Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 05:55 PM JST

PDB ID	:	5GSQ
Title	:	Crystal structure of IgG Fc with a homogeneous glycoform and Antibody-Dependent Cellular Cytotoxicity
Authors	:	Chen, C.-L.; Hsu, J.-C.; Lin, C.-W.; Wu, C.-Y.; Wong, C.-H.; Ma, C.
Deposited on	:	2016-08-17
Resolution	:	1.85 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:

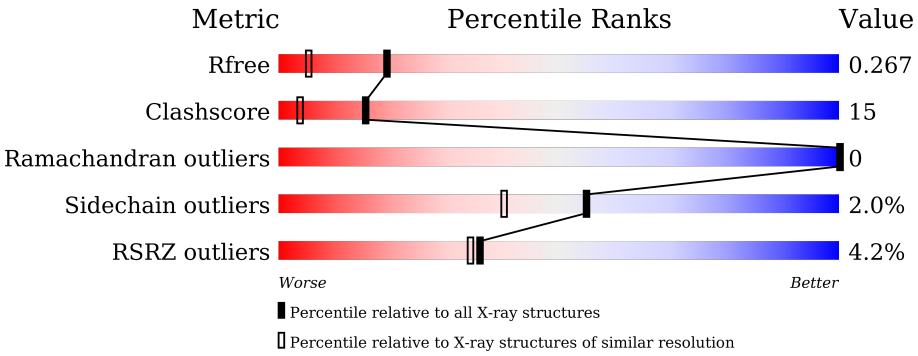
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	225	74% 16% 8%
1	B	225	76% 16% 8%
1	C	225	72% 21% 8%
1	D	225	11% 62% 22% 14%
2	E	7	71% 29%
2	F	7	71% 29%

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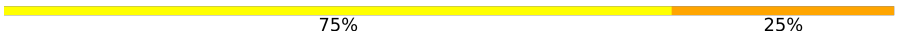
Mol	Chain	Length	Quality of chain
3	G	8	
4	H	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	E	7	-	-	X	-
4	NAG	H	1	-	-	X	X
4	NAG	H	5	-	-	X	-

2 Entry composition

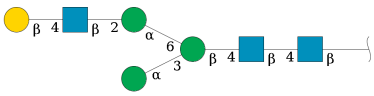
There are 5 unique types of molecules in this entry. The entry contains 7717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ig gamma-1 chain C region.

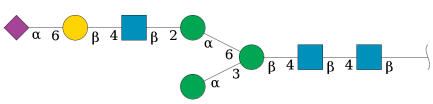
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	C	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			
1	D	194	Total	C	N	O	S	0	0	0
			1555	992	261	296	6			

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



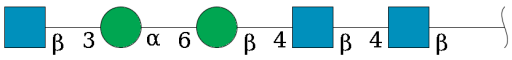
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	0	0	0
			86	48	3	35			
2	F	7	Total	C	N	O	0	0	0
			86	48	3	35			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
3	G	8	Total	C	N	O	0	0	0
			106	59	4	43			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-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	5	Total	C	N	O	0	0	0
			64	36	3	25			

- Molecule 5 is water.

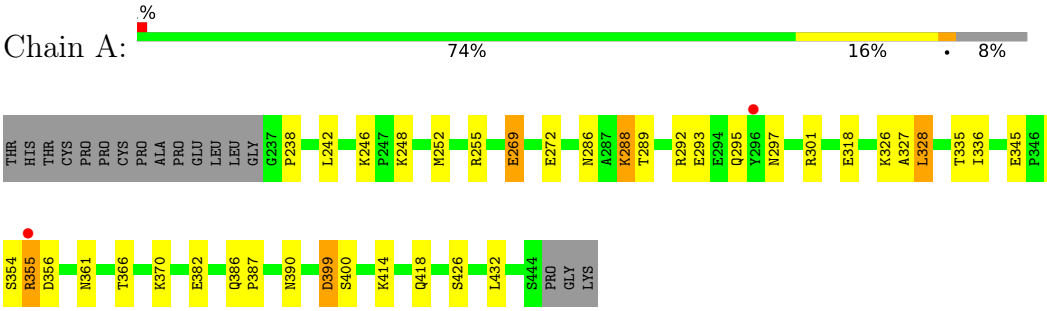
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total	O	0	0
			231	231		
5	B	221	Total	O	0	0
			221	221		
5	C	198	Total	O	0	0
			198	198		
5	D	178	Total	O	0	0
			178	178		

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.

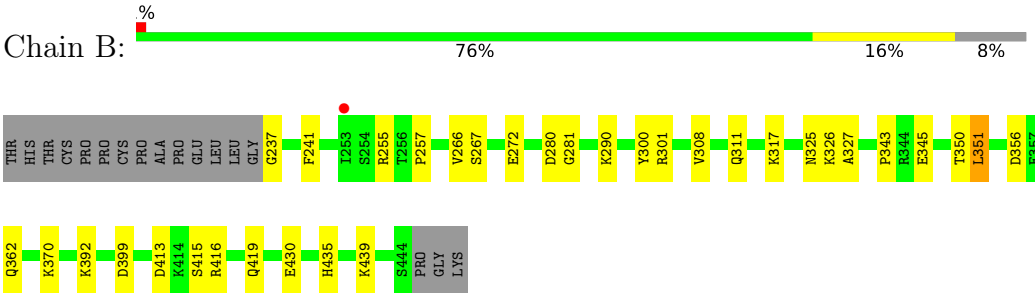
• Molecule 1: Ig gamma-1 chain C region

Chain A:



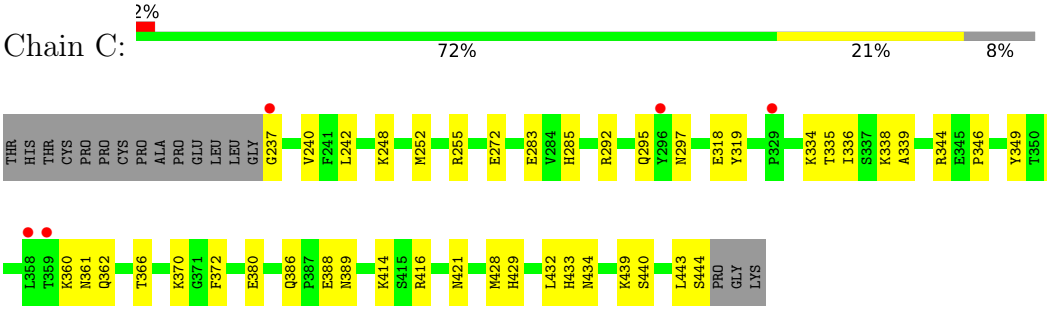
• Molecule 1: Ig gamma-1 chain C region

Chain B:



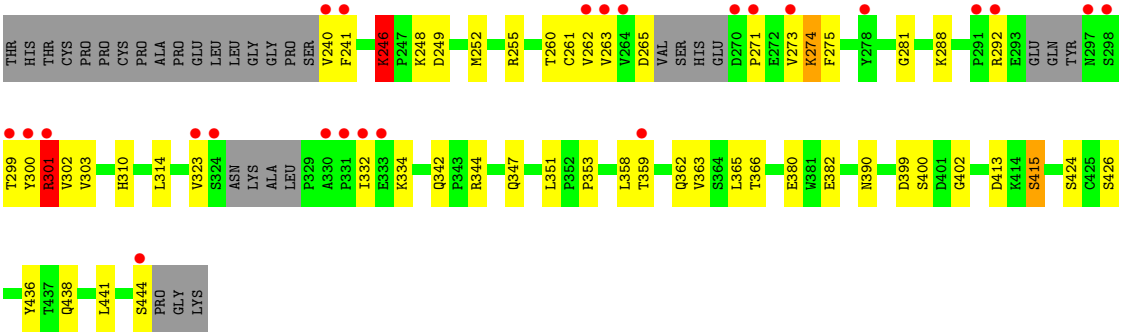
• Molecule 1: Ig gamma-1 chain C region

Chain C:



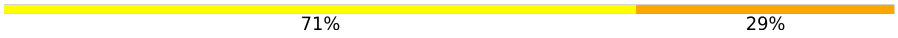
• Molecule 1: Ig gamma-1 chain C region

Chain D:



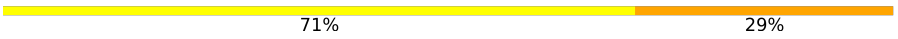
• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



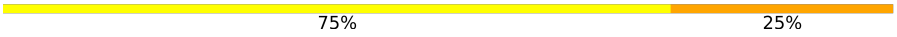
• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 G:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.18Å 158.41Å 66.91Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	49.42 – 1.85 49.42 – 1.85	Depositor EDS
% Data completeness (in resolution range)	86.8 (49.42-1.85) 84.0 (49.42-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.227 , 0.267 0.227 , 0.267	Depositor DCC
R_{free} test set	3640 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, GAL, SIA

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	0.61	3/1710 (0.2%)	0.69	2/2330 (0.1%)
1	B	0.44	0/1710	0.60	1/2330 (0.0%)
1	C	0.45	0/1710	0.58	0/2330
1	D	0.70	6/1595 (0.4%)	0.64	0/2168
All	All	0.56	9/6725 (0.1%)	0.63	3/9158 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	GLU	CD-OE1	-10.17	1.14	1.25
1	D	301	ARG	CZ-NH2	-9.86	1.20	1.33
1	D	301	ARG	NE-CZ	-9.18	1.21	1.33
1	A	269	GLU	CD-OE2	-8.78	1.16	1.25
1	D	301	ARG	CZ-NH1	-8.65	1.21	1.33
1	D	301	ARG	CD-NE	-7.96	1.32	1.46
1	D	246	LYS	CE-NZ	-7.82	1.29	1.49
1	D	246	LYS	CD-CE	-6.99	1.33	1.51
1	A	355	ARG	NE-CZ	-6.77	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	355	ARG	NE-CZ-NH1	-15.16	112.72	120.30
1	A	355	ARG	NH1-CZ-NH2	5.83	125.82	119.40
1	B	351	LEU	CA-CB-CG	5.30	127.49	115.30

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	1664	0	1630	38	0
1	B	1664	0	1630	38	0
1	C	1664	0	1630	38	0
1	D	1555	0	1528	69	1
2	E	86	0	73	7	0
2	F	86	0	73	2	0
3	G	106	0	89	2	0
4	H	64	0	53	25	0
5	A	231	0	0	26	1
5	B	221	0	0	22	1
5	C	198	0	0	19	1
5	D	178	0	0	20	0
All	All	7717	0	6706	201	2

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 15.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:N	5:A:603:HOH:O	1.95	0.99
1:D:344:ARG:NH2	5:D:601:HOH:O	1.93	0.99
1:C:370:LYS:NZ	5:C:601:HOH:O	1.97	0.96
1:D:301:ARG:HE	4:H:1:NAG:H81	1.25	0.96
1:C:338:LYS:NZ	1:C:339:ALA:O	2.02	0.91
1:D:248:LYS:NZ	1:D:380:GLU:OE2	2.04	0.91
1:B:267:SER:C	5:B:604:HOH:O	2.08	0.90
1:A:293:GLU:OE1	5:A:601:HOH:O	1.90	0.89
1:D:402:GLY:O	5:D:601:HOH:O	1.89	0.88
1:A:272:GLU:OE2	5:A:602:HOH:O	1.92	0.86
1:B:272:GLU:O	1:B:325:ASN:ND2	2.09	0.86
1:B:430:GLU:OE1	5:B:601:HOH:O	1.93	0.85
1:D:400:SER:O	5:D:602:HOH:O	1.96	0.84
1:D:390:ASN:ND2	5:D:605:HOH:O	2.11	0.83
1:D:246:LYS:NZ	4:H:5:NAG:HN2	1.76	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD1	5:B:602:HOH:O	1.95	0.82
5:D:603:HOH:O	4:H:5:NAG:O7	1.97	0.81
1:B:267:SER:OG	5:B:604:HOH:O	1.98	0.80
4:H:1:NAG:N2	4:H:1:NAG:O4	2.14	0.79
1:C:344:ARG:NH1	5:C:607:HOH:O	2.15	0.79
1:B:360:LYS:HD2	1:B:362:GLN:H	1.47	0.79
1:A:361:ASN:O	5:A:604:HOH:O	2.02	0.78
1:D:415:SER:HB2	5:D:728:HOH:O	1.84	0.78
1:D:301:ARG:HE	4:H:1:NAG:C8	1.97	0.77
1:D:246:LYS:HZ1	4:H:5:NAG:H3	1.48	0.77
1:C:386:GLN:OE1	5:C:602:HOH:O	2.03	0.77
1:D:240:VAL:O	1:D:334:LYS:NZ	2.12	0.77
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.65	0.77
1:B:360:LYS:HE3	1:B:362:GLN:HB2	1.66	0.76
1:B:317:LYS:HA	5:B:602:HOH:O	1.86	0.76
1:C:429:HIS:HB3	1:C:432:LEU:HD23	1.67	0.75
1:D:246:LYS:HZ2	4:H:5:NAG:HN2	1.31	0.75
1:C:252:MET:SD	5:C:745:HOH:O	2.44	0.74
1:D:246:LYS:HD3	1:D:246:LYS:H	1.52	0.74
1:B:326:LYS:O	5:B:605:HOH:O	2.03	0.74
1:D:275:PHE:N	5:D:608:HOH:O	2.20	0.74
1:D:301:ARG:CZ	4:H:1:NAG:O7	2.36	0.73
1:D:240:VAL:HG21	1:D:323:VAL:HG21	1.71	0.73
1:C:237:GLY:N	5:C:610:HOH:O	2.21	0.72
1:B:301:ARG:NH2	5:B:608:HOH:O	2.19	0.72
1:A:297:ASN:O	5:A:606:HOH:O	2.07	0.72
1:B:345:GLU:O	5:B:606:HOH:O	2.07	0.72
1:C:318:GLU:CD	1:C:335:THR:HG23	2.11	0.71
1:A:328:LEU:O	5:A:607:HOH:O	2.07	0.71
1:D:260:THR:OG1	4:H:5:NAG:H62	1.90	0.71
1:B:416:ARG:NH2	5:B:610:HOH:O	2.23	0.70
1:C:439:LYS:NZ	5:C:613:HOH:O	2.24	0.70
1:D:301:ARG:NH2	4:H:1:NAG:O7	2.25	0.70
1:A:382:GLU:OE1	5:A:609:HOH:O	2.10	0.69
1:B:281:GLY:O	5:B:607:HOH:O	2.09	0.69
1:B:435:HIS:NE2	5:B:611:HOH:O	2.25	0.69
5:C:603:HOH:O	3:G:7:SIA:O1B	2.09	0.69
1:D:246:LYS:HE2	5:D:607:HOH:O	1.94	0.68
1:D:246:LYS:CE	4:H:5:NAG:HN2	2.06	0.67
1:D:444:SER:O	5:D:606:HOH:O	2.12	0.67
1:D:261:CYS:SG	5:D:704:HOH:O	2.51	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:GLU:OE2	1:C:335:THR:HG23	1.95	0.66
1:A:386:GLN:NE2	1:A:387:PRO:HD2	2.10	0.66
1:C:421:ASN:ND2	5:C:615:HOH:O	2.25	0.66
5:D:603:HOH:O	4:H:5:NAG:C7	2.44	0.66
1:B:267:SER:O	5:B:604:HOH:O	2.07	0.66
1:B:290:LYS:HE3	5:B:706:HOH:O	1.96	0.65
1:D:246:LYS:NZ	4:H:5:NAG:H3	2.12	0.65
1:D:246:LYS:HD3	1:D:246:LYS:N	2.11	0.64
1:A:390:ASN:OD1	5:A:610:HOH:O	2.15	0.64
1:B:327:ALA:HB3	5:B:657:HOH:O	1.97	0.64
1:A:327:ALA:O	5:A:611:HOH:O	2.15	0.63
4:H:1:NAG:H4	4:H:2:NAG:N2	2.12	0.63
1:B:343:PRO:HG3	5:B:613:HOH:O	1.99	0.62
1:A:248:LYS:NZ	1:A:255:ARG:HH12	1.97	0.62
1:D:301:ARG:NE	4:H:1:NAG:O7	2.32	0.62
1:D:438:GLN:NE2	5:D:610:HOH:O	2.32	0.62
1:B:419:GLN:NE2	5:B:603:HOH:O	1.96	0.62
1:D:249:ASP:OD2	5:D:607:HOH:O	2.16	0.62
1:A:248:LYS:HZ2	1:A:255:ARG:HH12	1.47	0.61
1:A:295:GLN:O	1:A:297:ASN:N	2.32	0.61
1:D:299:THR:CG2	4:H:1:NAG:H2	2.32	0.60
5:A:638:HOH:O	2:E:5:NAG:H82	2.00	0.60
1:D:382:GLU:OE2	1:D:426:SER:OG	2.20	0.59
1:B:360:LYS:HE2	1:B:362:GLN:O	2.02	0.59
1:D:240:VAL:O	1:D:241:PHE:HD2	1.85	0.59
5:B:729:HOH:O	2:F:7:MAN:H62	2.02	0.59
1:D:292:ARG:HD2	1:D:300:TYR:CD1	2.38	0.59
1:A:361:ASN:OD1	5:A:612:HOH:O	2.17	0.59
5:C:691:HOH:O	3:G:8:MAN:H61	2.02	0.58
4:H:4:MAN:O4	4:H:5:NAG:H2	2.03	0.58
1:C:272:GLU:OE2	5:C:608:HOH:O	2.17	0.58
1:D:248:LYS:HD2	1:D:252:MET:SD	2.44	0.57
1:C:240:VAL:O	1:C:334:LYS:HE2	2.06	0.56
1:C:252:MET:HG3	1:C:428:MET:HE3	1.86	0.56
1:A:292:ARG:NH1	5:A:629:HOH:O	2.38	0.55
1:C:283:GLU:HG2	1:C:285:HIS:CE1	2.41	0.55
1:B:311:GLN:OE1	1:B:311:GLN:N	2.38	0.55
5:A:785:HOH:O	2:E:7:MAN:H2	2.07	0.55
5:A:605:HOH:O	2:E:7:MAN:O2	2.04	0.55
1:B:272:GLU:OE2	1:B:326:LYS:HB2	2.07	0.55
1:D:281:GLY:N	5:D:614:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:HG2	5:C:620:HOH:O	2.06	0.54
1:C:389:ASN:ND2	5:C:604:HOH:O	2.12	0.54
1:A:242:LEU:HD23	1:A:336:ILE:HG23	1.90	0.54
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.90	0.54
1:C:388:GLU:OE1	1:C:416:ARG:NH2	2.42	0.53
4:H:2:NAG:HO3	4:H:3:BMA:C2	2.19	0.53
1:B:360:LYS:HD2	1:B:361:ASN:N	2.23	0.53
1:D:362:GLN:OE1	1:D:413:ASP:HA	2.07	0.53
1:D:262:VAL:HG13	1:D:303:VAL:HG22	1.90	0.53
1:D:323:VAL:HG22	1:D:332:ILE:HG23	1.91	0.53
5:A:686:HOH:O	2:E:7:MAN:C3	2.57	0.53
1:A:289:THR:HG23	5:A:698:HOH:O	2.09	0.52
1:B:237:GLY:N	5:B:624:HOH:O	2.42	0.52
5:A:686:HOH:O	2:E:7:MAN:H2	2.10	0.51
1:B:255:ARG:NE	5:B:621:HOH:O	2.40	0.51
1:D:271:PRO:O	1:D:292:ARG:NH1	2.43	0.51
1:A:347:GLN:NE2	5:A:614:HOH:O	2.23	0.51
1:A:399:ASP:OD1	5:A:603:HOH:O	2.19	0.51
1:B:266:VAL:O	1:B:300:TYR:N	2.34	0.51
1:D:248:LYS:O	1:D:252:MET:HG3	2.11	0.51
1:C:292:ARG:NH1	5:C:629:HOH:O	2.44	0.51
1:A:361:ASN:HB3	5:A:718:HOH:O	2.11	0.50
1:A:326:LYS:N	5:A:602:HOH:O	2.45	0.50
1:C:255:ARG:NH1	5:C:622:HOH:O	2.36	0.50
1:B:272:GLU:OE2	1:B:326:LYS:N	2.40	0.50
1:D:301:ARG:HE	4:H:1:NAG:C7	2.24	0.50
1:A:355:ARG:HG3	1:A:356:ASP:H	1.78	0.49
1:C:338:LYS:NZ	5:C:621:HOH:O	2.36	0.49
1:D:353:PRO:HD3	1:D:365:LEU:CD2	2.43	0.49
1:D:359:THR:C	5:D:609:HOH:O	2.51	0.49
1:C:361:ASN:ND2	5:C:630:HOH:O	2.45	0.49
5:A:686:HOH:O	2:E:7:MAN:H3	2.13	0.48
1:D:288:LYS:NZ	5:D:618:HOH:O	2.46	0.48
1:D:301:ARG:NE	4:H:1:NAG:C7	2.77	0.48
1:D:252:MET:HB2	1:D:255:ARG:HG3	1.95	0.48
1:A:355:ARG:HG3	1:A:356:ASP:N	2.30	0.47
1:D:310:HIS:O	1:D:314:LEU:HD13	2.13	0.47
1:D:332:ILE:HD11	1:D:334:LYS:HE3	1.96	0.47
1:D:365:LEU:HB3	1:D:441:LEU:HD23	1.96	0.47
1:A:269:GLU:CD	1:A:269:GLU:H	2.18	0.47
1:D:275:PHE:HE1	5:D:704:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1:NAG:H4	4:H:2:NAG:C7	2.45	0.47
1:B:370:LYS:NZ	5:B:620:HOH:O	2.39	0.47
1:C:318:GLU:OE2	1:C:319:TYR:N	2.48	0.46
1:B:413:ASP:OD1	1:B:415:SER:OG	2.30	0.46
1:A:288:LYS:HD3	5:A:739:HOH:O	2.14	0.46
1:D:240:VAL:CG2	1:D:323:VAL:HG21	2.42	0.46
1:D:351:LEU:HB2	1:D:366:THR:HB	1.98	0.46
1:B:360:LYS:CD	1:B:362:GLN:H	2.24	0.46
1:D:359:THR:O	5:D:609:HOH:O	2.20	0.46
1:D:390:ASN:ND2	5:D:621:HOH:O	2.48	0.46
1:D:271:PRO:HB2	1:D:292:ARG:NH1	2.31	0.45
1:D:347:GLN:HG3	5:D:626:HOH:O	2.16	0.45
1:A:318:GLU:HG3	1:A:335:THR:CG2	2.46	0.45
1:B:241:PHE:CZ	2:F:2:NAG:H61	2.51	0.45
1:D:240:VAL:HG21	1:D:323:VAL:CG2	2.45	0.45
1:A:301:ARG:HD3	5:A:601:HOH:O	2.15	0.45
1:C:252:MET:HG3	1:C:428:MET:CE	2.46	0.45
1:D:248:LYS:HG2	1:D:255:ARG:NH2	2.32	0.45
1:D:358:LEU:HD23	1:D:363:VAL:HG11	2.00	0.44
1:C:388:GLU:OE2	5:C:609:HOH:O	2.20	0.44
1:A:246:LYS:HD3	1:A:246:LYS:HA	1.86	0.44
1:A:414:LYS:HD3	1:A:418:GLN:NE2	2.33	0.44
1:D:301:ARG:NE	4:H:1:NAG:H81	2.10	0.43
1:C:433:HIS:CE1	1:C:434:ASN:OD1	2.71	0.43
1:D:265:ASP:HA	1:D:299:THR:OG1	2.18	0.43
1:C:349:TYR:HD1	5:C:613:HOH:O	2.02	0.43
1:D:246:LYS:N	1:D:246:LYS:CD	2.79	0.43
1:B:392:LYS:HB3	5:B:663:HOH:O	2.19	0.42
1:A:414:LYS:O	1:A:414:LYS:HG2	2.19	0.42
1:B:311:GLN:H	1:B:311:GLN:CD	2.11	0.42
1:B:350:THR:HG23	1:B:439:LYS:HB3	2.02	0.42
1:B:360:LYS:CE	1:B:362:GLN:HB2	2.45	0.42
1:D:246:LYS:HE3	4:H:5:NAG:HN2	1.81	0.42
1:A:426:SER:OG	5:A:613:HOH:O	2.20	0.42
1:D:273:VAL:O	1:D:274:LYS:HD3	2.20	0.42
1:A:370:LYS:HB2	1:A:370:LYS:HE2	1.90	0.42
1:D:436:TYR:OH	1:D:438:GLN:NE2	2.48	0.42
1:B:356:ASP:O	1:B:359:THR:HG23	2.20	0.41
1:C:242:LEU:HG	1:C:336:ILE:HG12	2.02	0.41
1:D:263:VAL:HG12	1:D:302:VAL:O	2.20	0.41
1:D:353:PRO:HD3	1:D:365:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HE2	1:C:380:GLU:OE1	2.21	0.41
1:D:240:VAL:C	1:D:241:PHE:HD2	2.23	0.41
1:D:299:THR:HG23	4:H:1:NAG:H2	2.02	0.41
1:C:351:LEU:HB2	1:C:366:THR:HB	2.03	0.41
1:A:286:ASN:HD22	1:A:286:ASN:H	1.68	0.41
1:A:238:PRO:HD2	1:A:328:LEU:HD13	2.02	0.41
1:A:286:ASN:H	1:A:286:ASN:ND2	2.19	0.41
1:C:360:LYS:HG3	1:C:362:GLN:H	1.86	0.41
1:C:361:ASN:HA	1:C:414:LYS:HE2	2.03	0.41
1:C:295:GLN:O	1:C:297:ASN:N	2.51	0.41
1:C:444:SER:HB3	5:C:702:HOH:O	2.21	0.41
1:D:323:VAL:HG22	1:D:332:ILE:CG2	2.51	0.41
1:D:271:PRO:HB3	1:D:300:TYR:HE1	1.86	0.40
1:C:429:HIS:HB3	1:C:432:LEU:CD2	2.46	0.40
1:A:351:LEU:HB2	1:A:366:THR:HB	2.03	0.40
5:A:686:HOH:O	2:E:7:MAN:C2	2.68	0.40
1:B:257:PRO:HG2	1:B:308:VAL:O	2.22	0.40
1:C:443:LEU:O	1:C:444:SER:OG	2.36	0.40
4:H:5:NAG:N2	4:H:5:NAG:H5	2.36	0.40
1:A:248:LYS:HG3	1:A:252:MET:HE1	2.03	0.40
1:C:338:LYS:HZ2	1:C:338:LYS:HG3	1.71	0.40
1:B:267:SER:CA	5:B:604:HOH:O	2.61	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:MET:SD	5:A:807:HOH:O[1_655]	2.15	0.05
5:B:667:HOH:O	5:C:707:HOH:O[2_649]	2.17	0.03

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	206/225 (92%)	203 (98%)	3 (2%)	0	100	100
1	B	206/225 (92%)	203 (98%)	3 (2%)	0	100	100
1	C	206/225 (92%)	197 (96%)	9 (4%)	0	100	100
1	D	186/225 (83%)	183 (98%)	3 (2%)	0	100	100
All	All	804/900 (89%)	786 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/208 (93%)	190 (98%)	4 (2%)	53	38
1	B	194/208 (93%)	192 (99%)	2 (1%)	76	69
1	C	194/208 (93%)	192 (99%)	2 (1%)	76	69
1	D	182/208 (88%)	175 (96%)	7 (4%)	33	16
All	All	764/832 (92%)	749 (98%)	15 (2%)	55	40

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	328	LEU
1	A	354	SER
1	A	399	ASP
1	B	351	LEU
1	B	399	ASP
1	C	354	SER
1	C	440	SER
1	D	246	LYS
1	D	274	LYS
1	D	301	ARG
1	D	342	GLN
1	D	399	ASP

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Mol	Chain	Res	Type
1	D	415	SER
1	D	424	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	C	285	HIS
1	C	315	ASN
1	C	361	ASN
1	C	384	ASN
1	D	390	ASN
1	D	438	GLN

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)

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	1.84	3 (21%)	17,19,21	1.38	3 (17%)
2	NAG	E	2	2	14,14,15	1.91	4 (28%)	17,19,21	1.52	3 (17%)
2	BMA	E	3	2	11,11,12	1.50	2 (18%)	15,15,17	2.13	3 (20%)
2	MAN	E	4	2	11,11,12	1.80	3 (27%)	15,15,17	1.65	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	5	2	14,14,15	1.86	3 (21%)	17,19,21	1.19	2 (11%)
2	GAL	E	6	2	11,11,12	1.60	1 (9%)	15,15,17	1.28	1 (6%)
2	MAN	E	7	2	11,11,12	1.93	4 (36%)	15,15,17	1.47	3 (20%)
2	NAG	F	1	2,1	14,14,15	1.74	2 (14%)	17,19,21	1.43	2 (11%)
2	NAG	F	2	2	14,14,15	1.82	3 (21%)	17,19,21	1.13	1 (5%)
2	BMA	F	3	2	11,11,12	1.66	3 (27%)	15,15,17	1.55	3 (20%)
2	MAN	F	4	2	11,11,12	1.86	4 (36%)	15,15,17	1.17	1 (6%)
2	NAG	F	5	2	14,14,15	1.81	4 (28%)	17,19,21	1.37	3 (17%)
2	GAL	F	6	2	11,11,12	1.64	2 (18%)	15,15,17	0.97	1 (6%)
2	MAN	F	7	2	11,11,12	2.06	4 (36%)	15,15,17	1.87	3 (20%)
3	NAG	G	1	3,1	14,14,15	2.54	4 (28%)	17,19,21	1.78	7 (41%)
3	NAG	G	2	3	14,14,15	1.85	4 (28%)	17,19,21	1.27	1 (5%)
3	BMA	G	3	3	11,11,12	1.43	1 (9%)	15,15,17	1.68	3 (20%)
3	MAN	G	4	3	11,11,12	1.87	2 (18%)	15,15,17	1.08	2 (13%)
3	NAG	G	5	3	14,14,15	1.82	4 (28%)	17,19,21	1.61	4 (23%)
3	GAL	G	6	3	11,11,12	1.44	2 (18%)	15,15,17	1.22	2 (13%)
3	SIA	G	7	3	20,20,21	2.36	10 (50%)	24,28,31	1.42	4 (16%)
3	MAN	G	8	3	11,11,12	1.92	4 (36%)	15,15,17	0.84	0
4	NAG	H	1	4,1	14,14,15	1.65	3 (21%)	17,19,21	3.40	7 (41%)
4	NAG	H	2	4,1	14,14,15	2.12	5 (35%)	17,19,21	2.32	7 (41%)
4	BMA	H	3	4	11,11,12	1.85	1 (9%)	15,15,17	3.60	6 (40%)
4	MAN	H	4	4	11,11,12	2.12	3 (27%)	15,15,17	2.67	5 (33%)
4	NAG	H	5	4	14,14,15	2.33	4 (28%)	17,19,21	5.41	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	NAG	E	5	2	-	0/6/23/26	0/1/1/1
2	GAL	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	1/2/19/22	0/1/1/1
2	NAG	F	5	2	-	0/6/23/26	0/1/1/1
2	GAL	F	6	2	-	1/2/19/22	0/1/1/1
2	MAN	F	7	2	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
3	NAG	G	5	3	-	0/6/23/26	0/1/1/1
3	GAL	G	6	3	-	1/2/19/22	0/1/1/1
3	SIA	G	7	3	-	5/18/34/38	0/1/1/1
3	MAN	G	8	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4,1	-	3/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	2/2/19/22	0/1/1/1
4	NAG	H	5	4	-	3/6/23/26	0/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	6.98	1.54	1.43
4	H	5	NAG	O5-C1	5.63	1.52	1.43
3	G	7	SIA	C4-C5	-5.29	1.48	1.53
4	H	3	BMA	O5-C1	5.04	1.51	1.43
2	F	7	MAN	O5-C1	4.87	1.51	1.43
4	H	5	NAG	C7-N2	4.67	1.50	1.34
4	H	4	MAN	O5-C1	4.66	1.51	1.43
2	E	6	GAL	O5-C1	4.38	1.50	1.43
3	G	8	MAN	O5-C1	4.36	1.50	1.43
2	F	6	GAL	O5-C1	4.35	1.50	1.43
2	F	4	MAN	O5-C1	4.34	1.50	1.43
2	E	2	NAG	O5-C1	4.28	1.50	1.43
4	H	2	NAG	O5-C1	4.28	1.50	1.43
3	G	7	SIA	O6-C2	4.21	1.49	1.43
2	E	4	MAN	O5-C1	4.19	1.50	1.43
2	F	2	NAG	O5-C1	4.15	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	O5-C1	4.12	1.50	1.43
2	E	1	NAG	O5-C1	4.12	1.50	1.43
3	G	5	NAG	O5-C1	4.06	1.50	1.43
3	G	4	MAN	O5-C1	4.03	1.50	1.43
4	H	1	NAG	O5-C1	3.97	1.50	1.43
2	F	1	NAG	O5-C1	3.97	1.50	1.43
2	E	7	MAN	O5-C1	3.96	1.50	1.43
2	E	3	BMA	O5-C1	3.92	1.50	1.43
4	H	4	MAN	C2-C3	-3.88	1.46	1.52
3	G	7	SIA	C2-C1	3.86	1.55	1.52
2	E	5	NAG	O5-C1	3.72	1.49	1.43
4	H	2	NAG	C7-N2	3.71	1.47	1.34
3	G	3	BMA	O5-C1	3.62	1.49	1.43
2	E	2	NAG	C7-N2	3.62	1.46	1.34
2	E	1	NAG	C7-N2	3.61	1.46	1.34
2	E	5	NAG	C7-N2	3.60	1.46	1.34
3	G	1	NAG	C7-N2	3.55	1.46	1.34
3	G	5	NAG	C7-N2	3.55	1.46	1.34
3	G	4	MAN	C2-C3	-3.52	1.47	1.52
2	F	5	NAG	O5-C1	3.50	1.49	1.43
2	F	5	NAG	C7-N2	3.49	1.46	1.34
2	F	3	BMA	O5-C1	3.48	1.49	1.43
3	G	7	SIA	C10-N5	3.48	1.46	1.34
3	G	1	NAG	O5-C5	3.45	1.50	1.43
3	G	2	NAG	C7-N2	3.44	1.46	1.34
2	F	1	NAG	C7-N2	3.40	1.46	1.34
4	H	2	NAG	C2-N2	3.30	1.51	1.46
3	G	6	GAL	O5-C1	3.29	1.49	1.43
2	F	2	NAG	C7-N2	3.22	1.45	1.34
2	F	3	BMA	C2-C3	-3.19	1.47	1.52
2	E	7	MAN	C2-C3	-3.12	1.47	1.52
3	G	7	SIA	C5-N5	3.09	1.50	1.45
4	H	5	NAG	C8-C7	3.01	1.56	1.50
2	E	4	MAN	C2-C3	-2.94	1.48	1.52
3	G	8	MAN	C2-C3	-2.91	1.48	1.52
2	F	4	MAN	C2-C3	-2.89	1.48	1.52
2	F	7	MAN	O2-C2	2.82	1.49	1.43
2	E	7	MAN	O2-C2	2.80	1.49	1.43
2	F	7	MAN	C2-C3	-2.78	1.48	1.52
4	H	4	MAN	O2-C2	2.72	1.49	1.43
2	E	3	BMA	C2-C3	-2.67	1.48	1.52
2	E	5	NAG	C2-N2	2.67	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	C3-C2	-2.65	1.46	1.52
3	G	8	MAN	O2-C2	2.63	1.48	1.43
3	G	7	SIA	C3-C4	-2.48	1.48	1.52
2	E	7	MAN	O5-C5	2.42	1.48	1.43
3	G	1	NAG	C2-N2	2.42	1.50	1.46
3	G	7	SIA	O1B-C1	-2.41	1.22	1.30
3	G	7	SIA	O10-C10	-2.38	1.17	1.23
4	H	1	NAG	C3-C2	-2.36	1.47	1.52
3	G	6	GAL	C2-C3	-2.32	1.49	1.52
3	G	2	NAG	C2-N2	2.30	1.50	1.46
2	F	6	GAL	C2-C3	-2.29	1.49	1.52
4	H	5	NAG	O5-C5	2.28	1.48	1.43
2	F	5	NAG	C2-N2	2.27	1.50	1.46
2	F	2	NAG	C3-C2	-2.23	1.47	1.52
4	H	1	NAG	C7-N2	2.23	1.42	1.34
2	F	7	MAN	O5-C5	2.23	1.48	1.43
2	E	2	NAG	C2-N2	2.22	1.50	1.46
3	G	5	NAG	C2-N2	2.20	1.50	1.46
2	F	3	BMA	O5-C5	2.18	1.47	1.43
3	G	7	SIA	O6-C6	2.18	1.47	1.44
2	F	5	NAG	O5-C5	2.16	1.47	1.43
2	E	1	NAG	C2-N2	2.12	1.49	1.46
2	F	4	MAN	O5-C5	2.11	1.47	1.43
3	G	7	SIA	O1A-C1	2.11	1.28	1.22
3	G	8	MAN	O5-C5	2.07	1.47	1.43
3	G	5	NAG	C3-C2	-2.06	1.48	1.52
3	G	2	NAG	O5-C5	2.05	1.47	1.43
2	E	4	MAN	O5-C5	2.02	1.47	1.43
2	E	2	NAG	O5-C5	2.02	1.47	1.43
2	F	4	MAN	O2-C2	2.00	1.47	1.43
4	H	2	NAG	O5-C5	2.00	1.47	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	5	NAG	C2-N2-C7	13.07	141.52	122.90
4	H	3	BMA	C1-O5-C5	-12.07	95.83	112.19
4	H	5	NAG	C1-O5-C5	-11.38	96.77	112.19
4	H	5	NAG	C1-C2-N2	-10.15	93.15	110.49
4	H	1	NAG	C1-C2-N2	-9.95	93.49	110.49
4	H	4	MAN	O3-C3-C2	-8.57	93.58	109.99
4	H	5	NAG	O5-C5-C6	7.34	118.70	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	BMA	O3-C3-C2	-5.98	98.53	109.99
4	H	1	NAG	C2-N2-C7	-5.71	114.77	122.90
4	H	2	NAG	O3-C3-C2	-4.63	99.88	109.47
3	G	3	BMA	C1-C2-C3	4.55	115.26	109.67
2	F	7	MAN	C1-O5-C5	-4.49	106.10	112.19
4	H	2	NAG	C1-C2-N2	4.42	118.05	110.49
4	H	1	NAG	O7-C7-N2	-4.02	114.57	121.95
2	E	4	MAN	C1-O5-C5	-3.95	106.84	112.19
3	G	5	NAG	C2-N2-C7	-3.92	117.32	122.90
2	F	1	NAG	C2-N2-C7	-3.88	117.37	122.90
2	E	2	NAG	C2-N2-C7	-3.87	117.39	122.90
4	H	1	NAG	O7-C7-C8	3.86	129.22	122.06
4	H	2	NAG	O4-C4-C5	-3.75	99.99	109.30
2	F	3	BMA	O3-C3-C2	-3.66	102.99	109.99
4	H	1	NAG	C1-O5-C5	-3.58	107.34	112.19
2	E	3	BMA	C1-C2-C3	3.44	113.89	109.67
3	G	1	NAG	C2-N2-C7	-3.39	118.08	122.90
4	H	5	NAG	C3-C4-C5	-3.32	104.32	110.24
2	F	7	MAN	C6-C5-C4	-3.21	105.49	113.00
4	H	2	NAG	C4-C3-C2	3.17	115.66	111.02
2	E	4	MAN	O5-C5-C6	3.15	112.14	107.20
4	H	3	BMA	O5-C1-C2	-3.13	105.93	110.77
4	H	4	MAN	C1-O5-C5	-3.07	108.03	112.19
2	F	7	MAN	O5-C1-C2	-3.00	106.14	110.77
4	H	1	NAG	C4-C3-C2	-2.99	106.64	111.02
2	E	7	MAN	C1-O5-C5	-2.97	108.17	112.19
4	H	3	BMA	O5-C5-C6	2.92	111.78	107.20
2	E	7	MAN	O5-C5-C6	2.91	111.77	107.20
3	G	7	SIA	C4-C5-N5	-2.89	104.66	110.38
2	E	1	NAG	C2-N2-C7	-2.86	118.83	122.90
4	H	2	NAG	C2-N2-C7	2.79	126.87	122.90
3	G	1	NAG	C1-O5-C5	2.76	115.93	112.19
4	H	3	BMA	C2-C3-C4	2.75	115.66	110.89
4	H	5	NAG	C4-C3-C2	2.74	115.03	111.02
2	F	2	NAG	O4-C4-C3	-2.73	104.04	110.35
2	F	4	MAN	C1-C2-C3	2.67	112.95	109.67
3	G	3	BMA	O6-C6-C5	-2.63	102.25	111.29
2	F	3	BMA	C1-C2-C3	2.62	112.89	109.67
3	G	7	SIA	O1B-C1-C2	2.61	120.49	113.03
3	G	4	MAN	O2-C2-C1	-2.58	103.88	109.15
3	G	5	NAG	C1-C2-N2	-2.56	106.12	110.49
4	H	3	BMA	O6-C6-C5	-2.51	102.67	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C8-C7-N2	2.51	120.35	116.10
4	H	4	MAN	O2-C2-C1	-2.50	104.05	109.15
2	F	3	BMA	O2-C2-C1	-2.49	104.06	109.15
2	E	5	NAG	C8-C7-N2	2.48	120.31	116.10
4	H	5	NAG	O4-C4-C3	-2.46	104.65	110.35
2	F	5	NAG	C4-C3-C2	2.46	114.63	111.02
3	G	7	SIA	O1B-C1-O1A	-2.46	118.50	124.09
2	E	6	GAL	C1-C2-C3	2.46	112.69	109.67
4	H	2	NAG	C1-O5-C5	2.45	115.52	112.19
3	G	6	GAL	O6-C6-C5	-2.44	102.92	111.29
4	H	3	BMA	C1-C2-C3	2.41	112.63	109.67
2	E	2	NAG	C8-C7-N2	2.37	120.12	116.10
3	G	1	NAG	O5-C5-C4	2.36	116.56	110.83
2	F	5	NAG	C3-C4-C5	2.30	114.34	110.24
2	E	1	NAG	O5-C1-C2	-2.29	107.67	111.29
4	H	5	NAG	O5-C5-C4	-2.28	105.27	110.83
2	F	1	NAG	O4-C4-C5	-2.28	103.64	109.30
2	E	5	NAG	C2-N2-C7	-2.28	119.66	122.90
3	G	5	NAG	C4-C3-C2	2.26	114.33	111.02
3	G	1	NAG	O4-C4-C5	-2.24	103.73	109.30
3	G	2	NAG	C8-C7-N2	2.23	119.87	116.10
3	G	5	NAG	O4-C4-C3	-2.22	105.22	110.35
3	G	6	GAL	C1-C2-C3	2.21	112.38	109.67
3	G	1	NAG	C6-C5-C4	-2.20	107.85	113.00
3	G	3	BMA	O5-C5-C6	-2.19	103.77	107.20
4	H	2	NAG	O5-C5-C4	2.16	116.09	110.83
4	H	1	NAG	C3-C4-C5	2.15	114.07	110.24
2	E	1	NAG	C8-C7-N2	2.14	119.72	116.10
2	E	7	MAN	O5-C1-C2	-2.12	107.50	110.77
3	G	1	NAG	O5-C5-C6	-2.11	103.89	107.20
2	F	5	NAG	C8-C7-N2	2.07	119.60	116.10
3	G	7	SIA	C6-C5-N5	2.06	114.34	110.91
4	H	4	MAN	O5-C1-C2	-2.04	107.62	110.77
3	G	4	MAN	O5-C1-C2	2.03	113.91	110.77
2	E	2	NAG	C1-O5-C5	-2.03	109.44	112.19
2	F	6	GAL	O2-C2-C3	-2.02	106.09	110.14
4	H	4	MAN	O2-C2-C3	-2.02	106.09	110.14
2	E	3	BMA	O6-C6-C5	-2.00	104.42	111.29

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	7	SIA	C6-C7-C8-C9
3	G	7	SIA	O7-C7-C8-C9
3	G	7	SIA	O7-C7-C8-O8
3	G	8	MAN	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	E	7	MAN	O5-C5-C6-O6
4	H	4	MAN	O5-C5-C6-O6
3	G	8	MAN	C4-C5-C6-O6
2	F	7	MAN	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	H	4	MAN	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	F	7	MAN	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	E	7	MAN	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	5	NAG	C1-C2-N2-C7
2	E	4	MAN	C4-C5-C6-O6
3	G	7	SIA	O8-C8-C9-O9
4	H	2	NAG	C1-C2-N2-C7
3	G	7	SIA	C6-C7-C8-O8
4	H	5	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	G	6	GAL	O5-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
2	F	6	GAL	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
4	H	5	NAG	C3-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	7	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	3	0
4	H	3	BMA	1	0
2	F	2	NAG	1	0
3	G	8	MAN	1	0

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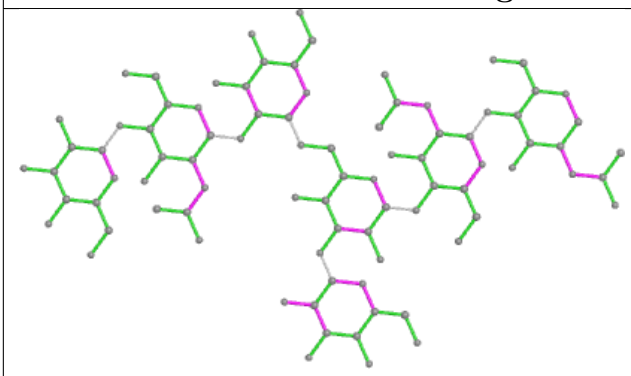
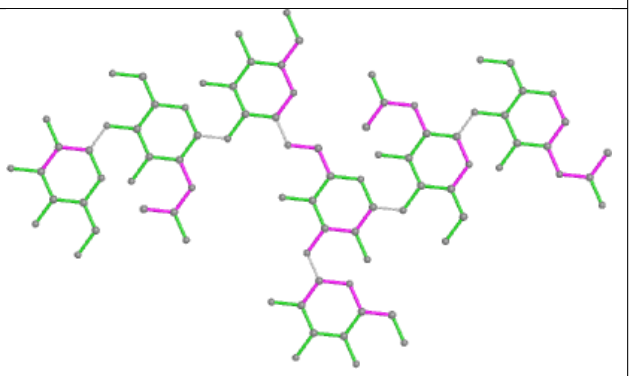
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	7	SIA	1	0
2	F	7	MAN	1	0
4	H	1	NAG	13	0
2	E	7	MAN	6	0
4	H	5	NAG	11	0
2	E	5	NAG	1	0
4	H	4	MAN	1	0

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

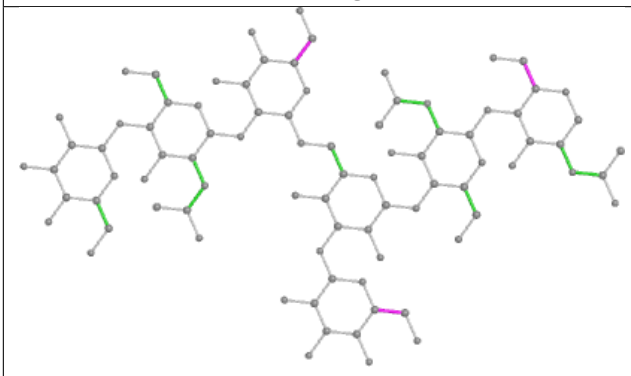
Oligosaccharide Chain E



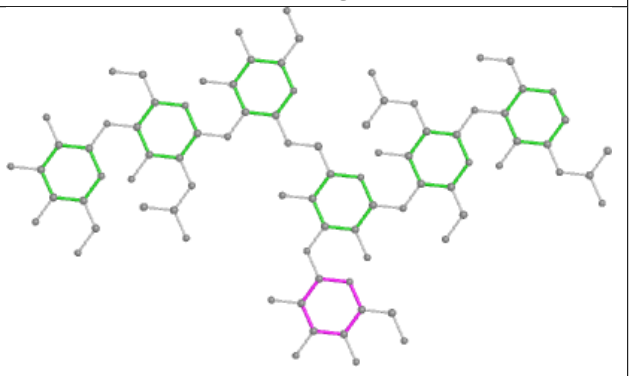
Bond lengths



Bond angles

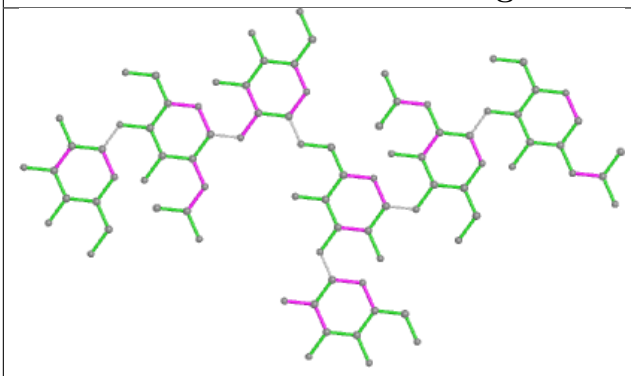


Torsions

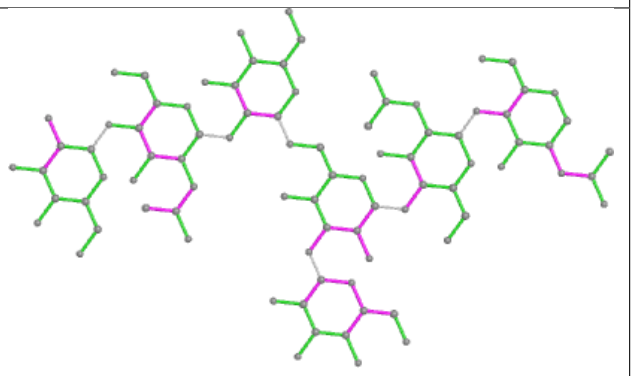


Rings

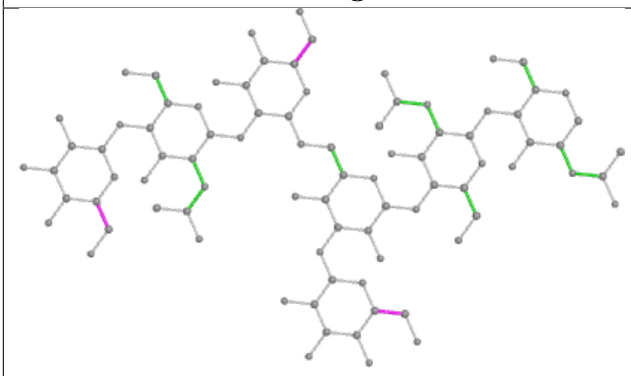
Oligosaccharide Chain F



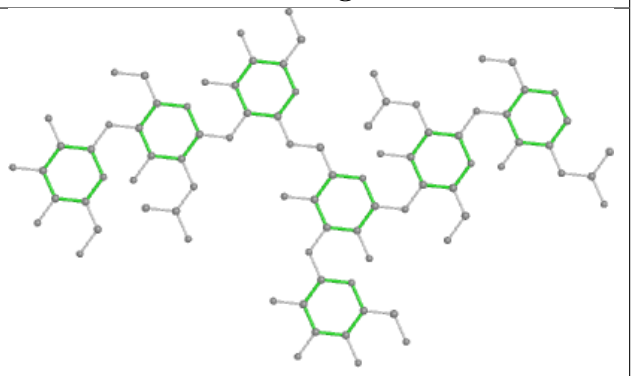
Bond lengths



Bond angles

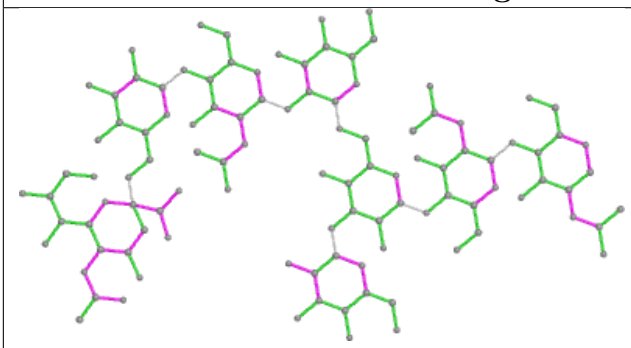


Torsions

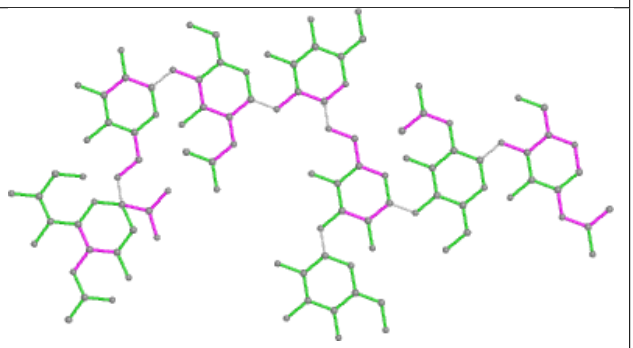


Rings

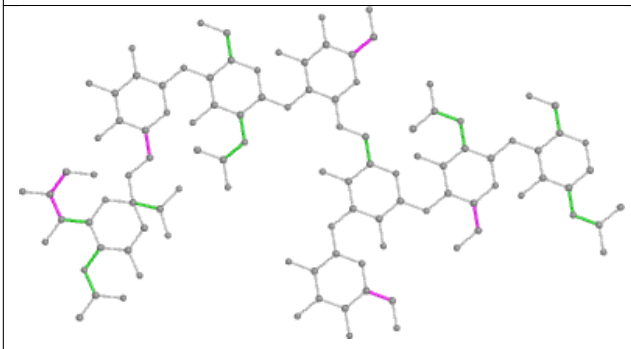
Oligosaccharide Chain G



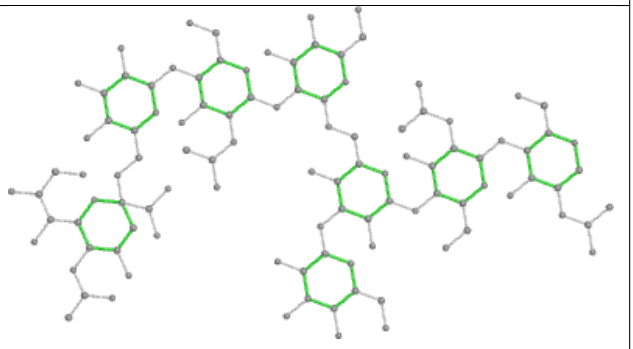
Bond lengths



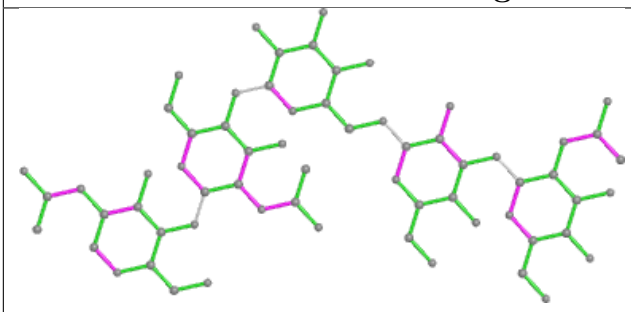
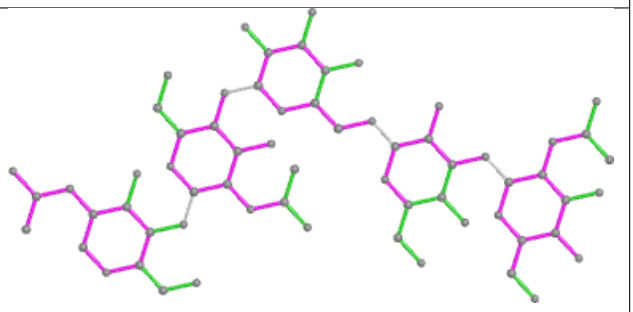
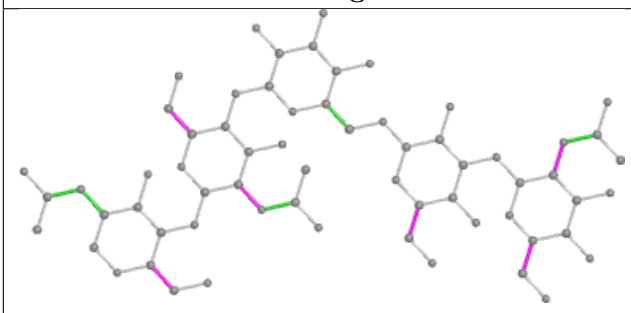
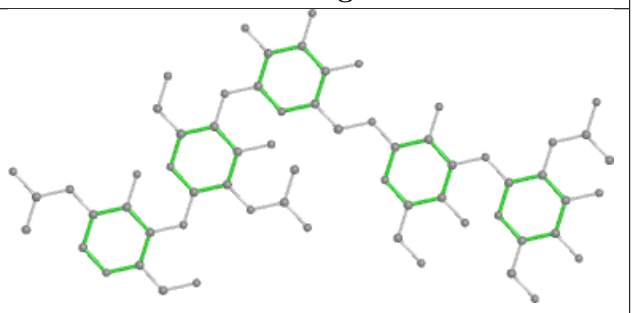
Bond angles



Torsions



Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	208/225 (92%)	-0.09	2 (0%) 82 82	7, 20, 41, 62	0
1	B	208/225 (92%)	-0.01	3 (1%) 75 76	9, 24, 41, 56	0
1	C	208/225 (92%)	0.17	5 (2%) 59 57	10, 28, 46, 56	0
1	D	194/225 (86%)	0.49	24 (12%) 4 4	7, 26, 72, 99	0
All	All	818/900 (90%)	0.13	34 (4%) 36 34	7, 25, 50, 99	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	300	TYR	6.4
1	D	264	VAL	5.2
1	C	296	TYR	5.0
1	D	332	ILE	4.9
1	D	330	ALA	4.7
1	C	359	THR	4.6
1	D	270	ASP	4.6
1	D	298	SER	4.5
1	D	263	VAL	4.2
1	D	273	VAL	4.1
1	D	323	VAL	4.0
1	A	296	TYR	3.9
1	D	262	VAL	3.8
1	D	444	SER	3.5
1	C	358	LEU	3.5
1	D	291	PRO	3.3
1	B	359	THR	3.2
1	D	301	ARG	3.1
1	C	329	PRO	3.0
1	D	324	SER	3.0
1	D	240	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	271	PRO	2.9
1	D	331	PRO	2.8
1	A	355	ARG	2.5
1	C	237	GLY	2.4
1	D	297	ASN	2.4
1	D	333	GLU	2.4
1	D	299	THR	2.2
1	D	278	TYR	2.2
1	B	253	ILE	2.2
1	D	292	ARG	2.2
1	D	241	PHE	2.0
1	B	358	LEU	2.0
1	D	359	THR	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, 95^{th} 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	H	1	14/15	0.51	0.46	90,95,101,101	0
2	MAN	F	7	11/12	0.54	0.36	41,52,57,59	0
4	NAG	H	2	14/15	0.54	0.29	79,86,91,91	0
4	NAG	H	5	14/15	0.65	0.22	40,50,59,60	0
4	BMA	H	3	11/12	0.67	0.27	68,71,75,79	0
4	MAN	H	4	11/12	0.67	0.23	57,65,67,69	0
2	MAN	E	7	11/12	0.67	0.26	34,43,47,51	0
3	MAN	G	8	11/12	0.77	0.17	43,50,54,58	0
2	MAN	F	4	11/12	0.78	0.18	29,33,41,50	0
3	SIA	G	7	20/21	0.86	0.12	16,23,29,42	0
3	MAN	G	4	11/12	0.87	0.15	30,32,37,39	0
3	NAG	G	1	14/15	0.87	0.15	36,41,49,49	0
3	BMA	G	3	11/12	0.88	0.12	31,36,46,52	0
2	GAL	F	6	11/12	0.89	0.11	21,28,33,38	0
2	NAG	F	1	14/15	0.89	0.12	26,32,36,38	0

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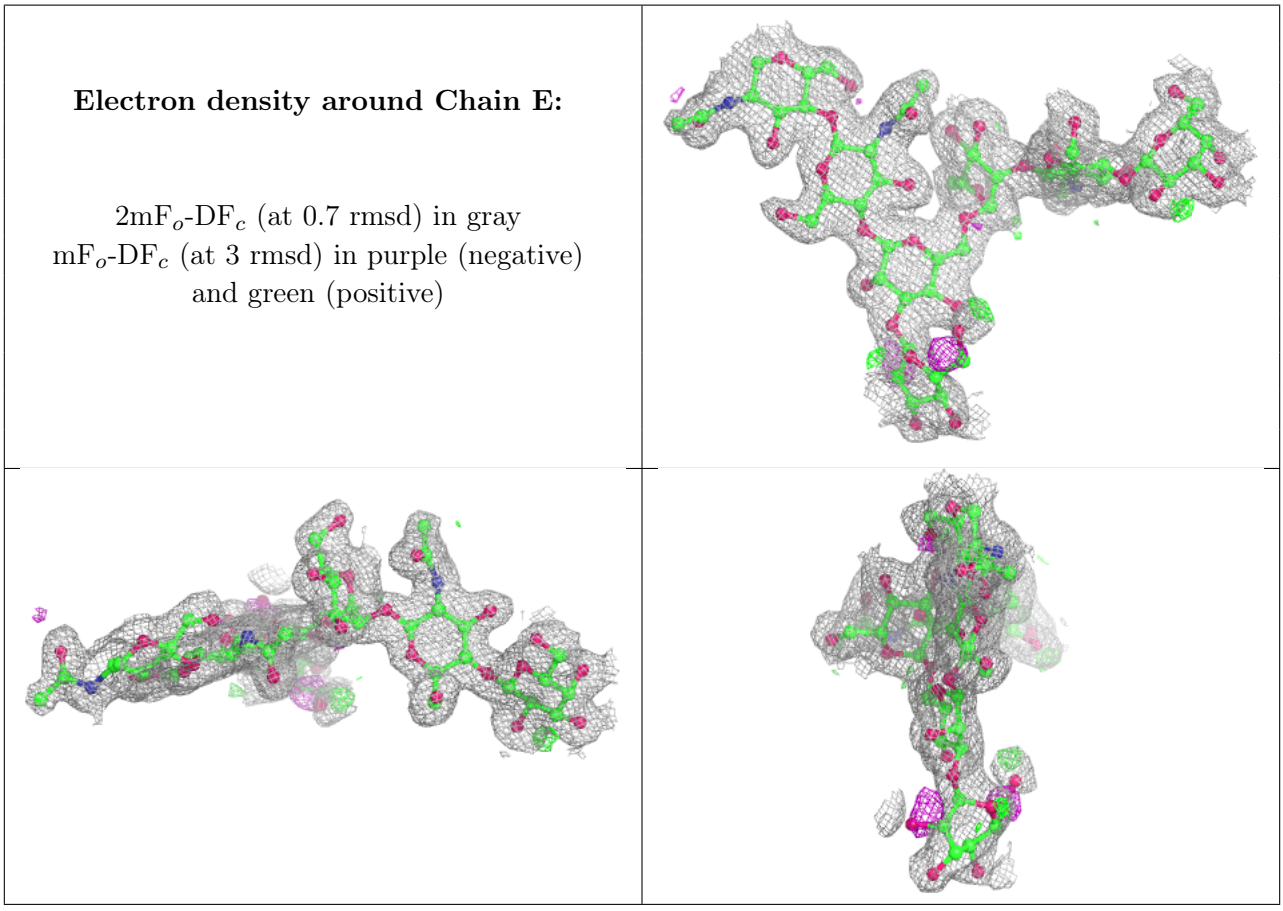
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	14/15	0.90	0.10	26,30,35,37	0
2	BMA	F	3	11/12	0.90	0.09	27,31,36,43	0
2	NAG	E	1	14/15	0.90	0.10	28,36,39,42	0
2	NAG	F	5	14/15	0.90	0.12	24,30,41,43	0
3	NAG	G	5	14/15	0.91	0.11	17,25,35,36	0
3	NAG	G	2	14/15	0.91	0.11	30,33,39,43	0
2	MAN	E	4	11/12	0.92	0.09	25,28,31,40	0
2	BMA	E	3	11/12	0.93	0.11	20,25,28,33	0
2	NAG	E	2	14/15	0.94	0.09	21,27,30,37	0
3	GAL	G	6	11/12	0.95	0.09	12,17,19,21	0
2	NAG	E	5	14/15	0.95	0.08	19,24,29,32	0
2	GAL	E	6	11/12	0.96	0.07	13,18,26,35	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.

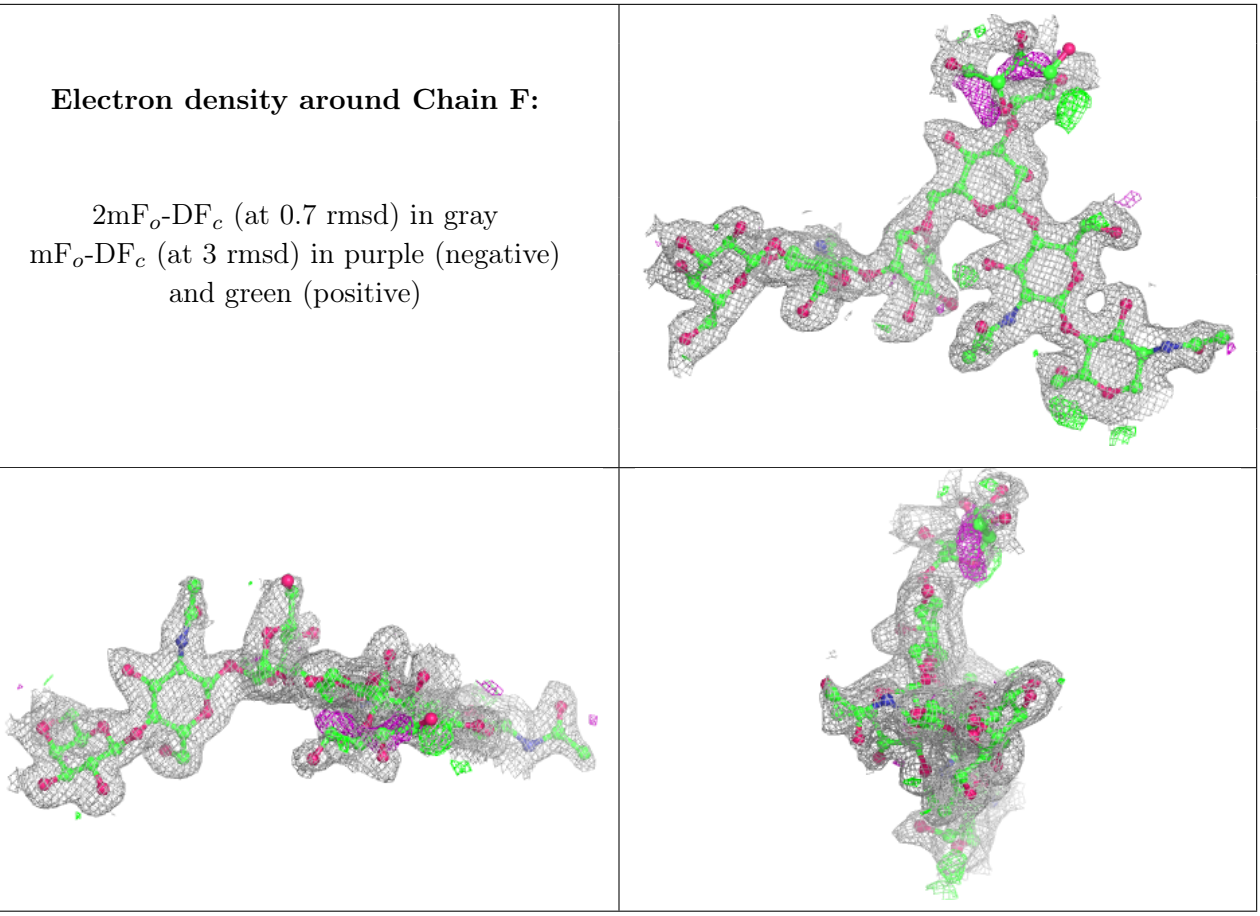
Electron density around Chain E:

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



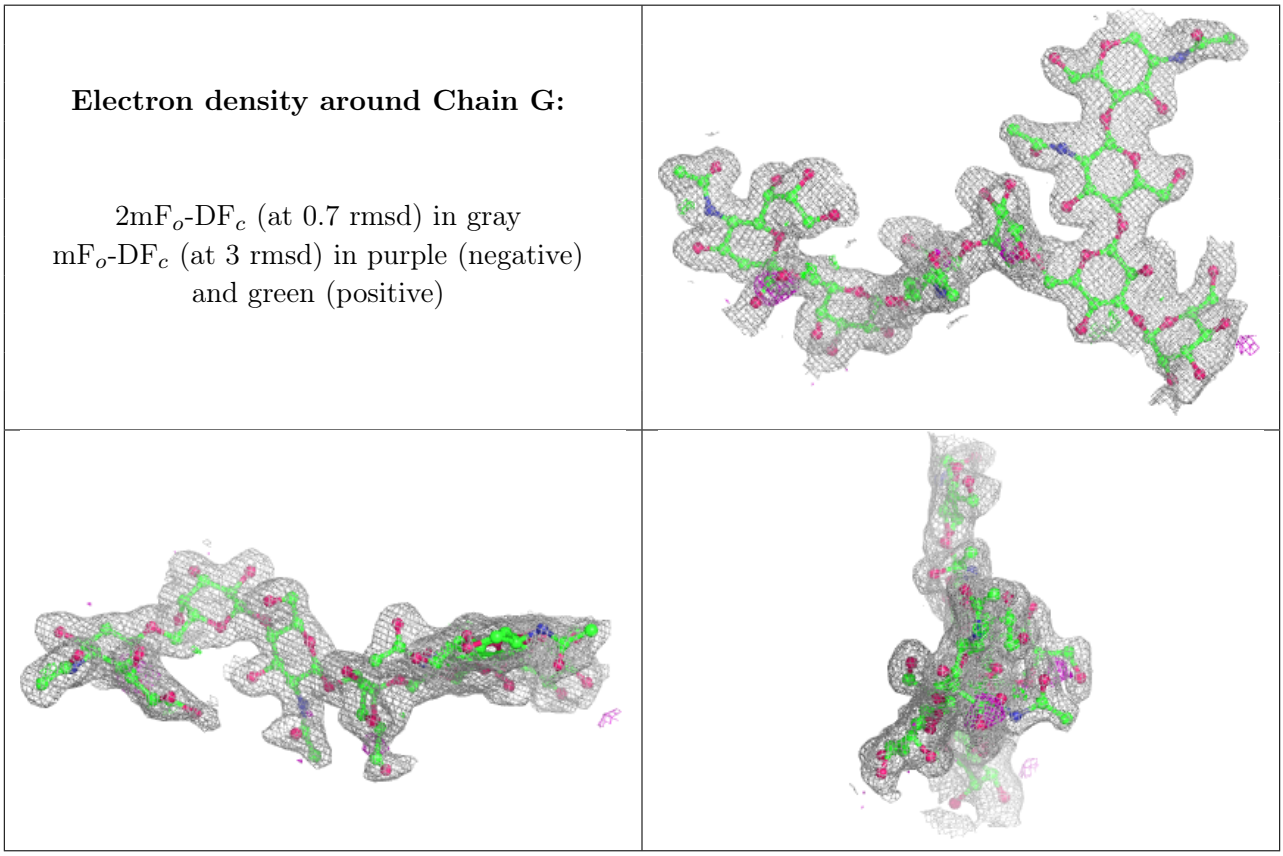
Electron density around Chain F:

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



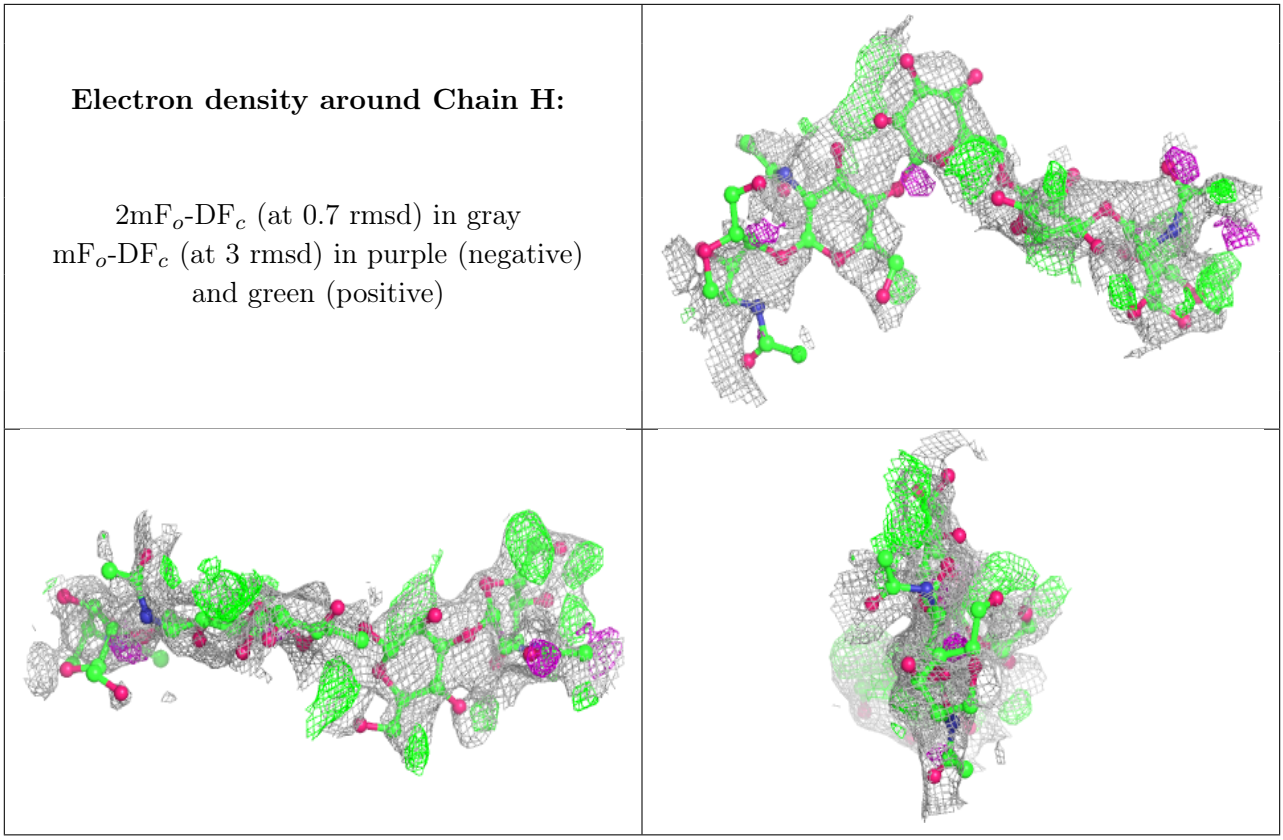
Electron density around Chain G:

$2mF_o$-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 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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.