



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:35 PM EDT

PDB ID : 6TJY / pdb_00006tjy
Title : Crystal structure of haemagglutinin from (A/seal/Germany/1/2014) seal H10N7 influenza virus
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on : 2019-11-27
Resolution : 2.82 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

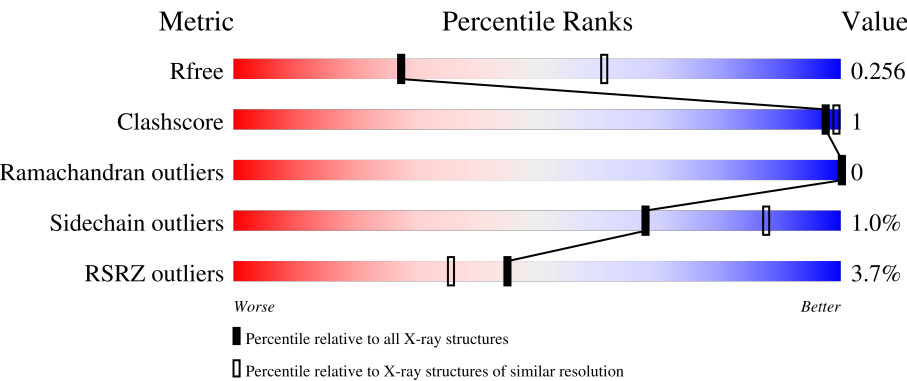
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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.



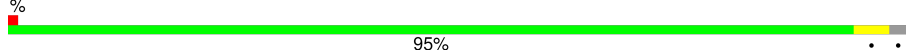
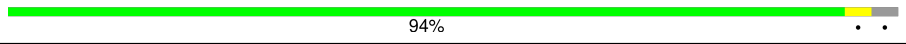
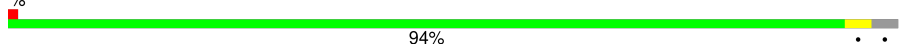
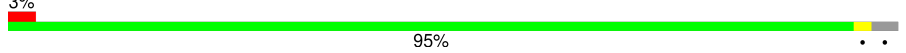
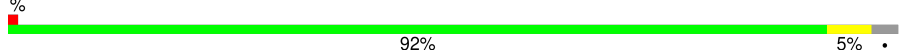
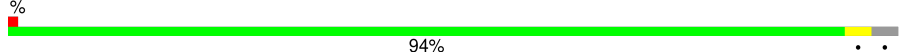
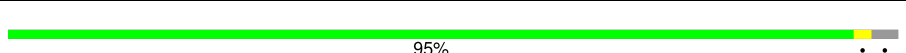
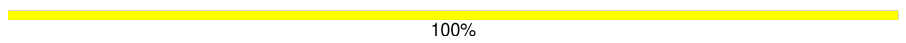
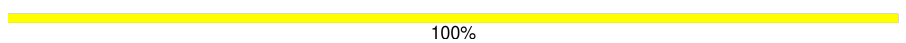
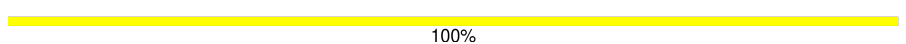
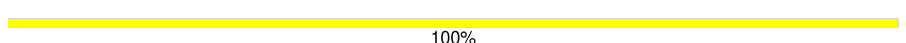
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	98% ..
1	C	325	4% 96% ..
1	E	325	4% 95% ..
1	G	325	18% 92% 5% .
1	I	325	4% 97% ..

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Mol	Chain	Length	Quality of chain
1	K	325	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	M	3	
4	N	2	
4	O	2	
4	P	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	1	0
			2446	1516	444	470	16			
1	C	320	Total	C	N	O	S	0	0	0
			2417	1501	437	463	16			
1	E	320	Total	C	N	O	S	0	1	0
			2423	1507	439	461	16			
1	G	317	Total	C	N	O	S	0	0	0
			2289	1411	420	442	16			
1	I	320	Total	C	N	O	S	0	1	0
			2411	1498	432	465	16			
1	K	320	Total	C	N	O	S	0	1	0
			2448	1518	444	470	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	219	GLN	LEU	conflict	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	219	GLN	LEU	conflict	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
E	219	GLN	LEU	conflict	UNP A0A0A7HR51
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
G	219	GLN	LEU	conflict	UNP A0A0A7HR51
I	-1	ASP	-	expression tag	UNP A0A0A7HR51
I	0	PRO	-	expression tag	UNP A0A0A7HR51
I	219	GLN	LEU	conflict	UNP A0A0A7HR51
K	-1	ASP	-	expression tag	UNP A0A0A7HR51
K	0	PRO	-	expression tag	UNP A0A0A7HR51

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Chain	Residue	Modelled	Actual	Comment	Reference
K	219	GLN	LEU	conflict	UNP A0A0A7HR51

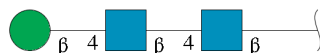
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	H	172	Total	C	N	O	S	0	0	0
			1379	854	240	277	8			
2	J	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	L	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HNL0
D	177	LYS	-	expression tag	UNP A0A0A7HNL0
F	177	LYS	-	expression tag	UNP A0A0A7HNL0
H	177	LYS	-	expression tag	UNP A0A0A7HNL0
J	177	LYS	-	expression tag	UNP A0A0A7HNL0
L	177	LYS	-	expression tag	UNP A0A0A7HNL0

- Molecule 3 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					ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O		0	0	0
			39	22	2	15				

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

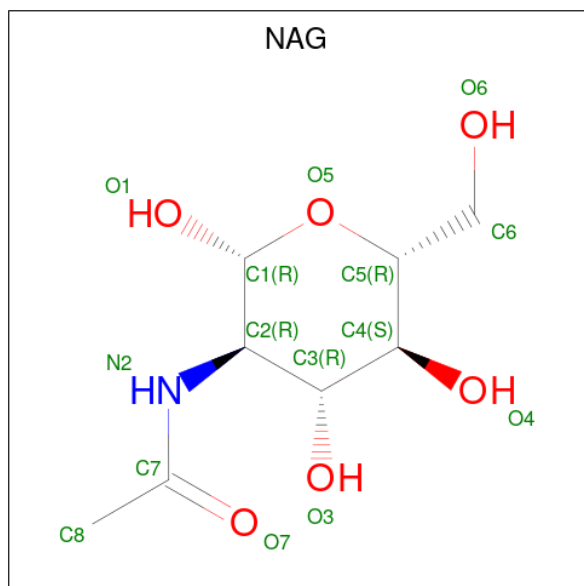


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

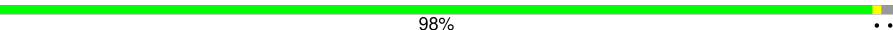
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	54	Total	O	0	0
			54	54		
7	B	31	Total	O	0	0
			31	31		
7	C	52	Total	O	0	0
			52	52		
7	D	59	Total	O	0	0
			59	59		
7	E	22	Total	O	0	0
			22	22		
7	F	38	Total	O	0	0
			38	38		
7	G	17	Total	O	0	0
			17	17		
7	H	40	Total	O	0	0
			40	40		
7	I	11	Total	O	0	0
			11	11		
7	J	30	Total	O	0	0
			30	30		
7	K	98	Total	O	0	0
			98	98		
7	L	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

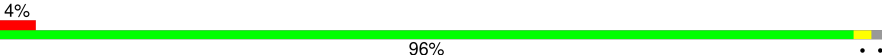
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Hemagglutinin HA1

Chain A:  98% ..

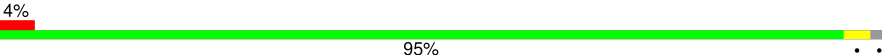


- Molecule 1: Hemagglutinin HA1

Chain C:  96% ..

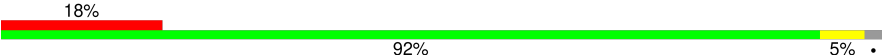


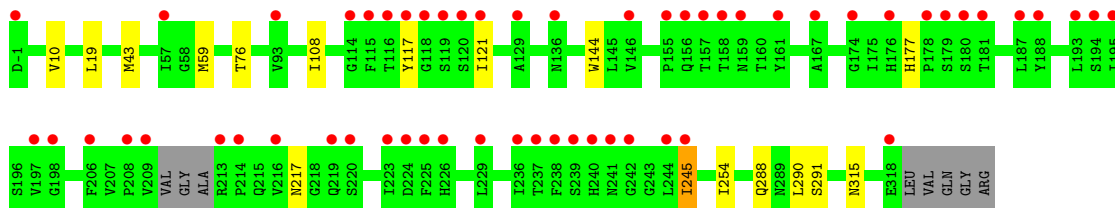
- Molecule 1: Hemagglutinin HA1

Chain E:  95% ..

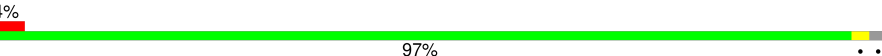


- Molecule 1: Hemagglutinin HA1

Chain G:  92% 5% .



- Molecule 1: Hemagglutinin HA1

Chain I:  97% ..



- Molecule 1: Hemagglutinin HA1



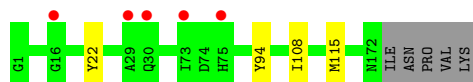
- Molecule 2: Hemagglutinin HA2



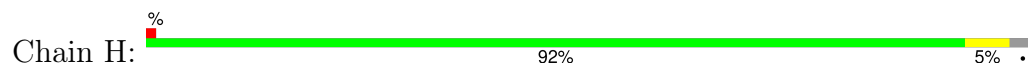
- Molecule 2: Hemagglutinin HA2



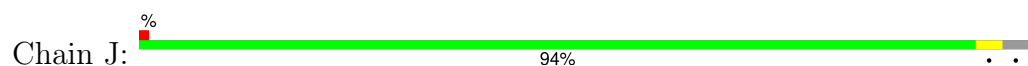
- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2

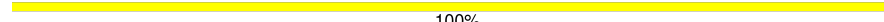


- Molecule 2: Hemagglutinin HA2

Chain L:  95% . .

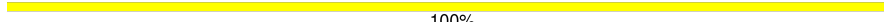


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

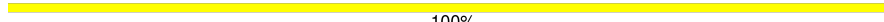


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

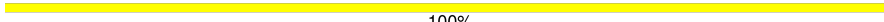


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



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

Chain P:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.42Å 212.93Å 156.90Å 90.00° 101.51° 90.00°	Depositor
Resolution (Å)	35.04 – 2.82 35.04 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.04-2.82) 98.1 (35.04-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.216 , 0.257 0.216 , 0.256	Depositor DCC
R_{free} test set	5255 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23432	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5657e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: BMA, CA, 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	0.51	0/2499	0.68	0/3385
1	C	0.52	0/2467	0.70	0/3346
1	E	0.54	0/2476	0.72	0/3356
1	G	0.57	0/2335	0.75	0/3174
1	I	0.55	0/2464	0.71	0/3342
1	K	0.52	0/2501	0.69	0/3388
2	B	0.51	0/1411	0.77	0/1903
2	D	0.52	0/1411	0.77	0/1903
2	F	0.51	0/1411	0.79	0/1903
2	H	0.50	0/1404	0.77	0/1894
2	J	0.51	0/1411	0.79	0/1903
2	L	0.50	0/1411	0.78	0/1903
All	All	0.53	0/23201	0.74	0/31400

There are no bond length outliers.

There are no bond angle outliers.

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	2446	0	2400	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2417	0	2346	2	0
1	E	2423	0	2357	6	0
1	G	2289	0	2091	9	0
1	I	2411	0	2341	1	0
1	K	2448	0	2407	7	0
2	B	1386	0	1290	4	0
2	D	1386	0	1291	3	0
2	F	1386	0	1291	4	0
2	H	1379	0	1283	5	0
2	J	1386	0	1292	3	0
2	L	1386	0	1291	2	0
3	M	39	0	34	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	B	28	0	26	0	0
6	C	14	0	13	0	0
6	G	14	0	13	0	0
6	J	14	0	13	0	0
7	A	54	0	0	0	0
7	B	31	0	0	0	0
7	C	52	0	0	0	0
7	D	59	0	0	0	0
7	E	22	0	0	0	0
7	F	38	0	0	0	0
7	G	17	0	0	0	0
7	H	40	0	0	0	0
7	I	11	0	0	0	0
7	J	30	0	0	0	0
7	K	98	0	0	0	0
7	L	41	0	0	0	0
All	All	23432	0	21854	37	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 1.

All (37) 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:E:43:MET:HE1	1:E:76:THR:HG21	1.70	0.72
1:G:144:TRP:HA	1:G:245:ILE:HG22	1.74	0.69
1:G:10:VAL:H	1:G:315:ASN:HD21	1.47	0.61
2:B:55:ILE:HG23	2:B:99:LEU:HD21	1.83	0.60
2:B:99:LEU:HD22	2:H:94:TYR:OH	2.02	0.60
1:G:43:MET:HE1	1:G:76:THR:HG21	1.84	0.57
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.37	0.57
1:G:59:MET:HE3	1:G:108:ILE:CD1	2.34	0.56
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.39	0.56
1:E:157:THR:HG23	1:E:240:HIS:CE1	2.44	0.53
1:G:59:MET:HE3	1:G:108:ILE:HD12	1.90	0.53
2:D:94:TYR:OH	2:L:99:LEU:HD22	2.09	0.52
1:E:56:PRO:HA	1:E:59:MET:HE2	1.95	0.49
2:H:6:ILE:HD12	2:H:112:ASP:HA	1.94	0.48
1:K:48:HIS:HE1	1:K:268:ASN:HD21	1.61	0.48
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.95	0.47
1:K:159:ASN:HD22	1:K:240:HIS:HE1	1.61	0.47
1:G:117:TYR:HB3	1:G:121:ILE:HG21	1.95	0.47
1:C:205:ASN:HB2	1:E:209:VAL:HG23	1.97	0.46
2:D:99:LEU:HD22	2:F:94:TYR:OH	2.16	0.46
1:E:314:ARG:HG3	2:F:108:ILE:HG23	1.97	0.46
2:F:22:TYR:CD1	2:F:115:MET:HE2	2.52	0.45
1:G:19:LEU:HB2	2:H:105:GLN:HE21	1.82	0.44
1:K:48:HIS:CE1	1:K:268:ASN:HD21	2.35	0.44
2:H:99:LEU:HD22	2:J:94:TYR:OH	2.17	0.43
1:K:281:ILE:HG22	1:K:283:THR:HG22	2.00	0.43
2:B:94:TYR:OH	2:J:99:LEU:HD22	2.18	0.43
1:G:288:GLN:HE21	1:G:290:LEU:H	1.67	0.43
1:K:101:LYS:HE2	1:K:229:LEU:HD11	2.00	0.43
1:E:7:HIS:HB3	2:F:115:MET:CE	2.49	0.43
1:I:281:ILE:HG22	1:I:283:THR:HG22	2.00	0.43
1:K:63:THR:HG22	1:K:64:PRO:HD2	2.02	0.42
1:K:5:LEU:HD13	2:L:119:TYR:HA	2.01	0.41
2:H:74:ASP:HB3	2:H:77:ILE:HG22	2.02	0.41
1:A:113:THR:HG21	1:A:247:PRO:O	2.20	0.41
1:C:100:GLN:HE21	1:C:104:GLU:HG3	1.86	0.41
1:G:288:GLN:NE2	1:G:291:SER:H	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	319/325 (98%)	311 (98%)	8 (2%)	0	100	100
1	C	318/325 (98%)	306 (96%)	12 (4%)	0	100	100
1	E	319/325 (98%)	307 (96%)	12 (4%)	0	100	100
1	G	313/325 (96%)	299 (96%)	14 (4%)	0	100	100
1	I	319/325 (98%)	306 (96%)	13 (4%)	0	100	100
1	K	319/325 (98%)	309 (97%)	10 (3%)	0	100	100
2	B	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	D	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	F	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	H	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
2	J	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	L	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
All	All	2927/3012 (97%)	2822 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	270/275 (98%)	269 (100%)	1 (0%)	84	94
1	C	262/275 (95%)	257 (98%)	5 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	260/275 (94%)	258 (99%)	2 (1%)	73	90
1	G	226/275 (82%)	222 (98%)	4 (2%)	51	80
1	I	262/275 (95%)	259 (99%)	3 (1%)	65	86
1	K	271/275 (98%)	270 (100%)	1 (0%)	84	94
2	B	146/151 (97%)	145 (99%)	1 (1%)	76	91
2	D	146/151 (97%)	145 (99%)	1 (1%)	76	91
2	F	146/151 (97%)	146 (100%)	0	100	100
2	H	144/151 (95%)	142 (99%)	2 (1%)	59	84
2	J	146/151 (97%)	144 (99%)	2 (1%)	59	84
2	L	146/151 (97%)	145 (99%)	1 (1%)	76	91
All	All	2425/2556 (95%)	2402 (99%)	23 (1%)	68	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
2	B	133	ASP
1	C	14	THR
1	C	22	GLU
1	C	148	LYS
1	C	205	ASN
1	C	219	GLN
2	D	32	THR
1	E	20	THR
1	E	244	LEU
1	G	177	HIS
1	G	217	ASN
1	G	245	ILE
1	G	254	ILE
2	H	113	SER
2	H	171	LEU
1	I	148	LYS
1	I	235	LYS
1	I	251	SER
2	J	30	GLN
2	J	95	GLN
1	K	203	LYS
2	L	95	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	39	ASN
1	A	48	HIS
1	A	53	ASN
1	A	185	ASN
1	A	205	ASN
1	A	231	GLN
2	B	27	GLN
2	B	105	GLN
2	B	125	GLN
1	C	23	GLN
1	C	48	HIS
1	C	94	ASN
1	C	100	GLN
1	C	191	GLN
1	C	205	ASN
1	C	268	ASN
1	C	297	GLN
2	D	159	HIS
1	E	23	GLN
1	E	69	HIS
1	E	100	GLN
1	E	231	GLN
1	E	240	HIS
1	E	241	ASN
1	E	282	ASN
1	E	303	ASN
2	F	30	GLN
2	F	95	GLN
2	F	106	HIS
1	G	48	HIS
1	G	159	ASN
1	G	268	ASN
1	G	288	GLN
1	G	289	ASN
1	G	315	ASN
2	H	47	GLN
2	H	95	GLN
2	H	105	GLN
2	H	161	GLN
2	H	169	ASN

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Mol	Chain	Res	Type
1	I	39	ASN
1	I	48	HIS
1	I	53	ASN
1	I	100	GLN
1	I	149	ASN
1	I	153	ASN
1	I	156	GLN
1	I	204	ASN
2	J	95	GLN
1	K	48	HIS
1	K	136	ASN
1	K	149	ASN
1	K	159	ASN
1	K	176	HIS
1	K	268	ASN
1	K	303	ASN
2	L	12	ASN
2	L	30	GLN
2	L	95	GLN
2	L	106	HIS
2	L	169	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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	M	1	5,3,2	14,14,15	0.29	0	17,19,21	1.08	1 (5%)
3	NAG	M	2	3	14,14,15	0.66	0	17,19,21	1.40	1 (5%)
3	BMA	M	3	3	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
4	NAG	N	1	2,4	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
4	NAG	N	2	4	14,14,15	0.33	0	17,19,21	0.75	1 (5%)
4	NAG	O	1	5,2,4	14,14,15	0.46	0	17,19,21	1.08	1 (5%)
4	NAG	O	2	4	14,14,15	0.40	0	17,19,21	1.59	3 (17%)
4	NAG	P	1	5,2,4	14,14,15	0.36	0	17,19,21	1.08	1 (5%)
4	NAG	P	2	4	14,14,15	0.39	0	17,19,21	0.84	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	M	1	5,3,2	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
4	NAG	N	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	5,2,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	5,2,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	2	NAG	C1-O5-C5	5.14	119.07	112.19
3	M	2	NAG	C4-C3-C2	4.32	117.35	111.02
3	M	1	NAG	C1-O5-C5	3.84	117.33	112.19
4	O	1	NAG	C1-O5-C5	2.96	116.15	112.19
4	N	1	NAG	C4-C3-C2	2.40	114.54	111.02
4	N	2	NAG	C1-O5-C5	2.20	115.13	112.19
4	P	1	NAG	C4-C3-C2	2.12	114.13	111.02
4	P	2	NAG	C1-O5-C5	2.12	115.03	112.19
4	O	2	NAG	C4-C3-C2	2.05	114.02	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	2	NAG	C3-C4-C5	2.03	113.91	110.23
3	M	3	BMA	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

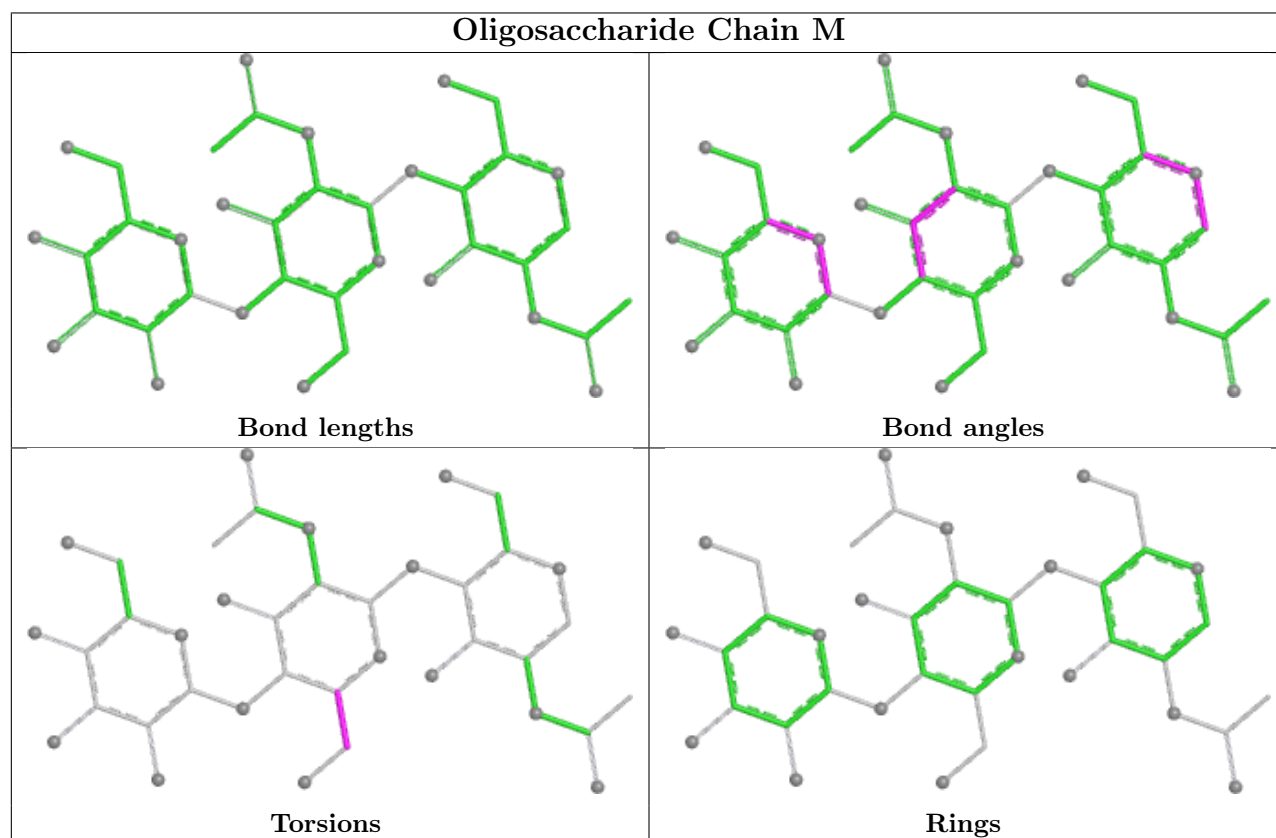
All (4) torsion outliers are listed below:

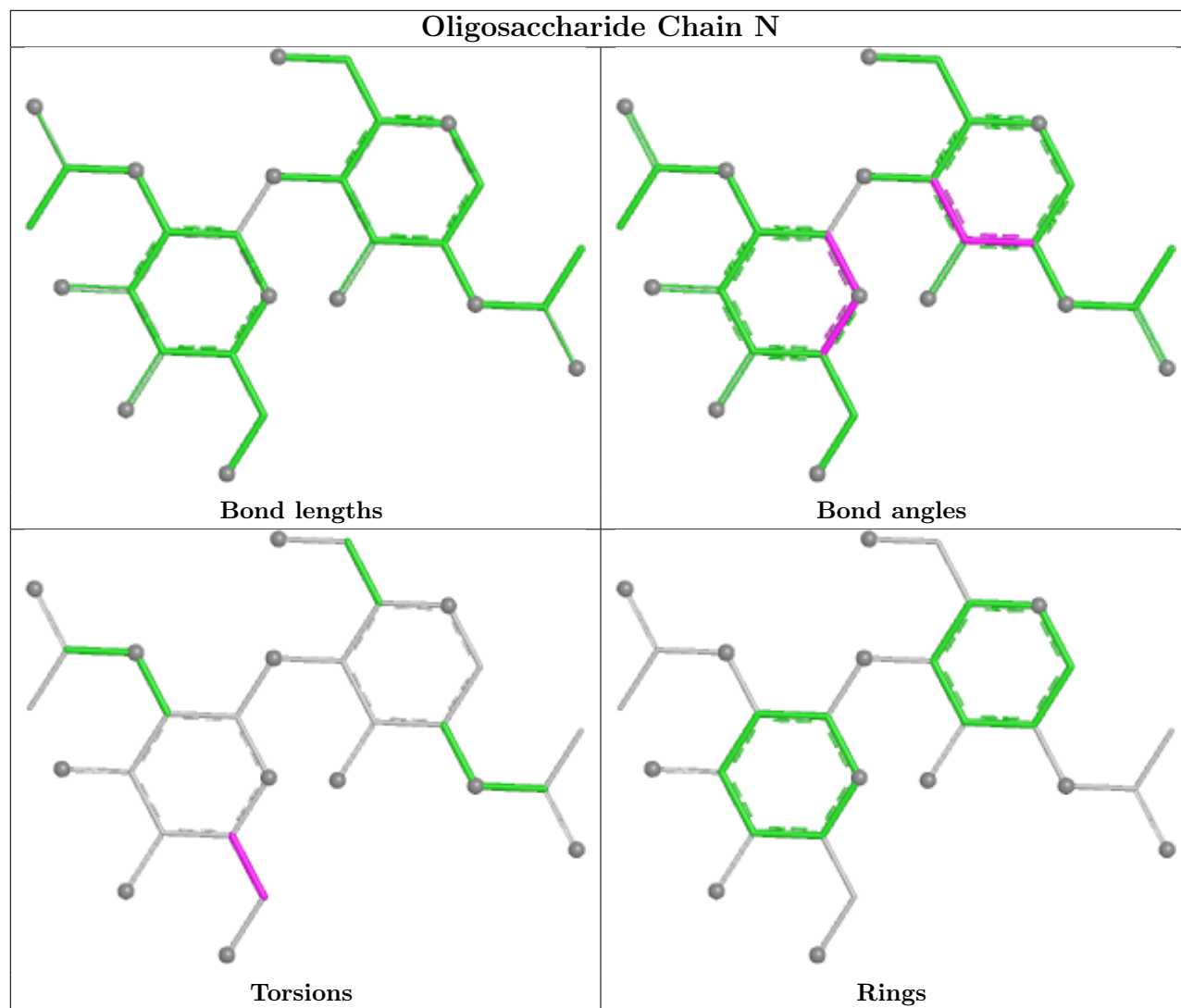
Mol	Chain	Res	Type	Atoms
4	N	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6

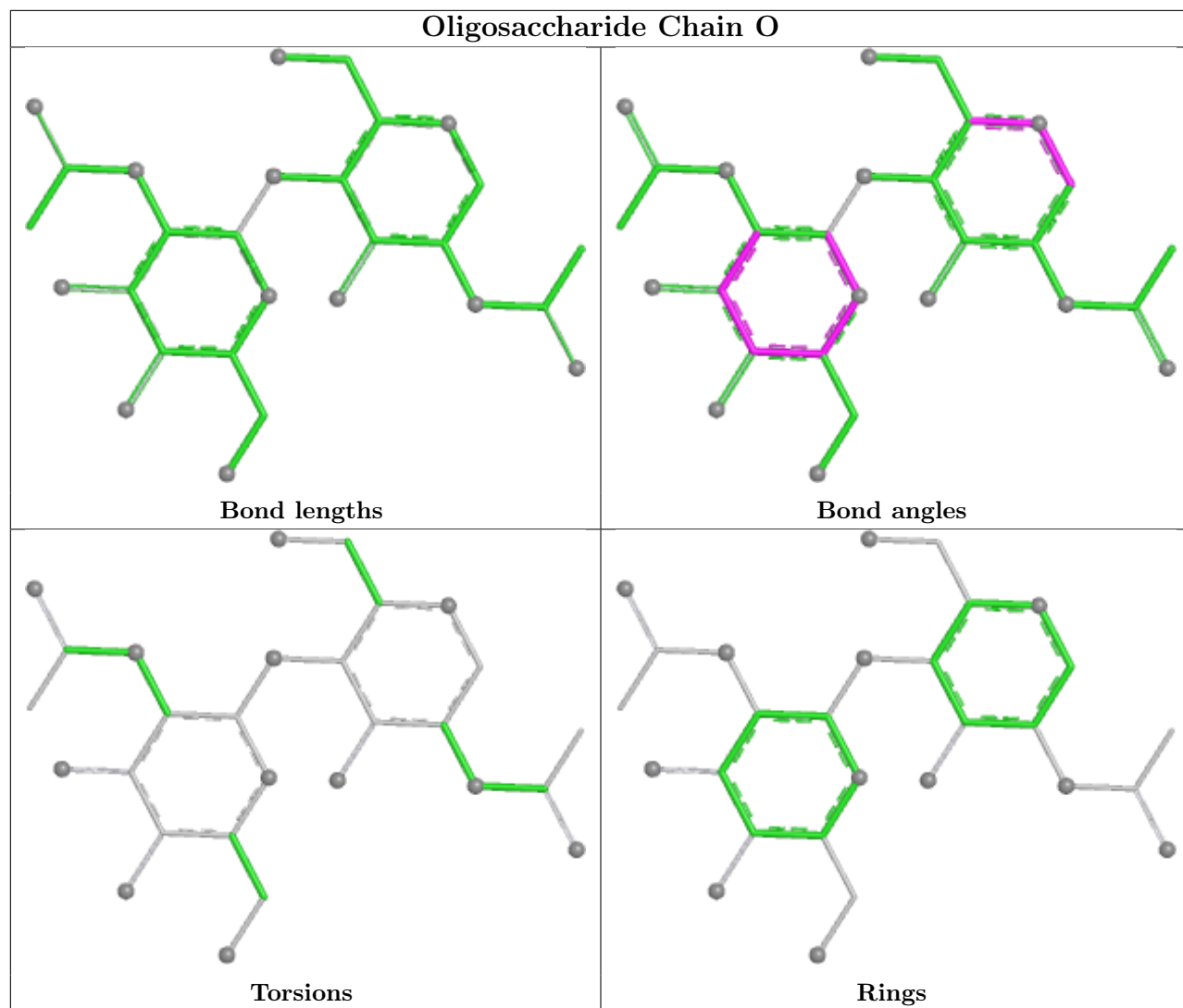
There are no ring outliers.

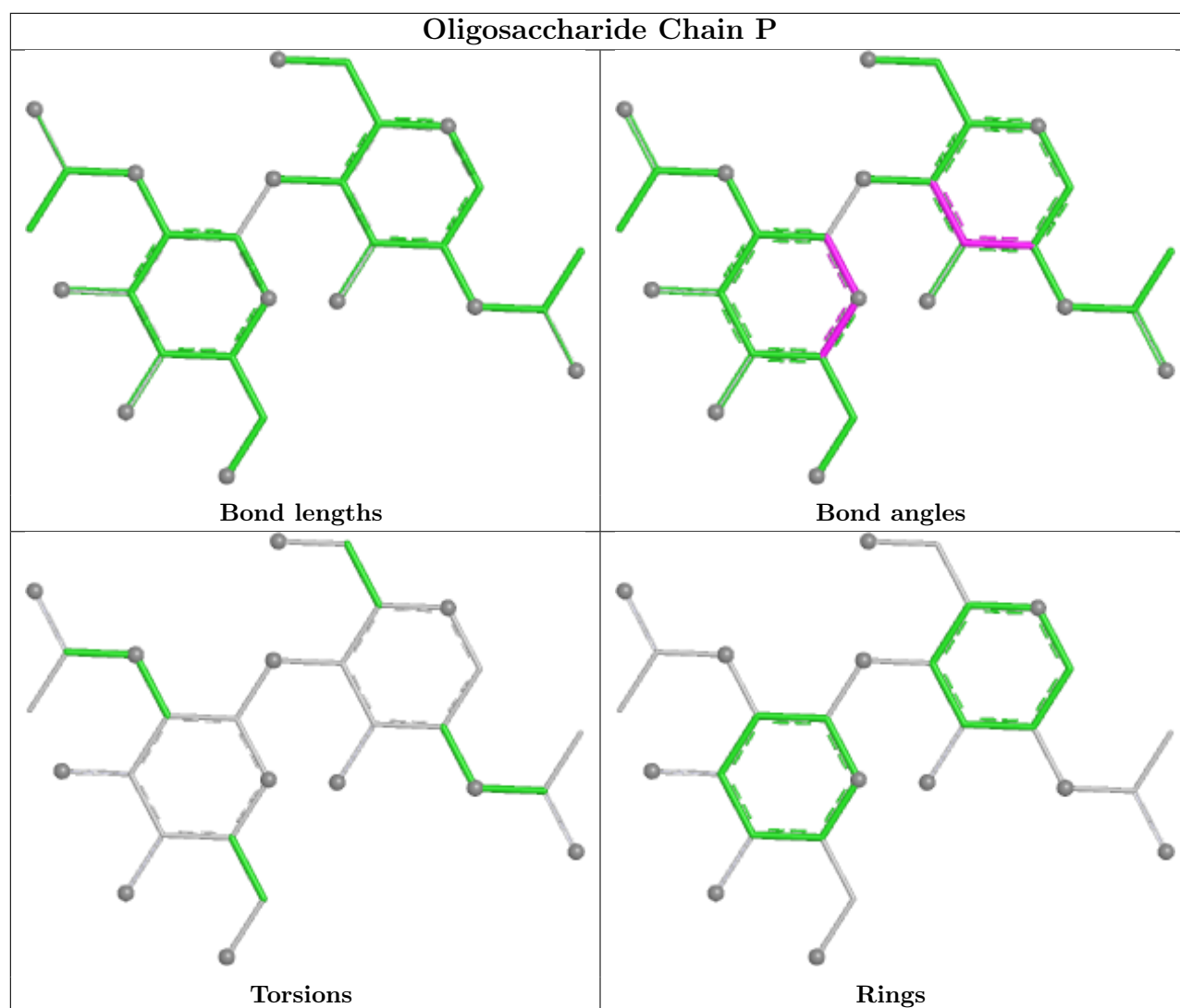
No monomer is involved in short contacts.

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 [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
6	NAG	B	201	2	14,14,15	0.39	0	17,19,21	1.10	0
6	NAG	G	401	1	14,14,15	0.47	0	17,19,21	1.00	1 (5%)
6	NAG	B	202	2	14,14,15	0.57	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	J	201	2	14,14,15	0.41	0	17,19,21	1.01	1 (5%)
6	NAG	C	401	1	14,14,15	0.39	0	17,19,21	1.27	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
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
6	NAG	G	401	1	-	0/6/23/26	0/1/1/1
6	NAG	B	202	2	-	0/6/23/26	0/1/1/1
6	NAG	J	201	2	-	0/6/23/26	0/1/1/1
6	NAG	C	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	401	NAG	C1-O5-C5	4.06	117.63	112.19
6	J	201	NAG	C1-O5-C5	3.23	116.52	112.19
6	G	401	NAG	C1-O5-C5	2.89	116.06	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	NAG	C3-C2-N2-C7
6	C	401	NAG	C1-C2-N2-C7
6	B	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/325 (98%)	0.00	1 (0%) 90 86	38, 58, 87, 94	1 (0%)
1	C	320/325 (98%)	0.20	12 (3%) 44 35	38, 64, 107, 118	0
1	E	320/325 (98%)	0.42	13 (4%) 41 32	46, 77, 110, 123	1 (0%)
1	G	317/325 (97%)	1.00	57 (17%) 3 2	42, 89, 138, 173	0
1	I	320/325 (98%)	0.60	14 (4%) 39 30	50, 81, 127, 151	1 (0%)
1	K	320/325 (98%)	-0.15	4 (1%) 75 66	34, 54, 74, 85	1 (0%)
2	B	172/177 (97%)	-0.09	0 100 100	42, 59, 85, 92	0
2	D	172/177 (97%)	-0.21	1 (0%) 85 80	35, 53, 68, 84	0
2	F	172/177 (97%)	0.15	5 (2%) 53 43	40, 62, 86, 106	0
2	H	172/177 (97%)	-0.09	2 (1%) 76 68	38, 56, 76, 99	0
2	J	172/177 (97%)	0.01	1 (0%) 85 80	45, 62, 80, 99	0
2	L	172/177 (97%)	-0.09	0 100 100	40, 55, 80, 88	0
All	All	2949/3012 (97%)	0.20	110 (3%) 45 36	34, 64, 112, 173	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	197	VAL	5.3
1	G	93	VAL	4.5
1	G	156	GLN	4.4
1	G	188	TYR	4.3
1	G	178	PRO	4.3
1	G	157	THR	4.2
1	G	119	SER	4.1
1	E	133	ASN	4.1
1	G	114	GLY	4.0
1	G	116	THR	4.0
1	G	158	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	179	SER	3.9
1	G	241	ASN	3.9
1	C	214	PRO	3.8
1	G	245	ILE	3.4
2	F	29	ALA	3.4
2	H	172	ASN	3.3
1	G	209	VAL	3.3
1	G	214	PRO	3.2
1	C	216	VAL	3.2
1	G	180	SER	3.2
1	G	244	LEU	3.2
1	G	120	SER	3.2
1	G	224	ASP	3.1
1	I	-1	ASP	3.0
2	F	30	GLN	3.0
1	G	206	PHE	3.0
1	I	271	GLU	3.0
1	C	217	ASN	2.9
1	K	-1	ASP	2.9
1	G	237	THR	2.9
1	G	174	GLY	2.9
1	G	117	TYR	2.9
1	G	195	ILE	2.9
1	I	243	GLY	2.9
1	G	155	PRO	2.9
1	E	120	SER	2.9
1	G	187	LEU	2.9
1	I	210	VAL	2.8
1	I	40	ARG	2.8
2	D	164	GLU	2.8
1	G	-1	ASP	2.8
1	C	119	SER	2.8
1	C	176	HIS	2.7
1	C	181	THR	2.7
1	G	240	HIS	2.7
1	E	146	VAL	2.7
1	G	146	VAL	2.7
2	J	73	ILE	2.6
1	G	216	VAL	2.6
1	G	176	HIS	2.6
1	E	138	PHE	2.6
1	G	239	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	242	GLY	2.6
1	G	229	LEU	2.6
1	G	121	ILE	2.6
1	G	208	PRO	2.5
1	G	238	PHE	2.5
1	C	39	ASN	2.4
1	G	136	ASN	2.4
1	E	121	ILE	2.4
1	K	278	GLY	2.4
1	G	220	SER	2.4
1	I	139	TYR	2.4
1	G	193	LEU	2.4
1	G	318	GLU	2.4
1	G	225	PHE	2.3
1	E	-1	ASP	2.3
1	C	187	LEU	2.3
1	G	118	GLY	2.3
1	G	242	GLY	2.3
1	I	211	GLY	2.3
1	C	270	CYS	2.3
1	E	181	THR	2.3
1	E	129	ALA	2.2
1	I	91	ALA	2.2
1	I	41	LEU	2.2
1	G	57	ILE	2.2
1	E	150	LYS	2.2
1	G	226	HIS	2.2
1	I	215	GLN	2.2
2	F	75	HIS	2.2
1	G	161	TYR	2.2
1	G	198	GLY	2.2
1	I	318	GLU	2.2
1	C	213	ARG	2.2
1	G	236	ILE	2.2
1	C	282	ASN	2.2
1	G	194	SER	2.2
1	G	129	ALA	2.2
1	I	159	ASN	2.1
1	A	-1	ASP	2.1
1	G	181	THR	2.1
1	G	115	PHE	2.1
1	G	223	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	167	ALA	2.1
1	E	119	SER	2.1
1	E	192	SER	2.1
1	E	117	TYR	2.1
2	F	73	ILE	2.1
1	I	125	GLY	2.1
1	G	213	ARG	2.1
1	G	219	GLN	2.0
1	G	159	ASN	2.0
1	C	224	ASP	2.0
2	H	73	ILE	2.0
1	I	124	ALA	2.0
1	E	208	PRO	2.0
1	K	270	CYS	2.0
2	F	16	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

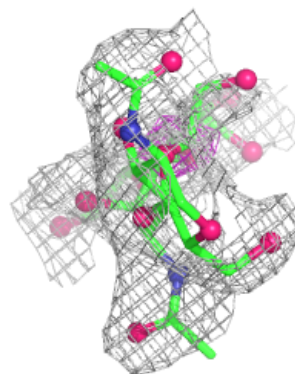
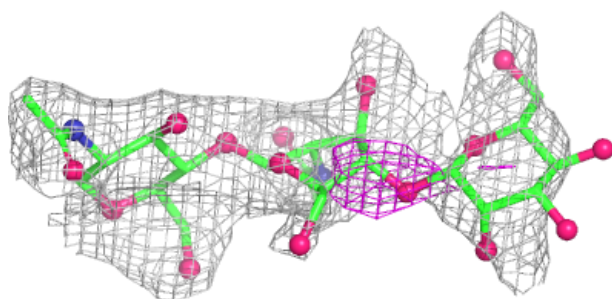
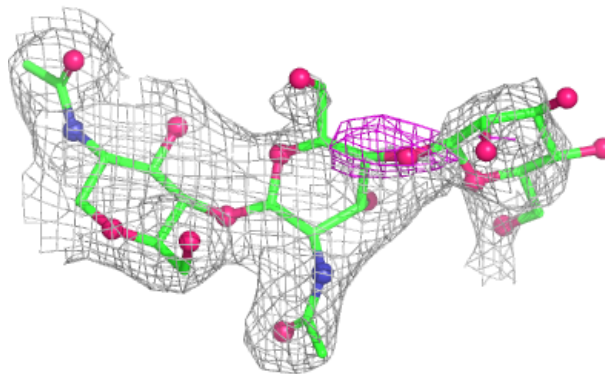
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	M	3	11/12	0.38	0.16	112,120,124,126	0
4	NAG	P	2	14/15	0.62	0.17	113,119,122,122	0
4	NAG	N	1	14/15	0.70	0.13	101,107,112,120	0
4	NAG	P	1	14/15	0.78	0.12	86,94,98,108	0
3	NAG	M	2	14/15	0.81	0.13	79,93,103,113	0
4	NAG	N	2	14/15	0.81	0.14	117,126,130,133	0
4	NAG	O	2	14/15	0.84	0.11	85,92,97,98	0
4	NAG	O	1	14/15	0.94	0.07	57,63,69,77	0
3	NAG	M	1	14/15	0.95	0.08	61,63,68,76	0

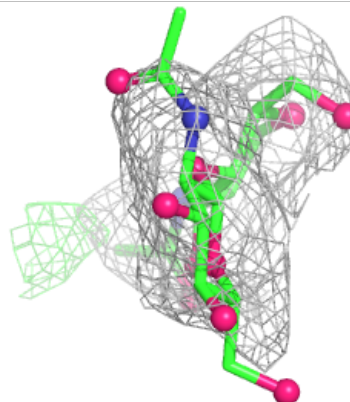
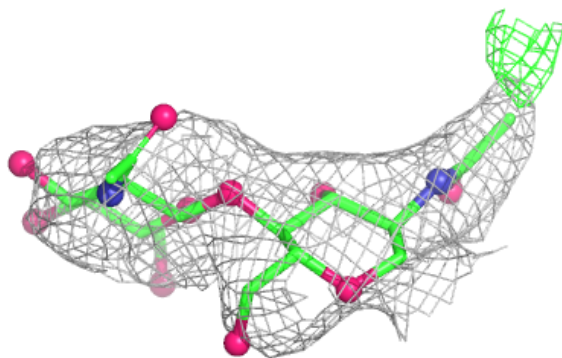
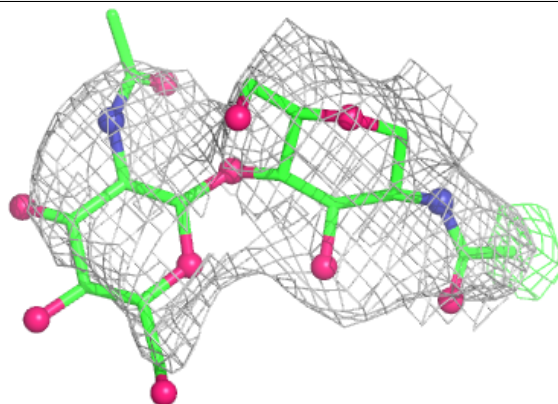
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

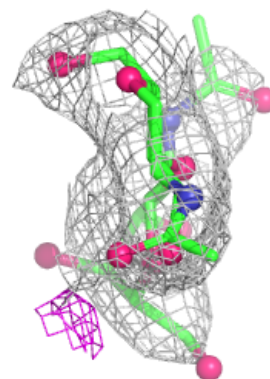
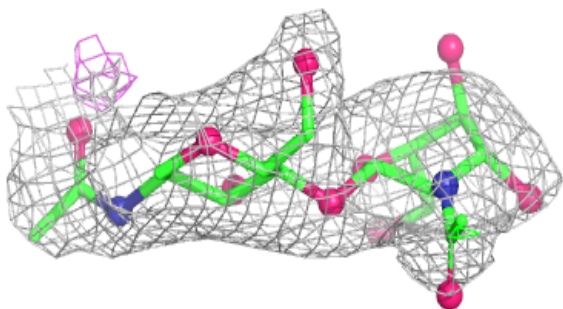
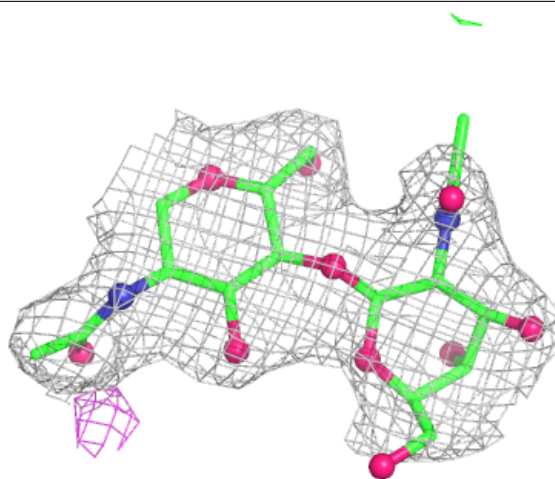
**Electron density around Chain N:**

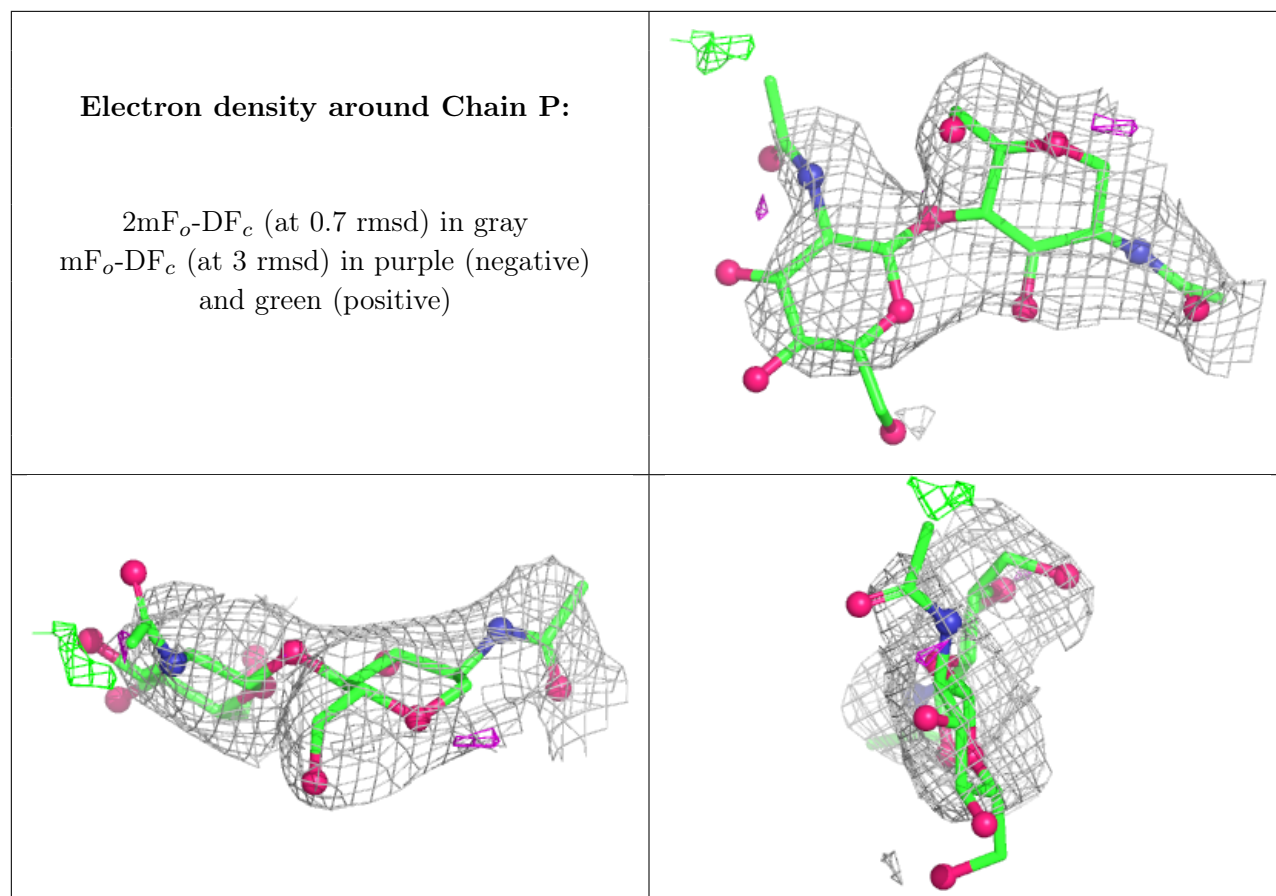
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	B	202	14/15	0.69	0.13	115,120,122,123	0
6	NAG	C	401	14/15	0.73	0.15	79,85,87,90	0
6	NAG	J	201	14/15	0.73	0.15	92,96,101,101	0
6	NAG	G	401	14/15	0.76	0.16	89,94,98,99	0
6	NAG	B	201	14/15	0.81	0.11	79,84,88,90	0
5	CA	E	401	1/1	0.91	0.08	103,103,103,103	0
5	CA	A	401	1/1	0.95	0.06	57,57,57,57	0
5	CA	D	204	1/1	0.95	0.06	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.