Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 04:23 PM EDT

PDB ID	:	2R9K
Title	:	Crystal Structure of Misteltoe Lectin I in Complex with Phloretamide
Authors	:	Meyer, A.; Rypniewski, W.; Celewicz, L.; Erdmann, V.A.; Voelter, W.; Betzel, C.
Deposited on	:	2007-09-13
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 (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:

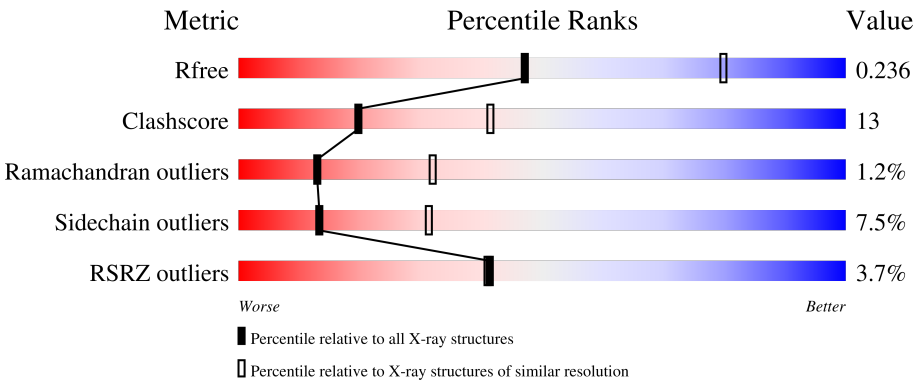
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	254	3% 67% 25% • • •
2	B	263	4% 68% 25% 6% •
3	C	2	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4135 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 Beta-galactoside-specific lectin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	1927	1218	330	375	4	0	1	0

- Molecule 2 is a protein called Beta-galactoside-specific lectin 1 chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	1995	1239	352	392	12	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	249	ALA	ASP	conflict	UNP P81446
B	253	THR	SER	conflict	UNP P81446
B	258	ILE	THR	conflict	UNP P81446
B	268	THR	CYS	conflict	UNP P81446
B	301	LYS	ARG	conflict	UNP P81446
B	337	ILE	LEU	conflict	UNP P81446
B	339	GLN	GLU	conflict	UNP P81446
B	390	THR	VAL	conflict	UNP P81446
B	403	ALA	ASN	conflict	UNP P81446
B	408	TYR	TRP	conflict	UNP P81446
B	413	THR	VAL	conflict	UNP P81446
B	414	ALA	ILE	conflict	UNP P81446
B	415	GLY	SER	conflict	UNP P81446
B	417	GLU	GLN	conflict	UNP P81446
B	434	LEU	ASN	conflict	UNP P81446
B	436	SER	ASP	conflict	UNP P81446
B	441	ASN	CYS	conflict	UNP P81446
B	446	ILE	VAL	conflict	UNP P81446
B	489	SER	LYS	conflict	UNP P81446
B	491	GLN	ARG	conflict	UNP P81446

Continued on next page...

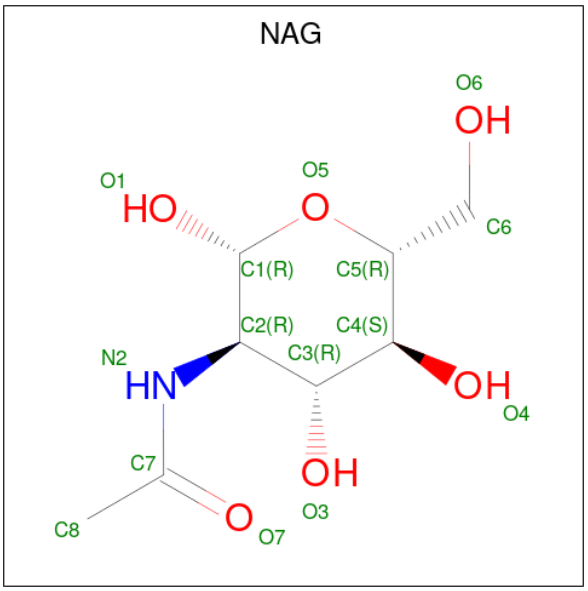
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	501	ASN	LYS	conflict	UNP P81446

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

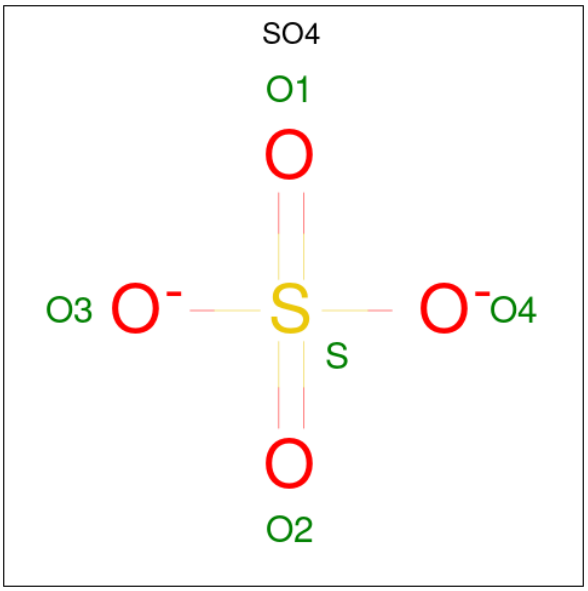
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



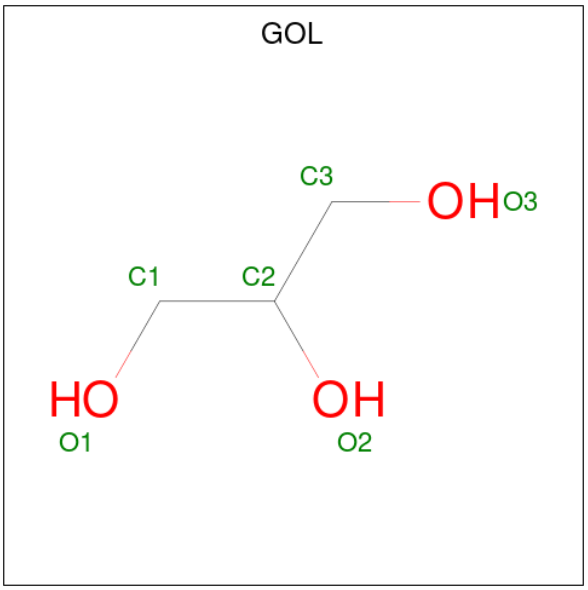
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

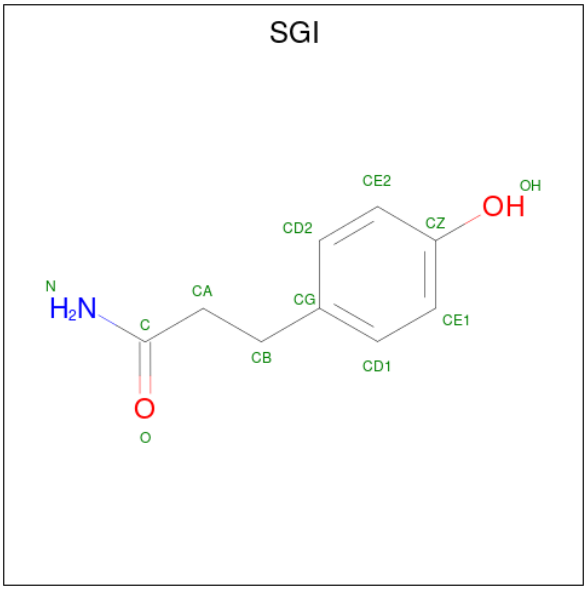


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0

- Molecule 8 is 3-(4-hydroxyphenyl)propanamide (three-letter code: SGI) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	12	9	1	2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	27	27	27	0	0

Continued on next page...

Continued from previous page...

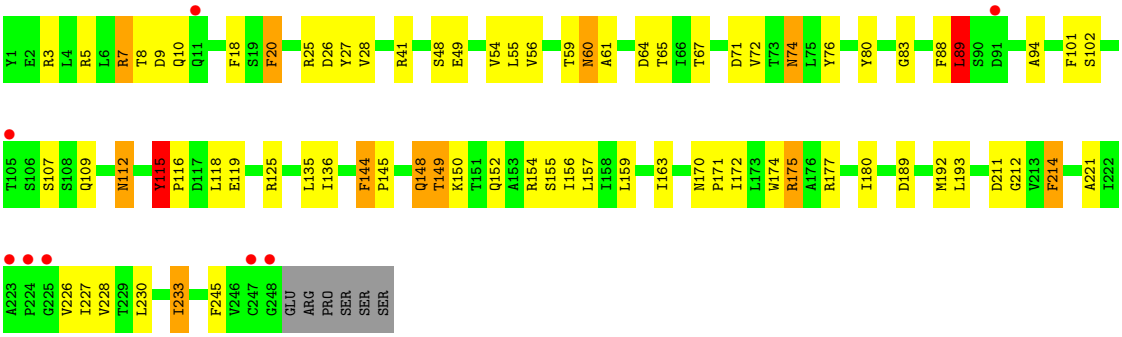
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	B	45	45	45	0	0

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.

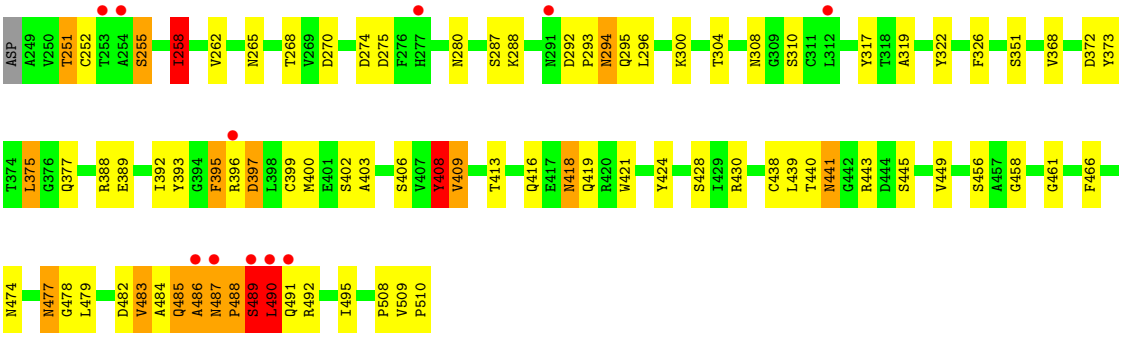
• Molecule 1: Beta-galactoside-specific lectin 1

Chain A:



• Molecule 2: Beta-galactoside-specific lectin 1 chain B

Chain B:



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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.06Å 107.06Å 312.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.74 – 2.70 19.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.74-2.70) 99.9 (19.93-2.70)	Depositor EDS
R_{merge}	0.60	Depositor
R_{sym}	0.47	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.267 0.225 , 0.236	Depositor DCC
R_{free} test set	1524 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 33.9	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	0.93	EDS
Total number of atoms	4135	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: SO4, SGI, NAG, CL, GOL

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	0.50	0/1965	0.65	0/2678
2	B	0.52	0/2034	0.68	0/2774
All	All	0.51	0/3999	0.66	0/5452

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	33
2	B	0	37
All	All	0	70

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	SER	Mainchain
1	A	115	TYR	Sidechain
1	A	116	PRO	Mainchain
1	A	118	LEU	Mainchain
1	A	135	LEU	Mainchain
1	A	144	PHE	Sidechain
1	A	154	ARG	Sidechain
1	A	156	ILE	Mainchain
1	A	171	PRO	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	174	TRP	Mainchain
1	A	175[A]	ARG	Sidechain
1	A	177	ARG	Mainchain
1	A	18	PHE	Sidechain
1	A	180	ILE	Mainchain
1	A	20	PHE	Sidechain
1	A	211	ASP	Mainchain
1	A	214	PHE	Sidechain
1	A	221	ALA	Mainchain
1	A	227	ILE	Mainchain
1	A	245	PHE	Sidechain
1	A	26	ASP	Mainchain
1	A	27	TYR	Sidechain
1	A	3	ARG	Mainchain
1	A	5	ARG	Sidechain
1	A	54	VAL	Mainchain
1	A	61	ALA	Mainchain
1	A	65	THR	Mainchain
1	A	7	ARG	Mainchain
1	A	83	GLY	Mainchain
1	A	88	PHE	Sidechain
1	A	89	LEU	Mainchain
1	A	94	ALA	Mainchain
2	B	251	THR	Mainchain
2	B	252	CYS	Mainchain
2	B	255	SER	Mainchain
2	B	258	ILE	Mainchain
2	B	270	ASP	Sidechain
2	B	274	ASP	Sidechain
2	B	287	SER	Mainchain
2	B	300	LYS	Mainchain
2	B	304	THR	Mainchain
2	B	317	TYR	Sidechain
2	B	319	ALA	Mainchain
2	B	322	TYR	Sidechain
2	B	351	SER	Mainchain
2	B	368	VAL	Mainchain
2	B	388	ARG	Sidechain
2	B	392	ILE	Mainchain
2	B	393	TYR	Sidechain
2	B	396	ARG	Sidechain
2	B	397	ASP	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	399	CYS	Mainchain
2	B	400	MET	Mainchain
2	B	408	TYR	Sidechain
2	B	409	VAL	Mainchain
2	B	438	CYS	Mainchain
2	B	441	ASN	Mainchain
2	B	443	ARG	Sidechain
2	B	445	SER	Mainchain
2	B	449	VAL	Mainchain
2	B	456	SER	Mainchain
2	B	482	ASP	Sidechain
2	B	483	VAL	Mainchain
2	B	485	GLN	Mainchain
2	B	486	ALA	Mainchain,Peptide
2	B	489	SER	Mainchain
2	B	490	LEU	Peptide
2	B	508	PRO	Mainchain

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	1927	0	1896	35	0
2	B	1995	0	1934	65	0
3	C	28	0	22	3	0
4	A	14	0	13	1	0
4	B	42	0	39	3	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	12	0	16	2	0
6	B	12	0	16	3	0
7	A	1	0	0	0	0
8	A	12	0	11	0	0
9	A	27	0	0	1	0
9	B	45	0	0	0	0
All	All	4135	0	3947	102	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 13.

All (102) 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)
2:B:489:SER:H	2:B:490:LEU:HA	1.29	0.98
1:A:148:GLN:HG2	1:A:150:LYS:HB3	1.46	0.96
2:B:408:TYR:HD2	2:B:491:GLN:O	1.48	0.95
2:B:489:SER:N	2:B:490:LEU:HA	1.80	0.94
2:B:488:PRO:HA	2:B:489:SER:HB2	1.50	0.93
1:A:148:GLN:HG3	1:A:150:LYS:H	1.35	0.91
2:B:288:LYS:H	2:B:295:GLN:HE22	1.14	0.90
2:B:265:ASN:HD22	2:B:430:ARG:HH22	1.22	0.87
1:A:115:TYR:O	1:A:119:GLU:OE2	1.92	0.86
1:A:148:GLN:CG	1:A:150:LYS:HB3	2.07	0.83
2:B:489:SER:N	2:B:490:LEU:CA	2.42	0.82
2:B:477:ASN:HD22	2:B:479:LEU:H	1.29	0.79
1:A:148:GLN:HG3	1:A:150:LYS:N	1.97	0.79
2:B:474:ASN:HD22	2:B:477:ASN:H	1.28	0.78
2:B:477:ASN:ND2	2:B:479:LEU:H	1.85	0.74
1:A:9:ASP:HA	1:A:136:ILE:HD11	1.69	0.72
2:B:262:VAL:HG22	2:B:268:THR:HG22	1.72	0.72
2:B:466:PHE:H	6:B:647:GOL:H11	1.54	0.71
2:B:490:LEU:H	2:B:491:GLN:CG	2.03	0.70
2:B:416:GLN:HE21	2:B:418:ASN:HD21	1.39	0.70
2:B:258:ILE:CD1	2:B:296:LEU:HB3	2.22	0.69
2:B:441:ASN:HD22	2:B:495:ILE:HD13	1.56	0.69
2:B:484:ALA:HA	2:B:485:GLN:HG3	1.73	0.69
1:A:25:ARG:HH12	1:A:170:ASN:HD21	1.46	0.63
2:B:408:TYR:CD2	2:B:491:GLN:O	2.40	0.62
2:B:477:ASN:HD22	2:B:477:ASN:C	2.02	0.62
2:B:484:ALA:CA	2:B:485:GLN:HG3	2.30	0.62
2:B:474:ASN:ND2	2:B:477:ASN:H	1.97	0.61
2:B:490:LEU:H	2:B:491:GLN:HG3	1.65	0.61
2:B:409:VAL:HG23	2:B:488:PRO:HG3	1.82	0.61
2:B:372:ASP:H	2:B:377:GLN:HE22	1.48	0.60
2:B:490:LEU:H	2:B:491:GLN:HG2	1.65	0.60
1:A:212:GLY:HA2	1:A:233:ILE:HG23	1.84	0.59
2:B:258:ILE:HD11	2:B:296:LEU:HB3	1.84	0.59
3:C:1:NAG:H3	3:C:1:NAG:H83	1.83	0.59
2:B:488:PRO:HA	2:B:489:SER:CB	2.29	0.58
1:A:71:ASP:HB3	1:A:74:ASN:HD21	1.70	0.57
2:B:490:LEU:N	2:B:491:GLN:HG2	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:ASN:ND2	2:B:430:ARG:HH22	1.98	0.57
1:A:170:ASN:ND2	6:A:649:GOL:H32	2.20	0.57
4:B:603:NAG:O4	4:B:604:NAG:H2	2.04	0.57
2:B:466:PHE:H	6:B:647:GOL:C1	2.17	0.56
2:B:488:PRO:HG2	2:B:488:PRO:O	2.06	0.55
2:B:492:ARG:HH11	2:B:492:ARG:HG3	1.71	0.55
2:B:490:LEU:CB	2:B:491:GLN:HG2	2.36	0.55
2:B:466:PHE:N	6:B:647:GOL:H11	2.19	0.55
2:B:490:LEU:HB3	2:B:491:GLN:HG2	1.90	0.54
1:A:112:ASN:OD1	4:A:500:NAG:C1	2.56	0.54
2:B:373:TYR:HE1	3:C:1:NAG:H81	1.73	0.53
1:A:25:ARG:HH22	1:A:170:ASN:ND2	2.07	0.53
1:A:74:ASN:ND2	1:A:76:TYR:H	2.07	0.52
2:B:492:ARG:HH11	2:B:492:ARG:CG	2.23	0.52
1:A:59:THR:HA	1:A:64:ASP:O	2.10	0.52
2:B:413:THR:H	2:B:419:GLN:HE22	1.59	0.51
2:B:288:LYS:NZ	2:B:294:ASN:HD21	2.08	0.51
2:B:490:LEU:CA	2:B:491:GLN:HG2	2.41	0.50
2:B:490:LEU:N	2:B:491:GLN:CG	2.73	0.50
1:A:56:VAL:HG11	1:A:163:ILE:HD13	1.94	0.50
1:A:149:THR:HA	1:A:152:GLN:HE21	1.78	0.49
2:B:488:PRO:CA	2:B:489:SER:HB2	2.33	0.48
1:A:71:ASP:HB3	1:A:74:ASN:ND2	2.27	0.48
2:B:308:ASN:HD21	4:B:600:NAG:C1	2.26	0.48
1:A:148:GLN:HE21	1:A:149:THR:H	1.63	0.47
1:A:175[A]:ARG:NH2	1:A:189:ASP:OD1	2.47	0.47
1:A:125:ARG:HG3	1:A:193:LEU:CD2	2.45	0.47
2:B:373:TYR:CE1	3:C:1:NAG:H81	2.49	0.47
2:B:477:ASN:HD22	2:B:478:GLY:N	2.13	0.46
1:A:148:GLN:HG3	1:A:150:LYS:HB3	1.94	0.46
2:B:486:ALA:O	2:B:487:ASN:ND2	2.49	0.46
1:A:67:THR:O	1:A:80:TYR:HA	2.16	0.46
2:B:490:LEU:C	2:B:491:GLN:HG2	2.37	0.46
2:B:509:VAL:HA	2:B:510:PRO:HD2	1.82	0.46
1:A:20:PHE:CZ	1:A:56:VAL:HG13	2.51	0.45
1:A:8:THR:O	1:A:60:ASN:HA	2.16	0.45
2:B:275:ASP:HB3	2:B:280:ASN:ND2	2.31	0.45
1:A:25:ARG:HH12	1:A:170:ASN:ND2	2.14	0.45
1:A:125:ARG:HG3	1:A:193:LEU:HD22	1.98	0.45
2:B:440:THR:HA	2:B:461:GLY:O	2.16	0.45
2:B:294:ASN:HD22	2:B:294:ASN:H	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:NH1	1:A:170:ASN:HD21	2.13	0.44
2:B:418:ASN:C	2:B:418:ASN:HD22	2.21	0.44
1:A:89:LEU:HD22	1:A:109:GLN:HE22	1.83	0.44
1:A:144:PHE:HA	1:A:145:PRO:HD3	1.85	0.44
2:B:488:PRO:CA	2:B:489:SER:CB	2.95	0.43
1:A:148:GLN:NE2	9:A:658:HOH:O	2.51	0.43
2:B:308:ASN:HD21	4:B:600:NAG:C2	2.31	0.43
2:B:402:SER:HB3	2:B:421:TRP:CH2	2.54	0.43
2:B:395:PHE:HE2	2:B:487:ASN:HA	1.83	0.42
2:B:416:GLN:HE21	2:B:418:ASN:ND2	2.11	0.42
2:B:424:TYR:HB2	2:B:428:SER:OG	2.19	0.42
2:B:477:ASN:ND2	2:B:477:ASN:C	2.72	0.42
2:B:484:ALA:CB	2:B:485:GLN:HG3	2.50	0.42
1:A:155:SER:O	1:A:159:LEU:HG	2.19	0.42
1:A:175[A]:ARG:NH1	6:A:650:GOL:O1	2.43	0.42
2:B:403:ALA:HB3	2:B:408:TYR:HE1	1.84	0.42
2:B:292:ASP:HA	2:B:293:PRO:HD3	1.84	0.41
1:A:28:VAL:HG12	1:A:72:VAL:HG22	2.02	0.41
2:B:375:LEU:HD22	2:B:458:GLY:HA2	2.03	0.41
1:A:214:PHE:HE1	1:A:233:ILE:HG22	1.85	0.41
2:B:488:PRO:O	2:B:488:PRO:CG	2.60	0.41
1:A:172:ILE:HG12	1:A:192:MET:HG3	2.04	0.40
2:B:310:SER:HB2	2:B:326:PHE:O	2.21	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	247/254 (97%)	234 (95%)	11 (4%)	2 (1%)	19 43
2	B	260/263 (99%)	241 (93%)	15 (6%)	4 (2%)	10 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	507/517 (98%)	475 (94%)	26 (5%)	6 (1%)	13 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	487	ASN
2	B	488	PRO
1	A	101	PHE
2	B	489	SER
1	A	115	TYR
2	B	395	PHE

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	210/215 (98%)	192 (91%)	18 (9%)	10 24
2	B	218/219 (100%)	204 (94%)	14 (6%)	17 39
All	All	428/434 (99%)	396 (92%)	32 (8%)	13 31

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	10	GLN
1	A	41	ARG
1	A	48	SER
1	A	49	GLU
1	A	55	LEU
1	A	60	ASN
1	A	74	ASN
1	A	89	LEU
1	A	102	SER
1	A	112	ASN
1	A	148	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	THR
1	A	157	LEU
1	A	226	VAL
1	A	228	VAL
1	A	230	LEU
1	A	233	ILE
2	B	251	THR
2	B	255	SER
2	B	258	ILE
2	B	294	ASN
2	B	375	LEU
2	B	389	GLU
2	B	397	ASP
2	B	406	SER
2	B	408	TYR
2	B	418	ASN
2	B	439	LEU
2	B	477	ASN
2	B	483	VAL
2	B	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	60	ASN
1	A	74	ASN
1	A	85	GLN
1	A	109	GLN
1	A	112	ASN
1	A	148	GLN
1	A	152	GLN
1	A	161	GLN
1	A	170	ASN
1	A	215	ASN
1	A	216	ASN
2	B	265	ASN
2	B	294	ASN
2	B	295	GLN
2	B	308	ASN
2	B	348	ASN
2	B	377	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	418	ASN
2	B	419	GLN
2	B	462	GLN
2	B	474	ASN
2	B	477	ASN
2	B	487	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	$\#\|Z\| > 2$
3	NAG	C	1	3,2	14,14,15	0.64	0	17,19,21	1.99	5 (29%)
3	NAG	C	2	3	14,14,15	0.77	0	17,19,21	1.53	5 (29%)

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	C	1	3,2	-	5/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	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})
3	C	1	NAG	C2-N2-C7	4.56	129.39	122.90
3	C	1	NAG	C1-O5-C5	3.83	117.38	112.19
3	C	1	NAG	C8-C7-N2	3.15	121.42	116.10
3	C	1	NAG	O4-C4-C5	3.04	116.84	109.30
3	C	2	NAG	C1-C2-N2	-2.66	105.94	110.49
3	C	2	NAG	O5-C1-C2	-2.63	107.14	111.29
3	C	2	NAG	C4-C3-C2	2.23	114.29	111.02
3	C	2	NAG	C1-O5-C5	2.17	115.14	112.19
3	C	1	NAG	C3-C4-C5	-2.17	106.38	110.24
3	C	2	NAG	O7-C7-C8	-2.12	118.11	122.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	C	1	NAG	O5-C5-C6-O6

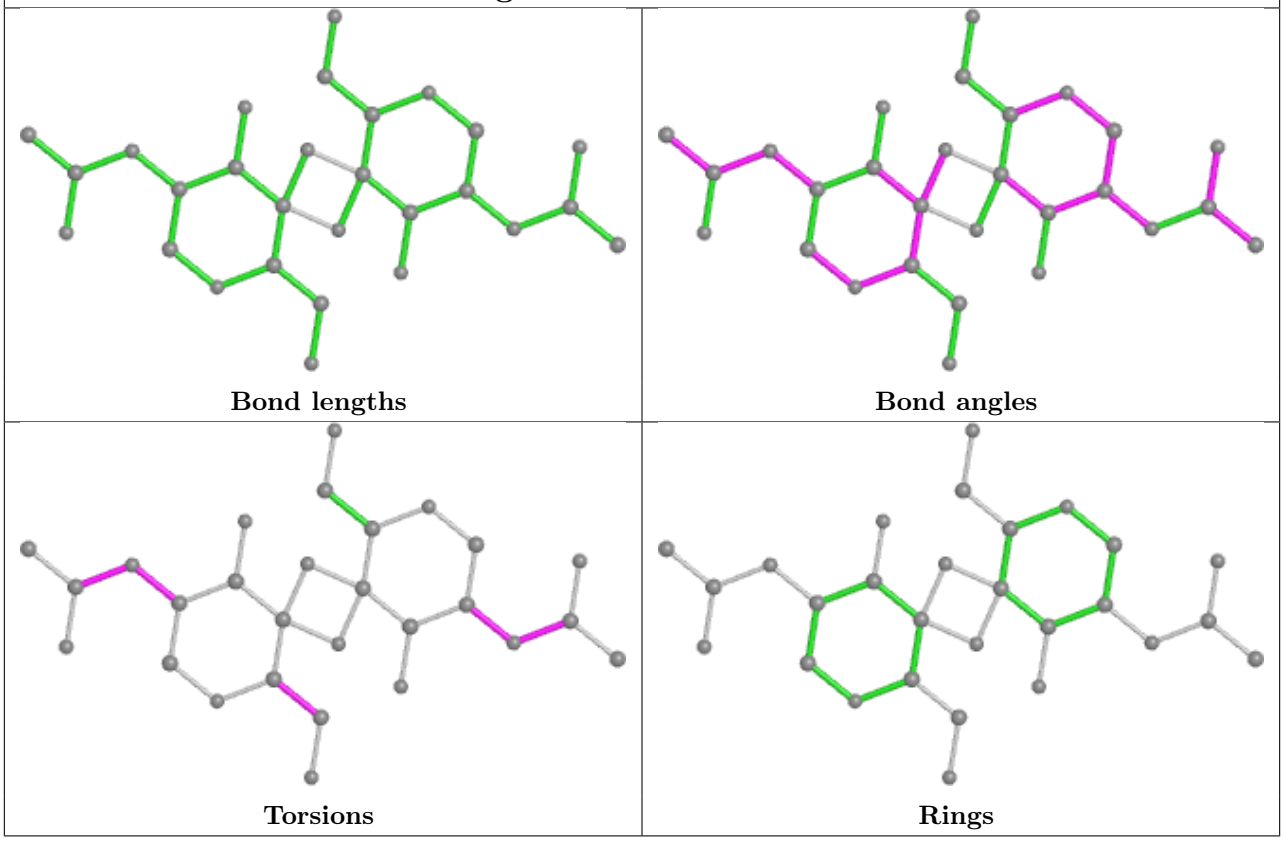
There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	NAG	B	600	-	14,14,15	0.62	0	17,19,21	1.40	2 (11%)
4	NAG	B	603	2	14,14,15	0.54	0	17,19,21	1.43	2 (11%)
6	GOL	B	648	-	5,5,5	0.34	0	5,5,5	1.08	0
5	SO4	B	3	-	4,4,4	0.09	0	6,6,6	0.34	0
6	GOL	B	647	-	5,5,5	0.33	0	5,5,5	0.50	0
5	SO4	A	256	-	4,4,4	0.17	0	6,6,6	0.42	0
8	SGI	A	600	-	12,12,12	0.51	0	15,15,15	0.62	0
5	SO4	A	257	-	4,4,4	0.14	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	255	-	4,4,4	0.13	0	6,6,6	0.12	0
6	GOL	A	649	-	5,5,5	0.32	0	5,5,5	0.32	0
4	NAG	B	604	-	14,14,15	0.47	0	17,19,21	1.89	5 (29%)
6	GOL	A	650	-	5,5,5	0.41	0	5,5,5	0.35	0
4	NAG	A	500	-	14,14,15	0.46	0	17,19,21	1.23	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
4	NAG	B	600	-	-	2/6/23/26	0/1/1/1
4	NAG	B	603	2	-	2/6/23/26	0/1/1/1
6	GOL	B	648	-	-	3/4/4/4	-
8	SGI	A	600	-	-	0/5/5/5	0/1/1/1
6	GOL	B	647	-	-	1/4/4/4	-
6	GOL	A	649	-	-	0/4/4/4	-
4	NAG	B	604	-	-	3/6/23/26	0/1/1/1
6	GOL	A	650	-	-	2/4/4/4	-
4	NAG	A	500	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	NAG	C1-O5-C5	4.48	118.26	112.19
4	B	604	NAG	C1-O5-C5	4.05	117.68	112.19
4	B	604	NAG	C3-C4-C5	3.73	116.90	110.24
4	B	600	NAG	C1-O5-C5	3.29	116.65	112.19
4	B	604	NAG	O5-C1-C2	-3.26	106.14	111.29
4	A	500	NAG	C1-C2-N2	-2.97	105.42	110.49
4	B	604	NAG	O5-C5-C4	2.84	117.74	110.83
4	B	600	NAG	C3-C4-C5	2.83	115.29	110.24
4	B	603	NAG	C6-C5-C4	-2.44	107.28	113.00
4	A	500	NAG	O5-C5-C6	2.30	110.81	107.20
4	A	500	NAG	C4-C3-C2	-2.13	107.90	111.02
4	B	604	NAG	C1-C2-N2	-2.12	106.86	110.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	NAG	C8-C7-N2-C2
6	A	650	GOL	C1-C2-C3-O3
6	B	648	GOL	O1-C1-C2-C3
6	B	648	GOL	C1-C2-C3-O3
4	A	500	NAG	O5-C5-C6-O6
4	B	603	NAG	O5-C5-C6-O6
4	B	604	NAG	C4-C5-C6-O6
4	B	604	NAG	O7-C7-N2-C2
4	B	600	NAG	O5-C5-C6-O6
4	B	600	NAG	C4-C5-C6-O6
4	B	603	NAG	C4-C5-C6-O6
4	A	500	NAG	O7-C7-N2-C2
4	A	500	NAG	C4-C5-C6-O6
4	B	604	NAG	O5-C5-C6-O6
6	B	647	GOL	C1-C2-C3-O3
6	B	648	GOL	O2-C2-C3-O3
6	A	650	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	600	NAG	2	0
4	B	603	NAG	1	0
6	B	647	GOL	3	0
6	A	649	GOL	1	0
4	B	604	NAG	1	0
6	A	650	GOL	1	0
4	A	500	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 (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	248/254 (97%)	-0.01	8 (3%)	47	48	35, 48, 68, 72	1 (0%)
2	B	262/263 (99%)	-0.01	11 (4%)	36	35	32, 41, 57, 72	0
All	All	510/517 (98%)	-0.01	19 (3%)	41	41	32, 44, 65, 72	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	486	ALA	7.9
2	B	487	ASN	6.7
1	A	224	PRO	5.0
2	B	491	GLN	4.9
1	A	223	ALA	4.7
2	B	253	THR	4.5
1	A	248	GLY	3.8
1	A	225	GLY	3.8
2	B	490	LEU	3.6
2	B	277	HIS	3.2
2	B	489	SER	2.7
1	A	105	THR	2.6
2	B	254	ALA	2.4
1	A	91	ASP	2.4
2	B	396	ARG	2.3
1	A	247	CYS	2.2
2	B	312	LEU	2.2
1	A	11	GLN	2.1
2	B	291	ASN	2.1

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

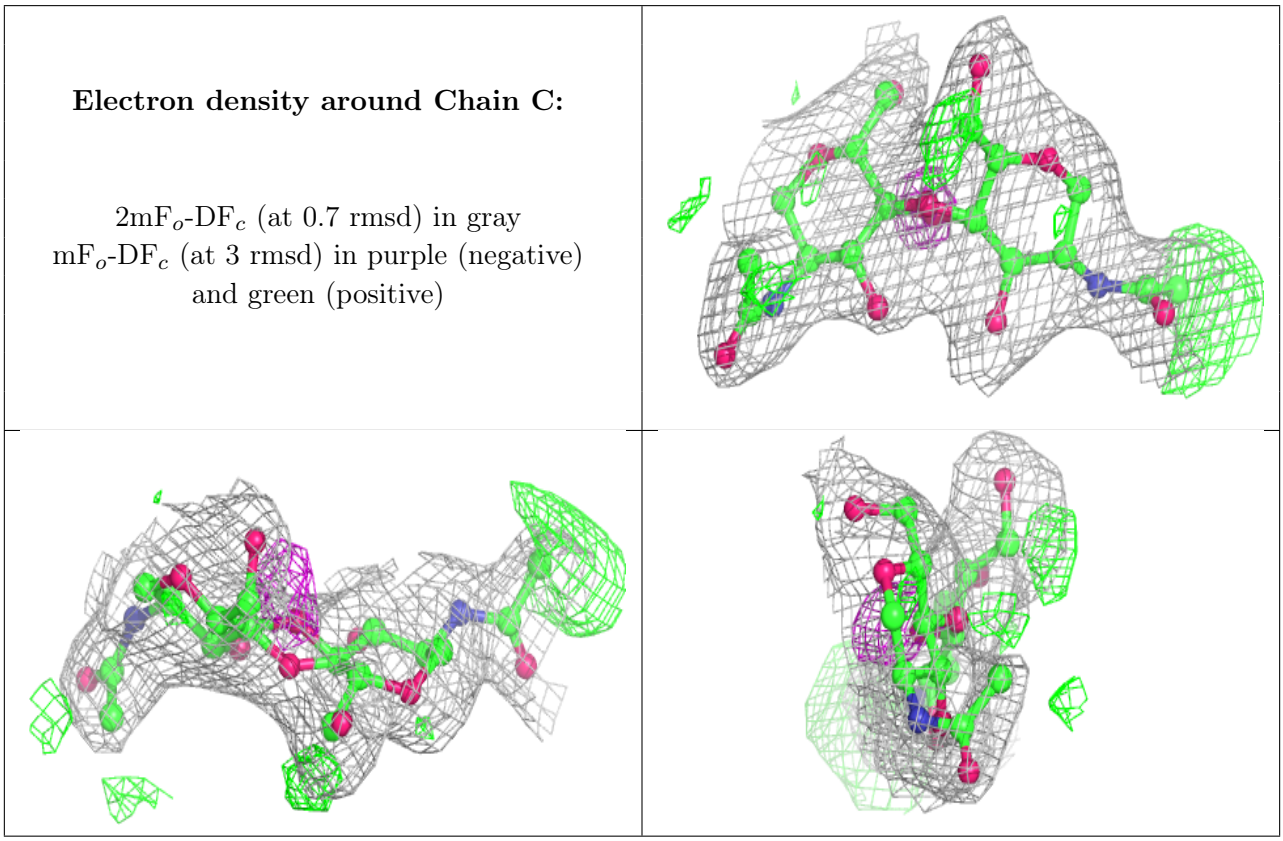
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	C	2	14/15	0.81	0.27	71,74,78,78	0
3	NAG	C	1	14/15	0.87	0.20	56,60,64,68	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
4	NAG	B	600	14/15	0.62	0.27	80,83,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	500	14/15	0.70	0.27	93,94,95,95	0
4	NAG	B	604	14/15	0.72	0.31	81,88,89,89	0
5	SO4	B	3	5/5	0.82	0.30	92,93,93,94	0
6	GOL	B	647	6/6	0.83	0.28	67,71,71,72	0
6	GOL	A	649	6/6	0.87	0.26	59,62,62,63	0
6	GOL	B	648	6/6	0.87	0.22	49,50,51,51	0
5	SO4	A	255	5/5	0.90	0.26	101,101,101,101	0
6	GOL	A	650	6/6	0.91	0.24	50,53,53,56	0
7	CL	A	258	1/1	0.92	0.19	77,77,77,77	0
8	SGI	A	600	12/12	0.93	0.19	41,42,43,43	0
4	NAG	B	603	14/15	0.96	0.14	40,43,47,48	0
5	SO4	A	256	5/5	0.97	0.09	54,55,55,55	0
5	SO4	A	257	5/5	0.98	0.27	86,86,86,87	0

6.5 Other polymers (i)

There are no such residues in this entry.