2/2
7	FWF	D	902	-	-	9/32/36/36	0/2/2/2
5	GLU	A	901	-	-	0/9/9/9	-
5	GLU	B	901	-	-	0/9/9/9	-
5	GLU	C	901	-	-	0/9/9/9	-
5	GLU	D	901	-	-	0/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	GLU	OXT-C	-2.46	1.22	1.30
5	D	901	GLU	OXT-C	-2.45	1.22	1.30
5	A	901	GLU	OXT-C	-2.37	1.23	1.30
5	C	901	GLU	OXT-C	-2.29	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	901	GLU	OXT-C-O	-3.06	117.15	124.08
5	A	901	GLU	OXT-C-O	-3.04	117.17	124.08
5	D	901	GLU	OXT-C-O	-3.03	117.21	124.08
5	B	901	GLU	OXT-C-O	-3.00	117.27	124.08

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	902	FWF	C24-C20-S2-O3
7	C	902	FWF	C23-C20-S2-O4
7	C	902	FWF	C24-C20-S2-O4
7	C	902	FWF	C21-C19-S1-O1
7	C	902	FWF	C22-C19-S1-O1
7	C	902	FWF	C21-C19-S1-O2
7	D	902	FWF	C24-C20-S2-O3
7	D	902	FWF	C23-C20-S2-O4
7	D	902	FWF	C24-C20-S2-O4
7	D	902	FWF	C21-C19-S1-O1
7	D	902	FWF	C22-C19-S1-O1
7	D	902	FWF	C21-C19-S1-O2
7	D	902	FWF	C22-C19-S1-O2
7	C	902	FWF	C6-C1-C14-C15
7	C	902	FWF	C18-N2-S1-C19
7	D	902	FWF	C18-N2-S1-C19
7	D	902	FWF	C15-N1-S2-C20

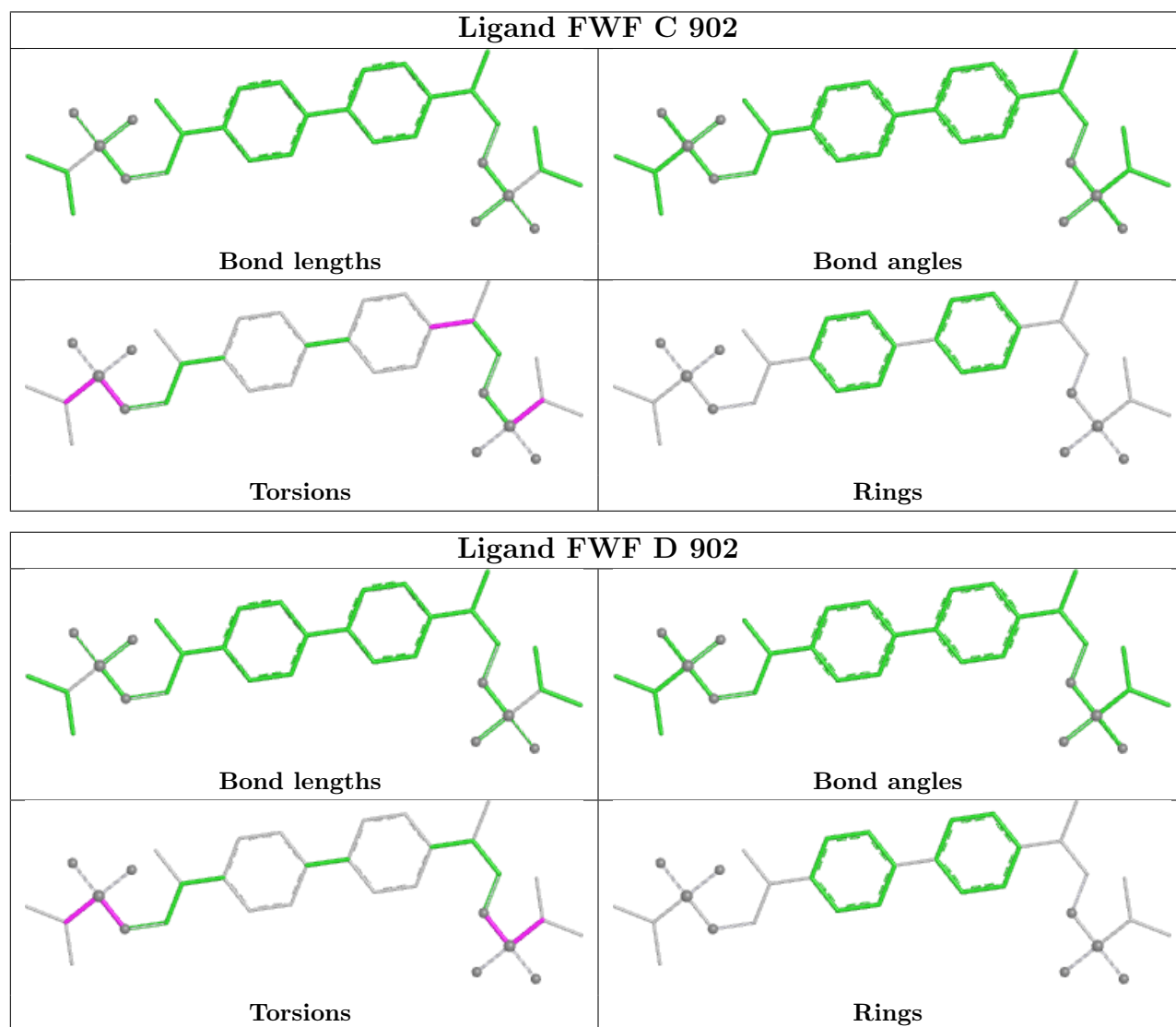
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	GLU	1	0
5	B	901	GLU	1	0
5	C	901	GLU	1	0
5	D	901	GLU	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

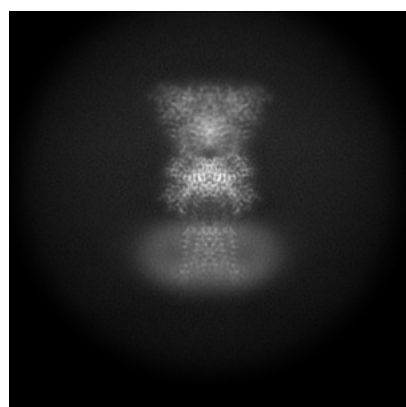
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70919. These allow visual inspection of the internal detail of the map and identification of artifacts.

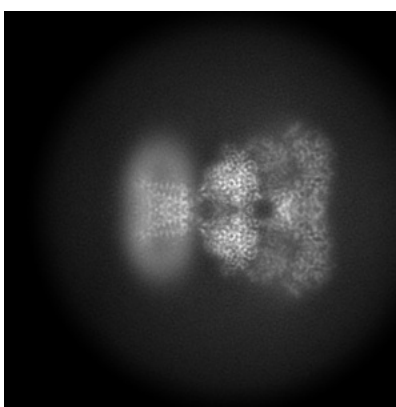
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

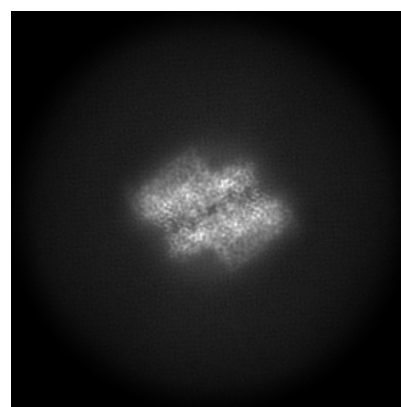
6.1.1 Primary map



X



Y

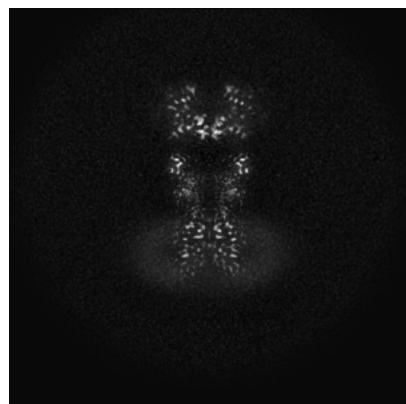


Z

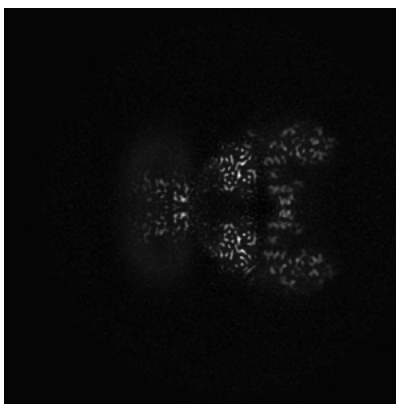
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

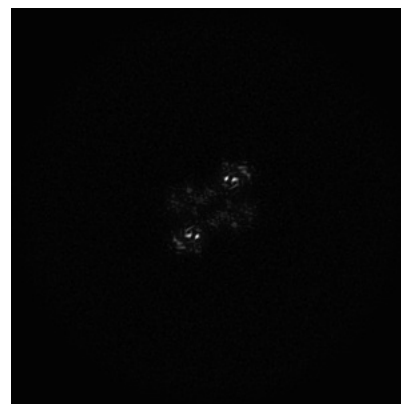
6.2.1 Primary map



X Index: 208



Y Index: 208

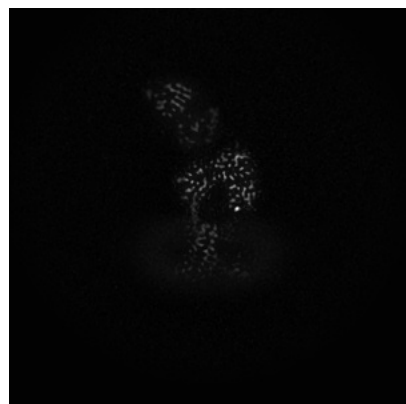


Z Index: 208

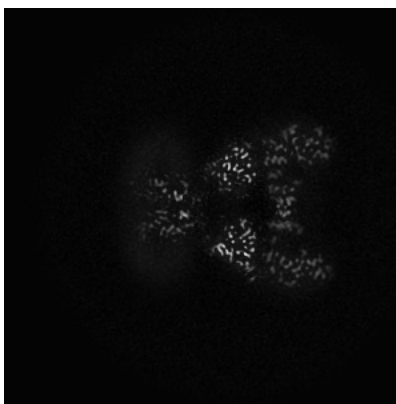
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

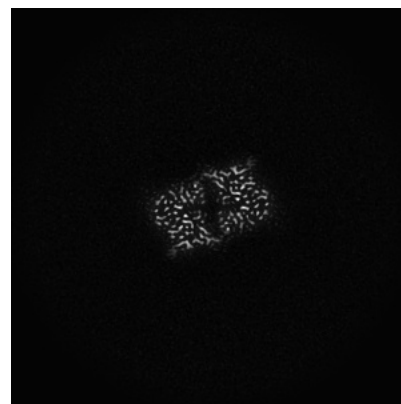
6.3.1 Primary map



X Index: 231



Y Index: 206

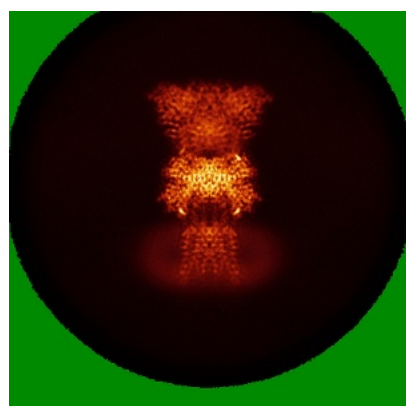


Z Index: 244

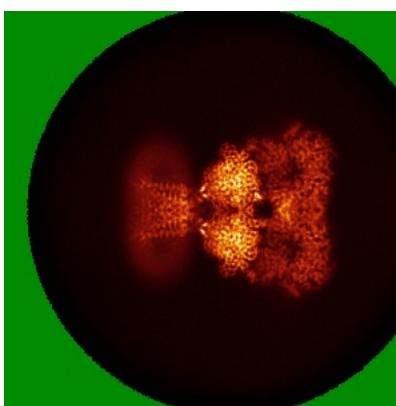
The images above show the largest variance slices of the map in three orthogonal directions.

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

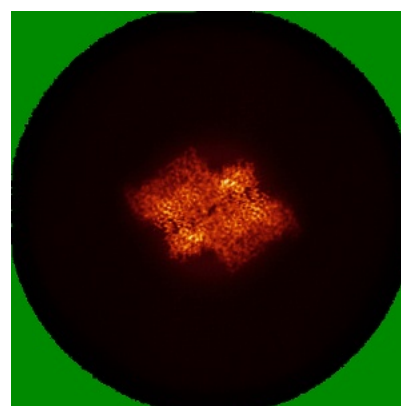
6.4.1 Primary map



X



Y

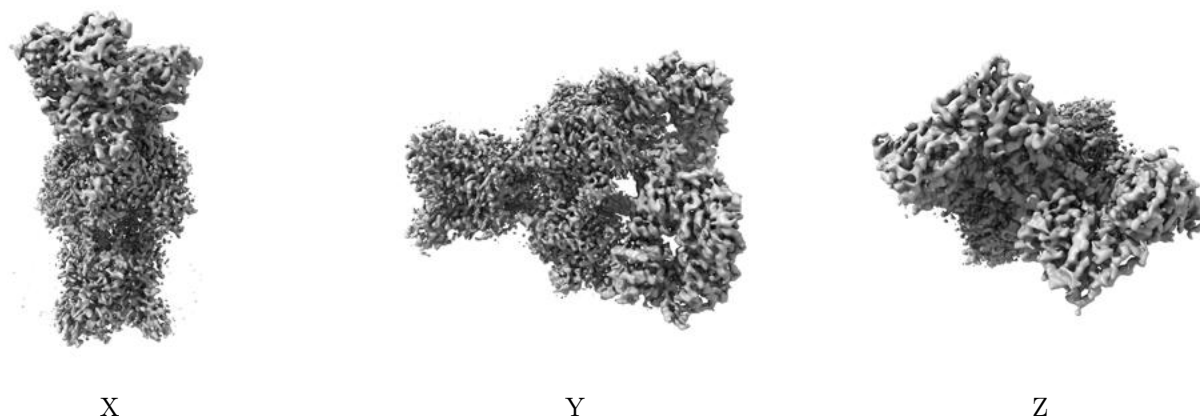


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

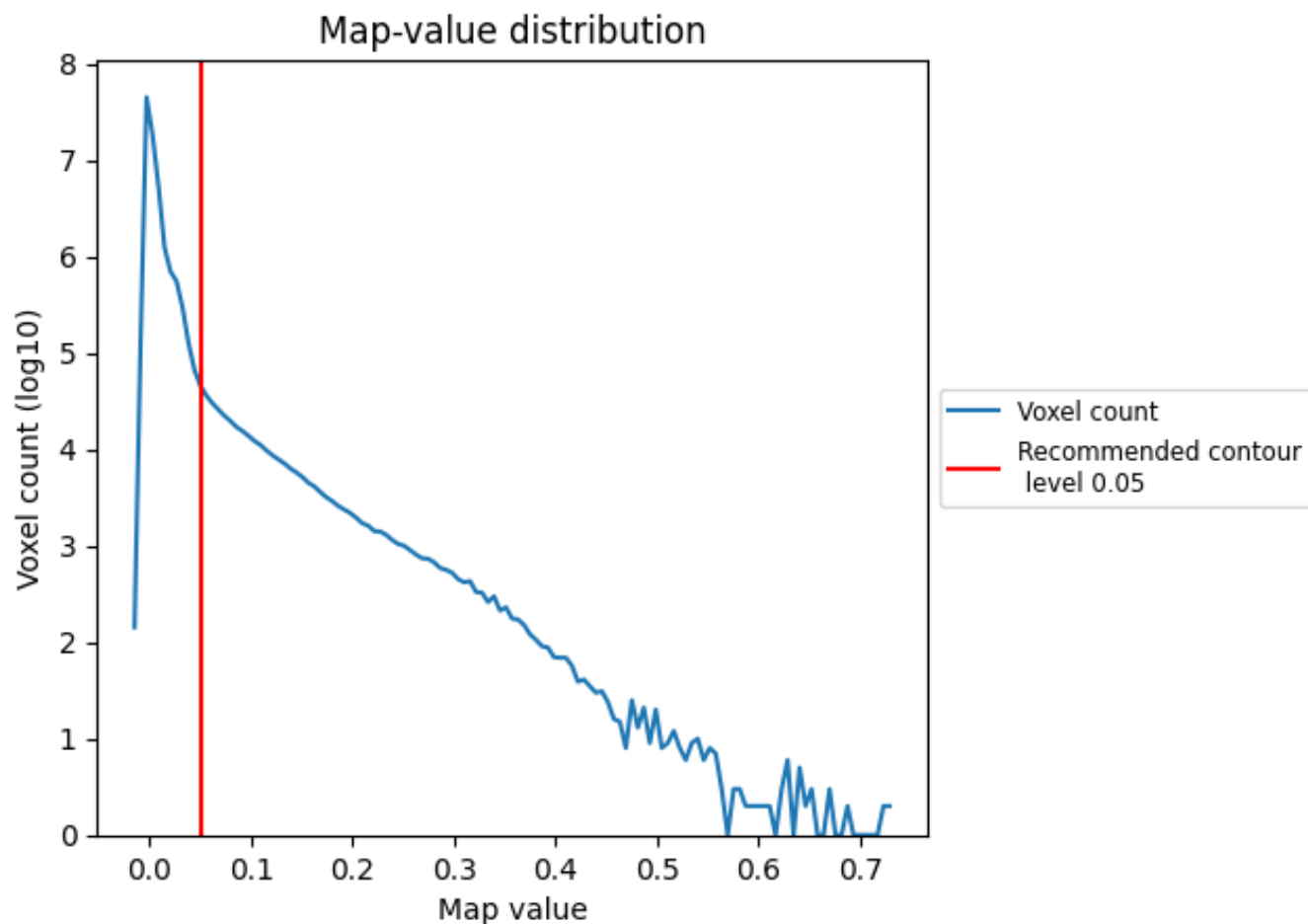
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

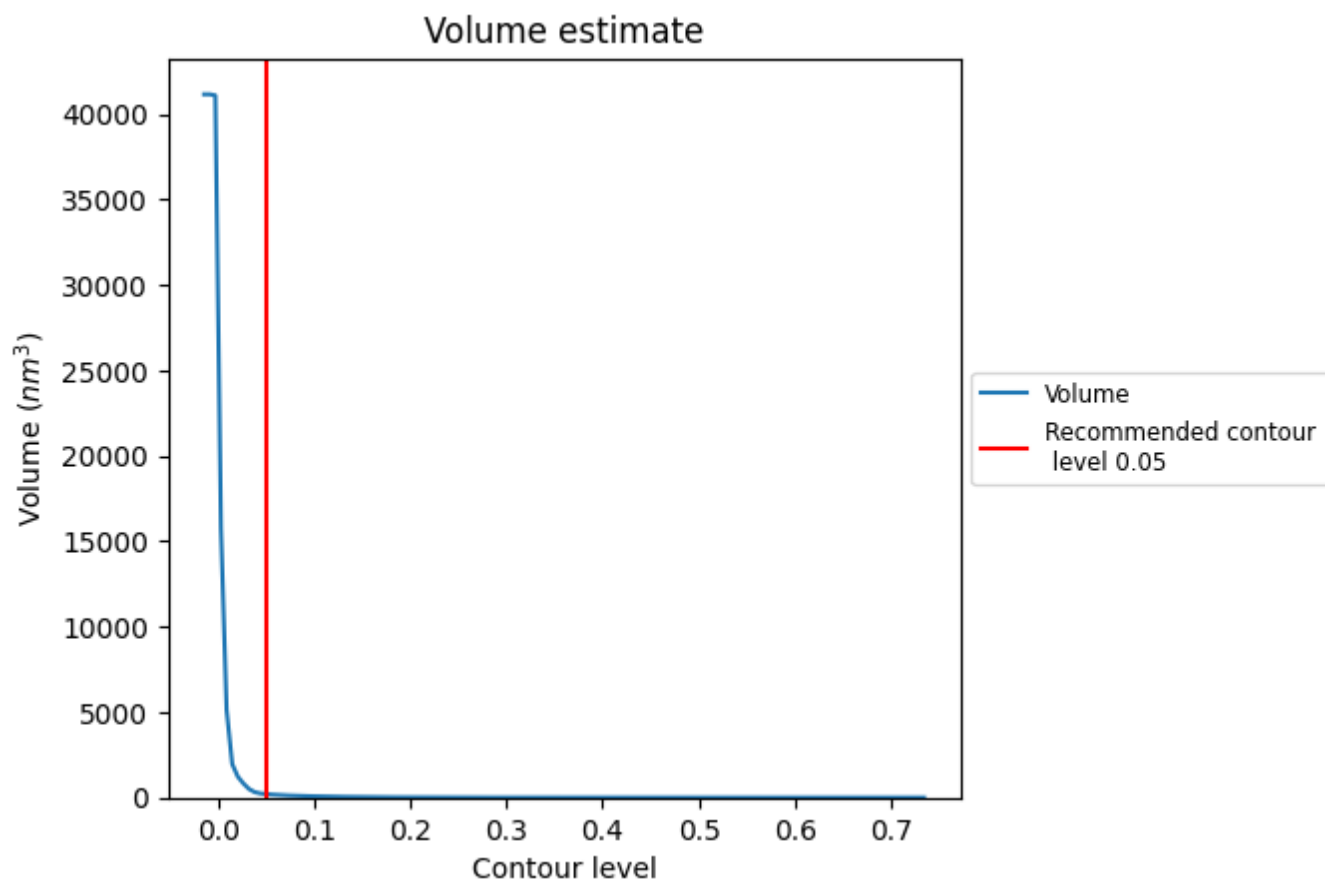
This section contains the results of statistical analysis of the map.

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.

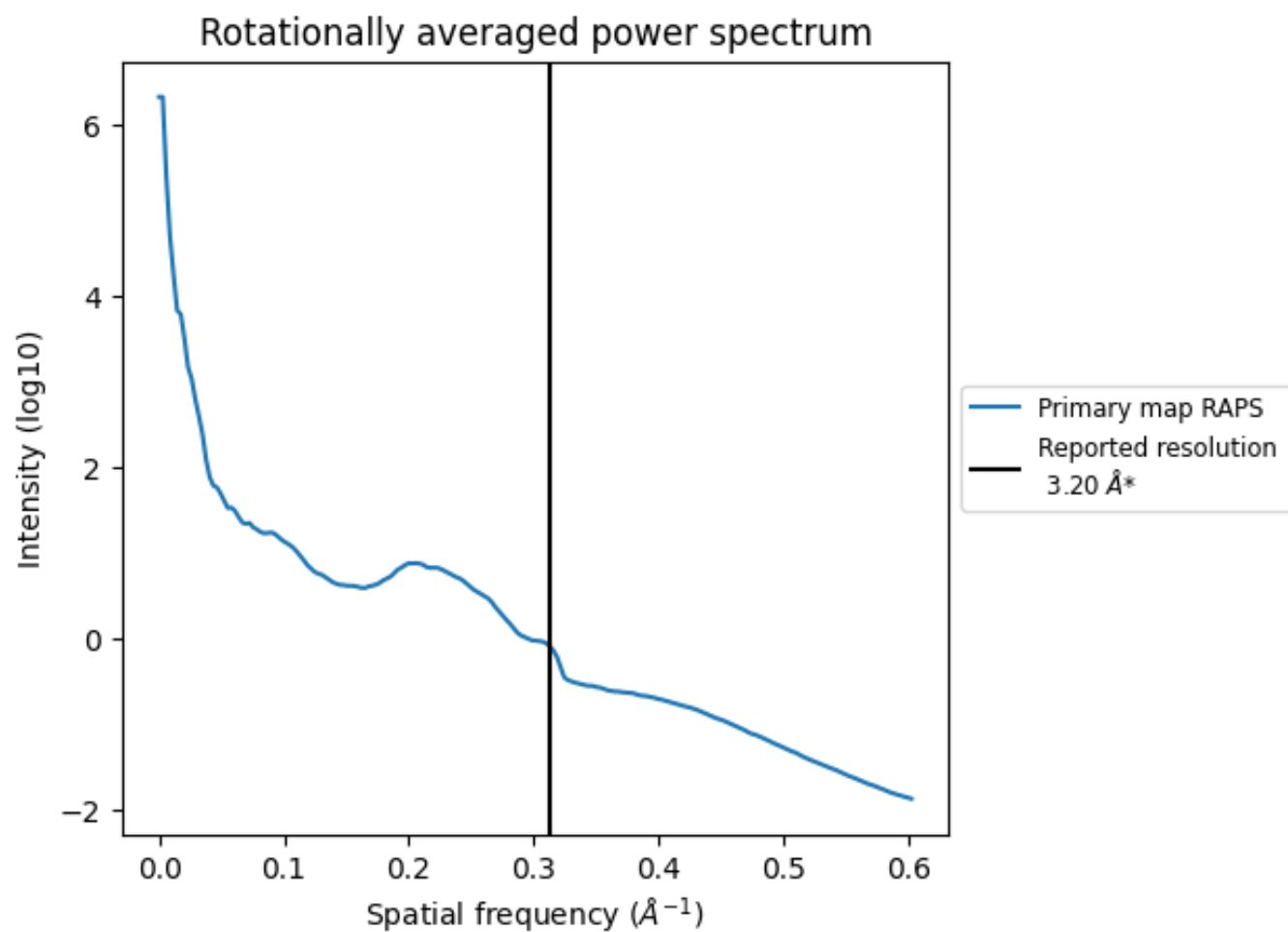
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm^3 ; this corresponds to an approximate mass of 180 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 0.312 Å⁻¹

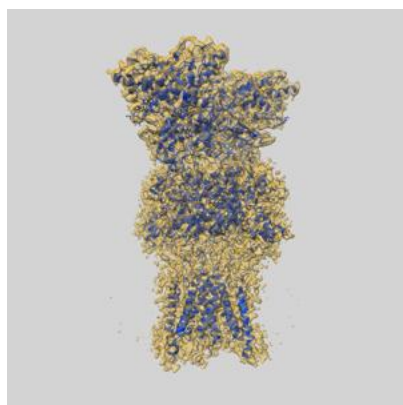
8 Fourier-Shell correlation

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

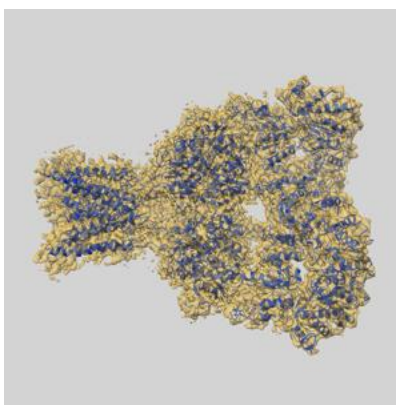
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70919 and PDB model 9OVU. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

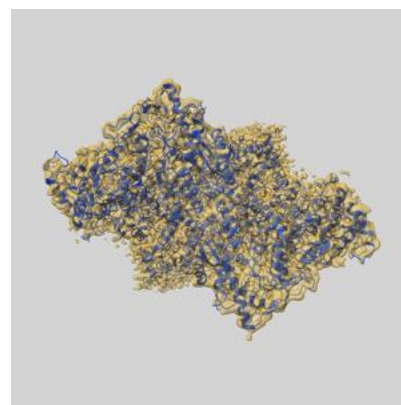
9.1 Map-model overlay [i](#)



X



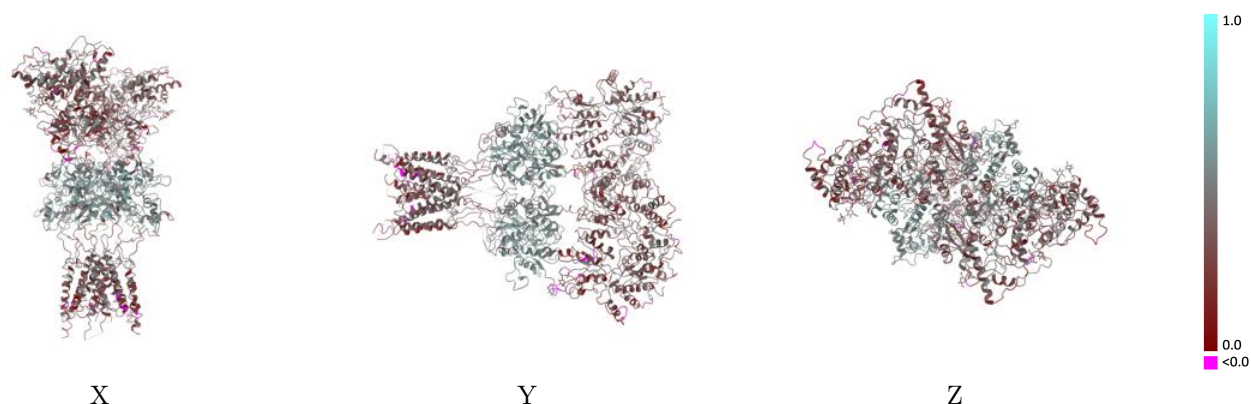
Y



Z

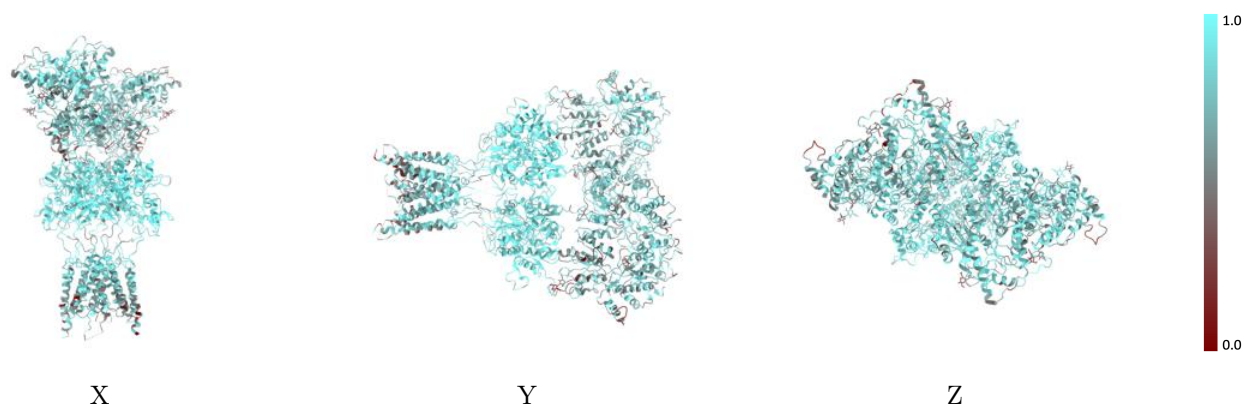
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



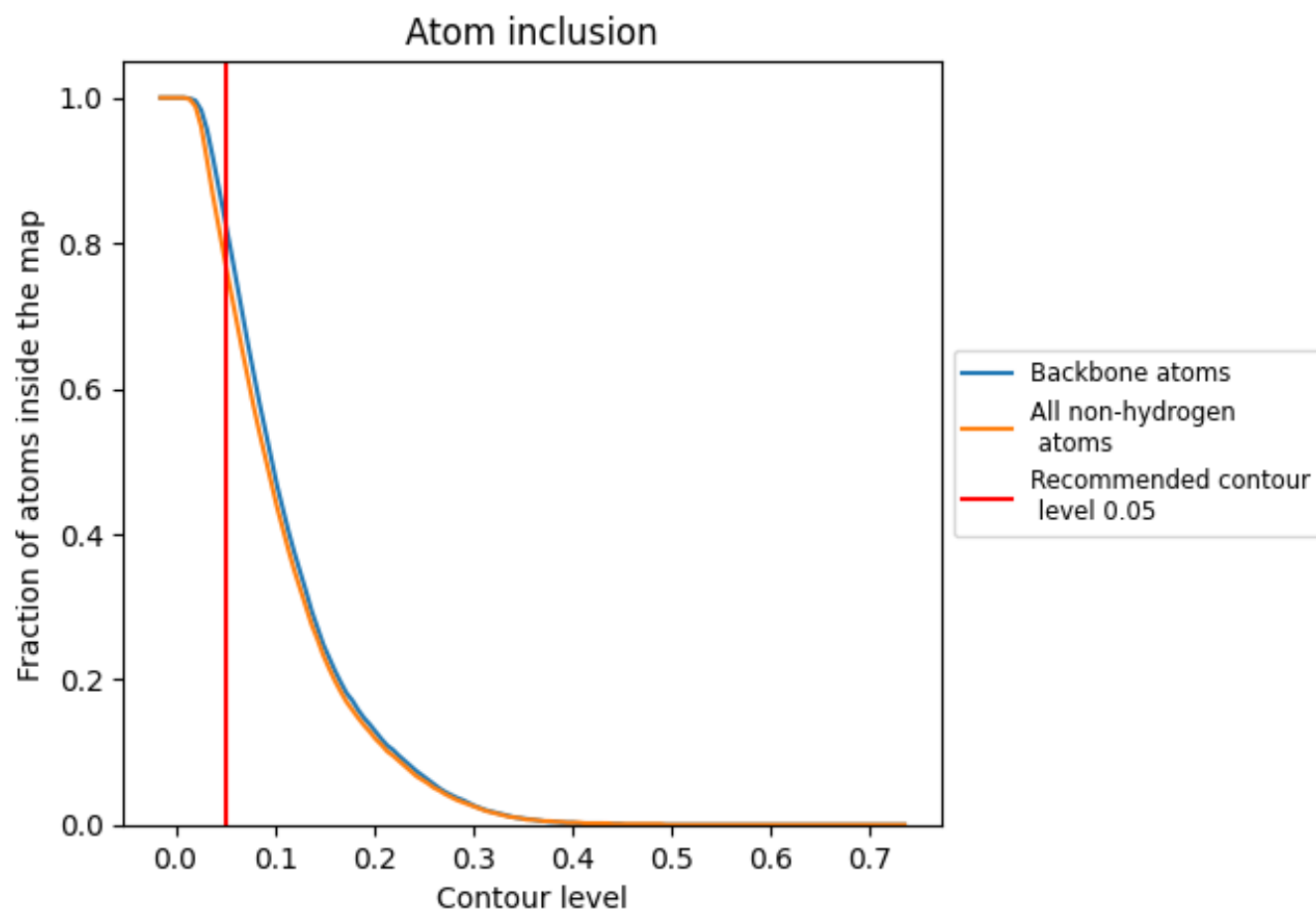
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.3870
A	0.7780	0.3850
B	0.8110	0.4040
C	0.7600	0.3720
D	0.7950	0.3890
E	0.3570	0.2950
F	0.6670	0.3140
G	0.7140	0.4300
H	0.3930	0.3350
I	0.2860	0.3330
J	0.3850	0.1020
K	0.6070	0.4210
L	0.3210	0.1830

