Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2021 – 01:19 AM EDT

PDB ID	:	3KEH
Title	:	Crystal Structure of N370S Glucocerebrosidase mutant at pH 7.4
Authors	:	Wei, R.R.; Boucher, S.; Pan, C.Q.; Edmunds, T.
Deposited on	:	2009-10-26
Resolution	:	2.80 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 following versions of software and data (see references (i)) were used in the production of this report:

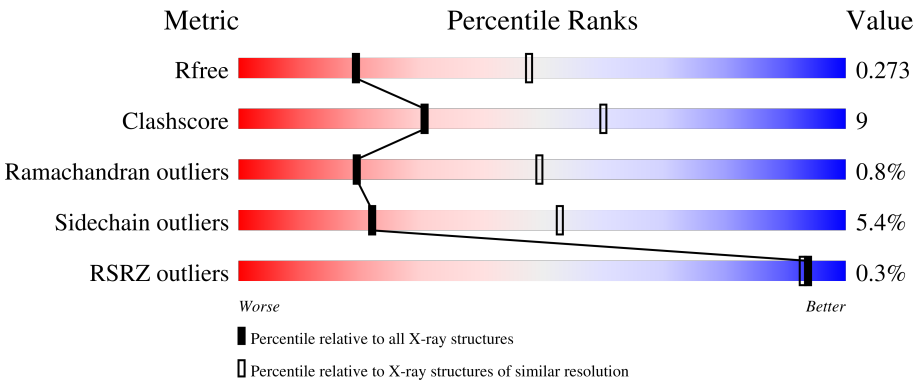
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	497	75% 22% •
1	B	497	% 75% 23% •
2	C	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1501	-	-	-	X
4	SO4	A	1502	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8008 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 Glucocerebrosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3928	2531	671	710	16	0	0	0
1	B	497	3929	2531	671	711	16	0	0	0

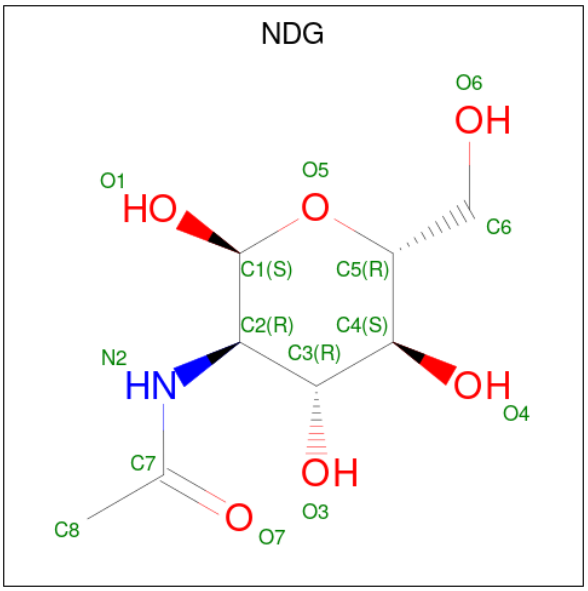
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	SER	ASN	engineered mutation	UNP P04062
B	370	SER	ASN	engineered mutation	UNP P04062

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

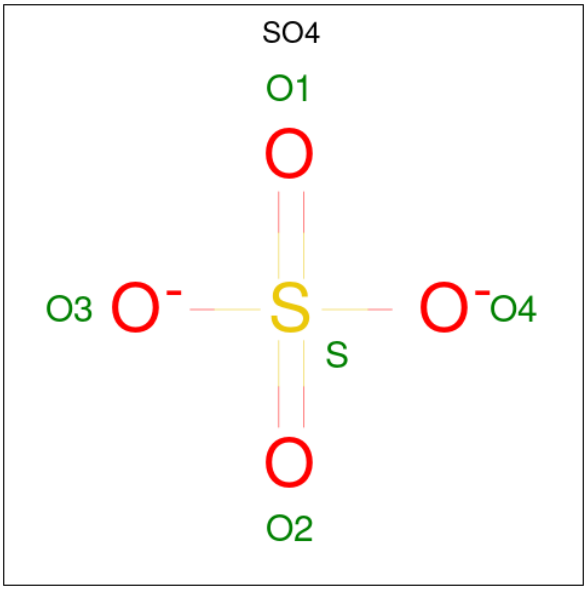
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
4	A	1	5	4	1		0	0
			Total	O	S			
4	A	1	5	4	1		0	0
			Total	O	S			
4	A	1	5	4	1		0	0

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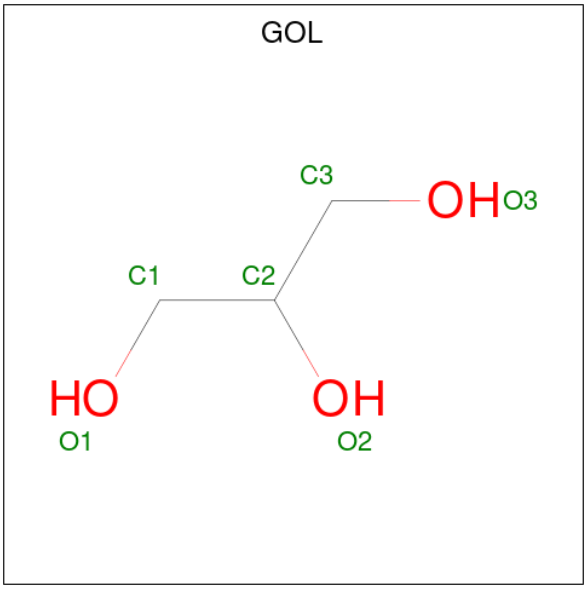
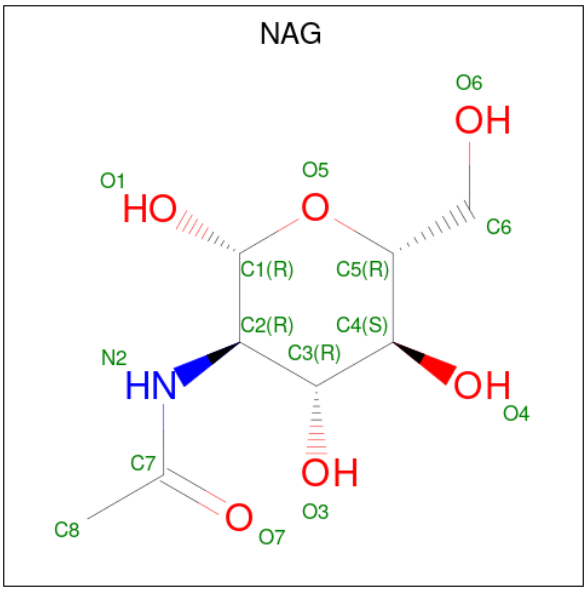
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
			Total	O	S		
4	A	1	5	4	1	0	0
			Total	O	S		
4	B	1	5	4	1	0	0
			Total	O	S		
4	B	1	5	4	1	0	0
			Total	O	S		
4	B	1	5	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	B	1	6	3	3	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

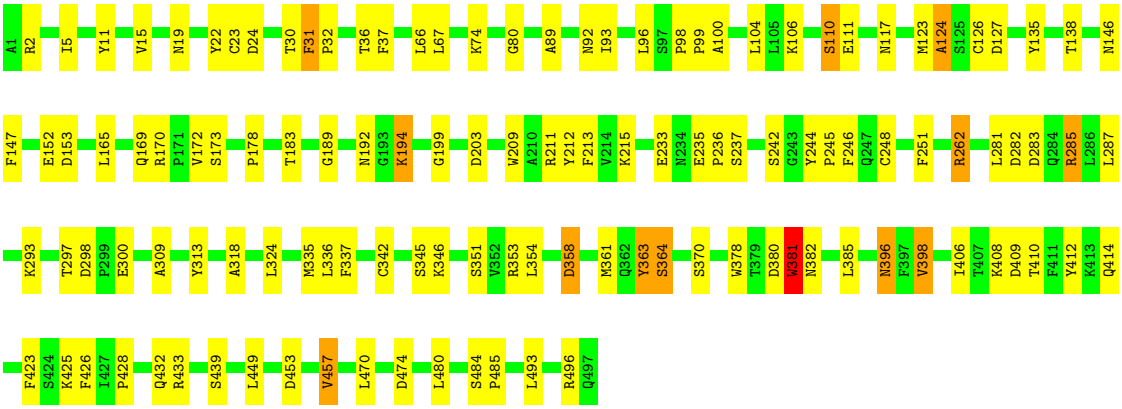
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	16	Total O 16 16	0	0
7	B	26	Total O 26 26	0	0

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.

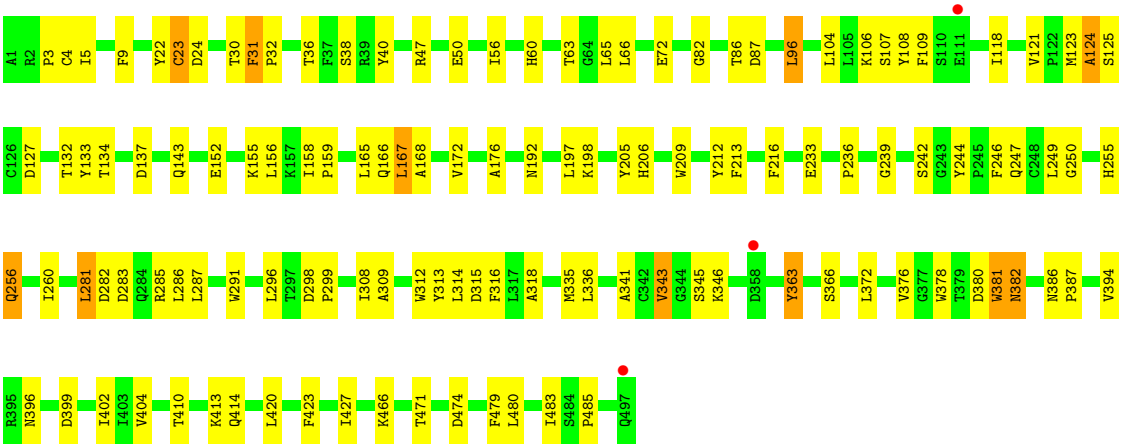
• Molecule 1: Glucocerebrosidase

Chain A:



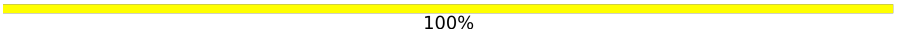
• Molecule 1: Glucocerebrosidase

Chain B:



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

Chain C:



NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.83Å 285.92Å 92.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 71.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.80) 94.2 (71.41-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.212 , 0.273 0.212 , 0.273	Depositor DCC
R_{free} test set	1698 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8008	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 4.74% 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: NDG, GOL, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.71	2/4048 (0.0%)	0.78	0/5519
1	B	0.76	1/4049 (0.0%)	0.78	2/5519 (0.0%)
All	All	0.73	3/8097 (0.0%)	0.78	2/11038 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	CYS	CB-SG	6.83	1.93	1.82
1	B	23	CYS	CB-SG	5.51	1.91	1.82
1	A	126	CYS	CB-SG	-5.16	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	LEU	CA-CB-CG	6.39	129.99	115.30
1	B	96	LEU	CB-CG-CD1	-5.02	102.46	111.00

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	3928	0	3849	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3929	0	3847	67	0
2	C	28	0	25	0	0
3	A	14	0	12	2	0
4	A	25	0	0	1	0
4	B	15	0	0	0	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
6	A	1	0	0	0	0
6	B	14	0	13	0	0
7	A	16	0	0	0	0
7	B	26	0	0	1	0
All	All	8008	0	7762	144	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 9.

All (144) 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:19:ASN:HD21	3:A:1997:NDG:C1	1.45	1.30
1:A:281:LEU:O	1:A:281:LEU:HG	1.60	1.00
1:A:19:ASN:ND2	3:A:1997:NDG:C1	2.28	0.95
1:A:169:GLN:HB3	1:A:170:ARG:HG3	1.53	0.89
1:B:256:GLN:O	1:B:260:ILE:HG13	1.74	0.87
1:A:74:LYS:HB3	1:A:432:GLN:NE2	1.94	0.82
1:B:312:TRP:CZ3	1:B:366:SER:HB2	2.14	0.81
1:B:206:HIS:NE2	1:B:255:HIS:HE1	1.85	0.74
1:B:316:PHE:CZ	1:B:346:LYS:HG3	2.23	0.74
1:A:67:LEU:HG	1:A:470:LEU:HD11	1.70	0.73
1:A:363:TYR:OH	1:A:380:ASP:OD1	2.06	0.73
1:B:281:LEU:O	1:B:309:ALA:O	2.08	0.71
1:A:281:LEU:O	1:A:281:LEU:CG	2.30	0.70
1:B:198:LYS:HD3	1:B:205:TYR:CE2	2.29	0.68
1:A:457:VAL:HB	1:A:493:LEU:HD23	1.78	0.65
1:A:211:ARG:O	1:A:215:LYS:HG2	1.98	0.64
1:A:111:GLU:HB2	1:A:169:GLN:HG3	1.79	0.64
1:A:285:ARG:NH2	1:A:318:ALA:HB3	2.15	0.62
1:A:11:TYR:CE2	1:A:353:ARG:HD3	2.35	0.61
1:B:104:LEU:HD23	1:B:104:LEU:O	2.00	0.61
1:A:244:TYR:HD2	1:A:248:CYS:HG	1.49	0.59
1:A:354:LEU:HA	1:A:414:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:HA	1:A:361:MET:HE2	1.84	0.59
1:B:104:LEU:HD23	1:B:104:LEU:C	2.23	0.59
1:B:5:ILE:HG12	1:B:22:TYR:CE2	2.38	0.58
1:B:3:PRO:O	1:B:22:TYR:OH	2.18	0.58
1:B:281:LEU:O	1:B:281:LEU:HG	2.03	0.58
1:A:194:LYS:HB2	1:A:242:SER:HA	1.86	0.58
1:A:32:PRO:HB2	1:A:36:THR:HB	1.86	0.57
1:A:293:LYS:O	1:A:297:THR:HG23	2.05	0.57
1:B:315:ASP:OD1	1:B:343:VAL:HG12	2.05	0.57
1:A:298:ASP:OD1	1:A:298:ASP:C	2.43	0.57
1:B:108:TYR:CE1	1:B:402:ILE:HD12	2.40	0.57
1:B:233:GLU:O	1:B:282:ASP:HB3	2.03	0.57
1:A:92:ASN:ND2	1:A:385:LEU:HA	2.20	0.57
1:B:336:LEU:O	1:B:376:VAL:HG22	2.05	0.56
1:A:5:ILE:HG12	1:A:22:TYR:CE2	2.40	0.56
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.40	0.56
1:A:345:SER:O	1:A:346:LYS:C	2.44	0.56
1:A:408:LYS:O	1:A:410:THR:HG23	2.06	0.55
1:A:474:ASP:OD1	1:A:496:ARG:NH2	2.31	0.55
1:B:127:ASP:HB3	1:B:246:PHE:CD1	2.41	0.55
1:A:281:LEU:O	1:A:309:ALA:O	2.25	0.54
1:B:4:CYS:HA	1:B:24:ASP:HB3	1.90	0.54
1:B:471:THR:HA	1:B:480:LEU:O	2.08	0.54
1:A:138:THR:HG21	1:A:146:ASN:HD22	1.73	0.54
1:A:111:GLU:HA	1:A:169:GLN:NE2	2.23	0.53
1:A:66:LEU:HB3	1:A:439:SER:HB3	1.89	0.53
1:B:239:GLY:HA3	1:B:250:GLY:CA	2.39	0.52
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.91	0.52
1:A:74:LYS:HB3	1:A:432:GLN:HE21	1.74	0.52
1:B:197:LEU:HD23	1:B:249:LEU:HD11	1.92	0.52
1:B:23:CYS:SG	1:B:413:LYS:HE2	2.50	0.51
1:A:262:ARG:HH11	1:A:262:ARG:HB3	1.75	0.51
1:A:24:ASP:HB2	5:A:1509:GOL:H11	1.92	0.51
1:B:96:LEU:HD21	1:B:404:VAL:HG13	1.92	0.51
1:A:324:LEU:HD22	1:A:336:LEU:HD13	1.93	0.51
1:B:121:VAL:O	1:B:176:ALA:HA	2.12	0.50
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.41	0.49
1:A:233:GLU:O	1:A:282:ASP:HB3	2.13	0.49
1:B:82:GLY:HA3	1:B:118:ILE:O	2.12	0.49
1:A:123:MET:O	1:A:124:ALA:HB3	2.13	0.49
1:B:109:PHE:O	1:B:168:ALA:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD11	1:B:209:TRP:CD1	2.48	0.49
1:A:236:PRO:HB2	1:A:251:PHE:HB2	1.94	0.49
1:B:285:ARG:CZ	1:B:318:ALA:HB3	2.43	0.48
1:A:235:GLU:OE2	1:A:313:TYR:OH	2.26	0.48
1:A:285:ARG:CZ	1:A:318:ALA:HB3	2.42	0.48
1:B:423:PHE:O	1:B:427:ILE:HG13	2.13	0.48
1:B:165:LEU:O	1:B:166:GLN:C	2.51	0.48
1:A:396:ASN:N	1:A:396:ASN:OD1	2.46	0.47
1:A:209:TRP:CZ3	1:A:212:TYR:CD2	3.02	0.47
1:A:474:ASP:CG	1:A:496:ARG:HH21	2.13	0.47
1:B:314:LEU:HD12	1:B:343:VAL:HG13	1.96	0.47
1:B:125:SER:HB3	1:B:133:TYR:CE2	2.50	0.47
1:B:363:TYR:OH	1:B:380:ASP:OD1	2.15	0.47
1:B:209:TRP:HA	1:B:209:TRP:CE3	2.51	0.46
1:B:152:GLU:O	1:B:156:LEU:HB2	2.16	0.46
1:A:117:ASN:HA	1:A:172:VAL:HG22	1.97	0.45
1:B:65:LEU:HD12	1:B:66:LEU:N	2.31	0.45
1:A:165:LEU:HD22	1:A:172:VAL:HB	1.97	0.45
1:A:178:PRO:HG3	1:A:213:PHE:CZ	2.51	0.45
1:A:363:TYR:CE2	1:A:378:TRP:CH2	3.04	0.45
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.52	0.45
1:A:474:ASP:OD1	1:A:474:ASP:C	2.56	0.45
1:A:138:THR:HG21	1:A:146:ASN:ND2	2.32	0.45
1:A:309:ALA:HA	1:A:337:PHE:O	2.17	0.44
1:A:244:TYR:HD2	1:A:248:CYS:SG	2.39	0.44
1:B:106:LYS:HG2	1:B:167:LEU:HD22	1.99	0.44
1:B:287:LEU:HB3	1:B:291:TRP:CD1	2.53	0.44
1:B:474:ASP:C	1:B:474:ASP:OD1	2.56	0.44
1:B:483:ILE:O	1:B:485:PRO:HD3	2.17	0.44
1:A:425:LYS:HD3	1:A:426:PHE:CZ	2.52	0.44
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.59	0.44
1:B:123:MET:O	1:B:124:ALA:HB3	2.17	0.44
1:B:213:PHE:O	1:B:216:PHE:HB3	2.18	0.44
1:B:382:ASN:H	1:B:382:ASN:HD22	1.66	0.44
1:A:192:ASN:HB2	1:A:244:TYR:O	2.18	0.43
1:B:399:ASP:OD1	1:B:414:GLN:NE2	2.51	0.43
1:A:96:LEU:HB3	1:A:100:ALA:HB3	2.00	0.43
1:A:199:GLY:HA3	1:A:203:ASP:OD2	2.19	0.43
1:A:127:ASP:HB3	1:A:246:PHE:HB3	2.00	0.43
1:A:428:PRO:HB3	4:A:1502:SO4:O1	2.19	0.43
1:B:314:LEU:HB2	1:B:343:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:O	1:A:147:PHE:HA	2.19	0.43
1:A:484:SER:HA	1:A:485:PRO:HD3	1.87	0.42
1:B:47:ARG:HD3	1:B:50:GLU:OE1	2.19	0.42
1:B:60:HIS:HB3	1:B:479:PHE:CD2	2.54	0.42
1:B:158:ILE:O	1:B:159:PRO:C	2.57	0.42
1:A:80:GLY:HA3	1:A:117:ASN:HD21	1.84	0.42
1:A:98:PRO:HB2	1:A:99:PRO:HD3	2.00	0.42
1:B:192:ASN:HB2	1:B:244:TYR:O	2.20	0.42
1:B:296:LEU:HD11	1:B:308:ILE:HD11	2.01	0.42
1:B:31:PHE:CD2	1:B:32:PRO:HD2	2.55	0.42
1:B:281:LEU:O	1:B:281:LEU:CG	2.63	0.42
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.83	0.42
1:B:298:ASP:HA	1:B:299:PRO:HD2	1.95	0.42
1:B:312:TRP:HB2	1:B:341:ALA:HB2	2.02	0.42
1:B:9:PHE:HB3	7:B:506:HOH:O	2.19	0.41
1:B:40:TYR:HA	1:B:50:GLU:O	2.20	0.41
1:A:298:ASP:OD1	1:A:300:GLU:N	2.53	0.41
1:A:364:SER:HB3	1:A:423:PHE:HE1	1.85	0.41
1:A:30:THR:CG2	1:A:31:PHE:N	2.82	0.41
1:A:37:PHE:CD2	1:A:480:LEU:HG	2.55	0.41
1:A:342:CYS:HB2	1:A:398:VAL:HG11	2.03	0.41
1:A:89:ALA:O	1:A:93:ILE:HG13	2.21	0.41
1:A:262:ARG:HB3	1:A:262:ARG:NH1	2.36	0.41
1:A:381:TRP:HA	1:A:381:TRP:HE3	1.85	0.41
1:B:134:THR:OG1	1:B:137:ASP:OD1	2.36	0.41
1:B:86:THR:O	1:B:87:ASP:C	2.59	0.41
1:B:313:TYR:HB3	1:B:316:PHE:HD1	1.85	0.41
1:B:394:VAL:HG23	1:B:396:ASN:HB2	2.02	0.41
1:A:15:VAL:HG21	1:A:412:TYR:HB3	2.03	0.40
1:A:183:THR:O	1:A:189:GLY:HA2	2.22	0.40
1:A:5:ILE:HD13	1:A:5:ILE:HA	1.87	0.40
1:A:453:ASP:OD1	1:A:453:ASP:C	2.59	0.40
1:B:247:GLN:OE1	1:B:247:GLN:N	2.44	0.40
1:A:31:PHE:HA	1:A:32:PRO:HD2	1.94	0.40
1:A:104:LEU:C	1:A:104:LEU:HD23	2.42	0.40
1:A:283:ASP:HB3	1:A:287:LEU:HD12	2.03	0.40
1:A:203:ASP:C	1:A:203:ASP:OD1	2.59	0.40
1:A:106:LYS:HA	1:A:110:SER:HB3	2.04	0.40
1:B:209:TRP:O	1:B:212:TYR:HB3	2.22	0.40
1:B:236:PRO:HD2	1:B:283:ASP:HB2	2.04	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	495/497 (100%)	448 (90%)	41 (8%)	6 (1%)	13	39
1	B	495/497 (100%)	460 (93%)	33 (7%)	2 (0%)	34	66
All	All	990/994 (100%)	908 (92%)	74 (8%)	8 (1%)	19	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	ALA
1	B	381	TRP
1	A	124	ALA
1	A	194	LYS
1	A	409	ASP
1	A	381	TRP
1	A	406	ILE
1	A	245	PRO

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	424/424 (100%)	402 (95%)	22 (5%)	23	55
1	B	424/424 (100%)	400 (94%)	24 (6%)	20	50
All	All	848/848 (100%)	802 (95%)	46 (5%)	22	53

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	31	PHE
1	A	110	SER
1	A	152	GLU
1	A	153	ASP
1	A	173	SER
1	A	237	SER
1	A	262	ARG
1	A	285	ARG
1	A	335	MET
1	A	351	SER
1	A	358	ASP
1	A	363	TYR
1	A	364	SER
1	A	370	SER
1	A	381	TRP
1	A	382	ASN
1	A	396	ASN
1	A	398	VAL
1	A	433	ARG
1	A	449	LEU
1	A	457	VAL
1	B	30	THR
1	B	31	PHE
1	B	36	THR
1	B	38	SER
1	B	56	ILE
1	B	63	THR
1	B	72	GLU
1	B	107	SER
1	B	132	THR
1	B	143	GLN
1	B	155	LYS
1	B	242	SER
1	B	256	GLN
1	B	281	LEU
1	B	335	MET
1	B	343	VAL
1	B	345	SER
1	B	363	TYR
1	B	378	TRP
1	B	381	TRP
1	B	382	ASN

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Mol	Chain	Res	Type
1	B	410	THR
1	B	420	LEU
1	B	466	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	146	ASN
1	A	169	GLN
1	A	306	HIS
1	A	382	ASN
1	B	166	GLN
1	B	255	HIS
1	B	365	HIS
1	B	374	HIS
1	B	382	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	C	1	1,2	14,14,15	0.69	0	17,19,21	1.61	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	2.64	6 (35%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	NAG	C1-O5-C5	7.88	122.87	112.19
2	C	2	NAG	C4-C3-C2	4.69	117.89	111.02
2	C	1	NAG	C1-C2-N2	-3.95	103.75	110.49
2	C	1	NAG	C4-C3-C2	3.35	115.93	111.02
2	C	1	NAG	O5-C5-C6	-2.62	103.10	107.20
2	C	2	NAG	O5-C5-C6	2.57	111.23	107.20
2	C	2	NAG	O5-C5-C4	2.37	116.60	110.83
2	C	2	NAG	C3-C4-C5	2.25	114.26	110.24
2	C	2	NAG	C1-C2-N2	-2.19	106.74	110.49
2	C	1	NAG	O4-C4-C5	2.15	114.63	109.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

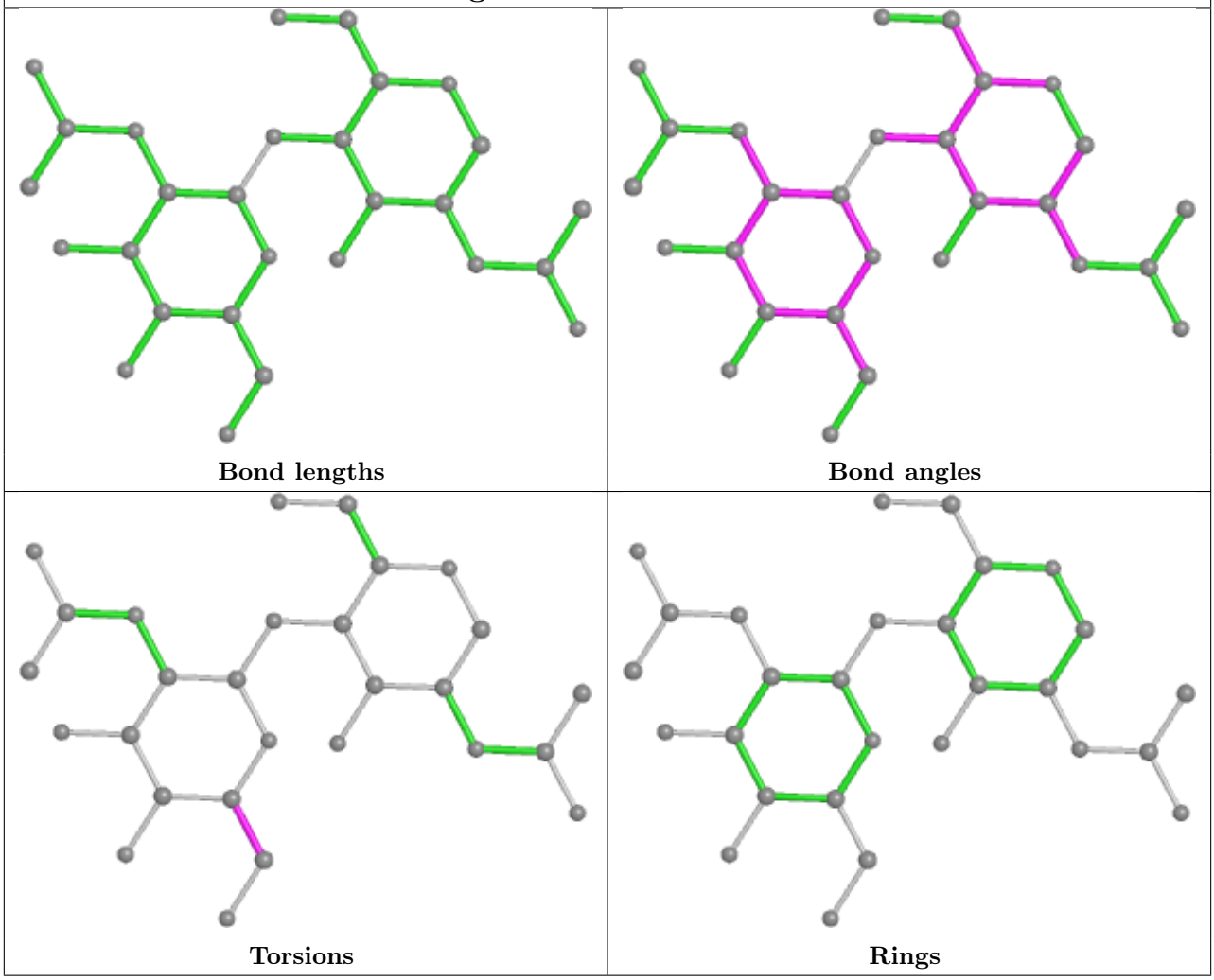
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is modelled with single atom - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	1502	-	4,4,4	0.16	0	6,6,6	0.14	0
4	SO4	B	1502	-	4,4,4	0.14	0	6,6,6	0.25	0
4	SO4	A	1501	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	1507	-	4,4,4	0.16	0	6,6,6	0.25	0
6	NAG	B	1505	1	14,14,15	0.90	0	17,19,21	2.02	4 (23%)
3	NDG	A	1997	-	14,14,15	0.57	0	17,19,21	1.32	2 (11%)
4	SO4	A	1506	-	4,4,4	0.16	0	6,6,6	0.17	0
5	GOL	A	1509	-	5,5,5	0.33	0	5,5,5	0.67	0
5	GOL	B	498	-	5,5,5	0.39	0	5,5,5	0.60	0
4	SO4	B	1499	-	4,4,4	0.20	0	6,6,6	0.29	0
4	SO4	A	1504	-	4,4,4	0.14	0	6,6,6	0.44	0
4	SO4	B	1500	-	4,4,4	0.24	0	6,6,6	0.43	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
5	GOL	A	1509	-	-	2/4/4/4	-
6	NAG	B	1505	1	-	2/6/23/26	0/1/1/1
3	NDG	A	1997	-	-	0/6/23/26	0/1/1/1
5	GOL	B	498	-	-	0/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1505	NAG	C1-O5-C5	5.97	120.28	112.19
6	B	1505	NAG	O4-C4-C5	3.41	117.76	109.30
3	A	1997	NDG	C1-C2-N2	-3.35	104.77	110.49
6	B	1505	NAG	C1-C2-N2	-2.82	105.68	110.49
3	A	1997	NDG	O4-C4-C5	2.33	115.09	109.30
6	B	1505	NAG	O3-C3-C2	2.15	113.91	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1509	GOL	C1-C2-C3-O3
5	A	1509	GOL	O2-C2-C3-O3
6	B	1505	NAG	C4-C5-C6-O6
6	B	1505	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1502	SO4	1	0
3	A	1997	NDG	2	0
5	A	1509	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	497/497 (100%)	-0.15	0	100	100	18, 30, 44, 52	5 (1%)
1	B	497/497 (100%)	-0.41	3 (0%)	89	86	11, 23, 38, 49	7 (1%)
All	All	994/994 (100%)	-0.28	3 (0%)	94	93	11, 27, 41, 52	12 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	ASP	3.0
1	B	497	GLN	2.8
1	B	111	GLU	2.1

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)

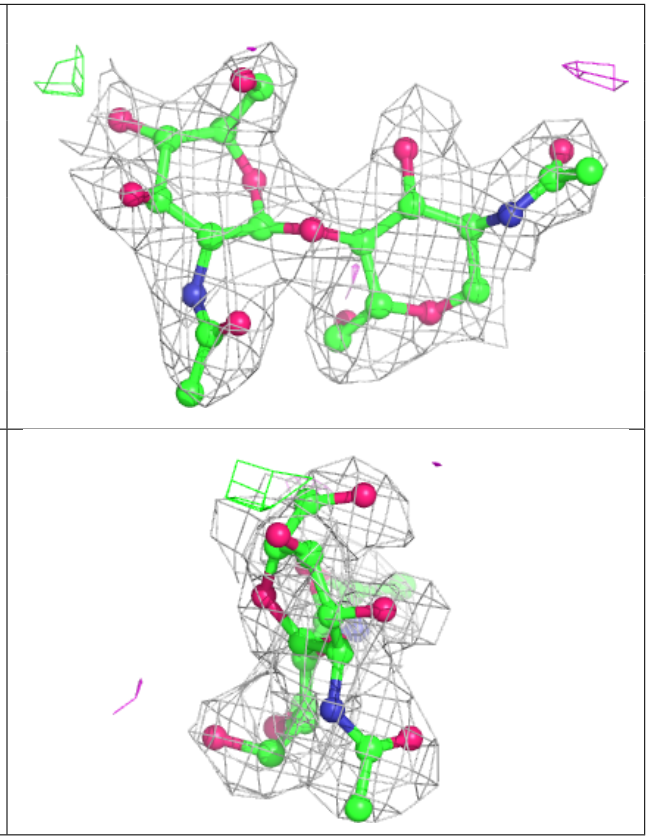
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.85	0.25	43,49,52,52	0
2	NAG	C	1	14/15	0.91	0.23	39,43,44,47	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 C:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1501	5/5	0.53	0.62	162,163,163,163	0
4	SO4	A	1502	5/5	0.70	0.54	125,126,126,126	0
4	SO4	B	1502	5/5	0.75	0.28	94,95,95,96	0
6	NAG	A	1998	1/15	0.76	0.24	29,29,29,29	0
6	NAG	B	1505	14/15	0.80	0.30	41,44,48,50	0
3	NDG	A	1997	14/15	0.86	0.27	55,58,59,61	0
5	GOL	A	1509	6/6	0.92	0.36	43,47,49,50	0
4	SO4	B	1499	5/5	0.93	0.21	57,57,59,59	0
4	SO4	A	1507	5/5	0.94	0.23	66,67,68,68	0
4	SO4	A	1506	5/5	0.94	0.23	64,64,65,66	0
5	GOL	B	498	6/6	0.97	0.16	35,36,37,37	0
4	SO4	B	1500	5/5	0.98	0.18	42,42,44,45	0
4	SO4	A	1504	5/5	0.98	0.11	34,36,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.