Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 09:29 PM EDT

PDB ID	:	1OQO
Title	:	Complex between G0 version of an Fc bound to a minimized version of Protein A called Mini-Z
Authors	:	Raju, T.S.; Mulkerrin, M.G.; Parker, M.; De Vos, A.M.; Gazzano-Santoro, H.; Totpal, K.; Ultsch, M.H.
Deposited on	:	2003-03-10
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

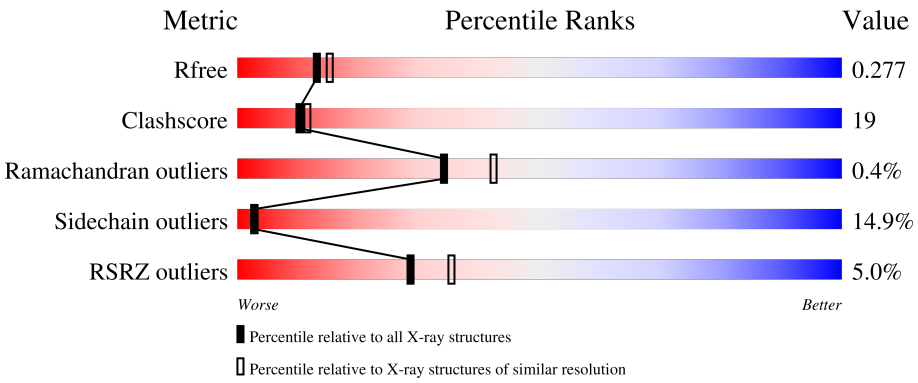
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	212	6% 57% 34% 7% •
1	B	212	4% 52% 40% 7% •
2	C	34	3% 74% 24% •
2	D	34	6% 65% 24% 12%
3	E	8	62% 38%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	8	12% 88%

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	FUC	F	8	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4246 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.

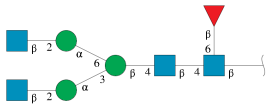
- Molecule 1 is a protein called immunoglobulin gamma-1 heavy chain constant region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1664	1059	280	319	6	0	0	0
1	B	208	1662	1058	280	318	6	0	0	0

- Molecule 2 is a protein called Minimized version of Protein A (Z34C).

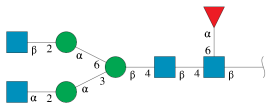
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	34	291	176	57	55	3	0	0	0
2	D	34	291	176	57	55	3	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	8	99	56	4	39	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	8	99	56	4	39	0	0	0

- Molecule 5 is water.

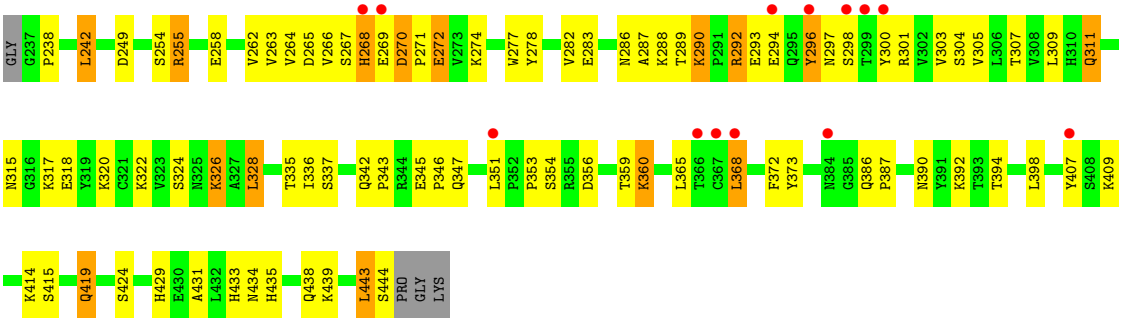
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	59	59	59	0	0
			Total	O		
5	C	18	18	18	0	0
			Total	O		
5	B	54	54	54	0	0
			Total	O		
5	D	9	9	9	0	0

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.

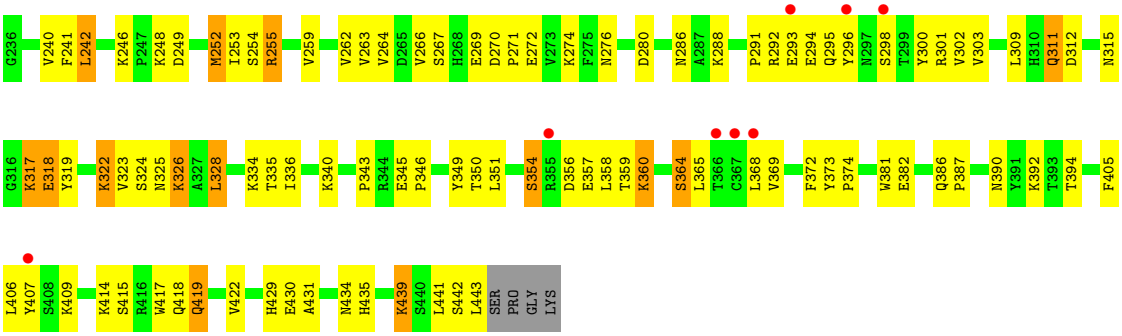
• Molecule 1: immunoglobulin gamma-1 heavy chain constant region

Chain A:



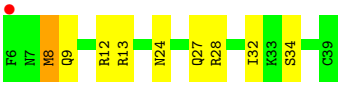
• Molecule 1: immunoglobulin gamma-1 heavy chain constant region

Chain B:



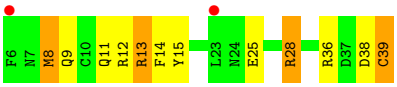
• Molecule 2: Minimized version of Protein A (Z34C)

Chain C:



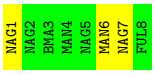
• Molecule 2: Minimized version of Protein A (Z34C)

Chain D:



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

Chain E:



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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.78Å 126.41Å 54.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 24.25 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.30) 99.6 (24.25-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.216 , 0.286 0.211 , 0.277	Depositor DCC
R_{free} test set	2673 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4246	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 7.58% 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 (i)

5.1 Standard geometry (i)

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

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	0.52	0/1710	0.70	0/2330
1	B	0.50	0/1708	0.69	0/2327
2	C	0.49	0/295	0.58	0/393
2	D	0.51	0/295	0.64	0/393
All	All	0.51	0/4008	0.69	0/5443

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1630	63	0
1	B	1662	0	1628	77	0
2	C	291	0	272	11	0
2	D	291	0	272	10	0
3	E	99	0	85	0	0
4	F	99	0	84	4	0
5	A	59	0	0	1	0
5	B	54	0	0	5	0
5	C	18	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	9	0	0	1	0
All	All	4246	0	3971	152	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 19.

All (152) 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:B:252:MET:HG2	5:B:538:HOH:O	1.69	0.93
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.52	0.88
1:A:292:ARG:HD3	1:A:300:TYR:CE2	2.10	0.87
1:B:269:GLU:O	1:B:271:PRO:HD3	1.75	0.85
1:A:386:GLN:HG3	1:A:387:PRO:HD2	1.59	0.81
2:C:8:MET:O	2:C:12:ARG:HG3	1.80	0.81
1:B:359:THR:HG23	1:B:360:LYS:HD2	1.63	0.79
1:A:356:ASP:O	1:A:359:THR:HG22	1.86	0.75
1:A:429:HIS:CD2	1:A:431:ALA:H	2.04	0.75
1:A:429:HIS:HD2	1:A:431:ALA:H	1.33	0.74
1:A:270:ASP:N	1:A:271:PRO:HD3	2.07	0.70
1:B:240:VAL:HG22	1:B:263:VAL:HG22	1.74	0.69
2:C:28:ARG:HD3	5:C:104:HOH:O	1.92	0.68
1:A:292:ARG:HD3	1:A:300:TYR:CD2	2.27	0.68
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.74	0.68
1:B:415:SER:O	1:B:419:GLN:HB2	1.94	0.68
1:B:248:LYS:NZ	1:B:255:ARG:HH12	1.91	0.68
1:B:359:THR:HG23	1:B:360:LYS:CD	2.24	0.67
2:D:38:ASP:O	2:D:39:CYS:HB3	1.94	0.67
1:A:359:THR:HG23	1:A:360:LYS:HE2	1.76	0.66
1:B:270:ASP:HA	1:B:326:LYS:HZ3	1.60	0.66
1:A:443:LEU:O	1:A:444:SER:HB2	1.95	0.66
2:D:8:MET:O	2:D:12:ARG:HG3	1.97	0.65
1:A:249:ASP:OD1	1:A:255:ARG:HD2	1.97	0.65
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.78	0.64
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.78	0.64
1:A:311:GLN:HG2	2:C:32:ILE:CD1	2.28	0.64
1:B:386:GLN:HG3	1:B:387:PRO:HD2	1.81	0.63
1:A:311:GLN:HG2	2:C:32:ILE:HD13	1.80	0.62
1:B:360:LYS:HD2	1:B:360:LYS:N	2.14	0.62
1:A:415:SER:O	1:A:419:GLN:HB2	1.99	0.62
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG13	1:B:336:ILE:HD11	1.81	0.61
1:B:381:TRP:O	1:B:382:GLU:HG3	2.01	0.60
1:B:269:GLU:C	1:B:271:PRO:HD3	2.22	0.60
1:A:290:LYS:HE3	1:A:305:VAL:HG23	1.83	0.60
1:B:262:VAL:HG22	1:B:303:VAL:HG22	1.84	0.58
1:A:360:LYS:O	1:A:414:LYS:HE2	2.03	0.58
1:B:294:GLU:HB3	5:B:507:HOH:O	2.03	0.58
1:B:318:GLU:HG2	1:B:335:THR:CG2	2.34	0.58
1:B:292:ARG:HB2	1:B:300:TYR:HD2	1.69	0.57
1:A:345:GLU:HG3	1:A:431:ALA:O	2.05	0.57
1:A:356:ASP:OD1	1:B:439:LYS:NZ	2.37	0.57
1:B:255:ARG:O	2:D:36:ARG:NH2	2.37	0.57
1:B:292:ARG:HB3	1:B:302:VAL:HG22	1.87	0.57
1:A:311:GLN:CG	2:C:32:ILE:HD13	2.35	0.56
2:D:13:ARG:NH2	5:D:101:HOH:O	2.39	0.56
1:B:345:GLU:HG3	1:B:431:ALA:O	2.06	0.55
1:B:358:LEU:HD22	1:B:418:GLN:HE21	1.71	0.55
1:B:280:ASP:OD2	1:B:317:LYS:HG3	2.06	0.55
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.88	0.55
1:B:292:ARG:HG3	1:B:300:TYR:CE2	2.42	0.55
1:B:374:PRO:O	1:B:429:HIS:HE1	1.91	0.54
1:A:271:PRO:HD2	1:A:326:LYS:NZ	2.23	0.54
1:A:289:THR:HA	1:A:304:SER:HA	1.90	0.54
1:A:262:VAL:HG13	1:A:303:VAL:HG22	1.89	0.53
1:B:325:ASN:HB3	1:B:328:LEU:HD22	1.91	0.53
1:B:291:PRO:HA	5:B:527:HOH:O	2.09	0.52
1:B:311:GLN:O	1:B:315:ASN:HB2	2.08	0.52
1:B:242:LEU:HD13	1:B:336:ILE:HG12	1.91	0.52
1:A:429:HIS:O	1:A:435:HIS:HA	2.10	0.52
1:A:270:ASP:HA	1:A:326:LYS:HZ3	1.75	0.52
1:B:343:PRO:HA	1:B:373:TYR:O	2.10	0.52
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.45	0.51
1:A:354:SER:CB	1:B:349:TYR:HB3	2.40	0.51
2:C:9:GLN:HG2	5:C:115:HOH:O	2.10	0.51
1:A:277:TRP:O	1:A:283:GLU:HA	2.11	0.51
1:B:252:MET:CG	5:B:538:HOH:O	2.42	0.51
2:C:9:GLN:O	2:C:13:ARG:HG3	2.09	0.51
1:A:272:GLU:H	1:A:326:LYS:NZ	2.09	0.51
1:A:292:ARG:HD3	1:A:300:TYR:HE2	1.72	0.51
1:A:343:PRO:HA	1:A:373:TYR:O	2.11	0.51
1:B:418:GLN:HA	1:B:443:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:THR:HG23	1:B:360:LYS:CE	2.41	0.50
1:B:292:ARG:HG3	1:B:300:TYR:HE2	1.75	0.50
1:B:356:ASP:O	1:B:359:THR:HG22	2.12	0.50
1:A:351:LEU:HB3	5:B:528:HOH:O	2.12	0.49
2:D:11:GLN:OE1	2:D:11:GLN:HA	2.12	0.49
1:A:266:VAL:HB	1:A:300:TYR:CB	2.40	0.49
1:A:438:GLN:O	1:A:439:LYS:HG2	2.12	0.49
1:A:278:TYR:CE2	1:A:283:GLU:HB2	2.47	0.49
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.95	0.48
1:A:297:ASN:O	1:A:298:SER:HB2	2.14	0.48
1:B:422:VAL:HG22	1:B:442:SER:HB3	1.94	0.48
1:B:429:HIS:CD2	1:B:431:ALA:H	2.32	0.48
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.14	0.48
1:B:350:THR:O	1:B:351:LEU:HD23	2.12	0.47
2:D:9:GLN:O	2:D:13:ARG:HG3	2.14	0.47
1:A:268:HIS:O	1:A:271:PRO:HG3	2.14	0.47
1:B:248:LYS:HZ3	1:B:255:ARG:HH12	1.60	0.47
1:A:433:HIS:O	1:A:434:ASN:HB2	2.14	0.47
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.97	0.47
1:A:290:LYS:HE3	1:A:305:VAL:CG2	2.44	0.47
1:B:312:ASP:O	1:B:317:LYS:HB2	2.15	0.47
1:B:318:GLU:HG2	1:B:335:THR:HG21	1.96	0.46
1:B:394:THR:HG23	1:B:407:TYR:O	2.15	0.46
1:B:241:PHE:CE2	4:F:2:NAG:H4	2.50	0.46
1:B:270:ASP:HA	1:B:326:LYS:NZ	2.30	0.46
1:B:248:LYS:HZ2	1:B:255:ARG:HH12	1.60	0.46
1:B:269:GLU:N	1:B:269:GLU:OE2	2.47	0.46
1:A:242:LEU:HD13	1:A:336:ILE:HG12	1.98	0.46
1:A:270:ASP:N	1:A:271:PRO:CD	2.73	0.46
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.35	0.45
1:B:295:GLN:OE1	4:F:1:NAG:H62	2.16	0.45
1:B:248:LYS:NZ	1:B:255:ARG:NH1	2.61	0.45
1:A:255:ARG:HH11	1:A:255:ARG:CG	2.28	0.45
1:A:270:ASP:OD1	1:A:326:LYS:HB2	2.16	0.45
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.99	0.45
1:B:294:GLU:HG2	1:B:300:TYR:CZ	2.52	0.45
1:B:429:HIS:HD2	1:B:431:ALA:HB3	1.81	0.45
2:D:25:GLU:HA	2:D:28:ARG:NH2	2.32	0.45
2:D:38:ASP:O	2:D:39:CYS:CB	2.65	0.45
2:C:28:ARG:HG2	2:C:32:ILE:HD12	1.99	0.45
1:B:358:LEU:HD22	1:B:418:GLN:NE2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HB2	1:A:407:TYR:CE1	2.52	0.44
1:B:253:ILE:HB	2:D:14:PHE:CG	2.53	0.44
2:C:9:GLN:CG	5:C:115:HOH:O	2.65	0.44
1:A:394:THR:HG23	1:A:407:TYR:O	2.18	0.44
1:B:350:THR:C	1:B:351:LEU:HD23	2.37	0.44
1:A:264:VAL:O	1:A:265:ASP:HB2	2.18	0.44
1:B:369:VAL:O	1:B:405:PHE:HA	2.18	0.43
1:B:241:PHE:CZ	4:F:2:NAG:H61	2.53	0.43
1:B:417:TRP:CE2	1:B:443:LEU:HD13	2.54	0.43
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.54	0.43
1:B:240:VAL:HG21	1:B:323:VAL:HG21	2.00	0.43
1:A:320:LYS:HG3	1:A:335:THR:OG1	2.19	0.43
1:B:325:ASN:O	1:B:328:LEU:HB2	2.19	0.43
1:A:294:GLU:HG2	1:A:300:TYR:CZ	2.54	0.43
1:A:278:TYR:CD2	1:A:283:GLU:HB2	2.53	0.43
2:C:8:MET:SD	2:C:12:ARG:NH2	2.78	0.43
1:B:364:SER:HB3	1:B:409:LYS:HD2	2.01	0.43
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.54	0.42
1:A:398:LEU:O	1:B:392:LYS:HD2	2.19	0.42
1:A:263:VAL:O	1:A:301:ARG:HA	2.19	0.42
1:A:318:GLU:HG3	1:A:337:SER:HB3	2.00	0.42
1:B:266:VAL:O	1:B:300:TYR:HB2	2.19	0.42
1:B:414:LYS:HB3	1:B:414:LYS:HE2	1.87	0.42
4:F:2:NAG:H82	4:F:8:FUC:C1	2.49	0.42
1:A:270:ASP:HA	1:A:326:LYS:NZ	2.34	0.42
1:A:311:GLN:O	1:A:315:ASN:N	2.52	0.42
1:A:278:TYR:HA	1:A:282:VAL:O	2.20	0.41
1:B:357:GLU:OE2	1:B:364:SER:OG	2.37	0.41
1:A:277:TRP:CD1	1:A:287:ALA:HB2	2.55	0.41
1:B:259:VAL:CG1	1:B:336:ILE:HD11	2.47	0.41
5:A:540:HOH:O	1:B:354:SER:HA	2.20	0.41
1:A:354:SER:HB2	1:B:349:TYR:HB3	2.02	0.41
1:B:246:LYS:O	1:B:249:ASP:HB2	2.20	0.41
1:B:365:LEU:HB3	1:B:441:LEU:HD23	2.03	0.41
1:B:434:ASN:HA	2:D:15:TYR:CG	2.56	0.41
2:C:24:ASN:OD1	2:C:27:GLN:HG3	2.21	0.40
1:A:255:ARG:CG	1:A:255:ARG:NH1	2.82	0.40
1:B:272:GLU:HB3	1:B:326:LYS:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	206/212 (97%)	198 (96%)	6 (3%)	2 (1%)	15	17
1	B	206/212 (97%)	200 (97%)	6 (3%)	0	100	100
2	C	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
2	D	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	476/492 (97%)	460 (97%)	14 (3%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ARG
1	A	296	TYR

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	194/196 (99%)	161 (83%)	33 (17%)	2	2
1	B	193/196 (98%)	165 (86%)	28 (14%)	3	3
2	C	32/32 (100%)	30 (94%)	2 (6%)	18	24
2	D	32/32 (100%)	28 (88%)	4 (12%)	4	5
All	All	451/456 (99%)	384 (85%)	67 (15%)	3	3

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	254	SER
1	A	255	ARG
1	A	258	GLU
1	A	267	SER
1	A	268	HIS
1	A	269	GLU
1	A	270	ASP
1	A	272	GLU
1	A	274	LYS
1	A	286	ASN
1	A	288	LYS
1	A	290	LYS
1	A	293	GLU
1	A	296	TYR
1	A	307	THR
1	A	309	LEU
1	A	311	GLN
1	A	317	LYS
1	A	322	LYS
1	A	324	SER
1	A	326	LYS
1	A	328	LEU
1	A	342	GLN
1	A	347	GLN
1	A	360	LYS
1	A	368	LEU
1	A	390	ASN
1	A	392	LYS
1	A	409	LYS
1	A	419	GLN
1	A	424	SER
1	A	443	LEU
2	C	8	MET
2	C	34	SER
1	B	242	LEU
1	B	252	MET
1	B	254	SER
1	B	255	ARG
1	B	267	SER
1	B	274	LYS
1	B	286	ASN
1	B	288	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	293	GLU
1	B	296	TYR
1	B	298	SER
1	B	309	LEU
1	B	311	GLN
1	B	317	LYS
1	B	318	GLU
1	B	322	LYS
1	B	324	SER
1	B	326	LYS
1	B	328	LEU
1	B	334	LYS
1	B	340	LYS
1	B	354	SER
1	B	360	LYS
1	B	364	SER
1	B	390	ASN
1	B	406	LEU
1	B	419	GLN
1	B	439	LYS
2	D	8	MET
2	D	13	ARG
2	D	28	ARG
2	D	39	CYS

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

Mol	Chain	Res	Type
1	A	361	ASN
1	A	390	ASN
1	A	429	HIS
1	A	434	ASN
2	C	19	HIS
1	B	361	ASN
1	B	362	GLN
1	B	384	ASN
1	B	390	ASN
1	B	418	GLN
1	B	429	HIS
1	B	434	ASN
2	D	19	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)

16 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	E	1	1,3	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
3	NAG	E	2	3	14,14,15	0.63	0	17,19,21	0.56	0
3	BMA	E	3	3	11,11,12	0.47	0	15,15,17	0.63	0
3	MAN	E	4	3	11,11,12	0.54	0	15,15,17	0.63	0
3	NAG	E	5	3	14,14,15	0.61	0	17,19,21	0.65	0
3	MAN	E	6	3	11,11,12	0.55	0	15,15,17	0.91	1 (6%)
3	NAG	E	7	3	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
3	FUL	E	8	3	10,10,11	0.71	0	14,14,16	0.72	0
4	NAG	F	1	1,4	14,14,15	0.58	0	17,19,21	0.69	0
4	NAG	F	2	4	14,14,15	0.54	0	17,19,21	0.75	0
4	BMA	F	3	4	11,11,12	0.44	0	15,15,17	1.04	2 (13%)
4	MAN	F	4	4	11,11,12	1.00	1 (9%)	15,15,17	1.57	2 (13%)
4	NDG	F	5	4	14,14,15	0.66	0	17,19,21	0.85	1 (5%)
4	MAN	F	6	4	11,11,12	0.57	0	15,15,17	0.73	1 (6%)
4	NAG	F	7	4	14,14,15	0.51	0	17,19,21	0.57	0
4	FUC	F	8	4	10,10,11	0.78	0	14,14,16	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	1/6/23/26	0/1/1/1
3	MAN	E	6	3	-	2/2/19/22	0/1/1/1
3	NAG	E	7	3	-	2/6/23/26	0/1/1/1
3	FUL	E	8	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NDG	F	5	4	-	2/6/23/26	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	NAG	F	7	4	-	0/6/23/26	0/1/1/1
4	FUC	F	8	4	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	C2-C3	2.86	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4	MAN	C1-C2-C3	4.94	115.74	109.67
3	E	7	NAG	C2-N2-C7	-2.46	119.40	122.90
3	E	1	NAG	C2-N2-C7	-2.29	119.64	122.90
4	F	4	MAN	O2-C2-C3	2.28	114.71	110.14
4	F	6	MAN	C1-O5-C5	2.28	115.28	112.19
4	F	3	BMA	O3-C3-C4	-2.25	105.14	110.35
4	F	3	BMA	C2-C3-C4	2.11	114.54	110.89
4	F	5	NDG	C2-N2-C7	-2.08	119.94	122.90
3	E	6	MAN	C1-O5-C5	2.02	114.93	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	8	FUC	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	7	NAG	O5-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
3	E	7	NAG	C4-C5-C6-O6
4	F	5	NDG	C4-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
4	F	5	NDG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6

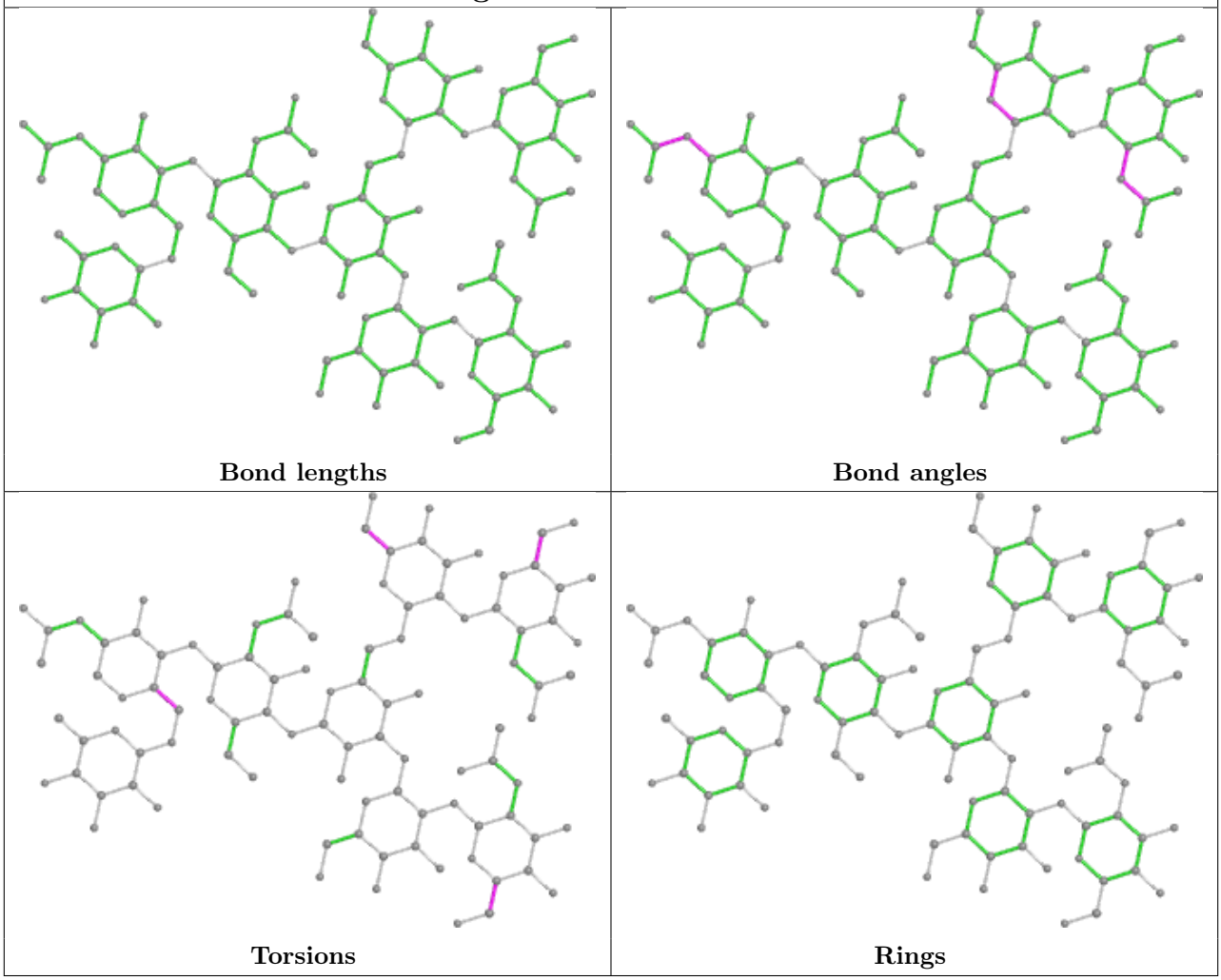
There are no ring outliers.

3 monomers are involved in 4 short contacts:

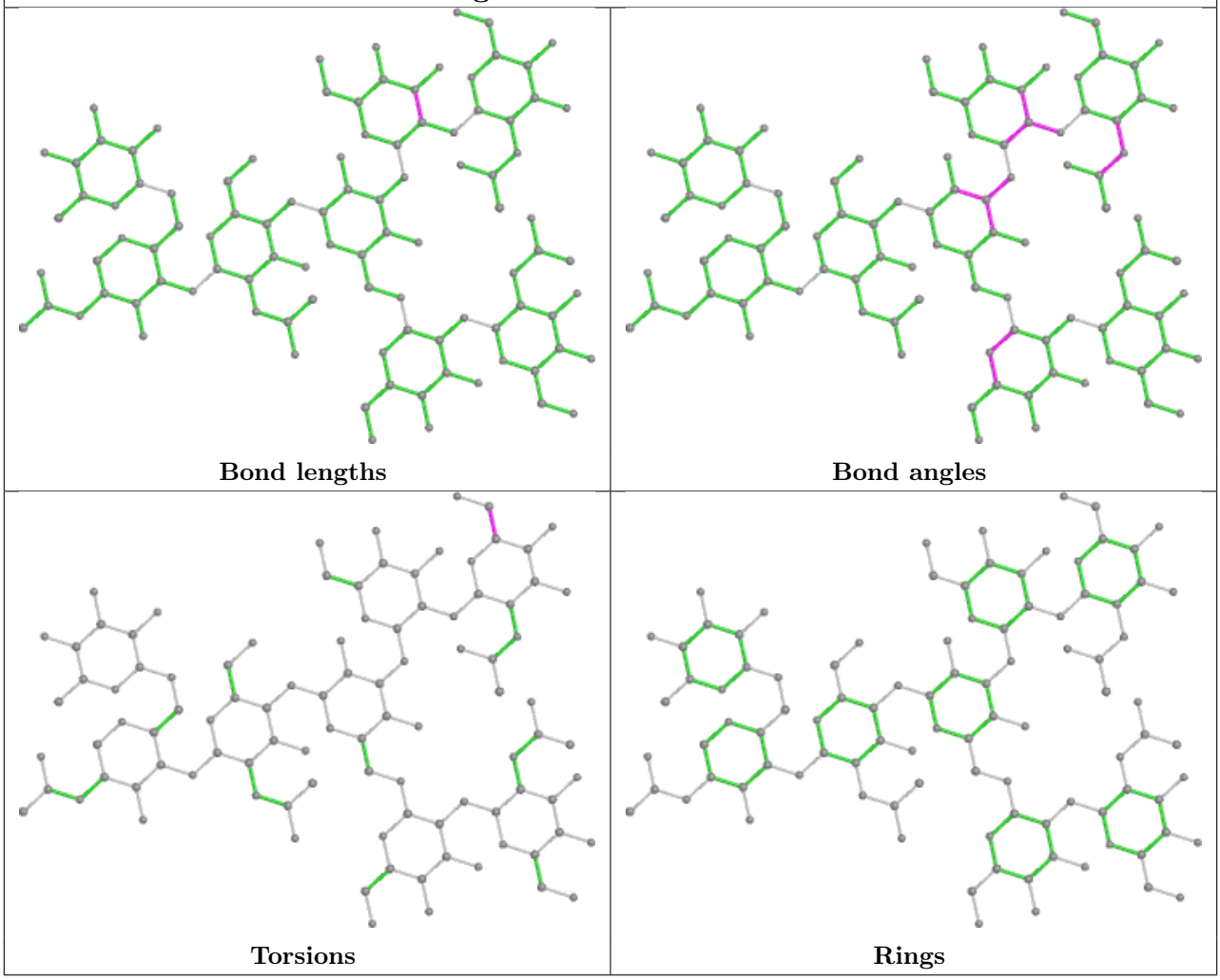
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	3	0
4	F	8	FUC	1	0
4	F	1	NAG	1	0

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



Oligosaccharide Chain F



5.6 Ligand geometry (i)

There are no ligands in this entry.

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	208/212 (98%)	-0.03	13 (6%)	20	25	19, 36, 72, 96	0
1	B	208/212 (98%)	0.05	8 (3%)	40	47	21, 36, 72, 92	0
2	C	34/34 (100%)	0.05	1 (2%)	51	58	25, 42, 71, 99	0
2	D	34/34 (100%)	0.36	2 (5%)	22	28	29, 48, 73, 88	0
All	All	484/492 (98%)	0.04	24 (4%)	28	35	19, 38, 73, 99	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	6	PHE	10.5
1	A	296	TYR	7.8
1	B	296	TYR	5.6
2	D	6	PHE	5.6
1	B	366	THR	3.6
1	A	299	THR	3.4
1	B	368	LEU	3.0
1	A	300	TYR	2.9
1	B	407	TYR	2.8
2	D	23	LEU	2.6
1	A	368	LEU	2.6
1	B	367	CYS	2.5
1	A	351	LEU	2.5
1	A	294	GLU	2.4
1	A	366	THR	2.4
1	B	298	SER	2.2
1	A	269	GLU	2.2
1	A	407	TYR	2.2
1	A	268	HIS	2.2
1	A	367	CYS	2.1
1	B	355	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	384	ASN	2.1
1	B	293	GLU	2.1
1	A	298	SER	2.0

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

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

6.3 Carbohydrates (i)

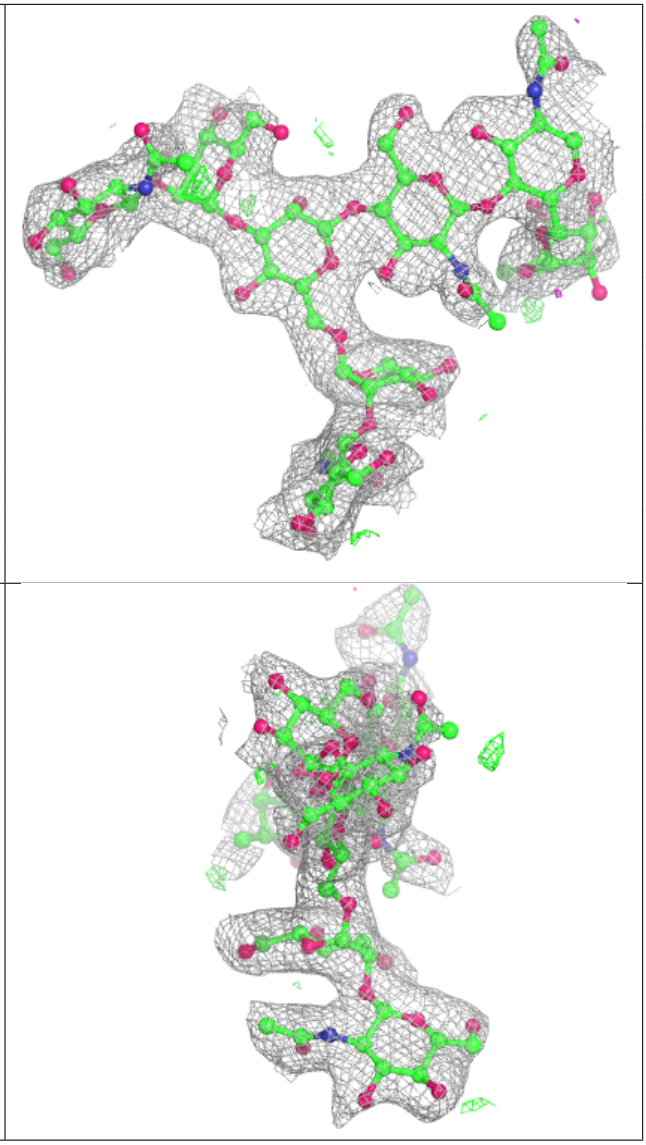
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	1	14/15	0.79	0.17	62,75,83,87	0
3	FUL	E	8	10/11	0.82	0.31	80,85,91,97	0
3	NAG	E	7	14/15	0.84	0.14	60,65,68,75	0
4	NDG	F	5	14/15	0.85	0.24	75,84,90,93	0
4	MAN	F	4	11/12	0.86	0.13	49,57,62,71	0
4	FUC	F	8	10/11	0.86	0.25	66,71,75,90	0
4	NAG	F	1	14/15	0.87	0.14	49,56,66,71	0
3	NAG	E	5	14/15	0.90	0.24	84,91,95,99	0
3	MAN	E	4	11/12	0.92	0.14	59,67,76,78	0
3	NAG	E	2	14/15	0.92	0.15	52,57,62,62	0
4	MAN	F	6	11/12	0.92	0.09	33,41,48,50	0
4	NAG	F	7	14/15	0.92	0.10	33,36,41,42	0
3	MAN	E	6	11/12	0.92	0.15	49,56,65,66	0
4	NAG	F	2	14/15	0.93	0.11	38,47,50,60	0
3	BMA	E	3	11/12	0.94	0.11	37,46,51,52	0
4	BMA	F	3	11/12	0.95	0.07	44,46,55,57	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.

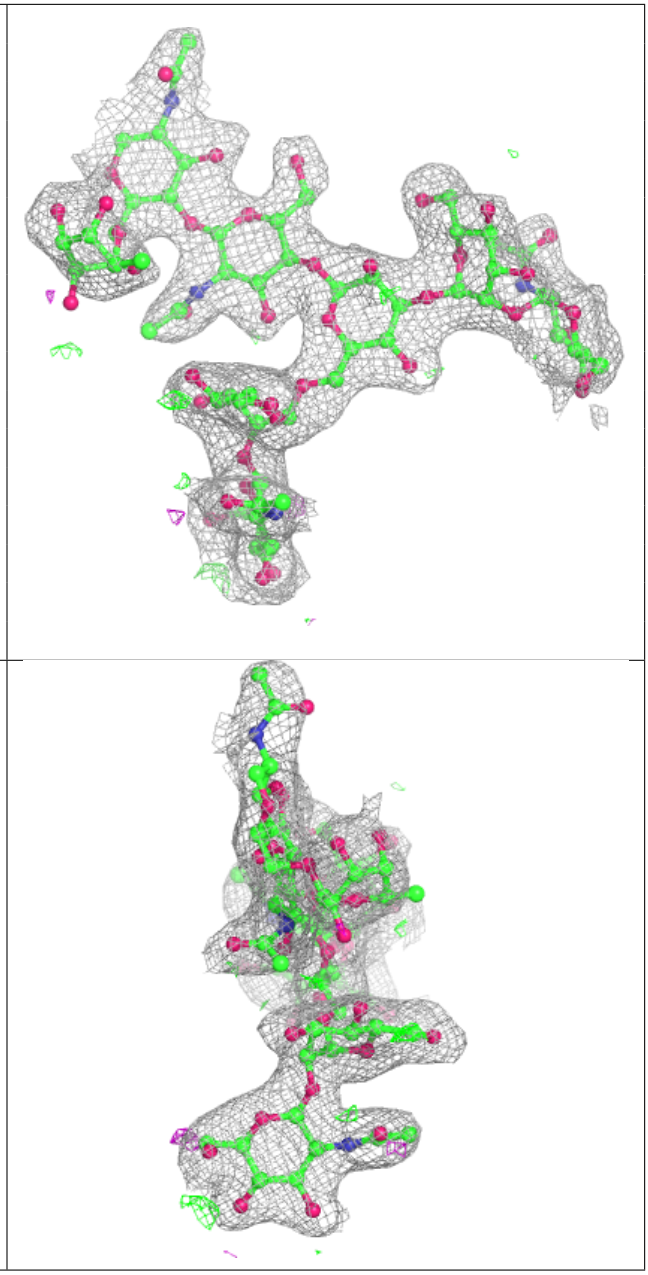
Electron density around Chain E:

$2mF_o$-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)



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.