Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 01:35 PM EDT

PDB ID	:	1ZBA
Title	:	Foot-and-Mouth Disease virus serotype A1061 complexed with oligosaccharide receptor.
Authors	:	Fry, E.E.; Newman, J.W.; Curry, S.; Najjam, S.; Jackson, T.; Blakemore, W.; Lea, S.M.; Miller, L.; Burman, A.; King, A.M.; Stuart, D.I.
Deposited on	:	2005-04-08
Resolution	:	2.00 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 following versions of software and data (see references (i)) were used in the production of this report:

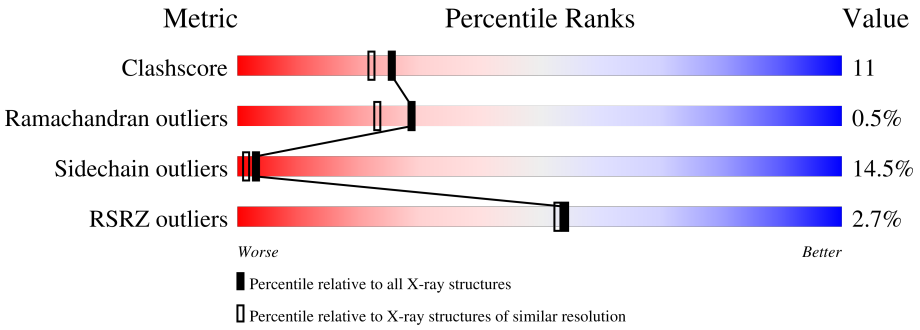
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	1	212	3%, 67%, 17%, 6%, 10%
2	2	218	%, 70%, 19%, 6%, 5%
3	3	221	76%, 19%, 5%
4	4	85	8%, 46%, 7%, • •, 42%
5	A	3	67%, 33%

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
5	SGN	A	3	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5732 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 Coat protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	191	1492	944	266	278	4	0	0	0

- Molecule 2 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	207	1652	1061	280	306	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	14	LEU	ILE	engineered mutation	UNP Q84769

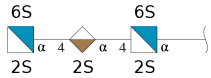
- Molecule 3 is a protein called Coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	221	1708	1089	277	335	7	0	0	0

- Molecule 4 is a protein called Coat protein VP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	49	375	235	62	76	2	0	0	0

- Molecule 5 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	3	55	18	2	30	5	0	0	0

- Molecule 6 is water.

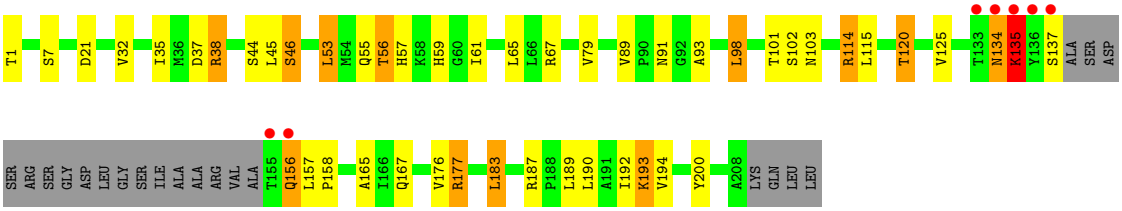
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	1	154	154	154	0	0
6	2	109	109	109	0	0
6	3	157	157	157	0	0
6	4	30	30	30	0	0

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.

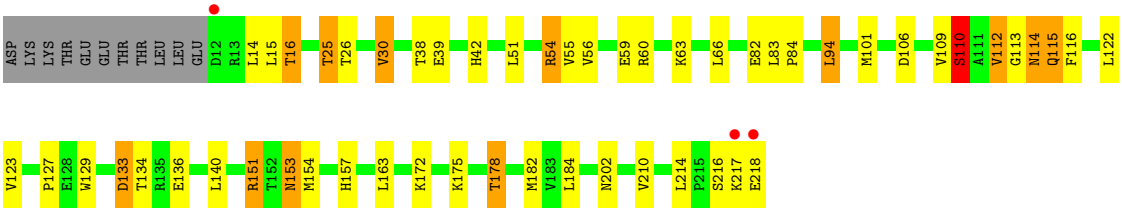
- Molecule 1: Coat protein VP1

Chain 1:



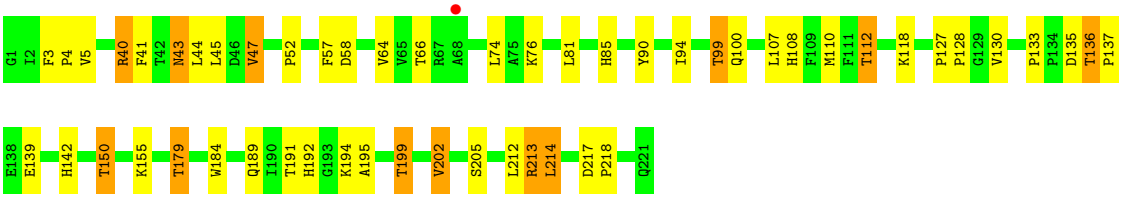
- Molecule 2: Coat protein VP2

Chain 2:



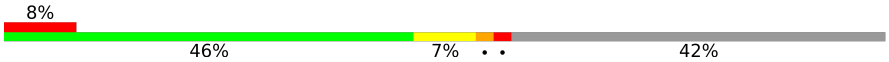
- Molecule 3: Coat protein VP3

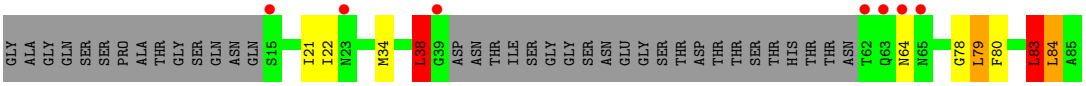
Chain 3:



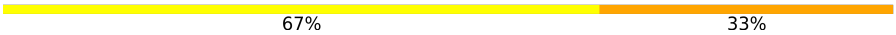
- Molecule 4: Coat protein VP4

Chain 4:





• Molecule 5: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-id opyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain A: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	307.00Å 307.00Å 715.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 24.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 26.8 (24.88-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.016 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.017 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.017 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.017 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.015 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.074 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5732	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: SGN, IDS

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	1	0.50	0/1527	0.79	0/2083
2	2	0.49	1/1701 (0.1%)	0.82	4/2322 (0.2%)
3	3	0.51	1/1757 (0.1%)	0.79	0/2405
4	4	0.53	0/381	0.86	2/513 (0.4%)
All	All	0.50	2/5366 (0.0%)	0.81	6/7323 (0.1%)

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
2	2	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	182	MET	SD-CE	-6.00	1.44	1.77
3	3	110	MET	SD-CE	-5.09	1.49	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	38	LEU	CA-CB-CG	6.61	130.51	115.30
2	2	110	SER	O-C-N	-6.09	112.96	122.70
4	4	83	LEU	CA-CB-CG	5.61	128.20	115.30
2	2	113	GLY	N-CA-C	-5.39	99.61	113.10
2	2	109	VAL	C-N-CA	5.29	134.93	121.70
2	2	109	VAL	O-C-N	-5.01	114.68	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	110	SER	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	1	1492	0	1485	44	0
2	2	1652	0	1607	37	0
3	3	1708	0	1631	32	0
4	4	375	0	348	6	1
5	A	55	0	23	1	0
6	1	154	0	0	5	2
6	2	109	0	0	5	3
6	3	157	0	0	2	0
6	4	30	0	0	2	0
All	All	5732	0	5094	110	3

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 11.

All (110) 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)
2:2:129:TRP:HB2	2:2:178:THR:HG21	1.52	0.91
1:1:57:HIS:HD2	1:1:59:HIS:H	1.18	0.88
1:1:156:GLN:HE21	1:1:156:GLN:HA	1.42	0.84
1:1:135:LYS:NZ	1:1:158:PRO:HA	1.93	0.83
2:2:115:GLN:NE2	2:2:115:GLN:H	1.78	0.81
2:2:218:GLU:HB2	3:3:139:GLU:HG2	1.62	0.80
1:1:193:LYS:HE2	5:A:1:SGN:H4	1.64	0.80
1:1:103:ASN:HD21	3:3:217:ASP:H	1.32	0.77
3:3:136:THR:HG22	3:3:139:GLU:H	1.50	0.76
2:2:42:HIS:HB2	6:4:113:HOH:O	1.85	0.76
2:2:115:GLN:H	2:2:115:GLN:HE21	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:56:THR:HG22	1:1:67:ARG:NH2	2.03	0.73
1:1:165:ALA:HB3	6:1:606:HOH:O	1.88	0.73
1:1:56:THR:HG22	1:1:67:ARG:HH21	1.54	0.72
3:3:43:ASN:HD22	3:3:45:LEU:H	1.38	0.71
1:1:91:ASN:HB3	1:1:120:THR:HG23	1.73	0.71
2:2:16:THR:HB	2:2:25:THR:HB	1.71	0.70
3:3:112:THR:HG22	6:3:373:HOH:O	1.92	0.68
2:2:129:TRP:HB2	2:2:178:THR:CG2	2.22	0.68
1:1:53:LEU:O	1:1:56:THR:HB	1.94	0.68
1:1:57:HIS:CD2	1:1:59:HIS:H	2.07	0.68
1:1:135:LYS:HZ2	1:1:158:PRO:HA	1.57	0.67
2:2:106:ASP:OD2	2:2:157:HIS:HE1	1.79	0.66
1:1:37:ASP:OD2	1:1:177:ARG:HD3	1.98	0.63
1:1:135:LYS:HD2	6:1:624:HOH:O	1.98	0.62
2:2:25:THR:HG21	6:2:235:HOH:O	1.98	0.62
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.31	0.61
3:3:213:ARG:HD3	3:3:214:LEU:HD22	1.81	0.61
4:4:34:MET:HG3	6:4:100:HOH:O	2.01	0.61
3:3:99:THR:HG22	3:3:100:GLN:HG3	1.83	0.61
3:3:112:THR:HB	3:3:199:THR:HG22	1.81	0.60
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.83	0.60
1:1:134:ASN:O	1:1:135:LYS:HD3	2.02	0.60
1:1:91:ASN:O	3:3:99:THR:HG21	2.01	0.60
4:4:83:LEU:HD22	4:4:84:LEU:N	2.17	0.59
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.84	0.59
3:3:108:HIS:HE1	3:3:205:SER:OG	1.85	0.59
4:4:21:ILE:HG22	4:4:22:ILE:HD12	1.85	0.59
1:1:135:LYS:O	1:1:135:LYS:HG2	2.03	0.58
1:1:91:ASN:H	1:1:120:THR:CG2	2.17	0.58
3:3:133:PRO:HG3	3:3:184:TRP:CD2	2.39	0.57
2:2:216:SER:HB3	3:3:142:HIS:CD2	2.40	0.57
2:2:63:LYS:HZ3	2:2:202:ASN:HD21	1.52	0.57
2:2:84:PRO:O	2:2:175:LYS:HE3	2.05	0.56
3:3:179:THR:HG21	6:3:330:HOH:O	2.05	0.56
1:1:55:GLN:HG2	6:1:576:HOH:O	2.06	0.56
2:2:115:GLN:HE21	2:2:115:GLN:N	2.01	0.56
1:1:91:ASN:H	1:1:120:THR:HG21	1.70	0.56
1:1:156:GLN:HA	1:1:156:GLN:NE2	2.19	0.56
2:2:114:ASN:ND2	2:2:116:PHE:H	2.04	0.55
3:3:99:THR:CG2	3:3:100:GLN:HG3	2.36	0.55
1:1:35:ILE:O	1:1:38:ARG:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:153:ASN:HD22	2:2:153:ASN:N	2.05	0.55
3:3:90:TYR:CE1	3:3:94:ILE:HD11	2.42	0.55
1:1:89:VAL:HB	6:1:606:HOH:O	2.07	0.55
1:1:7:SER:HA	2:2:30:VAL:HG13	1.90	0.54
1:1:56:THR:CG2	1:1:67:ARG:HH21	2.21	0.53
1:1:187:ARG:NH2	2:2:127:PRO:O	2.41	0.53
2:2:122:LEU:HB2	2:2:184:LEU:HD22	1.90	0.52
3:3:118:LYS:HA	3:3:150:THR:HG21	1.90	0.52
2:2:129:TRP:HH2	6:2:230:HOH:O	1.92	0.52
1:1:134:ASN:O	1:1:135:LYS:HB3	2.09	0.52
1:1:135:LYS:HZ3	1:1:158:PRO:HA	1.72	0.51
1:1:46:SER:HB2	6:1:580:HOH:O	2.11	0.50
2:2:217:LYS:N	2:2:217:LYS:HD2	2.27	0.50
2:2:133:ASP:HB2	2:2:136:GLU:HG3	1.94	0.50
1:1:194:VAL:HG22	1:1:200:TYR:HB2	1.94	0.49
3:3:43:ASN:ND2	3:3:45:LEU:H	2.07	0.49
1:1:98:LEU:HG	1:1:167:GLN:HB2	1.93	0.49
2:2:63:LYS:NZ	2:2:202:ASN:ND2	2.61	0.49
2:2:151:ARG:HD3	6:2:327:HOH:O	2.13	0.48
2:2:114:ASN:C	2:2:114:ASN:HD22	2.16	0.48
2:2:63:LYS:NZ	2:2:202:ASN:HD21	2.11	0.48
2:2:157:HIS:HD2	6:2:237:HOH:O	1.95	0.48
1:1:44:SER:O	1:1:45:LEU:HD23	2.14	0.47
3:3:108:HIS:HB3	3:3:155:LYS:HE3	1.97	0.47
2:2:94:LEU:HG	2:2:210:VAL:HG11	1.97	0.47
1:1:89:VAL:CG1	1:1:93:ALA:CB	2.92	0.46
2:2:153:ASN:HD22	2:2:153:ASN:H	1.62	0.46
2:2:82:GLU:HA	2:2:178:THR:HB	1.95	0.46
2:2:175:LYS:HE2	6:2:277:HOH:O	2.15	0.46
3:3:136:THR:HB	3:3:139:GLU:OE1	2.16	0.46
4:4:83:LEU:HD22	4:4:84:LEU:H	1.80	0.46
3:3:40:ARG:HG3	3:3:41:PHE:N	2.31	0.45
3:3:57:PHE:CE2	3:3:202:VAL:HG13	2.52	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE2	2.48	0.45
1:1:135:LYS:HG3	1:1:158:PRO:HG3	1.99	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE1	2.51	0.44
1:1:79:VAL:HG22	1:1:114:ARG:HG3	1.99	0.44
4:4:38:LEU:O	4:4:38:LEU:HD12	2.18	0.44
1:1:91:ASN:CB	1:1:120:THR:HG23	2.46	0.43
3:3:192:HIS:HB2	3:3:195:ALA:HB3	1.99	0.43
3:3:47:VAL:HG22	3:3:90:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:VAL:HG13	1:1:183:LEU:HD22	2.00	0.43
1:1:91:ASN:CB	1:1:120:THR:CG2	2.97	0.43
1:1:56:THR:O	1:1:67:ARG:NH2	2.52	0.43
1:1:91:ASN:HB3	1:1:120:THR:CG2	2.45	0.43
3:3:136:THR:HA	3:3:137:PRO:HD3	1.95	0.42
3:3:213:ARG:O	3:3:214:LEU:HB2	2.19	0.42
3:3:85:HIS:H	3:3:85:HIS:CD2	2.37	0.42
2:2:202:ASN:HD22	2:2:202:ASN:HA	1.70	0.42
3:3:66:THR:HB	3:3:189:GLN:OE1	2.19	0.42
2:2:110:SER:HA	2:2:154:MET:O	2.19	0.42
1:1:1:THR:HG23	4:4:79:LEU:HA	2.01	0.42
3:3:3:PHE:HA	3:3:4:PRO:HD3	1.82	0.42
1:1:102:SER:HB2	3:3:217:ASP:OD2	2.20	0.41
3:3:127:PRO:HB2	3:3:128:PRO:HD2	2.02	0.41
1:1:35:ILE:HD11	1:1:61:ILE:HD11	2.03	0.40
2:2:112:VAL:HB	2:2:154:MET:SD	2.61	0.40
3:3:52:PRO:HB3	3:3:205:SER:HB3	2.04	0.40

All (3) 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)
6:1:525:HOH:O	6:2:235:HOH:O[2_555]	0.77	1.43
4:4:80:PHE:O	6:2:236:HOH:O[2_555]	1.93	0.27
6:1:653:HOH:O	6:2:221:HOH:O[2_555]	2.12	0.08

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	1	187/212 (88%)	179 (96%)	7 (4%)	1 (0%)	29 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	205/218 (94%)	195 (95%)	10 (5%)	0	100	100
3	3	219/221 (99%)	208 (95%)	10 (5%)	1 (0%)	29	23
4	4	45/85 (53%)	41 (91%)	3 (7%)	1 (2%)	6	2
All	All	656/736 (89%)	623 (95%)	30 (5%)	3 (0%)	29	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	78	GLY
1	1	135	LYS
3	3	58	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	1	161/176 (92%)	137 (85%)	24 (15%)	3	1
2	2	181/192 (94%)	153 (84%)	28 (16%)	2	1
3	3	183/183 (100%)	158 (86%)	25 (14%)	3	2
4	4	40/68 (59%)	35 (88%)	5 (12%)	4	2
All	All	565/619 (91%)	483 (86%)	82 (14%)	3	1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	21	ASP
1	1	38	ARG
1	1	46	SER
1	1	53	LEU
1	1	56	THR
1	1	65	LEU
1	1	98	LEU
1	1	101	THR

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Mol	Chain	Res	Type
1	1	114	ARG
1	1	115	LEU
1	1	120	THR
1	1	125	VAL
1	1	134	ASN
1	1	135	LYS
1	1	137	SER
1	1	156	GLN
1	1	157	LEU
1	1	176	VAL
1	1	177	ARG
1	1	183	LEU
1	1	189	LEU
1	1	190	LEU
1	1	192	ILE
1	1	193	LYS
2	2	14	LEU
2	2	15	LEU
2	2	16	THR
2	2	25	THR
2	2	26	THR
2	2	30	VAL
2	2	38	THR
2	2	39	GLU
2	2	51	LEU
2	2	54	ARG
2	2	55	VAL
2	2	56	VAL
2	2	60	ARG
2	2	66	LEU
2	2	83	LEU
2	2	94	LEU
2	2	112	VAL
2	2	114	ASN
2	2	115	GLN
2	2	123	VAL
2	2	133	ASP
2	2	134	THR
2	2	140	LEU
2	2	151	ARG
2	2	153	ASN
2	2	163	LEU

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Mol	Chain	Res	Type
2	2	172	LYS
2	2	178	THR
3	3	5	VAL
3	3	40	ARG
3	3	43	ASN
3	3	44	LEU
3	3	47	VAL
3	3	64	VAL
3	3	74	LEU
3	3	76	LYS
3	3	81	LEU
3	3	99	THR
3	3	107	LEU
3	3	112	THR
3	3	130	VAL
3	3	135	ASP
3	3	136	THR
3	3	150	THR
3	3	179	THR
3	3	191	THR
3	3	194	LYS
3	3	199	THR
3	3	202	VAL
3	3	212	LEU
3	3	213	ARG
3	3	214	LEU
3	3	218	PRO
4	4	38	LEU
4	4	64	ASN
4	4	79	LEU
4	4	83	LEU
4	4	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	28	HIS
1	1	57	HIS
1	1	103	ASN
1	1	156	GLN
1	1	169	GLN
2	2	114	ASN

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Mol	Chain	Res	Type
2	2	115	GLN
2	2	153	ASN
2	2	157	HIS
2	2	166	ASN
2	2	202	ASN
3	3	36	ASN
3	3	43	ASN
3	3	85	HIS
3	3	108	HIS
3	3	153	ASN
3	3	180	ASN
4	4	17	ASN
4	4	64	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)

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	$\#\|Z\| > 2$
5	SGN	A	1	5	19,20,20	3.86	4 (21%)	24,31,31	1.12	2 (8%)
5	IDS	A	2	5	13,16,17	2.10	2 (15%)	15,24,26	1.76	4 (26%)
5	SGN	A	3	5	18,19,20	4.11	4 (22%)	22,29,31	1.16	1 (4%)

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
5	SGN	A	1	5	-	4/11/31/31	0/1/1/1
5	IDS	A	2	5	-	3/5/26/29	0/1/1/1
5	SGN	A	3	5	-	5/11/28/31	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3	SGN	S1-N2	13.36	1.77	1.59
5	A	1	SGN	S1-N2	12.85	1.76	1.59
5	A	3	SGN	O6-S2	7.61	1.77	1.56
5	A	1	SGN	O6-S2	7.11	1.76	1.56
5	A	2	IDS	O2-S	6.73	1.77	1.57
5	A	1	SGN	O2S-S1	5.70	1.48	1.42
5	A	3	SGN	O2S-S1	5.68	1.48	1.42
5	A	3	SGN	O1S-S1	5.60	1.48	1.42
5	A	1	SGN	O1S-S1	5.38	1.48	1.42
5	A	2	IDS	O2-C2	-2.91	1.42	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2	IDS	C1-O5-C5	4.92	120.86	112.17
5	A	3	SGN	O2S-S1-O1S	-4.44	109.67	120.16
5	A	1	SGN	O2S-S1-O1S	-4.36	109.86	120.16
5	A	2	IDS	C3-C4-C5	2.65	114.47	109.02
5	A	1	SGN	C6-C5-C4	-2.23	107.45	112.09
5	A	2	IDS	O2-C2-C3	2.07	109.84	106.95
5	A	2	IDS	C6-C5-C4	-2.02	108.00	113.04

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	IDS	C2-O2-S-O1S
5	A	2	IDS	C2-O2-S-O3S
5	A	3	SGN	C4-C5-C6-O6
5	A	3	SGN	O5-C5-C6-O6
5	A	3	SGN	C2-N2-S1-O1S

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Mol	Chain	Res	Type	Atoms
5	A	3	SGN	C2-N2-S1-O2S
5	A	3	SGN	C2-N2-S1-O3S
5	A	1	SGN	C6-O6-S2-O6S
5	A	2	IDS	C2-O2-S-O2S
5	A	1	SGN	C6-O6-S2-O4S
5	A	1	SGN	C6-O6-S2-O5S
5	A	1	SGN	C2-N2-S1-O1S

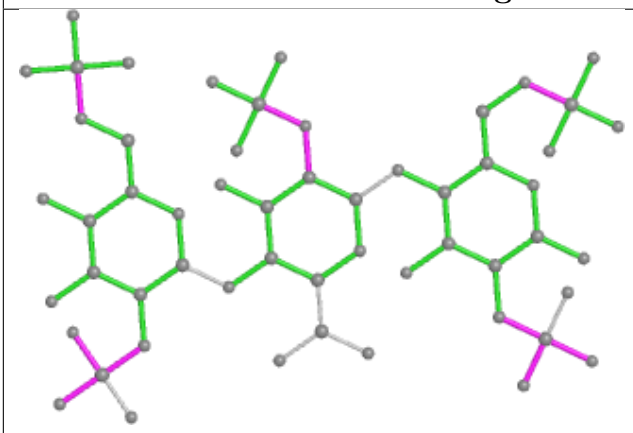
There are no ring outliers.

1 monomer is involved in 1 short contact:

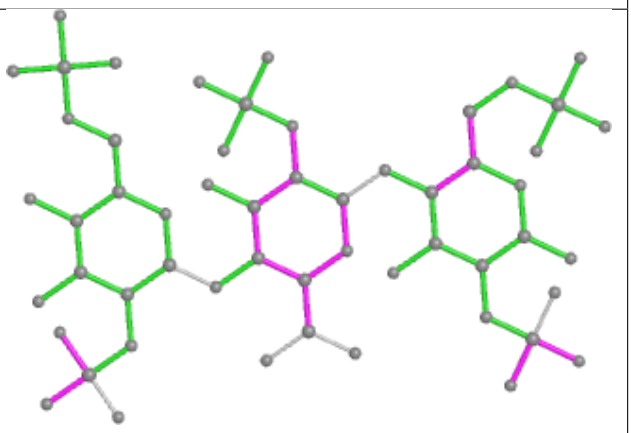
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	SGN	1	0

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

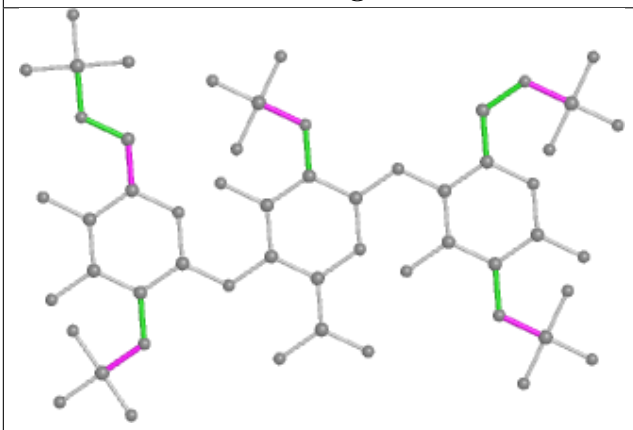
Oligosaccharide Chain A



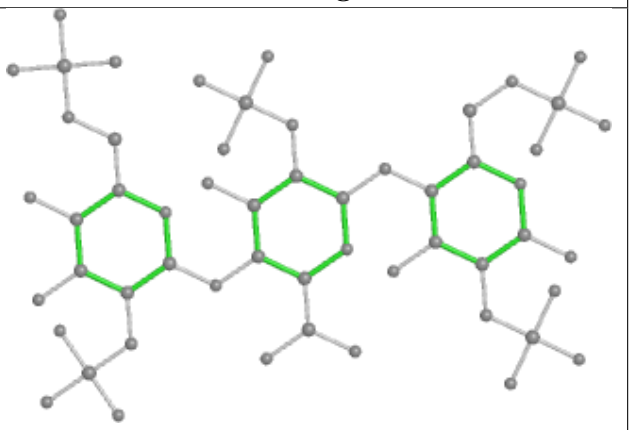
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	1	191/212 (90%)	-0.65	7 (3%)	41	41	13, 21, 59, 151	0
2	2	207/218 (94%)	-0.92	3 (1%)	75	74	14, 21, 44, 104	0
3	3	221/221 (100%)	-0.85	1 (0%)	91	90	14, 20, 48, 86	0
4	4	49/85 (57%)	0.41	7 (14%)	2	2	17, 43, 109, 138	0
All	All	668/736 (90%)	-0.72	18 (2%)	54	53	13, 21, 61, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	136	TYR	13.5
1	1	137	SER	11.6
1	1	134	ASN	7.7
4	4	62	THR	6.5
1	1	135	LYS	5.8
4	4	64	ASN	5.4
4	4	63	GLN	5.0
1	1	155	THR	4.6
4	4	15	SER	3.9
2	2	218	GLU	3.7
2	2	217	LYS	3.6
4	4	65	ASN	3.3
2	2	12	ASP	3.0
4	4	39	GLY	2.7
3	3	68	ALA	2.5
1	1	133	THR	2.5
1	1	156	GLN	2.4
4	4	23	ASN	2.3

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)

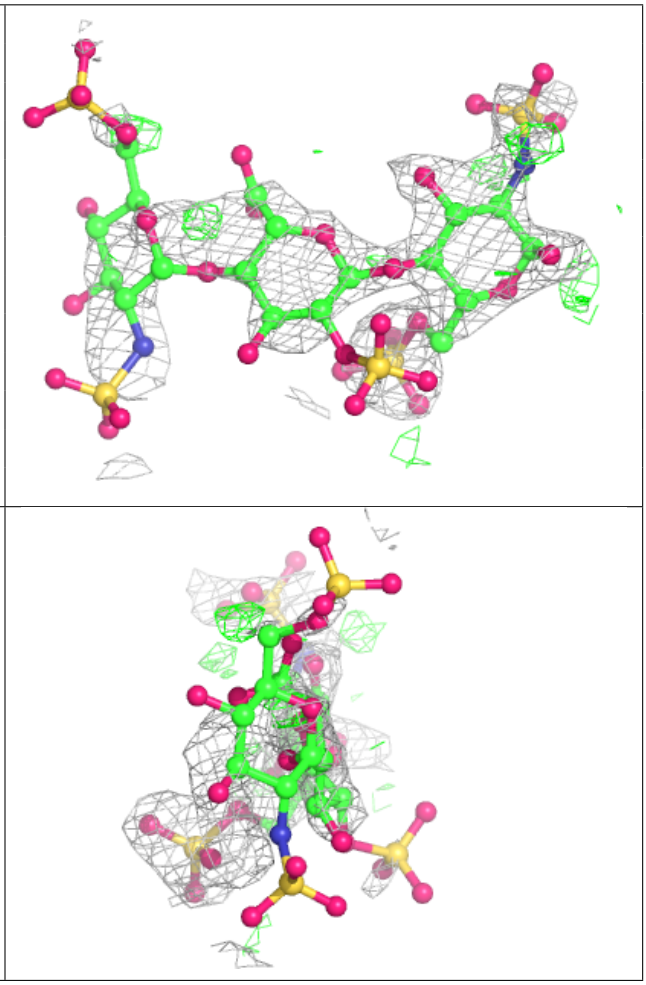
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SGN	A	3	19/20	0.68	0.56	66,78,118,125	19
5	IDS	A	2	16/17	0.78	0.39	34,61,83,91	16
5	SGN	A	1	20/20	0.90	0.21	10,42,81,86	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 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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.