



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:49 AM UTC

PDB ID : 7QCL / pdb_00007qcl
EMDB ID : EMD-13896
Title : Structure of the MUCIN-2 Cterminal domains
Authors : Gallego, P.; Hansson, G.C.
Deposited on : 2021-11-24
Resolution : 3.36 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:

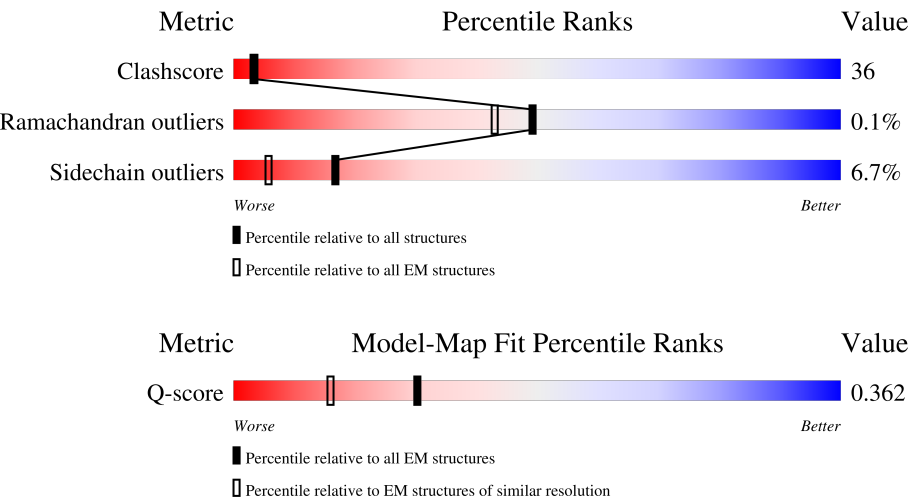
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	583	
1	B	583	
2	C	10	
2	F	10	

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Mol	Chain	Length	Quality of chain
2	G	10	
2	J	10	
2	L	10	
2	Q	10	
3	D	14	
4	E	4	
4	M	4	
4	N	4	
5	H	9	
5	K	9	
6	I	5	
7	O	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	L	10	-	-	X	-
3	BMA	D	3	-	-	X	-
3	MAN	D	9	-	-	X	-
5	NAG	K	2	-	-	X	-

2 Entry composition [i](#)

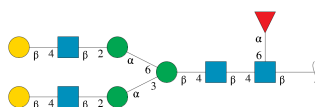
There are 9 unique types of molecules in this entry. The entry contains 9884 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mucin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	546	Total	C	N	O	S	0	0
			4177	2602	691	814	70		
1	B	546	Total	C	N	O	S	0	0
			4177	2602	691	814	70		

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	10	Total	C	N	O	0	0
			121	68	4	49		
2	F	10	Total	C	N	O	0	0
			121	68	4	49		
2	G	10	Total	C	N	O	0	0
			121	68	4	49		
2	J	10	Total	C	N	O	0	0
			121	68	4	49		
2	L	10	Total	C	N	O	0	0
			121	68	4	49		
2	Q	10	Total	C	N	O	0	0
			121	68	4	49		

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-aceta

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	14	Total	C	N	O	0	0
			171	96	6	69		

-
- A diagram of a 1D lattice with three sites. The first site has a green circle, the second has a blue square, and the third has a blue square with a red triangle on top. The sites are labeled β , 4, β , 4, β from left to right. The red triangle is labeled α and the number 6 is written below it.

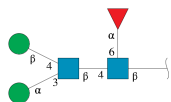
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	4	Total 49	C 28	N 2	O 19	0	0
4	M	4	Total 49	C 28	N 2	O 19	0	0
4	N	4	Total 49	C 28	N 2	O 19	0	0

-

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	9	Total 111	C 62	N 4	O 45	0	0
5	K	9	Total 111	C 62	N 4	O 45	0	0

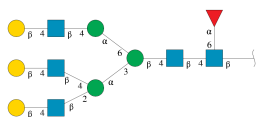
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se-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



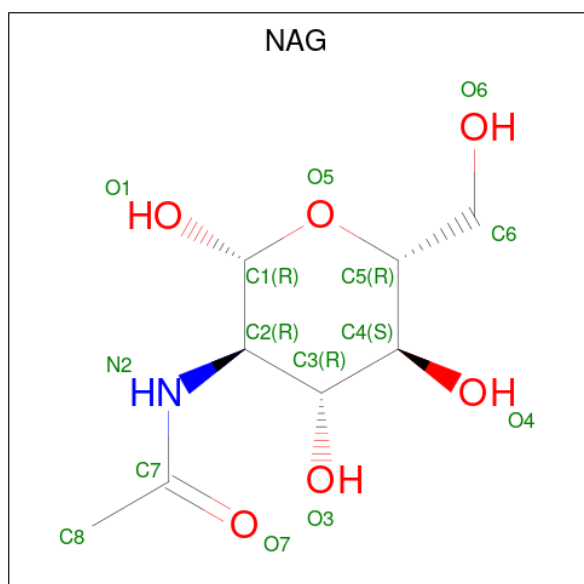
Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 7 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	12	Total	C	N	O	0	0
			146	82	5	59		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

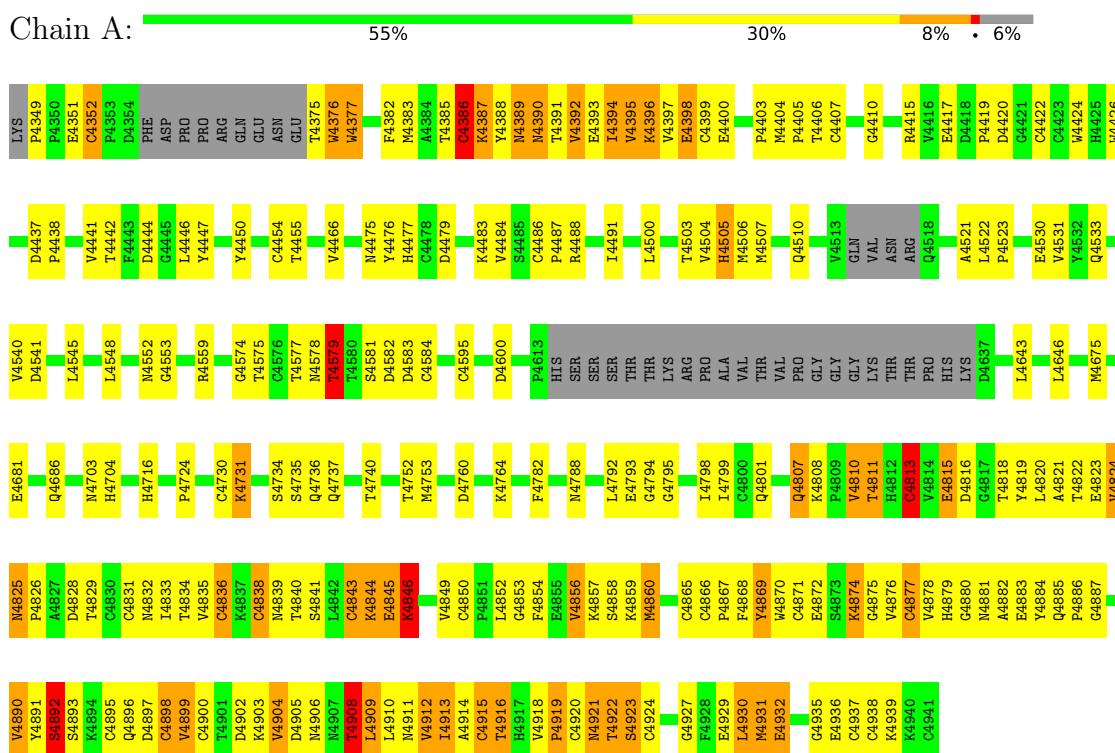
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

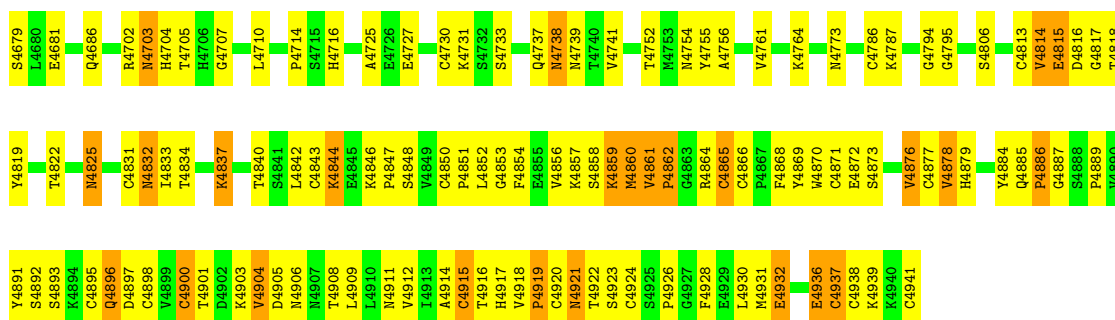
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Ca	0
			1	1	
9	B	1	Total	Ca	0
			1	1	

3 Residue-property plots

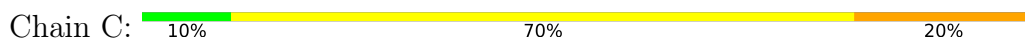
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mucin-2

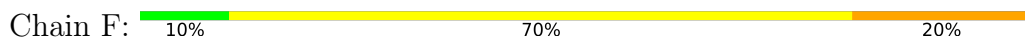




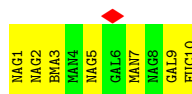
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



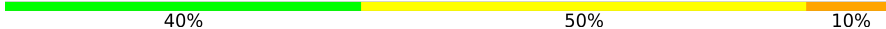
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

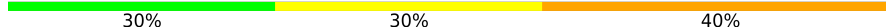


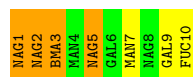
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

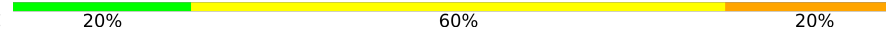


- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

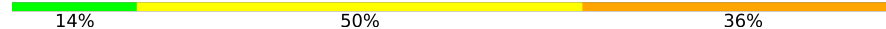


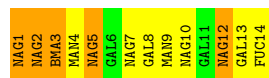
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

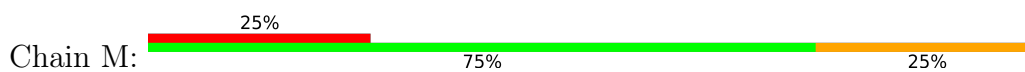


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

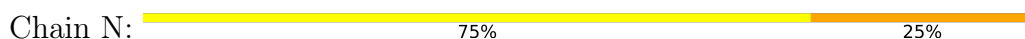
Chain E: 



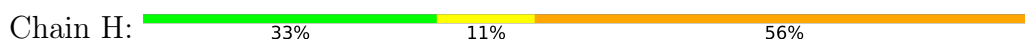
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
BMA3
MAN4
NAG5
GAL6
NAG7
GAL8
MAN9
NAG10
GAL11
FUC12

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	369150	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 ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.643	Depositor
Minimum map value	-0.273	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	495.36002, 495.36002, 495.36002	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: CA, BMA, GAL, FUC, 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	0.68	0/4290	1.28	55/5853 (0.9%)
1	B	0.67	1/4290 (0.0%)	1.10	29/5853 (0.5%)
All	All	0.68	1/8580 (0.0%)	1.19	84/11706 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4861	VAL	CA-C	6.69	1.59	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4927	GLY	N-CA-C	-11.93	100.81	113.58
1	A	4904	VAL	N-CA-C	10.58	120.37	110.74
1	B	4825	ASN	N-CA-C	-10.35	94.11	109.42
1	A	4904	VAL	N-CA-CB	-10.15	98.46	110.64
1	B	4844	LYS	N-CA-C	9.89	122.14	111.36
1	B	4825	ASN	N-CA-CB	9.28	124.37	109.90
1	A	4919	PRO	N-CA-C	9.04	126.00	111.26
1	B	4477	HIS	N-CA-C	-8.98	101.49	111.28
1	A	4813	CYS	N-CA-C	-8.89	95.63	108.60
1	A	4843	CYS	CB-CA-C	-8.51	92.83	109.68
1	A	4930	LEU	N-CA-C	-8.17	102.31	111.71
1	A	4892	SER	N-CA-C	-8.13	102.42	111.28
1	B	4814	VAL	N-CA-C	7.58	117.70	110.42
1	A	4398	GLU	CA-C-O	-7.52	113.05	121.25
1	A	4387	LYS	N-CA-C	-7.30	103.98	114.12
1	A	4579	THR	N-CA-CB	7.27	122.77	110.49
1	A	4845	GLU	N-CA-C	-7.15	104.17	113.17
1	A	4825	ASN	N-CA-C	-7.08	100.87	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4731	LYS	N-CA-C	-7.00	103.65	111.28
1	B	4862	PRO	N-CA-C	-6.94	105.19	113.86
1	A	4397	VAL	CA-C-O	-6.92	114.40	121.67
1	B	4886	PRO	N-CA-C	6.78	123.85	113.75
1	A	4860	MET	N-CA-C	6.71	118.50	108.31
1	A	4935	GLY	N-CA-C	-6.65	105.68	115.72
1	A	4923	SER	N-CA-C	6.64	118.70	109.15
1	A	4581	SER	N-CA-C	6.62	118.50	111.28
1	A	4931	MET	CA-C-O	-6.53	113.97	121.54
1	A	4825	ASN	N-CA-CB	6.50	120.74	109.57
1	A	4929	GLU	CB-CA-C	6.43	121.84	111.36
1	B	4846	LYS	N-CA-CB	-6.42	98.89	110.39
1	A	4377	TRP	N-CA-C	-6.38	100.20	109.59
1	A	4807	GLN	N-CA-C	6.33	119.85	109.72
1	A	4811	THR	N-CA-C	6.23	118.95	107.99
1	A	4816	ASP	N-CA-C	-6.17	101.14	110.28
1	B	4919	PRO	N-CA-C	-6.14	106.67	114.35
1	A	4815	GLU	N-CA-CB	6.12	119.06	109.69
1	A	4376	TRP	N-CA-CB	-6.12	101.71	111.43
1	B	4928	PHE	CB-CA-C	6.05	119.78	109.80
1	A	4815	GLU	N-CA-C	-6.03	101.11	110.10
1	B	4376	TRP	N-CA-C	6.02	118.27	108.76
1	A	4395	VAL	CA-C-O	-5.96	114.64	121.44
1	A	4843	CYS	CA-C-N	-5.91	114.77	123.05
1	A	4843	CYS	C-N-CA	-5.91	114.77	123.05
1	A	4869	TYR	N-CA-C	5.89	118.83	109.24
1	A	4860	MET	CB-CA-C	-5.80	109.87	116.54
1	B	4937	CYS	N-CA-C	-5.78	100.63	109.41
1	A	4484	VAL	N-CA-C	-5.76	105.24	110.82
1	A	4932	GLU	CA-C-O	-5.74	114.86	122.03
1	B	4398	GLU	CA-C-O	-5.71	115.34	121.45
1	B	4387	LYS	N-CA-C	-5.68	105.17	111.36
1	B	4483	LYS	N-CA-C	-5.61	106.23	112.57
1	A	4846	LYS	CA-C-O	-5.58	116.18	120.48
1	B	4419	PRO	N-CA-C	-5.55	101.05	112.47
1	A	4920	CYS	CB-CA-C	-5.54	100.33	110.62
1	B	4494	HIS	CB-CA-C	-5.49	102.61	110.62
1	B	4853	GLY	N-CA-C	5.46	119.28	112.73
1	A	4386	CYS	N-CA-C	5.44	117.26	108.34
1	A	4810	VAL	N-CA-C	5.43	116.31	108.48
1	A	4853	GLY	CA-C-N	-5.42	115.31	122.85
1	A	4853	GLY	C-N-CA	-5.42	115.31	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4378	LEU	N-CA-C	5.42	117.18	111.28
1	B	4425	HIS	CA-C-O	-5.35	115.13	121.66
1	A	4824	VAL	N-CA-C	5.34	120.44	109.34
1	B	4876	VAL	CA-C-O	-5.32	116.11	121.49
1	A	4908	THR	N-CA-C	-5.32	106.05	112.54
1	A	4396	LYS	N-CA-C	-5.30	100.46	108.46
1	B	4584	CYS	CA-C-N	-5.30	114.74	122.58
1	B	4584	CYS	C-N-CA	-5.30	114.74	122.58
1	A	4394	ILE	N-CA-C	5.29	116.41	109.58
1	A	4816	ASP	N-CA-CB	5.28	117.72	109.97
1	A	4844	LYS	N-CA-C	-5.25	99.97	108.52
1	A	4422	CYS	N-CA-C	5.23	116.98	111.28
1	B	4738	ASN	N-CA-C	-5.22	101.92	109.59
1	A	4410	GLY	N-CA-C	-5.19	108.46	115.36
1	A	4921	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	4733	SER	N-CA-C	-5.13	105.38	111.69
1	A	4505	HIS	N-CA-C	5.11	117.52	111.33
1	A	4376	TRP	N-CA-C	5.11	117.18	109.41
1	B	4419	PRO	CB-CA-C	-5.08	103.17	111.56
1	B	4394	ILE	N-CA-C	-5.08	104.52	110.05
1	B	4505	HIS	N-CA-C	5.07	118.24	111.75
1	A	4579	THR	N-CA-C	-5.05	100.05	110.80
1	B	4485	SER	N-CA-C	5.03	116.46	111.07
1	A	4922	THR	CA-CB-OG1	-5.01	102.08	109.60

There are no chirality outliers.

There are no planarity outliers.

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	4177	0	3850	306	0
1	B	4177	0	3849	300	0
2	C	121	0	103	12	0
2	F	121	0	103	12	0
2	G	121	0	103	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	121	0	103	6	0
2	L	121	0	103	14	0
2	Q	121	0	103	16	0
3	D	171	0	145	18	0
4	E	49	0	43	2	0
4	M	49	0	43	2	0
4	N	49	0	43	5	0
5	H	111	0	94	8	0
5	K	111	0	94	10	0
6	I	60	0	52	8	0
7	O	146	0	124	15	0
8	A	28	0	26	7	0
8	B	28	0	26	6	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
All	All	9884	0	9007	685	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 36.

All (685) 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:4505:HIS:CE1	1:A:4506:MET:HE3	1.43	1.49
1:B:4885:GLN:HG3	1:B:4886:PRO:CD	1.42	1.49
1:A:4505:HIS:ND1	1:A:4506:MET:HE3	1.27	1.44
1:A:4505:HIS:CE1	1:A:4506:MET:CE	2.10	1.31
1:A:4376:TRP:CE3	1:A:4377:TRP:O	1.87	1.26
1:B:4885:GLN:OE1	1:B:4886:PRO:HD3	1.18	1.26
1:B:4885:GLN:CG	1:B:4886:PRO:HD2	1.67	1.25
1:A:4505:HIS:ND1	1:A:4506:MET:CE	2.00	1.25
1:B:4885:GLN:CG	1:B:4886:PRO:CD	2.16	1.22
1:B:4885:GLN:CD	1:B:4886:PRO:HD3	1.65	1.20
1:B:4905:ASP:HB3	1:B:4908:THR:HB	1.27	1.14
1:B:4939:LYS:HE3	1:B:4941:CYS:HB3	1.29	1.13
1:B:4378:LEU:HD12	1:B:4379:CYS:N	1.66	1.08
1:B:4879:HIS:HA	1:B:4884:TYR:HB3	1.37	1.07
2:G:1:NAG:H4	2:G:10:FUC:H5	1.37	1.06
1:A:4898:CYS:HA	1:A:4915:CYS:HA	1.37	1.03
1:A:4885:GLN:OE1	1:B:4886:PRO:HG2	1.56	1.02
1:B:4815:GLU:HG2	1:B:4865:CYS:HB2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4822:THR:HA	1:B:4834:THR:HA	1.40	1.02
1:A:4900:CYS:HB2	1:A:4913:ILE:HB	1.44	1.00
1:A:4895:CYS:HB3	1:A:4919:PRO:HD3	1.41	0.99
1:B:4885:GLN:OE1	1:B:4886:PRO:CD	2.12	0.97
1:A:4398:GLU:OE2	1:A:4399:CYS:O	1.82	0.96
1:A:4819:TYR:HE2	1:A:4839:ASN:HB2	1.29	0.96
1:A:4391:THR:HA	1:B:4392:VAL:O	1.65	0.96
1:A:4376:TRP:CZ3	1:A:4377:TRP:O	2.18	0.95
1:B:4378:LEU:CD1	1:B:4379:CYS:SG	2.55	0.94
1:B:4856:VAL:HG13	1:B:4870:TRP:HB2	1.48	0.94
1:B:4476:TYR:HB3	1:B:4480:PRO:HA	1.49	0.93
1:B:4857:LYS:H	1:B:4871:CYS:H	1.03	0.92
1:A:4405:PRO:HD2	5:K:2:NAG:C7	2.00	0.92
1:A:4398:GLU:CD	1:A:4399:CYS:N	2.27	0.91
2:Q:3:BMA:H3	2:Q:8:NAG:H61	1.52	0.91
1:B:4857:LYS:H	1:B:4871:CYS:N	1.68	0.90
1:B:4483:LYS:HB2	1:B:4487:PRO:HA	1.52	0.90
1:A:4385:THR:HB	1:A:4393:GLU:HB2	1.52	0.89
1:A:4852:LEU:HD12	1:A:4884:TYR:CE1	2.06	0.89
1:A:4388:TYR:HB2	1:A:4391:THR:O	1.73	0.88
1:A:4388:TYR:HB3	8:A:5002:NAG:H2	1.52	0.88
2:C:5:NAG:H5	2:C:8:NAG:H3	1.53	0.88
1:B:4922:THR:HB	1:B:4939:LYS:H	1.39	0.87
1:A:4730:CYS:SG	1:A:4753:MET:SD	2.74	0.86
1:B:4885:GLN:CG	1:B:4886:PRO:HD3	1.95	0.86
4:E:1:NAG:H4	4:E:4:FUC:H5	1.57	0.86
1:A:4919:PRO:HA	1:A:4937:CYS:HA	1.56	0.85
1:A:4852:LEU:HD12	1:A:4884:TYR:CD1	2.11	0.85
1:B:4905:ASP:HB3	1:B:4908:THR:CB	2.07	0.85
1:B:4848:SER:H	1:B:4857:LYS:HZ2	1.24	0.85
1:A:4856:VAL:HG23	1:A:4870:TRP:HB2	1.59	0.84
2:Q:1:NAG:H4	2:Q:2:NAG:N2	1.92	0.84
1:B:4474:ASP:HB3	1:B:4489:THR:HG22	1.59	0.84
1:B:4505:HIS:ND1	1:B:4506:MET:HG2	1.92	0.84
1:B:4905:ASP:CB	1:B:4908:THR:HB	2.06	0.84
1:A:4383:MET:HB3	1:A:4395:VAL:HB	1.59	0.83
1:A:4921:ASN:ND2	1:A:4932:GLU:HG3	1.93	0.83
1:B:4922:THR:HB	1:B:4939:LYS:N	1.93	0.82
3:D:3:BMA:H5	3:D:9:MAN:H2	1.60	0.82
1:A:4406:THR:HG23	5:K:1:NAG:H61	1.62	0.82
1:A:4859:LYS:C	1:A:4868:PHE:HB3	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4505:HIS:CE1	1:A:4506:MET:HE1	2.15	0.80
1:A:4921:ASN:CG	1:A:4932:GLU:HG3	2.07	0.80
2:Q:3:BMA:H5	2:Q:7:MAN:H2	1.65	0.79
1:A:4389:ASN:HD22	1:A:4390:ASN:H	1.31	0.79
1:A:4395:VAL:HG12	1:A:4396:LYS:N	1.98	0.78
1:A:4822:THR:HA	1:A:4834:THR:HA	1.63	0.78
1:B:4857:LYS:N	1:B:4871:CYS:H	1.80	0.78
1:A:4859:LYS:NZ	1:A:4869:TYR:HB3	1.98	0.78
1:B:4857:LYS:HE2	1:B:4859:LYS:HG2	1.64	0.78
7:O:3:BMA:H5	7:O:5:NAG:HN2	1.48	0.78
7:O:4:MAN:H2	7:O:7:NAG:C1	2.12	0.78
1:B:4908:THR:HG23	1:B:4912:VAL:HA	1.64	0.78
1:A:4815:GLU:HB3	1:A:4818:THR:HG23	1.63	0.78
1:A:4904:VAL:HG13	1:A:4905:ASP:H	1.49	0.77
1:A:4825:ASN:OD1	1:A:4826:PRO:HD2	1.84	0.77
2:L:1:NAG:H4	2:L:10:FUC:H5	1.66	0.77
1:B:4876:VAL:HG23	1:B:4878:VAL:HG13	1.65	0.76
1:A:4578:ASN:O	1:A:4579:THR:HG22	1.86	0.75
1:B:4376:TRP:CD1	1:B:4378:LEU:HA	2.21	0.74
1:A:4922:THR:HG22	1:A:4923:SER:H	1.51	0.74
1:B:4877:CYS:HB3	1:B:4912:VAL:H	1.51	0.74
1:B:4378:LEU:HD12	1:B:4379:CYS:SG	2.28	0.74
1:B:4405:PRO:HD3	5:H:7:MAN:H4	1.70	0.74
1:B:4885:GLN:HG3	1:B:4886:PRO:HD2	0.75	0.73
1:A:4487:PRO:O	1:A:4488:ARG:HG3	1.88	0.73
1:B:4905:ASP:H	1:B:4909:LEU:HB2	1.53	0.73
1:B:4444:ASP:HB2	1:B:4583:ASP:OD2	1.89	0.72
1:A:4859:LYS:CB	1:A:4868:PHE:HB3	2.19	0.72
1:A:4398:GLU:CD	1:A:4399:CYS:H	1.95	0.72
1:A:4921:ASN:ND2	8:A:5001:NAG:C1	2.52	0.72
1:A:4819:TYR:CE2	1:A:4839:ASN:HB2	2.20	0.72
1:B:4466:VAL:HG21	1:B:4545:LEU:HD21	1.72	0.72
1:B:4901:THR:HG22	1:B:4903:LYS:HE2	1.72	0.72
1:A:4885:GLN:HG3	1:B:4886:PRO:HB2	1.72	0.72
1:A:4883:GLU:O	1:A:4884:TYR:CD2	2.43	0.71
3:D:3:BMA:H5	3:D:9:MAN:C2	2.20	0.71
1:B:4860:MET:HA	1:B:4868:PHE:O	1.90	0.71
1:B:4819:TYR:HE2	2:F:10:FUC:H3	1.55	0.71
1:B:4859:LYS:HB3	1:B:4868:PHE:HB3	1.72	0.71
1:B:4879:HIS:HA	1:B:4884:TYR:CB	2.18	0.71
1:A:4395:VAL:HG12	1:A:4396:LYS:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:MAN:H4	2:C:5:NAG:H82	1.71	0.71
7:O:4:MAN:C2	7:O:7:NAG:C1	2.68	0.71
1:A:4828:ASP:CG	1:A:4831:CYS:HB2	2.17	0.70
1:A:4891:TYR:HB3	1:A:4893:SER:O	1.90	0.70
1:A:4904:VAL:HG23	1:A:4909:LEU:HB3	1.73	0.70
1:A:4859:LYS:HB2	1:A:4869:TYR:N	2.06	0.70
1:A:4736:GLN:HB3	6:I:1:NAG:HN2	1.55	0.70
1:A:4390:ASN:HA	1:B:4394:ILE:HG13	1.73	0.70
1:B:4406:THR:HG22	1:B:4407:CYS:H	1.56	0.70
2:Q:5:NAG:H3	2:Q:8:NAG:H5	1.74	0.69
2:C:3:BMA:H3	2:C:8:NAG:H5	1.74	0.69
1:A:4908:THR:O	1:A:4912:VAL:N	2.26	0.69
3:D:3:BMA:O4	3:D:10:NAG:H4	1.91	0.69
2:J:5:NAG:H3	2:J:8:NAG:H83	1.74	0.69
1:B:4645:GLN:NE2	1:B:4648:LYS:HB2	2.07	0.69
1:B:4896:GLN:HA	1:B:4917:HIS:CD2	2.28	0.69
6:I:2:NAG:HN2	6:I:3:MAN:H5	1.57	0.69
1:A:4897:ASP:OD2	1:A:4916:THR:HB	1.93	0.69
1:B:4885:GLN:CD	1:B:4886:PRO:CD	2.43	0.69
1:A:4883:GLU:O	1:A:4884:TYR:CG	2.46	0.68
1:A:4415:ARG:HH21	1:A:4424:TRP:CG	2.11	0.68
3:D:2:NAG:H5	3:D:14:FUC:H4	1.75	0.68
1:A:4522:LEU:HB3	1:A:4523:PRO:HD3	1.76	0.68
1:A:4857:LYS:HG2	1:A:4859:LYS:HD2	1.77	0.67
1:B:4383:MET:HG3	1:B:4384:ALA:N	2.09	0.67
1:A:4857:LYS:HG3	1:A:4859:LYS:HG3	1.77	0.67
1:B:4900:CYS:HB2	1:B:4912:VAL:HG13	1.76	0.67
7:O:1:NAG:H4	7:O:12:FUC:H5	1.76	0.67
1:B:4381:CYS:HB3	1:B:4397:VAL:CG1	2.24	0.67
1:A:4825:ASN:OD1	1:A:4826:PRO:CD	2.43	0.67
1:A:4856:VAL:HG22	1:A:4858:SER:N	2.09	0.67
2:L:1:NAG:H2	2:L:10:FUC:H61	1.77	0.67
2:F:6:GAL:H5	2:F:8:NAG:H3	1.77	0.67
2:G:5:NAG:H61	2:G:7:MAN:H62	1.77	0.67
1:A:4859:LYS:HE2	1:A:4869:TYR:H	1.59	0.66
1:A:4882:ALA:O	1:A:4885:GLN:HG2	1.95	0.66
1:B:4878:VAL:HA	1:B:4885:GLN:C	2.20	0.66
1:A:4877:CYS:HB2	1:A:4887:GLY:H	1.59	0.66
1:A:4788:ASN:HB2	1:A:4801:GLN:HE21	1.60	0.66
1:A:4895:CYS:HB3	1:A:4919:PRO:CD	2.22	0.66
1:A:4841:SER:HB3	2:J:10:FUC:H3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4415:ARG:HH21	1:B:4424:TRP:CD1	2.14	0.66
1:B:4893:SER:HB3	1:B:4896:GLN:HB2	1.77	0.66
1:A:4921:ASN:ND2	1:A:4932:GLU:HA	2.11	0.65
1:B:4930:LEU:H	8:B:5001:NAG:H62	1.61	0.65
1:A:4921:ASN:ND2	1:A:4932:GLU:CA	2.59	0.65
1:A:4815:GLU:HG2	1:A:4838:CYS:SG	2.36	0.65
1:B:4703:ASN:ND2	2:L:1:NAG:C7	2.59	0.65
1:A:4902:ASP:HA	1:A:4912:VAL:HG11	1.78	0.65
1:B:4862:PRO:HG3	1:B:4868:PHE:CD1	2.30	0.65
1:B:4405:PRO:HG3	5:H:7:MAN:HO3	1.61	0.65
3:D:3:BMA:O2	3:D:7:NAG:H5	1.97	0.65
1:A:4822:THR:CA	1:A:4834:THR:HA	2.26	0.65
1:A:4905:ASP:HB2	1:A:4908:THR:CG2	2.27	0.65
1:A:4931:MET:HA	8:A:5001:NAG:H4	1.76	0.65
1:B:4350:PRO:HA	1:B:4388:TYR:HA	1.76	0.65
1:B:4378:LEU:CD1	1:B:4379:CYS:N	2.54	0.65
1:B:4505:HIS:CE1	1:B:4506:MET:HG2	2.31	0.65
1:B:4815:GLU:HB3	1:B:4818:THR:HG23	1.79	0.65
1:A:4921:ASN:HD22	1:A:4932:GLU:H	1.45	0.65
1:B:4552:ASN:ND2	1:B:4686:GLN:OE1	2.29	0.64
1:B:4860:MET:HG2	1:B:4861:VAL:HG12	1.79	0.64
1:A:4876:VAL:HB	1:A:4902:ASP:HB3	1.77	0.64
1:A:4822:THR:HA	1:A:4833:ILE:C	2.22	0.64
1:A:4921:ASN:HD22	1:A:4932:GLU:HA	1.63	0.64
1:A:4921:ASN:HD22	1:A:4932:GLU:N	1.96	0.64
1:A:4491:ILE:HG12	1:A:4500:LEU:HD22	1.78	0.64
1:A:4552:ASN:ND2	1:A:4686:GLN:OE1	2.30	0.64
1:A:4886:PRO:HG2	1:B:4885:GLN:HG2	1.80	0.64
1:B:4567:ASN:HD22	7:O:1:NAG:H62	1.62	0.64
1:A:4349:PRO:N	1:A:4389:ASN:HB3	2.13	0.64
1:A:4466:VAL:HG21	1:A:4545:LEU:HD21	1.80	0.64
1:A:4852:LEU:HD12	1:A:4884:TYR:HE1	1.59	0.64
1:B:4898:CYS:HA	1:B:4914:ALA:O	1.97	0.64
1:B:4815:GLU:CG	1:B:4865:CYS:HB2	2.22	0.63
1:A:4505:HIS:O	1:A:4506:MET:HE2	1.97	0.63
1:A:4487:PRO:HG3	1:A:4553:GLY:O	1.98	0.63
2:C:2:NAG:H3	2:C:10:FUC:H3	1.80	0.63
1:B:4386:CYS:HA	1:B:4392:VAL:HB	1.80	0.63
1:A:4898:CYS:O	1:A:4913:ILE:HG13	1.99	0.63
1:A:4822:THR:HA	1:A:4834:THR:CA	2.28	0.63
1:A:4795:GLY:H	1:B:4521:ALA:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4505:HIS:ND1	1:A:4506:MET:HE2	2.06	0.62
1:B:4375:THR:HG22	1:B:4375:THR:O	1.98	0.62
1:B:4906:ASN:C	1:B:4908:THR:H	2.07	0.62
1:B:4381:CYS:HB3	1:B:4397:VAL:HG12	1.79	0.62
1:B:4376:TRP:HD1	1:B:4378:LEU:HA	1.61	0.62
1:B:4908:THR:CG2	1:B:4912:VAL:HG23	2.29	0.62
1:A:4388:TYR:HD2	1:A:4391:THR:HB	1.65	0.62
1:B:4822:THR:HA	1:B:4834:THR:CA	2.23	0.62
1:A:4859:LYS:HZ2	1:A:4869:TYR:HB3	1.64	0.62
1:B:4912:VAL:HG13	1:B:4912:VAL:O	2.00	0.62
5:K:1:NAG:O3	5:K:2:NAG:H2	2.00	0.62
1:A:4844:LYS:HZ3	1:A:4846:LYS:HA	1.65	0.62
2:F:2:NAG:H2	2:F:7:MAN:H62	1.82	0.62
2:L:3:BMA:H3	2:L:5:NAG:H5	1.82	0.62
1:A:4904:VAL:HG13	1:A:4905:ASP:N	2.14	0.61
1:A:4405:PRO:HD2	5:K:2:NAG:N2	2.15	0.61
1:A:4877:CYS:CB	1:A:4887:GLY:H	2.12	0.61
1:B:4378:LEU:HG	1:B:4382:PHE:O	2.00	0.61
1:A:4483:LYS:HD3	1:A:4487:PRO:HB3	1.81	0.61
1:A:4821:ALA:HB3	1:A:4835:VAL:CG1	2.31	0.61
1:B:4922:THR:CB	1:B:4939:LYS:H	2.11	0.61
1:A:4821:ALA:HB1	1:A:4823:GLU:HG2	1.81	0.61
1:A:4902:ASP:CA	1:A:4912:VAL:HG11	2.30	0.61
1:A:4921:ASN:HD22	1:A:4932:GLU:CA	2.14	0.61
1:A:4811:THR:O	1:A:4811:THR:HG23	2.01	0.61
2:Q:2:NAG:H5	2:Q:3:BMA:O5	2.01	0.61
1:A:4877:CYS:SG	1:A:4912:VAL:HG13	2.41	0.61
1:B:4752:THR:HG22	1:B:4764:LYS:HG2	1.83	0.60
1:A:4860:MET:O	1:A:4868:PHE:HB2	2.01	0.60
1:B:4862:PRO:HG3	1:B:4868:PHE:HD1	1.66	0.60
1:A:4395:VAL:CG1	1:A:4396:LYS:N	2.65	0.60
1:B:4877:CYS:HB3	1:B:4912:VAL:HG12	1.83	0.60
1:B:4904:VAL:HA	1:B:4909:LEU:HD13	1.83	0.60
1:B:4383:MET:HG3	1:B:4384:ALA:H	1.66	0.60
1:B:4851:PRO:HD2	1:B:4854:PHE:CD2	2.36	0.60
1:B:4896:GLN:HA	1:B:4917:HIS:HD2	1.67	0.60
1:A:4395:VAL:CG1	1:A:4396:LYS:H	2.14	0.60
1:B:4900:CYS:HB2	1:B:4912:VAL:O	2.01	0.60
1:B:4435:TRP:O	1:B:4439:HIS:HB2	2.01	0.60
2:C:5:NAG:H61	2:C:6:GAL:O2	2.02	0.60
1:A:4921:ASN:ND2	1:A:4932:GLU:N	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4531:VAL:HG22	1:B:4540:VAL:HG22	1.84	0.59
1:B:4887:GLY:C	1:B:4889:PRO:HD3	2.26	0.59
2:C:1:NAG:H4	2:C:10:FUC:H5	1.83	0.59
1:B:4859:LYS:CB	1:B:4868:PHE:HB3	2.31	0.59
2:J:4:MAN:H61	2:J:5:NAG:H82	1.84	0.59
2:L:2:NAG:H4	2:L:7:MAN:H5	1.83	0.59
1:A:4884:TYR:CD1	1:A:4884:TYR:O	2.55	0.59
1:B:4900:CYS:HA	1:B:4903:LYS:HE3	1.84	0.59
3:D:3:BMA:O2	3:D:8:GAL:H5	2.02	0.59
1:A:4921:ASN:ND2	1:A:4932:GLU:CG	2.64	0.59
1:A:4922:THR:HG22	1:A:4923:SER:N	2.16	0.59
1:B:4378:LEU:HD12	1:B:4379:CYS:CA	2.31	0.59
1:A:4389:ASN:HD22	1:A:4389:ASN:N	2.00	0.59
5:H:8:NAG:O3	5:H:9:GAL:H2	2.03	0.59
1:A:4875:GLY:O	1:A:4909:LEU:HB2	2.01	0.59
1:B:4474:ASP:HB3	1:B:4489:THR:CG2	2.31	0.59
1:A:4820:LEU:HD11	1:A:4834:THR:HB	1.84	0.59
1:A:4859:LYS:HB3	1:A:4868:PHE:HB3	1.85	0.59
1:A:4876:VAL:O	1:A:4912:VAL:HG12	2.03	0.59
1:A:4860:MET:SD	1:A:4870:TRP:HB3	2.42	0.58
1:A:4891:TYR:H	1:B:4891:TYR:HE1	1.51	0.58
1:A:4735:SER:HB2	6:I:1:NAG:H82	1.85	0.58
7:O:1:NAG:H5	7:O:2:NAG:H83	1.85	0.58
1:A:4389:ASN:ND2	1:A:4390:ASN:H	1.98	0.58
1:B:4898:CYS:HA	1:B:4915:CYS:HA	1.85	0.58
1:B:4898:CYS:CA	1:B:4915:CYS:HA	2.33	0.58
6:I:2:NAG:N2	6:I:3:MAN:H5	2.17	0.58
1:B:4856:VAL:HG12	1:B:4858:SER:H	1.69	0.58
1:A:4807:GLN:N	1:A:4807:GLN:OE1	2.36	0.58
1:B:4425:HIS:CD2	1:B:4427:GLU:HG2	2.39	0.58
1:B:4459:VAL:HG12	1:B:4471:VAL:HB	1.83	0.58
2:C:7:MAN:H61	2:C:8:NAG:H82	1.85	0.58
1:B:4819:TYR:CE2	2:F:10:FUC:H3	2.38	0.58
1:B:4837:LYS:HE2	1:B:4837:LYS:HA	1.85	0.58
1:A:4856:VAL:HG22	1:A:4858:SER:H	1.69	0.58
1:A:4505:HIS:HE1	1:A:4506:MET:HE3	1.49	0.58
1:A:4522:LEU:HD11	1:A:4533:GLN:HG3	1.86	0.58
1:A:4521:ALA:HB3	1:B:4795:GLY:H	1.68	0.57
1:B:4738:ASN:ND2	4:N:4:FUC:C1	2.67	0.57
1:A:4404:MET:HG2	1:A:4426:TRP:HB2	1.85	0.57
1:A:4406:THR:CG2	5:K:1:NAG:H61	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4429:ASP:OD2	1:B:4559:ARG:NH1	2.37	0.57
1:A:4740:THR:HG21	6:I:5:FUC:H63	1.86	0.57
1:A:4881:ASN:HD21	1:A:4892:SER:HB3	1.69	0.57
1:B:4415:ARG:HH21	1:B:4424:TRP:CG	2.23	0.57
1:A:4782:PHE:HZ	1:A:4798:ILE:HD12	1.69	0.57
1:A:4903:LYS:HG2	1:A:4912:VAL:CG2	2.33	0.57
1:A:4388:TYR:CB	8:A:5002:NAG:H2	2.30	0.57
1:B:4483:LYS:HD2	1:B:4487:PRO:CA	2.35	0.57
1:A:4824:VAL:HG23	1:A:4824:VAL:O	2.04	0.57
1:B:4378:LEU:HD12	1:B:4378:LEU:C	2.28	0.57
1:A:4859:LYS:HB2	1:A:4869:TYR:H	1.70	0.57
1:B:4848:SER:HB2	1:B:4857:LYS:NZ	2.19	0.56
1:B:4908:THR:O	1:B:4912:VAL:N	2.37	0.56
1:A:4808:LYS:H	1:A:4833:ILE:HB	1.69	0.56
1:A:4918:VAL:HG22	1:A:4938:CYS:H	1.70	0.56
1:B:4386:CYS:SG	1:B:4392:VAL:HB	2.45	0.56
1:B:4483:LYS:HD2	1:B:4487:PRO:HB3	1.87	0.56
1:A:4375:THR:HB	1:A:4386:CYS:HB2	1.86	0.56
1:B:4725:ALA:HB3	1:B:4739:ASN:HD21	1.69	0.56
1:B:4859:LYS:HG3	1:B:4868:PHE:HB3	1.87	0.56
1:B:4437:ASP:OD1	1:B:4476:TYR:OH	2.23	0.56
1:B:4857:LYS:HD3	1:B:4869:TYR:O	2.04	0.56
1:A:4389:ASN:HD22	1:A:4390:ASN:N	2.00	0.56
1:B:4580:THR:HA	1:B:4583:ASP:OD2	2.05	0.56
1:B:4437:ASP:OD2	1:B:4476:TYR:OH	2.23	0.56
1:A:4918:VAL:O	1:A:4938:CYS:HB2	2.06	0.56
1:B:4859:LYS:NZ	1:B:4862:PRO:HB3	2.20	0.56
6:I:1:NAG:H62	6:I:2:NAG:N2	2.20	0.56
1:A:4476:TYR:HA	1:A:4479:ASP:O	2.05	0.56
1:A:4841:SER:HB3	2:J:10:FUC:H5	1.88	0.56
1:A:4859:LYS:HD3	1:A:4869:TYR:O	2.05	0.56
1:A:4883:GLU:C	1:A:4884:TYR:CD2	2.84	0.56
1:A:4919:PRO:HA	1:A:4937:CYS:CA	2.31	0.56
1:A:4857:LYS:HB3	1:A:4869:TYR:O	2.06	0.55
3:D:3:BMA:H5	3:D:9:MAN:C3	2.36	0.55
1:A:4857:LYS:HG2	1:A:4859:LYS:CD	2.36	0.55
1:A:4487:PRO:HD2	1:A:4503:THR:OG1	2.06	0.55
1:B:4918:VAL:O	1:B:4937:CYS:SG	2.60	0.55
4:N:1:NAG:C8	4:N:1:NAG:C1	2.84	0.55
1:A:4383:MET:CB	1:A:4395:VAL:HB	2.32	0.55
1:B:4405:PRO:HG3	5:H:7:MAN:O3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4897:ASP:N	1:A:4916:THR:O	2.40	0.55
1:A:4352:CYS:HB2	1:A:4375:THR:HG22	1.88	0.55
1:A:4575:THR:HB	1:A:4577:THR:HG23	1.88	0.55
1:B:4825:ASN:HB2	1:B:4833:ILE:HG23	1.88	0.55
1:B:4852:LEU:HD12	1:B:4884:TYR:O	2.07	0.55
3:D:2:NAG:C1	3:D:14:FUC:H3	2.36	0.55
1:B:4505:HIS:O	1:B:4506:MET:HE2	2.07	0.55
1:A:4400:GLU:HG2	1:A:4424:TRP:CZ2	2.41	0.54
1:B:4931:MET:CG	1:B:4931:MET:O	2.55	0.54
1:A:4531:VAL:HG22	1:A:4540:VAL:HG22	1.88	0.54
1:B:4939:LYS:HG3	1:B:4941:CYS:SG	2.47	0.54
1:A:4852:LEU:HD12	1:A:4884:TYR:HD1	1.68	0.54
1:B:4817:GLY:HA3	1:B:4865:CYS:HB3	1.89	0.54
1:B:4921:ASN:HB3	1:B:4936:GLU:HB3	1.89	0.54
7:O:9:MAN:O3	7:O:10:NAG:H2	2.08	0.54
1:A:4349:PRO:CD	1:A:4389:ASN:HB3	2.37	0.54
1:A:4922:THR:CG2	1:A:4923:SER:H	2.19	0.54
1:B:4859:LYS:O	1:B:4868:PHE:HB2	2.08	0.54
1:B:4923:SER:N	8:B:5001:NAG:H2	2.22	0.54
1:A:4394:ILE:HD11	1:B:4389:ASN:O	2.07	0.54
1:A:4857:LYS:CG	1:A:4859:LYS:HD2	2.38	0.54
1:B:4437:ASP:CG	1:B:4476:TYR:OH	2.51	0.54
1:B:4378:LEU:HD12	1:B:4379:CYS:CB	2.37	0.54
1:B:4483:LYS:CB	1:B:4487:PRO:HA	2.31	0.54
1:B:4816:ASP:HB3	1:B:4844:LYS:HG2	1.88	0.54
1:B:4848:SER:CB	1:B:4857:LYS:HZ1	2.21	0.54
1:B:4921:ASN:CG	1:B:4932:GLU:H	2.16	0.54
1:B:4893:SER:HB3	1:B:4896:GLN:CB	2.38	0.54
1:A:4904:VAL:CG1	1:A:4905:ASP:H	2.19	0.54
1:B:4487:PRO:HD2	1:B:4503:THR:OG1	2.08	0.53
1:B:4848:SER:N	1:B:4857:LYS:HZ2	2.02	0.53
1:A:4389:ASN:N	1:A:4389:ASN:ND2	2.51	0.53
1:A:4918:VAL:N	1:A:4919:PRO:HD2	2.22	0.53
2:F:2:NAG:H2	2:F:7:MAN:C6	2.39	0.53
1:A:4885:GLN:OE1	1:B:4886:PRO:CG	2.45	0.53
1:A:4898:CYS:H	1:A:4916:THR:H	1.57	0.53
2:F:6:GAL:H5	2:F:8:NAG:HN2	1.74	0.53
2:C:2:NAG:H4	2:C:7:MAN:H2	1.91	0.53
7:O:3:BMA:H3	7:O:4:MAN:O2	2.09	0.53
1:A:4505:HIS:HE1	1:A:4506:MET:CE	2.04	0.53
1:A:4898:CYS:CA	1:A:4915:CYS:HA	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4378:LEU:HD11	1:B:4379:CYS:SG	2.46	0.53
1:B:4852:LEU:O	1:B:4873:SER:HB2	2.09	0.53
1:B:4832:ASN:OD1	2:Q:10:FUC:H61	2.09	0.53
2:L:2:NAG:H2	2:L:7:MAN:H62	1.90	0.53
1:A:4821:ALA:HB3	1:A:4835:VAL:HG13	1.91	0.52
1:B:4703:ASN:HB3	2:L:10:FUC:H61	1.90	0.52
1:B:4818:THR:HA	1:B:4837:LYS:O	2.09	0.52
1:B:4877:CYS:SG	1:B:4912:VAL:HG12	2.49	0.52
1:A:4389:ASN:ND2	1:A:4389:ASN:H	2.07	0.52
1:A:4844:LYS:NZ	1:A:4846:LYS:HA	2.24	0.52
1:A:4877:CYS:SG	1:A:4913:ILE:HG22	2.50	0.52
1:B:4545:LEU:HD23	1:B:4565:PHE:HZ	1.74	0.52
1:B:4923:SER:CA	8:B:5001:NAG:H2	2.38	0.52
1:A:4483:LYS:CD	1:A:4487:PRO:HB3	2.39	0.52
1:A:4899:VAL:O	1:A:4913:ILE:HA	2.10	0.52
1:A:4392:VAL:HG23	1:A:4393:GLU:N	2.25	0.52
7:O:3:BMA:H5	7:O:5:NAG:N2	2.20	0.52
1:A:4521:ALA:HB3	1:B:4794:GLY:HA3	1.92	0.52
1:A:4870:TRP:CZ2	1:A:4872:GLU:HA	2.45	0.52
1:B:4761:VAL:CG1	1:B:4773:ASN:HB3	2.40	0.52
1:B:4860:MET:CB	1:B:4870:TRP:HD1	2.23	0.52
1:B:4906:ASN:C	1:B:4908:THR:N	2.68	0.52
1:A:4879:HIS:CE1	1:A:4913:ILE:HD13	2.44	0.52
2:C:5:NAG:C5	2:C:8:NAG:H3	2.32	0.52
2:C:2:NAG:H2	2:C:7:MAN:O3	2.09	0.51
1:A:4475:ASN:HA	1:A:4488:ARG:HG2	1.92	0.51
1:A:4479:ASP:HB2	1:A:4486:CYS:O	2.11	0.51
1:B:4387:LYS:H	1:B:4392:VAL:HA	1.75	0.51
1:B:4731:LYS:HB2	1:B:4756:ALA:HB2	1.93	0.51
1:B:4458:LEU:HG	1:B:4473:ILE:HG22	1.92	0.51
1:A:4643:LEU:HD23	1:A:4681:GLU:HG2	1.92	0.51
1:B:4895:CYS:HB2	1:B:4918:VAL:C	2.36	0.51
1:B:4848:SER:CB	1:B:4857:LYS:NZ	2.73	0.51
1:B:4879:HIS:CD2	1:B:4911:ASN:HD21	2.29	0.51
1:B:4860:MET:O	1:B:4861:VAL:HG12	2.11	0.51
1:B:4904:VAL:HA	1:B:4909:LEU:HB2	1.92	0.51
1:B:4645:GLN:HE21	1:B:4648:LYS:HB2	1.75	0.51
1:B:4816:ASP:CB	1:B:4844:LYS:HG2	2.41	0.51
1:A:4398:GLU:CG	1:A:4399:CYS:N	2.73	0.51
1:A:4574:GLY:HA2	1:A:4583:ASP:O	2.10	0.51
1:B:4908:THR:HG22	1:B:4912:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GAL:H5	2:F:8:NAG:N2	2.26	0.51
1:A:4349:PRO:HD2	1:A:4389:ASN:HB3	1.93	0.50
1:B:4703:ASN:HB3	2:L:10:FUC:C6	2.40	0.50
1:A:4388:TYR:CD2	1:A:4391:THR:HB	2.45	0.50
1:A:4906:ASN:CB	4:M:1:NAG:H82	2.41	0.50
1:A:4924:CYS:HB2	8:A:5001:NAG:H83	1.94	0.50
1:B:4378:LEU:HD13	1:B:4379:CYS:SG	2.49	0.50
1:A:4424:TRP:HZ3	1:A:4426:TRP:CZ2	2.28	0.50
1:B:4870:TRP:CZ3	1:B:4872:GLU:HA	2.46	0.50
1:B:4923:SER:HB2	8:B:5001:NAG:H2	1.92	0.50
3:D:5:NAG:H82	3:D:12:NAG:H61	1.93	0.50
1:A:4815:GLU:HB3	1:A:4818:THR:CG2	2.38	0.50
2:Q:4:MAN:H4	2:Q:5:NAG:H83	1.94	0.50
1:A:4404:MET:HE2	1:A:4426:TRP:HB2	1.94	0.50
1:A:4903:LYS:HG2	1:A:4912:VAL:HG23	1.94	0.50
1:B:4473:ILE:HD12	1:B:4489:THR:O	2.12	0.50
1:B:4876:VAL:HG21	1:B:4886:PRO:HG3	1.94	0.49
1:B:4455:THR:HG23	1:B:4604:VAL:HG13	1.93	0.49
1:B:4920:CYS:O	1:B:4938:CYS:N	2.45	0.49
1:B:4923:SER:HB2	8:B:5001:NAG:O3	2.12	0.49
1:A:4822:THR:HA	1:A:4833:ILE:O	2.11	0.49
1:A:4906:ASN:HB2	4:M:1:NAG:H82	1.94	0.49
1:A:4913:ILE:HG12	1:A:4914:ALA:O	2.11	0.49
1:B:4375:THR:N	1:B:4386:CYS:SG	2.86	0.49
1:B:4704:HIS:CD2	2:L:10:FUC:H62	2.47	0.49
1:A:4450:TYR:OH	1:A:4600:ASP:OD1	2.25	0.49
1:A:4908:THR:HB	1:A:4912:VAL:HA	1.95	0.49
1:B:4424:TRP:HZ3	1:B:4426:TRP:NE1	2.10	0.49
1:B:4452:GLY:O	1:B:4476:TYR:CD2	2.65	0.49
1:A:4643:LEU:HA	1:A:4646:LEU:HD13	1.95	0.49
1:B:4642:PRO:O	1:B:4645:GLN:HB3	2.12	0.49
1:B:4859:LYS:HG3	1:B:4868:PHE:HD2	1.77	0.49
7:O:4:MAN:H2	7:O:7:NAG:C2	2.43	0.49
1:B:4931:MET:O	1:B:4931:MET:HG3	2.13	0.48
1:A:4393:GLU:HA	1:B:4390:ASN:O	2.13	0.48
1:A:4897:ASP:HB2	1:A:4916:THR:HB	1.95	0.48
1:B:4737:GLN:H	1:B:4737:GLN:CD	2.20	0.48
1:B:4577:THR:O	1:B:4578:ASN:CB	2.61	0.48
1:B:4904:VAL:HG23	1:B:4909:LEU:HD22	1.94	0.48
1:A:4387:LYS:O	1:A:4388:TYR:CD1	2.66	0.48
1:A:4857:LYS:H	1:A:4871:CYS:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4878:VAL:O	1:A:4884:TYR:HB2	2.14	0.48
1:B:4905:ASP:HB3	1:B:4908:THR:CG2	2.44	0.48
1:B:4905:ASP:H	1:B:4909:LEU:CB	2.25	0.48
4:N:1:NAG:C1	4:N:1:NAG:H83	2.42	0.48
1:B:4387:LYS:HG2	1:B:4388:TYR:CE2	2.48	0.48
1:A:4420:ASP:OD1	1:A:4420:ASP:C	2.57	0.48
1:A:4704:HIS:CE1	2:G:9:GAL:O3	2.67	0.48
1:A:4857:LYS:CG	1:A:4859:LYS:CD	2.92	0.48
2:J:2:NAG:O3	2:J:7:MAN:H2	2.14	0.48
1:A:4398:GLU:CG	1:A:4399:CYS:H	2.27	0.48
1:A:4919:PRO:CA	1:A:4937:CYS:HA	2.36	0.48
1:B:4893:SER:HB2	1:B:4917:HIS:CE1	2.48	0.48
2:F:2:NAG:H4	2:F:7:MAN:H5	1.96	0.48
1:B:4392:VAL:HG22	1:B:4394:ILE:HG23	1.96	0.48
1:B:4852:LEU:HD13	1:B:4885:GLN:NE2	2.29	0.48
1:A:4398:GLU:OE2	1:A:4399:CYS:C	2.57	0.47
1:A:4821:ALA:HB3	1:A:4835:VAL:HG12	1.96	0.47
1:A:4885:GLN:CD	1:B:4886:PRO:HG2	2.31	0.47
1:B:4452:GLY:O	1:B:4476:TYR:CE2	2.67	0.47
3:D:3:BMA:H5	3:D:9:MAN:H3	1.96	0.47
7:O:2:NAG:H3	7:O:9:MAN:H62	1.96	0.47
1:A:4444:ASP:HB2	1:A:4583:ASP:OD2	2.14	0.47
1:B:4381:CYS:HB3	1:B:4397:VAL:HG13	1.96	0.47
2:Q:2:NAG:H3	2:Q:3:BMA:O5	2.13	0.47
1:B:4859:LYS:CG	1:B:4868:PHE:HB3	2.43	0.47
1:B:4900:CYS:O	1:B:4900:CYS:SG	2.72	0.47
1:A:4716:HIS:NE2	1:A:4760:ASP:OD1	2.34	0.47
1:B:4530:GLU:HB3	1:B:4541:ASP:OD1	2.14	0.47
1:B:4862:PRO:HG3	1:B:4868:PHE:H	1.80	0.47
2:J:2:NAG:H2	2:J:8:NAG:H5	1.96	0.47
1:A:4390:ASN:HB3	1:B:4394:ILE:O	2.15	0.47
1:A:4577:THR:HG21	1:A:4582:ASP:CG	2.39	0.47
1:A:4903:LYS:O	1:A:4912:VAL:HB	2.14	0.47
1:B:4413:PRO:HB3	1:B:4428:CYS:HB3	1.95	0.47
1:B:4815:GLU:HG3	1:B:4817:GLY:H	1.80	0.47
2:F:4:MAN:H2	2:F:5:NAG:H2	1.58	0.47
1:A:4404:MET:N	1:A:4404:MET:SD	2.88	0.47
1:A:4845:GLU:HB3	1:A:4867:PRO:HD2	1.97	0.47
1:B:4405:PRO:HG2	5:H:1:NAG:O4	2.13	0.47
1:B:4741:VAL:O	1:B:4741:VAL:HG23	2.14	0.47
1:B:4814:VAL:HG13	1:B:4815:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:NAG:O6	2:F:8:NAG:H5	2.15	0.47
1:A:4504:VAL:HG22	1:A:4507:MET:O	2.14	0.47
1:A:4840:THR:HG22	1:A:4865:CYS:O	2.14	0.47
2:Q:4:MAN:H4	2:Q:5:NAG:C8	2.45	0.47
1:A:4392:VAL:HG22	1:A:4394:ILE:HG23	1.96	0.47
1:A:4487:PRO:O	1:A:4488:ARG:CG	2.60	0.47
1:A:4877:CYS:HB3	1:A:4886:PRO:HA	1.96	0.47
1:B:4483:LYS:HD2	1:B:4487:PRO:CB	2.44	0.46
1:B:4918:VAL:HG13	1:B:4937:CYS:SG	2.54	0.46
3:D:1:NAG:H2	3:D:13:GAL:H62	1.96	0.46
1:A:4455:THR:O	1:A:4455:THR:HG23	2.14	0.46
1:B:4424:TRP:HZ3	1:B:4426:TRP:CE2	2.34	0.46
1:B:4473:ILE:HD11	1:B:4488:ARG:HB3	1.96	0.46
1:B:4478:CYS:SG	1:B:4479:ASP:N	2.88	0.46
1:B:4920:CYS:O	1:B:4937:CYS:C	2.57	0.46
3:D:9:MAN:O3	3:D:10:NAG:N2	2.47	0.46
1:A:4486:CYS:HB3	1:A:4503:THR:O	2.16	0.46
1:A:4859:LYS:HD3	1:A:4869:TYR:HB3	1.97	0.46
1:B:4870:TRP:HZ3	1:B:4872:GLU:HA	1.80	0.46
1:B:4876:VAL:O	1:B:4878:VAL:N	2.49	0.46
2:Q:1:NAG:H4	2:Q:2:NAG:C7	2.44	0.46
1:A:4859:LYS:HB3	1:A:4868:PHE:CD2	2.51	0.46
1:B:4727:GLU:OE2	1:B:4754:ASN:ND2	2.46	0.46
3:D:3:BMA:H2	3:D:4:MAN:C5	2.46	0.46
1:A:4921:ASN:ND2	1:A:4932:GLU:H	2.08	0.46
1:A:4822:THR:O	1:A:4832:ASN:HB2	2.16	0.46
1:A:4921:ASN:HB3	1:A:4936:GLU:HG2	1.98	0.46
1:B:4815:GLU:HG2	1:B:4865:CYS:CB	2.29	0.46
1:B:4879:HIS:CA	1:B:4884:TYR:HB3	2.26	0.46
1:B:4930:LEU:H	8:B:5001:NAG:C6	2.27	0.46
1:B:4429:ASP:OD1	1:B:4429:ASP:N	2.48	0.46
1:B:4878:VAL:O	1:B:4885:GLN:N	2.48	0.46
4:E:2:NAG:H3	4:E:4:FUC:H3	1.98	0.46
2:G:2:NAG:H3	2:G:10:FUC:H3	1.98	0.46
1:A:4846:LYS:HB2	1:A:4846:LYS:HE2	1.69	0.46
1:A:4874:LYS:HE3	1:A:4874:LYS:HB3	1.67	0.46
1:A:4913:ILE:O	1:A:4914:ALA:C	2.58	0.46
5:K:2:NAG:H4	5:K:3:BMA:H2	1.47	0.46
1:A:4881:ASN:HD21	1:A:4892:SER:CB	2.28	0.45
1:B:4483:LYS:HD2	1:B:4487:PRO:HA	1.98	0.45
1:B:4852:LEU:HB3	1:B:4878:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4848:SER:H	1:B:4857:LYS:NZ	2.06	0.45
2:Q:2:NAG:H83	2:Q:7:MAN:O4	2.15	0.45
1:B:4891:TYR:CD1	1:B:4891:TYR:N	2.84	0.45
6:I:1:NAG:H62	6:I:2:NAG:C1	2.46	0.45
1:B:4383:MET:CG	1:B:4384:ALA:N	2.79	0.45
1:A:4487:PRO:C	1:A:4488:ARG:HG3	2.40	0.45
1:A:4813:CYS:HB2	1:A:4836:CYS:HB3	1.63	0.45
1:A:4859:LYS:CE	1:A:4869:TYR:H	2.25	0.45
1:B:4859:LYS:HZ1	1:B:4862:PRO:HB3	1.81	0.45
1:B:4859:LYS:HE3	1:B:4868:PHE:CD2	2.51	0.45
1:B:4869:TYR:N	1:B:4869:TYR:CD1	2.83	0.45
1:B:4905:ASP:N	1:B:4909:LEU:HB2	2.28	0.45
1:A:4387:LYS:O	1:A:4388:TYR:HD1	2.00	0.45
1:A:4828:ASP:OD1	1:A:4831:CYS:HB2	2.17	0.45
1:B:4349:PRO:HD2	1:B:4389:ASN:HB3	1.99	0.45
2:L:3:BMA:H5	2:L:5:NAG:H5	1.98	0.45
2:Q:5:NAG:H3	2:Q:8:NAG:H3	1.99	0.45
1:A:4575:THR:CB	1:A:4577:THR:HG23	2.47	0.45
1:A:4815:GLU:CG	1:A:4838:CYS:SG	3.05	0.45
1:A:4903:LYS:H	1:A:4912:VAL:HG21	1.82	0.45
1:A:4930:LEU:HB3	8:A:5001:NAG:H2	1.99	0.45
1:B:4400:GLU:HG2	1:B:4424:TRP:CZ2	2.52	0.45
1:A:4903:LYS:HG2	1:A:4912:VAL:HG21	1.99	0.45
1:A:4420:ASP:OD1	1:A:4420:ASP:O	2.34	0.44
1:A:4905:ASP:HB2	1:A:4908:THR:HG23	1.96	0.44
1:A:4891:TYR:HA	1:A:4896:GLN:NE2	2.32	0.44
1:B:4378:LEU:HD12	1:B:4379:CYS:H	1.68	0.44
1:B:4389:ASN:CG	1:B:4390:ASN:N	2.75	0.44
1:B:4704:HIS:HA	2:L:10:FUC:O4	2.17	0.44
1:A:4820:LEU:CG	1:A:4834:THR:HB	2.47	0.44
1:A:4877:CYS:O	1:A:4886:PRO:HA	2.17	0.44
1:A:4883:GLU:C	1:A:4884:TYR:CG	2.96	0.44
1:B:4856:VAL:HG12	1:B:4858:SER:N	2.31	0.44
1:B:4859:LYS:HG3	1:B:4868:PHE:CD2	2.53	0.44
3:D:1:NAG:H3	3:D:12:NAG:O7	2.18	0.44
1:B:4898:CYS:HA	1:B:4914:ALA:C	2.42	0.44
1:B:4737:GLN:CD	1:B:4737:GLN:N	2.76	0.44
1:A:4382:PHE:HA	1:A:4396:LYS:HA	2.00	0.44
1:A:4441:VAL:HG12	1:A:4447:TYR:HB2	2.00	0.44
1:A:4897:ASP:HB2	1:A:4916:THR:CB	2.47	0.44
1:A:4931:MET:HE3	1:A:4931:MET:HB3	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4662:GLN:NE2	1:B:4666:ASP:OD2	2.51	0.44
1:A:4885:GLN:CG	1:B:4886:PRO:HB2	2.46	0.44
2:F:6:GAL:H5	2:F:8:NAG:C3	2.47	0.44
2:L:1:NAG:H2	2:L:10:FUC:C6	2.46	0.44
1:A:4510:GLN:NE2	1:A:4522:LEU:HA	2.33	0.44
1:A:4548:LEU:HB2	1:A:4559:ARG:HB3	2.00	0.44
1:B:4819:TYR:CZ	1:B:4837:LYS:HB3	2.53	0.44
2:G:2:NAG:C1	2:G:10:FUC:H3	2.47	0.44
1:A:4375:THR:HA	1:A:4385:THR:HA	1.99	0.44
7:O:1:NAG:H4	7:O:12:FUC:C5	2.44	0.44
7:O:4:MAN:O5	7:O:7:NAG:C1	2.66	0.44
1:A:4831:CYS:O	1:A:4833:ILE:HG23	2.18	0.43
1:A:4859:LYS:CA	1:A:4868:PHE:HB3	2.48	0.43
1:A:4890:VAL:HG11	1:B:4889:PRO:HG2	2.00	0.43
1:B:4893:SER:HB3	1:B:4896:GLN:CA	2.48	0.43
2:Q:5:NAG:C3	2:Q:8:NAG:H3	2.48	0.43
1:A:4892:SER:H	1:A:4896:GLN:NE2	2.15	0.43
1:A:4904:VAL:CG1	1:A:4905:ASP:N	2.80	0.43
1:B:4813:CYS:HB3	1:B:4818:THR:OG1	2.19	0.43
1:B:4877:CYS:CB	1:B:4912:VAL:HG12	2.46	0.43
3:D:2:NAG:H2	3:D:12:NAG:H2	2.01	0.43
1:A:4349:PRO:HB2	1:A:4351:GLU:O	2.19	0.43
1:A:4577:THR:O	1:A:4578:ASN:HB3	2.18	0.43
1:A:4881:ASN:ND2	1:A:4892:SER:HB3	2.31	0.43
1:B:4377:TRP:HA	1:B:4383:MET:HA	2.00	0.43
1:B:4437:ASP:O	1:B:4488:ARG:NH2	2.52	0.43
1:B:4476:TYR:O	1:B:4477:HIS:C	2.61	0.43
1:B:4707:GLY:HA2	1:B:4710:LEU:HD11	2.01	0.43
1:B:4786:CYS:O	1:B:4787:LYS:HG3	2.19	0.43
1:A:4792:LEU:HD21	1:A:4799:ILE:HD12	2.00	0.43
1:A:4820:LEU:CD1	1:A:4834:THR:HB	2.47	0.43
1:A:4859:LYS:CE	1:A:4869:TYR:HB3	2.48	0.43
1:A:4417:GLU:OE2	1:A:4424:TRP:HB3	2.19	0.43
1:A:4577:THR:O	1:A:4578:ASN:CB	2.67	0.43
1:A:4854:PHE:HB3	1:A:4871:CYS:SG	2.59	0.43
1:B:4761:VAL:HG11	1:B:4773:ASN:HB3	2.00	0.43
1:B:4437:ASP:HB3	1:B:4438:PRO:HD3	1.99	0.43
1:B:4857:LYS:C	1:B:4859:LYS:H	2.26	0.43
1:A:4811:THR:O	1:A:4811:THR:CG2	2.67	0.43
1:A:4823:GLU:N	1:A:4833:ILE:O	2.52	0.43
2:Q:4:MAN:H61	2:Q:5:NAG:H83	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4474:ASP:OD2	1:B:4477:HIS:HB2	2.19	0.43
1:B:4859:LYS:HB3	1:B:4869:TYR:N	2.33	0.43
7:O:3:BMA:H3	7:O:5:NAG:C1	2.49	0.43
1:A:4404:MET:HB3	5:K:2:NAG:O7	2.18	0.42
1:B:4643:LEU:HA	1:B:4646:LEU:HD13	2.01	0.42
1:B:4922:THR:HB	1:B:4939:LYS:C	2.44	0.42
1:A:4724:PRO:HB2	1:A:4737:GLN:HE22	1.85	0.42
1:A:4752:THR:HG22	1:A:4764:LYS:HG3	2.02	0.42
1:A:4879:HIS:CG	1:A:4880:GLY:N	2.87	0.42
1:B:4861:VAL:HG13	1:B:4861:VAL:O	2.19	0.42
2:F:1:NAG:O3	2:F:7:MAN:H3	2.18	0.42
1:A:4475:ASN:O	1:A:4476:TYR:HB2	2.18	0.42
1:A:4808:LYS:HB2	1:A:4833:ILE:HD12	2.00	0.42
1:B:4378:LEU:HD11	1:B:4382:PHE:HB2	2.00	0.42
1:B:4487:PRO:C	1:B:4488:ARG:HG3	2.45	0.42
3:D:9:MAN:O3	3:D:12:NAG:O5	2.36	0.42
2:Q:1:NAG:H4	2:Q:2:NAG:H82	2.02	0.42
1:B:4479:ASP:HB3	1:B:4483:LYS:HA	2.00	0.42
1:B:4912:VAL:O	1:B:4912:VAL:CG1	2.67	0.42
5:H:1:NAG:H62	5:H:2:NAG:N2	2.34	0.42
1:B:4738:ASN:HB3	4:N:4:FUC:H2	2.00	0.42
1:A:4530:GLU:HB3	1:A:4541:ASP:OD1	2.18	0.42
1:B:4376:TRP:HD1	1:B:4378:LEU:CA	2.30	0.42
1:B:4567:ASN:HD22	7:O:1:NAG:C6	2.31	0.42
1:B:4905:ASP:CG	1:B:4908:THR:HB	2.44	0.42
2:L:2:NAG:H82	2:L:10:FUC:H3	2.01	0.42
1:A:4405:PRO:HD2	5:K:2:NAG:HN2	1.84	0.42
1:A:4829:THR:O	1:A:4831:CYS:SG	2.78	0.42
1:B:4376:TRP:CD1	1:B:4378:LEU:CA	2.98	0.42
1:B:4857:LYS:N	1:B:4871:CYS:HB2	2.35	0.42
1:A:4403:PRO:O	1:A:4404:MET:C	2.62	0.42
1:A:4505:HIS:C	1:A:4506:MET:HE2	2.44	0.42
1:A:4904:VAL:O	1:A:4909:LEU:N	2.53	0.42
1:B:4390:ASN:OD1	1:B:4391:THR:N	2.52	0.42
1:B:4679:SER:O	1:B:4679:SER:OG	2.33	0.42
1:B:4822:THR:O	2:Q:10:FUC:H63	2.20	0.42
1:B:4876:VAL:CG2	1:B:4878:VAL:HG13	2.43	0.42
1:B:4895:CYS:SG	1:B:4919:PRO:HA	2.60	0.42
5:H:3:BMA:H4	5:H:8:NAG:H2	2.01	0.42
1:A:4406:THR:HG23	5:K:1:NAG:C6	2.42	0.41
1:B:4860:MET:O	1:B:4861:VAL:CG1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4714:PRO:HB2	1:B:4716:HIS:CE1	2.55	0.41
1:B:4825:ASN:HB2	1:B:4833:ILE:H	1.85	0.41
1:B:4860:MET:HB3	1:B:4870:TRP:HB3	2.03	0.41
1:B:4879:HIS:ND1	1:B:4884:TYR:HB3	2.35	0.41
1:A:4442:THR:OG1	1:A:4446:LEU:HB3	2.20	0.41
1:B:4754:ASN:OD1	1:B:4755:TYR:N	2.53	0.41
1:B:4860:MET:C	1:B:4861:VAL:HG12	2.45	0.41
1:B:4908:THR:O	1:B:4909:LEU:C	2.62	0.41
1:A:4822:THR:H	1:A:4835:VAL:H	1.69	0.41
1:A:4824:VAL:O	1:A:4825:ASN:C	2.64	0.41
1:A:4832:ASN:ND2	2:C:10:FUC:H61	2.36	0.41
1:A:4887:GLY:HA2	1:A:4900:CYS:SG	2.59	0.41
1:A:4931:MET:HA	8:A:5001:NAG:O6	2.20	0.41
1:B:4862:PRO:HG2	1:B:4864:ARG:H	1.86	0.41
1:A:4454:CYS:HA	1:A:4477:HIS:CD2	2.56	0.41
1:A:4764:LYS:HE2	1:A:4764:LYS:HB2	1.81	0.41
1:A:4794:GLY:HA3	1:B:4521:ALA:HB3	2.03	0.41
1:B:4897:ASP:OD2	1:B:4916:THR:O	2.38	0.41
3:D:1:NAG:O3	3:D:12:NAG:H2	2.20	0.41
1:A:4392:VAL:O	1:B:4391:THR:HA	2.20	0.41
1:A:4884:TYR:O	1:A:4884:TYR:HD1	2.01	0.41
1:B:4377:TRP:NE1	1:B:4381:CYS:HA	2.36	0.41
1:B:4859:LYS:NZ	1:B:4859:LYS:HA	2.35	0.41
1:B:4643:LEU:HD23	1:B:4681:GLU:HG2	2.02	0.41
1:B:4702:ARG:O	1:B:4705:THR:OG1	2.32	0.41
1:B:4704:HIS:HA	2:L:10:FUC:H63	2.03	0.41
6:I:3:MAN:H2	6:I:4:BMA:O6	2.20	0.41
1:A:4405:PRO:HG2	5:K:2:NAG:HN2	1.85	0.41
1:A:4675:MET:HE2	1:A:4675:MET:HB3	2.01	0.41
1:A:4808:LYS:HZ1	1:A:4810:VAL:HB	1.85	0.41
1:A:4896:GLN:N	1:A:4918:VAL:HG12	2.35	0.41
1:A:4821:ALA:CB	1:A:4823:GLU:HG2	2.49	0.41
2:C:1:NAG:H61	2:C:2:NAG:C7	2.50	0.41
3:D:2:NAG:O3	3:D:9:MAN:H3	2.21	0.41
1:A:4909:LEU:HG	1:A:4910:LEU:H	1.85	0.40
1:A:4930:LEU:HD21	1:A:4939:LYS:CE	2.51	0.40
1:B:4847:PRO:HA	1:B:4869:TYR:CD1	2.56	0.40
1:B:4859:LYS:HA	1:B:4859:LYS:HD2	1.54	0.40
1:B:4892:SER:N	1:B:4896:GLN:OE1	2.53	0.40
1:A:4793:GLU:HG3	1:B:4520:VAL:HG12	2.02	0.40
1:B:4376:TRP:CG	1:B:4377:TRP:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4879:HIS:HA	1:B:4884:TYR:CG	2.56	0.40
4:N:1:NAG:H4	4:N:2:NAG:H2	1.81	0.40
1:A:4419:PRO:HB2	1:A:4420:ASP:H	1.73	0.40
1:A:4437:ASP:HB3	1:A:4438:PRO:HD3	2.04	0.40
1:A:4541:ASP:HB3	1:A:4548:LEU:HD13	2.04	0.40
1:B:4462:ILE:HG12	1:B:4570:LYS:HD3	2.03	0.40
1:B:4815:GLU:HG3	1:B:4817:GLY:N	2.36	0.40
1:A:4909:LEU:HG	1:A:4910:LEU:N	2.36	0.40
1:B:4479:ASP:HB2	1:B:4486:CYS:SG	2.62	0.40
1:B:4816:ASP:CG	1:B:4843:CYS:HA	2.46	0.40
5:H:7:MAN:O3	5:H:7:MAN:H61	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/583 (92%)	490 (91%)	48 (9%)	0	100	100
1	B	538/583 (92%)	478 (89%)	59 (11%)	1 (0%)	43	70
All	All	1076/1166 (92%)	968 (90%)	107 (10%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4926	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	488/521 (94%)	454 (93%)	34 (7%)	14	40
1	B	488/521 (94%)	457 (94%)	31 (6%)	16	42
All	All	976/1042 (94%)	911 (93%)	65 (7%)	17	41

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4352	CYS
1	A	4386	CYS
1	A	4389	ASN
1	A	4390	ASN
1	A	4392	VAL
1	A	4407	CYS
1	A	4579	THR
1	A	4584	CYS
1	A	4595	CYS
1	A	4703	ASN
1	A	4731	LYS
1	A	4734	SER
1	A	4813	CYS
1	A	4836	CYS
1	A	4838	CYS
1	A	4843	CYS
1	A	4846	LYS
1	A	4849	VAL
1	A	4850	CYS
1	A	4856	VAL
1	A	4866	CYS
1	A	4874	LYS
1	A	4877	CYS
1	A	4890	VAL
1	A	4892	SER
1	A	4898	CYS
1	A	4899	VAL
1	A	4908	THR
1	A	4909	LEU
1	A	4911	ASN
1	A	4912	VAL
1	A	4913	ILE
1	A	4915	CYS

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Mol	Chain	Res	Type
1	A	4916	THR
1	B	4351	GLU
1	B	4352	CYS
1	B	4389	ASN
1	B	4392	VAL
1	B	4406	THR
1	B	4478	CYS
1	B	4584	CYS
1	B	4604	VAL
1	B	4703	ASN
1	B	4730	CYS
1	B	4806	SER
1	B	4815	GLU
1	B	4831	CYS
1	B	4832	ASN
1	B	4837	LYS
1	B	4840	THR
1	B	4842	LEU
1	B	4850	CYS
1	B	4859	LYS
1	B	4860	MET
1	B	4865	CYS
1	B	4866	CYS
1	B	4878	VAL
1	B	4896	GLN
1	B	4900	CYS
1	B	4904	VAL
1	B	4915	CYS
1	B	4921	ASN
1	B	4924	CYS
1	B	4932	GLU
1	B	4936	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4390	ASN
1	A	4601	GLN
1	A	4704	HIS
1	A	4754	ASN
1	A	4801	GLN
1	A	4896	GLN

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Mol	Chain	Res	Type
1	A	4921	ASN
1	B	4425	HIS
1	B	4611	HIS
1	B	4645	GLN
1	B	4694	GLN
1	B	4706	HIS
1	B	4736	GLN

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 ⓘ

121 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.31	0	17,19,21	1.09	1 (5%)
2	FUC	C	10	2	10,10,11	0.22	0	14,14,16	0.59	0
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.76	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	1.03	0
2	MAN	C	4	2	11,11,12	0.21	0	15,15,17	0.50	0
2	NAG	C	5	2	14,14,15	0.30	0	17,19,21	0.72	0
2	GAL	C	6	2	11,11,12	0.21	0	15,15,17	0.57	0
2	MAN	C	7	2	11,11,12	0.22	0	15,15,17	0.56	0
2	NAG	C	8	2	14,14,15	0.30	0	17,19,21	0.80	1 (5%)
2	GAL	C	9	2	11,11,12	0.21	0	15,15,17	0.59	0
3	NAG	D	1	1,3	14,14,15	0.36	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	10	3	14,14,15	0.30	0	17,19,21	0.73	0
3	GAL	D	11	3	11,11,12	0.20	0	15,15,17	0.52	0
3	NAG	D	12	3	14,14,15	0.25	0	17,19,21	1.03	1 (5%)
3	GAL	D	13	3	11,11,12	0.16	0	15,15,17	0.56	0
3	FUC	D	14	3	10,10,11	0.21	0	14,14,16	0.55	0
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.91	1 (5%)
3	BMA	D	3	3	11,11,12	0.29	0	15,15,17	1.22	3 (20%)
3	MAN	D	4	3	11,11,12	0.24	0	15,15,17	0.66	0
3	NAG	D	5	3	14,14,15	0.33	0	17,19,21	1.07	2 (11%)
3	GAL	D	6	3	11,11,12	0.24	0	15,15,17	0.60	0
3	NAG	D	7	3	14,14,15	0.28	0	17,19,21	0.62	0
3	GAL	D	8	3	11,11,12	0.21	0	15,15,17	0.68	0
3	MAN	D	9	3	11,11,12	0.28	0	15,15,17	1.00	0
4	NAG	E	1	4,1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
4	NAG	E	2	4	14,14,15	0.39	0	17,19,21	0.58	0
4	BMA	E	3	4	11,11,12	0.24	0	15,15,17	0.55	0
4	FUC	E	4	4	10,10,11	0.21	0	14,14,16	0.50	0
2	NAG	F	1	2,1	14,14,15	0.80	1 (7%)	17,19,21	1.21	3 (17%)
2	FUC	F	10	2	10,10,11	0.22	0	14,14,16	0.54	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.88	0
2	BMA	F	3	2	11,11,12	0.27	0	15,15,17	0.74	0
2	MAN	F	4	2	11,11,12	0.21	0	15,15,17	0.50	0
2	NAG	F	5	2	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
2	GAL	F	6	2	11,11,12	0.19	0	15,15,17	0.59	0
2	MAN	F	7	2	11,11,12	0.23	0	15,15,17	0.56	0
2	NAG	F	8	2	14,14,15	0.29	0	17,19,21	0.56	0
2	GAL	F	9	2	11,11,12	0.27	0	15,15,17	1.10	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.31	0	17,19,21	0.72	0
2	FUC	G	10	2	10,10,11	0.23	0	14,14,16	0.54	0
2	NAG	G	2	2	14,14,15	0.32	0	17,19,21	0.64	0
2	BMA	G	3	2	11,11,12	0.33	0	15,15,17	1.20	1 (6%)
2	MAN	G	4	2	11,11,12	0.21	0	15,15,17	0.62	0
2	NAG	G	5	2	14,14,15	0.28	0	17,19,21	0.56	0
2	GAL	G	6	2	11,11,12	0.21	0	15,15,17	0.53	0
2	MAN	G	7	2	11,11,12	0.21	0	15,15,17	0.54	0
2	NAG	G	8	2	14,14,15	0.29	0	17,19,21	0.72	0
2	GAL	G	9	2	11,11,12	0.22	0	15,15,17	0.52	0
5	NAG	H	1	5,1	14,14,15	0.39	0	17,19,21	0.91	2 (11%)
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	1.42	2 (11%)
5	BMA	H	3	5	11,11,12	0.24	0	15,15,17	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	H	4	5	11,11,12	0.24	0	15,15,17	0.78	0
5	NAG	H	5	5	14,14,15	0.36	0	17,19,21	0.48	0
5	GAL	H	6	5	11,11,12	0.23	0	15,15,17	0.60	0
5	MAN	H	7	5	11,11,12	0.40	0	15,15,17	0.81	0
5	NAG	H	8	5	14,14,15	0.37	0	17,19,21	1.44	2 (11%)
5	GAL	H	9	5	11,11,12	0.35	0	15,15,17	1.19	1 (6%)
6	NAG	I	1	1,6	14,14,15	0.40	0	17,19,21	0.72	0
6	NAG	I	2	6	14,14,15	0.28	0	17,19,21	0.64	0
6	MAN	I	3	6	11,11,12	0.18	0	15,15,17	0.57	0
6	BMA	I	4	6	11,11,12	0.21	0	15,15,17	0.56	0
6	FUC	I	5	6	10,10,11	0.23	0	14,14,16	0.55	0
2	NAG	J	1	2,1	14,14,15	0.26	0	17,19,21	0.66	0
2	FUC	J	10	2	10,10,11	0.24	0	14,14,16	0.55	0
2	NAG	J	2	2	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
2	BMA	J	3	2	11,11,12	0.22	0	15,15,17	0.52	0
2	MAN	J	4	2	11,11,12	0.20	0	15,15,17	0.52	0
2	NAG	J	5	2	14,14,15	0.29	0	17,19,21	0.63	0
2	GAL	J	6	2	11,11,12	0.20	0	15,15,17	0.55	0
2	MAN	J	7	2	11,11,12	0.24	0	15,15,17	0.57	0
2	NAG	J	8	2	14,14,15	0.27	0	17,19,21	0.68	0
2	GAL	J	9	2	11,11,12	0.21	0	15,15,17	0.56	0
5	NAG	K	1	5,1	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
5	NAG	K	2	5	14,14,15	0.27	0	17,19,21	0.67	0
5	BMA	K	3	5	11,11,12	0.24	0	15,15,17	0.62	0
5	MAN	K	4	5	11,11,12	0.21	0	15,15,17	0.62	0
5	NAG	K	5	5	14,14,15	0.29	0	17,19,21	0.62	0
5	GAL	K	6	5	11,11,12	0.21	0	15,15,17	0.54	0
5	MAN	K	7	5	11,11,12	0.21	0	15,15,17	0.53	0
5	NAG	K	8	5	14,14,15	0.28	0	17,19,21	0.62	0
5	GAL	K	9	5	11,11,12	0.19	0	15,15,17	0.51	0
2	NAG	L	1	2,1	14,14,15	0.36	0	17,19,21	1.26	2 (11%)
2	FUC	L	10	2	10,10,11	0.21	0	14,14,16	0.62	0
2	NAG	L	2	2	14,14,15	0.32	0	17,19,21	0.99	2 (11%)
2	BMA	L	3	2	11,11,12	0.23	0	15,15,17	1.12	1 (6%)
2	MAN	L	4	2	11,11,12	0.25	0	15,15,17	0.68	0
2	NAG	L	5	2	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
2	GAL	L	6	2	11,11,12	0.22	0	15,15,17	0.57	0
2	MAN	L	7	2	11,11,12	0.24	0	15,15,17	0.62	0
2	NAG	L	8	2	14,14,15	0.32	0	17,19,21	0.58	0
2	GAL	L	9	2	11,11,12	0.42	0	15,15,17	1.75	4 (26%)
4	NAG	M	1	4,1	14,14,15	0.32	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.64	0
4	BMA	M	3	4	11,11,12	0.19	0	15,15,17	0.55	0
4	FUC	M	4	4	10,10,11	0.33	0	14,14,16	0.82	0
4	NAG	N	1	4,1	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
4	NAG	N	2	4	14,14,15	0.26	0	17,19,21	0.71	0
4	BMA	N	3	4	11,11,12	0.28	0	15,15,17	1.17	1 (6%)
4	FUC	N	4	4	10,10,11	0.24	0	14,14,16	0.56	0
7	NAG	O	1	1,7	14,14,15	0.27	0	17,19,21	1.32	3 (17%)
7	NAG	O	10	7	14,14,15	0.35	0	17,19,21	1.38	1 (5%)
7	GAL	O	11	7	11,11,12	0.25	0	15,15,17	0.57	0
7	FUC	O	12	7	10,10,11	0.24	0	14,14,16	0.54	0
7	NAG	O	2	7	14,14,15	0.28	0	17,19,21	0.66	0
7	BMA	O	3	7	11,11,12	0.29	0	15,15,17	1.04	2 (13%)
7	MAN	O	4	7	11,11,12	0.30	0	15,15,17	1.77	3 (20%)
7	NAG	O	5	7	14,14,15	0.29	0	17,19,21	0.70	0
7	GAL	O	6	7	11,11,12	0.23	0	15,15,17	0.53	0
7	NAG	O	7	7	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
7	GAL	O	8	7	11,11,12	0.46	0	15,15,17	1.73	4 (26%)
7	MAN	O	9	7	11,11,12	0.53	0	15,15,17	1.63	2 (13%)
2	NAG	Q	1	2,1	14,14,15	0.27	0	17,19,21	0.78	0
2	FUC	Q	10	2	10,10,11	0.22	0	14,14,16	0.61	0
2	NAG	Q	2	2	14,14,15	0.44	0	17,19,21	1.10	2 (11%)
2	BMA	Q	3	2	11,11,12	0.24	0	15,15,17	0.72	1 (6%)
2	MAN	Q	4	2	11,11,12	0.22	0	15,15,17	0.56	0
2	NAG	Q	5	2	14,14,15	0.33	0	17,19,21	0.60	0
2	GAL	Q	6	2	11,11,12	0.22	0	15,15,17	0.53	0
2	MAN	Q	7	2	11,11,12	0.20	0	15,15,17	0.58	0
2	NAG	Q	8	2	14,14,15	0.27	0	17,19,21	0.71	0
2	GAL	Q	9	2	11,11,12	0.21	0	15,15,17	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	C	10	2	-	-	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	GAL	C	6	2	-	1/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	NAG	C	8	2	-	2/6/23/26	0/1/1/1
2	GAL	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	10	3	-	3/6/23/26	0/1/1/1
3	GAL	D	11	3	-	0/2/19/22	0/1/1/1
3	NAG	D	12	3	-	4/6/23/26	0/1/1/1
3	GAL	D	13	3	-	1/2/19/22	0/1/1/1
3	FUC	D	14	3	-	-	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	1/2/19/22	0/1/1/1
3	NAG	D	7	3	-	4/6/23/26	0/1/1/1
3	GAL	D	8	3	-	1/2/19/22	0/1/1/1
3	MAN	D	9	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	FUC	F	10	2	-	-	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
2	MAN	F	4	2	-	1/2/19/22	0/1/1/1
2	NAG	F	5	2	-	3/6/23/26	0/1/1/1
2	GAL	F	6	2	-	1/2/19/22	0/1/1/1
2	MAN	F	7	2	-	0/2/19/22	0/1/1/1
2	NAG	F	8	2	-	0/6/23/26	0/1/1/1
2	GAL	F	9	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	4/6/23/26	0/1/1/1
2	FUC	G	10	2	-	-	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	5	2	-	2/6/23/26	0/1/1/1
2	GAL	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	0/2/19/22	0/1/1/1
2	NAG	G	8	2	-	2/6/23/26	0/1/1/1
2	GAL	G	9	2	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	2/6/23/26	0/1/1/1
5	GAL	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	0/2/19/22	0/1/1/1
5	NAG	H	8	5	-	0/6/23/26	0/1/1/1
5	GAL	H	9	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	MAN	I	3	6	-	0/2/19/22	0/1/1/1
6	BMA	I	4	6	-	0/2/19/22	0/1/1/1
6	FUC	I	5	6	-	-	0/1/1/1
2	NAG	J	1	2,1	-	3/6/23/26	0/1/1/1
2	FUC	J	10	2	-	-	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	NAG	J	5	2	-	2/6/23/26	0/1/1/1
2	GAL	J	6	2	-	0/2/19/22	0/1/1/1
2	MAN	J	7	2	-	0/2/19/22	0/1/1/1
2	NAG	J	8	2	-	0/6/23/26	0/1/1/1
2	GAL	J	9	2	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	NAG	K	5	5	-	2/6/23/26	0/1/1/1
5	GAL	K	6	5	-	0/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1
5	NAG	K	8	5	-	2/6/23/26	0/1/1/1
5	GAL	K	9	5	-	1/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	L	10	2	-	-	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1
2	MAN	L	4	2	-	0/2/19/22	0/1/1/1
2	NAG	L	5	2	-	2/6/23/26	0/1/1/1
2	GAL	L	6	2	-	1/2/19/22	0/1/1/1
2	MAN	L	7	2	-	0/2/19/22	0/1/1/1
2	NAG	L	8	2	-	2/6/23/26	0/1/1/1
2	GAL	L	9	2	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	FUC	M	4	4	-	-	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	FUC	N	4	4	-	-	0/1/1/1
7	NAG	O	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	O	10	7	-	2/6/23/26	0/1/1/1
7	GAL	O	11	7	-	0/2/19/22	0/1/1/1
7	FUC	O	12	7	-	-	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	NAG	O	5	7	-	3/6/23/26	0/1/1/1
7	GAL	O	6	7	-	1/2/19/22	0/1/1/1
7	NAG	O	7	7	-	3/6/23/26	0/1/1/1
7	GAL	O	8	7	-	0/2/19/22	0/1/1/1
7	MAN	O	9	7	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	2,1	-	4/6/23/26	0/1/1/1
2	FUC	Q	10	2	-	-	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
2	NAG	Q	5	2	-	2/6/23/26	0/1/1/1
2	GAL	Q	6	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	7	2	-	1/2/19/22	0/1/1/1
2	NAG	Q	8	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	Q	9	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	2.74	1.56	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	4	MAN	C1-O5-C5	5.14	119.07	112.19
7	O	10	NAG	C1-O5-C5	4.87	118.71	112.19
2	L	9	GAL	C1-O5-C5	4.84	118.68	112.19
7	O	8	GAL	C1-O5-C5	4.70	118.48	112.19
5	H	2	NAG	C2-N2-C7	-4.48	116.89	122.90
7	O	9	MAN	C2-C3-C4	-4.03	103.78	110.86
5	H	8	NAG	C4-C3-C2	-3.99	105.18	111.02
5	H	9	GAL	C1-O5-C5	3.53	116.91	112.19
4	N	3	BMA	C1-O5-C5	3.36	116.68	112.19
2	Q	2	NAG	C1-O5-C5	3.34	116.66	112.19
2	F	9	GAL	C1-O5-C5	3.20	116.47	112.19
2	G	3	BMA	C1-O5-C5	2.97	116.17	112.19
5	H	3	BMA	O5-C5-C6	2.86	113.23	107.66
2	F	1	NAG	C1-O5-C5	2.85	116.01	112.19
7	O	1	NAG	C1-O5-C5	2.81	115.95	112.19
7	O	4	MAN	O2-C2-C3	-2.81	104.34	110.15
2	F	5	NAG	C4-C3-C2	-2.75	106.99	111.02
2	L	3	BMA	C1-C2-C3	-2.66	105.76	109.64
4	N	1	NAG	C1-O5-C5	2.65	115.74	112.19
3	D	1	NAG	C1-O5-C5	2.65	115.74	112.19
7	O	8	GAL	C3-C4-C5	2.62	114.97	110.23
5	H	2	NAG	C4-C3-C2	-2.59	107.23	111.02
2	L	1	NAG	O4-C4-C5	-2.56	103.01	109.32
2	L	9	GAL	C3-C4-C5	2.56	114.87	110.23
7	O	3	BMA	C1-C2-C3	-2.55	105.94	109.64
7	O	7	NAG	C4-C3-C2	-2.50	107.36	111.02
2	C	1	NAG	C4-C3-C2	-2.49	107.37	111.02
2	L	1	NAG	O4-C4-C3	2.47	116.20	110.38
5	H	1	NAG	C2-N2-C7	-2.46	119.60	122.90
2	Q	2	NAG	C1-C2-N2	2.45	114.30	110.43
7	O	4	MAN	C1-C2-C3	2.39	113.13	109.64
3	D	5	NAG	C4-C3-C2	-2.38	107.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	8	GAL	O5-C5-C6	2.33	112.20	107.66
2	L	9	GAL	O5-C5-C6	2.33	112.20	107.66
2	L	2	NAG	C4-C3-C2	-2.32	107.62	111.02
7	O	1	NAG	C3-C4-C5	2.30	114.40	110.23
7	O	1	NAG	O5-C1-C2	2.28	114.83	111.29
3	D	3	BMA	C2-C3-C4	-2.27	106.86	110.86
5	H	8	NAG	O5-C1-C2	-2.26	107.80	111.29
7	O	8	GAL	C1-C2-C3	2.25	112.92	109.64
2	F	1	NAG	C6-C5-C4	-2.24	107.53	113.02
3	D	5	NAG	C1-O5-C5	-2.23	109.19	112.19
2	L	9	GAL	C1-C2-C3	2.21	112.86	109.64
5	H	3	BMA	C2-C3-C4	-2.20	106.98	110.86
2	J	2	NAG	C4-C3-C2	-2.20	107.79	111.02
3	D	3	BMA	C3-C4-C5	-2.20	106.25	110.23
3	D	3	BMA	O5-C5-C6	2.19	111.93	107.66
2	L	5	NAG	O5-C1-C2	2.13	114.59	111.29
2	F	1	NAG	O5-C1-C2	-2.11	108.03	111.29
3	D	2	NAG	C4-C3-C2	-2.10	107.94	111.02
7	O	9	MAN	C1-O5-C5	-2.10	109.38	112.19
2	L	2	NAG	C2-N2-C7	-2.09	120.09	122.90
4	E	1	NAG	C4-C3-C2	-2.09	107.96	111.02
4	M	1	NAG	C1-O5-C5	2.06	114.95	112.19
7	O	3	BMA	O5-C5-C6	2.06	111.68	107.66
5	K	1	NAG	O3-C3-C2	-2.04	105.16	109.40
2	Q	3	BMA	C1-O5-C5	2.03	114.91	112.19
5	H	1	NAG	C4-C3-C2	-2.01	108.07	111.02
3	D	12	NAG	O5-C1-C2	-2.01	108.18	111.29
2	C	8	NAG	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	5	NAG	C8-C7-N2-C2
2	C	5	NAG	O7-C7-N2-C2
2	F	5	NAG	C1-C2-N2-C7
2	F	5	NAG	C8-C7-N2-C2
2	F	5	NAG	O7-C7-N2-C2
2	J	1	NAG	C1-C2-N2-C7
2	J	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	J	1	NAG	O7-C7-N2-C2
2	L	5	NAG	C8-C7-N2-C2
2	L	5	NAG	O7-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	Q	5	NAG	C8-C7-N2-C2
2	Q	5	NAG	O7-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	D	7	NAG	C3-C2-N2-C7
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
3	D	10	NAG	C1-C2-N2-C7
3	D	10	NAG	C8-C7-N2-C2
3	D	10	NAG	O7-C7-N2-C2
3	D	12	NAG	C3-C2-N2-C7
3	D	12	NAG	C8-C7-N2-C2
3	D	12	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-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
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C1-C2-N2-C7
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C1-C2-N2-C7
7	O	5	NAG	C8-C7-N2-C2
7	O	5	NAG	O7-C7-N2-C2
7	O	7	NAG	C8-C7-N2-C2
7	O	7	NAG	O7-C7-N2-C2
7	O	10	NAG	C8-C7-N2-C2
7	O	10	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	D	5	NAG	C8-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
5	K	5	NAG	C8-C7-N2-C2
4	E	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C8-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
2	F	3	BMA	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
2	G	5	NAG	C8-C7-N2-C2
2	J	5	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
5	H	5	NAG	C8-C7-N2-C2
5	K	5	NAG	O7-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
2	L	3	BMA	O5-C5-C6-O6
2	G	5	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	5	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
5	H	5	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
2	C	8	NAG	C8-C7-N2-C2
2	G	8	NAG	C8-C7-N2-C2
7	O	3	BMA	C4-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
3	D	8	GAL	O5-C5-C6-O6
3	D	13	GAL	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
5	K	9	GAL	O5-C5-C6-O6
2	Q	8	NAG	O5-C5-C6-O6
2	Q	9	GAL	O5-C5-C6-O6
5	H	9	GAL	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	O	6	GAL	O5-C5-C6-O6
3	D	6	GAL	O5-C5-C6-O6
2	Q	7	MAN	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	L	6	GAL	O5-C5-C6-O6
7	O	7	NAG	O5-C5-C6-O6
3	D	7	NAG	O5-C5-C6-O6
2	F	6	GAL	O5-C5-C6-O6
2	G	8	NAG	O7-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
5	K	8	NAG	C8-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C3-C2-N2-C7
2	Q	2	NAG	O5-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	C	8	NAG	O7-C7-N2-C2
5	K	8	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
2	L	8	NAG	C8-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	C4-C5-C6-O6
2	L	8	NAG	O7-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7
7	O	5	NAG	C1-C2-N2-C7
2	G	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	D	12	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6

There are no ring outliers.

85 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	8	NAG	4	0
6	I	5	FUC	1	0
4	N	4	FUC	2	0
6	I	1	NAG	4	0

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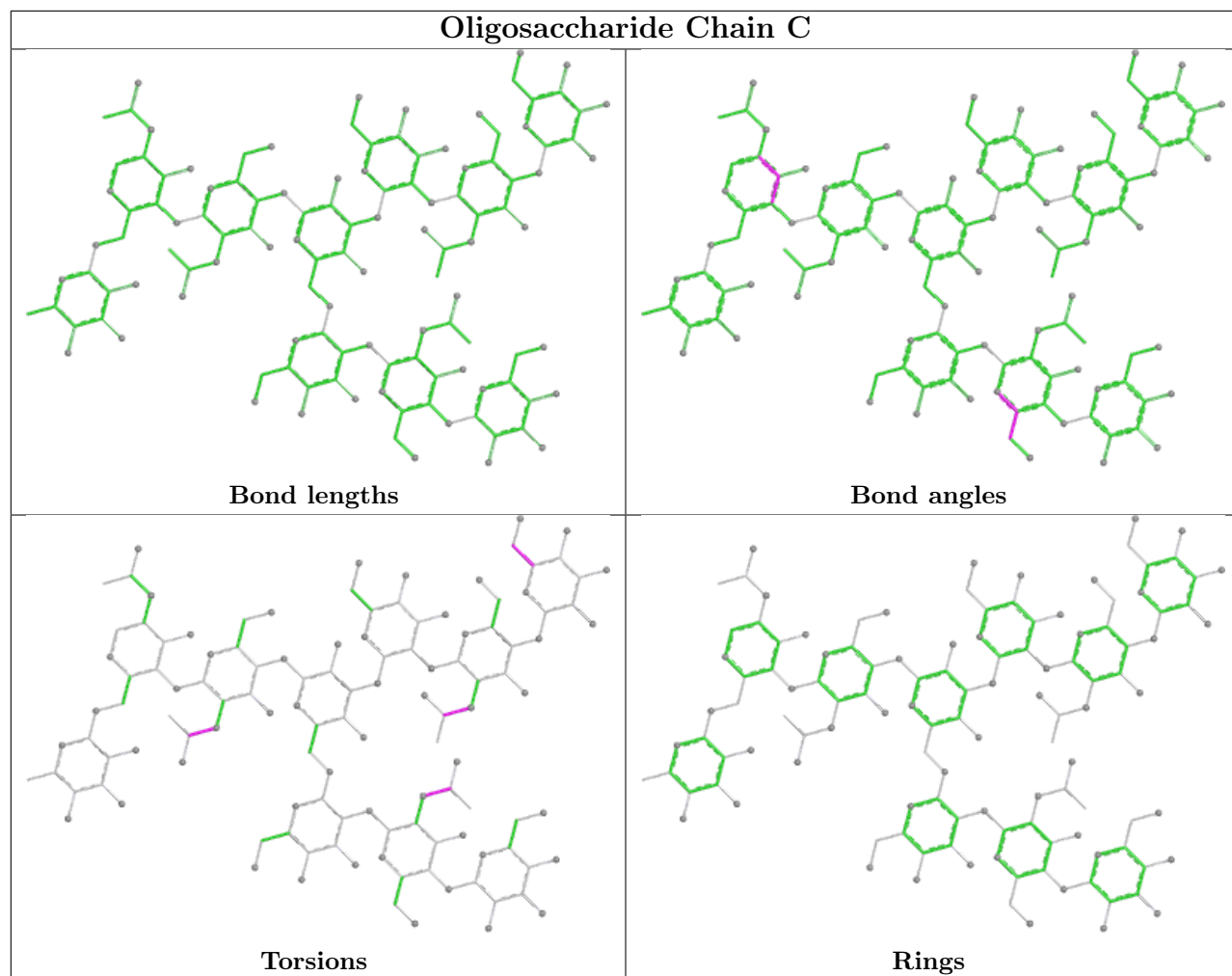
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	MAN	3	0
2	J	2	NAG	2	0
2	J	7	MAN	1	0
7	O	5	NAG	3	0
3	D	9	MAN	7	0
4	E	4	FUC	2	0
3	D	14	FUC	2	0
5	H	2	NAG	1	0
4	E	1	NAG	1	0
2	F	2	NAG	3	0
2	F	10	FUC	2	0
2	L	2	NAG	3	0
7	O	7	NAG	4	0
2	G	2	NAG	2	0
5	H	3	BMA	1	0
7	O	2	NAG	2	0
5	K	1	NAG	4	0
2	F	7	MAN	4	0
2	L	7	MAN	2	0
2	F	6	GAL	4	0
4	E	2	NAG	1	0
2	G	7	MAN	1	0
2	F	4	MAN	1	0
7	O	4	MAN	5	0
2	C	3	BMA	1	0
3	D	1	NAG	3	0
3	D	10	NAG	2	0
5	H	8	NAG	2	0
6	I	2	NAG	4	0
2	G	9	GAL	1	0
3	D	4	MAN	1	0
2	Q	3	BMA	4	0
3	D	12	NAG	5	0
2	C	1	NAG	2	0
3	D	3	BMA	8	0
2	Q	10	FUC	2	0
2	F	5	NAG	2	0
5	K	2	NAG	7	0
2	G	10	FUC	3	0
3	D	13	GAL	1	0
5	H	7	MAN	4	0
5	K	3	BMA	1	0

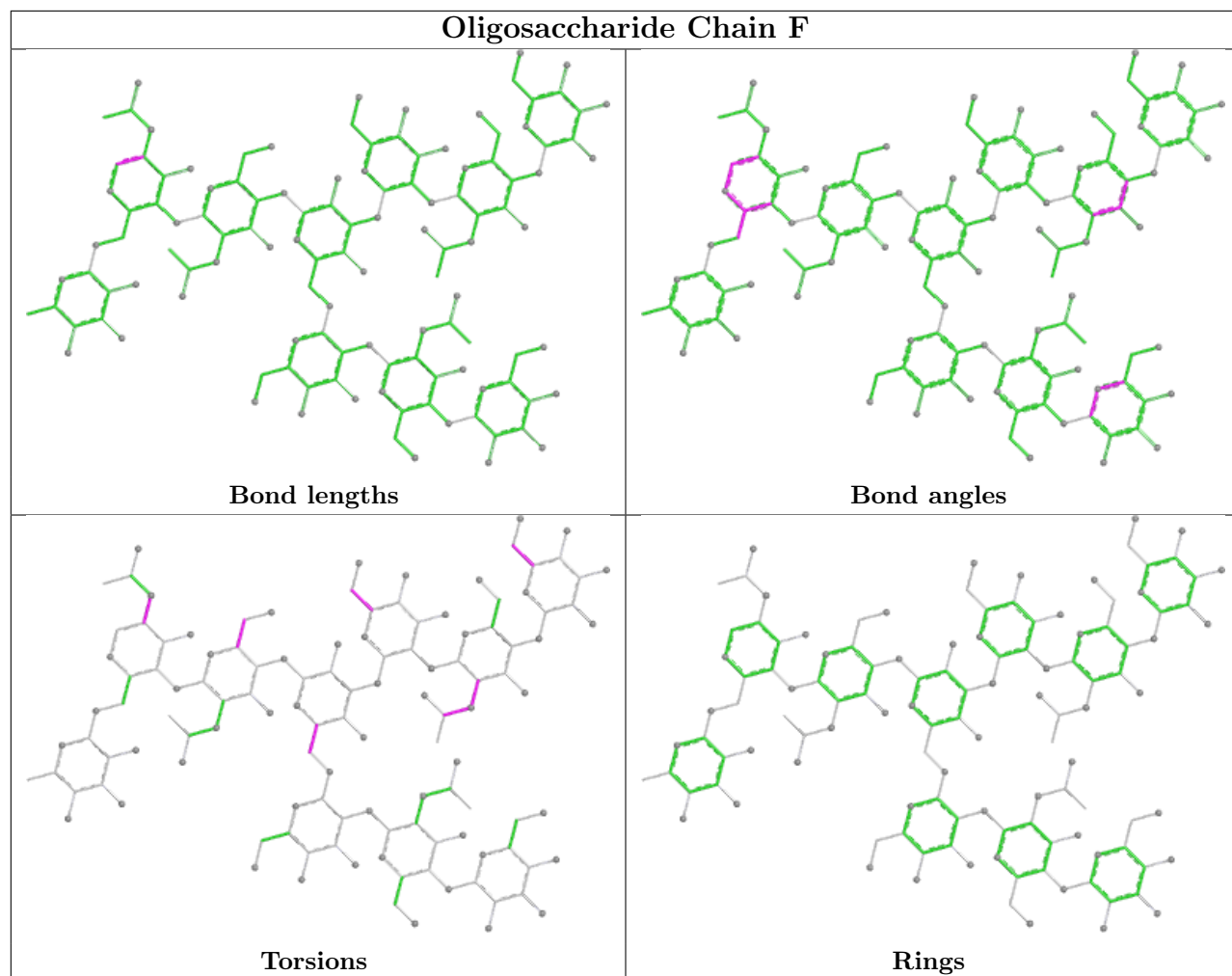
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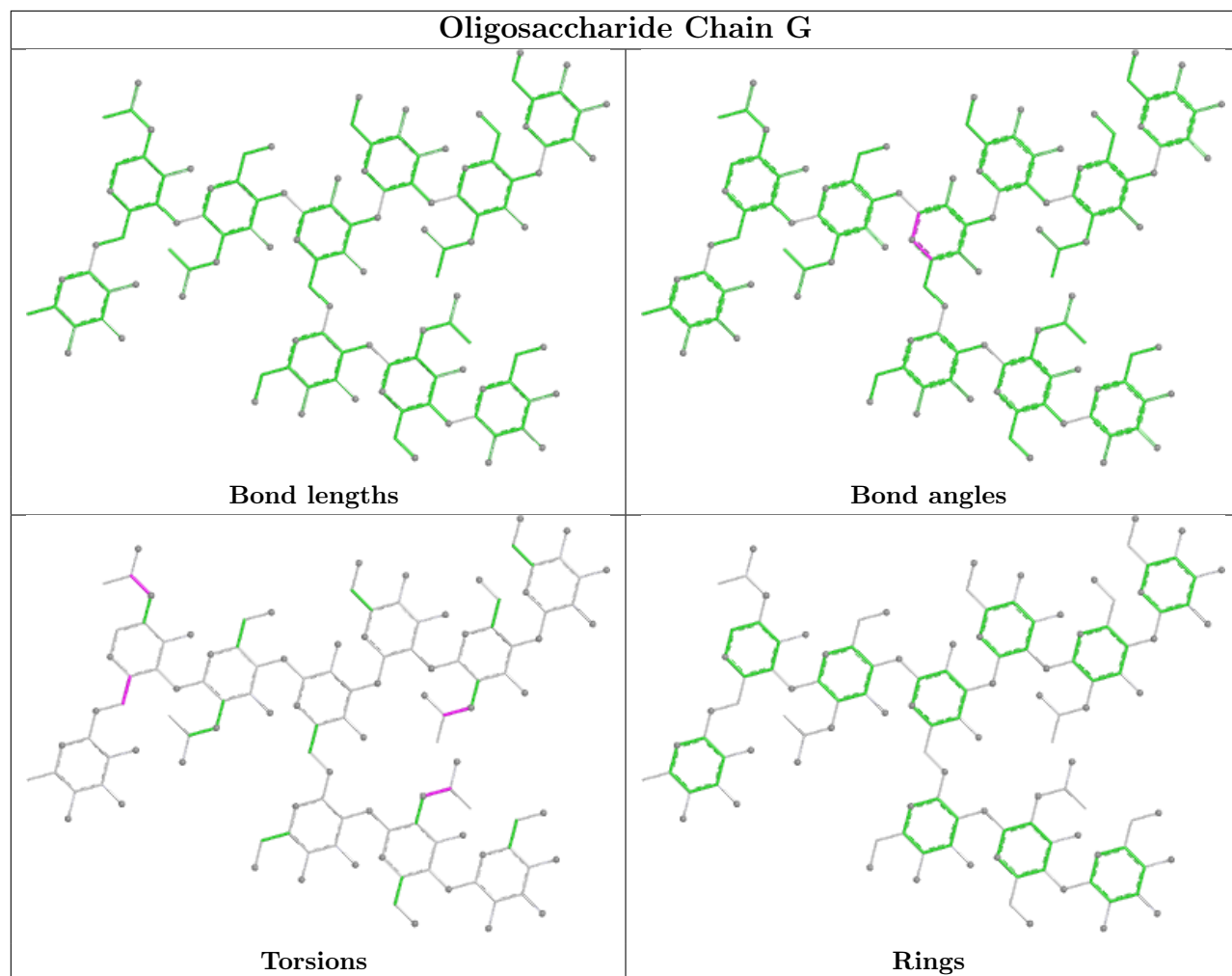
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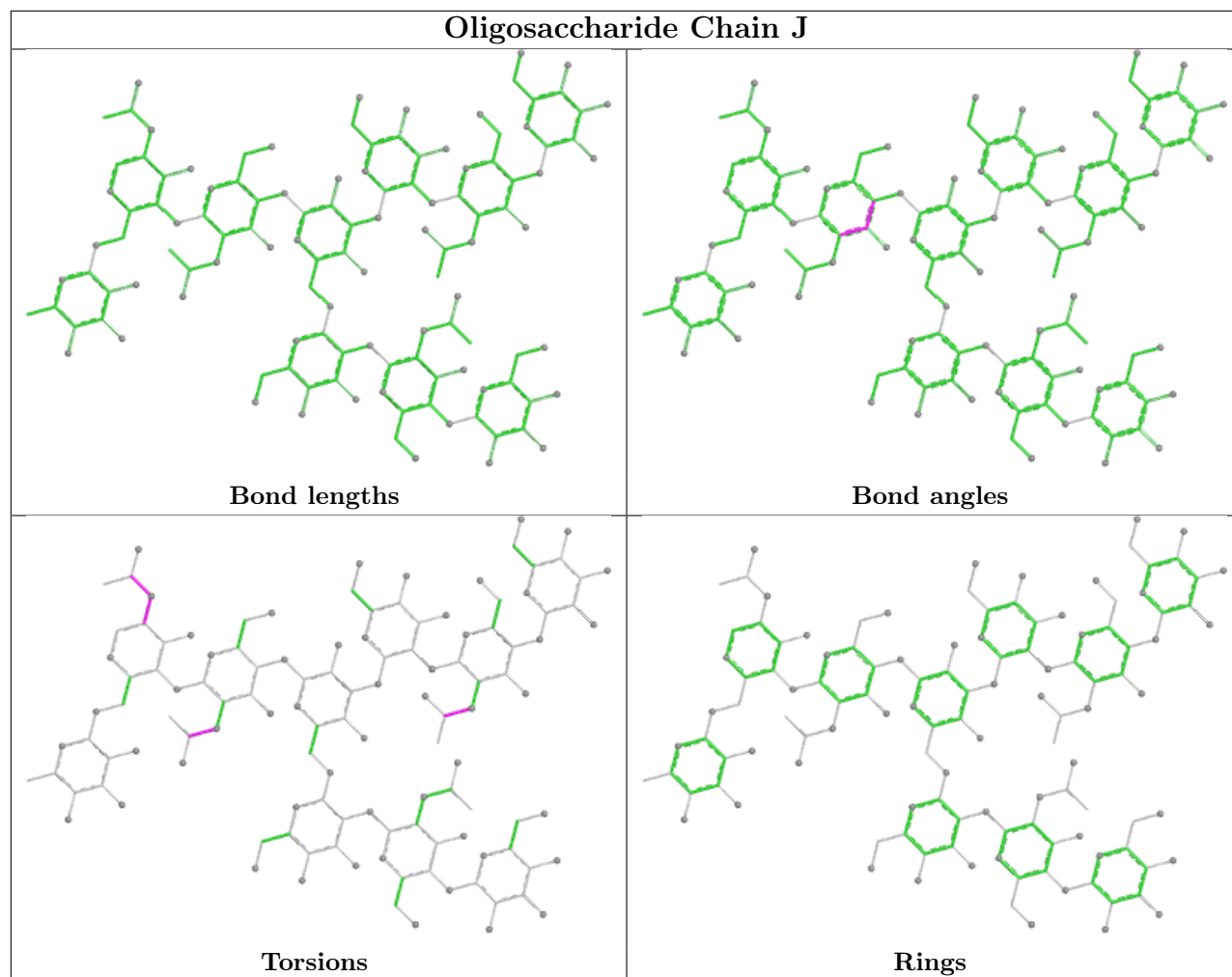
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	10	FUC	2	0
3	D	5	NAG	1	0
2	G	5	NAG	1	0
2	C	5	NAG	4	0
3	D	8	GAL	1	0
2	J	4	MAN	1	0
2	L	5	NAG	2	0
2	L	10	FUC	9	0
2	Q	5	NAG	6	0
7	O	12	FUC	2	0
2	L	3	BMA	2	0
7	O	1	NAG	5	0
2	F	8	NAG	5	0
2	Q	1	NAG	3	0
2	J	5	NAG	2	0
2	C	8	NAG	4	0
2	C	10	FUC	3	0
2	G	1	NAG	1	0
2	C	2	NAG	4	0
2	Q	4	MAN	3	0
2	J	8	NAG	2	0
4	N	2	NAG	1	0
6	I	3	MAN	3	0
2	C	4	MAN	1	0
3	D	7	NAG	1	0
6	I	4	BMA	1	0
7	O	9	MAN	2	0
7	O	10	NAG	1	0
2	F	1	NAG	1	0
2	L	1	NAG	4	0
2	Q	7	MAN	2	0
3	D	2	NAG	4	0
5	H	1	NAG	2	0
4	M	1	NAG	2	0
2	C	6	GAL	1	0
2	Q	2	NAG	6	0
4	N	1	NAG	3	0
7	O	3	BMA	4	0
5	H	9	GAL	1	0

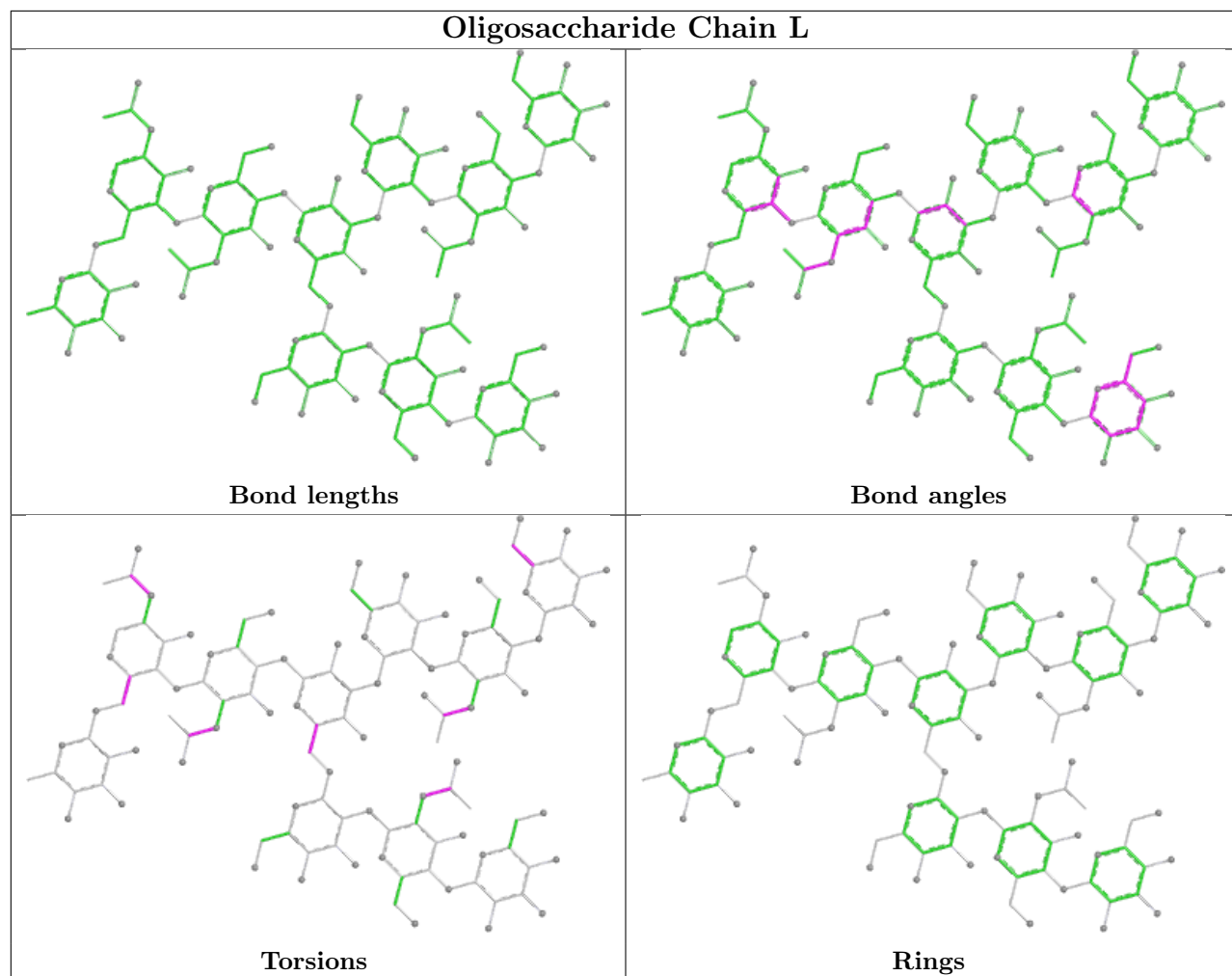
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

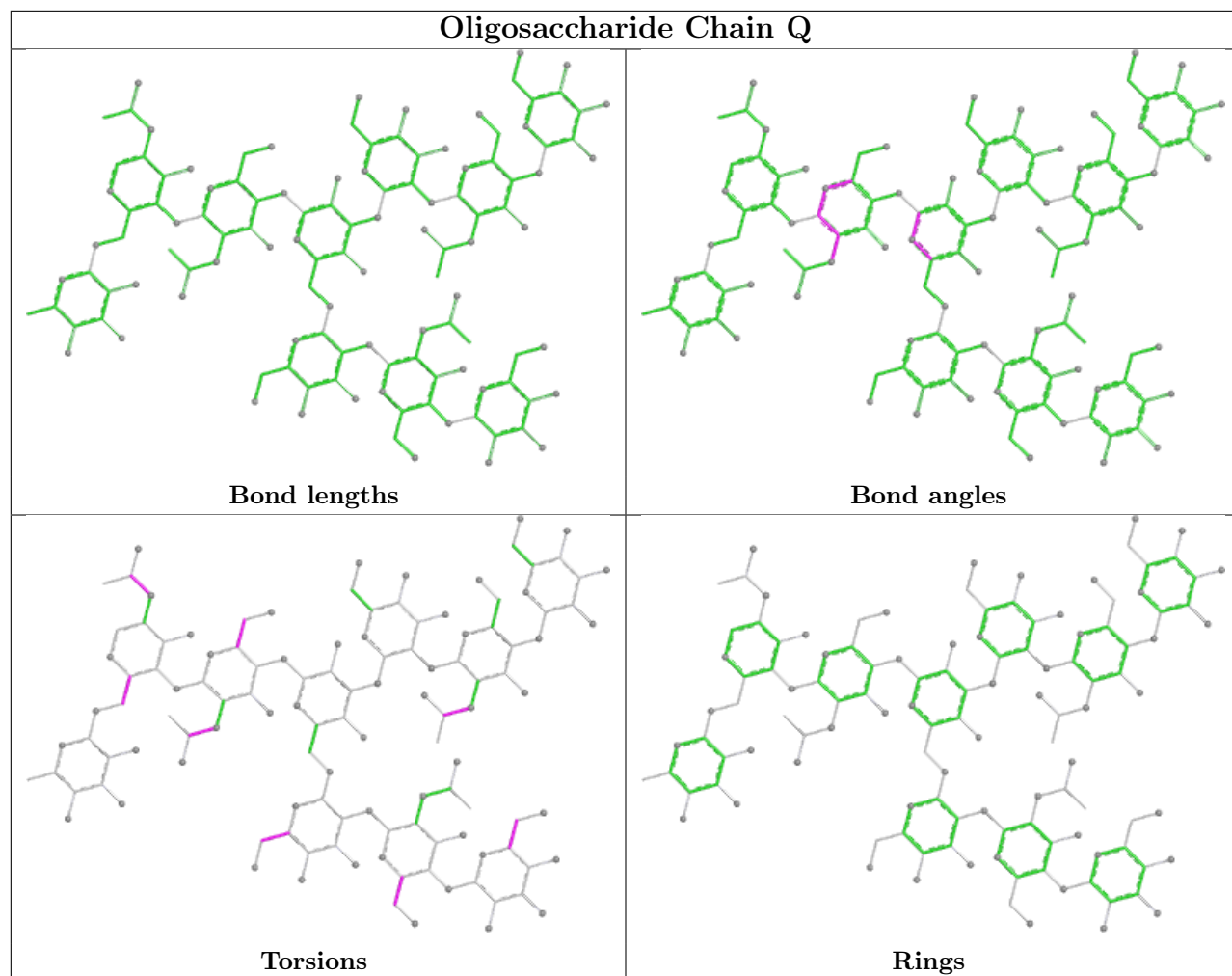


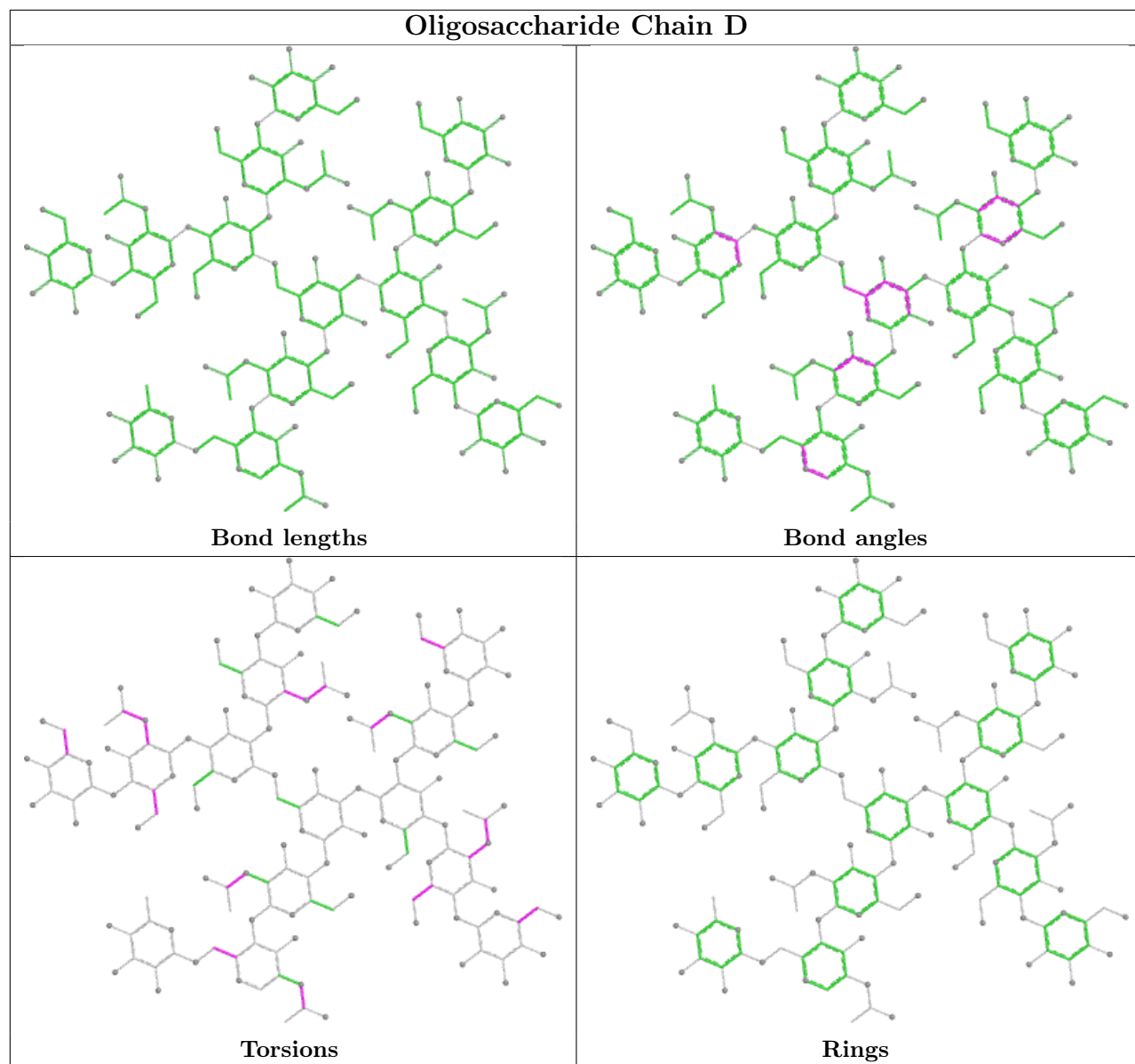


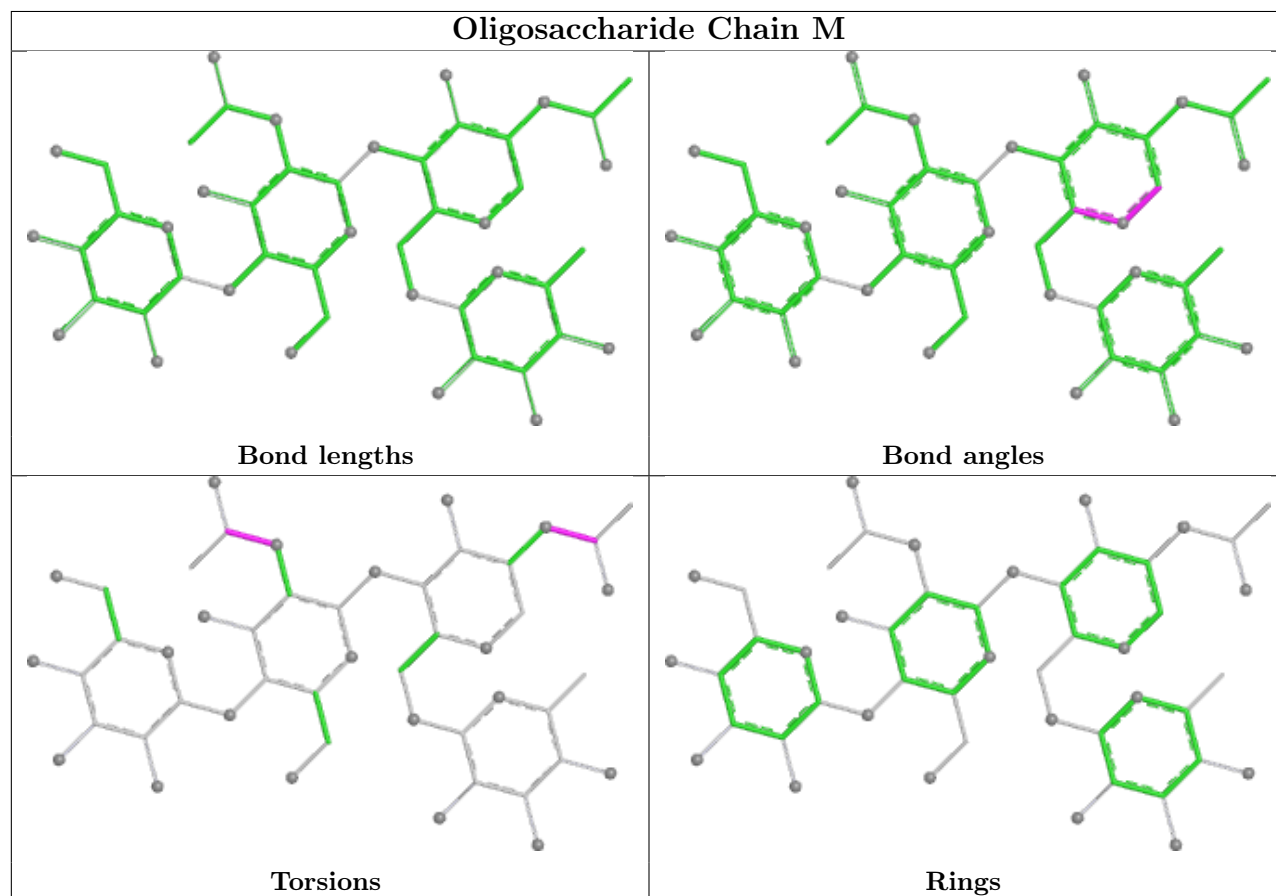
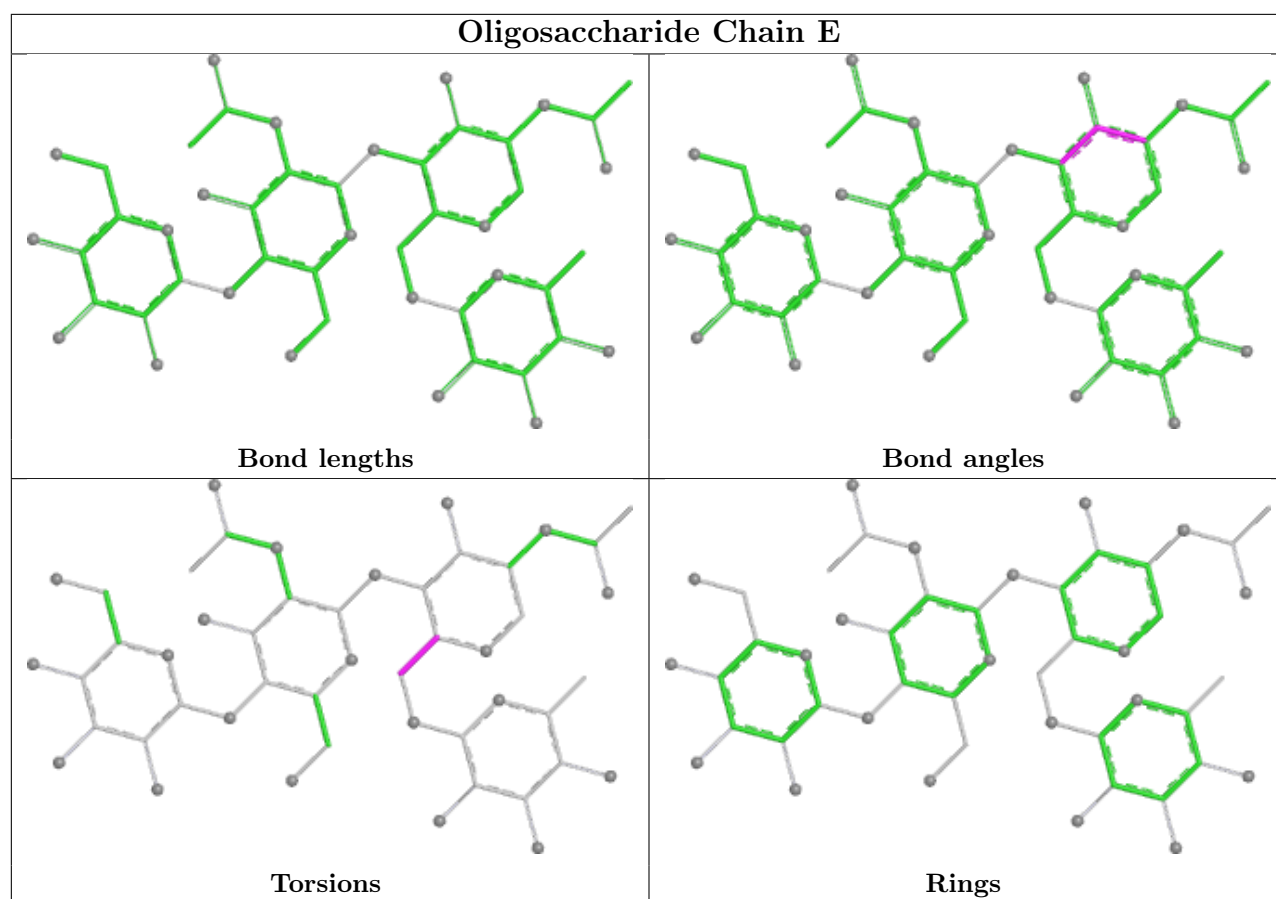


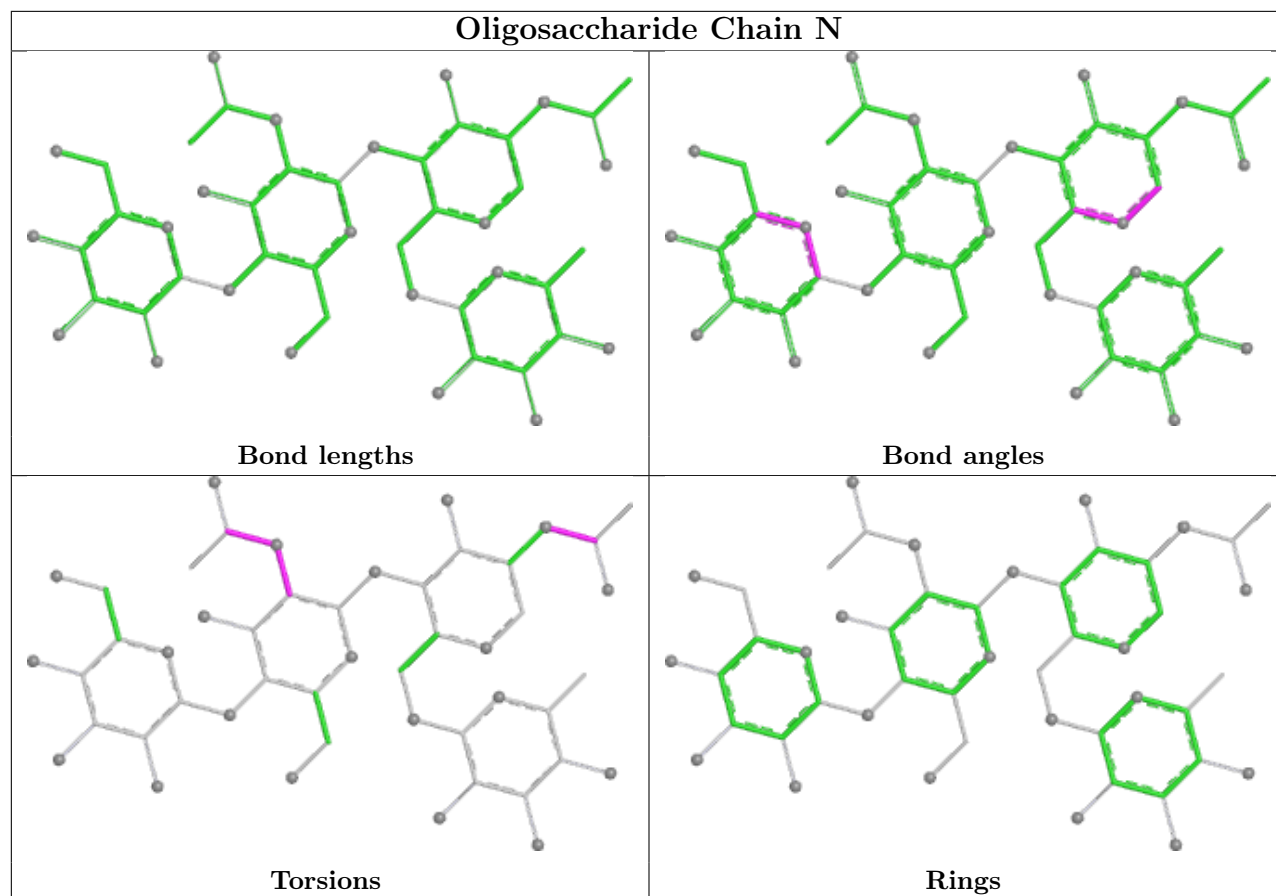


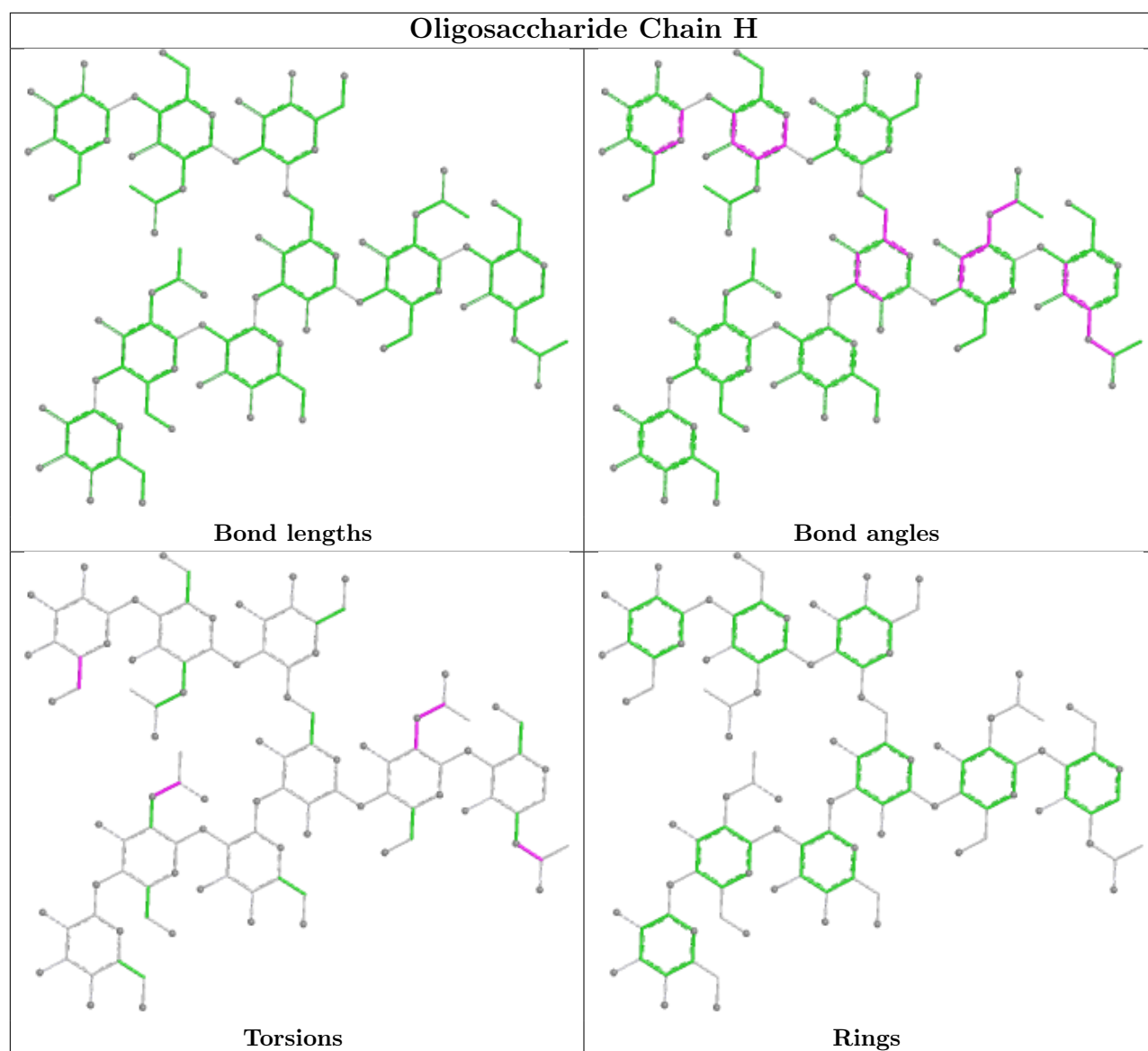


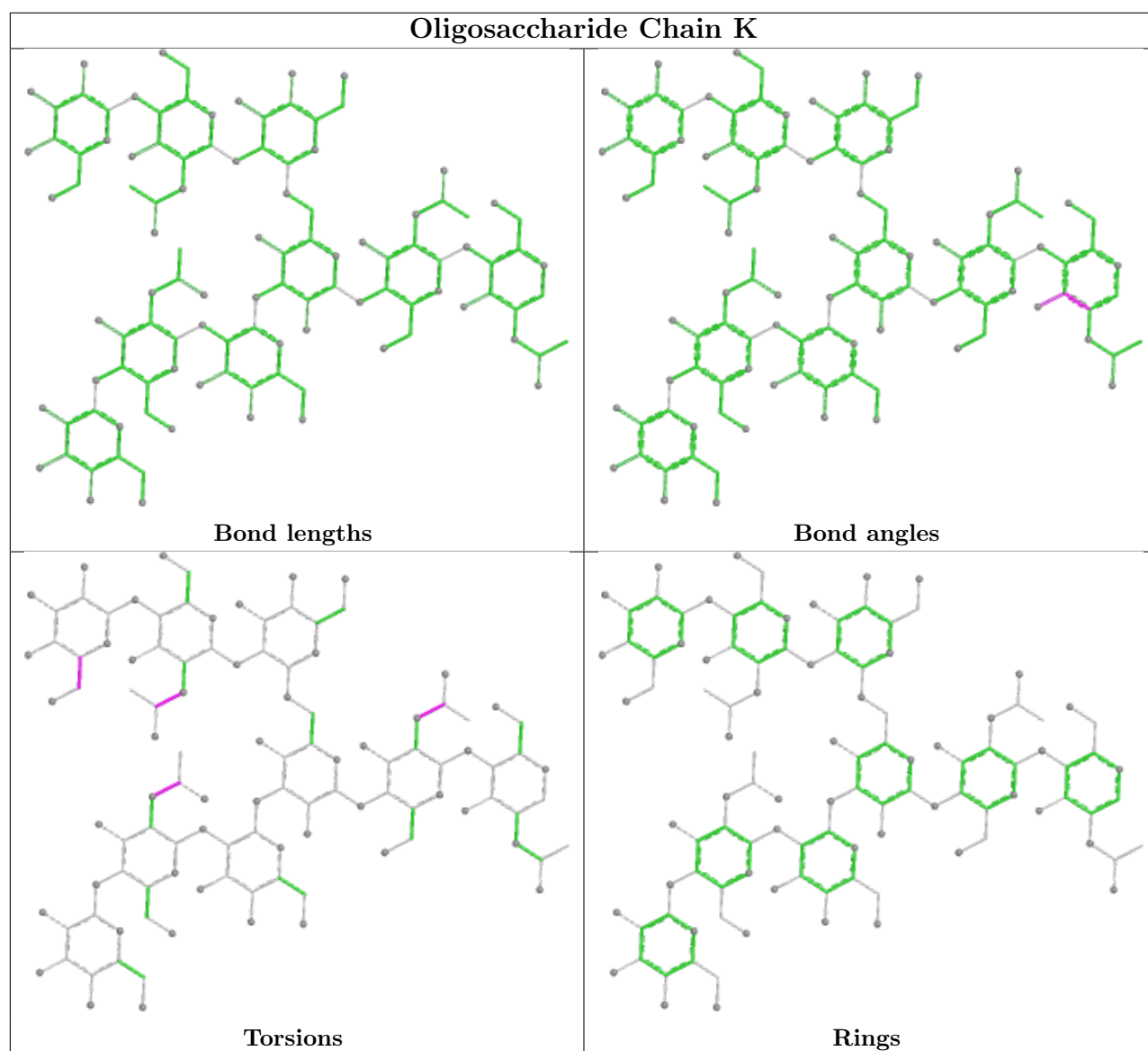


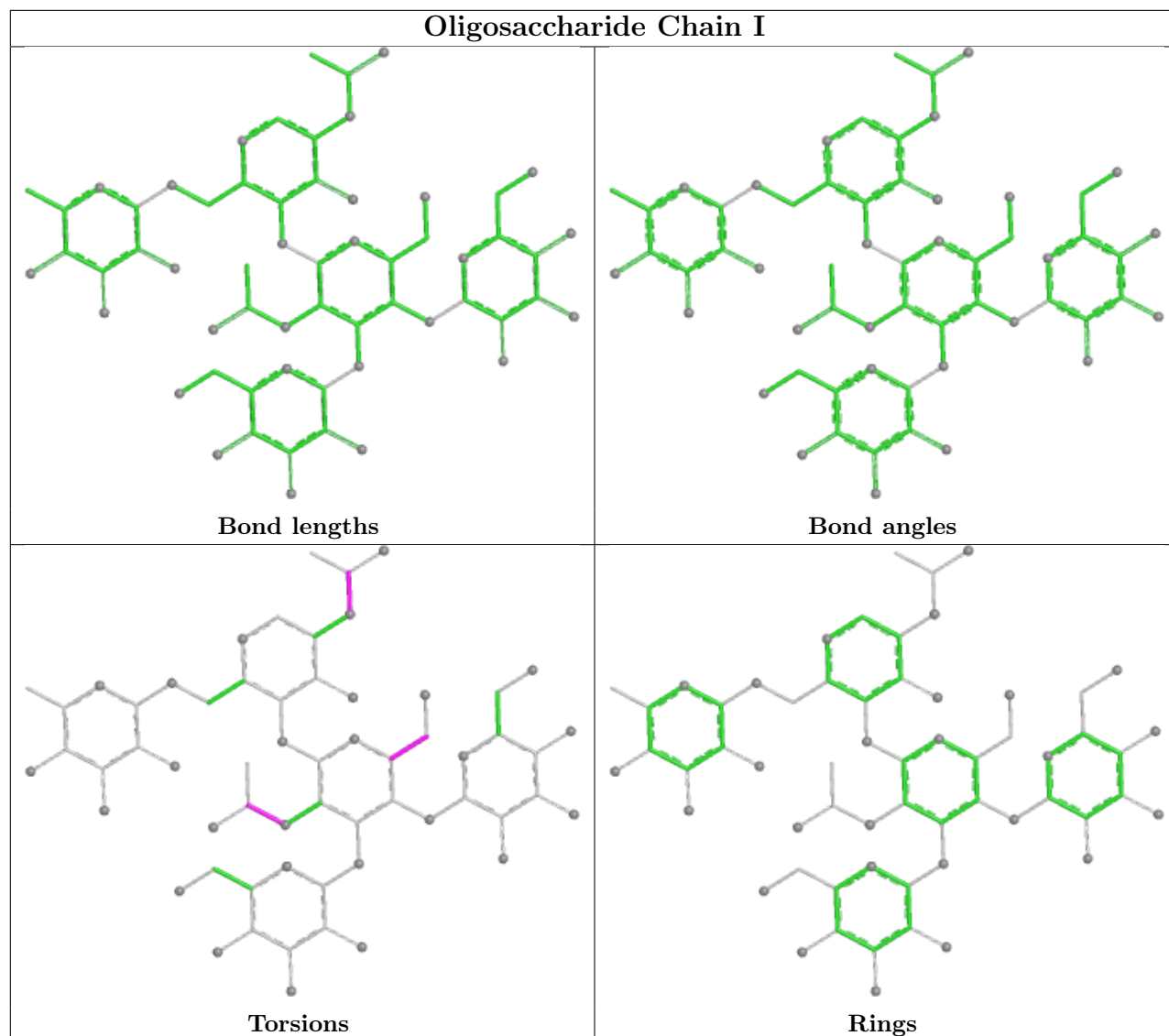


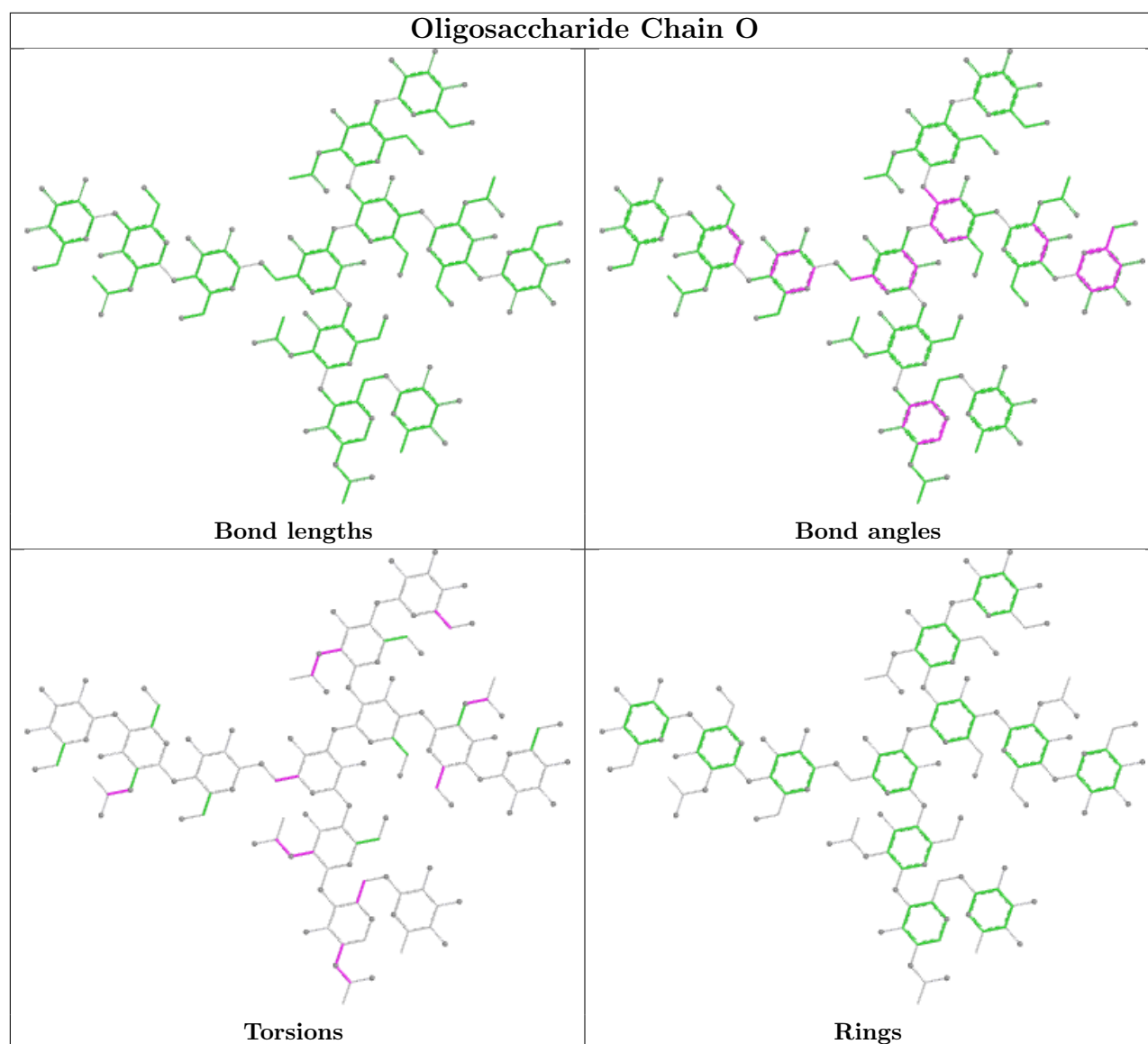












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
8	NAG	B	5002	1	14,14,15	0.35	0	17,19,21	1.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	5001	-	14,14,15	0.24	0	17,19,21	0.78	0
8	NAG	A	5001	-	14,14,15	0.23	0	17,19,21	0.90	1 (5%)
8	NAG	A	5002	1	14,14,15	0.33	0	17,19,21	1.14	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
8	NAG	B	5002	1	-	0/6/23/26	0/1/1/1
8	NAG	B	5001	-	-	3/6/23/26	0/1/1/1
8	NAG	A	5001	-	-	5/6/23/26	0/1/1/1
8	NAG	A	5002	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	5002	NAG	O5-C1-C2	-3.36	106.09	111.29
8	A	5002	NAG	C4-C3-C2	-2.44	107.45	111.02
8	A	5002	NAG	O5-C1-C2	-2.33	107.69	111.29
8	B	5002	NAG	C4-C3-C2	-2.23	107.75	111.02
8	B	5002	NAG	C2-N2-C7	-2.19	119.97	122.90
8	A	5001	NAG	C1-C2-N2	-2.15	107.04	110.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	5001	NAG	C3-C2-N2-C7
8	A	5001	NAG	C8-C7-N2-C2
8	A	5001	NAG	O7-C7-N2-C2
8	A	5002	NAG	C1-C2-N2-C7
8	A	5002	NAG	C8-C7-N2-C2
8	A	5002	NAG	O7-C7-N2-C2
8	B	5001	NAG	C8-C7-N2-C2
8	B	5001	NAG	O7-C7-N2-C2
8	B	5001	NAG	C3-C2-N2-C7
8	A	5001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	5001	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	5001	NAG	6	0
8	A	5001	NAG	5	0
8	A	5002	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.

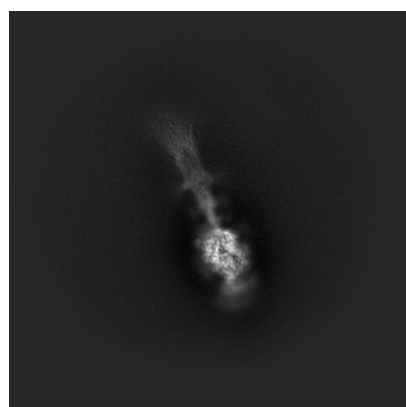
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13896. These allow visual inspection of the internal detail of the map and identification of artifacts.

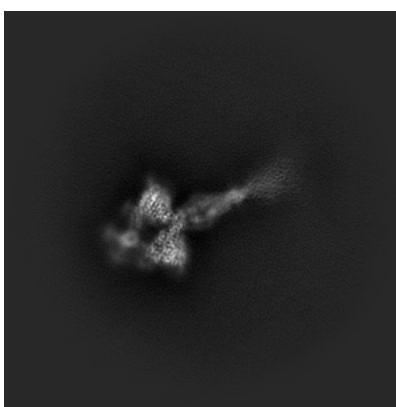
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

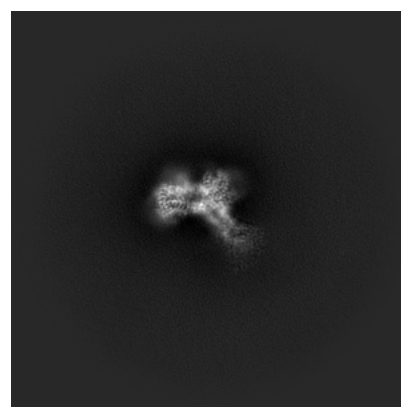
6.1.1 Primary map



X



Y



Z

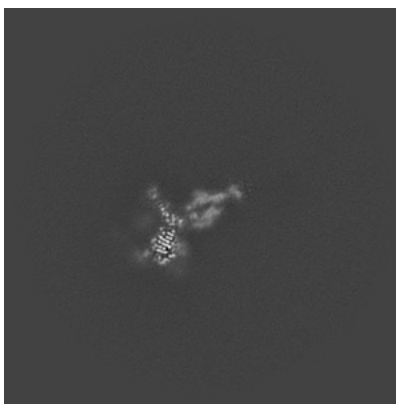
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

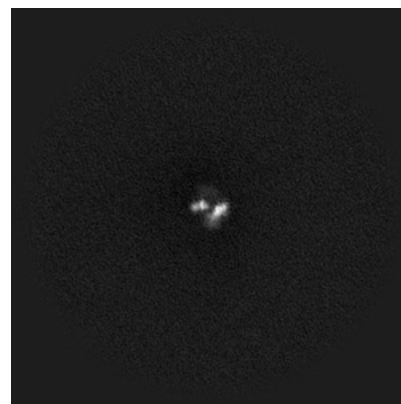
6.2.1 Primary map



X Index: 288



Y Index: 288

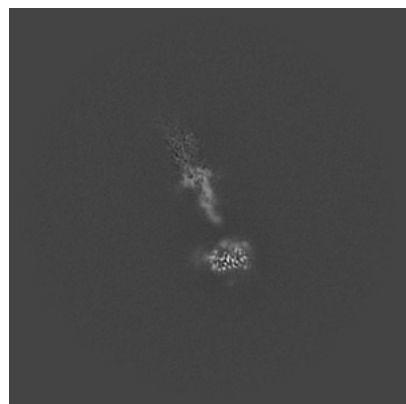


Z Index: 288

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

6.3 Largest variance slices [i](#)

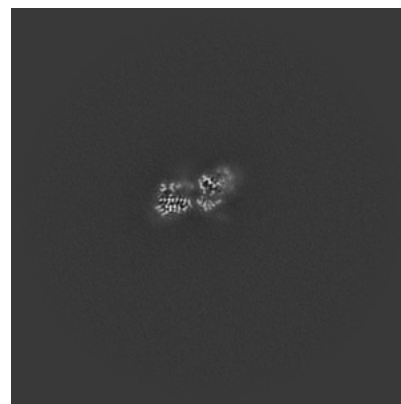
6.3.1 Primary map



X Index: 305



Y Index: 300

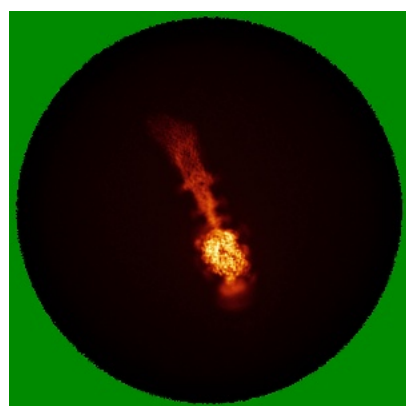


Z Index: 230

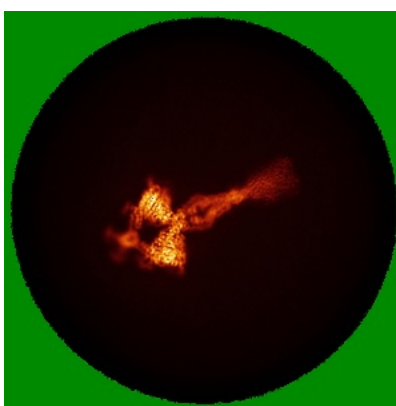
The images above show the largest variance slices of the map in three orthogonal directions.

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

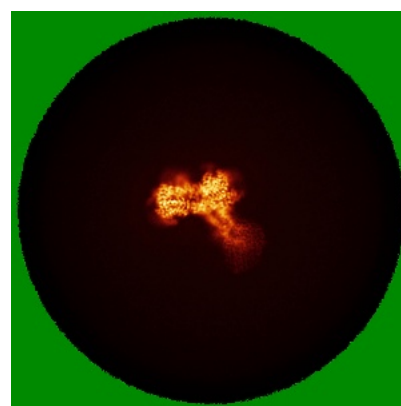
6.4.1 Primary map



X



Y

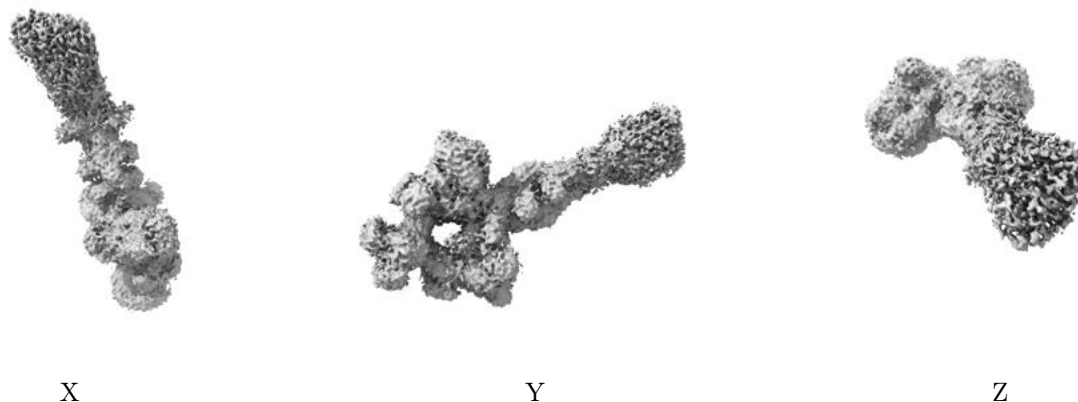


Z

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

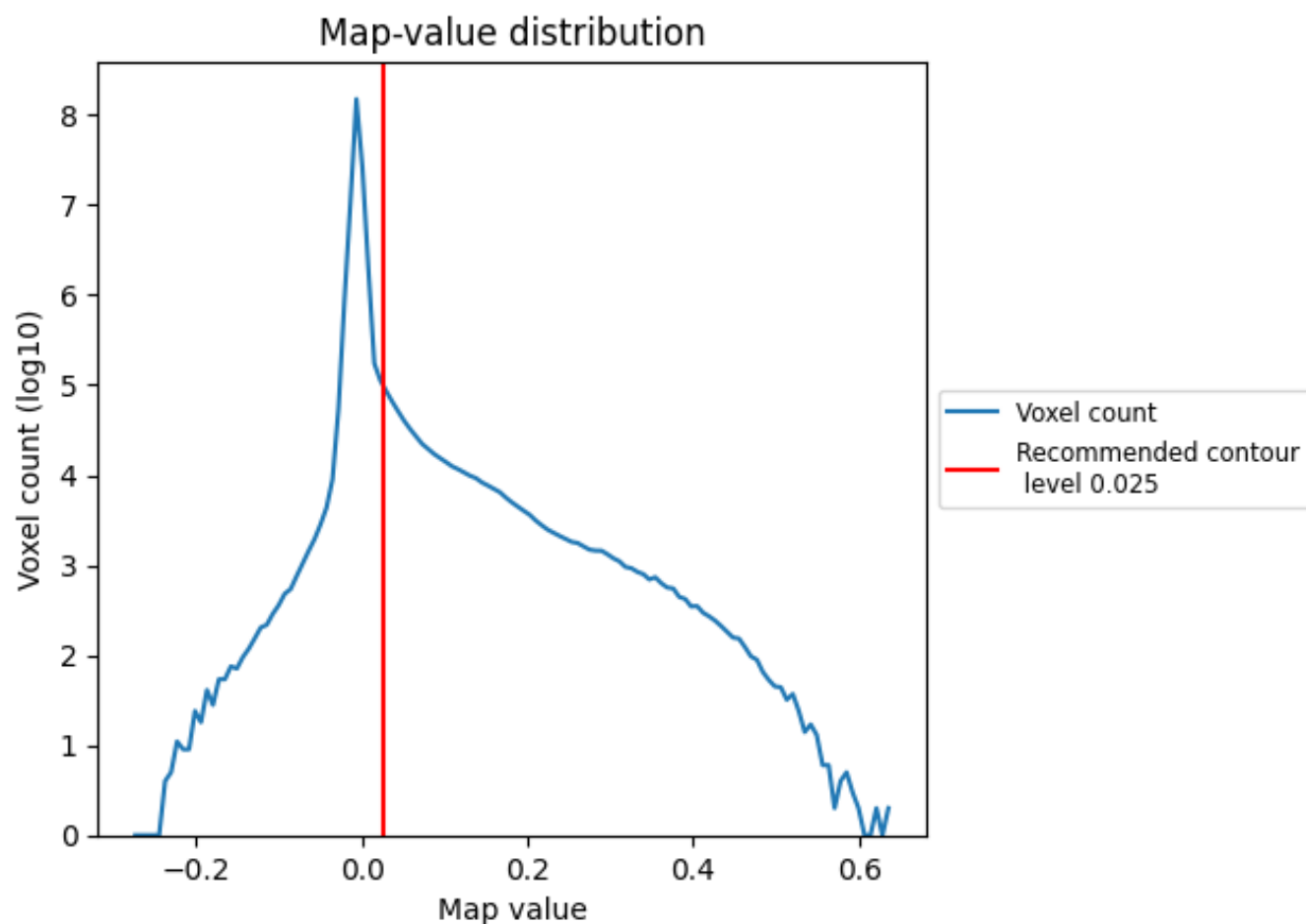
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

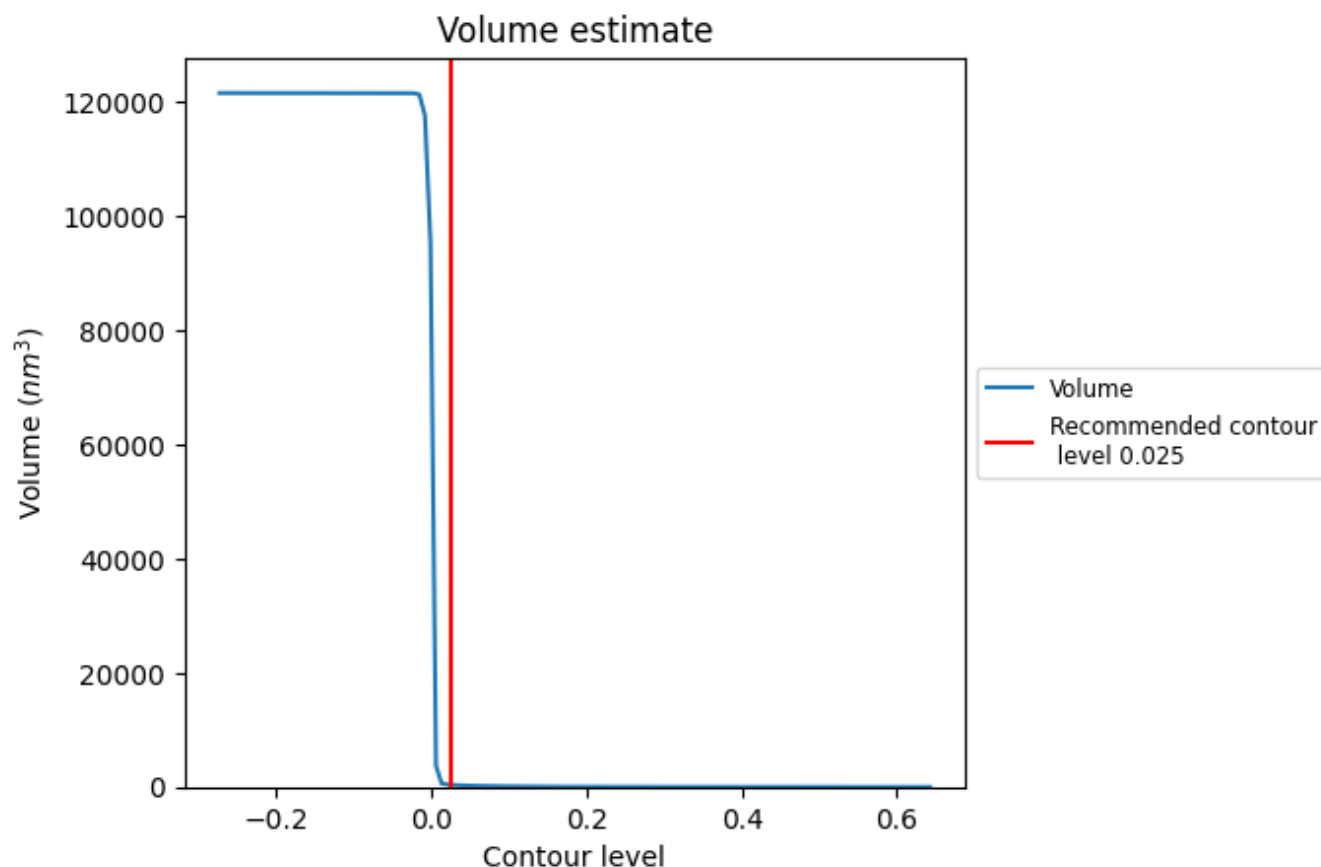
This section contains the results of statistical analysis of the map.

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.

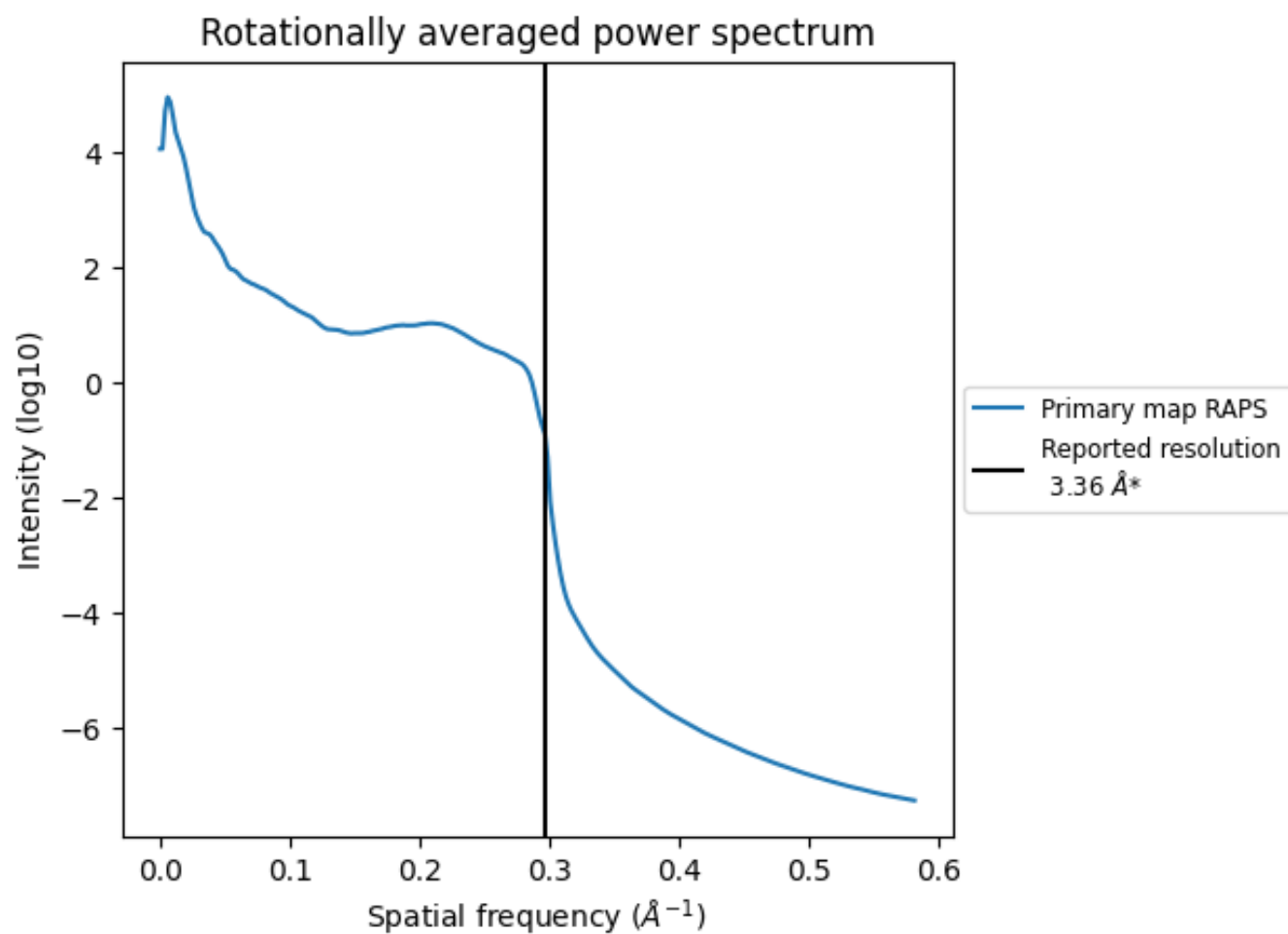
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 387 nm³; this corresponds to an approximate mass of 350 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 0.298 Å⁻¹

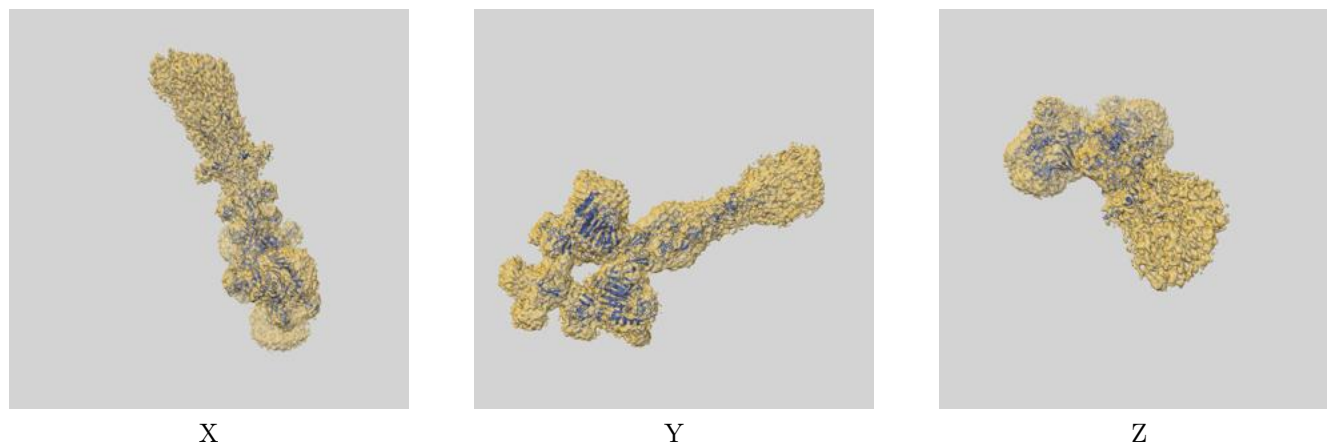
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

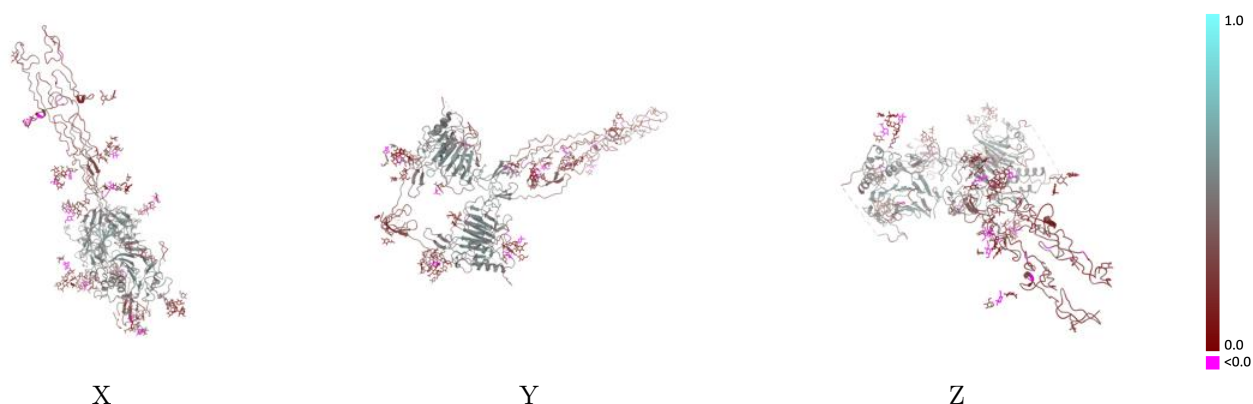
This section contains information regarding the fit between EMDB map EMD-13896 and PDB model 7QCL. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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](#)

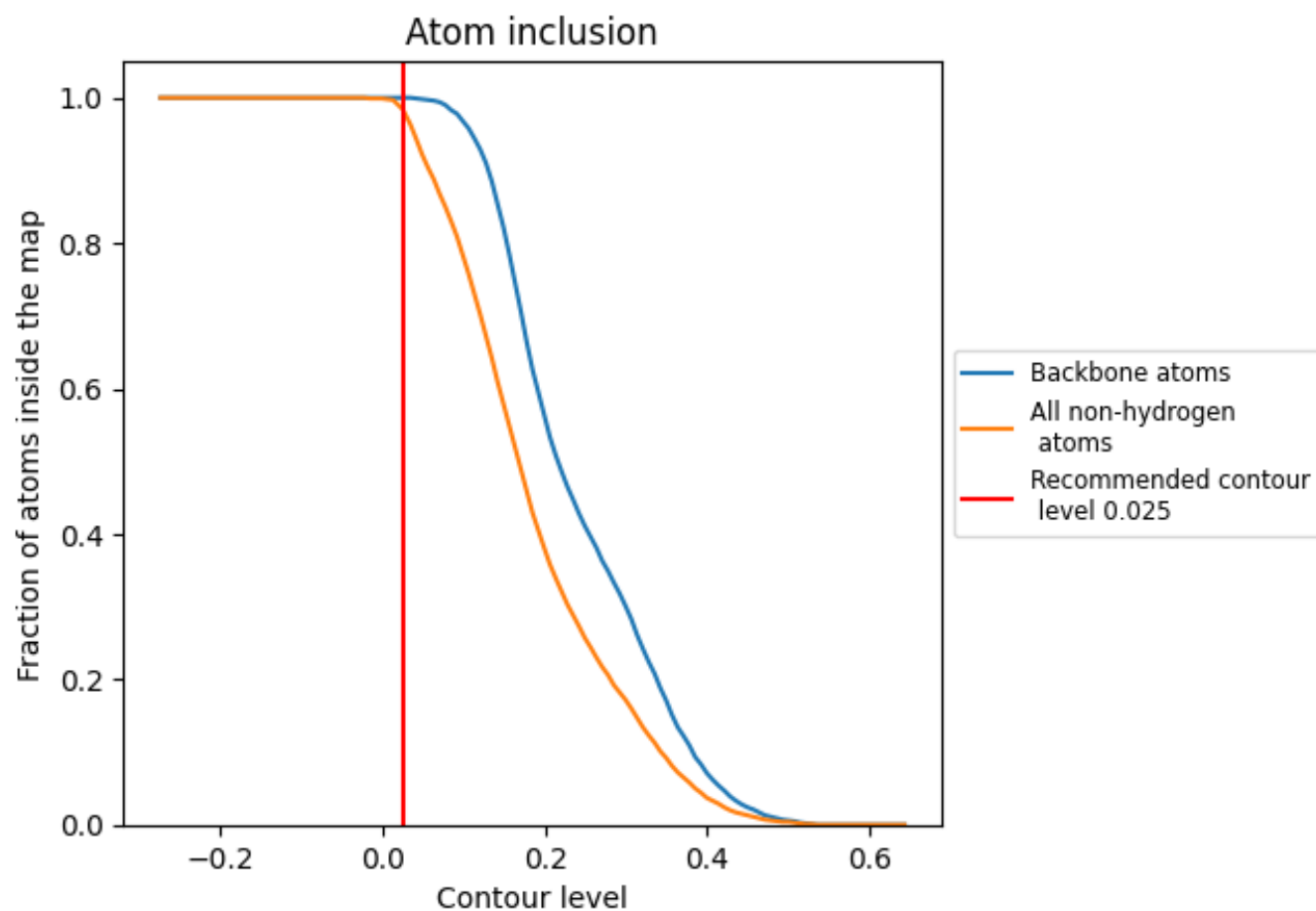


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9840	 0.3620
A	 0.9950	 0.3990
B	 0.9980	 0.4040
C	 0.8930	 0.1560
D	 0.9940	 0.1640
E	 0.7140	 0.0950
F	 0.9420	 0.1420
G	 0.8510	 0.0610
H	 0.9640	 0.2150
I	 0.8330	 0.1270
J	 0.8760	 0.1020
K	 0.8920	 0.1150
L	 0.9090	 0.1580
M	 0.7350	 0.1590
N	 0.8780	 0.1270
O	 0.9660	 0.1510
Q	 0.9840	 0.1030

