



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:10 PM UTC

PDB ID : 5JCE / pdb_00005jce
Title : Crystal structure of OsCEBiP complex
Authors : Chai, J.J.; Liu, S.M.; Wang, J.Z.
Deposited on : 2016-04-15
Resolution : 2.51 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

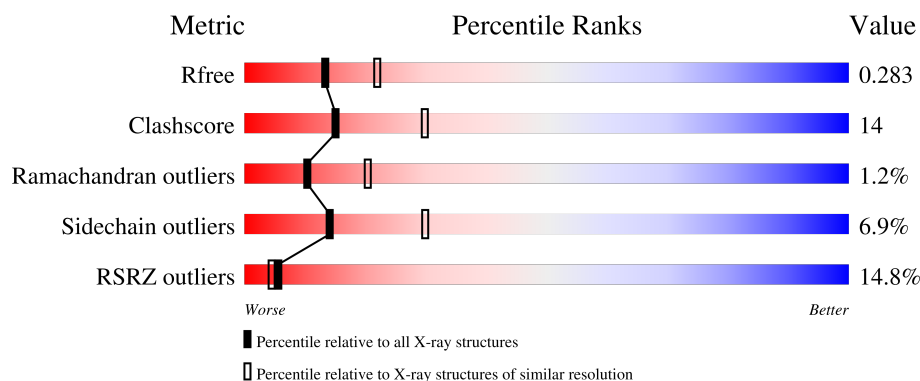
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	297	15% 73% 22% ...
1	B	297	14% 70% 24% 6%
2	C	3	33% 67%

2 Entry composition [i](#)

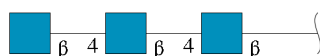
There are 3 unique types of molecules in this entry. The entry contains 4407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chitin elicitor-binding protein.

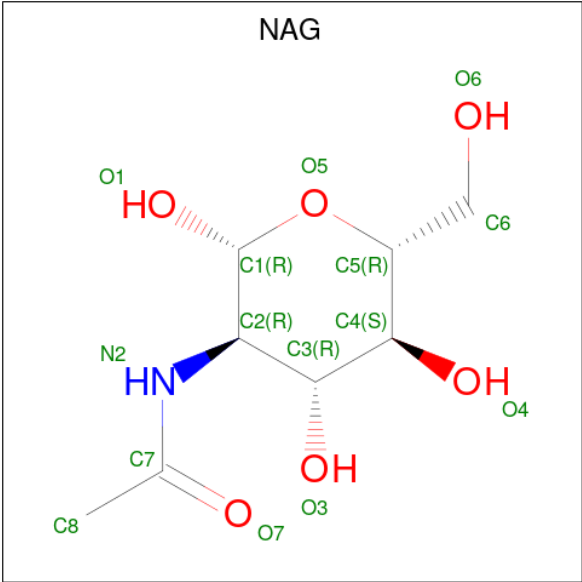
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2137	1317	366	436	18			
1	B	297	Total	C	N	O	S	0	0	0
			2171	1336	372	444	19			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	C	3	Total	C	N	O	0	0	0
			43	24	3	16			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

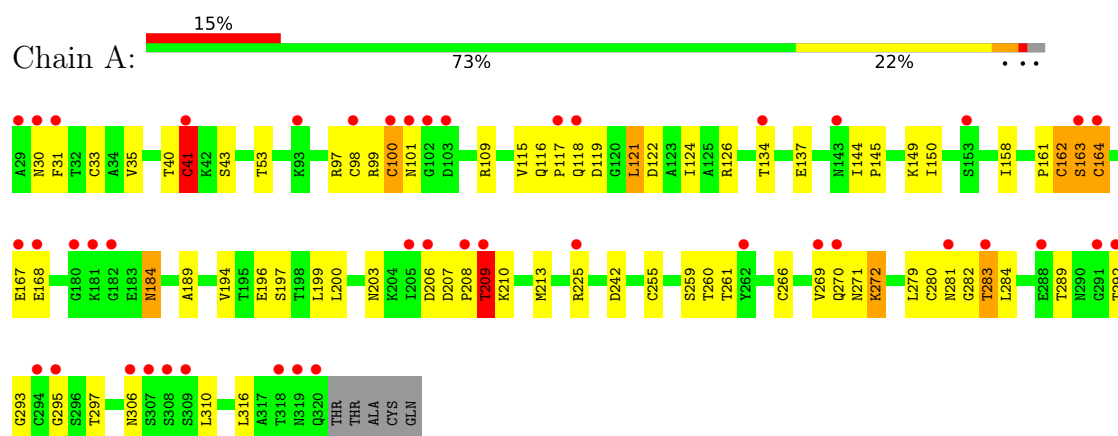


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

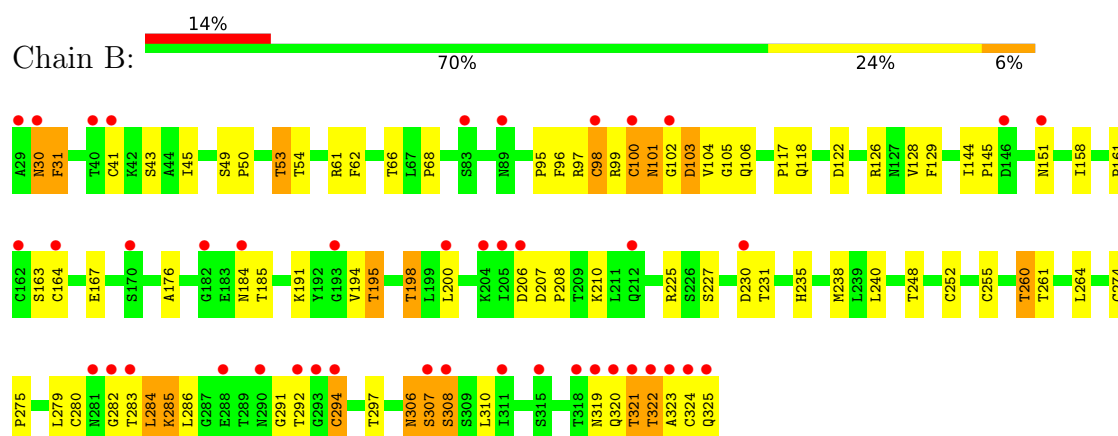
3 Residue-property plots [i](#)

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: Chitin elicitor-binding protein



• Molecule 1: Chitin elicitor-binding protein



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.45Å 99.77Å 87.65Å 90.00° 103.73° 90.00°	Depositor
Resolution (Å)	39.16 – 2.51 39.16 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.16-2.51) 92.9 (39.16-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.256 0.265 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (5.79%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.0	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	0.90	EDS
Total number of atoms	4407	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: 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	0.86	6/2173 (0.3%)	1.05	12/2969 (0.4%)
1	B	0.88	5/2207 (0.2%)	1.02	9/3016 (0.3%)
All	All	0.87	11/4380 (0.3%)	1.04	21/5985 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	SER	C-O	-9.33	1.12	1.23
1	A	97	ARG	C-O	-7.86	1.14	1.24
1	A	162	CYS	C-O	-7.48	1.16	1.24
1	A	163	SER	C-O	-6.43	1.16	1.23
1	B	97	ARG	C-O	-6.02	1.16	1.24
1	B	98	CYS	CA-CB	5.75	1.62	1.53
1	A	99	ARG	CZ-NH2	-5.73	1.26	1.33
1	B	96	PHE	C-O	-5.50	1.17	1.23
1	A	158	ILE	CA-C	-5.40	1.48	1.53
1	A	100	CYS	C-O	-5.34	1.17	1.24
1	B	161	PRO	C-O	-5.23	1.17	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	SER	N-CA-C	-9.43	93.81	108.14
1	B	98	CYS	N-CA-C	9.08	120.94	111.14
1	B	102	GLY	N-CA-C	7.74	123.57	113.27
1	A	163	SER	CA-C-O	-6.88	113.91	121.28
1	A	306	ASN	N-CA-C	6.86	122.61	112.94
1	B	321	THR	N-CA-C	6.76	120.21	112.57
1	B	306	ASN	N-CA-C	6.72	119.49	110.88
1	B	101	ASN	N-CA-C	-6.68	99.51	109.86
1	A	163	SER	O-C-N	-6.43	116.86	123.29
1	A	283	THR	CB-CA-C	-6.11	103.78	109.83
1	A	116	GLN	CA-C-N	6.01	127.35	119.84
1	A	116	GLN	C-N-CA	6.01	127.35	119.84
1	B	98	CYS	N-CA-CB	6.01	118.78	110.07
1	B	151	ASN	N-CA-C	5.80	119.17	109.95
1	A	271	ASN	N-CA-C	-5.68	102.63	110.35
1	B	128	VAL	N-CA-C	-5.61	107.36	111.90
1	A	41	CYS	N-CA-CB	-5.57	102.75	111.56
1	B	31	PHE	N-CA-C	-5.49	100.08	109.24
1	A	162	CYS	N-CA-C	5.47	115.60	107.88
1	A	163	SER	CA-C-N	5.01	130.72	121.70
1	A	163	SER	C-N-CA	5.01	130.72	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	GLN	Peptide
1	B	103	ASP	Peptide

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	2137	0	2095	51	1
1	B	2171	0	2126	64	1
2	C	43	0	39	1	0
3	A	14	0	13	1	0
3	B	42	0	39	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4407	0	4312	116	1

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 14.

All (116) 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:41:CYS:SG	1:B:164:CYS:HB3	1.45	1.56
1:B:306:ASN:ND2	3:B:400:NAG:C1	1.70	1.52
1:B:294:CYS:SG	1:B:324:CYS:SG	1.24	1.24
1:B:294:CYS:SG	1:B:324:CYS:CB	2.26	1.23
1:B:41:CYS:SG	1:B:164:CYS:CB	2.41	1.07
1:B:306:ASN:ND2	3:B:400:NAG:O5	1.99	0.95
1:B:225:ARG:NH1	1:B:320:GLN:O	2.02	0.92
1:A:41:CYS:HB2	1:A:164:CYS:SG	2.13	0.88
1:A:100:CYS:SG	1:A:164:CYS:CB	2.64	0.85
1:A:293:GLY:O	1:A:295:GLY:N	2.08	0.84
1:B:306:ASN:ND2	3:B:400:NAG:C2	2.40	0.83
1:A:282:GLY:O	1:A:283:THR:OG1	1.96	0.82
1:B:307:SER:O	1:B:308:SER:OG	1.99	0.80
1:B:322:THR:HA	1:B:325:GLN:HG3	1.64	0.78
1:B:319:ASN:OD1	1:B:321:THR:HG23	1.84	0.77
1:B:306:ASN:CG	3:B:400:NAG:C1	2.57	0.76
1:A:279:LEU:HD13	1:A:283:THR:H	1.52	0.74
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.51	0.73
1:A:33:CYS:SG	1:A:164:CYS:HB3	2.29	0.73
1:A:209:THR:OG1	1:A:210:LYS:N	2.13	0.73
1:B:321:THR:O	1:B:323:ALA:N	2.20	0.70
1:B:322:THR:HA	1:B:325:GLN:CG	2.22	0.69
1:A:100:CYS:SG	1:A:164:CYS:HB2	2.32	0.69
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.08	0.68
1:B:291:GLY:C	1:B:292:THR:HG23	2.19	0.67
1:A:98:CYS:CB	1:A:162:CYS:SG	2.83	0.66
1:B:282:GLY:O	1:B:283:THR:OG1	2.13	0.66
1:B:294:CYS:SG	1:B:324:CYS:HB3	2.31	0.66
1:B:122:ASP:OD1	1:B:126:ARG:NH1	2.28	0.66
1:A:33:CYS:SG	1:A:164:CYS:CB	2.85	0.65
1:B:321:THR:O	1:B:322:THR:HG23	1.98	0.63
1:A:209:THR:HG1	1:A:210:LYS:H	1.45	0.63
1:B:30:ASN:OD1	1:B:30:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:OG1	1:A:293:GLY:N	2.24	0.62
1:B:184:ASN:HD21	3:B:402:NAG:C1	2.13	0.61
1:B:240:LEU:HD12	1:B:264:LEU:HD11	1.81	0.61
1:B:291:GLY:O	1:B:292:THR:HG23	2.01	0.61
1:A:293:GLY:C	1:A:295:GLY:H	2.06	0.60
1:B:195:THR:OG1	1:B:198:THR:OG1	2.20	0.60
1:A:30:ASN:OD1	1:A:31:PHE:N	2.33	0.59
1:A:207:ASP:CG	1:A:209:THR:CG2	2.77	0.58
1:B:206:ASP:HB2	1:B:210:LYS:NZ	2.19	0.57
1:B:206:ASP:HB2	1:B:210:LYS:HZ3	1.68	0.57
1:A:242:ASP:OD1	1:A:259:SER:N	2.32	0.56
2:C:2:NAG:H61	2:C:3:NAG:C1	2.35	0.56
1:B:194:VAL:HG12	1:B:195:THR:N	2.22	0.55
1:B:252:CYS:SG	1:B:275:PRO:HD2	2.46	0.55
1:A:184:ASN:HD21	3:A:403:NAG:C1	2.20	0.54
1:A:30:ASN:HB2	1:A:161:PRO:HB3	1.90	0.54
1:A:260:THR:HG22	1:A:261:THR:HG23	1.88	0.54
1:A:98:CYS:HB2	1:A:162:CYS:SG	2.47	0.54
1:B:45:ILE:HG22	1:B:176:ALA:HB3	1.90	0.53
1:A:282:GLY:C	1:A:283:THR:HG1	2.07	0.53
1:B:194:VAL:CG1	1:B:195:THR:N	2.73	0.52
1:B:207:ASP:H	1:B:210:LYS:HE2	1.75	0.52
1:B:279:LEU:HD13	1:B:283:THR:HA	1.90	0.51
1:B:66:THR:HB	1:B:68:PRO:HD2	1.91	0.51
1:B:98:CYS:SG	1:B:105:GLY:C	2.94	0.51
1:A:33:CYS:SG	1:A:164:CYS:HB2	2.52	0.50
1:B:100:CYS:SG	1:B:101:ASN:O	2.53	0.49
1:B:261:THR:O	1:B:322:THR:HG22	2.11	0.49
1:A:189:ALA:HB1	1:A:194:VAL:O	2.12	0.49
1:A:255:CYS:HG	1:A:266:CYS:HG	1.59	0.49
1:B:306:ASN:ND2	3:B:400:NAG:H2	2.25	0.49
1:B:321:THR:C	1:B:322:THR:CG2	2.85	0.49
1:A:293:GLY:C	1:A:295:GLY:N	2.65	0.49
1:B:185:THR:HG21	1:B:200:LEU:HD21	1.96	0.48
1:B:235:HIS:CD2	1:B:235:HIS:C	2.91	0.48
1:A:282:GLY:C	1:A:283:THR:HG23	2.38	0.48
1:B:167:GLU:OE1	1:B:198:THR:HG22	2.13	0.48
1:B:98:CYS:SG	1:B:106:GLN:N	2.87	0.47
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.71	0.47
1:B:61:ARG:HG2	1:B:62:PHE:CD1	2.49	0.47
1:A:134:THR:HG23	1:A:137:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:O	1:B:286:LEU:C	2.54	0.47
1:B:282:GLY:C	1:B:283:THR:HG1	2.17	0.47
1:A:280:CYS:O	1:A:281:ASN:HB2	2.13	0.47
1:A:41:CYS:CB	1:A:164:CYS:SG	2.98	0.47
1:B:200:LEU:HD11	1:B:208:PRO:HG3	1.97	0.46
1:A:121:LEU:HD13	1:A:150:ILE:HG21	1.96	0.46
1:A:119:ASP:HB3	1:A:124:ILE:HD11	1.98	0.46
1:B:321:THR:C	1:B:323:ALA:N	2.74	0.46
1:A:207:ASP:C	1:A:209:THR:HG23	2.41	0.46
1:B:129:PHE:CE2	1:B:158:ILE:HG13	2.51	0.46
1:B:195:THR:HG1	1:B:198:THR:HG1	1.57	0.45
1:A:43:SER:OG	1:A:163:SER:O	2.35	0.45
1:B:260:THR:HG22	1:B:261:THR:HG23	1.97	0.45
1:B:53:THR:HB	1:B:54:THR:H	1.55	0.45
1:A:33:CYS:SG	1:A:35:VAL:HG22	2.57	0.44
1:A:207:ASP:OD1	1:A:209:THR:HG22	2.17	0.44
1:B:307:SER:C	1:B:308:SER:HG	2.11	0.44
1:B:117:PRO:O	1:B:118:GLN:HB2	2.17	0.44
1:B:282:GLY:C	1:B:283:THR:HG23	2.42	0.43
1:A:199:LEU:O	1:A:203:ASN:HB2	2.19	0.43
1:B:30:ASN:CG	1:B:31:PHE:H	2.27	0.43
1:B:43:SER:O	1:B:95:PRO:HA	2.18	0.43
1:A:163:SER:HA	1:A:164:CYS:HB2	2.01	0.43
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.43	0.43
1:A:167:GLU:O	1:A:168:GLU:HB2	2.17	0.43
1:B:230:ASP:OD1	1:B:235:HIS:NE2	2.52	0.43
1:B:279:LEU:HD13	1:B:283:THR:H	1.84	0.42
1:A:144:ILE:HA	1:A:145:PRO:HD3	1.75	0.42
1:B:49:SER:HA	1:B:50:PRO:HD2	1.93	0.42
1:A:196:GLU:O	1:A:200:LEU:HG	2.19	0.42
1:A:289:THR:HG23	1:A:297:THR:O	2.20	0.42
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.83	0.41
1:B:144:ILE:HA	1:B:145:PRO:HD3	1.71	0.41
1:A:40:THR:HA	1:A:98:CYS:O	2.21	0.41
1:B:98:CYS:SG	1:B:105:GLY:CA	3.08	0.41
1:A:115:VAL:HG13	1:A:119:ASP:HB2	2.03	0.41
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.93	0.41
1:B:194:VAL:HG12	1:B:195:THR:O	2.21	0.41
1:B:238:MET:HE3	1:B:248:THR:HB	2.02	0.41
1:A:101:ASN:OD1	1:A:101:ASN:C	2.64	0.41
1:A:122:ASP:O	1:A:126:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:CYS:SG	1:A:266:CYS:SG	3.17	0.40

All (1) 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:A:281:ASN:OD1	1:B:227:SER:OG[2_545]	1.99	0.21

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	290/297 (98%)	265 (91%)	20 (7%)	5 (2%)	7	13
1	B	295/297 (99%)	274 (93%)	19 (6%)	2 (1%)	18	34
All	All	585/594 (98%)	539 (92%)	39 (7%)	7 (1%)	10	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	CYS
1	B	99	ARG
1	A	117	PRO
1	A	206	ASP
1	A	209	THR
1	B	308	SER
1	A	208	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	244/248 (98%)	230 (94%)	14 (6%)	18	39
1	B	248/248 (100%)	228 (92%)	20 (8%)	11	23
All	All	492/496 (99%)	458 (93%)	34 (7%)	14	30

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	CYS
1	A	53	THR
1	A	118	GLN
1	A	121	LEU
1	A	149	LYS
1	A	184	ASN
1	A	197	SER
1	A	209	THR
1	A	213	MET
1	A	225	ARG
1	A	269	VAL
1	A	272	LYS
1	A	284	LEU
1	A	310	LEU
1	B	30	ASN
1	B	53	THR
1	B	100	CYS
1	B	103	ASP
1	B	104	VAL
1	B	191	LYS
1	B	195	THR
1	B	198	THR
1	B	231	THR
1	B	255	CYS
1	B	260	THR
1	B	274	CYS
1	B	280	CYS
1	B	284	LEU
1	B	285	LYS
1	B	294	CYS
1	B	297	THR

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Mol	Chain	Res	Type
1	B	307	SER
1	B	310	LEU
1	B	322	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	290	ASN
1	B	184	ASN
1	B	235	HIS
1	B	236	ASN
1	B	251	ASN

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 ⓘ

3 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	2	15,15,15	0.83	0	21,21,21	1.22	2 (9%)
2	NAG	C	2	2	14,14,15	0.99	1 (7%)	17,19,21	1.64	4 (23%)
2	NAG	C	3	2	14,14,15	1.34	1 (7%)	17,19,21	1.64	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	C	3	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	NAG	C2-N2	-2.25	1.42	1.46
2	C	2	NAG	O5-C5	-2.02	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAG	C1-O5-C5	4.36	118.03	112.19
2	C	2	NAG	O5-C5-C6	-3.21	101.42	107.66
2	C	2	NAG	O6-C6-C5	-2.95	101.30	111.33
2	C	2	NAG	C1-O5-C5	2.64	115.72	112.19
2	C	1	NAG	O5-C1-C2	-2.47	107.03	109.52
2	C	2	NAG	O5-C5-C4	-2.42	104.94	110.83
2	C	3	NAG	C1-C2-N2	-2.28	106.83	110.43
2	C	3	NAG	C3-C4-C5	-2.05	106.52	110.23
2	C	1	NAG	O6-C6-C5	-2.00	104.52	111.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

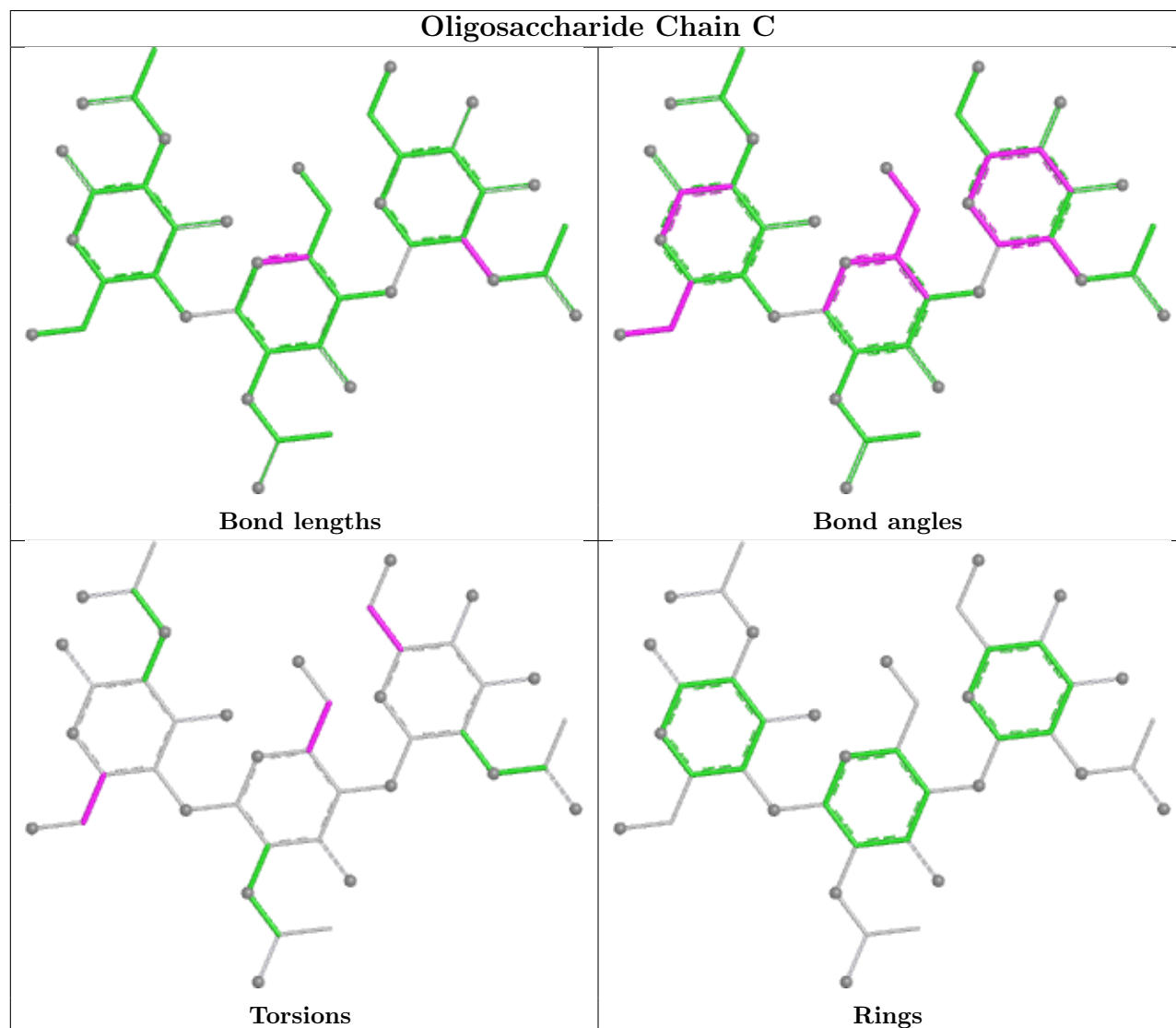
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	3	NAG	O5-C5-C6-O6
2	C	3	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

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



5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	NAG	B	401	-	14,14,15	0.86	1 (7%)	17,19,21	0.81	0
3	NAG	B	400	-	14,14,15	1.56	2 (14%)	17,19,21	1.21	2 (11%)
3	NAG	A	403	-	14,14,15	0.27	0	17,19,21	0.36	0
3	NAG	B	402	-	14,14,15	0.48	0	17,19,21	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
3	NAG	B	401	-	-	2/6/23/26	0/1/1/1
3	NAG	B	400	-	-	0/6/23/26	0/1/1/1
3	NAG	A	403	-	-	2/6/23/26	0/1/1/1
3	NAG	B	402	-	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	NAG	O5-C1	-5.19	1.35	1.43
3	B	400	NAG	C1-C2	-2.54	1.48	1.52
3	B	401	NAG	C1-C2	-2.19	1.49	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	NAG	C3-C4-C5	2.89	115.48	110.23
3	B	400	NAG	C1-O5-C5	-2.75	108.50	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	C4-C5-C6-O6
3	B	401	NAG	O5-C5-C6-O6
3	A	403	NAG	O5-C5-C6-O6
3	A	403	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	NAG	5	0
3	A	403	NAG	1	0
3	B	402	NAG	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

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, 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	292/297 (98%)	1.10	44 (15%) 5 4	27, 53, 82, 103	0
1	B	297/297 (100%)	1.08	43 (14%) 6 5	27, 52, 75, 98	0
All	All	589/594 (99%)	1.09	87 (14%) 5 4	27, 52, 78, 103	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	SER	9.9
1	B	29	ALA	7.3
1	B	98	CYS	7.3
1	B	322	THR	7.0
1	B	30	ASN	6.3
1	B	294	CYS	6.3
1	B	307	SER	5.9
1	A	292	THR	5.9
1	A	29	ALA	5.9
1	B	162	CYS	5.7
1	A	206	ASP	5.4
1	B	281	ASN	5.3
1	B	325	GLN	5.3
1	A	100	CYS	5.2
1	A	180	GLY	5.1
1	A	308	SER	4.9
1	B	283	THR	4.8
1	A	205	ILE	4.7
1	A	320	GLN	4.7
1	A	209	THR	4.7
1	A	283	THR	4.4
1	A	269	VAL	4.1
1	B	230	ASP	4.0
1	B	100	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	320	GLN	3.8
1	A	164	CYS	3.6
1	A	30	ASN	3.5
1	A	41	CYS	3.5
1	B	288	GLU	3.4
1	B	324	CYS	3.4
1	A	102	GLY	3.3
1	A	163	SER	3.3
1	A	291	GLY	3.1
1	B	206	ASP	3.1
1	A	309	SER	3.1
1	A	281	ASN	3.1
1	B	321	THR	3.0
1	A	103	ASP	3.0
1	B	282	GLY	2.9
1	B	292	THR	2.9
1	B	318	THR	2.9
1	B	164	CYS	2.8
1	B	205	ILE	2.7
1	A	181	LYS	2.7
1	A	182	GLY	2.7
1	A	318	THR	2.7
1	A	168	GLU	2.7
1	A	319	ASN	2.7
1	A	270	GLN	2.6
1	B	151	ASN	2.6
1	B	293	GLY	2.6
1	A	167	GLU	2.6
1	A	101	ASN	2.6
1	A	288	GLU	2.5
1	A	118	GLN	2.5
1	A	93	LYS	2.5
1	B	311	ILE	2.5
1	B	290	ASN	2.5
1	B	182	GLY	2.4
1	B	170	SER	2.4
1	B	204	LYS	2.4
1	A	294	CYS	2.4
1	B	83	SER	2.4
1	A	295	GLY	2.4
1	A	306	ASN	2.4
1	A	134	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASN	2.3
1	A	225	ARG	2.3
1	A	117	PRO	2.3
1	B	319	ASN	2.3
1	A	31	PHE	2.3
1	B	41	CYS	2.3
1	B	193	GLY	2.2
1	B	308	SER	2.2
1	A	98	CYS	2.2
1	A	143	ASN	2.2
1	B	212	GLN	2.2
1	B	89	ASN	2.1
1	B	323	ALA	2.1
1	B	200	LEU	2.1
1	A	208	PRO	2.1
1	A	153	SER	2.1
1	B	146	ASP	2.1
1	B	40	THR	2.1
1	B	102	GLY	2.1
1	A	262	TYR	2.1
1	B	315	SER	2.0

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

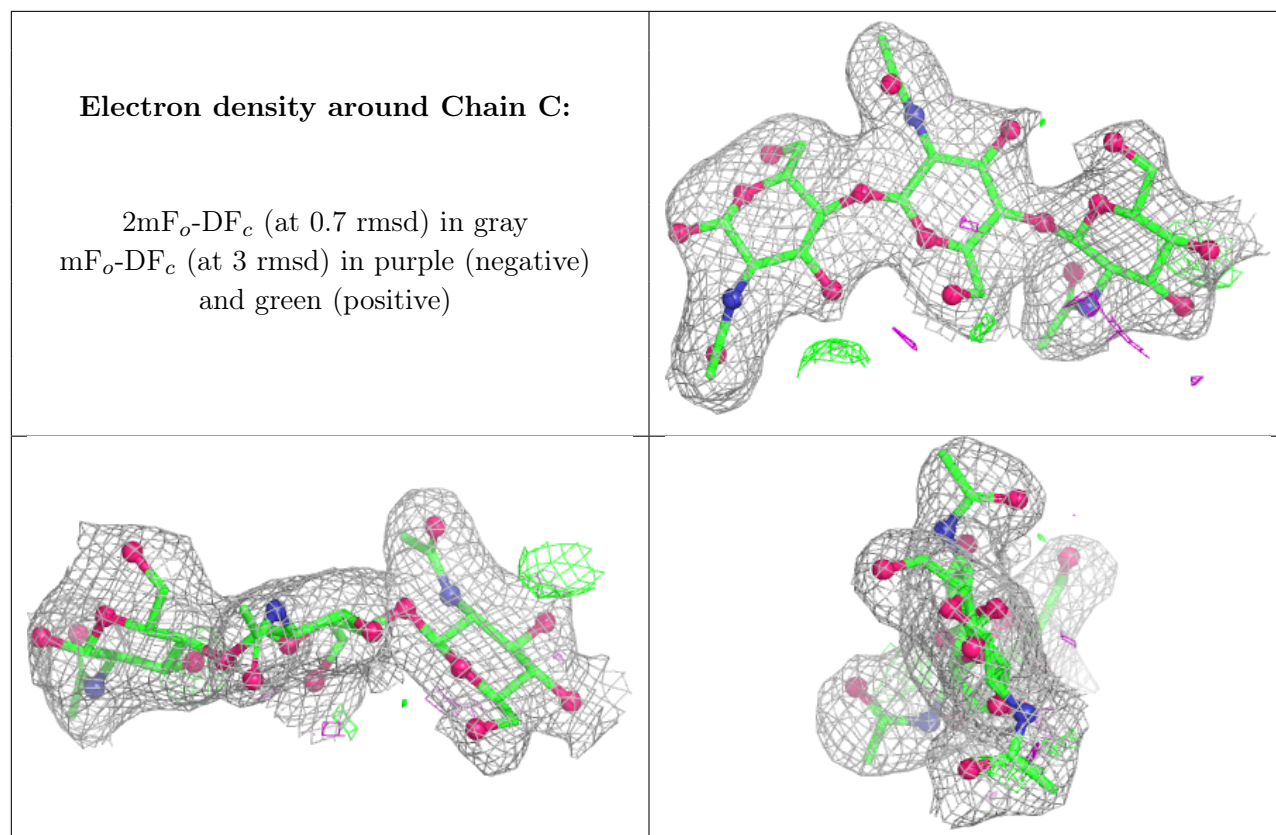
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.85	0.12	50,60,67,68	0
2	NAG	C	1	15/15	0.89	0.11	49,61,71,72	0
2	NAG	C	3	14/15	0.93	0.12	46,51,57,59	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
3	NAG	A	403	14/15	0.54	0.26	75,82,86,90	0
3	NAG	B	401	14/15	0.77	0.16	54,67,70,74	0
3	NAG	B	402	14/15	0.81	0.17	58,63,70,75	0
3	NAG	B	400	14/15	0.88	0.14	57,61,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.