



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:42 AM UTC

PDB ID : 3KE0 / pdb_00003ke0
Title : Crystal structure of N370S Glucocerebrosidase at acidic pH.
Authors : Wei, R.R.; Boucher, S.; Pan, C.Q.; Edmunds, T.
Deposited on : 2009-10-23
Resolution : 2.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

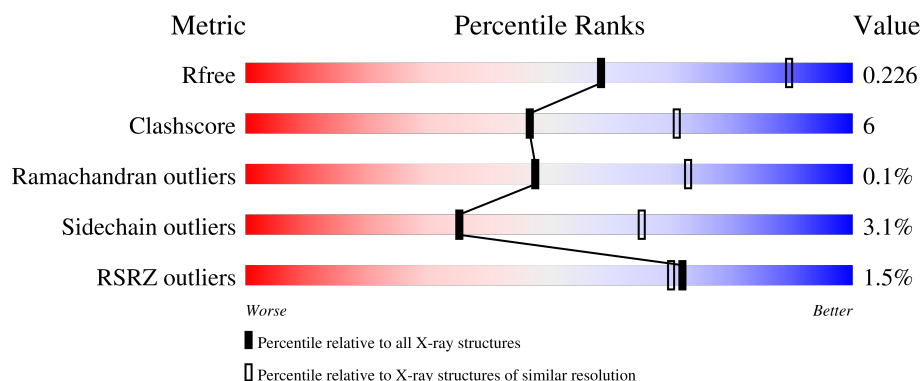
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	83% 14% .
1	B	497	2% 82% 17% .
2	C	2	100%
3	D	2	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8262 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 Glucosylceramidase.

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

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-alpha-D-glucopyranose.



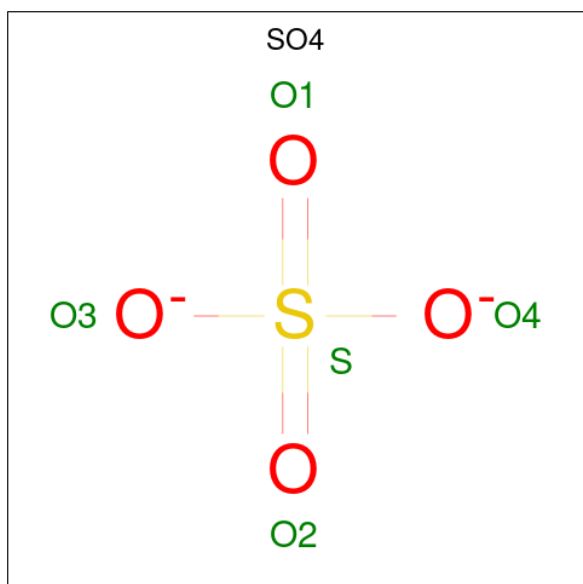
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



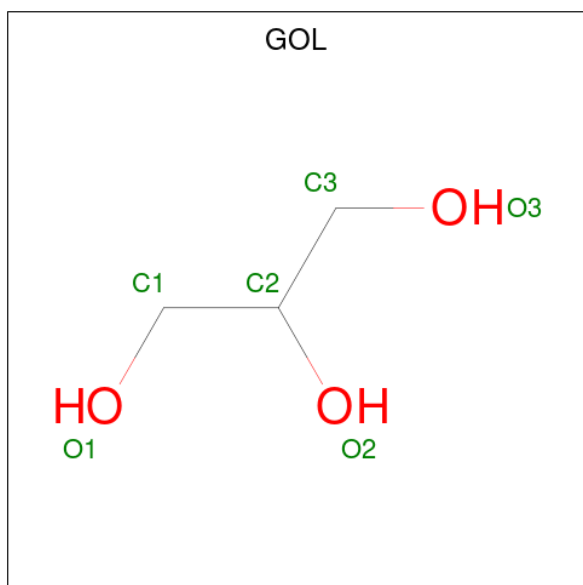
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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



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

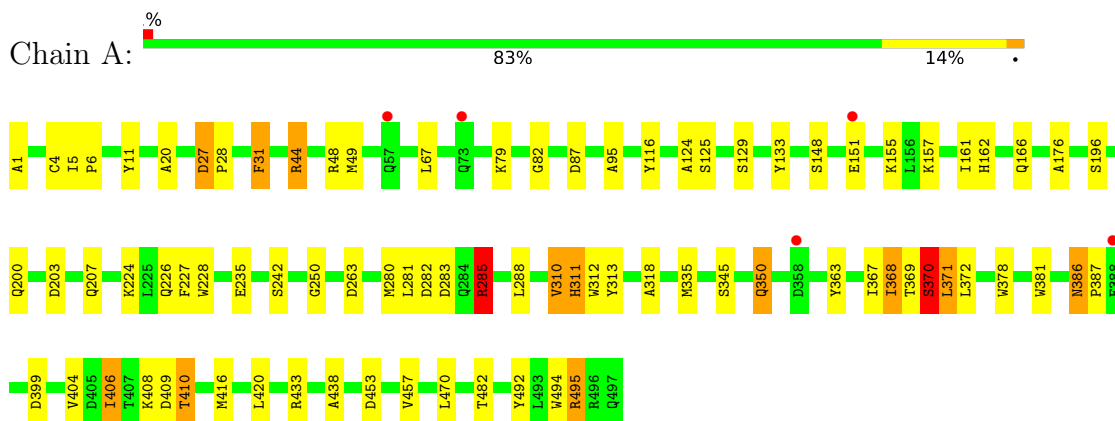
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	118	Total	O	0	0
			118	118		
7	B	134	Total	O	0	0
			134	134		

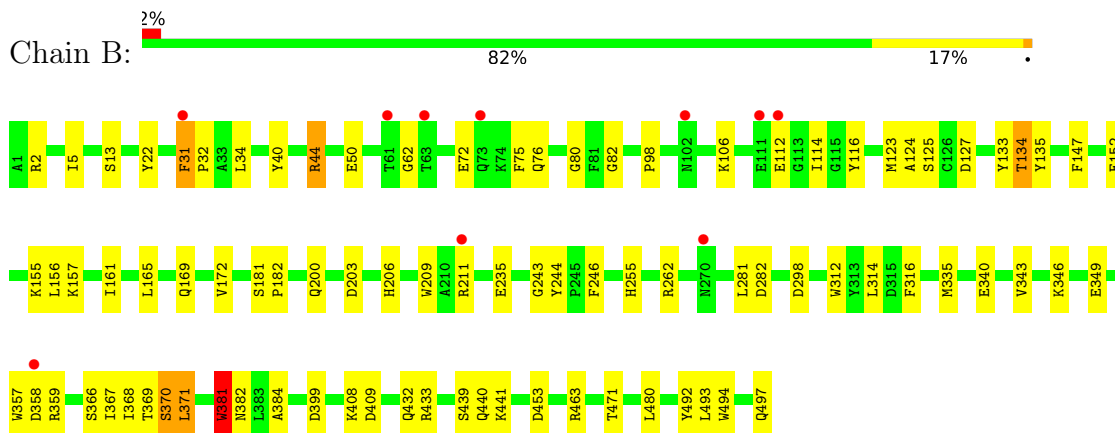
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glucosylceramidase



- Molecule 1: Glucosylceramidase



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

Chain C: 



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

Chain D:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	109.47Å 285.06Å 92.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.5 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.172 , 0.229 0.171 , 0.226	Depositor DCC
R_{free} test set	1997 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, NDG, SO4

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	1.14	13/4048 (0.3%)	1.12	16/5519 (0.3%)
1	B	1.13	11/4049 (0.3%)	1.14	15/5519 (0.3%)
All	All	1.13	24/8097 (0.3%)	1.13	31/11038 (0.3%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	VAL	C-O	-8.21	1.15	1.24
1	B	493	LEU	C-O	-7.45	1.14	1.23
1	B	370	SER	C-O	-7.44	1.15	1.24
1	B	369	THR	C-O	-7.08	1.15	1.24
1	B	492	TYR	C-O	-6.94	1.15	1.24
1	A	370	SER	C-O	-6.70	1.16	1.24
1	B	381	TRP	C-O	-6.54	1.15	1.24
1	A	494	TRP	C-O	-6.46	1.16	1.23
1	A	495	ARG	C-O	-6.22	1.16	1.23
1	B	367	ILE	C-O	-6.15	1.17	1.24
1	B	494	TRP	C-O	-6.14	1.16	1.23
1	B	371	LEU	C-O	-6.02	1.16	1.24
1	A	369	THR	C-O	-5.82	1.17	1.24
1	A	312	TRP	C-O	-5.73	1.17	1.24
1	A	372	LEU	N-CA	-5.71	1.38	1.46
1	A	350	GLN	CG-CD	5.67	1.66	1.52
1	B	384	ALA	C-O	-5.64	1.17	1.23
1	A	311	HIS	C-O	-5.46	1.17	1.23
1	B	368	ILE	C-O	-5.40	1.17	1.24
1	A	368	ILE	C-O	-5.39	1.17	1.24
1	B	155	LYS	CD-CE	5.37	1.68	1.52
1	A	350	GLN	CB-CG	5.28	1.68	1.52
1	A	371	LEU	C-O	-5.25	1.17	1.24
1	A	482	THR	CA-CB	5.21	1.62	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CA-C-N	-12.32	110.79	119.66
1	A	27	ASP	C-N-CA	-12.32	110.79	119.66
1	B	76	GLN	N-CA-C	9.35	123.44	110.35
1	B	124	ALA	N-CA-C	8.98	121.29	108.00
1	A	372	LEU	N-CA-C	-8.24	103.36	113.50
1	B	80	GLY	N-CA-C	7.05	119.61	110.45
1	A	124	ALA	N-CA-C	6.57	117.73	108.00
1	B	203	ASP	N-CA-C	6.55	119.39	110.35
1	A	28	PRO	CA-C-N	5.91	125.85	119.76
1	A	28	PRO	C-N-CA	5.91	125.85	119.76
1	A	494	TRP	N-CA-C	5.90	117.82	108.79
1	B	62	GLY	N-CA-C	5.73	119.36	110.88
1	B	200	GLN	N-CA-C	5.72	113.37	108.22
1	A	5	ILE	CA-C-N	5.59	125.77	119.90
1	A	5	ILE	C-N-CA	5.59	125.77	119.90
1	B	134	THR	N-CA-C	-5.56	101.28	109.18
1	B	2	ARG	CA-C-N	5.55	125.75	120.31
1	B	2	ARG	C-N-CA	5.55	125.75	120.31
1	A	406	ILE	N-CA-C	5.51	116.90	110.62
1	A	386	ASN	CA-C-N	-5.44	114.22	119.87
1	A	386	ASN	C-N-CA	-5.44	114.22	119.87
1	A	200	GLN	N-CA-C	5.41	114.36	108.14
1	A	285	ARG	N-CA-C	5.28	118.98	112.54
1	A	28	PRO	O-C-N	5.21	123.60	121.15
1	B	155	LYS	CB-CG-CD	5.20	123.26	111.30
1	A	148	SER	N-CA-C	5.16	116.36	108.42
1	B	235	GLU	CA-C-N	5.15	124.94	119.28
1	B	235	GLU	C-N-CA	5.15	124.94	119.28
1	B	123	MET	N-CA-C	-5.10	100.76	108.67
1	B	98	PRO	N-CA-C	5.03	116.84	110.70
1	B	114	ILE	N-CA-C	5.02	116.94	112.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3928	0	3847	43	0
1	B	3929	0	3847	44	0
2	C	28	0	23	3	0
3	D	28	0	25	0	0
4	A	40	0	0	1	0
4	B	25	0	0	2	0
5	A	12	0	16	0	0
5	B	6	0	8	1	0
6	B	14	0	13	0	0
7	A	118	0	0	3	0
7	B	134	0	0	1	0
All	All	8262	0	7779	90	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 6.

All (90) 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:31:PHE:HD2	1:B:32:PRO:HD2	1.22	1.03
1:B:31:PHE:CD2	1:B:32:PRO:HD2	2.09	0.88
1:B:206:HIS:NE2	1:B:255:HIS:HE1	1.84	0.77
1:A:31:PHE:HB2	1:A:495:ARG:HH21	1.53	0.74
1:A:408:LYS:O	1:A:410:THR:HG23	1.90	0.70
1:B:314:LEU:HB2	1:B:343:VAL:CG1	2.22	0.70
1:A:95:ALA:HB1	1:A:406:ILE:HD12	1.74	0.70
1:B:340:GLU:OE2	5:B:498:GOL:H11	2.00	0.62
1:B:381:TRP:HA	1:B:381:TRP:CE3	2.34	0.61
1:B:314:LEU:HB2	1:B:343:VAL:HG13	1.83	0.60
1:A:371:LEU:O	1:A:433:ARG:HD2	2.01	0.60
7:A:572:HOH:O	2:C:1:NDG:H2	2.03	0.59
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.85	0.59
1:B:381:TRP:HA	1:B:381:TRP:HE3	1.67	0.58
1:B:125:SER:HB3	1:B:133:TYR:CE2	2.38	0.58
1:B:82:GLY:HA2	1:B:116:TYR:CD1	2.39	0.57
1:A:408:LYS:O	1:A:410:THR:CG2	2.54	0.56
1:B:40:TYR:HA	1:B:50:GLU:O	2.07	0.55
1:B:358:ASP:HB2	4:B:1500:SO4:O4	2.08	0.53
1:A:1:ALA:HB2	1:A:27:ASP:OD1	2.08	0.53
1:B:314:LEU:HB2	1:B:343:VAL:HG12	1.90	0.53
1:A:67:LEU:HD23	1:A:438:ALA:HA	1.90	0.53
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:NDG:H6C1	2:C:2:NAG:H2	1.92	0.52
1:A:453:ASP:OD1	1:A:453:ASP:C	2.52	0.52
1:A:125:SER:HB3	1:A:133:TYR:CE2	2.45	0.52
1:B:371:LEU:O	1:B:433:ARG:HD2	2.10	0.51
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.41	0.50
1:B:314:LEU:HD12	1:B:343:VAL:HG13	1.94	0.49
1:A:235:GLU:OE2	1:A:313:TYR:OH	2.19	0.49
1:B:471:THR:HA	1:B:480:LEU:O	2.13	0.49
1:A:44:ARG:NH1	4:A:1503:SO4:O2	2.31	0.48
1:B:298:ASP:C	1:B:298:ASP:OD1	2.57	0.48
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.94	0.48
1:A:226:GLN:NE2	7:A:580:HOH:O	2.44	0.48
1:A:82:GLY:HA2	1:A:116:TYR:CD1	2.48	0.48
1:B:134:THR:HG21	1:B:182:PRO:HA	1.96	0.48
1:B:206:HIS:NE2	1:B:255:HIS:CE1	2.73	0.48
1:B:281:LEU:O	1:B:282:ASP:C	2.57	0.47
2:C:1:NDG:C6	2:C:2:NAG:H2	2.44	0.47
1:B:5:ILE:HG12	1:B:22:TYR:CE2	2.49	0.47
1:A:399:ASP:CG	1:A:416:MET:HE1	2.41	0.46
1:A:386:ASN:OD1	1:A:386:ASN:C	2.59	0.46
1:B:44:ARG:NH2	4:B:1501:SO4:O1	2.45	0.46
1:B:312:TRP:HD1	1:B:314:LEU:HD23	1.81	0.46
1:A:4:CYS:O	1:A:6:PRO:HD3	2.16	0.46
1:B:82:GLY:HA2	1:B:116:TYR:CG	2.51	0.46
1:A:281:LEU:HD22	1:A:288:LEU:HD21	1.98	0.46
1:A:157:LYS:O	1:A:161:ILE:HG13	2.17	0.45
1:A:203:ASP:OD1	1:A:203:ASP:C	2.60	0.45
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.52	0.45
1:B:480:LEU:HD12	1:B:480:LEU:N	2.32	0.45
1:A:235:GLU:OE2	1:A:311:HIS:ND1	2.48	0.45
1:B:255:HIS:HD2	7:B:541:HOH:O	1.99	0.44
1:A:11:TYR:OH	1:A:350:GLN:HG2	2.18	0.44
1:A:363:TYR:CD2	1:A:378:TRP:CH2	3.06	0.44
1:A:285:ARG:CZ	1:A:318:ALA:HB3	2.48	0.44
1:B:157:LYS:O	1:B:161:ILE:HG13	2.18	0.44
1:B:181:SER:HA	1:B:209:TRP:CZ3	2.53	0.44
1:A:67:LEU:HD12	1:A:470:LEU:HD11	1.99	0.43
1:A:285:ARG:H	1:A:285:ARG:HG2	1.60	0.43
1:A:399:ASP:HB3	1:A:416:MET:HE1	1.99	0.43
1:A:280:MET:O	1:A:281:LEU:HB3	2.19	0.43
1:A:116:TYR:OH	1:A:420:LEU:HD13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.53	0.43
1:B:135:TYR:O	1:B:147:PHE:HA	2.17	0.43
1:B:13:SER:HB2	1:B:357:TRP:HB2	2.01	0.43
1:A:48:ARG:O	1:A:49:MET:C	2.62	0.43
1:A:387:PRO:HD3	1:A:404:VAL:O	2.19	0.43
1:B:106:LYS:HE2	1:B:112:GLU:OE2	2.19	0.42
1:A:20:ALA:HB2	1:A:409:ASP:OD2	2.19	0.42
1:A:151:GLU:HB2	7:A:558:HOH:O	2.19	0.42
1:A:162:HIS:O	1:A:166:GLN:HG3	2.19	0.42
1:A:367:ILE:O	1:A:370:SER:HB2	2.19	0.42
1:B:463:ARG:HE	1:B:463:ARG:HB2	1.65	0.42
1:B:439:SER:O	1:B:440:GLN:HB3	2.18	0.42
1:A:378:TRP:CZ3	1:A:420:LEU:HD21	2.55	0.41
1:A:87:ASP:HB2	1:A:129:SER:HA	2.01	0.41
1:A:196:SER:HB3	1:A:250:GLY:O	2.20	0.41
1:B:408:LYS:O	1:B:409:ASP:C	2.63	0.41
1:B:359:ARG:NH1	1:B:399:ASP:OD2	2.44	0.41
1:B:453:ASP:OD1	1:B:453:ASP:C	2.64	0.41
1:A:368:ILE:HG21	1:A:368:ILE:HD13	1.77	0.41
1:B:75:PHE:O	1:B:432:GLN:HG3	2.20	0.41
1:B:181:SER:HA	1:B:209:TRP:CH2	2.56	0.41
1:A:457:VAL:HA	1:A:492:TYR:O	2.21	0.41
1:B:316:PHE:CE2	1:B:346:LYS:HE3	2.56	0.41
1:B:382:ASN:ND2	1:B:382:ASN:H	2.18	0.40
1:A:281:LEU:O	1:A:283:ASP:HB2	2.22	0.40
1:B:243:GLY:O	1:B:244:TYR:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	468 (94%)	26 (5%)	1 (0%)	43	68
1	B	495/497 (100%)	467 (94%)	28 (6%)	0	100	100
All	All	990/994 (100%)	935 (94%)	54 (6%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP

5.3.2 Protein sidechains ⓘ

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%)	412 (97%)	12 (3%)	38	68
1	B	424/424 (100%)	410 (97%)	14 (3%)	33	63
All	All	848/848 (100%)	822 (97%)	26 (3%)	35	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	44	ARG
1	A	155	LYS
1	A	224	LYS
1	A	242	SER
1	A	285	ARG
1	A	310	VAL
1	A	335	MET
1	A	345	SER
1	A	370	SER
1	A	381	TRP
1	A	410	THR
1	B	31	PHE
1	B	34	LEU
1	B	44	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	GLU
1	B	169	GLN
1	B	211	ARG
1	B	262	ARG
1	B	335	MET
1	B	349	GLU
1	B	366	SER
1	B	370	SER
1	B	381	TRP
1	B	441	LYS
1	B	497	GLN

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	57	GLN
1	A	73	GLN
1	A	226	GLN
1	A	362	GLN
1	A	432	GLN
1	B	166	GLN
1	B	223	HIS
1	B	255	HIS
1	B	365	HIS
1	B	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	NDG	C	1	2	14,14,15	0.86	0	17,19,21	1.99	5 (29%)
2	NAG	C	2	2	14,14,15	1.55	3 (21%)	17,19,21	2.39	8 (47%)
3	NAG	D	1	3,1	14,14,15	0.66	0	17,19,21	1.82	2 (11%)
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	2.28	2 (11%)

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	NDG	C	1	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	3.84	1.57	1.52
2	C	2	NAG	C2-N2	2.58	1.50	1.46
2	C	2	NAG	O7-C7	2.36	1.28	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	7.81	122.66	112.19
3	D	1	NAG	C2-N2-C7	-5.57	115.44	122.90
2	C	2	NAG	C3-C4-C5	-4.68	101.74	110.23
2	C	2	NAG	C1-O5-C5	4.12	117.71	112.19
2	C	1	NDG	C2-N2-C7	-3.77	117.84	122.90
2	C	1	NDG	O5-C1-C2	-3.70	105.57	111.29
2	C	2	NAG	C1-C2-N2	3.57	116.05	110.43
3	D	1	NAG	O5-C1-C2	-3.46	105.93	111.29
2	C	2	NAG	O5-C5-C6	3.17	113.83	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NDG	O4-C4-C5	3.15	117.08	109.32
2	C	1	NDG	C1-C2-N2	-3.11	105.54	110.43
3	D	2	NAG	C1-C2-N2	3.05	115.25	110.43
2	C	1	NDG	C1-O5-C5	2.76	115.88	112.19
2	C	2	NAG	O5-C1-C2	2.38	114.98	111.29
2	C	2	NAG	O4-C4-C5	2.34	115.08	109.32
2	C	2	NAG	O3-C3-C2	2.09	113.74	109.40
2	C	2	NAG	C4-C3-C2	-2.08	107.97	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

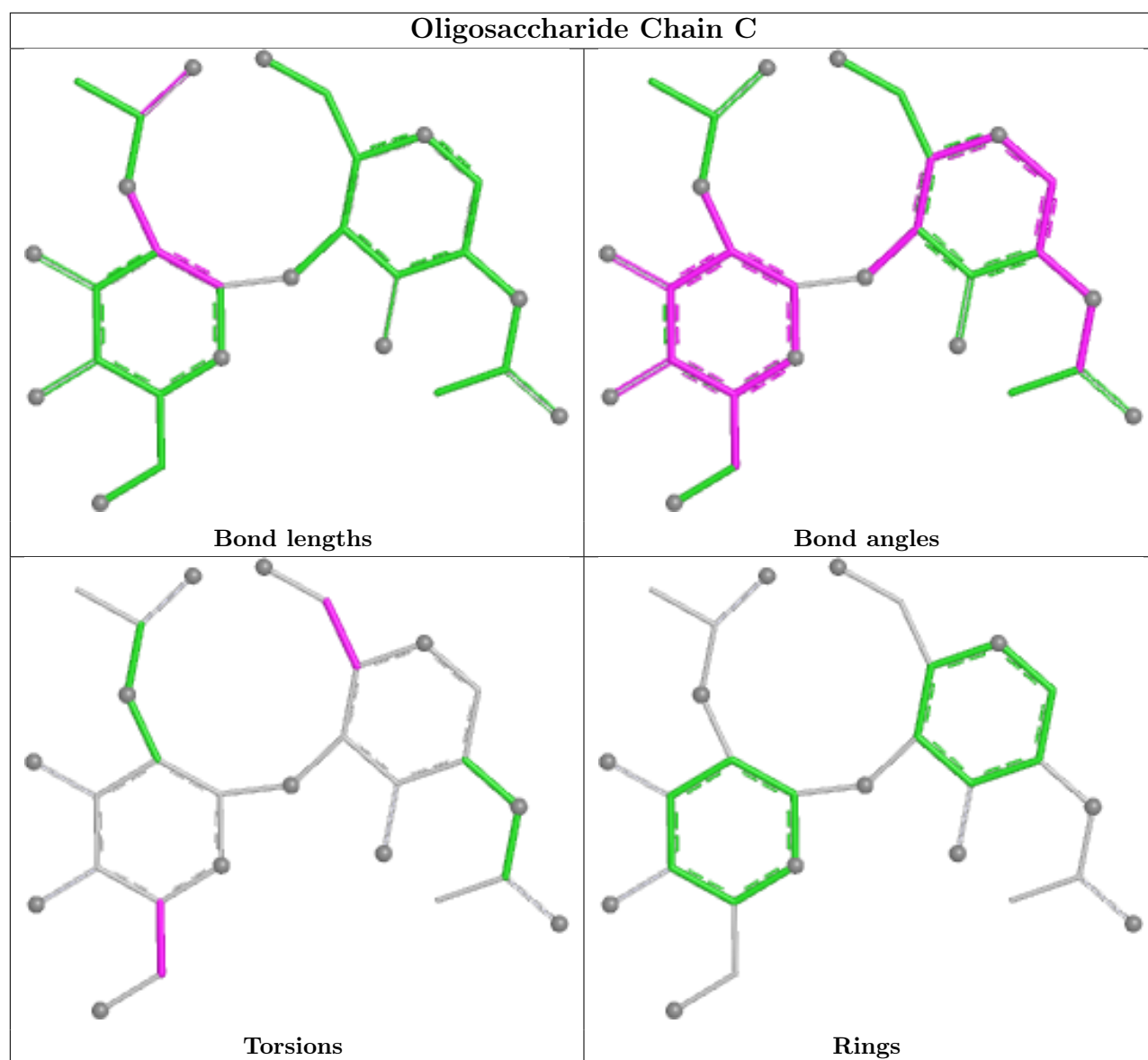
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NDG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NDG	C4-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7

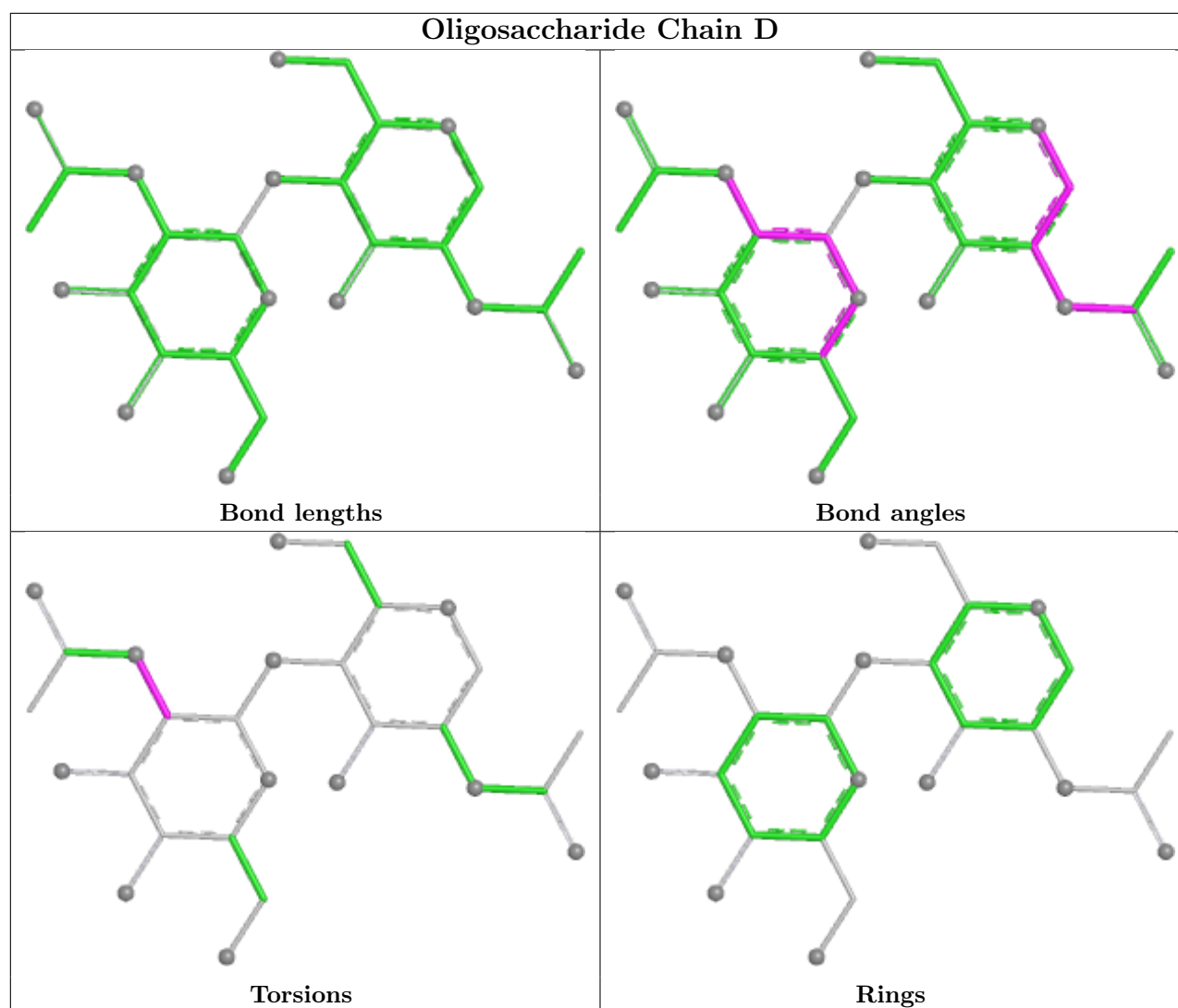
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	1	NDG	3	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.





5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	1507	-	4,4,4	0.23	0	6,6,6	0.67	0
5	GOL	B	498	-	5,5,5	0.57	0	5,5,5	0.53	0
4	SO4	A	1503	-	4,4,4	0.35	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1504	-	4,4,4	0.15	0	6,6,6	0.61	0
4	SO4	A	1502	-	4,4,4	0.22	0	6,6,6	0.50	0
4	SO4	A	1505	-	4,4,4	0.22	0	6,6,6	0.24	0
4	SO4	B	1501	-	4,4,4	0.28	0	6,6,6	0.46	0
6	NAG	B	1505	1	14,14,15	0.87	0	17,19,21	2.34	4 (23%)
4	SO4	B	1502	-	4,4,4	0.33	0	6,6,6	0.44	0
5	GOL	A	1509	-	5,5,5	0.40	0	5,5,5	0.63	0
4	SO4	B	1499	-	4,4,4	0.26	0	6,6,6	0.82	0
5	GOL	A	1508	-	5,5,5	0.60	0	5,5,5	0.53	0
4	SO4	B	1498	-	4,4,4	0.33	0	6,6,6	0.28	0
4	SO4	A	1500	-	4,4,4	0.26	0	6,6,6	0.40	0
4	SO4	A	1506	-	4,4,4	0.34	0	6,6,6	0.78	0
4	SO4	B	1500	-	4,4,4	0.25	0	6,6,6	1.01	0
4	SO4	A	1501	-	4,4,4	0.31	0	6,6,6	0.49	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
6	NAG	B	1505	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1508	-	-	2/4/4/4	-
5	GOL	A	1509	-	-	4/4/4/4	-
5	GOL	B	498	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1505	NAG	C1-O5-C5	7.42	122.14	112.19
6	B	1505	NAG	C4-C3-C2	3.10	115.56	111.02
6	B	1505	NAG	O4-C4-C5	2.80	116.22	109.32
6	B	1505	NAG	O5-C1-C2	-2.34	107.67	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1509	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1508	GOL	C1-C2-C3-O3
5	A	1508	GOL	O2-C2-C3-O3
5	B	498	GOL	O1-C1-C2-C3
5	A	1509	GOL	O2-C2-C3-O3
6	B	1505	NAG	C4-C5-C6-O6
5	B	498	GOL	O1-C1-C2-O2
5	A	1509	GOL	O1-C1-C2-O2
5	A	1509	GOL	O1-C1-C2-C3
6	B	1505	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	498	GOL	1	0
4	A	1503	SO4	1	0
4	B	1501	SO4	1	0
4	B	1500	SO4	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%)	-0.65	5 (1%) 79 78	3, 13, 25, 37	5 (1%)
1	B	497/497 (100%)	-0.63	10 (2%) 65 62	3, 12, 26, 44	7 (1%)
All	All	994/994 (100%)	-0.64	15 (1%) 72 70	3, 12, 26, 44	12 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	ASN	6.5
1	B	211	ARG	6.3
1	A	57	GLN	6.1
1	A	73	GLN	6.1
1	B	112	GLU	6.0
1	A	358	ASP	5.9
1	B	73	GLN	5.7
1	B	111	GLU	5.5
1	A	151	GLU	5.3
1	B	358	ASP	5.3
1	B	102	ASN	5.2
1	A	388	GLU	4.4
1	B	63	THR	2.9
1	B	31	PHE	2.7
1	B	61	THR	2.1

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

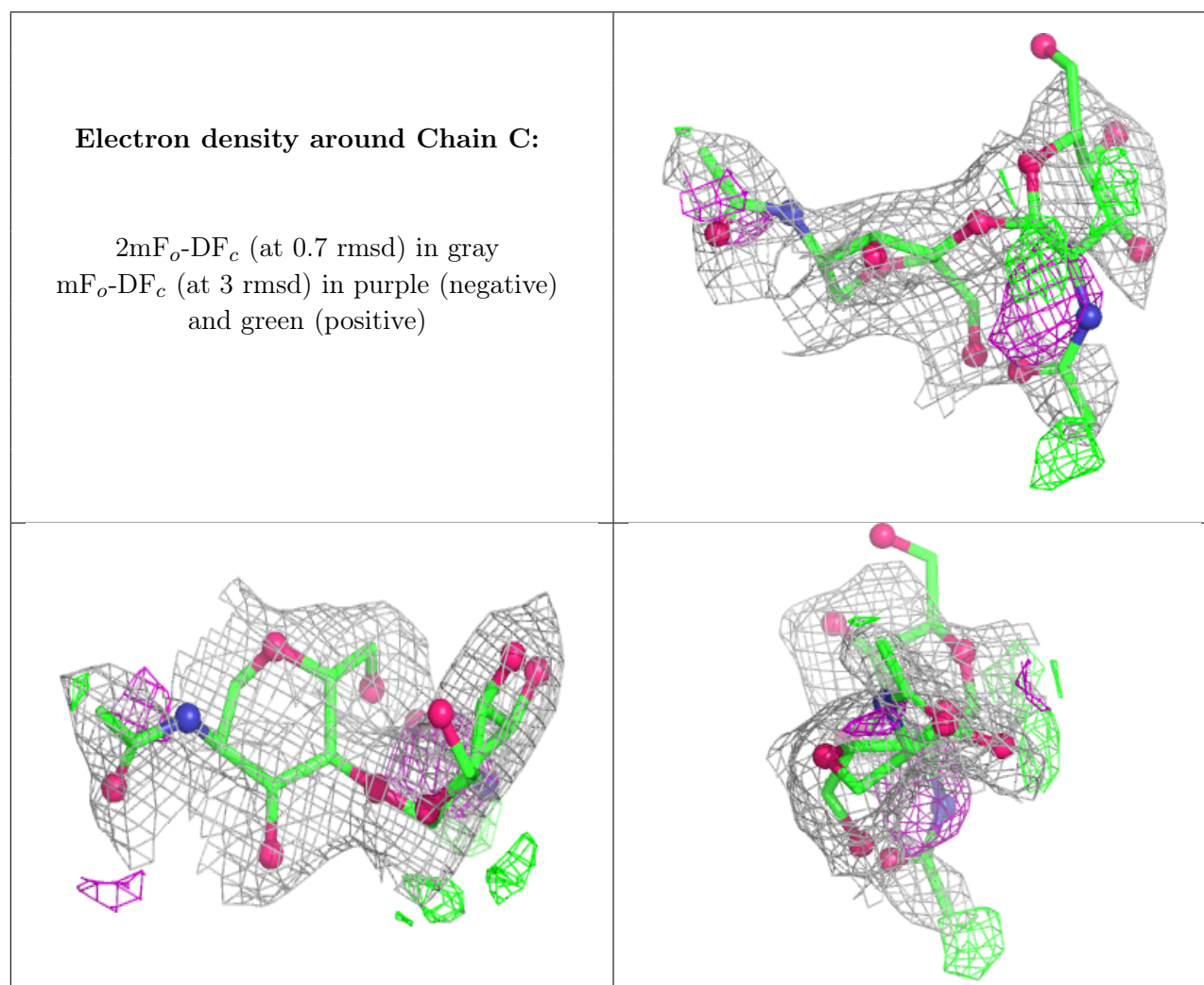
There are no non-standard protein/DNA/RNA residues in this entry.

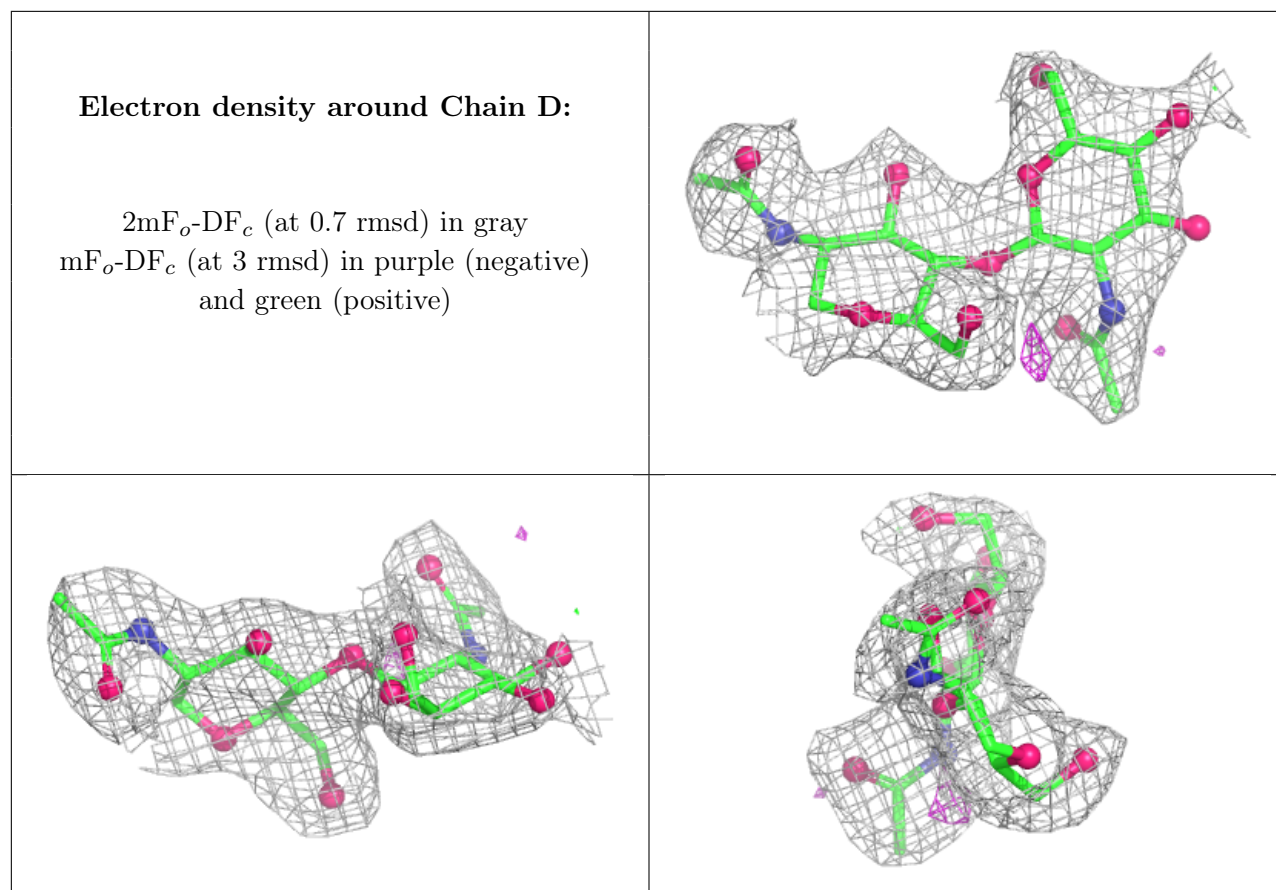
6.3 Carbohydrates ⓘ

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	0.57	0.29	62,66,71,72	0
2	NDG	C	1	14/15	0.80	0.18	43,48,54,54	0
3	NAG	D	2	14/15	0.83	0.15	41,44,48,51	0
3	NAG	D	1	14/15	0.95	0.07	25,29,31,36	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.





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
6	NAG	B	1505	14/15	0.81	0.14	40,44,49,49	0
4	SO4	A	1500	5/5	0.85	0.24	75,76,77,78	0
4	SO4	A	1502	5/5	0.86	0.20	86,86,86,87	0
4	SO4	A	1501	5/5	0.86	0.18	78,79,79,79	0
4	SO4	B	1502	5/5	0.87	0.16	69,70,71,71	0
4	SO4	A	1503	5/5	0.89	0.13	49,50,52,54	0
4	SO4	A	1505	5/5	0.90	0.16	65,65,66,67	0
5	GOL	A	1509	6/6	0.91	0.12	31,32,33,34	0
4	SO4	B	1501	5/5	0.91	0.12	50,51,53,53	0
4	SO4	A	1507	5/5	0.92	0.12	53,53,54,55	0
4	SO4	B	1498	5/5	0.92	0.11	60,60,61,62	0
5	GOL	A	1508	6/6	0.94	0.09	19,21,21,22	0
4	SO4	A	1506	5/5	0.94	0.11	33,37,37,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	1499	5/5	0.95	0.09	33,34,37,39	0
5	GOL	B	498	6/6	0.96	0.07	14,18,21,23	0
4	SO4	A	1504	5/5	0.99	0.05	15,16,17,18	0
4	SO4	B	1500	5/5	0.99	0.04	13,13,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.