Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 01:30 pm GMT

PDB ID	:	6R43
Title	:	Structure of P110 from Mycoplasma Genitalium complexed with 6'-SL
Authors	:	Aparicio, D.; Fita, I.
Deposited on	:	2019-03-21
Resolution	:	2.52 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:

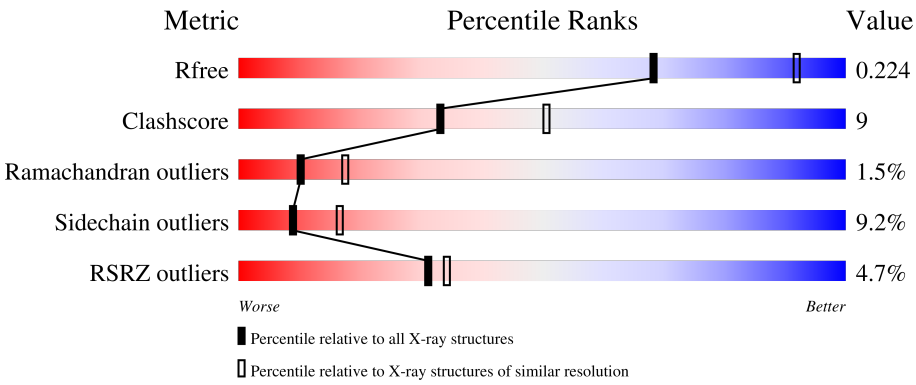
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	916	5%, 73%, 20%, • •
2	B	3	67%, 33%

2 Entry composition (i)

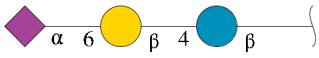
There are 5 unique types of molecules in this entry. The entry contains 6981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	887	6833	4285	1140	1402	6	0	1	0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.

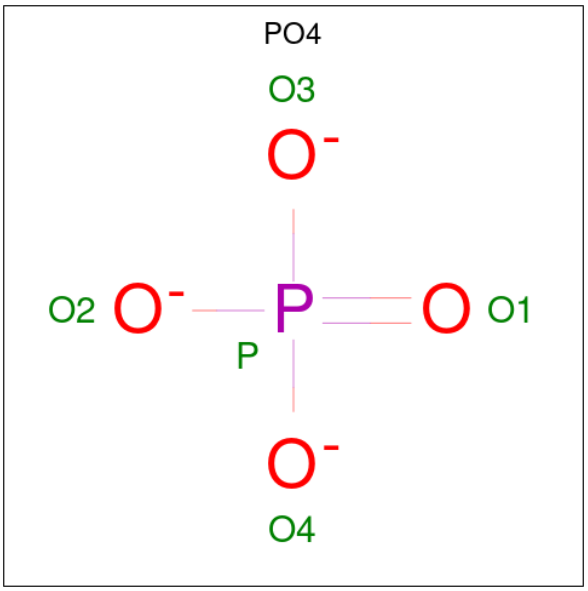


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	43	23	1	19	0	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	1	1	1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

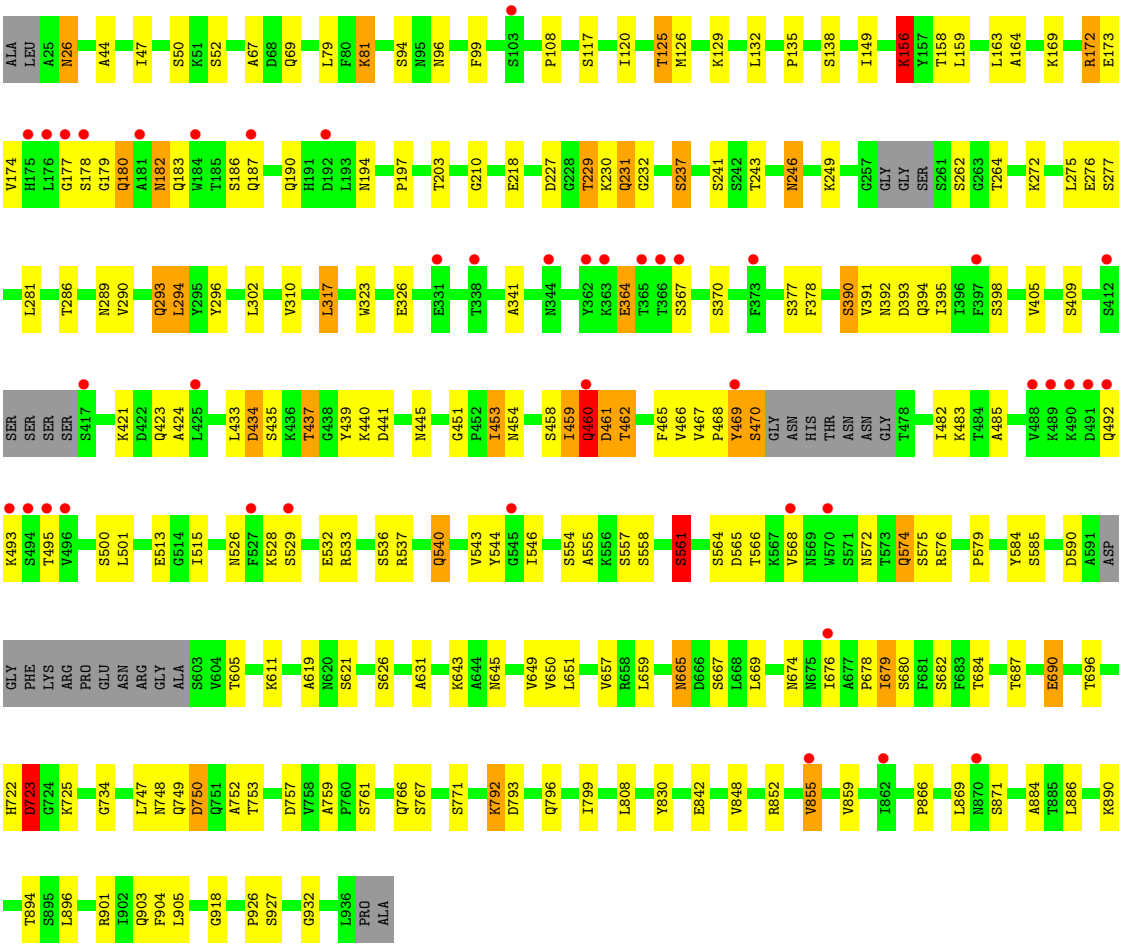
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	99	Total O 99 99	0	0

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: Mgp-operon protein 3

Chain A:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.69Å 152.69Å 176.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.70 – 2.52 57.70 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.9 (57.70-2.52) 98.0 (57.70-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.224 0.190 , 0.224	Depositor DCC
R_{free} test set	2474 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6981	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: BGC, GAL, SIA, K, PO4

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	0.83	4/6972 (0.1%)	1.00	4/9483 (0.0%)

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	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	927	SER	C-O	-5.55	1.12	1.23
1	A	842	GLU	CD-OE2	5.35	1.31	1.25
1	A	690	GLU	CD-OE2	-5.27	1.19	1.25
1	A	326	GLU	CD-OE2	5.19	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	584	TYR	CB-CG-CD1	6.08	124.65	121.00
1	A	723	ASP	CB-CA-C	-6.06	98.28	110.40
1	A	903	GLN	CB-CA-C	-5.30	99.79	110.40
1	A	392	ASN	CB-CA-C	5.18	120.77	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	PRO	Peptide
1	A	178	SER	Peptide
1	A	179	GLY	Peptide
1	A	243	THR	Peptide
1	A	722	HIS	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	6833	0	6611	116	0
2	B	43	0	37	1	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	99	0	0	2	0
All	All	6981	0	6648	116	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 (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:A:281:LEU:H	1:A:293:GLN:HE22	1.21	0.88
1:A:682:SER:OG	1:A:761:SER:HB3	1.76	0.84
1:A:749:GLN:N	1:A:753:THR:OG1	2.15	0.77
1:A:665:ASN:HD22	1:A:665:ASN:H	1.34	0.73
1:A:855:VAL:HG22	1:A:932:GLY:O	1.90	0.71
1:A:272:LYS:NZ	1:A:276:GLU:OE1	2.24	0.71
1:A:513:GLU:HG3	1:A:515:ILE:HG22	1.70	0.71
1:A:540:GLN:HG2	1:A:579:PRO:HA	1.74	0.70
1:A:364:GLU:HG2	1:A:367:SER:HB2	1.77	0.67
1:A:67:ALA:HB2	1:A:81:LYS:HD3	1.80	0.64
1:A:174:VAL:HG21	1:A:203:THR:HG21	1.81	0.62
1:A:869:LEU:C	1:A:869:LEU:HD12	2.20	0.61
1:A:665:ASN:HD22	1:A:665:ASN:N	1.99	0.61
1:A:459:ILE:O	1:A:461:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:HG22	1:A:501:LEU:HB3	1.83	0.60
1:A:117:SER:HB3	1:A:125:THR:HG21	1.83	0.59
1:A:465:PHE:HB3	1:A:515:ILE:HD13	1.83	0.59
1:A:246:ASN:N	1:A:246:ASN:OD1	2.35	0.58
1:A:848:VAL:HG22	1:A:852:ARG:HD3	1.84	0.58
1:A:852:ARG:NH1	1:A:871:SER:OG	2.37	0.58
1:A:470:SER:HA	1:A:482:ILE:HD13	1.86	0.58
1:A:194:ASN:HD22	1:A:483:LYS:HD2	1.68	0.58
1:A:227:ASP:OD1	1:A:229:THR:HB	2.04	0.58
1:A:440:LYS:HB2	1:A:674:ASN:HB3	1.86	0.57
1:A:465:PHE:CB	1:A:515:ILE:HD13	2.34	0.57
1:A:561:SER:OG	1:A:564:SER:O	2.21	0.57
1:A:194:ASN:ND2	1:A:483:LYS:HD2	2.19	0.57
1:A:859:VAL:HG11	1:A:890:LYS:HG3	1.87	0.57
1:A:687:THR:OG1	1:A:690:GLU:OE1	2.22	0.56
1:A:574:GLN:HE21	1:A:575:SER:H	1.51	0.56
1:A:156:LYS:HE2	5:A:1109:HOH:O	2.05	0.55
1:A:555:ALA:HA	1:A:568:VAL:HG21	1.89	0.55
1:A:460:GLN:OE1	1:A:462:THR:OG1	2.25	0.54
1:A:626:SER:HA	1:A:651:LEU:O	2.08	0.54
1:A:734:GLY:HA3	1:A:771:SER:O	2.08	0.54
1:A:501:LEU:C	1:A:501:LEU:HD12	2.28	0.53
1:A:290:VAL:HG12	1:A:294:LEU:HD22	1.90	0.53
1:A:281:LEU:HD11	1:A:296:TYR:CD1	2.43	0.53
1:A:317:LEU:HD23	1:A:317:LEU:N	2.23	0.52
1:A:585:SER:HG	1:A:621:SER:HG	1.56	0.52
1:A:544:TYR:CD2	1:A:659:LEU:HD22	2.46	0.51
1:A:341:ALA:HB1	1:A:378:PHE:HB3	1.92	0.51
1:A:229:THR:HG22	1:A:230:LYS:HG3	1.93	0.50
1:A:650:VAL:CG1	1:A:657:VAL:HG22	2.41	0.50
1:A:650:VAL:HG12	1:A:657:VAL:HG22	1.94	0.50
1:A:723:ASP:HB3	1:A:725:LYS:H	1.77	0.50
1:A:554:SER:HB2	1:A:568:VAL:HG13	1.94	0.50
1:A:138:SER:OG	1:A:565:ASP:OD1	2.17	0.50
1:A:173:GLU:O	1:A:177:GLY:HA2	2.13	0.49
1:A:390:SER:HA	1:A:394:GLN:O	2.11	0.49
1:A:454:ASN:OD1	1:A:467:VAL:HG23	2.12	0.49
1:A:901:ARG:NE	5:A:1101:HOH:O	2.41	0.49
1:A:26[B]:ASN:O	1:A:26[B]:ASN:ND2	2.45	0.49
1:A:210:GLY:O	1:A:232:GLY:HA3	2.13	0.48
1:A:904:PHE:CG	1:A:905:LEU:N	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:HA	1:A:96:ASN:OD1	2.14	0.47
1:A:218:GLU:O	1:A:289:ASN:HA	2.15	0.47
1:A:679:ILE:HD11	1:A:757:ASP:C	2.35	0.47
1:A:197:PRO:HB2	2:B:3:SIA:C9	2.45	0.47
1:A:433:LEU:HD12	1:A:468:PRO:HA	1.96	0.47
1:A:182:ASN:HD22	1:A:182:ASN:N	2.11	0.47
1:A:423:GLN:HG2	1:A:424:ALA:O	2.14	0.47
1:A:172:ARG:HH11	1:A:172:ARG:HG2	1.80	0.46
1:A:558:SER:O	1:A:561:SER:HB3	2.15	0.46
1:A:310:VAL:HA	1:A:323:TRP:O	2.16	0.46
1:A:180:GLN:O	1:A:183:GLN:HG2	2.16	0.46
1:A:451:GLY:HA3	1:A:485:ALA:O	2.15	0.46
1:A:453:ILE:O	1:A:467:VAL:HG22	2.16	0.46
1:A:158:THR:O	1:A:619:ALA:HB3	2.15	0.45
1:A:669:LEU:HD23	1:A:679:ILE:HG23	1.98	0.45
1:A:230:LYS:HB3	1:A:231:GLN:HE22	1.81	0.45
1:A:435:SER:HB2	1:A:445:ASN:ND2	2.31	0.45
1:A:558:SER:HA	1:A:566:THR:HB	2.00	0.44
1:A:230:LYS:CB	1:A:231:GLN:NE2	2.80	0.44
1:A:159:LEU:HD23	1:A:619:ALA:HB1	1.98	0.44
1:A:439:TYR:CD2	1:A:678:PRO:HD3	2.53	0.44
1:A:310:VAL:HG21	1:A:395:ILE:HG13	2.00	0.44
1:A:869:LEU:HD13	1:A:886:LEU:HB2	2.00	0.43
1:A:884:ALA:HA	1:A:901:ARG:O	2.19	0.43
1:A:574:GLN:HE21	1:A:575:SER:N	2.16	0.43
1:A:132:LEU:HD22	1:A:323:TRP:CD1	2.53	0.43
1:A:99:PHE:CZ	1:A:108:PRO:HB3	2.53	0.43
1:A:434:ASP:CG	1:A:469:TYR:HA	2.38	0.43
1:A:649:VAL:HA	1:A:657:VAL:O	2.18	0.43
1:A:679:ILE:HG12	1:A:759:ALA:HB2	2.01	0.43
1:A:398:SER:HA	1:A:544:TYR:HA	2.01	0.42
1:A:540:GLN:CG	1:A:579:PRO:HA	2.44	0.42
1:A:370:SER:O	1:A:370:SER:OG	2.34	0.42
1:A:665:ASN:ND2	1:A:667:SER:OG	2.50	0.42
1:A:767:SER:O	1:A:808:LEU:HD12	2.18	0.42
1:A:364:GLU:HG2	1:A:367:SER:CB	2.46	0.42
1:A:156:LYS:HE2	1:A:696:THR:OG1	2.20	0.42
1:A:526:ASN:ND2	1:A:532:GLU:O	2.51	0.42
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.02	0.42
1:A:317:LEU:N	1:A:317:LEU:CD2	2.82	0.42
1:A:117:SER:HB3	1:A:125:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:CG2	1:A:631:ALA:HB1	2.50	0.42
1:A:682:SER:HG	1:A:761:SER:HB3	1.83	0.41
1:A:187:GLN:HE21	1:A:187:GLN:HB3	1.70	0.41
1:A:132:LEU:HD22	1:A:323:TRP:CG	2.55	0.41
1:A:210:GLY:H	1:A:232:GLY:HA3	1.85	0.41
1:A:44:ALA:HB3	1:A:799:ILE:HD13	2.01	0.41
1:A:830:TYR:CE1	1:A:926:PRO:HD3	2.55	0.41
1:A:645:ASN:ND2	1:A:747:LEU:O	2.37	0.41
1:A:866:PRO:HA	1:A:869:LEU:HG	2.02	0.41
1:A:138:SER:CB	1:A:565:ASP:OD1	2.68	0.41
1:A:453:ILE:HG12	1:A:467:VAL:HG21	2.02	0.41
1:A:120:ILE:HD13	1:A:918:GLY:O	2.20	0.41
1:A:546:ILE:O	1:A:572:ASN:HB2	2.21	0.41
1:A:554:SER:O	1:A:557:SER:HB3	2.20	0.41
1:A:792:LYS:HA	1:A:796:GLN:O	2.20	0.41
1:A:47:ILE:HG22	1:A:50:SER:HB3	2.03	0.40
1:A:126:MET:HE2	1:A:129:LYS:HB2	2.02	0.40
1:A:750:ASP:O	1:A:752:ALA:N	2.54	0.40
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.94	0.40
1:A:896:LEU:C	1:A:896:LEU:HD12	2.42	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	878/916 (96%)	804 (92%)	61 (7%)	13 (2%)	10 17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER

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Mol	Chain	Res	Type
1	A	460	GLN
1	A	723	ASP
1	A	461	ASP
1	A	748	ASN
1	A	156	LYS
1	A	164	ALA
1	A	237	SER
1	A	561	SER
1	A	437	THR
1	A	453	ILE
1	A	529	SER
1	A	590	ASP

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	776/795 (98%)	704 (91%)	72 (9%)	9 16

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26[A]	ASN
1	A	26[B]	ASN
1	A	52	SER
1	A	69	GLN
1	A	79	LEU
1	A	81	LYS
1	A	125	THR
1	A	156	LYS
1	A	163	LEU
1	A	169	LYS
1	A	172	ARG
1	A	180	GLN
1	A	182	ASN
1	A	186	SER

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	229	THR
1	A	231	GLN
1	A	237	SER
1	A	241	SER
1	A	246	ASN
1	A	249	LYS
1	A	264	THR
1	A	275	LEU
1	A	277	SER
1	A	286	THR
1	A	293	GLN
1	A	294	LEU
1	A	302	LEU
1	A	317	LEU
1	A	364	GLU
1	A	377	SER
1	A	390	SER
1	A	393	ASP
1	A	409	SER
1	A	421	LYS
1	A	434	ASP
1	A	437	THR
1	A	441	ASP
1	A	458	SER
1	A	459	ILE
1	A	460	GLN
1	A	462	THR
1	A	466	VAL
1	A	469	TYR
1	A	470	SER
1	A	492	GLN
1	A	493	LYS
1	A	495	THR
1	A	500	SER
1	A	528	LYS
1	A	533	ARG
1	A	536	SER
1	A	537	ARG
1	A	540	GLN
1	A	543	VAL
1	A	561	SER

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Mol	Chain	Res	Type
1	A	574	GLN
1	A	576	ARG
1	A	605	THR
1	A	611	LYS
1	A	643	LYS
1	A	665	ASN
1	A	676	ILE
1	A	679	ILE
1	A	680	SER
1	A	684	THR
1	A	750	ASP
1	A	766	GLN
1	A	792	LYS
1	A	793	ASP
1	A	855	VAL
1	A	894	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	182	ASN
1	A	183	GLN
1	A	187	GLN
1	A	189	ASN
1	A	194	ASN
1	A	231	GLN
1	A	250	ASN
1	A	293	GLN
1	A	330	GLN
1	A	574	GLN
1	A	665	ASN
1	A	674	ASN
1	A	748	ASN
1	A	770	GLN

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)

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	BGC	B	1	2	12,12,12	0.86	0	17,17,17	1.15	2 (11%)
2	GAL	B	2	2	11,11,12	0.80	1 (9%)	15,15,17	2.84	11 (73%)
2	SIA	B	3	2	20,20,21	0.74	0	24,28,31	1.60	6 (25%)

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	BGC	B	1	2	-	2/2/22/22	0/1/1/1
2	GAL	B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	B	3	2	-	4/18/34/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GAL	C4-C5	2.34	1.58	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	GAL	C1-C2-C3	-5.44	102.98	109.67
2	B	2	GAL	O5-C5-C6	-4.59	100.01	107.20
2	B	3	SIA	C8-C7-C6	-3.40	106.59	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	SIA	C6-O6-C2	3.22	118.23	111.34
2	B	2	GAL	C2-C3-C4	-3.05	105.61	110.89
2	B	2	GAL	O6-C6-C5	-3.04	100.85	111.29
2	B	2	GAL	C1-O5-C5	2.91	116.13	112.19
2	B	2	GAL	C3-C4-C5	2.81	115.25	110.24
2	B	2	GAL	O5-C5-C4	2.74	117.50	110.83
2	B	2	GAL	O4-C4-C3	-2.47	104.63	110.35
2	B	3	SIA	O1B-C1-C2	2.46	120.06	113.03
2	B	3	SIA	C4-C3-C2	2.44	114.18	109.81
2	B	2	GAL	O2-C2-C1	2.26	113.77	109.15
2	B	3	SIA	O1B-C1-O1A	-2.25	118.98	124.09
2	B	2	GAL	C6-C5-C4	2.25	118.27	113.00
2	B	3	SIA	C6-C5-N5	-2.24	107.20	110.91
2	B	1	BGC	C3-C4-C5	2.20	114.16	110.24
2	B	1	BGC	O2-C2-C1	2.14	114.11	109.16
2	B	2	GAL	O3-C3-C4	2.07	115.13	110.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	BGC	C4-C5-C6-O6
2	B	1	BGC	O5-C5-C6-O6
2	B	2	GAL	O5-C5-C6-O6
2	B	3	SIA	C6-C7-C8-O8
2	B	3	SIA	C6-C7-C8-C9
2	B	3	SIA	O1A-C1-C2-O6
2	B	3	SIA	O7-C7-C8-C9

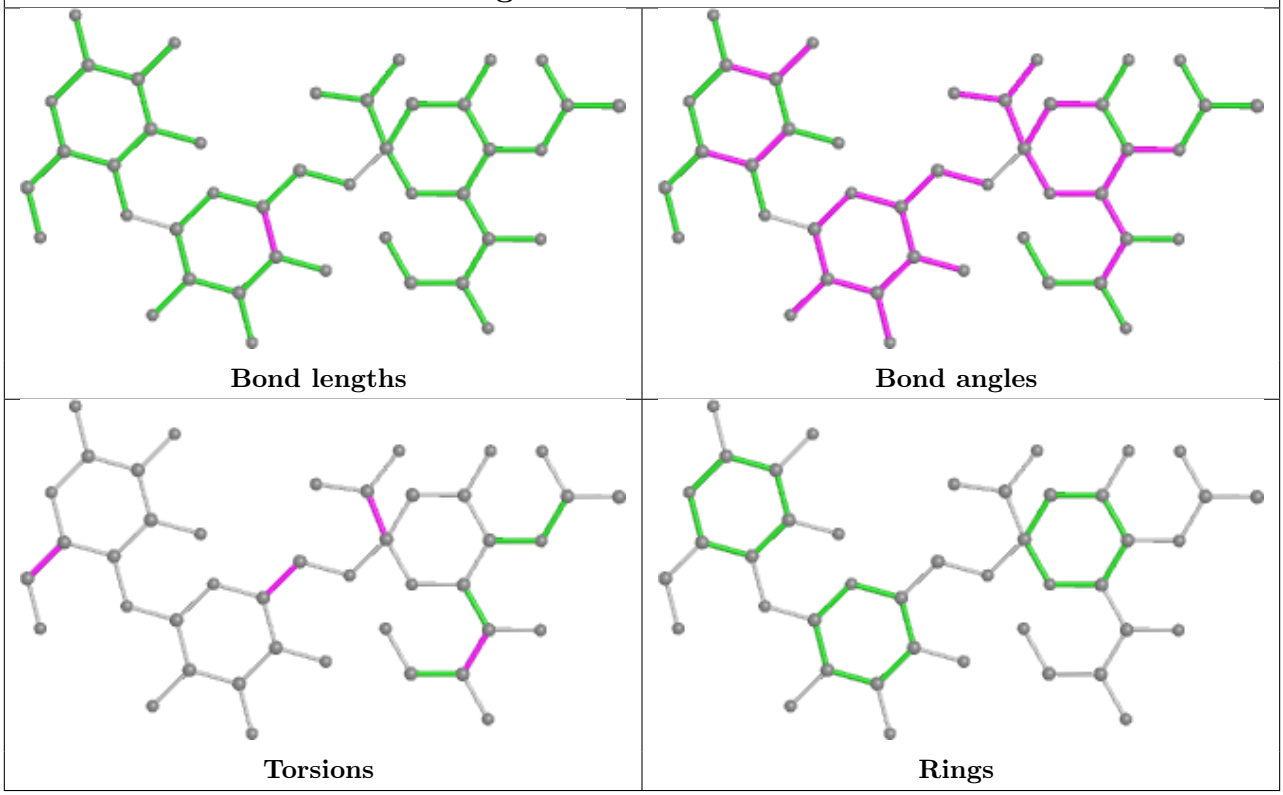
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	SIA	1	0

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PO4	A	1002	-	4,4,4	0.57	0	6,6,6	0.48	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	887/916 (96%)	0.26	42 (4%) 31 34	46, 100, 165, 237	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	SER	6.9
1	A	494	SER	6.8
1	A	493	LYS	5.1
1	A	855	VAL	4.9
1	A	529	SER	4.4
1	A	676	ILE	4.0
1	A	176	LEU	3.8
1	A	496	VAL	3.7
1	A	492	GLN	3.7
1	A	362	TYR	3.6
1	A	488	VAL	3.6
1	A	862	ILE	3.5
1	A	469	TYR	3.5
1	A	425	LEU	3.4
1	A	175	HIS	3.3
1	A	331	GLU	3.3
1	A	489	LYS	3.1
1	A	363	LYS	3.1
1	A	527	PHE	3.0
1	A	184	TRP	2.9
1	A	397	PHE	2.7
1	A	367	SER	2.6
1	A	366	THR	2.6
1	A	177	GLY	2.6
1	A	103	SER	2.5
1	A	178	SER	2.5
1	A	181	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	412	SER	2.5
1	A	460	GLN	2.4
1	A	373	PHE	2.4
1	A	187	GLN	2.4
1	A	870	ASN	2.4
1	A	495	THR	2.3
1	A	570	TRP	2.2
1	A	491	ASP	2.2
1	A	192	ASP	2.2
1	A	344	ASN	2.1
1	A	338	THR	2.1
1	A	365	THR	2.1
1	A	490	LYS	2.1
1	A	568	VAL	2.0
1	A	545	GLY	2.0

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

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

6.3 Carbohydrates (i)

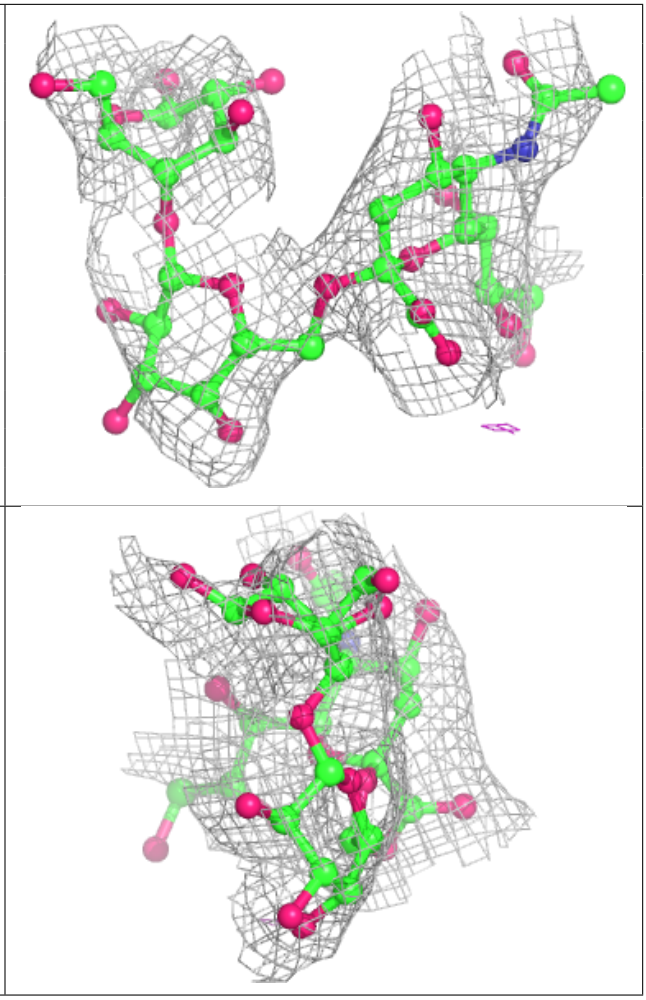
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	B	2	11/12	0.83	0.16	160,177,182,188	11
2	BGC	B	1	12/12	0.88	0.16	163,175,179,179	12
2	SIA	B	3	20/21	0.91	0.15	135,150,155,160	20

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 B:

$2mF_o$-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	PO4	A	1002	5/5	0.95	0.17	67,74,84,92	5
3	K	A	1001	1/1	0.99	0.15	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.