Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:02 PM EDT

PDB ID	:	3V0W
Title	:	Crystal structure of Fab WN1 222-5 in complex with LPS
Authors	:	Gomery, K.; Evans, S.V.
Deposited on	:	2011-12-08
Resolution	:	1.73 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:

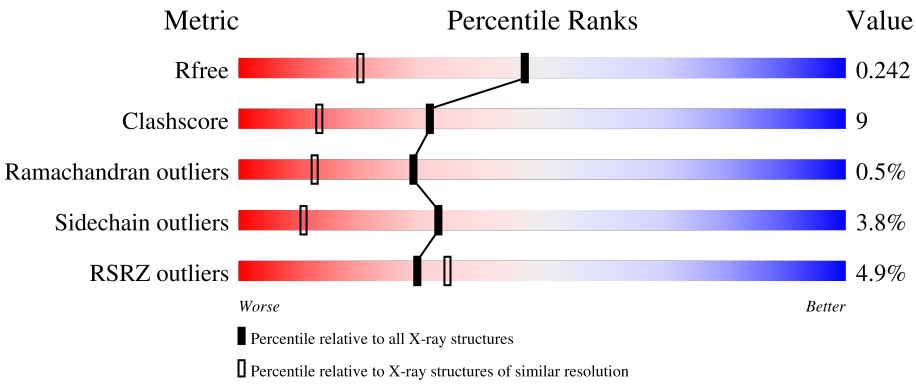
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	L	212	5%, 78%, 18%, •
2	H	219	5%, 83%, 12%, • •
3	A	10	10%, 70%, 20%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	H	315	-	-	-	X
4	SO4	L	303	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3953 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.

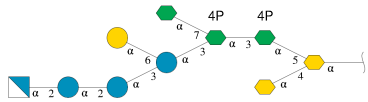
- Molecule 1 is a protein called WN1 222-5 Fab (IgG2a) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1632	1019	277	330	6	0	0	0

- Molecule 2 is a protein called WN1 222-5 Fab (IgG2a) heavy chain.

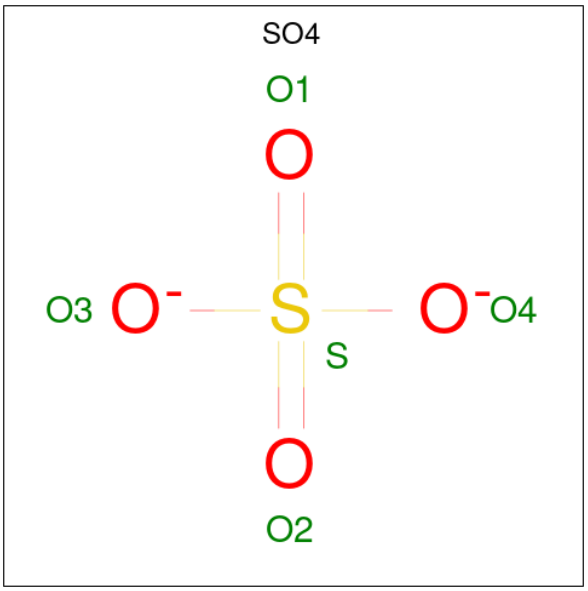
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	214	1612	1017	273	316	6	0	0	0

- Molecule 3 is an oligosaccharide called 2-amino-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]4-O-phosphono-L-glycero-alpha-D-manno-heptopyranose-(1-3)-4-O-phosphono-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	A	10	133	67	1	63	2	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

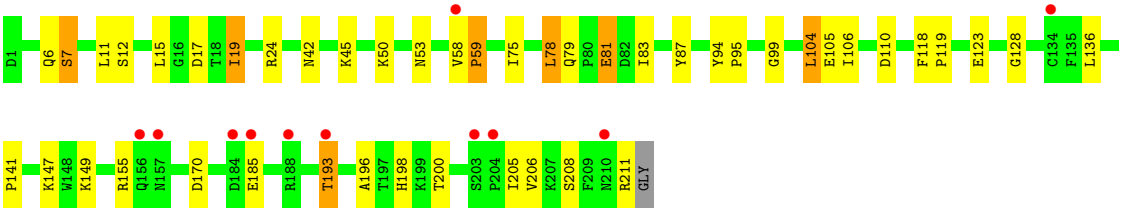
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	220	Total O 220 220	0	0
5	H	306	Total O 306 306	0	0

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.

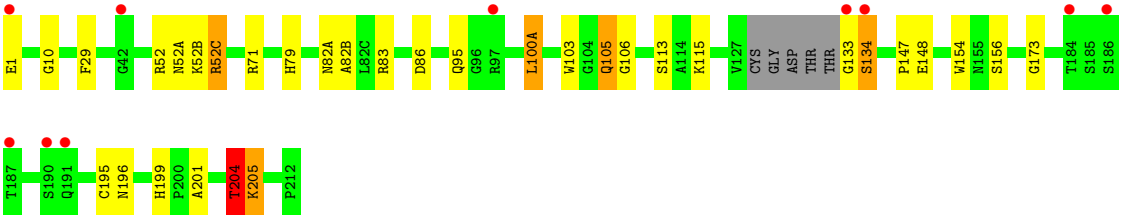
• Molecule 1: WN1 222-5 Fab (IgG2a) light chain

Chain L:



• Molecule 2: WN1 222-5 Fab (IgG2a) heavy chain

Chain H:



• Molecule 3: 2-amino-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-[L-glycero-alpha-D-manno-heptopyranose-(1-7)]4-O-phosphono-L-glycero-alpha-D-manno-heptopyranose-(1-3)-4-O-phosphono-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.85Å 101.85Å 118.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.73 29.85 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-1.73) 98.8 (29.85-1.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.182 , 0.231 0.208 , 0.242	Depositor DCC
R_{free} test set	3288 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3953	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: KDO, GLC, GLA, GMH, PA1, SO4, GM0

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	L	1.26	1/1669 (0.1%)	1.15	7/2267 (0.3%)
2	H	1.31	8/1651 (0.5%)	1.09	4/2251 (0.2%)
All	All	1.29	9/3320 (0.3%)	1.12	11/4518 (0.2%)

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	L	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	204	THR	CB-CG2	-5.96	1.32	1.52
2	H	113	SER	CB-OG	-5.82	1.34	1.42
2	H	195	CYS	CB-SG	-5.75	1.72	1.81
2	H	82(B)	ALA	CA-CB	5.70	1.64	1.52
2	H	148	GLU	CD-OE2	5.29	1.31	1.25
2	H	29	PHE	CD1-CE1	5.12	1.49	1.39
1	L	104	LEU	C-O	-5.11	1.13	1.23
2	H	103	TRP	CZ3-CH2	5.05	1.48	1.40
2	H	154	TRP	CZ3-CH2	5.02	1.48	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	115	LYS	CD-CE-NZ	-5.93	98.06	111.70
1	L	81	GLU	CA-CB-CG	5.92	126.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	78	LEU	CB-CG-CD1	-5.84	101.08	111.00
2	H	100(A)	LEU	CB-CG-CD1	5.74	120.75	111.00
1	L	17	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	H	71	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	L	110	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	L	128	GLY	CA-C-O	-5.26	111.12	120.60
1	L	170	ASP	CB-CG-OD1	5.16	122.94	118.30
2	H	52	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	L	205	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	7	SER	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	L	1632	0	1580	31	0
2	H	1612	0	1583	24	1
3	A	133	0	100	5	0
4	H	30	0	0	0	0
4	L	20	0	0	1	0
5	H	306	0	0	18	1
5	L	220	0	0	8	2
All	All	3953	0	3263	60	2

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 (60) 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:H:82(A):ASN:HB3	5:H:444:HOH:O	1.14	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82(A):ASN:ND2	5:H:436:HOH:O	1.67	1.23
5:H:605:HOH:O	3:A:2:GM0:O8	1.57	1.19
2:H:95:GLN:O	5:H:536:HOH:O	1.62	1.16
2:H:52(C):ARG:HH11	2:H:52(C):ARG:CG	1.66	1.08
5:H:605:HOH:O	3:A:2:GM0:P	2.03	1.08
2:H:82(A):ASN:CB	5:H:444:HOH:O	1.77	1.06
2:H:52(C):ARG:HG2	2:H:52(C):ARG:NH1	1.64	0.97
2:H:82(A):ASN:CG	5:H:436:HOH:O	1.91	0.96
2:H:52(C):ARG:HH11	2:H:52(C):ARG:HG2	0.80	0.95
1:L:123:GLU:HG3	5:L:534:HOH:O	1.71	0.90
2:H:156:SER:H	2:H:196:ASN:HD21	1.16	0.89
5:H:448:HOH:O	3:A:3:GM0:O9	1.97	0.82
2:H:105:GLN:HB3	5:H:540:HOH:O	1.86	0.75
2:H:199:HIS:CD2	5:H:518:HOH:O	2.42	0.72
2:H:156:SER:H	2:H:196:ASN:ND2	1.89	0.69
1:L:79:GLN:CD	5:L:544:HOH:O	2.37	0.62
1:L:19:ILE:HD11	1:L:78:LEU:HD13	1.82	0.62
1:L:45:LYS:NZ	4:L:301:SO4:O4	2.33	0.61
1:L:11:LEU:O	1:L:105:GLU:HG2	2.00	0.60
2:H:205:LYS:HE2	5:H:590:HOH:O	2.01	0.59
2:H:204:THR:HG21	5:H:541:HOH:O	2.03	0.59
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.87	0.58
1:L:79:GLN:HB3	5:L:544:HOH:O	2.03	0.57
2:H:133:GLY:O	2:H:134:SER:HB3	2.04	0.57
1:L:19:ILE:HD13	1:L:19:ILE:N	2.19	0.57
2:H:105:GLN:HG2	2:H:106:GLY:N	2.18	0.57
1:L:19:ILE:CD1	1:L:78:LEU:HD13	2.36	0.55
5:H:605:HOH:O	3:A:2:GM0:O4	2.14	0.55
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.74	0.52
1:L:79:GLN:CG	5:L:544:HOH:O	2.58	0.52
1:L:24:ARG:NH1	5:L:513:HOH:O	2.43	0.51
2:H:83:ARG:O	2:H:86:ASP:HB2	2.12	0.50
2:H:133:GLY:O	2:H:134:SER:CB	2.60	0.50
1:L:141:PRO:O	1:L:198:HIS:HE1	1.95	0.50
1:L:78:LEU:HD11	1:L:104:LEU:HD21	1.94	0.49
1:L:6:GLN:HE22	1:L:87:TYR:HA	1.78	0.49
1:L:147:LYS:HD3	1:L:149:LYS:HE3	1.95	0.48
1:L:136:LEU:CD2	1:L:196:ALA:HB2	2.43	0.48
2:H:82(A):ASN:HB2	5:H:444:HOH:O	1.76	0.47
1:L:79:GLN:NE2	5:L:544:HOH:O	2.47	0.47
1:L:11:LEU:HD21	5:L:499:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:ILE:HG12	1:L:106:ILE:HG12	1.97	0.47
1:L:50:LYS:HB2	1:L:53:ASN:HD22	1.81	0.45
2:H:52(C):ARG:CG	2:H:52(C):ARG:NH1	2.39	0.45
2:H:79:HIS:HE1	5:H:488:HOH:O	2.00	0.45
1:L:155:ARG:NH2	1:L:185:GLU:OE1	2.34	0.45
1:L:12:SER:HA	1:L:105:GLU:HG2	2.00	0.44
1:L:79:GLN:CB	5:L:544:HOH:O	2.65	0.44
2:H:173:GLY:HA3	5:H:579:HOH:O	2.17	0.44
1:L:211:ARG:HG2	1:L:211:ARG:HH11	1.83	0.43
2:H:147:PRO:HD2	2:H:201:ALA:CB	2.49	0.43
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.92	0.43
1:L:58:VAL:O	1:L:59:PRO:C	2.58	0.42
5:H:448:HOH:O	3:A:3:GM0:P	2.73	0.42
1:L:94:TYR:HA	1:L:95:PRO:C	2.41	0.41
1:L:19:ILE:HD11	1:L:75:ILE:HB	2.02	0.41
1:L:193:THR:HB	1:L:208:SER:CB	2.51	0.40
1:L:211:ARG:HG2	1:L:211:ARG:NH1	2.36	0.40
2:H:10:GLY:HA2	5:H:600:HOH:O	2.22	0.40

All (2) 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)
2:H:52(B):LYS:CD	5:L:513:HOH:O[4_545]	1.78	0.42
5:L:588:HOH:O	5:H:583:HOH:O[5_444]	2.09	0.11

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	L	209/212 (99%)	204 (98%)	4 (2%)	1 (0%)	29 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	210/219 (96%)	206 (98%)	3 (1%)	1 (0%)	29	12
All	All	419/431 (97%)	410 (98%)	7 (2%)	2 (0%)	29	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	134	SER
1	L	59	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	L	188/188 (100%)	181 (96%)	7 (4%)	34	11
2	H	180/184 (98%)	173 (96%)	7 (4%)	32	10
All	All	368/372 (99%)	354 (96%)	14 (4%)	33	11

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	15	LEU
1	L	19	ILE
1	L	42	ASN
1	L	81	GLU
1	L	193	THR
1	L	206	VAL
2	H	1	GLU
2	H	52(A)	ASN
2	H	52(C)	ARG
2	H	100(A)	LEU
2	H	105	GLN
2	H	204	THR
2	H	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	27	GLN
1	L	53	ASN
1	L	92	GLN
1	L	198	HIS
2	H	52(A)	ASN
2	H	53	ASN
2	H	164	HIS
2	H	191	GLN
2	H	196	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)

10 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	KDO	A	1	3	16,16,16	3.10	7 (43%)	17,24,24	2.51	7 (41%)
3	KDO	A	10	3	15,15,16	2.55	7 (46%)	17,21,24	2.58	7 (41%)
3	GM0	A	2	3	17,17,18	2.45	9 (52%)	24,25,27	1.97	8 (33%)
3	GM0	A	3	3	17,17,18	1.51	3 (17%)	24,25,27	1.46	4 (16%)
3	GLC	A	4	3	11,11,12	2.21	5 (45%)	15,15,17	2.28	5 (33%)
3	GLC	A	5	3	11,11,12	2.06	4 (36%)	15,15,17	1.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	A	6	3	11,11,12	0.88	0	15,15,17	1.01	0
3	PA1	A	7	3	11,11,12	1.51	3 (27%)	13,15,17	1.15	1 (7%)
3	GLA	A	8	3	11,11,12	2.17	5 (45%)	15,15,17	1.44	3 (20%)
3	GMH	A	9	3	13,13,14	1.21	1 (7%)	16,18,20	1.26	1 (6%)

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	KDO	A	1	3	-	2/12/30/30	0/1/1/1
3	KDO	A	10	3	-	6/10/26/30	0/1/1/1
3	GM0	A	2	3	-	1/11/28/31	0/1/1/1
3	GM0	A	3	3	-	1/11/28/31	0/1/1/1
3	GLC	A	4	3	-	2/2/19/22	0/1/1/1
3	GLC	A	5	3	-	0/2/19/22	0/1/1/1
3	GLC	A	6	3	-	0/2/19/22	0/1/1/1
3	PA1	A	7	3	-	0/2/19/22	0/1/1/1
3	GLA	A	8	3	-	0/2/19/22	0/1/1/1
3	GMH	A	9	3	-	0/6/23/26	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	KDO	O2-C2	7.34	1.50	1.39
3	A	2	GM0	C2-C3	5.85	1.61	1.52
3	A	1	KDO	C4-C5	5.82	1.61	1.52
3	A	10	KDO	C4-C5	-5.12	1.44	1.52
3	A	1	KDO	O6-C6	-5.04	1.36	1.44
3	A	10	KDO	O6-C6	4.31	1.50	1.44
3	A	4	GLC	O5-C1	4.21	1.50	1.43
3	A	5	GLC	C4-C5	4.00	1.61	1.53
3	A	1	KDO	C3-C2	3.97	1.57	1.51
3	A	2	GM0	O5-C1	3.95	1.50	1.43
3	A	8	GLA	O4-C4	3.76	1.52	1.43
3	A	4	GLC	O5-C5	3.47	1.50	1.43
3	A	10	KDO	O4-C4	-3.38	1.36	1.43
3	A	10	KDO	O5-C5	3.13	1.50	1.43
3	A	2	GM0	P-O8	3.09	1.66	1.54
3	A	8	GLA	C4-C5	-3.05	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	8	GLA	O5-C5	3.02	1.49	1.43
3	A	1	KDO	C7-C6	2.98	1.59	1.52
3	A	5	GLC	O5-C5	2.95	1.49	1.43
3	A	7	PA1	O5-C1	2.91	1.48	1.43
3	A	4	GLC	C2-C3	2.91	1.56	1.52
3	A	3	GM0	O3-C3	-2.89	1.35	1.43
3	A	2	GM0	C6-C5	2.86	1.58	1.52
3	A	10	KDO	C3-C4	2.77	1.58	1.52
3	A	10	KDO	O6-C2	2.76	1.48	1.43
3	A	2	GM0	O2-C2	2.64	1.48	1.43
3	A	5	GLC	O4-C4	2.63	1.49	1.43
3	A	4	GLC	O4-C4	2.50	1.49	1.43
3	A	2	GM0	O3-C3	-2.49	1.36	1.43
3	A	3	GM0	O5-C1	2.46	1.47	1.43
3	A	2	GM0	P-O9	-2.40	1.43	1.50
3	A	7	PA1	O5-C5	2.29	1.47	1.43
3	A	9	GMH	O7-C7	2.29	1.52	1.42
3	A	8	GLA	C1-C2	-2.26	1.46	1.52
3	A	2	GM0	O7-C7	2.20	1.51	1.42
3	A	3	GM0	C3-C4	2.19	1.58	1.52
3	A	4	GLC	C4-C3	2.18	1.58	1.52
3	A	2	GM0	O4-C4	2.18	1.51	1.44
3	A	1	KDO	C2-C1	-2.15	1.50	1.53
3	A	8	GLA	O2-C2	2.09	1.47	1.43
3	A	1	KDO	O5-C5	2.07	1.48	1.43
3	A	10	KDO	C3-C2	2.05	1.55	1.52
3	A	7	PA1	C1-C2	2.01	1.54	1.52
3	A	5	GLC	C1-C2	2.01	1.57	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	10	KDO	O7-C7-C6	5.96	123.41	109.18
3	A	1	KDO	C3-C4-C5	-5.59	105.41	110.84
3	A	1	KDO	O1A-C1-C2	-5.48	114.70	123.85
3	A	4	GLC	C1-O5-C5	-5.22	105.19	112.19
3	A	10	KDO	O6-C6-C7	4.57	115.49	106.60
3	A	2	GM0	O4-P-O9	4.05	123.78	109.33
3	A	10	KDO	C3-C4-C5	3.94	116.34	110.67
3	A	2	GM0	O7-C7-C6	-3.78	103.21	111.16
3	A	1	KDO	O6-C6-C5	3.78	113.78	108.50
3	A	10	KDO	O8-C8-C7	-3.54	103.71	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	9	GMH	O7-C7-C6	-3.53	103.74	111.16
3	A	4	GLC	C2-C3-C4	-3.50	104.71	110.86
3	A	2	GM0	O4-C4-C5	-3.47	101.38	108.76
3	A	2	GM0	O2-C2-C3	-3.44	103.02	110.15
3	A	5	GLC	O5-C5-C6	-3.31	101.22	107.66
3	A	3	GM0	O5-C1-C2	3.27	118.60	110.79
3	A	8	GLA	O3-C3-C2	-3.19	103.53	110.05
3	A	1	KDO	O5-C5-C4	-3.15	103.63	110.05
3	A	5	GLC	C1-O5-C5	-3.14	107.98	112.19
3	A	4	GLC	C1-C2-C3	-3.00	105.28	109.64
3	A	2	GM0	C3-C4-C5	-2.90	105.19	111.72
3	A	3	GM0	O7-C7-C6	-2.90	105.07	111.16
3	A	2	GM0	O8-P-O9	-2.87	99.64	110.83
3	A	4	GLC	O4-C4-C3	-2.77	103.85	110.38
3	A	10	KDO	O6-C2-C1	2.74	112.88	107.72
3	A	10	KDO	O5-C5-C6	2.72	116.90	109.94
3	A	7	PA1	C1-O5-C5	-2.63	108.66	112.19
3	A	3	GM0	O3-C3-C2	-2.53	104.89	110.05
3	A	2	GM0	C1-O5-C5	2.48	115.53	111.48
3	A	1	KDO	O4-C4-C5	-2.45	105.07	110.15
3	A	8	GLA	O2-C2-C3	2.38	115.09	110.15
3	A	2	GM0	O8-P-O1A	2.38	116.72	107.80
3	A	8	GLA	O3-C3-C4	2.32	115.83	110.38
3	A	4	GLC	O3-C3-C2	2.27	114.69	110.05
3	A	1	KDO	O2-C2-C3	-2.26	106.03	109.44
3	A	1	KDO	C8-C7-C6	-2.23	107.61	112.05
3	A	3	GM0	O4-C4-C5	-2.22	104.04	108.76
3	A	10	KDO	O1A-C1-C2	-2.07	118.38	122.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	GM0	O5-C5-C6-C7
3	A	10	KDO	C5-C6-C7-O7
3	A	10	KDO	C5-C6-C7-C8
3	A	10	KDO	O6-C6-C7-O7
3	A	10	KDO	O6-C6-C7-C8
3	A	10	KDO	O7-C7-C8-O8
3	A	4	GLC	C4-C5-C6-O6
3	A	1	KDO	O1A-C1-C2-O6
3	A	4	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	3	GM0	C4-O4-P-O8
3	A	10	KDO	C6-C7-C8-O8
3	A	1	KDO	O1B-C1-C2-O6

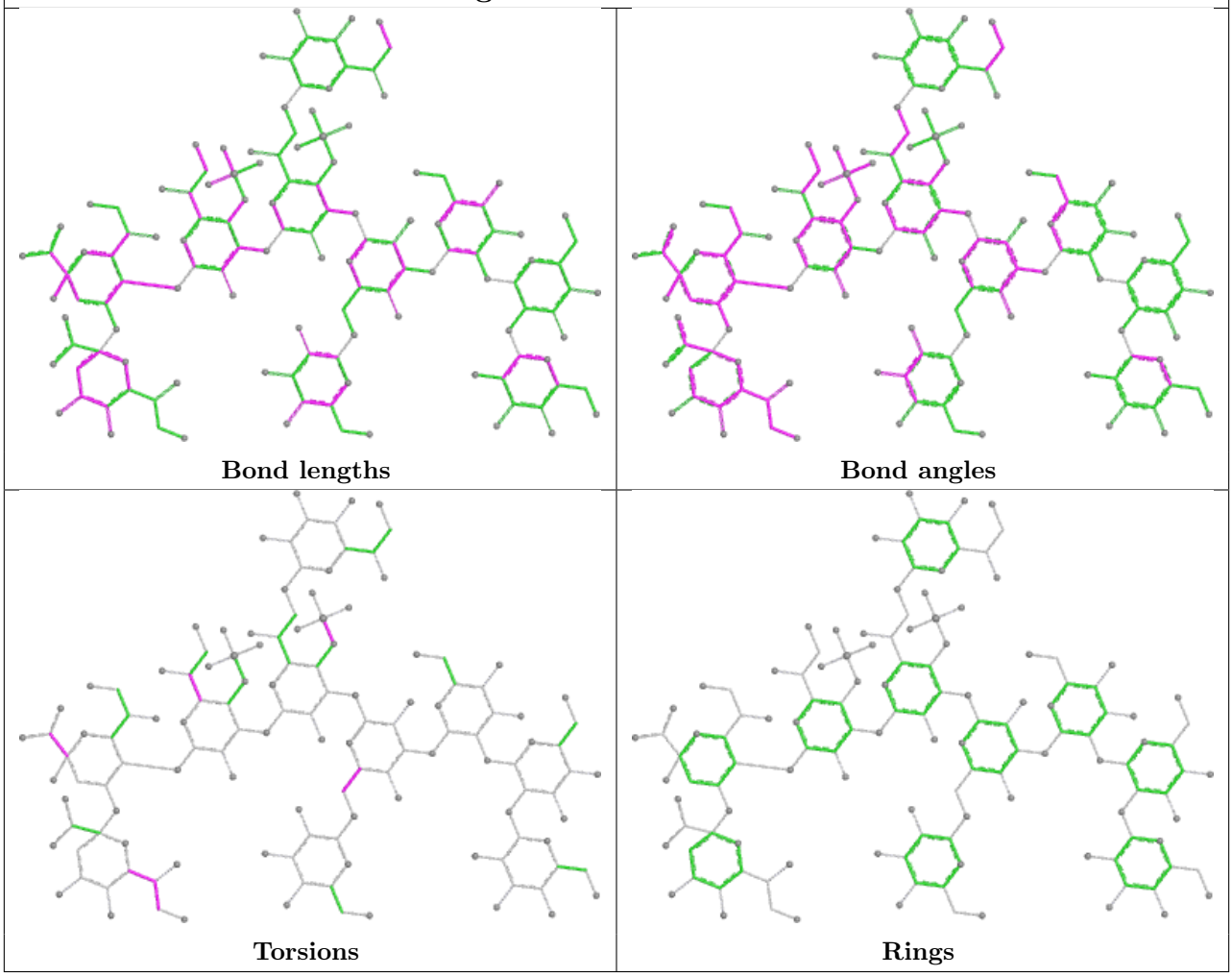
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	GM0	2	0
3	A	2	GM0	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 A



5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	H	312	-	4,4,4	0.34	0	6,6,6	0.73	0
4	SO4	H	315	-	4,4,4	0.26	0	6,6,6	0.27	0
4	SO4	L	304	-	4,4,4	0.31	0	6,6,6	0.43	0
4	SO4	H	311	-	4,4,4	0.32	0	6,6,6	0.53	0
4	SO4	H	313	-	4,4,4	0.30	0	6,6,6	0.78	0
4	SO4	H	314	-	4,4,4	0.71	0	6,6,6	0.65	0
4	SO4	L	303	-	4,4,4	0.27	0	6,6,6	0.23	0
4	SO4	L	302	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.19	0
4	SO4	H	316	-	4,4,4	0.52	0	6,6,6	0.89	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	211/212 (99%)	0.33	11 (5%)	27	32	11, 21, 42, 52	0
2	H	214/219 (97%)	0.13	10 (4%)	31	36	11, 17, 38, 50	0
All	All	425/431 (98%)	0.23	21 (4%)	29	34	11, 19, 39, 52	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	203	SER	4.5
2	H	133	GLY	4.3
1	L	157	ASN	4.3
1	L	188	ARG	3.9
2	H	1	GLU	3.5
2	H	187	THR	3.1
1	L	184	ASP	3.1
1	L	58	VAL	3.0
2	H	134	SER	2.9
1	L	210	ASN	2.9
2	H	42	GLY	2.7
1	L	193	THR	2.5
2	H	186	SER	2.4
2	H	191	GLN	2.4
2	H	190	SER	2.4
1	L	204	PRO	2.3
1	L	134	CYS	2.2
1	L	185	GLU	2.2
1	L	156	GLN	2.2
2	H	97	ARG	2.1
2	H	184	THR	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)

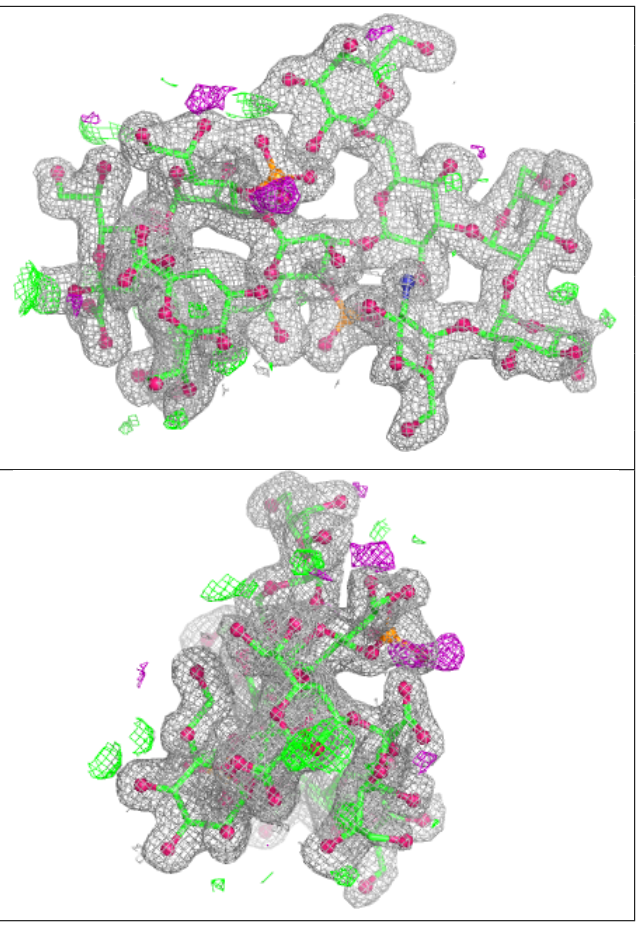
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	KDO	A	10	15/16	0.85	0.18	28,34,39,42	0
3	GLC	A	6	11/12	0.91	0.21	28,33,40,42	0
3	GLC	A	5	11/12	0.92	0.10	17,26,34,34	0
3	GLA	A	8	11/12	0.93	0.08	17,22,26,26	0
3	PA1	A	7	11/12	0.94	0.17	22,28,34,36	0
3	KDO	A	1	16/16	0.94	0.10	19,23,26,38	0
3	GM0	A	2	17/18	0.94	0.10	15,20,27,30	0
3	GMH	A	9	13/14	0.96	0.07	14,16,19,19	0
3	GLC	A	4	11/12	0.96	0.06	15,18,20,21	0
3	GM0	A	3	17/18	0.98	0.06	13,15,18,18	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 A:

$2mF_o$-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	SO4	L	303	5/5	0.27	0.54	121,122,122,122	0
4	SO4	H	315	5/5	0.60	0.49	123,123,123,124	0
4	SO4	L	304	5/5	0.74	0.29	72,73,74,75	0
4	SO4	H	313	5/5	0.78	0.29	39,55,57,58	0
4	SO4	H	314	5/5	0.84	0.34	36,37,43,47	0
4	SO4	L	301	5/5	0.84	0.33	78,78,79,80	0
4	SO4	H	316	5/5	0.89	0.26	35,36,46,48	0
4	SO4	L	302	5/5	0.93	0.20	64,65,67,67	0
4	SO4	H	312	5/5	0.98	0.06	19,22,24,27	0
4	SO4	H	311	5/5	0.99	0.04	17,18,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.