Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 12:17 PM GMT

PDB ID	:	6TLZ
Title	:	N-Domain P40/P90 Mycoplasma pneumoniae complexed with 3'SL
Authors	:	Vizarraga, D.; Aparicio, D.; Illanes, R.; Fita, I.; Perez-Luque, R.; Martin, J.
Deposited on	:	2019-12-03
Resolution	:	3.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

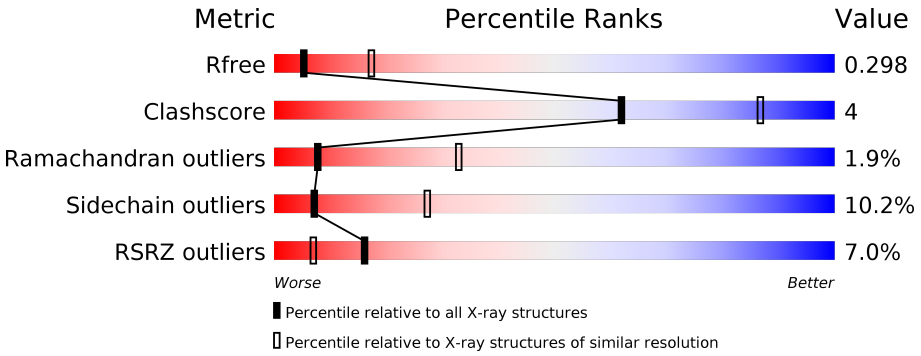
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	976	6% 68% 13% • 18%
1	B	976	6% 69% 13% • 17%
2	C	3	67% 33%
3	D	2	50% 50%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	C	2	-	-	-	X
3	GAL	D	2	-	-	X	-
4	SIA	B	1001	-	-	X	-

2 Entry composition

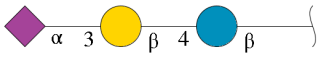
There are 4 unique types of molecules in this entry. The entry contains 12559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	803	Total	C	N	O	S	0	0	0
			6190	3897	1043	1246	4			
1	B	810	Total	C	N	O	S	0	2	0
			6283	3949	1073	1257	4			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.

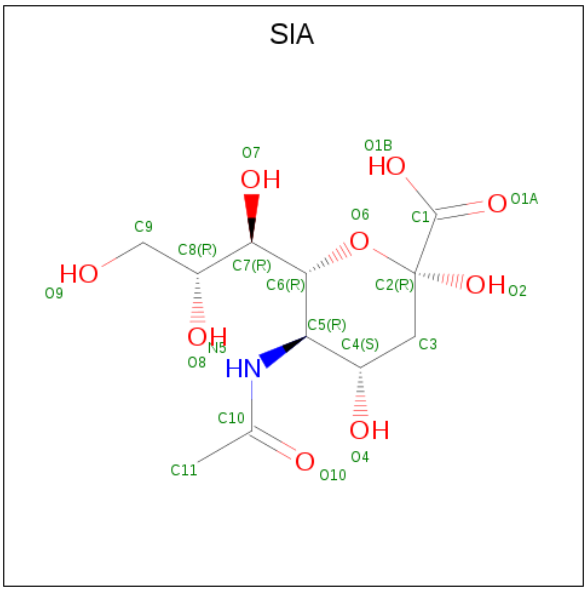


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by author).



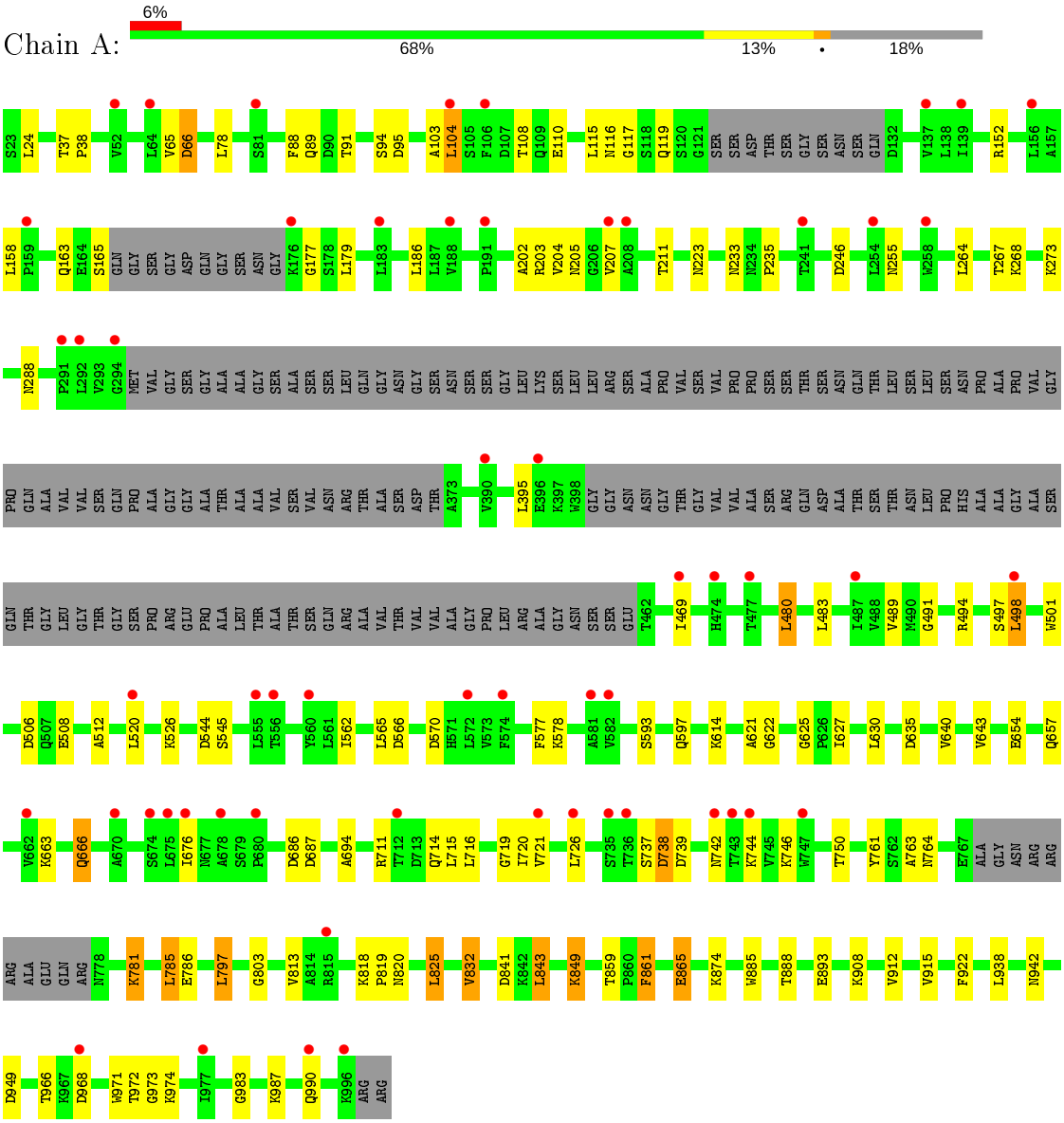
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	20	11	1	8	0	0

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.

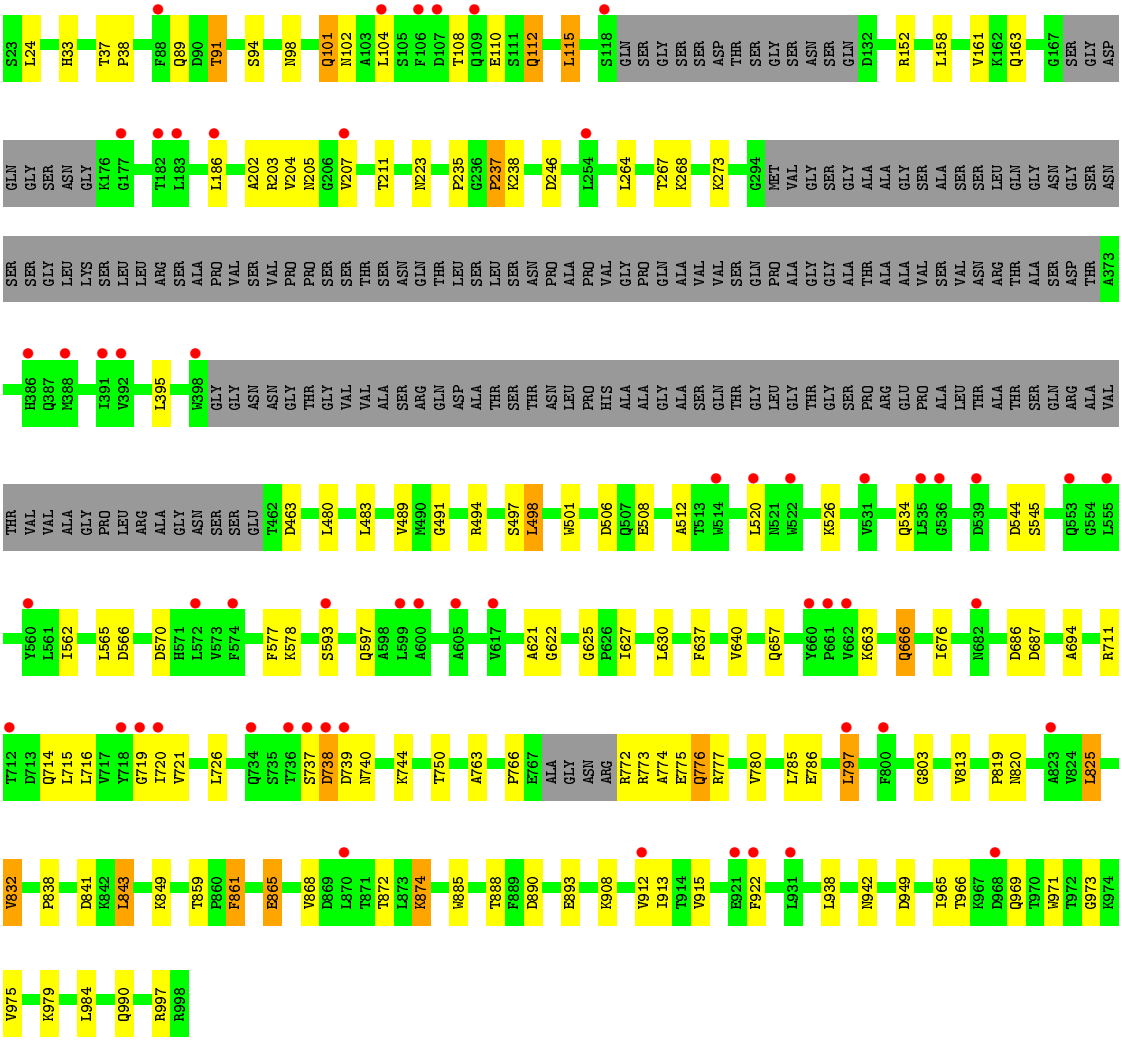
- Molecule 1: Mgp-operon protein 3

Chain A:



- Molecule 1: Mgp-operon protein 3

Chain B:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:

• Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.21Å 107.31Å 162.01Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	81.01 – 3.10 81.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (81.01-3.10) 96.5 (81.01-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.244 , 0.279 0.260 , 0.298	Depositor DCC
R_{free} test set	1779 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	97.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.367 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12559	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, BGC, GAL

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	0.40	0/6319	0.62	0/8597
1	B	0.39	0/6413	0.62	0/8719
All	All	0.40	0/12732	0.62	0/17316

There are no bond length outliers.

There are no bond angle outliers.

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	6190	0	6012	40	0
1	B	6283	0	6109	53	0
2	C	43	0	37	0	0
3	D	23	0	20	9	0
4	B	20	0	17	28	0
All	All	12559	0	12195	109	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 4.

All (109) 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)
4:B:1001:SIA:C2	3:D:2:GAL:O3	1.66	1.40
1:B:238:LYS:HB2	4:B:1001:SIA:C11	1.70	1.19
1:B:238:LYS:CB	4:B:1001:SIA:H111	1.77	1.14
1:B:238:LYS:HG2	4:B:1001:SIA:O10	1.52	1.10
1:B:238:LYS:HB2	4:B:1001:SIA:H111	1.32	1.02
1:B:238:LYS:CG	4:B:1001:SIA:O10	2.10	0.98
1:B:238:LYS:HB2	4:B:1001:SIA:C10	1.97	0.94
1:B:238:LYS:CG	4:B:1001:SIA:H111	2.04	0.87
1:B:235:PRO:O	4:B:1001:SIA:O9	1.95	0.83
1:B:238:LYS:CB	4:B:1001:SIA:O10	2.27	0.83
1:B:238:LYS:CB	4:B:1001:SIA:C11	2.46	0.81
4:B:1001:SIA:C1	3:D:2:GAL:O3	2.29	0.80
1:B:238:LYS:HG3	4:B:1001:SIA:H111	1.64	0.79
1:A:861:PHE:HB2	1:A:865:GLU:HG3	1.67	0.74
1:B:861:PHE:HB2	1:B:865:GLU:HG3	1.68	0.73
4:B:1001:SIA:C2	3:D:2:GAL:C3	2.67	0.73
1:B:238:LYS:CG	4:B:1001:SIA:C10	2.69	0.71
1:B:238:LYS:CG	4:B:1001:SIA:C11	2.71	0.68
1:B:238:LYS:CB	4:B:1001:SIA:C10	2.65	0.68
4:B:1001:SIA:H113	4:B:1001:SIA:C4	2.25	0.67
1:B:813:VAL:HG11	1:B:819:PRO:HA	1.77	0.66
1:A:813:VAL:HG11	1:A:819:PRO:HA	1.76	0.66
4:B:1001:SIA:O4	4:B:1001:SIA:H113	1.96	0.66
4:B:1001:SIA:O7	4:B:1001:SIA:N5	2.27	0.65
1:B:238:LYS:HG3	4:B:1001:SIA:C11	2.27	0.63
1:B:205:ASN:HD21	1:B:687:ASP:HB2	1.66	0.61
1:A:205:ASN:HD21	1:A:687:ASP:HB2	1.66	0.61
3:D:2:GAL:H61	3:D:2:GAL:H2	1.83	0.60
1:B:238:LYS:N	4:B:1001:SIA:O10	2.33	0.60
3:D:2:GAL:H61	3:D:2:GAL:O3	2.03	0.57
1:A:233:ASN:HD21	1:A:654:GLU:HB3	1.70	0.57
4:B:1001:SIA:C1	3:D:2:GAL:C3	2.82	0.56
1:A:66:ASP:HB3	1:A:480:LEU:HD23	1.88	0.56
1:B:820:ASN:HD21	1:B:922:PHE:HB3	1.71	0.55
4:B:1001:SIA:C11	4:B:1001:SIA:C4	2.85	0.54
1:A:820:ASN:HD21	1:A:922:PHE:HB3	1.72	0.54
1:A:78:LEU:HB2	1:A:480:LEU:HD22	1.91	0.53
4:B:1001:SIA:C11	4:B:1001:SIA:H4	2.38	0.53
1:A:152:ARG:HH12	1:A:508:GLU:HG3	1.73	0.53
1:A:483:LEU:HD11	1:A:570:ASP:HA	1.90	0.53
4:B:1001:SIA:O6	4:B:1001:SIA:O8	2.09	0.52
1:B:102:ASN:HD21	1:B:161:VAL:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LEU:HD11	1:B:570:ASP:HA	1.90	0.51
1:A:763:ALA:HB3	1:A:786:GLU:HB3	1.92	0.51
1:B:520:LEU:HD22	1:B:750:THR:HG21	1.92	0.50
1:B:820:ASN:HA	1:B:838:PRO:HG3	1.93	0.50
4:B:1001:SIA:H4	4:B:1001:SIA:H113	1.94	0.50
1:B:763:ALA:HB3	1:B:786:GLU:HB3	1.93	0.49
1:A:104:LEU:HD21	1:A:469:ILE:HD11	1.93	0.49
1:A:103:ALA:HB2	1:A:163:GLN:HG3	1.94	0.49
1:A:966:THR:OG1	1:A:974:LYS:HB3	2.12	0.48
1:A:489:VAL:HB	1:A:501:TRP:HB2	1.94	0.48
1:A:520:LEU:HD22	1:A:750:THR:HG21	1.95	0.48
1:B:112:GLN:HA	1:B:115:LEU:HD12	1.96	0.48
1:B:719:GLY:HA3	1:B:750:THR:HG22	1.96	0.47
3:D:2:GAL:C2	3:D:2:GAL:H61	2.41	0.47
1:A:764:ASN:HD21	1:A:785:LEU:HD12	1.80	0.46
1:A:825:LEU:HG	1:A:832:VAL:HG13	1.97	0.46
1:B:785:LEU:HD22	1:B:797:LEU:HD23	1.98	0.46
1:B:872:THR:HA	1:B:893:GLU:HB3	1.98	0.46
1:A:498:LEU:HD11	1:A:676:ILE:HD13	1.98	0.46
1:B:766:PRO:HD2	1:B:772:ARG:HG3	1.97	0.46
1:B:498:LEU:HD11	1:B:676:ILE:HD13	1.99	0.45
1:B:885:TRP:HB2	1:B:915:VAL:HB	1.98	0.45
3:D:1:BGC:H4	3:D:1:BGC:O1	2.17	0.45
1:B:98:ASN:HB3	1:B:101:GLN:HG2	1.99	0.45
1:A:785:LEU:HD22	1:A:797:LEU:HD23	1.98	0.45
1:B:825:LEU:HG	1:B:832:VAL:HG13	1.98	0.45
1:B:491:GLY:HA3	1:B:497:SER:HB3	1.97	0.45
1:B:874:LYS:HG2	1:B:890:ASP:HB2	1.99	0.45
1:A:491:GLY:HA3	1:A:497:SER:HB3	1.98	0.45
1:A:885:TRP:HB2	1:A:915:VAL:HB	1.99	0.44
1:A:719:GLY:HA3	1:A:750:THR:HG22	1.98	0.44
1:A:207:VAL:HG11	1:A:593:SER:HB3	2.00	0.43
1:A:94:SER:HA	1:A:165:SER:HB2	1.99	0.43
1:A:720:ILE:HG22	1:A:843:LEU:HD12	2.00	0.43
1:A:88:PHE:HD2	1:A:255:ASN:HD21	1.65	0.43
1:B:622:GLY:HA2	1:B:625:GLY:O	2.17	0.43
1:B:207:VAL:HG11	1:B:593:SER:HB3	2.00	0.43
1:B:720:ILE:HG22	1:B:843:LEU:HD12	2.01	0.43
1:B:912:VAL:HG12	1:B:942:ASN:HD21	1.82	0.43
1:B:663:LYS:HB3	1:B:666:GLN:HB2	2.01	0.42
1:A:663:LYS:HB3	1:A:666:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HA	1:B:38:PRO:HD3	1.95	0.42
1:B:776:GLN:HE22	1:B:780:VAL:HB	1.84	0.42
1:A:912:VAL:HG12	1:A:942:ASN:HD21	1.83	0.42
1:A:233:ASN:ND2	1:A:654:GLU:HB3	2.35	0.42
1:B:719:GLY:HA2	1:B:843:LEU:HD11	2.02	0.42
1:B:237:PRO:HD2	4:B:1001:SIA:O7	2.19	0.42
1:A:614:LYS:HD2	1:A:849:LYS:HB3	2.02	0.42
1:A:204:VAL:HG22	1:A:267:THR:HG23	2.02	0.41
1:B:721:VAL:HG22	1:B:726:LEU:HG	2.02	0.41
1:A:687:ASP:HA	1:A:781:LYS:HB3	2.03	0.41
1:B:694:ALA:HA	1:B:714:GLN:HG3	2.02	0.41
1:A:177:GLY:HA2	1:A:742:ASN:HD21	1.86	0.41
1:A:719:GLY:HA2	1:A:843:LEU:HD11	2.02	0.41
1:B:152:ARG:HH12	1:B:508:GLU:HG2	1.84	0.41
1:A:694:ALA:HA	1:A:714:GLN:HG3	2.02	0.41
1:A:37:THR:HA	1:A:38:PRO:HD3	1.95	0.41
1:A:501:TRP:CE2	1:A:512:ALA:HB2	2.55	0.41
1:A:721:VAL:HG22	1:A:726:LEU:HG	2.03	0.41
1:B:489:VAL:HB	1:B:501:TRP:HB2	2.03	0.41
1:B:868:VAL:HG21	1:B:913:ILE:HD11	2.01	0.41
1:B:204:VAL:HG22	1:B:267:THR:HG23	2.02	0.41
3:D:2:GAL:C2	3:D:2:GAL:C6	2.94	0.40
1:B:965:ILE:HG13	1:B:975:VAL:HG22	2.02	0.40
1:A:622:GLY:HA2	1:A:625:GLY:O	2.22	0.40
1:A:235:PRO:HG3	1:A:643:VAL:HB	2.03	0.40
1:B:501:TRP:CE2	1:B:512:ALA:HB2	2.55	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	791/976 (81%)	703 (89%)	72 (9%)	16 (2%)	7 31
1	B	800/976 (82%)	714 (89%)	71 (9%)	15 (2%)	8 33
All	All	1591/1952 (82%)	1417 (89%)	143 (9%)	31 (2%)	8 33

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	ILE
1	A	621	ALA
1	A	686	ASP
1	A	737	SER
1	A	803	GLY
1	A	968	ASP
1	B	562	ILE
1	B	621	ALA
1	B	686	ASP
1	B	737	SER
1	B	803	GLY
1	A	202	ALA
1	A	738	ASP
1	A	973	GLY
1	B	94	SER
1	B	202	ALA
1	B	738	ASP
1	B	774	ALA
1	B	973	GLY
1	A	91	THR
1	A	95	ASP
1	A	116	ASN
1	A	983	GLY
1	A	972	THR
1	B	33[A]	HIS
1	B	33[B]	HIS
1	B	91	THR
1	A	627	ILE
1	B	627	ILE
1	A	117	GLY
1	B	237	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	675/800 (84%)	608 (90%)	67 (10%)	8 29
1	B	683/800 (85%)	612 (90%)	71 (10%)	7 27
All	All	1358/1600 (85%)	1220 (90%)	138 (10%)	7 27

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	65	VAL
1	A	66	ASP
1	A	89	GLN
1	A	104	LEU
1	A	108	THR
1	A	110	GLU
1	A	115	LEU
1	A	119	GLN
1	A	158	LEU
1	A	179	LEU
1	A	186	LEU
1	A	203	ARG
1	A	211	THR
1	A	223	ASN
1	A	246	ASP
1	A	264	LEU
1	A	268	LYS
1	A	273	LYS
1	A	288	ASN
1	A	395	LEU
1	A	480	LEU
1	A	494	ARG
1	A	498	LEU
1	A	506	ASP
1	A	526	LYS
1	A	544	ASP

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Mol	Chain	Res	Type
1	A	545	SER
1	A	565	LEU
1	A	566	ASP
1	A	577	PHE
1	A	578	LYS
1	A	597	GLN
1	A	630	LEU
1	A	635	ASP
1	A	640	VAL
1	A	657	GLN
1	A	666	GLN
1	A	711	ARG
1	A	715	LEU
1	A	716	LEU
1	A	738	ASP
1	A	739	ASP
1	A	744	LYS
1	A	746	LYS
1	A	761	TYR
1	A	781	LYS
1	A	785	LEU
1	A	797	LEU
1	A	818	LYS
1	A	825	LEU
1	A	832	VAL
1	A	841	ASP
1	A	843	LEU
1	A	849	LYS
1	A	859	THR
1	A	861	PHE
1	A	865	GLU
1	A	874	LYS
1	A	888	THR
1	A	893	GLU
1	A	908	LYS
1	A	938	LEU
1	A	949	ASP
1	A	971	TRP
1	A	987	LYS
1	A	990	GLN
1	B	24	LEU
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	91	THR
1	B	101	GLN
1	B	104	LEU
1	B	108	THR
1	B	110	GLU
1	B	112	GLN
1	B	115	LEU
1	B	158	LEU
1	B	163	GLN
1	B	186	LEU
1	B	203	ARG
1	B	211	THR
1	B	223	ASN
1	B	246	ASP
1	B	264	LEU
1	B	268	LYS
1	B	273	LYS
1	B	395	LEU
1	B	463	ASP
1	B	480	LEU
1	B	494	ARG
1	B	498	LEU
1	B	506	ASP
1	B	526	LYS
1	B	534	GLN
1	B	544	ASP
1	B	545	SER
1	B	565	LEU
1	B	566	ASP
1	B	577	PHE
1	B	578	LYS
1	B	597	GLN
1	B	630	LEU
1	B	637	PHE
1	B	640	VAL
1	B	657	GLN
1	B	666	GLN
1	B	711	ARG
1	B	715	LEU
1	B	716	LEU
1	B	738	ASP
1	B	739	ASP

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Mol	Chain	Res	Type
1	B	740	ASN
1	B	744	LYS
1	B	773	ARG
1	B	775	GLU
1	B	776	GLN
1	B	777	ARG
1	B	797	LEU
1	B	825	LEU
1	B	832	VAL
1	B	841	ASP
1	B	843	LEU
1	B	849	LYS
1	B	859	THR
1	B	861	PHE
1	B	865	GLU
1	B	874	LYS
1	B	888	THR
1	B	908	LYS
1	B	938	LEU
1	B	949	ASP
1	B	966	THR
1	B	969	GLN
1	B	971	TRP
1	B	979	LYS
1	B	984	LEU
1	B	990	GLN
1	B	997	ARG

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

Mol	Chain	Res	Type
1	A	47	ASN
1	A	205	ASN
1	A	233	ASN
1	A	553	GLN
1	A	732	ASN
1	A	734	GLN
1	A	742	ASN
1	A	820	ASN
1	A	942	ASN
1	B	47	ASN
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	205	ASN
1	B	233	ASN
1	B	534	GLN
1	B	624	ASN
1	B	714	GLN
1	B	732	ASN
1	B	734	GLN
1	B	740	ASN
1	B	776	GLN
1	B	820	ASN
1	B	942	ASN
1	B	980	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)

5 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	C	1	2	12,12,12	0.25	0	17,17,17	0.38	0
2	GAL	C	2	2	11,11,12	0.37	0	15,15,17	0.62	0
2	SIA	C	3	2	17,20,21	0.26	0	21,28,31	0.80	1 (4%)
3	BGC	D	1	3	12,12,12	0.41	0	17,17,17	0.63	0
3	GAL	D	2	3	11,11,12	0.33	0	15,15,17	1.22	2 (13%)

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	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	SIA	C	3	2	-	0/14/34/38	0/1/1/1
3	BGC	D	1	3	-	2/2/22/22	0/1/1/1
3	GAL	D	2	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	GAL	C1-C2-C3	3.48	113.95	109.67
2	C	3	SIA	C6-O6-C2	2.31	116.28	111.34
3	D	2	GAL	C2-C3-C4	-2.30	106.92	110.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	BGC	O5-C5-C6-O6
3	D	1	BGC	C4-C5-C6-O6
3	D	2	GAL	O5-C5-C6-O6

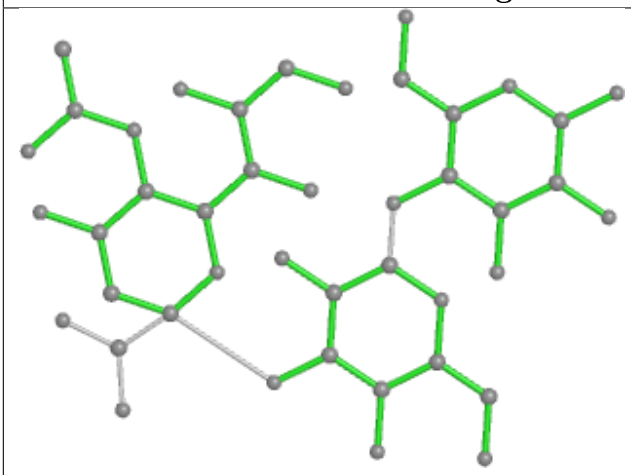
There are no ring outliers.

2 monomers are involved in 9 short contacts:

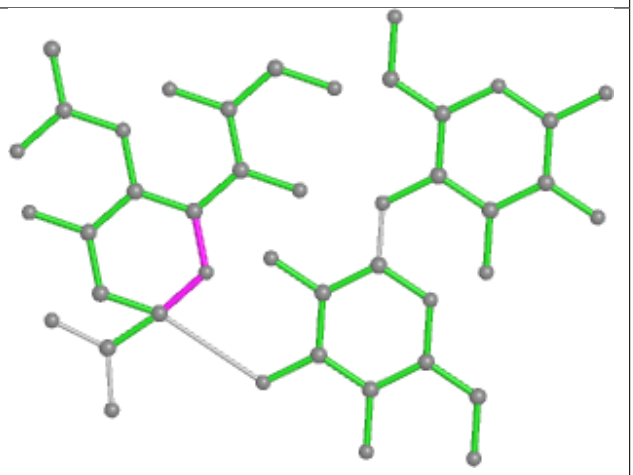
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	BGC	1	0
3	D	2	GAL	8	0

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

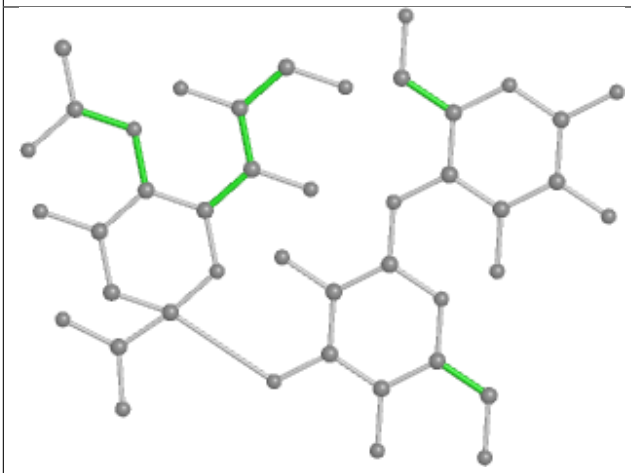
Oligosaccharide Chain C



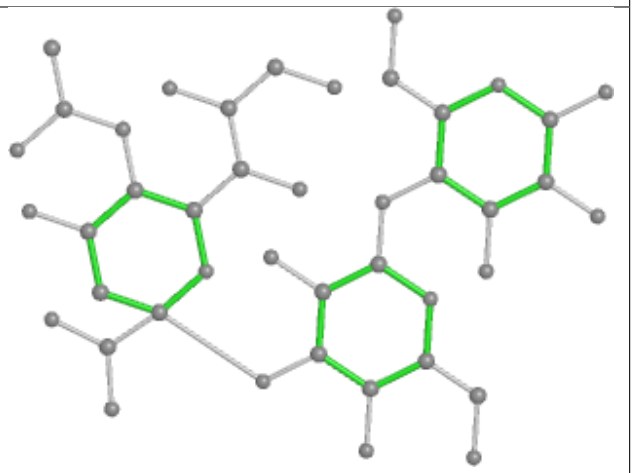
Bond lengths



Bond angles

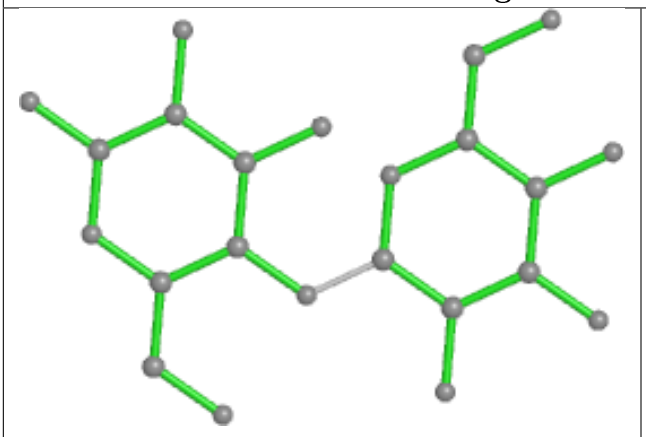


Torsions

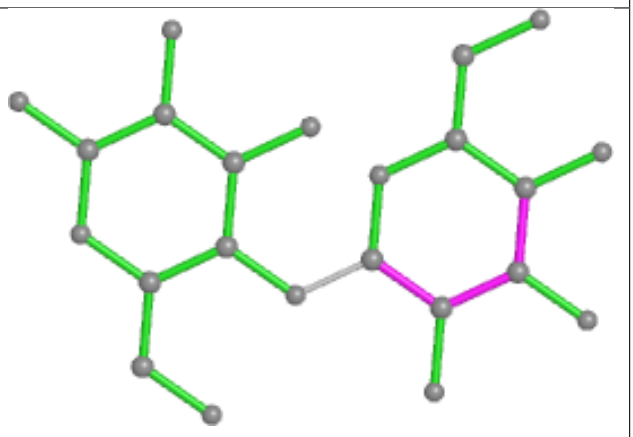


Rings

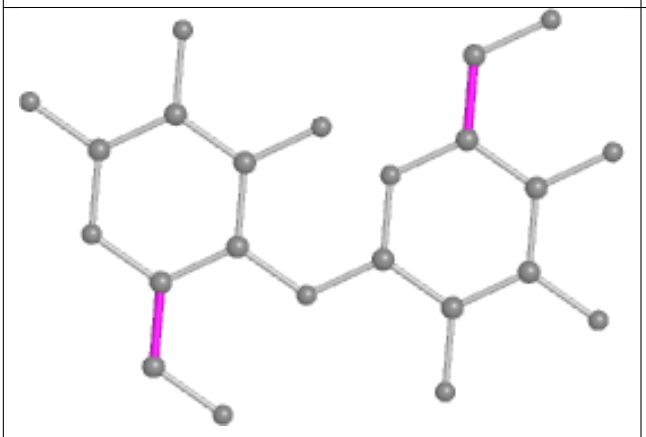
Oligosaccharide Chain D



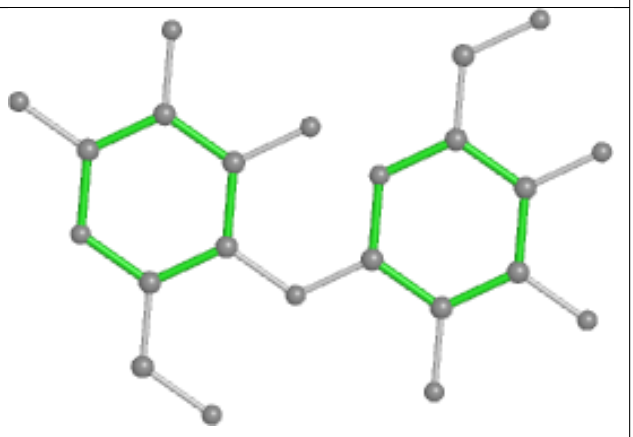
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

1 ligand is 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	SIA	B	1001	-	17,20,21	0.63	0	21,28,31	1.67	3 (14%)

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	SIA	B	1001	-	-	8/14/34/38	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	SIA	C3-C2-C1	-5.29	100.37	111.93
4	B	1001	SIA	O6-C2-C3	-3.34	104.02	109.87
4	B	1001	SIA	C6-O6-C2	3.29	118.38	111.34

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	SIA	C5-C6-C7-C8
4	B	1001	SIA	C7-C8-C9-O9
4	B	1001	SIA	O8-C8-C9-O9
4	B	1001	SIA	C11-C10-N5-C5
4	B	1001	SIA	O10-C10-N5-C5
4	B	1001	SIA	C6-C5-N5-C10
4	B	1001	SIA	C4-C5-N5-C10
4	B	1001	SIA	O6-C6-C7-C8

There are no ring outliers.

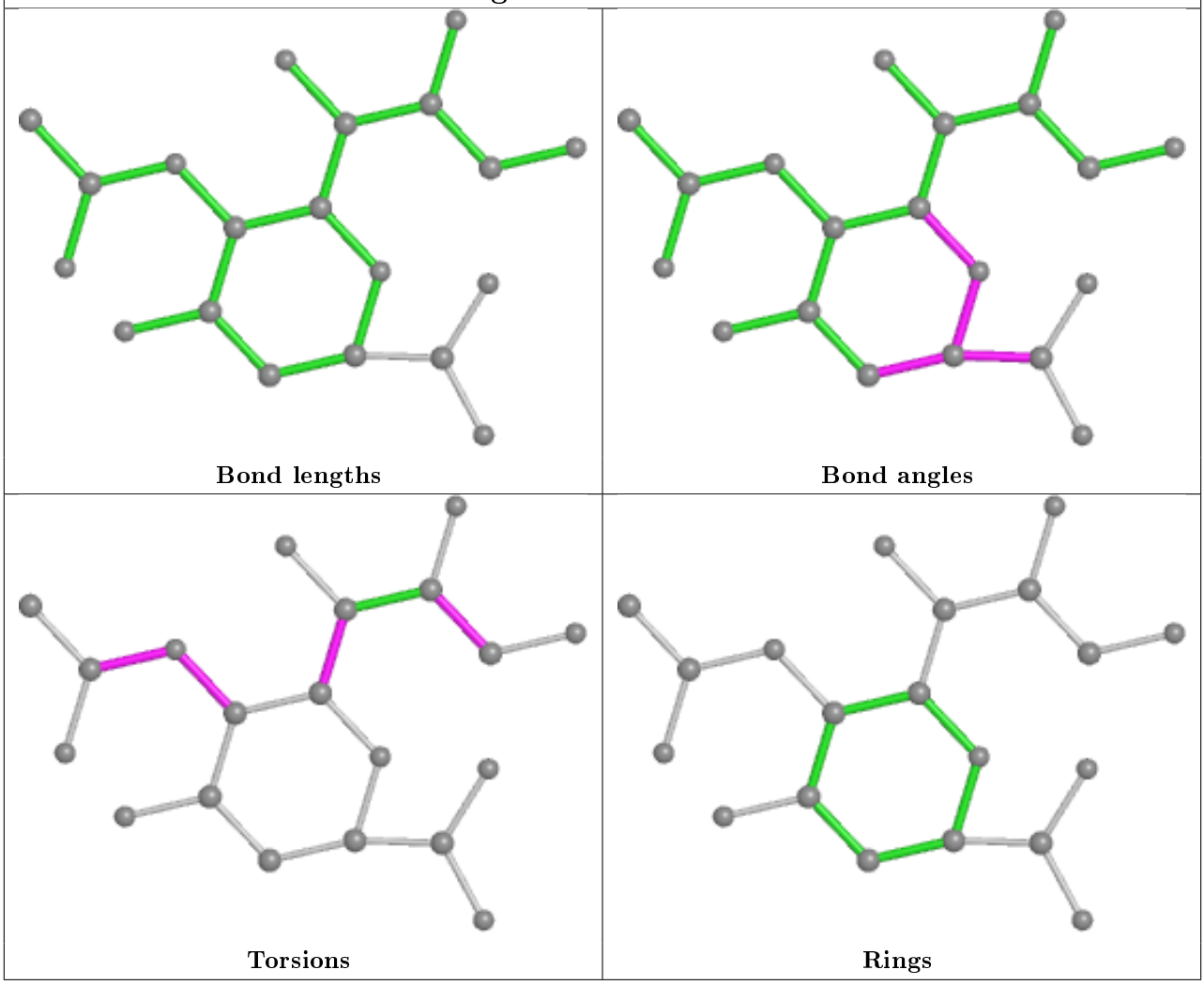
1 monomer is involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	SIA	28	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand SIA B 1001



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	803/976 (82%)	0.38	57 (7%) 16 6	79, 149, 192, 220	0
1	B	810/976 (82%)	0.38	56 (6%) 16 7	88, 146, 199, 230	0
All	All	1613/1952 (82%)	0.38	113 (7%) 16 7	79, 148, 196, 230	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	7.7
1	A	556	THR	5.4
1	A	159	PRO	5.2
1	A	662	VAL	5.2
1	B	931	LEU	5.1
1	B	520	LEU	4.8
1	A	555	LEU	4.5
1	B	254	LEU	4.5
1	B	662	VAL	4.5
1	B	535	LEU	4.5
1	A	815	ARG	4.4
1	A	183	LEU	4.2
1	A	207	VAL	4.1
1	B	712	THR	4.0
1	B	599	LEU	4.0
1	B	736	THR	3.9
1	A	582	VAL	3.8
1	A	254	LEU	3.8
1	B	600	ALA	3.7
1	A	477	THR	3.5
1	A	721	VAL	3.4
1	B	391	ILE	3.4
1	A	968	ASP	3.4
1	A	574	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	682	ASN	3.3
1	A	581	ALA	3.2
1	A	747	TRP	3.2
1	B	392	VAL	3.2
1	A	104	LEU	3.2
1	A	676	ILE	3.2
1	B	536	GLY	3.2
1	B	555	LEU	3.1
1	B	388	MET	3.1
1	B	739	ASP	3.0
1	A	742	ASN	3.0
1	B	118	SER	3.0
1	A	572	LEU	3.0
1	A	292	LEU	2.9
1	A	735	SER	2.9
1	A	208	ALA	2.9
1	B	386	HIS	2.9
1	B	572	LEU	2.9
1	A	726	LEU	2.9
1	B	514	TRP	2.9
1	B	593	SER	2.8
1	B	737	SER	2.7
1	B	921	GLU	2.7
1	A	258	TRP	2.7
1	B	605	ALA	2.7
1	A	743	THR	2.7
1	A	712	THR	2.7
1	A	674	SER	2.7
1	B	560	TYR	2.7
1	B	104	LEU	2.7
1	B	797	LEU	2.7
1	B	398	TRP	2.6
1	A	487	ILE	2.6
1	A	744	LYS	2.6
1	B	800	PHE	2.6
1	A	675	LEU	2.6
1	B	661	PRO	2.6
1	B	522	TRP	2.6
1	B	574	PHE	2.5
1	B	107	ASP	2.5
1	B	109	GLN	2.5
1	A	106	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	870	LEU	2.5
1	A	241	THR	2.4
1	B	660	TYR	2.4
1	A	560	TYR	2.4
1	A	678	ALA	2.4
1	B	734	GLN	2.4
1	A	474	HIS	2.4
1	B	177	GLY	2.3
1	B	719	GLY	2.3
1	B	553	GLN	2.3
1	B	539	ASP	2.3
1	B	823	ALA	2.3
1	A	137	VAL	2.3
1	B	88	PHE	2.3
1	B	738	ASP	2.3
1	A	156	LEU	2.3
1	B	718	TYR	2.3
1	A	469	ILE	2.2
1	B	922	PHE	2.2
1	B	720	ILE	2.2
1	B	912	VAL	2.2
1	B	186	LEU	2.2
1	A	294	GLY	2.2
1	A	996	LYS	2.2
1	A	498	LEU	2.2
1	A	81	SER	2.2
1	B	617	VAL	2.1
1	B	106	PHE	2.1
1	A	390	VAL	2.1
1	B	531	VAL	2.1
1	A	139	ILE	2.1
1	A	396	GLU	2.1
1	A	990	GLN	2.1
1	A	736	THR	2.1
1	A	291	PRO	2.1
1	A	680	PRO	2.1
1	A	670	ALA	2.1
1	B	182	THR	2.1
1	A	188	VAL	2.1
1	A	520	LEU	2.1
1	A	52	VAL	2.1
1	A	191	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	968	ASP	2.1
1	A	176	LYS	2.0
1	A	977	ILE	2.0
1	B	183	LEU	2.0
1	A	64	LEU	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)

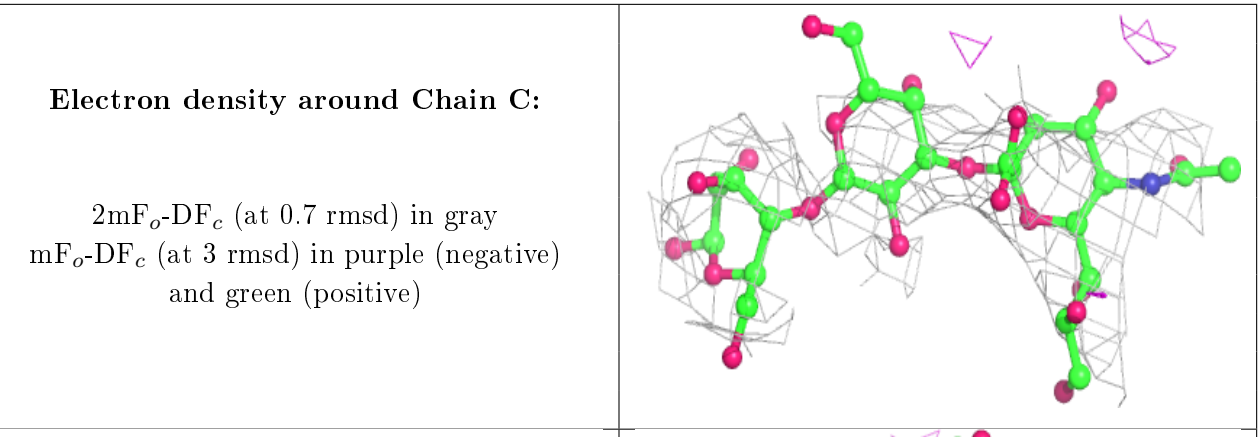
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BGC	D	1	12/12	0.56	0.30	244,244,244,244	0
2	GAL	C	2	11/12	0.65	0.42	245,246,247,247	0
3	GAL	D	2	11/12	0.69	0.22	243,244,245,245	0
2	BGC	C	1	12/12	0.82	0.21	244,244,245,245	0
2	SIA	C	3	20/21	0.85	0.35	242,244,245,245	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

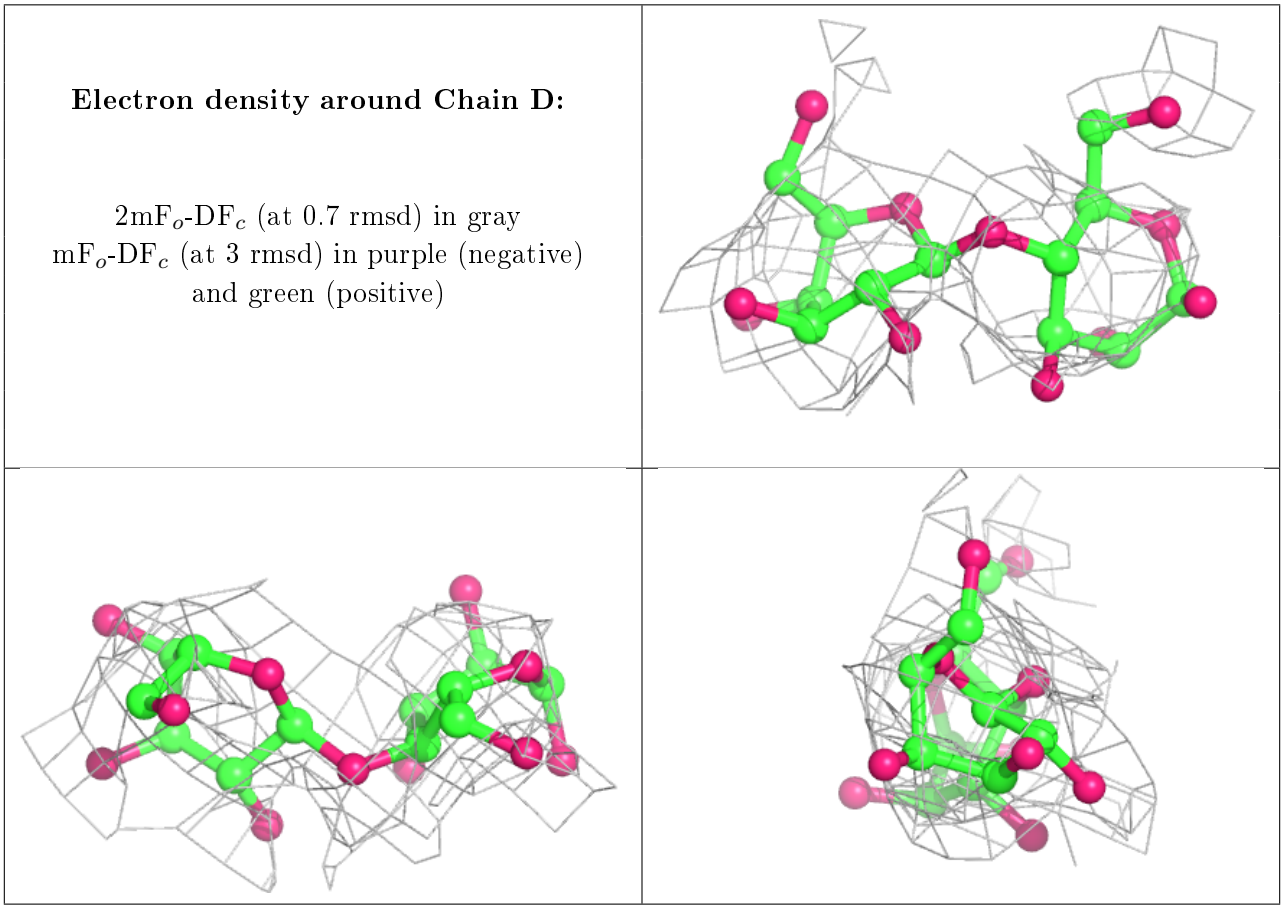
Electron density around Chain C:

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



Electron density around Chain D:

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



6.4 Ligands

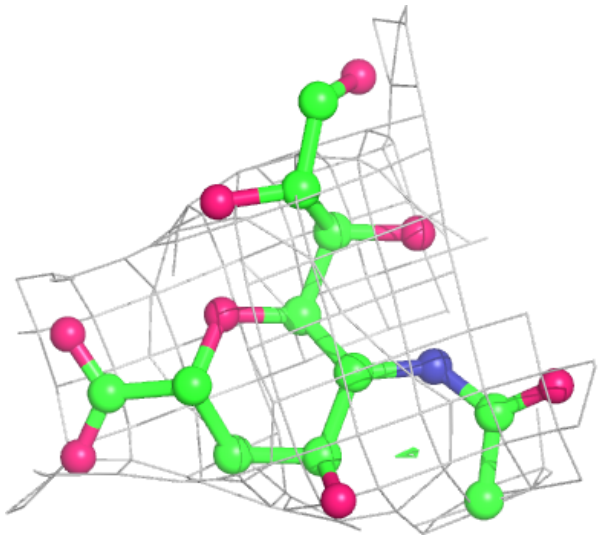
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

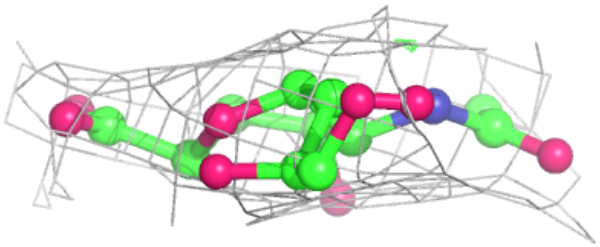
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SIA	B	1001	20/21	0.82	0.22	244,245,246,246	0

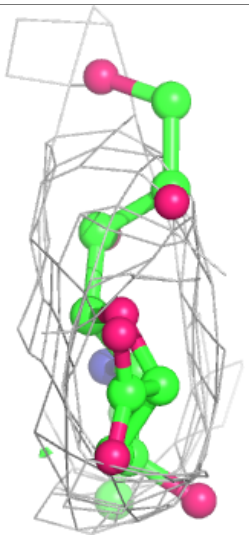
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA B 1001:

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







6.5 Other polymers (i)

There are no such residues in this entry.