Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:54 AM BST

PDB ID	:	3WPB
Title	:	Crystal structure of horse TLR9 (unliganded form)
Authors	:	Ohto, U.; Tanji, H.; Shimizu, T.
Deposited on	:	2014-01-11
Resolution	:	2.40 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:

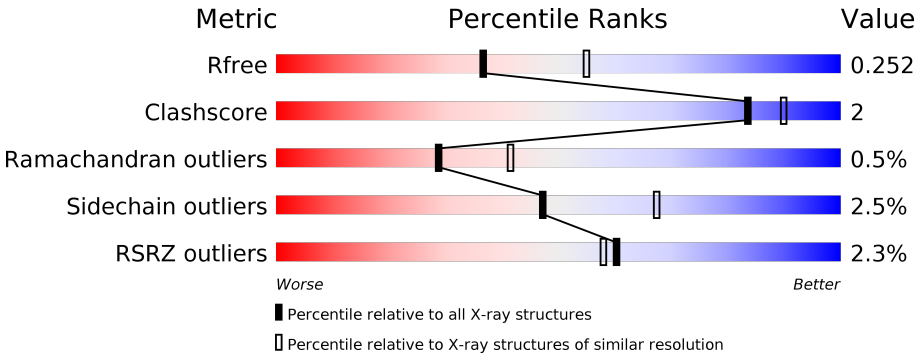
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	802	2% 85% 8% 6%
2	B	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6087 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 Toll-like receptor 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	16	0	0
			5909	3777	1040	1063	29			

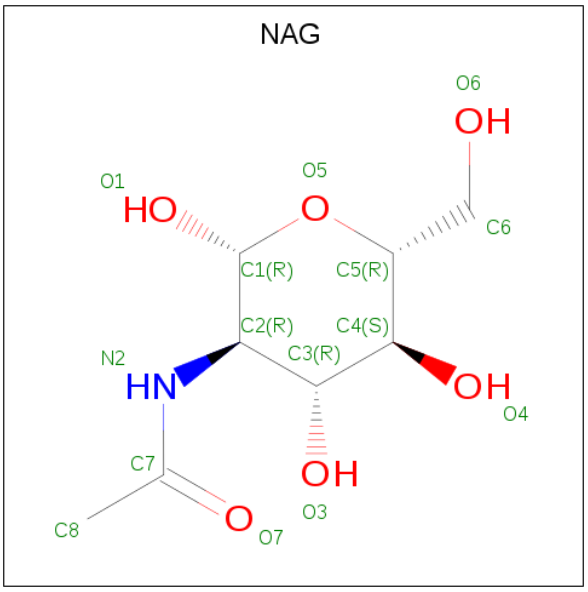
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q2EEY0
A	23	SER	-	expression tag	UNP Q2EEY0
A	24	PRO	-	expression tag	UNP Q2EEY0
A	25	TRP	-	expression tag	UNP Q2EEY0
A	818	GLU	-	expression tag	UNP Q2EEY0
A	819	PHE	-	expression tag	UNP Q2EEY0
A	820	LEU	-	expression tag	UNP Q2EEY0
A	821	VAL	-	expression tag	UNP Q2EEY0
A	822	PRO	-	expression tag	UNP Q2EEY0
A	823	ARG	-	expression tag	UNP Q2EEY0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

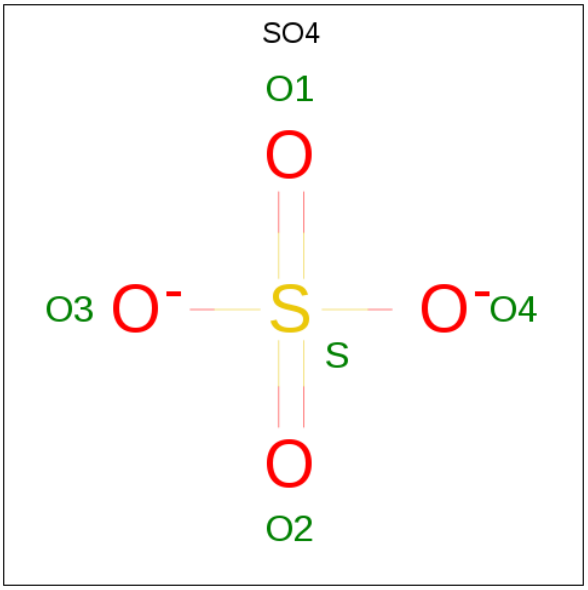
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

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



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

- Molecule 5 is water.

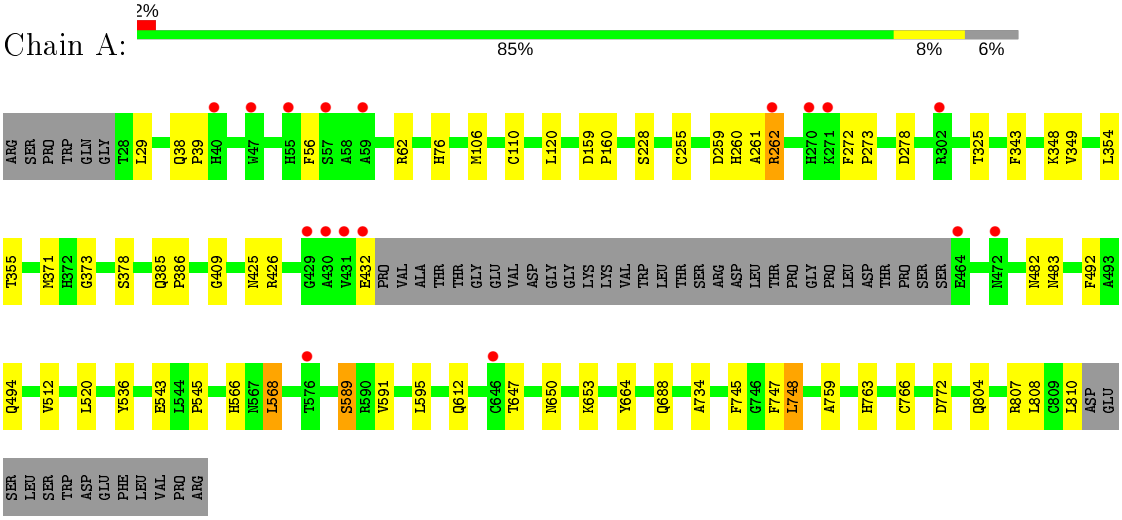
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	112	Total O 112 112	0	0

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.

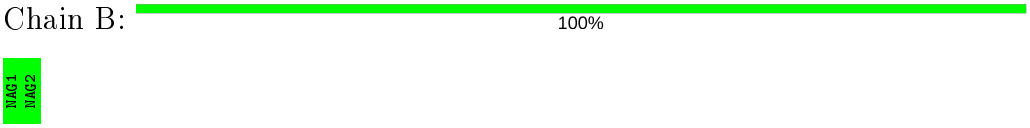
• Molecule 1: Toll-like receptor 9

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 118.84Å 77.75Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	36.85 – 2.40 36.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.85-2.40) 100.0 (36.67-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.197 , 0.250 0.201 , 0.252	Depositor DCC
R_{free} test set	1675 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.010 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: NAG, SO4

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	0.38	1/6048 (0.0%)	0.61	2/8228 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	804	GLN	CA-CB	-7.26	1.38	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	GLU	CB-CA-C	-5.47	99.47	110.40
1	A	804	GLN	N-CA-CB	5.13	119.83	110.60

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	5909	0	5941	28	0
2	B	28	0	25	0	0
3	A	28	0	26	1	0
4	A	10	0	0	1	0
5	A	112	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6087	0	5992	29	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 2.

All (29) 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:56:PHE:O	1:A:62:ARG:NH1	2.20	0.74
1:A:261:ALA:HA	1:A:262:ARG:HB2	1.73	0.70
1:A:492:PHE:HB3	1:A:520:LEU:HD21	1.81	0.62
1:A:745:PHE:O	1:A:747:PHE:O	2.19	0.60
1:A:536:TYR:H	1:A:566:HIS:HD2	1.51	0.57
1:A:747:PHE:O	1:A:748:LEU:HB2	2.06	0.56
1:A:568:LEU:HD22	1:A:591:VAL:CG2	2.37	0.55
3:A:902:NAG:H61	4:A:905:SO4:O2	2.09	0.52
1:A:278:ASP:OD1	1:A:278:ASP:N	2.44	0.50
1:A:747:PHE:O	1:A:748:LEU:CB	2.59	0.50
1:A:409:GLY:HA2	1:A:494:GLN:HB2	1.96	0.48
1:A:259:ASP:OD2	1:A:260:HIS:HD2	1.98	0.47
1:A:385:GLN:HB3	1:A:386:PRO:HD3	1.98	0.46
1:A:38:GLN:HB3	1:A:39:PRO:CD	2.46	0.45
1:A:425:ASN:O	1:A:482:ASN:HA	2.17	0.45
1:A:426:ARG:HD2	1:A:483:ASN:ND2	2.32	0.45
1:A:272:PHE:HB3	1:A:273:PRO:HA	1.99	0.44
1:A:664:TYR:HA	1:A:688:GLN:OE1	2.18	0.44
1:A:354:LEU:HD21	1:A:371:MET:CE	2.48	0.43
1:A:568:LEU:HD23	1:A:595:LEU:HD21	2.01	0.43
1:A:543:GLU:O	1:A:545:PRO:HD3	2.20	0.42
1:A:343:PHE:HA	1:A:373:GLY:O	2.18	0.42
1:A:76:HIS:CD2	1:A:110:CYS:SG	3.13	0.41
1:A:734:ALA:HA	1:A:759:ALA:O	2.20	0.41
1:A:325:THR:HA	1:A:355:THR:O	2.21	0.41
1:A:512:VAL:O	1:A:512:VAL:HG23	2.21	0.41
1:A:536:TYR:H	1:A:566:HIS:CD2	2.35	0.40
1:A:159:ASP:HB2	1:A:160:PRO:CD	2.51	0.40
1:A:29:LEU:HD21	1:A:810:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	748/802 (93%)	696 (93%)	48 (6%)	4 (0%)	29 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ARG
1	A	589	SER
1	A	748	LEU
1	A	349	VAL

5.3.2 Protein sidechains

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	668/712 (94%)	651 (98%)	17 (2%)	47 67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	MET
1	A	120	LEU
1	A	228	SER
1	A	255	CYS
1	A	348	LYS
1	A	378	SER
1	A	568	LEU

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Mol	Chain	Res	Type
1	A	589	SER
1	A	612	GLN
1	A	647	THR
1	A	650	ASN
1	A	653	LYS
1	A	763	HIS
1	A	766	CYS
1	A	772	ASP
1	A	807	ARG
1	A	808	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	111	HIS
1	A	117	ASN
1	A	260	HIS
1	A	309	ASN
1	A	566	HIS
1	A	585	ASN
1	A	588	HIS
1	A	650	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)

2 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	NAG	B	1	1,2	14,14,15	0.48	0	17,19,21	0.83	0
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	0.94	0

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

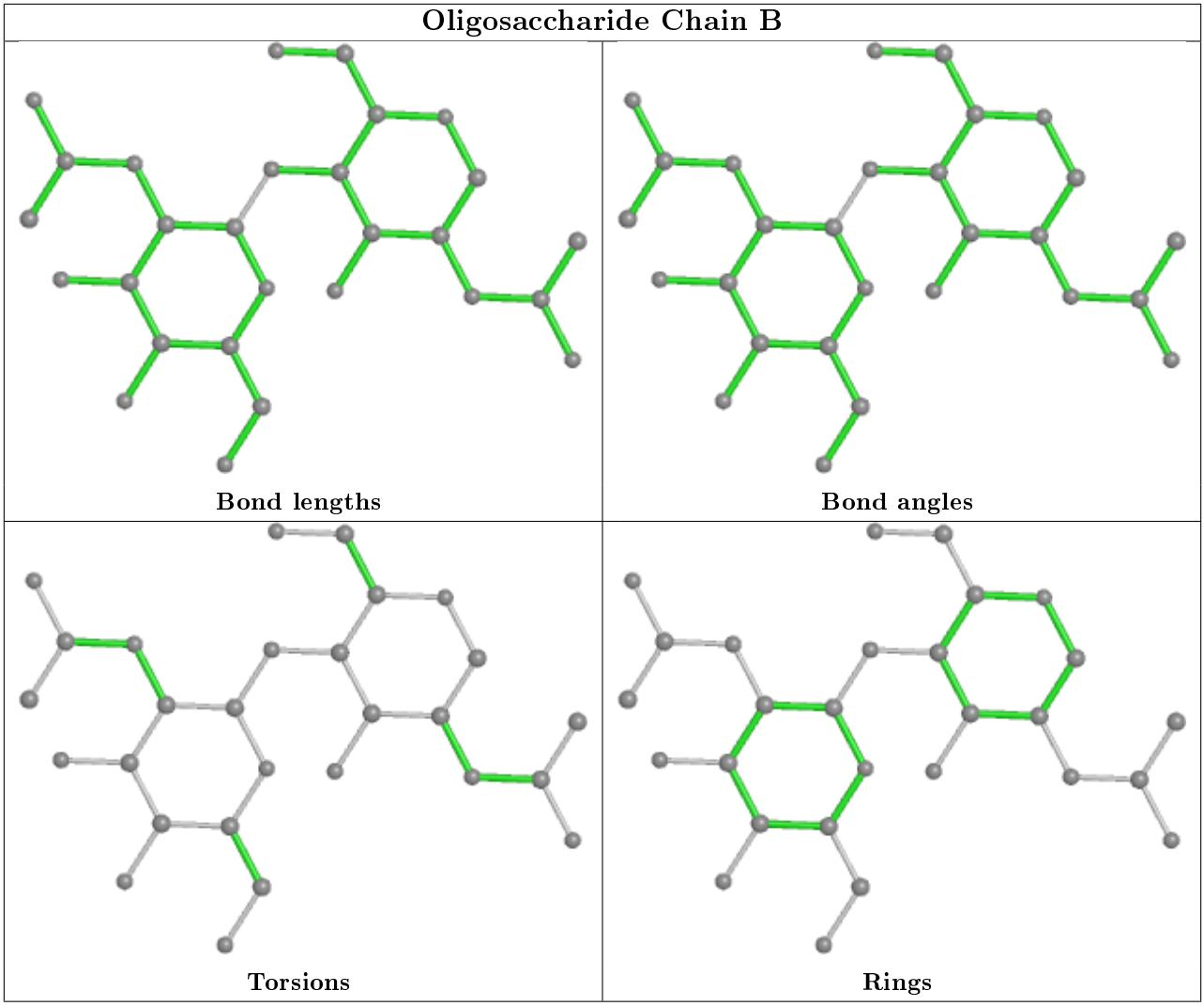
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry (i)

4 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	A	905	-	4,4,4	0.26	0	6,6,6	0.13	0
4	SO4	A	906	-	4,4,4	0.29	0	6,6,6	0.30	0
3	NAG	A	901	1	14,14,15	0.55	0	17,19,21	0.81	0
3	NAG	A	902	1	14,14,15	0.44	0	17,19,21	2.43	3 (17%)

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	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	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	A	902	NAG	C1-O5-C5	8.36	123.52	112.19
3	A	902	NAG	C4-C3-C2	-3.77	105.49	111.02
3	A	902	NAG	O7-C7-C8	-2.28	117.82	122.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	NAG	C4-C5-C6-O6
3	A	901	NAG	O5-C5-C6-O6
3	A	901	NAG	C4-C5-C6-O6
3	A	902	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	905	SO4	1	0
3	A	902	NAG	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

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	752/802 (93%)	-0.19	17 (2%) 60 58	13, 27, 53, 115	6 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	9.0
1	A	270	HIS	5.0
1	A	432	GLU	4.2
1	A	430	ALA	3.7
1	A	646	CYS	3.5
1	A	576	THR	2.9
1	A	59	ALA	2.8
1	A	429	GLY	2.8
1	A	262	ARG	2.8
1	A	40	HIS	2.4
1	A	464	GLU	2.3
1	A	55	HIS	2.3
1	A	47	TRP	2.3
1	A	57	SER	2.2
1	A	472	ASN	2.1
1	A	271	LYS	2.1
1	A	302	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

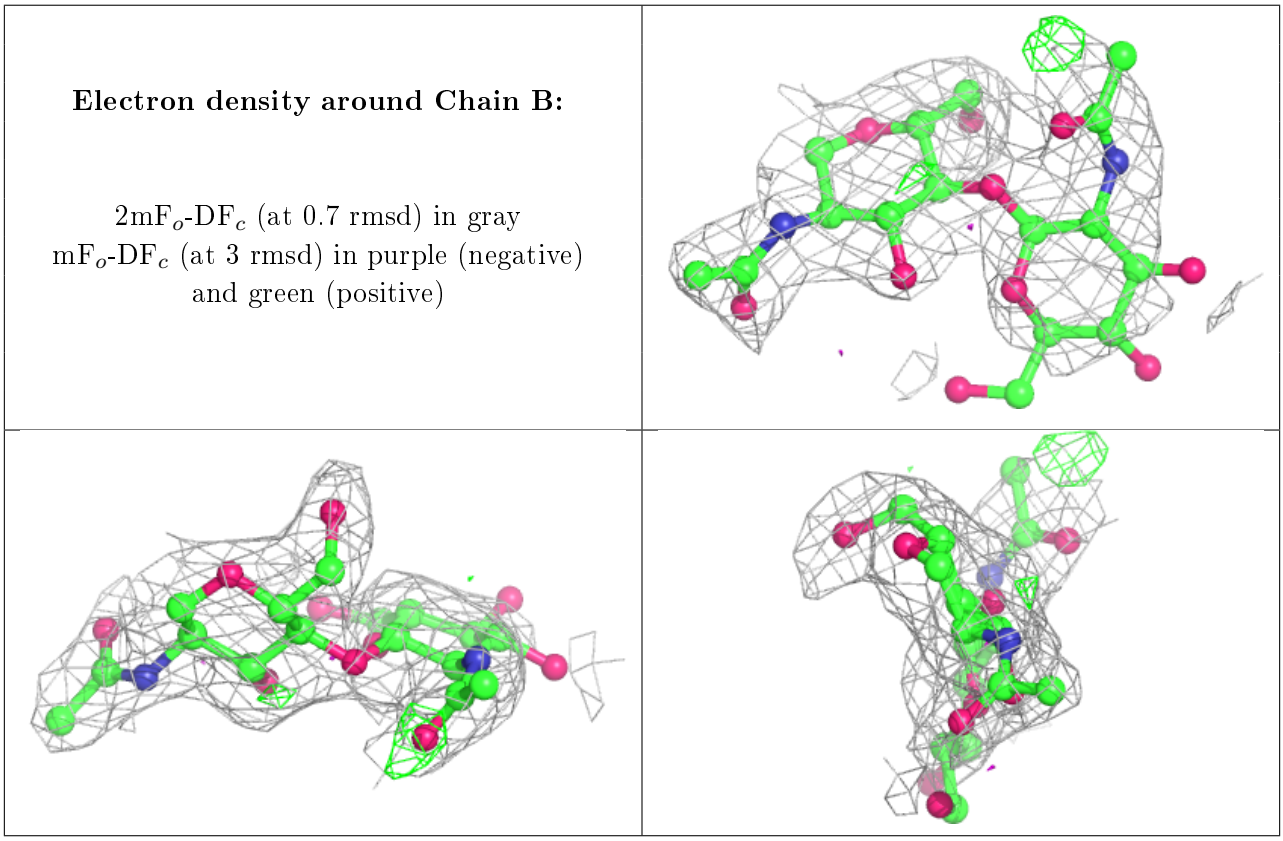
6.3 Carbohydrates

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
2	NAG	B	2	14/15	0.81	0.33	57,67,78,78	0
2	NAG	B	1	14/15	0.90	0.14	35,40,45,53	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.



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
3	NAG	A	901	14/15	0.91	0.16	39,41,43,45	0
3	NAG	A	902	14/15	0.95	0.15	30,34,38,41	0
4	SO4	A	906	5/5	0.97	0.12	38,40,43,44	0
4	SO4	A	905	5/5	0.98	0.14	43,43,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.