WORLD WIDE
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:24 AM BST

PDB ID	:	1RD8
Title	:	Crystal Structure of the 1918 Human H1 Hemagglutinin Precursor (HA0)
Authors	:	Stevens, J.; Corper, A.L.; Basler, C.F.; Taubenberger, J.K.; Palese, P.; Wilson, I.A.
Deposited on	:	2003-11-05
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

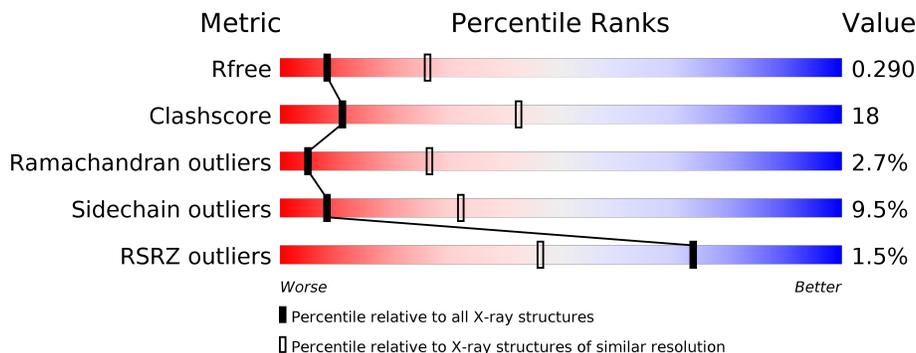|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.00 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.
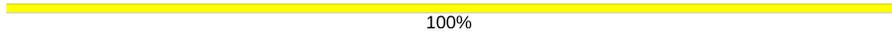
Metric	Percentile Ranks	Value
Rfree		0.290
Clashscore		18
Ramachandran outliers		2.7%
Sidechain outliers		9.5%
RSRZ outliers		1.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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 <=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	335	64% 28% 6% ·
1	C	335	2% 61% 32% 6% ·
1	E	335	2% 63% 29% 6% ·
2	B	182	2% 54% 33% 8% · ·
2	D	182	2% 57% 31% 8% · ·
2	F	182	57% 31% 8% · ·

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Mol	Chain	Length	Quality of chain
3	G	3	100%
3	I	3	33% 67%
4	H	4	25% 75%

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	H	2	-	-	-	X
4	MAN	H	4	-	-	-	X
5	NAG	A	1	X	-	-	-
5	NAG	A	2	X	-	-	-
5	NAG	B	183	X	-	-	-
5	NAG	C	330	X	-	-	X
5	NAG	C	335	-	-	-	X
5	NAG	E	330	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12082 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
1	A	328	Total 2549	C 1605	N 439	O 494	S 11	23	0	0
1	C	328	Total 2549	C 1605	N 439	O 494	S 11	46	0	0
1	E	328	Total 2549	C 1605	N 439	O 494	S 11	44	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	cloning artifact	GB 4325039
A	4	ASP	-	cloning artifact	GB 4325039
A	5	PRO	-	cloning artifact	GB 4325039
A	6	GLY	-	cloning artifact	GB 4325039
A	7	TYR	-	cloning artifact	GB 4325039
A	8	LEU	-	cloning artifact	GB 4325039
A	9	LEU	-	cloning artifact	GB 4325039
A	10	GLU	-	cloning artifact	GB 4325039
C	3	ALA	-	cloning artifact	GB 4325039
C	4	ASP	-	cloning artifact	GB 4325039
C	5	PRO	-	cloning artifact	GB 4325039
C	6	GLY	-	cloning artifact	GB 4325039
C	7	TYR	-	cloning artifact	GB 4325039
C	8	LEU	-	cloning artifact	GB 4325039
C	9	LEU	-	cloning artifact	GB 4325039
C	10	GLU	-	cloning artifact	GB 4325039
E	3	ALA	-	cloning artifact	GB 4325039
E	4	ASP	-	cloning artifact	GB 4325039
E	5	PRO	-	cloning artifact	GB 4325039
E	6	GLY	-	cloning artifact	GB 4325039
E	7	TYR	-	cloning artifact	GB 4325039
E	8	LEU	-	cloning artifact	GB 4325039
E	9	LEU	-	cloning artifact	GB 4325039

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLU	-	cloning artifact	GB 4325039

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total 1406	C 877	N 241	O 282	S 6	16	0	0
2	D	175	Total 1406	C 877	N 241	O 282	S 6	29	0	0
2	F	175	Total 1406	C 877	N 241	O 282	S 6	35	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	LYS	cloning artifact	GB 4325039
B	178	SER	-	cloning artifact	GB 4325039
B	179	LEU	-	cloning artifact	GB 4325039
B	180	VAL	-	cloning artifact	GB 4325039
B	181	PRO	-	cloning artifact	GB 4325039
B	182	ARG	-	cloning artifact	GB 4325039
D	177	ARG	LYS	cloning artifact	GB 4325039
D	178	SER	-	cloning artifact	GB 4325039
D	179	LEU	-	cloning artifact	GB 4325039
D	180	VAL	-	cloning artifact	GB 4325039
D	181	PRO	-	cloning artifact	GB 4325039
D	182	ARG	-	cloning artifact	GB 4325039
F	177	ARG	LYS	cloning artifact	GB 4325039
F	178	SER	-	cloning artifact	GB 4325039
F	179	LEU	-	cloning artifact	GB 4325039
F	180	VAL	-	cloning artifact	GB 4325039
F	181	PRO	-	cloning artifact	GB 4325039
F	182	ARG	-	cloning artifact	GB 4325039

- 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.
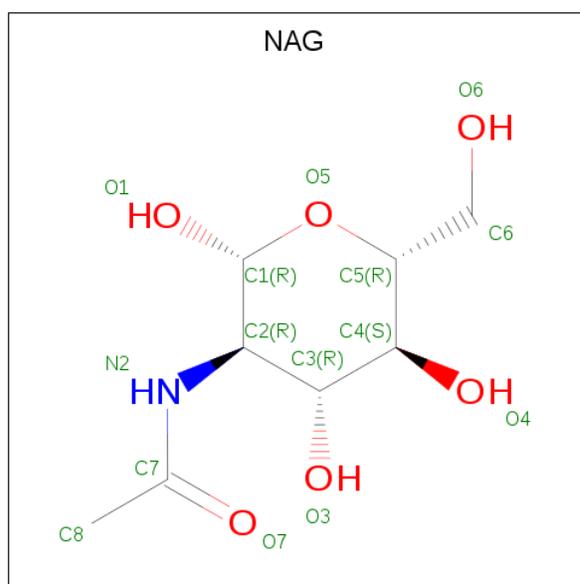
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
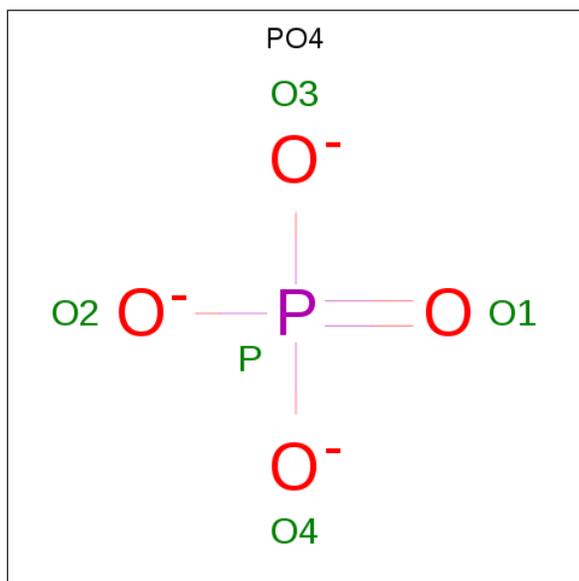
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 5	O 4	P 1	0	0

3 Residue-property plots ⓘ

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

Chain A:

- Molecule 1: hemagglutinin

Chain C:

- Molecule 1: hemagglutinin
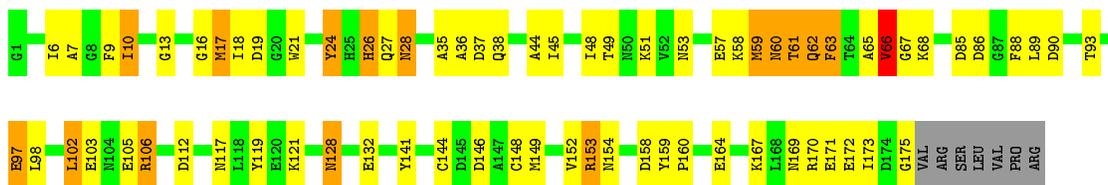
Chain E:

• Molecule 2: hemagglutinin

Chain B:

• Molecule 2: hemagglutinin

Chain D:

• Molecule 2: hemagglutinin

Chain F:

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

Chain G: 100%

NAG1 NAG2 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 I: 33% 67%

NAG1 NAG2 BMA3

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

Chain H: 25% 75%

NAG1 NAG2 BMA3 MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.53Å 109.95Å 136.24Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 49.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-3.00) 96.1 (49.49-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.270 , 0.295 0.266 , 0.290	Depositor DCC
R_{free} test set	2573 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, BMA, NAG, MAN

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	0.91	2/2613 (0.1%)	0.96	8/3558 (0.2%)
1	C	0.87	3/2613 (0.1%)	0.97	9/3558 (0.3%)
1	E	1.06	6/2613 (0.2%)	0.96	8/3558 (0.2%)
2	B	0.98	2/1433 (0.1%)	1.03	7/1929 (0.4%)
2	D	1.01	2/1433 (0.1%)	1.23	13/1929 (0.7%)
2	F	1.09	4/1433 (0.3%)	1.10	11/1929 (0.6%)
All	All	0.98	19/12138 (0.2%)	1.02	56/16461 (0.3%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	LYS	CD-CE	-20.71	0.99	1.51
1	E	133(A)	LYS	CG-CD	19.43	2.18	1.52
1	E	192	GLN	CA-CB	-9.37	1.33	1.53
2	F	175	GLY	N-CA	-9.17	1.32	1.46
1	C	133(A)	LYS	CA-CB	-8.69	1.34	1.53

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	PHE	CB-CG-CD2	-20.79	106.25	120.80
2	D	9	PHE	CB-CG-CD1	19.17	134.22	120.80
2	B	112	ASP	CB-CG-OD2	9.63	126.97	118.30
2	F	112	ASP	CB-CG-OD2	9.06	126.46	118.30
2	D	112	ASP	CB-CG-OD2	8.55	125.99	118.30

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	2549	0	2468	89	0
1	C	2549	0	2468	99	0
1	E	2549	0	2470	95	0
2	B	1406	0	1315	75	0
2	D	1406	0	1316	60	0
2	F	1406	0	1316	63	0
3	G	39	0	34	0	0
3	I	39	0	34	5	0
4	H	50	0	43	4	0
5	A	28	0	26	0	0
5	B	14	0	13	2	0
5	C	28	0	26	0	0
5	E	14	0	13	1	0
6	B	5	0	0	0	0
All	All	12082	0	11542	417	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 18.

The worst 5 of 417 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)
2:B:106:ARG:HD3	2:F:106:ARG:HH12	1.34	0.90
2:B:106:ARG:HH12	2:D:106:ARG:HD3	1.36	0.89
2:D:106:ARG:HH12	2:F:106:ARG:HD3	1.37	0.88
2:B:117:ASN:HD21	2:B:121:LYS:HE2	1.37	0.88
1:A:15:ILE:HD11	2:B:119:TYR:HB2	1.55	0.88

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	326/335 (97%)	290 (89%)	33 (10%)	3 (1%)	17	55
1	C	326/335 (97%)	292 (90%)	31 (10%)	3 (1%)	17	55
1	E	326/335 (97%)	291 (89%)	32 (10%)	3 (1%)	17	55
2	B	173/182 (95%)	151 (87%)	12 (7%)	10 (6%)	1	10
2	D	173/182 (95%)	151 (87%)	11 (6%)	11 (6%)	1	7
2	F	173/182 (95%)	151 (87%)	12 (7%)	10 (6%)	1	10
All	All	1497/1551 (96%)	1326 (89%)	131 (9%)	40 (3%)	5	26

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA
2	B	10	ILE
2	B	60	ASN
2	B	62	GLN
2	B	66	VAL

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	284/289 (98%)	257 (90%)	27 (10%)	8	32
1	C	284/289 (98%)	258 (91%)	26 (9%)	9	34
1	E	284/289 (98%)	260 (92%)	24 (8%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	149/156 (96%)	133 (89%)	16 (11%)	6	26
2	D	149/156 (96%)	134 (90%)	15 (10%)	7	29
2	F	149/156 (96%)	134 (90%)	15 (10%)	7	29
All	All	1299/1335 (97%)	1176 (90%)	123 (10%)	8	32

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	THR
1	C	309	VAL
2	F	63	PHE
1	C	225	ASP
1	C	260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	GLN
2	D	27	GLN
2	F	30	GLN
1	C	231	ASN
1	C	275	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 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	G	1	1,3	14,14,15	0.82	1 (7%)	17,19,21	2.39	7 (41%)
3	NAG	G	2	3	14,14,15	0.64	0	17,19,21	1.59	4 (23%)
3	BMA	G	3	3	11,11,12	0.64	0	15,15,17	1.42	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.75	0	17,19,21	1.47	3 (17%)
4	NAG	H	2	4	14,14,15	0.93	0	17,19,21	2.19	6 (35%)
4	BMA	H	3	4	11,11,12	0.76	0	15,15,17	2.12	5 (33%)
4	MAN	H	4	4	11,11,12	0.75	0	15,15,17	2.11	4 (26%)
3	NAG	I	1	1,3	14,14,15	0.72	0	17,19,21	1.67	3 (17%)
3	NAG	I	2	3	14,14,15	0.77	0	17,19,21	2.14	7 (41%)
3	BMA	I	3	3	11,11,12	0.93	0	15,15,17	1.31	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	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	5/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O3-C3	-2.07	1.38	1.43

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-O5-C5	5.07	119.06	112.19
4	H	4	MAN	C1-O5-C5	4.87	118.79	112.19
4	H	3	BMA	O5-C1-C2	-4.65	103.60	110.77
3	G	1	NAG	O7-C7-C8	-4.64	113.43	122.06
4	H	2	NAG	C4-C3-C2	4.62	117.79	111.02

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C3-C2-N2-C7
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	2	0
3	I	2	NAG	1	0
4	H	2	NAG	2	0
4	H	3	BMA	2	0
3	I	1	NAG	5	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.

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
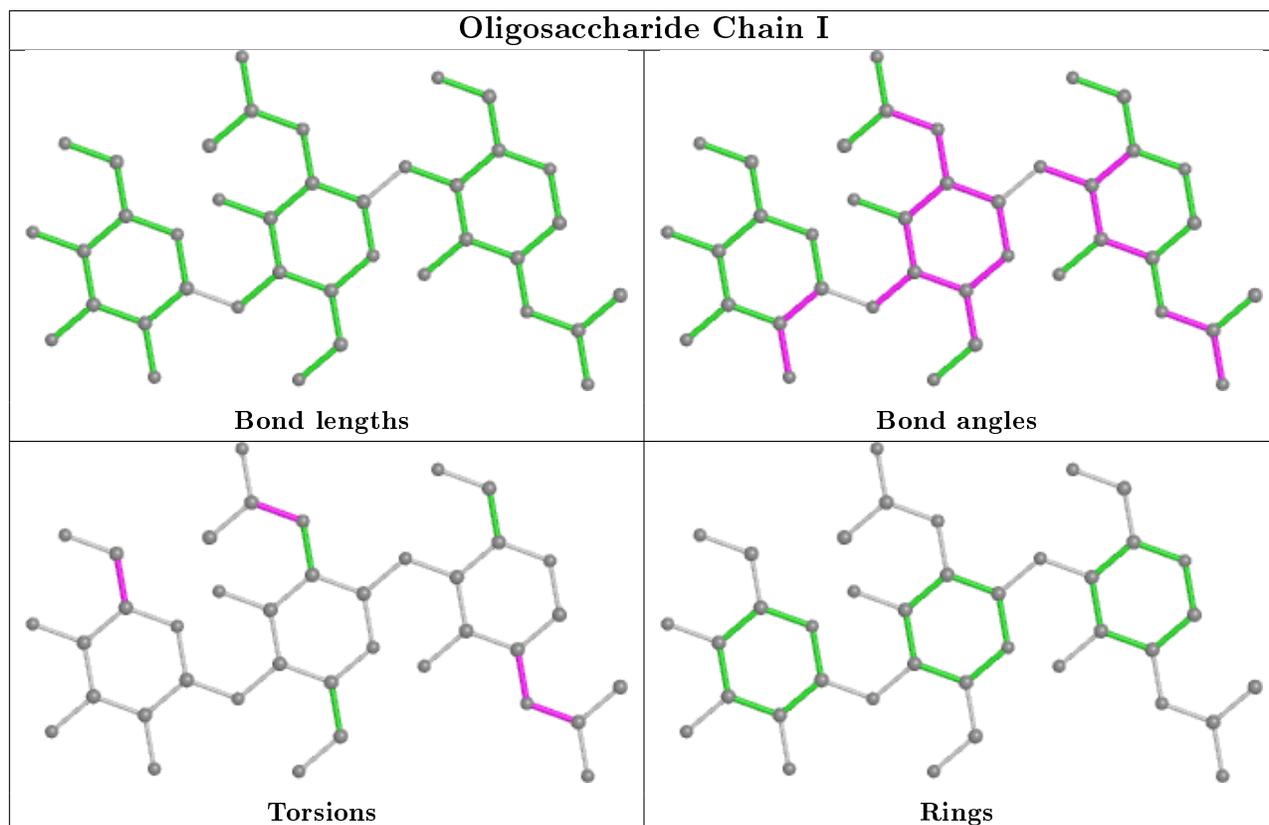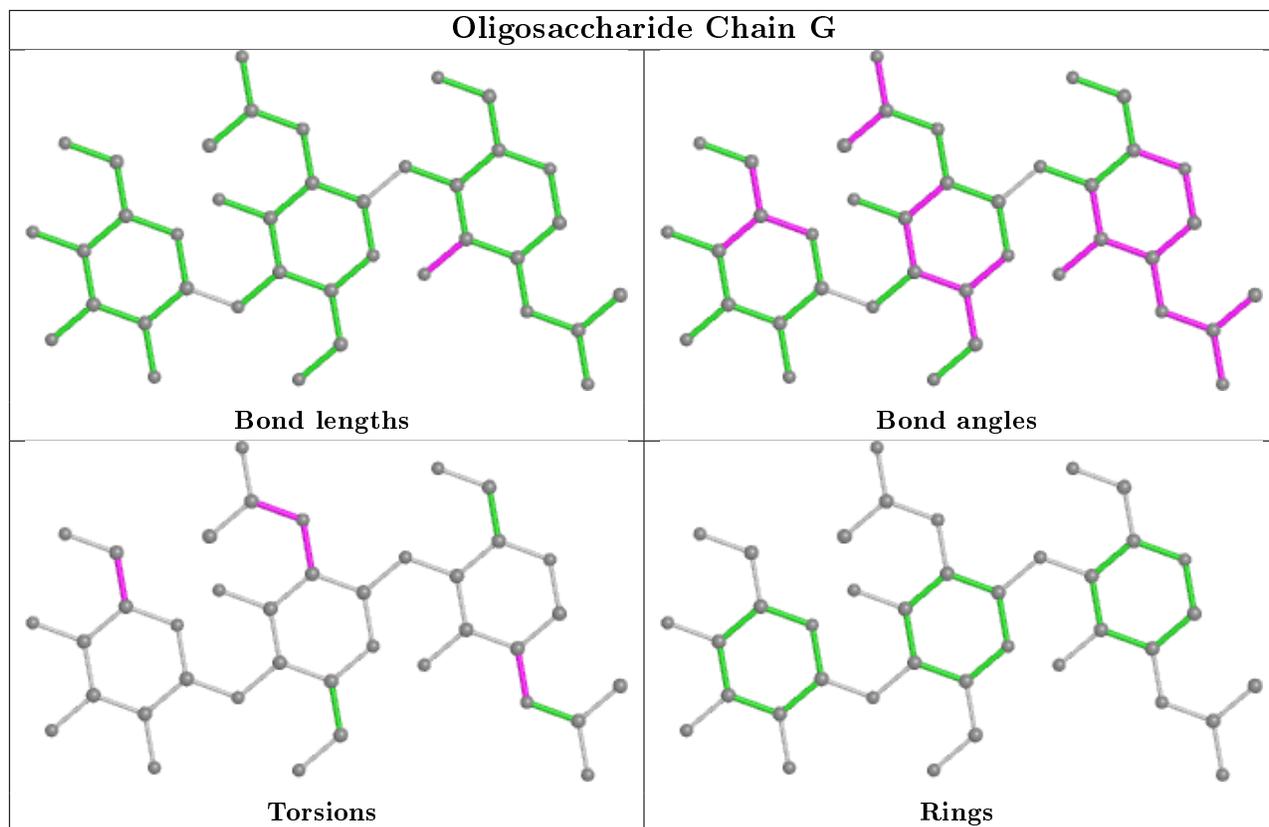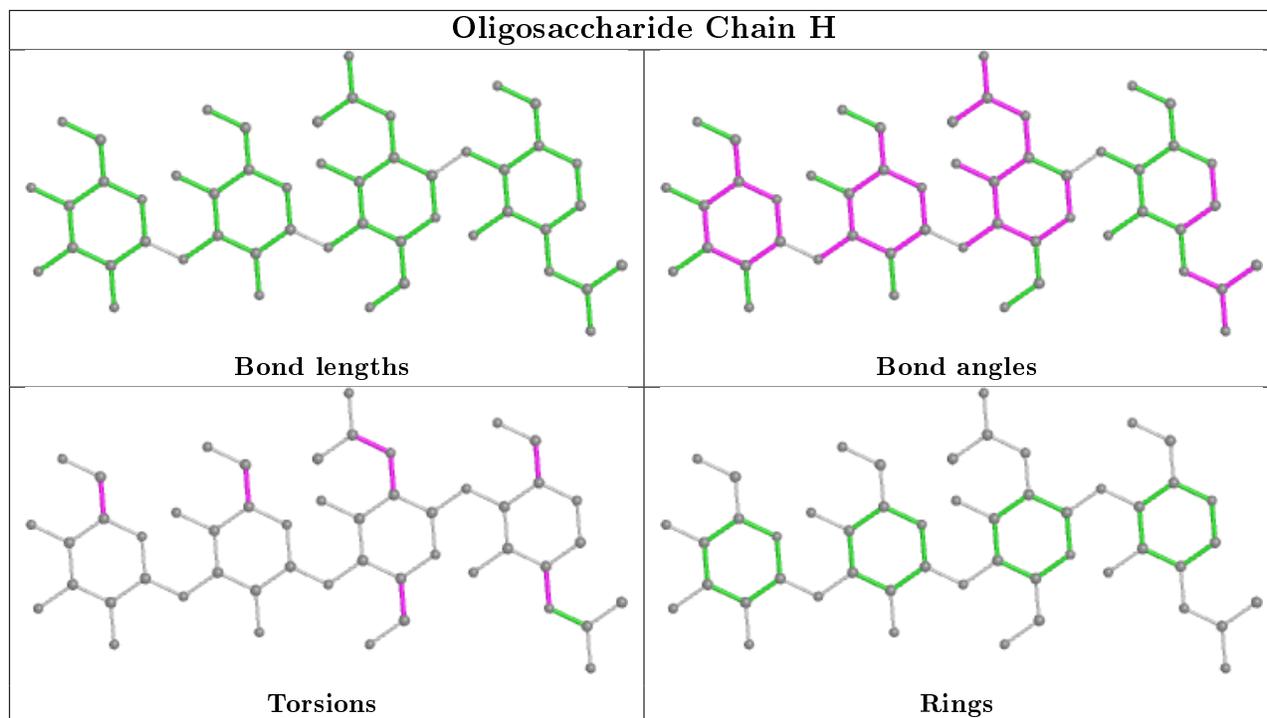
5.6 Ligand geometry ⓘ

7 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	#$|Z| > 2$
5	NAG	C	335	1	14,14,15	0.73	0	17,19,21	1.40	3 (17%)
6	PO4	B	301	-	4,4,4	1.01	0	6,6,6	0.51	0
5	NAG	C	330	1	14,14,15	1.02	1 (7%)	17,19,21	2.03	7 (41%)
5	NAG	E	330	1	14,14,15	1.46	3 (21%)	17,19,21	2.56	7 (41%)
5	NAG	B	183	2	14,14,15	0.56	0	17,19,21	1.53	4 (23%)
5	NAG	A	1	1	14,14,15	1.03	1 (7%)	17,19,21	1.99	6 (35%)
5	NAG	A	2	1	14,14,15	0.55	0	17,19,21	1.66	3 (17%)

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
5	NAG	C	335	1	-	2/6/23/26	0/1/1/1
5	NAG	C	330	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	E	330	1	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	B	183	2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	1	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	2	1	1/1/5/7	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	330	NAG	C1-C2	3.14	1.57	1.52
5	A	1	NAG	C1-C2	2.83	1.56	1.52
5	E	330	NAG	C1-C2	2.72	1.56	1.52
5	E	330	NAG	C3-C2	2.48	1.57	1.52
5	E	330	NAG	C2-N2	2.19	1.50	1.46

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2	NAG	C1-O5-C5	5.17	119.20	112.19
5	E	330	NAG	O5-C1-C2	-4.79	103.72	111.29
5	E	330	NAG	C2-N2-C7	4.46	129.25	122.90
5	E	330	NAG	O3-C3-C2	4.26	118.28	109.47
5	A	1	NAG	C1-C2-N2	3.95	117.23	110.49

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	330	NAG	C1
5	E	330	NAG	C1
5	B	183	NAG	C1
5	A	1	NAG	C1
5	A	2	NAG	C1

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	335	NAG	C8-C7-N2-C2
5	C	335	NAG	O7-C7-N2-C2
5	C	330	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	C	330	NAG	O7-C7-N2-C2
5	E	330	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	330	NAG	1	0
5	B	183	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 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	328/335 (97%)	-0.08	4 (1%)	79	54	25, 42, 66, 97	6 (1%)
1	C	328/335 (97%)	-0.03	7 (2%)	63	34	25, 42, 65, 97	13 (3%)
1	E	328/335 (97%)	-0.13	6 (1%)	68	40	25, 42, 65, 97	14 (4%)
2	B	175/182 (96%)	-0.27	3 (1%)	70	41	21, 36, 82, 108	4 (2%)
2	D	175/182 (96%)	-0.17	3 (1%)	70	41	21, 36, 82, 108	7 (4%)
2	F	175/182 (96%)	-0.20	0	100	100	21, 36, 82, 108	10 (5%)
All	All	1509/1551 (97%)	-0.13	23 (1%)	73	46	21, 40, 70, 108	54 (3%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	SER	4.0
1	C	159	SER	3.7
1	E	171	ASN	3.2
1	E	239	PRO	2.9
1	C	116	SER	2.9

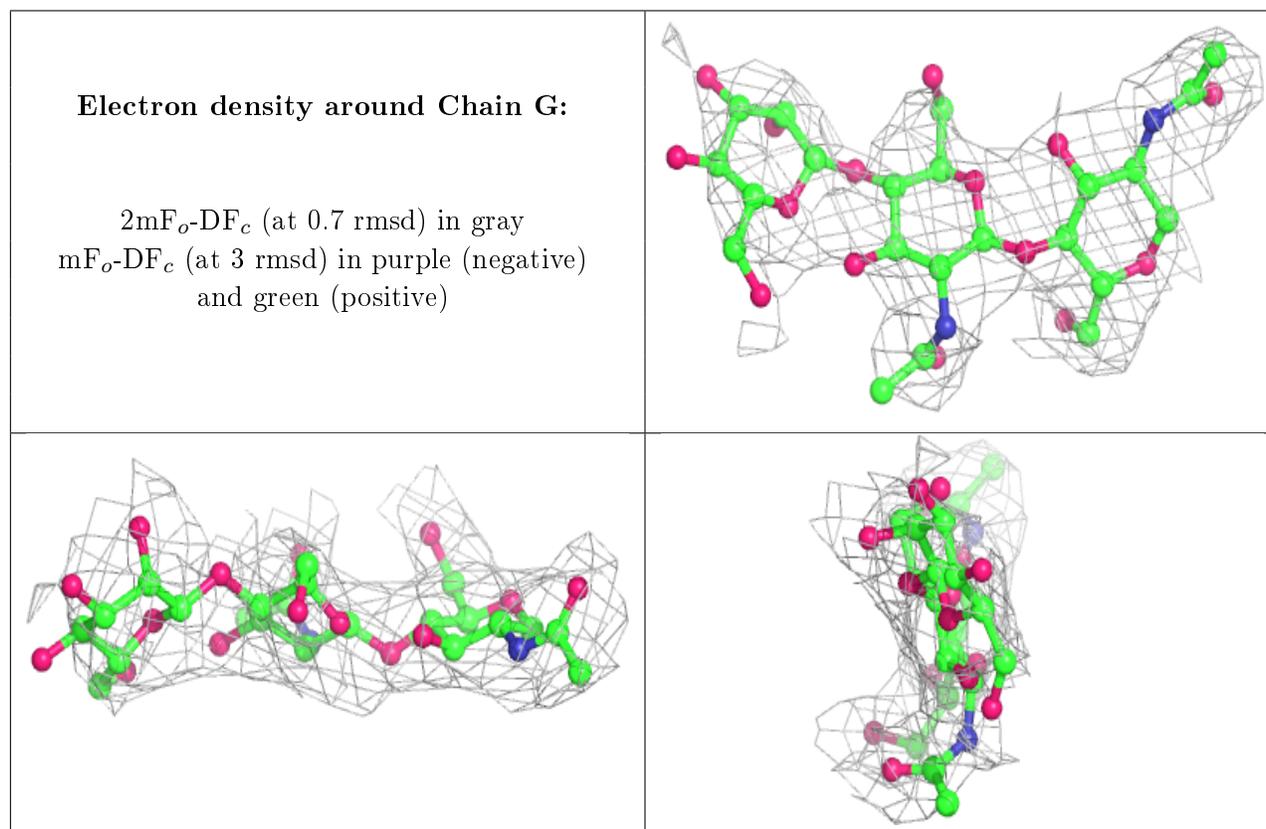## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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
4	MAN	H	4	11/12	0.50	0.60	93,95,98,99	0
3	BMA	G	3	11/12	0.65	0.40	91,96,97,98	0
3	BMA	I	3	11/12	0.66	0.35	83,85,89,89	0
4	BMA	H	3	11/12	0.72	0.30	78,81,85,89	0
4	NAG	H	2	14/15	0.74	0.40	76,84,88,89	0
3	NAG	G	2	14/15	0.81	0.39	71,77,82,89	0
3	NAG	I	2	14/15	0.84	0.34	64,70,73,79	0
3	NAG	G	1	14/15	0.93	0.19	44,45,53,62	0
4	NAG	H	1	14/15	0.96	0.23	45,48,54,65	0
3	NAG	I	1	14/15	0.96	0.20	41,47,53,56	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.
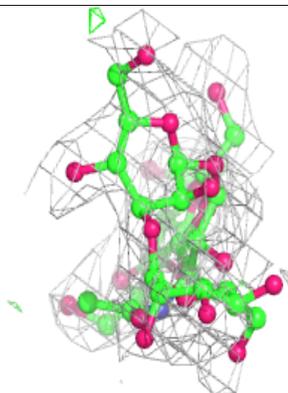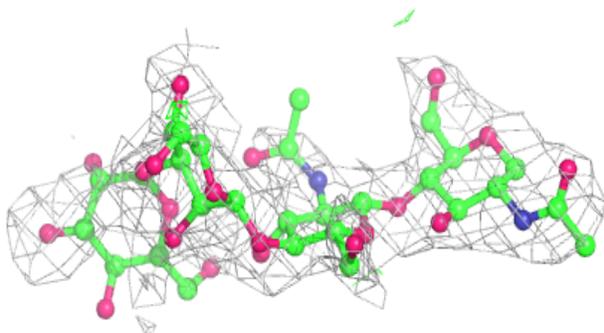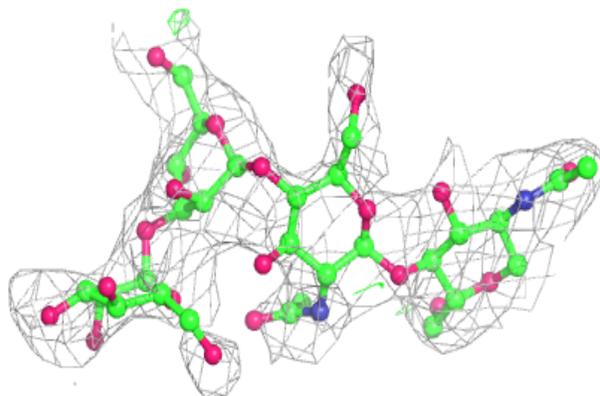

Electron density around Chain G:

$2mF_o$-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 I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
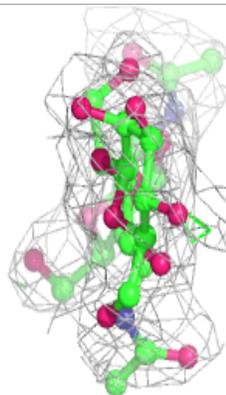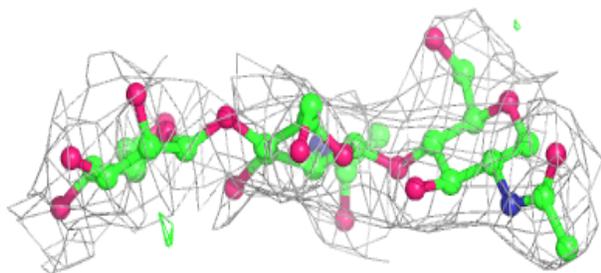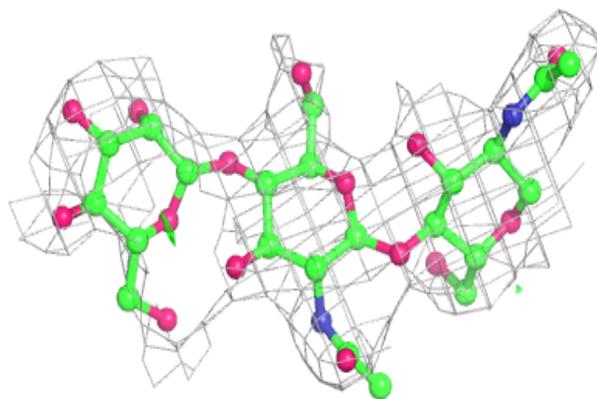
Electron density around Chain H:

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
5	NAG	C	335	14/15	0.48	0.42	90,95,95,96	0
5	NAG	A	2	14/15	0.61	0.34	70,78,79,81	0
5	NAG	E	330	14/15	0.69	0.30	63,66,70,71	0
5	NAG	C	330	14/15	0.76	0.46	71,76,78,78	0
5	NAG	A	1	14/15	0.83	0.41	71,75,78,78	0
5	NAG	B	183	14/15	0.83	0.40	74,82,84,86	0
6	PO4	B	301	5/5	0.88	0.25	61,62,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.