wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2024 – 10:39 pm BST

PDB ID	:	2WMI
Title	:	Crystal structure of the catalytic module of a family 98 glycoside hydrolase from Streptococcus pneumoniae SP3-BS71 in complex with the A-trisaccharide blood group antigen.
Authors	:	Higgins, M.A.; Whitworth, G.E.; El Warry, N.; Randriantsoa, M.; Samain, E.; Burke, R.D.; Vocadlo, D.J.; Boraston, A.B.
Deposited on	:	2009-06-30
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

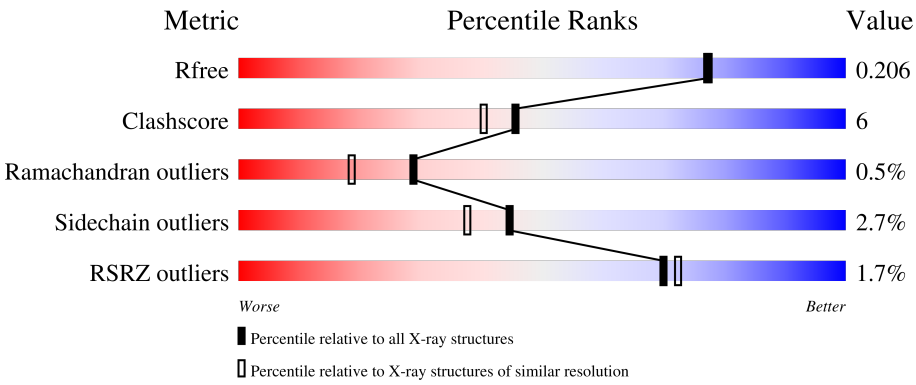
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	606	2%, 79%, 13%, • 6%
2	B	606	%, 83%, 10%, • 6%
3	C	3	100%
3	D	3	33%, 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10447 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 FUCOLECTIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	572	4681	3009	783	876	13	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	MET	-	expression tag	UNP A5LBQ0
A	399	GLY	-	expression tag	UNP A5LBQ0
A	400	SER	-	expression tag	UNP A5LBQ0
A	401	SER	-	expression tag	UNP A5LBQ0
A	402	HIS	-	expression tag	UNP A5LBQ0
A	403	HIS	-	expression tag	UNP A5LBQ0
A	404	HIS	-	expression tag	UNP A5LBQ0
A	405	HIS	-	expression tag	UNP A5LBQ0
A	406	HIS	-	expression tag	UNP A5LBQ0
A	407	HIS	-	expression tag	UNP A5LBQ0
A	408	SER	-	expression tag	UNP A5LBQ0
A	409	SER	-	expression tag	UNP A5LBQ0
A	410	GLY	-	expression tag	UNP A5LBQ0
A	411	LEU	-	expression tag	UNP A5LBQ0
A	412	VAL	-	expression tag	UNP A5LBQ0
A	413	PRO	-	expression tag	UNP A5LBQ0
A	414	ARG	-	expression tag	UNP A5LBQ0
A	415	GLY	-	expression tag	UNP A5LBQ0
A	416	SER	-	expression tag	UNP A5LBQ0
A	417	HIS	-	expression tag	UNP A5LBQ0
A	418	MET	-	expression tag	UNP A5LBQ0
A	419	ALA	-	expression tag	UNP A5LBQ0
A	420	SER	-	expression tag	UNP A5LBQ0

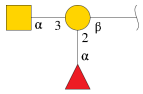
- Molecule 2 is a protein called FUCOLECTIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	571	4670	3003	782	872	13	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	398	MET	-	expression tag	UNP A5LBQ0
B	399	GLY	-	expression tag	UNP A5LBQ0
B	400	SER	-	expression tag	UNP A5LBQ0
B	401	SER	-	expression tag	UNP A5LBQ0
B	402	HIS	-	expression tag	UNP A5LBQ0
B	403	HIS	-	expression tag	UNP A5LBQ0
B	404	HIS	-	expression tag	UNP A5LBQ0
B	405	HIS	-	expression tag	UNP A5LBQ0
B	406	HIS	-	expression tag	UNP A5LBQ0
B	407	HIS	-	expression tag	UNP A5LBQ0
B	408	SER	-	expression tag	UNP A5LBQ0
B	409	SER	-	expression tag	UNP A5LBQ0
B	410	GLY	-	expression tag	UNP A5LBQ0
B	411	LEU	-	expression tag	UNP A5LBQ0
B	412	VAL	-	expression tag	UNP A5LBQ0
B	413	PRO	-	expression tag	UNP A5LBQ0
B	414	ARG	-	expression tag	UNP A5LBQ0
B	415	GLY	-	expression tag	UNP A5LBQ0
B	416	SER	-	expression tag	UNP A5LBQ0
B	417	HIS	-	expression tag	UNP A5LBQ0
B	418	MET	-	expression tag	UNP A5LBQ0
B	419	ALA	-	expression tag	UNP A5LBQ0
B	420	SER	-	expression tag	UNP A5LBQ0
B	746	SER	GLU	conflict	UNP A5LBQ0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	36	20	1	15	0	0	0
3	D	3	36	20	1	15	0	0	0

- Molecule 4 is water.

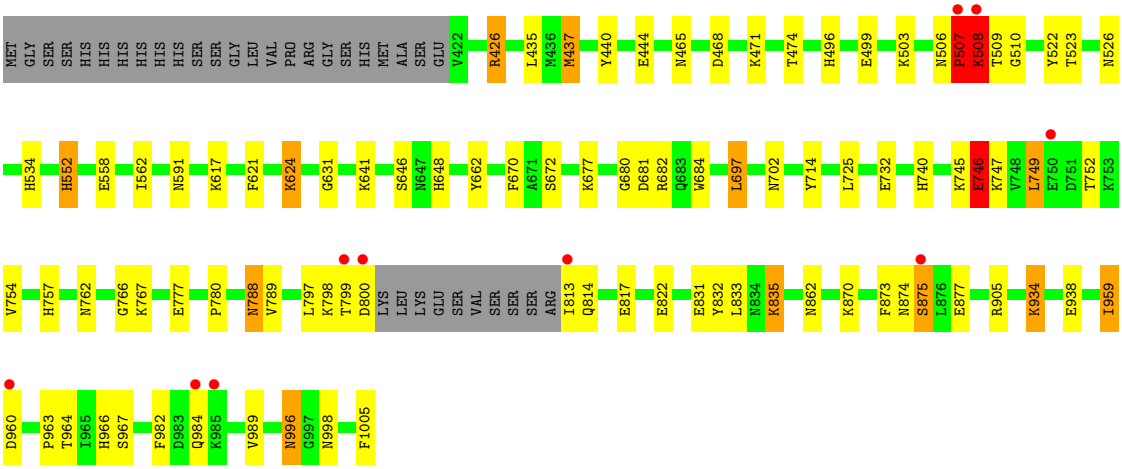
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	478	478	478	0	0
			Total	O		
4	B	546	546	546	0	0

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.

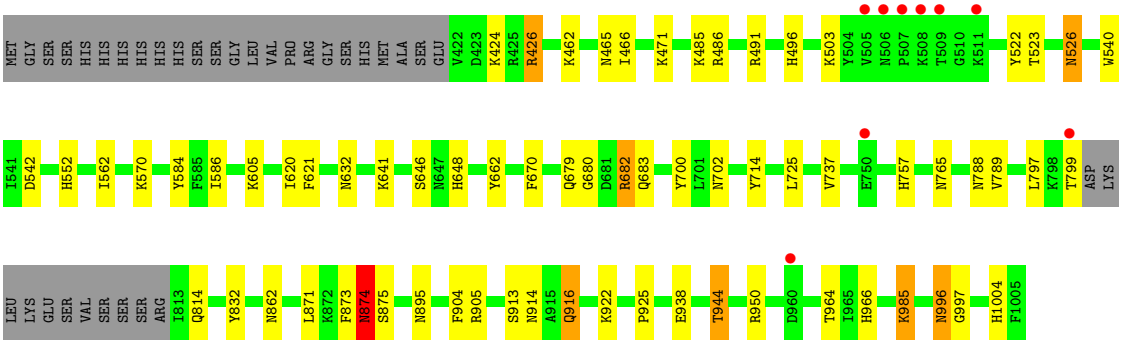
• Molecule 1: FUCOLECTIN-RELATED PROTEIN

Chain A:

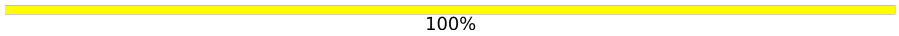


• Molecule 2: FUCOLECTIN-RELATED PROTEIN

Chain B:



• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain C: 

• Molecule 3: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.72Å 153.80Å 91.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.46 – 1.90 38.45 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (38.46-1.90) 96.7 (38.45-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.206 0.165 , 0.206	Depositor DCC
R_{free} test set	5245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.4	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	0.96	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3574e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: A2G, FUC, 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	0.88	2/4813 (0.0%)	0.79	6/6520 (0.1%)
2	B	0.90	0/4802	0.80	10/6505 (0.2%)
All	All	0.89	2/9615 (0.0%)	0.79	16/13025 (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
1	A	0	3
2	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	TYR	CD1-CE1	5.15	1.47	1.39
1	A	746	GLU	CG-CD	5.15	1.59	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	426	ARG	NE-CZ-NH2	-11.69	114.45	120.30
2	B	426	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	426	ARG	NE-CZ-NH2	-9.25	115.68	120.30
2	B	486	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	B	682	ARG	NE-CZ-NH1	-8.93	115.83	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	507	PRO	Peptide
1	A	799	THR	Peptide
1	A	874	ASN	Peptide
2	B	874	ASN	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	4681	0	4522	69	0
2	B	4670	0	4517	50	0
3	C	36	0	32	0	0
3	D	36	0	32	0	0
4	A	478	0	0	15	4
4	B	546	0	0	11	4
All	All	10447	0	9103	119	4

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 6.

The worst 5 of 119 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:905:ARG:H	1:A:996:ASN:HD21	1.20	0.88
1:A:1005:PHE:HB2	4:A:3430:HOH:O	1.78	0.83
1:A:670:PHE:H	1:A:862:ASN:HD21	1.26	0.83
1:A:762:ASN:ND2	4:A:3274:HOH:O	2.13	0.81
1:A:757:HIS:HE1	1:A:797:LEU:O	1.64	0.80

All (4) 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)
4:A:3287:HOH:O	4:B:3058:HOH:O[3_554]	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3286:HOH:O	4:B:3058:HOH:O[3_554]	1.81	0.39
4:A:3288:HOH:O	4:B:3058:HOH:O[3_554]	1.92	0.28
4:A:3456:HOH:O	4:B:3510:HOH:O[2_564]	2.00	0.20

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	568/606 (94%)	540 (95%)	23 (4%)	5 (1%)	17 7
2	B	567/606 (94%)	546 (96%)	20 (4%)	1 (0%)	47 38
All	All	1135/1212 (94%)	1086 (96%)	43 (4%)	6 (0%)	29 18

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	PRO
1	A	508	LYS
1	A	591	ASN
2	B	562	ILE
1	A	875	SER

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	502/532 (94%)	483 (96%)	19 (4%)	33 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	501/532 (94%)	493 (98%)	8 (2%)	62	60
All	All	1003/1064 (94%)	976 (97%)	27 (3%)	44	38

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	934	LYS
1	A	996	ASN
2	B	944	THR
1	A	967	SER
1	A	998	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	581	ASN
2	B	757	HIS
2	B	618	ASN
2	B	683	GLN
2	B	788	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)

6 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	GAL	C	1	3	12,12,12	0.88	0	17,17,17	1.33	1 (5%)
3	FUC	C	2	3	10,10,11	0.91	1 (10%)	14,14,16	1.14	0
3	A2G	C	3	3	14,14,15	1.35	3 (21%)	17,19,21	0.84	1 (5%)
3	GAL	D	1	3	12,12,12	0.83	0	17,17,17	1.32	1 (5%)
3	FUC	D	2	3	10,10,11	0.81	0	14,14,16	0.97	0
3	A2G	D	3	3	14,14,15	1.21	2 (14%)	17,19,21	0.78	1 (5%)

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	GAL	C	1	3	-	2/2/22/22	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	A2G	C	3	3	-	0/6/23/26	0/1/1/1
3	GAL	D	1	3	-	0/2/22/22	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	A2G	D	3	3	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	A2G	O5-C5	2.90	1.49	1.43
3	C	3	A2G	C8-C7	2.64	1.56	1.50
3	D	3	A2G	C8-C7	2.35	1.55	1.50
3	C	2	FUC	O5-C1	-2.29	1.40	1.43
3	D	3	A2G	C1-C2	2.26	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	GAL	O1-C1-O5	-3.56	99.71	110.38
3	D	1	GAL	O1-C1-O5	-3.49	99.91	110.38
3	C	3	A2G	C2-N2-C7	-2.17	119.81	122.90
3	D	3	A2G	O5-C5-C6	2.15	110.58	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

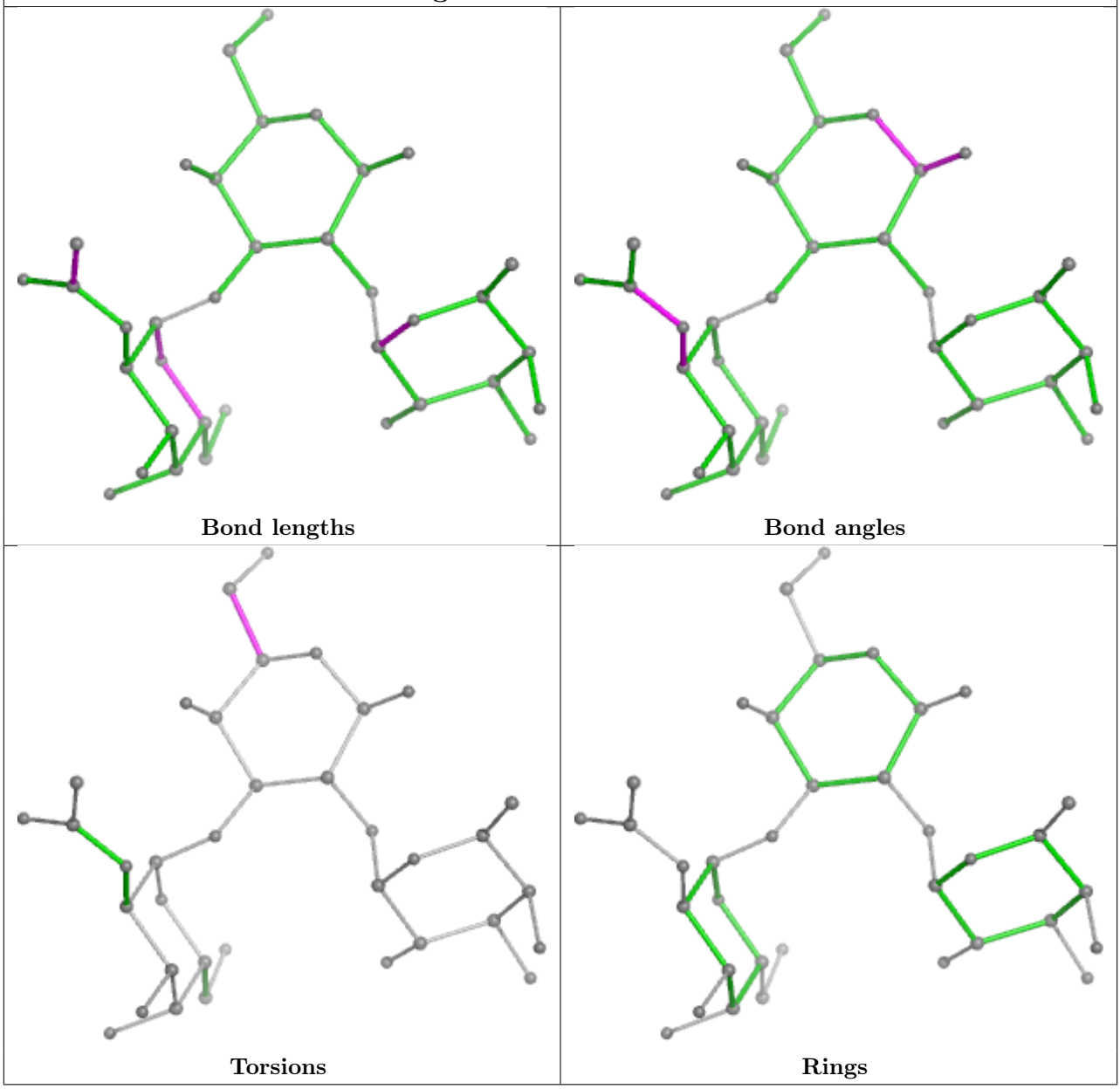
Mol	Chain	Res	Type	Atoms
3	C	1	GAL	C4-C5-C6-O6
3	C	1	GAL	O5-C5-C6-O6

There are no ring outliers.

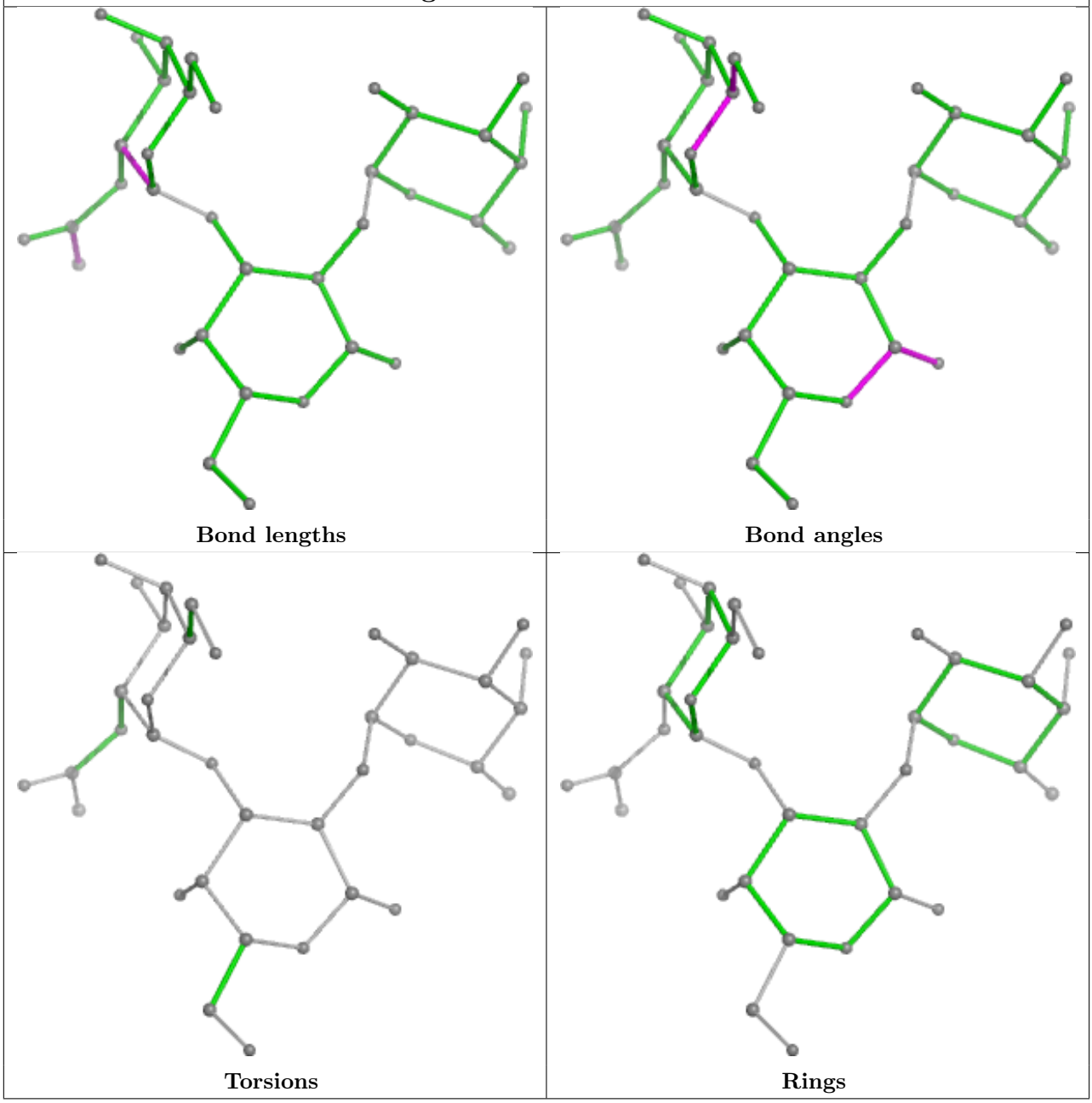
No monomer is involved in short contacts.

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



Oligosaccharide Chain D



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	A	572/606 (94%)	-0.28	10 (1%)	70	72	7, 14, 32, 51	0
2	B	571/606 (94%)	-0.31	9 (1%)	72	74	6, 13, 28, 51	0
All	All	1143/1212 (94%)	-0.29	19 (1%)	70	72	6, 13, 30, 51	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	799	THR	5.2
1	A	800	ASP	4.6
1	A	508	LYS	4.6
2	B	507	PRO	4.3
2	B	508	LYS	4.1

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GAL	C	1	12/12	0.96	0.09	7,9,19,23	0
3	GAL	D	1	12/12	0.96	0.08	8,10,15,18	0
3	A2G	C	3	14/15	0.97	0.09	9,11,20,23	0
3	FUC	D	2	10/11	0.98	0.11	7,9,11,11	0
3	A2G	D	3	14/15	0.98	0.09	7,8,17,20	0

Continued on next page...

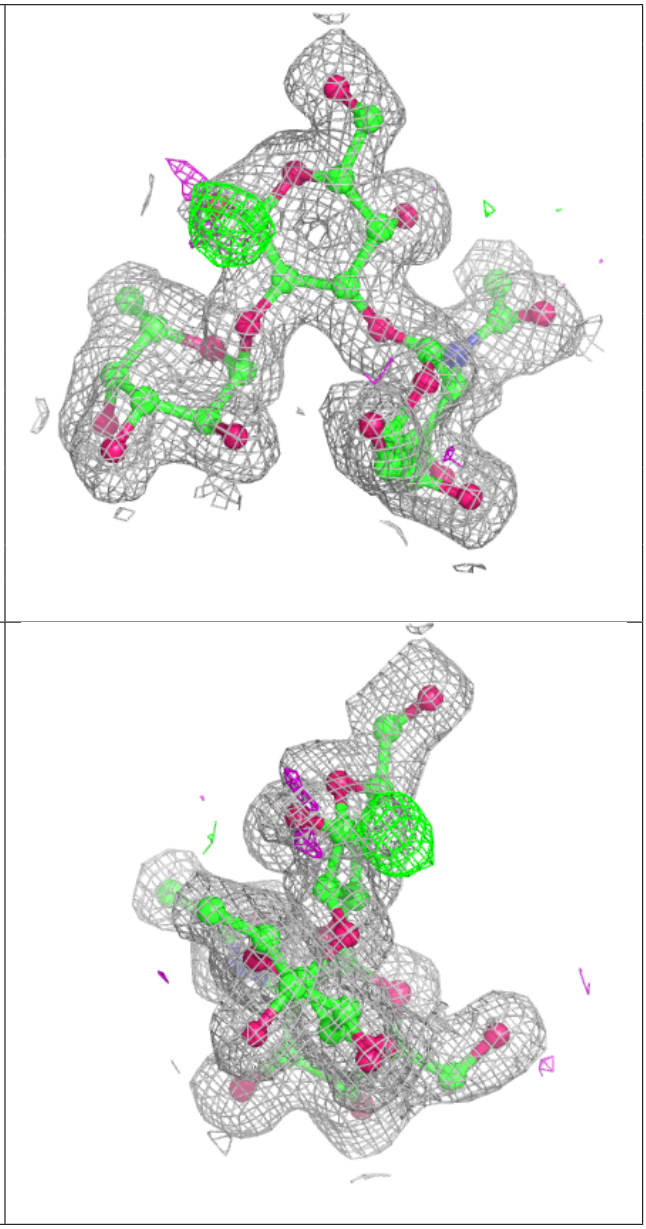
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	C	2	10/11	0.99	0.10	6,9,12,13	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.

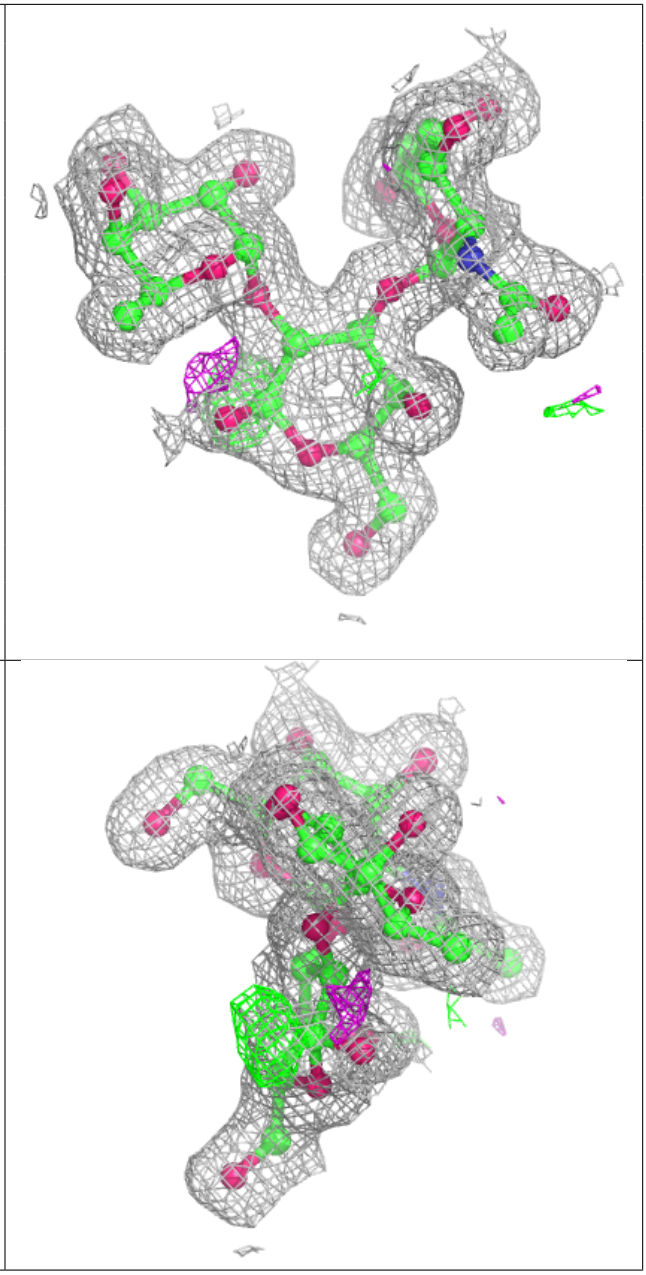
Electron density around Chain C:

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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.