



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 06:38 AM EDT

PDB ID : 4LN3
Title : The crystal structure of hemagglutinin from a H7N9 influenza virus (A/Shanghai/1/2013)
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2013-07-11
Resolution : 2.65 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

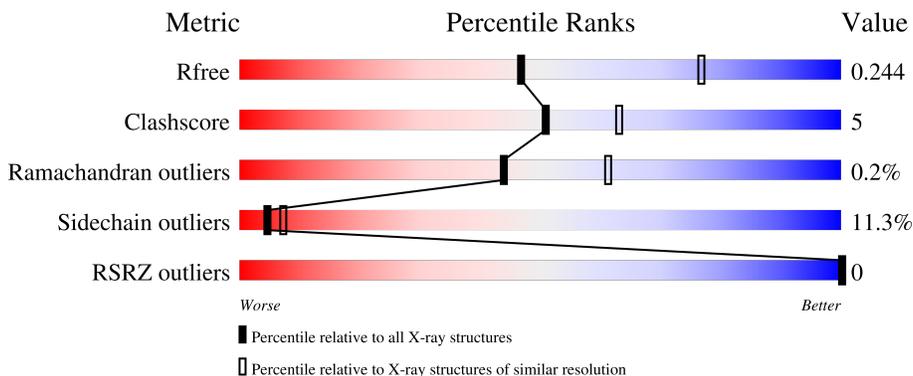
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



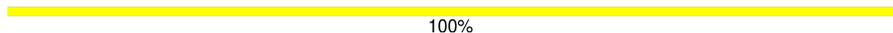
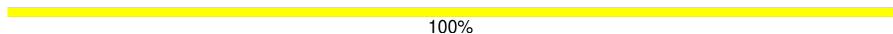
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	
1	C	325	
1	E	325	
1	G	325	
1	I	325	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	325	 77% 17% . .
2	B	181	 79% 12% .. 8%
2	D	181	 77% 14% .. 8%
2	F	181	 77% 14% .. 8%
2	H	181	 77% 12% .. 9%
2	J	181	 78% 10% .. 9%
2	L	181	 78% 10% .. 9%
3	M	3	 33% 67%
3	N	3	 100%
3	O	3	 100%

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
4	NAG	A	404	X	-	-	-
4	NAG	E	404	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23076 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2410	1494	435	466	15	0	0	0
1	C	316	2410	1494	435	466	15	0	0	0
1	E	316	2410	1494	435	466	15	0	0	0
1	G	316	2410	1494	435	466	15	0	0	0
1	I	316	2410	1494	435	466	15	0	0	0
1	K	316	2410	1494	435	466	15	0	0	0

- Molecule 2 is a protein called Hemagglutinin.

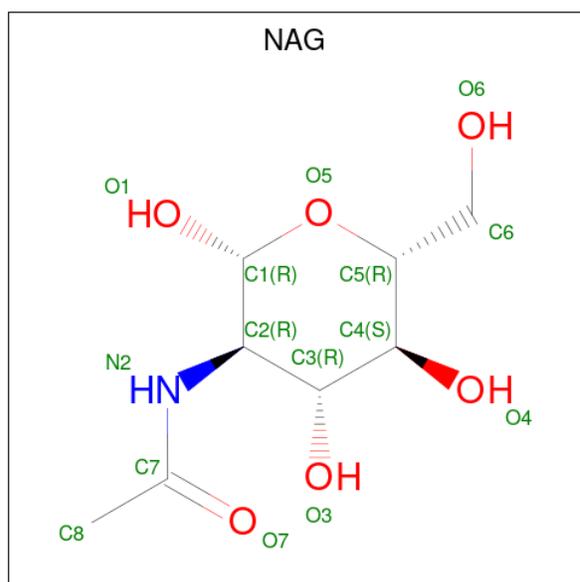
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	167	1359	838	237	277	7	0	0	0
2	D	167	1359	838	237	277	7	0	0	0
2	F	167	1359	838	237	277	7	0	0	0
2	H	164	1335	823	231	274	7	0	0	0
2	J	164	1335	823	231	274	7	0	0	0
2	L	164	1335	823	231	274	7	0	0	0

- 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			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

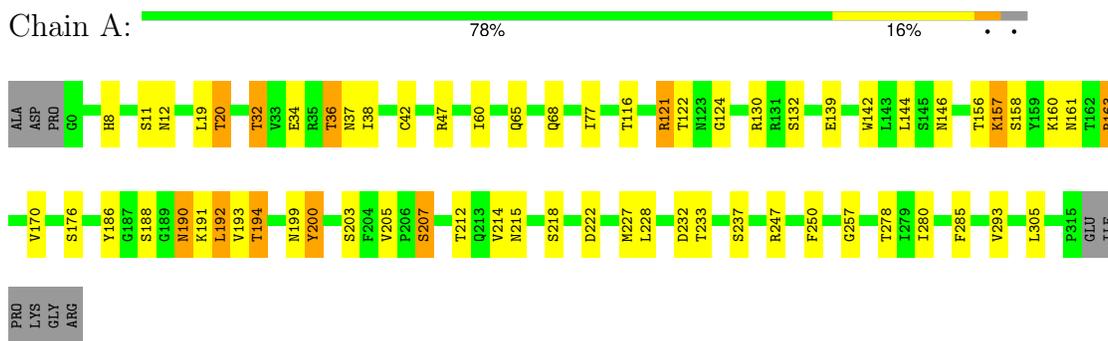
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	17	Total	O	0	0
			17	17		
5	C	38	Total	O	0	0
			38	38		
5	D	24	Total	O	0	0
			24	24		
5	E	40	Total	O	0	0
			40	40		
5	F	20	Total	O	0	0
			20	20		
5	G	22	Total	O	0	0
			22	22		
5	H	13	Total	O	0	0
			13	13		
5	I	21	Total	O	0	0
			21	21		
5	J	8	Total	O	0	0
			8	8		
5	K	17	Total	O	0	0
			17	17		
5	L	6	Total	O	0	0
			6	6		

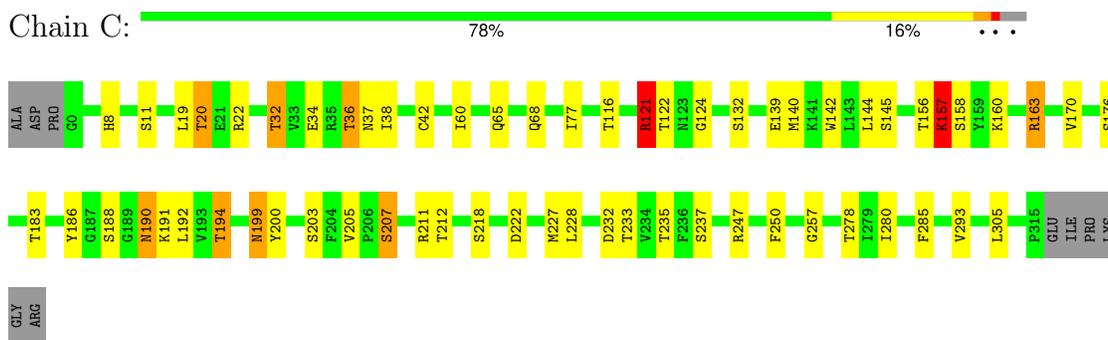
3 Residue-property plots [i](#)

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.

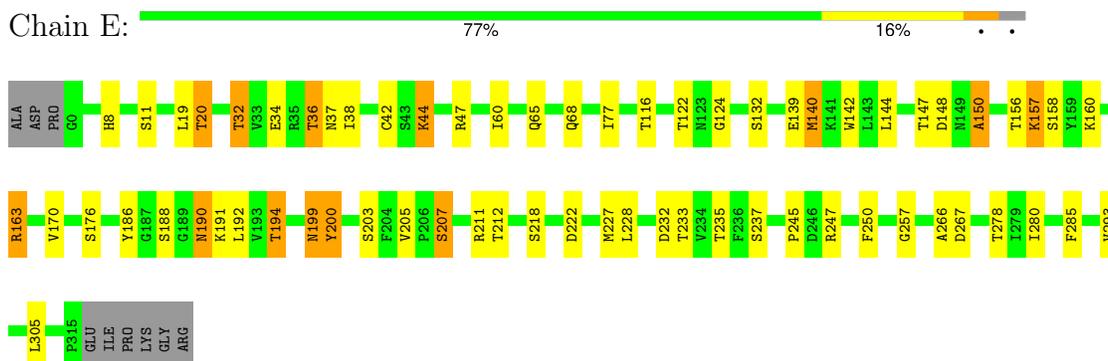
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin



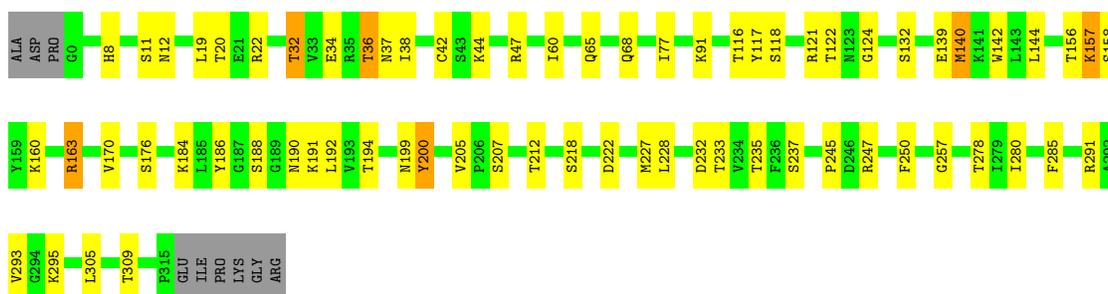
- Molecule 1: Hemagglutinin

Chain G: 78% 17% ..



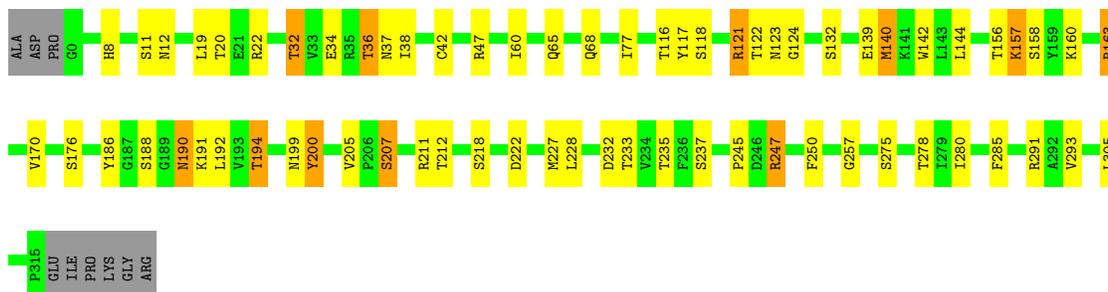
- Molecule 1: Hemagglutinin

Chain I: 76% 19% ..



- Molecule 1: Hemagglutinin

Chain K: 77% 17% ..



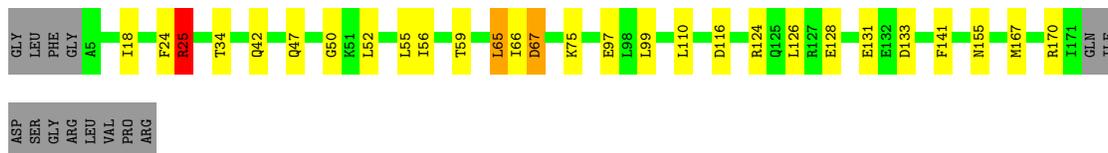
- Molecule 2: Hemagglutinin

Chain B: 79% 12% .. 8%



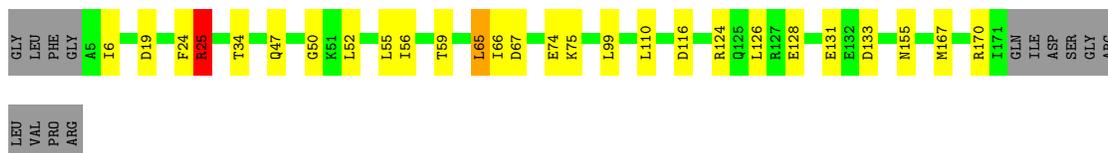
- Molecule 2: Hemagglutinin

Chain D: 77% 14% .. 8%



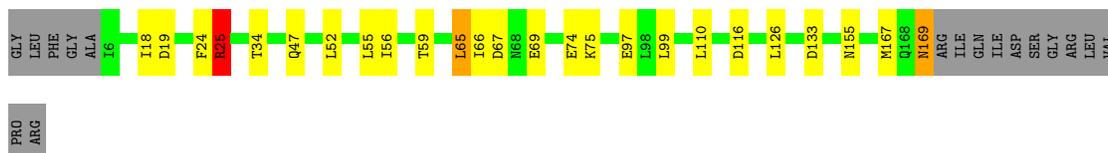
- Molecule 2: Hemagglutinin

Chain F: 77% 14% 8%



- Molecule 2: Hemagglutinin

Chain H: 77% 12% 9%



- Molecule 2: Hemagglutinin

Chain J: 78% 10% 9%



- Molecule 2: Hemagglutinin

Chain L: 78% 10% 9%



- 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: 33% 67%



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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain O:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.30Å 154.29Å 154.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.65 49.02 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.02-2.65) 98.7 (49.02-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.244 0.213 , 0.244	Depositor DCC
R_{free} test set	5388 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h 0.020 for -h,-l,-k 0.019 for k,h,-l 0.459 for l,h,k 0.459 for k,l,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23076	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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, 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	0.71	0/2455	0.84	3/3316 (0.1%)
1	C	0.72	0/2455	0.85	3/3316 (0.1%)
1	E	0.71	0/2455	0.83	2/3316 (0.1%)
1	G	0.62	0/2455	0.80	2/3316 (0.1%)
1	I	0.63	0/2455	0.81	2/3316 (0.1%)
1	K	0.63	0/2455	0.81	3/3316 (0.1%)
2	B	0.71	0/1382	0.89	4/1863 (0.2%)
2	D	0.69	0/1382	0.87	3/1863 (0.2%)
2	F	0.70	0/1382	0.87	3/1863 (0.2%)
2	H	0.59	0/1358	0.80	2/1831 (0.1%)
2	J	0.59	0/1358	0.81	2/1831 (0.1%)
2	L	0.60	0/1358	0.81	2/1831 (0.1%)
All	All	0.66	0/22950	0.83	31/30978 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ARG	CG-CD-NE	7.16	126.84	111.80
2	D	25	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	E	222	ASP	CB-CG-OD1	6.35	124.02	118.30
2	B	25	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	I	295	LYS	CD-CE-NZ	6.25	126.08	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2410	0	2361	29	0
1	C	2410	0	2362	27	0
1	E	2410	0	2361	34	0
1	G	2410	0	2362	25	0
1	I	2410	0	2362	25	0
1	K	2410	0	2362	30	0
2	B	1359	0	1263	12	0
2	D	1359	0	1263	15	0
2	F	1359	0	1263	15	0
2	H	1335	0	1234	10	0
2	J	1335	0	1234	10	0
2	L	1335	0	1234	10	0
3	M	39	0	34	0	0
3	N	39	0	34	0	0
3	O	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
4	L	14	0	13	0	0
5	A	37	0	0	1	0
5	B	17	0	0	1	0
5	C	38	0	0	1	0
5	D	24	0	0	1	0
5	E	40	0	0	2	0
5	F	20	0	0	0	0
5	G	22	0	0	3	0
5	H	13	0	0	0	0
5	I	21	0	0	3	0
5	J	8	0	0	1	0
5	K	17	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	6	0	0	0	0
All	All	23076	0	21906	226	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 5.

The worst 5 of 226 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:NH1	1:C:145:SER:O	1.99	0.96
2:D:131:GLU:OE1	2:D:170:ARG:HD2	1.66	0.95
2:F:131:GLU:OE1	2:F:170:ARG:HD2	1.67	0.94
1:K:47:ARG:NH1	5:K:906:HOH:O	1.89	0.86
1:I:117:TYR:HA	5:I:902:HOH:O	1.79	0.81

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 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	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	37	53
1	C	314/325 (97%)	295 (94%)	18 (6%)	1 (0%)	37	53
1	E	314/325 (97%)	296 (94%)	16 (5%)	2 (1%)	22	35
1	G	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	37	53
1	I	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	37	53
1	K	314/325 (97%)	297 (95%)	16 (5%)	1 (0%)	37	53
2	B	165/181 (91%)	159 (96%)	6 (4%)	0	100	100
2	D	165/181 (91%)	159 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	165/181 (91%)	159 (96%)	6 (4%)	0	100	100
2	H	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
2	J	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
2	L	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
All	All	2865/3036 (94%)	2727 (95%)	131 (5%)	7 (0%)	44	61

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	C	199	ASN
1	E	199	ASN
1	G	199	ASN
1	I	199	ASN

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 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	264/271 (97%)	238 (90%)	26 (10%)	6	10
1	C	264/271 (97%)	233 (88%)	31 (12%)	4	6
1	E	264/271 (97%)	235 (89%)	29 (11%)	5	8
1	G	264/271 (97%)	232 (88%)	32 (12%)	4	6
1	I	264/271 (97%)	229 (87%)	35 (13%)	3	4
1	K	264/271 (97%)	234 (89%)	30 (11%)	4	7
2	B	144/155 (93%)	131 (91%)	13 (9%)	8	12
2	D	144/155 (93%)	129 (90%)	15 (10%)	5	9
2	F	144/155 (93%)	130 (90%)	14 (10%)	6	10
2	H	142/155 (92%)	125 (88%)	17 (12%)	4	6
2	J	142/155 (92%)	125 (88%)	17 (12%)	4	6
2	L	142/155 (92%)	126 (89%)	16 (11%)	4	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2442/2556 (96%)	2167 (89%)	275 (11%)	4 7

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	12	ASN
1	K	65	GLN
2	L	25	ARG
1	E	140	MET
1	E	68	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	165	ASN
1	G	37	ASN
1	K	37	ASN
1	I	37	ASN
1	E	37	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	1,3	14,14,15	0.59	0	17,19,21	1.42	3 (17%)
3	NAG	M	2	3	14,14,15	0.80	1 (7%)	17,19,21	1.64	3 (17%)
3	BMA	M	3	3	11,11,12	0.58	0	15,15,17	0.87	0
3	NAG	N	1	1,3	14,14,15	0.84	1 (7%)	17,19,21	1.35	3 (17%)
3	NAG	N	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.53	4 (23%)
3	BMA	N	3	3	11,11,12	0.58	0	15,15,17	1.50	1 (6%)
3	NAG	O	1	1,3	14,14,15	0.56	0	17,19,21	1.40	1 (5%)
3	NAG	O	2	3	14,14,15	0.71	0	17,19,21	1.34	2 (11%)
3	BMA	O	3	3	11,11,12	0.51	0	15,15,17	1.04	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	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	-	2/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	C1-C2	2.55	1.55	1.52
3	N	2	NAG	C1-C2	2.35	1.55	1.52
3	M	2	NAG	C1-C2	2.28	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	BMA	O5-C5-C6	4.54	116.51	107.66
3	M	2	NAG	C1-C2-N2	3.90	116.58	110.43
3	O	1	NAG	C1-O5-C5	3.83	117.33	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C1-O5-C5	3.60	117.01	112.19
3	M	1	NAG	C1-C2-N2	-3.37	105.13	110.43

There are no chirality outliers.

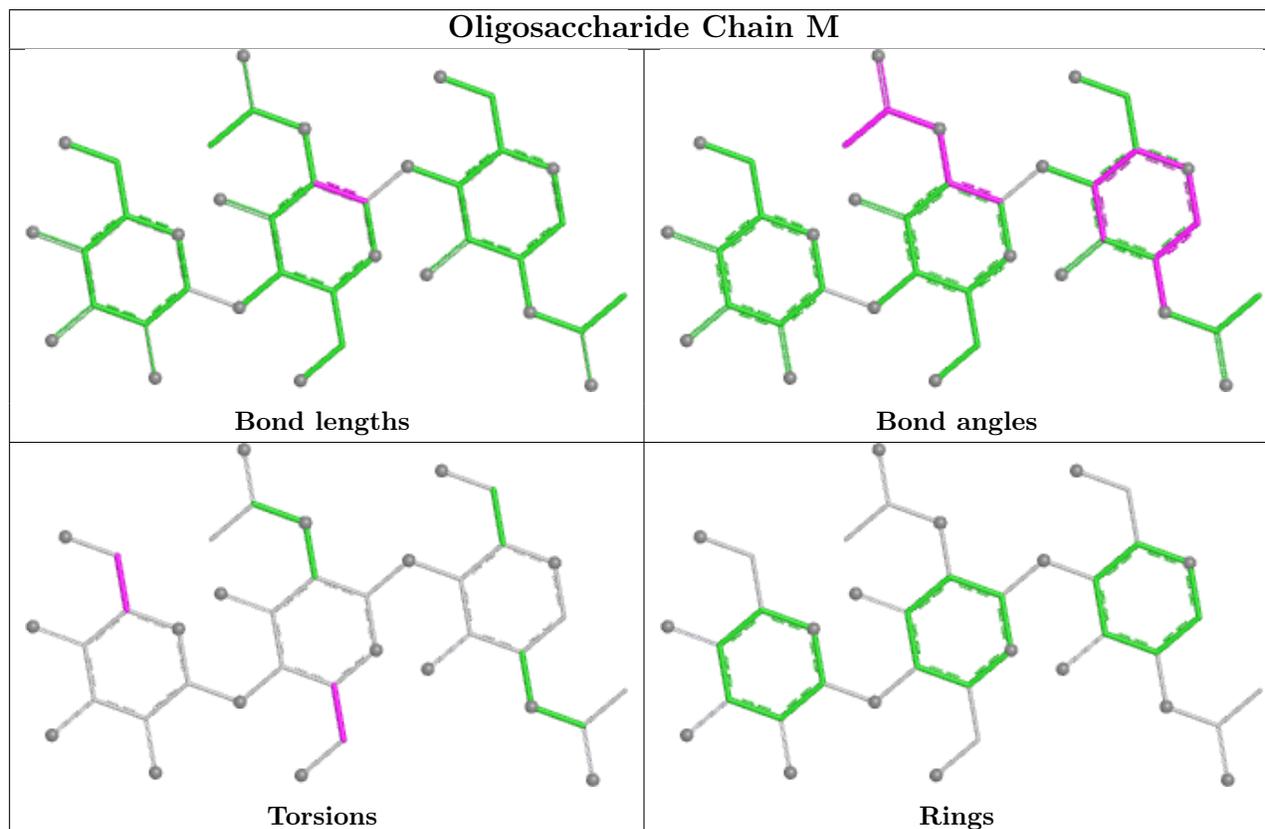
5 of 14 torsion outliers are listed below:

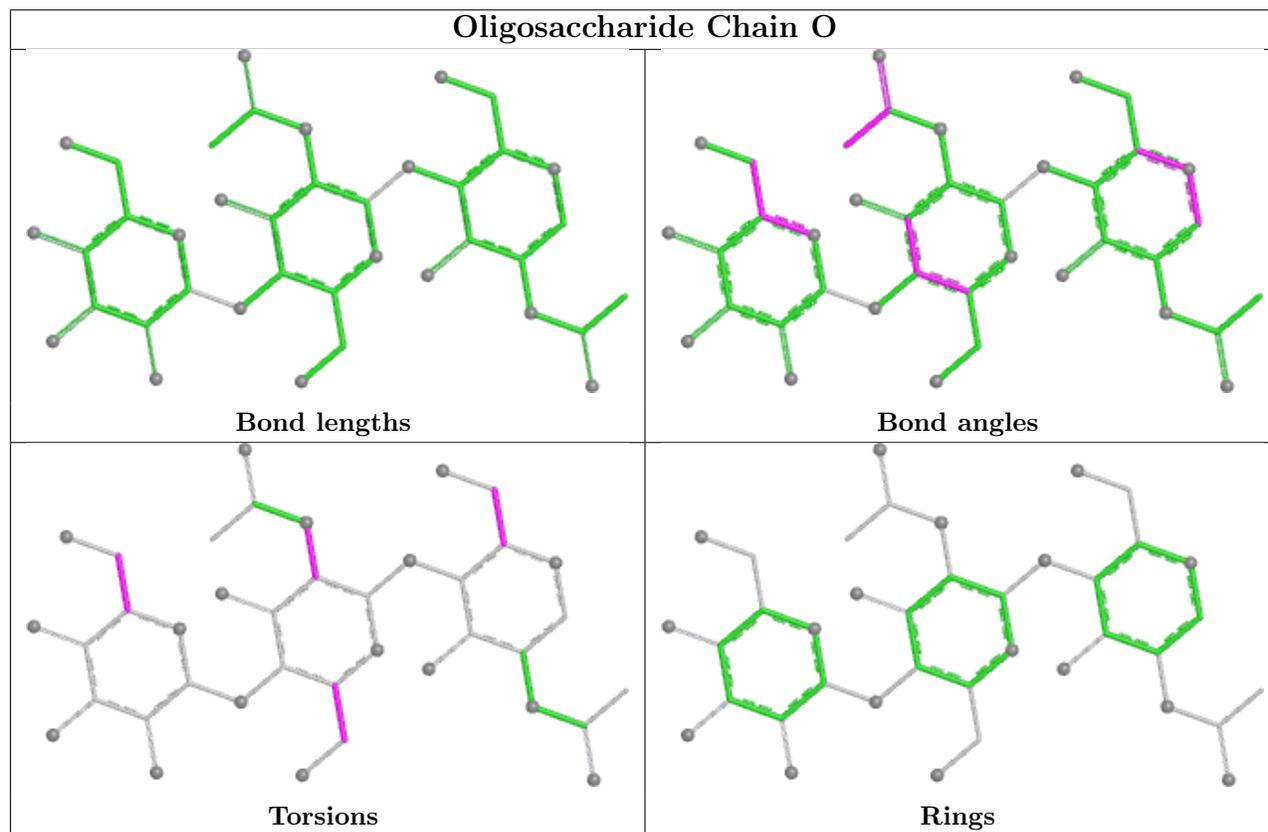
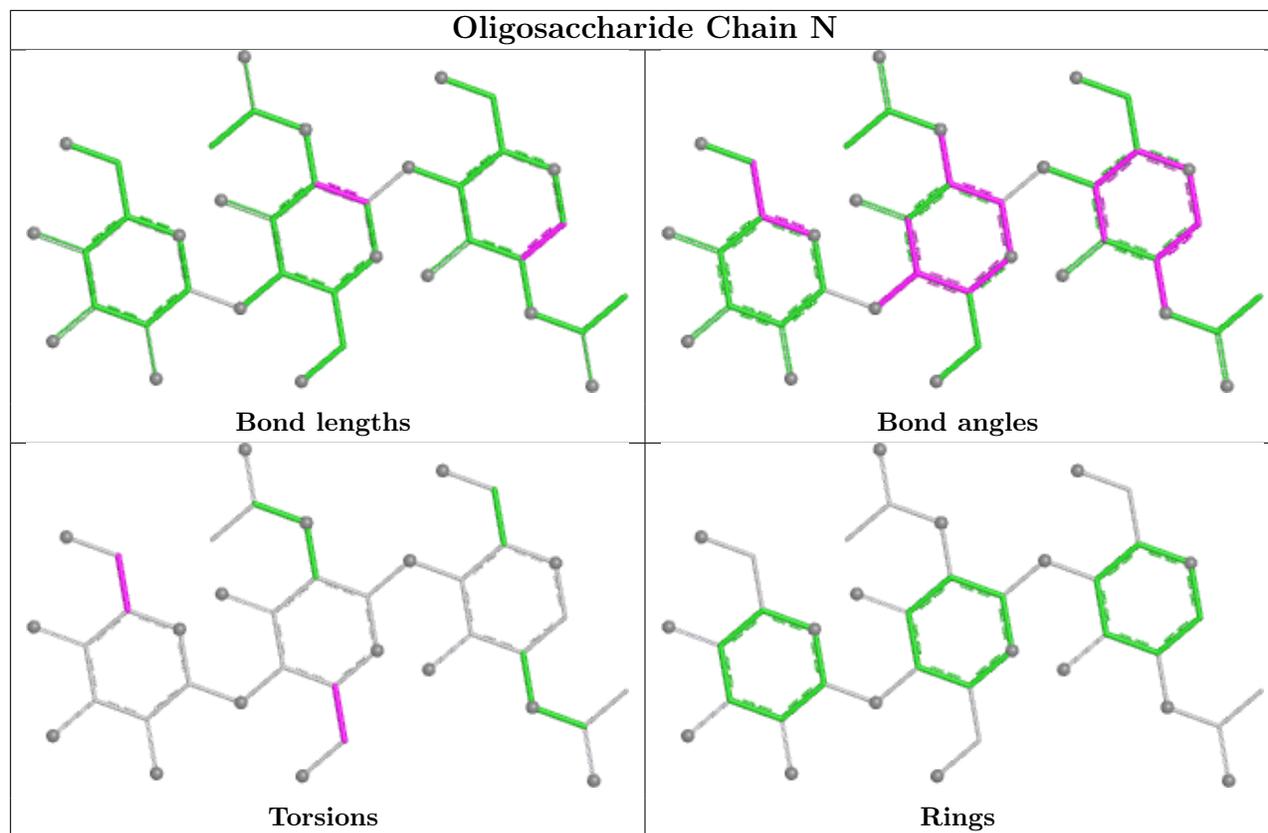
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6

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

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	404	1	14,14,15	0.82	1 (7%)	17,19,21	1.32	2 (11%)
4	NAG	F	500	2	14,14,15	0.63	0	17,19,21	2.13	2 (11%)
4	NAG	L	500	2	14,14,15	0.60	0	17,19,21	1.76	5 (29%)
4	NAG	A	404	1	14,14,15	0.64	1 (7%)	17,19,21	1.95	3 (17%)
4	NAG	K	800	1	14,14,15	0.44	0	17,19,21	1.83	3 (17%)
4	NAG	B	500	2	14,14,15	0.72	0	17,19,21	2.12	5 (29%)
4	NAG	J	500	2	14,14,15	0.71	1 (7%)	17,19,21	1.47	2 (11%)
4	NAG	G	800	1	14,14,15	0.38	0	17,19,21	1.50	3 (17%)
4	NAG	H	500	2	14,14,15	0.67	0	17,19,21	1.40	3 (17%)
4	NAG	D	500	2	14,14,15	0.71	0	17,19,21	2.04	4 (23%)
4	NAG	I	800	1	14,14,15	0.38	0	17,19,21	2.33	5 (29%)

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
4	NAG	E	404	1	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	F	500	2	-	2/6/23/26	0/1/1/1
4	NAG	L	500	2	-	0/6/23/26	0/1/1/1
4	NAG	A	404	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	K	800	1	-	2/6/23/26	0/1/1/1
4	NAG	B	500	2	-	1/6/23/26	0/1/1/1
4	NAG	J	500	2	-	0/6/23/26	0/1/1/1
4	NAG	G	800	1	-	2/6/23/26	0/1/1/1
4	NAG	H	500	2	-	0/6/23/26	0/1/1/1
4	NAG	D	500	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	800	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	404	NAG	C1-C2	2.29	1.55	1.52
4	A	404	NAG	C1-C2	2.04	1.55	1.52
4	J	500	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	500	NAG	C1-O5-C5	6.52	120.93	112.19
4	I	800	NAG	C1-O5-C5	6.51	120.92	112.19
4	A	404	NAG	C1-O5-C5	6.12	120.38	112.19
4	B	500	NAG	C1-O5-C5	5.90	120.09	112.19
4	K	800	NAG	C1-O5-C5	5.45	119.49	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	404	NAG	C1
4	E	404	NAG	C1

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	800	NAG	O5-C5-C6-O6
4	I	800	NAG	O5-C5-C6-O6
4	I	800	NAG	C4-C5-C6-O6
4	G	800	NAG	O5-C5-C6-O6
4	K	800	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	800	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	316/325 (97%)	-1.58	0 100 100	38, 59, 84, 103	1 (0%)
1	C	316/325 (97%)	-1.60	0 100 100	40, 59, 84, 104	1 (0%)
1	E	316/325 (97%)	-1.56	0 100 100	37, 58, 85, 106	1 (0%)
1	G	316/325 (97%)	-1.51	0 100 100	50, 73, 100, 128	1 (0%)
1	I	316/325 (97%)	-1.52	0 100 100	49, 72, 99, 124	1 (0%)
1	K	316/325 (97%)	-1.51	0 100 100	49, 72, 99, 127	1 (0%)
2	B	167/181 (92%)	-1.60	0 100 100	33, 59, 82, 125	0
2	D	167/181 (92%)	-1.61	0 100 100	34, 60, 83, 122	0
2	F	167/181 (92%)	-1.60	0 100 100	32, 60, 81, 125	0
2	H	164/181 (90%)	-1.43	0 100 100	47, 83, 103, 130	0
2	J	164/181 (90%)	-1.46	0 100 100	46, 82, 105, 133	0
2	L	164/181 (90%)	-1.44	0 100 100	46, 83, 104, 120	0
All	All	2889/3036 (95%)	-1.54	0 100 100	32, 67, 97, 133	6 (0%)

There are no RSRZ outliers to report.

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

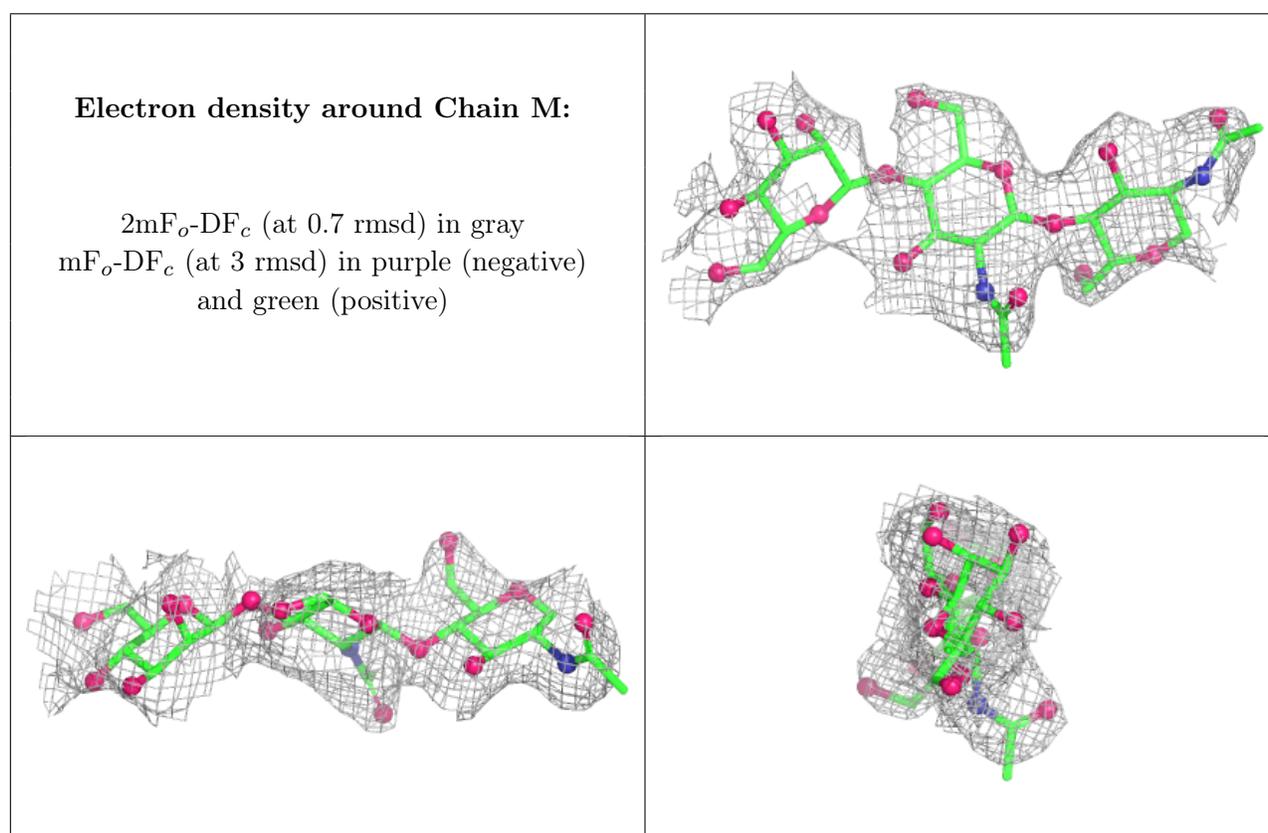
There are no non-standard protein/DNA/RNA residues in this entry.

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.

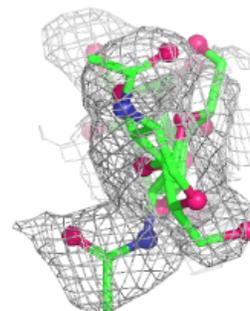
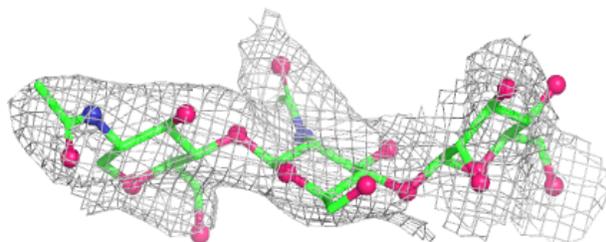
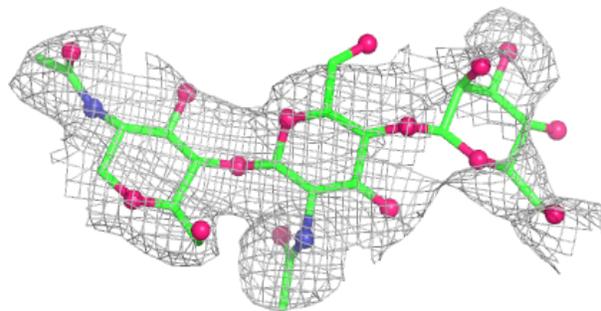
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	M	3	11/12	0.95	0.05	113,138,144,151	0
3	BMA	O	3	11/12	0.95	0.06	124,145,156,158	0
3	BMA	N	3	11/12	0.96	0.04	124,143,151,161	0
3	NAG	O	2	14/15	0.97	0.05	86,122,138,146	0
3	NAG	N	2	14/15	0.98	0.04	80,105,126,134	0
3	NAG	M	2	14/15	0.98	0.04	85,110,124,140	0
3	NAG	O	1	14/15	0.99	0.06	82,89,96,105	0
3	NAG	M	1	14/15	0.99	0.05	79,90,93,100	0
3	NAG	N	1	14/15	0.99	0.04	74,89,94,95	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.

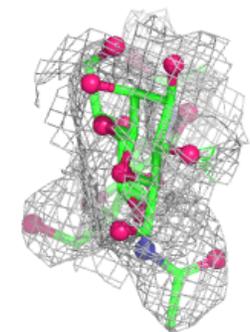
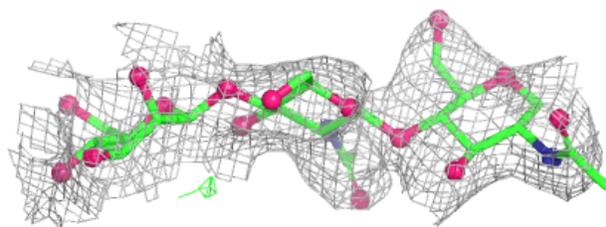
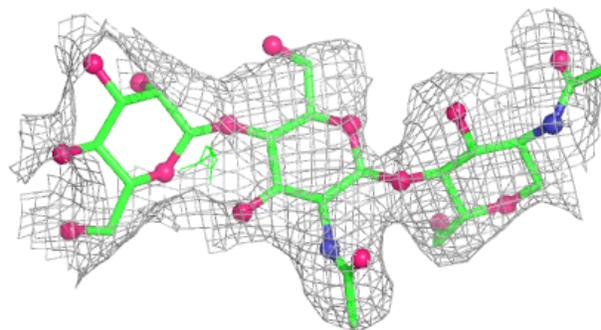


Electron density around Chain N:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	NAG	A	404	14/15	0.94	0.08	125,139,162,165	0
4	NAG	E	404	14/15	0.96	0.08	123,141,151,160	0
4	NAG	F	500	14/15	0.97	0.06	70,86,90,107	0
4	NAG	J	500	14/15	0.97	0.05	82,91,98,98	0
4	NAG	D	500	14/15	0.98	0.05	70,84,92,93	0
4	NAG	G	800	14/15	0.98	0.05	98,111,114,115	0
4	NAG	H	500	14/15	0.98	0.04	81,89,95,96	0
4	NAG	B	500	14/15	0.98	0.06	66,80,90,97	0
4	NAG	L	500	14/15	0.98	0.04	83,92,97,99	0
4	NAG	K	800	14/15	0.99	0.04	92,107,110,111	0
4	NAG	I	800	14/15	0.99	0.04	95,110,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.