wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 08:23 am GMT

PDB ID	:	5IIC
Title	:	Crystal structure of red abalone VERL repeat 3 at 2.9 A resolution
Authors	:	Sadat Al-Hosseini, H.; Raj, I.; Nishimura, K.; Jovine, L.
Deposited on	:	2016-03-01
Resolution	:	2.90 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:

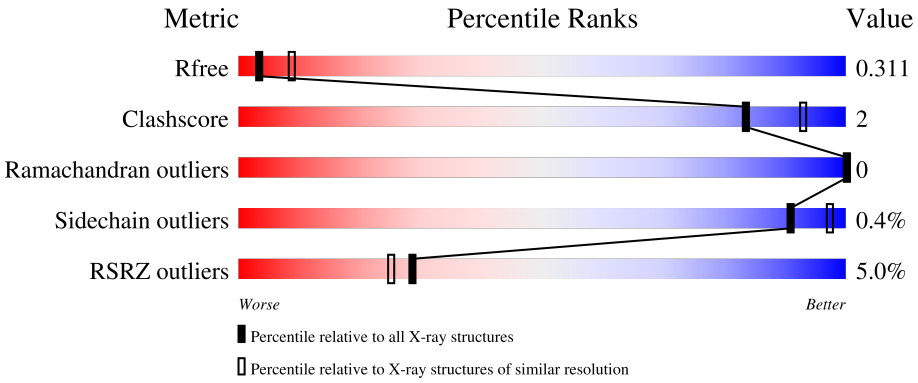
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	496	3% 88% 7% 5%
1	B	496	7% 88% 6% 6%
2	C	2	100%
2	D	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14603 atoms, of which 7243 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 Maltose-binding periplasmic protein,Vitelline envelope sperm lysin receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	H	N	O	S	0	0	0
			7244	2349	3596	593	692	14			
1	B	467	Total	C	H	N	O	S	0	0	0
			7159	2322	3549	588	686	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3966	GLU	-	expression tag	UNP P0AEX9
A	3967	THR	-	expression tag	UNP P0AEX9
A	3968	GLY	-	expression tag	UNP P0AEX9
A	3969	THR	-	expression tag	UNP P0AEX9
A	4051	ALA	ASP	engineered mutation	UNP P0AEX9
A	4052	ALA	LYS	engineered mutation	UNP P0AEX9
A	4141	ALA	GLU	engineered mutation	UNP P0AEX9
A	4142	ALA	ASN	engineered mutation	UNP P0AEX9
A	4184	HIS	ALA	engineered mutation	UNP P0AEX9
A	4188	HIS	LYS	engineered mutation	UNP P0AEX9
A	4208	ALA	LYS	engineered mutation	UNP P0AEX9
A	4281	VAL	ALA	engineered mutation	UNP P0AEX9
A	4286	VAL	ILE	engineered mutation	UNP P0AEX9
A	4328	ALA	GLU	engineered mutation	UNP P0AEX9
A	4331	ALA	LYS	engineered mutation	UNP P0AEX9
A	4332	ALA	ASP	engineered mutation	UNP P0AEX9
A	4336	ASN	ARG	engineered mutation	UNP P0AEX9
A	4337	ALA	-	linker	UNP P0AEX9
A	4338	ALA	-	linker	UNP P0AEX9
A	4339	ALA	-	linker	UNP P0AEX9
A	4454	LEU	-	expression tag	UNP Q8WR62
A	4455	GLU	-	expression tag	UNP Q8WR62
A	4456	HIS	-	expression tag	UNP Q8WR62
A	4457	HIS	-	expression tag	UNP Q8WR62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	4458	HIS	-	expression tag	UNP Q8WR62
A	4459	HIS	-	expression tag	UNP Q8WR62
A	4460	HIS	-	expression tag	UNP Q8WR62
A	4461	HIS	-	expression tag	UNP Q8WR62
B	3966	GLU	-	expression tag	UNP P0AEX9
B	3967	THR	-	expression tag	UNP P0AEX9
B	3968	GLY	-	expression tag	UNP P0AEX9
B	3969	THR	-	expression tag	UNP P0AEX9
B	4051	ALA	ASP	engineered mutation	UNP P0AEX9
B	4052	ALA	LYS	engineered mutation	UNP P0AEX9
B	4141	ALA	GLU	engineered mutation	UNP P0AEX9
B	4142	ALA	ASN	engineered mutation	UNP P0AEX9
B	4184	HIS	ALA	engineered mutation	UNP P0AEX9
B	4188	HIS	LYS	engineered mutation	UNP P0AEX9
B	4208	ALA	LYS	engineered mutation	UNP P0AEX9
B	4281	VAL	ALA	engineered mutation	UNP P0AEX9
B	4286	VAL	ILE	engineered mutation	UNP P0AEX9
B	4328	ALA	GLU	engineered mutation	UNP P0AEX9
B	4331	ALA	LYS	engineered mutation	UNP P0AEX9
B	4332	ALA	ASP	engineered mutation	UNP P0AEX9
B	4336	ASN	ARG	engineered mutation	UNP P0AEX9
B	4337	ALA	-	linker	UNP P0AEX9
B	4338	ALA	-	linker	UNP P0AEX9
B	4339	ALA	-	linker	UNP P0AEX9
B	4454	LEU	-	expression tag	UNP Q8WR62
B	4455	GLU	-	expression tag	UNP Q8WR62
B	4456	HIS	-	expression tag	UNP Q8WR62
B	4457	HIS	-	expression tag	UNP Q8WR62
B	4458	HIS	-	expression tag	UNP Q8WR62
B	4459	HIS	-	expression tag	UNP Q8WR62
B	4460	HIS	-	expression tag	UNP Q8WR62
B	4461	HIS	-	expression tag	UNP Q8WR62

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

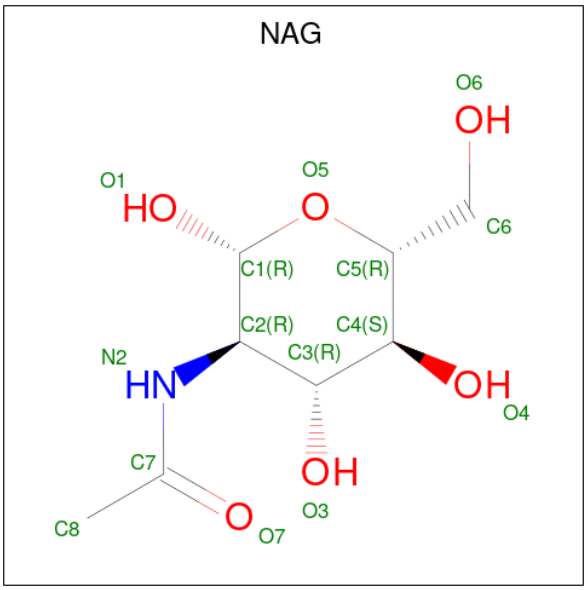
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			44	12	21	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total 44	C 12	H 21	O 11	0	0	0

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



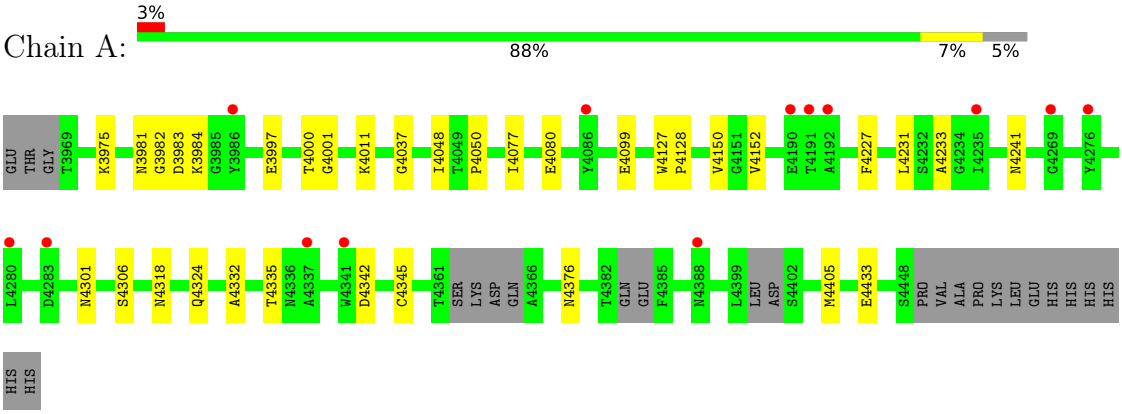
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
3	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
3	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
3	B	1	Total 28	C 8	H 14	N 1	O 5	0	0

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.

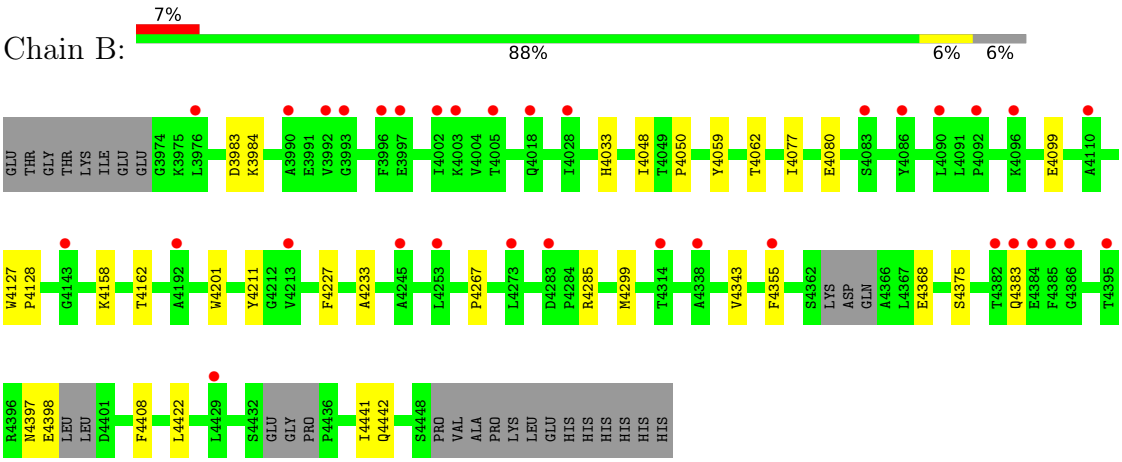
• Molecule 1: Maltose-binding periplasmic protein,Vitelline envelope sperm lysin receptor

Chain A:



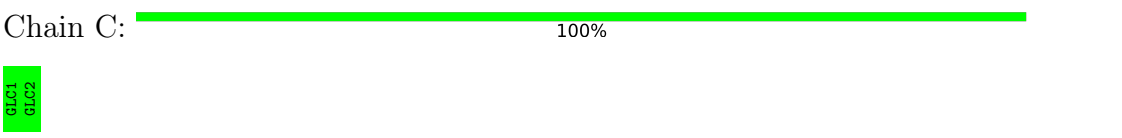
• Molecule 1: Maltose-binding periplasmic protein,Vitelline envelope sperm lysin receptor

Chain B:



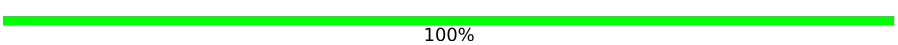
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:




CL2
CL1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.33Å 81.64Å 111.63Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	47.02 – 2.90 47.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.02-2.90) 85.4 (47.81-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.251 , 0.310 0.254 , 0.311	Depositor DCC
R_{free} test set	1192 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.6	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	0.91	EDS
Total number of atoms	14603	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, GLC

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	0.25	0/3738	0.41	0/5086
1	B	0.25	0/3699	0.41	0/5032
All	All	0.25	0/7437	0.41	0/10118

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3648	3596	3596	19	0
1	B	3610	3549	3550	16	0
2	C	23	21	21	0	0
2	D	23	21	21	0	0
3	A	28	28	26	0	0
3	B	28	28	26	0	0
All	All	7360	7243	7240	35	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.

The worst 5 of 35 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:B:3984:LYS:NZ	1:B:4080:GLU:OE2	2.22	0.72
1:A:4011:LYS:NZ	1:A:4345:CYS:O	2.22	0.72
1:A:3984:LYS:NZ	1:A:4080:GLU:OE2	2.35	0.60
1:A:4433:GLU:N	1:A:4433:GLU:OE1	2.35	0.60
1:A:4376:ASN:ND2	1:A:4405:MET:O	2.35	0.58

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/496 (94%)	457 (98%)	7 (2%)	0	100	100
1	B	459/496 (92%)	448 (98%)	11 (2%)	0	100	100
All	All	923/992 (93%)	905 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	382/404 (95%)	381 (100%)	1 (0%)	92	98
1	B	378/404 (94%)	376 (100%)	2 (0%)	88	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	760/808 (94%)	757 (100%)	3 (0%)	91 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4227	PHE
1	B	4227	PHE
1	B	4355	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	GLC	C	1	2	12,12,12	0.53	0	17,17,17	0.44	0
2	GLC	C	2	2	11,11,12	0.61	0	15,15,17	0.80	0
2	GLC	D	1	2	12,12,12	0.54	0	17,17,17	0.52	0
2	GLC	D	2	2	11,11,12	0.62	0	15,15,17	0.60	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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

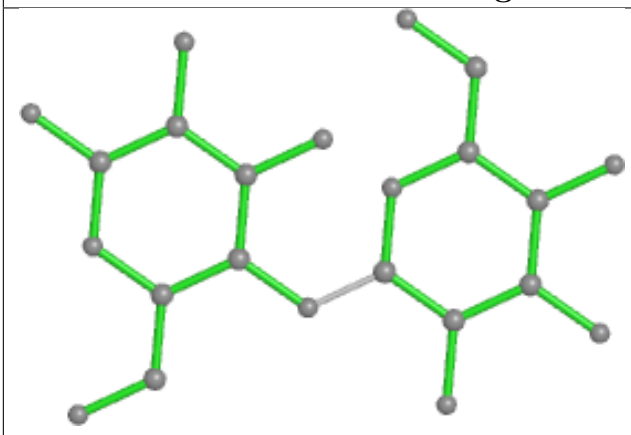
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6

There are no ring outliers.

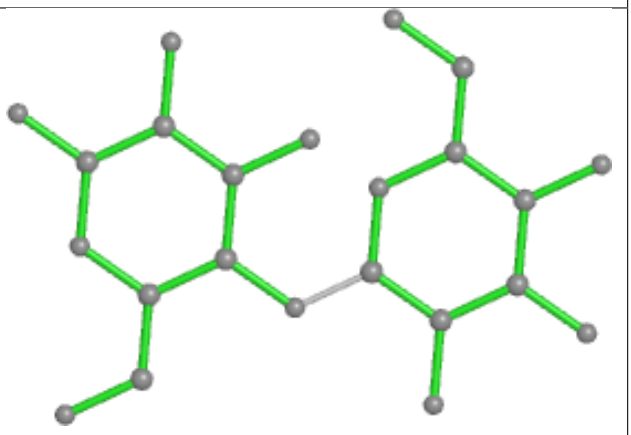
No monomer is involved in short contacts.

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

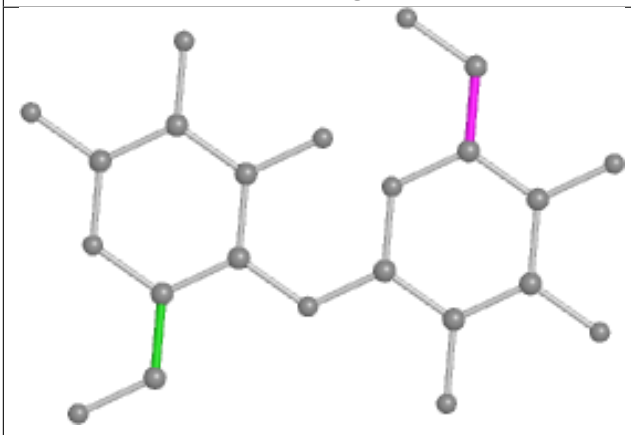
Oligosaccharide Chain C



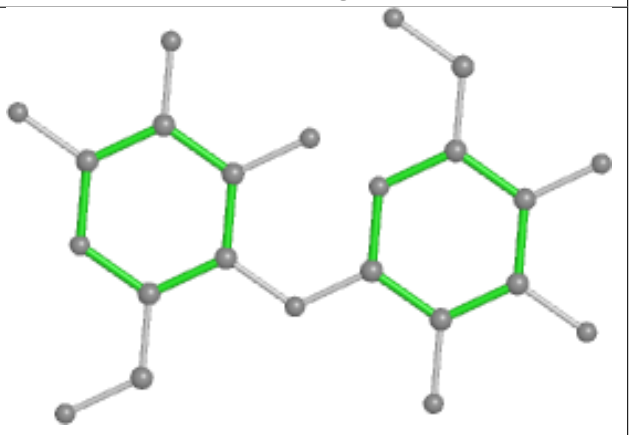
Bond lengths



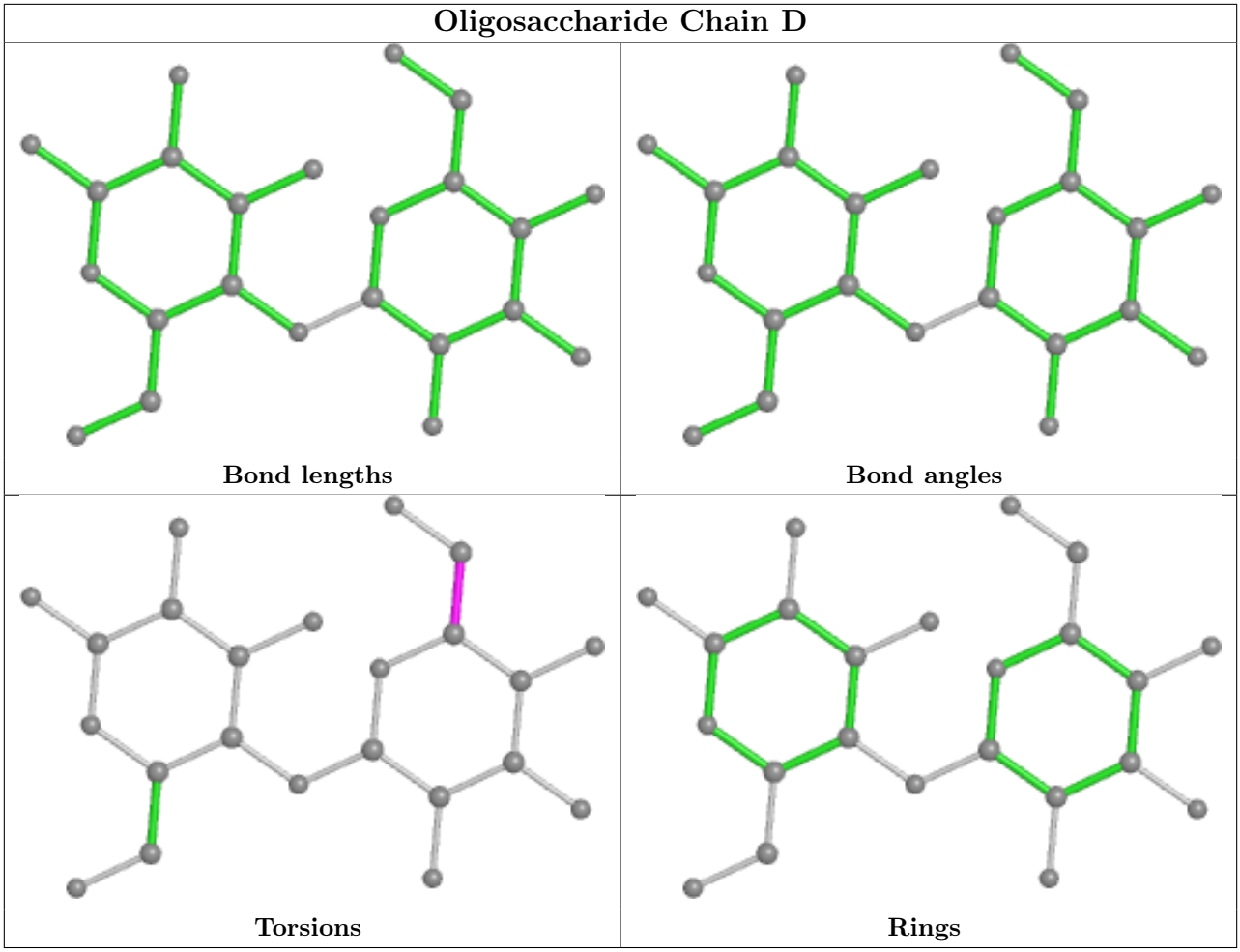
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
3	NAG	B	4502	1	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	B	4503	1	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	A	4502	1	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	A	4503	1	14,14,15	0.27	0	17,19,21	0.76	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	NAG	B	4502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	4503	1	-	2/6/23/26	0/1/1/1
3	NAG	A	4502	1	-	1/6/23/26	0/1/1/1
3	NAG	A	4503	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4503	NAG	C1-O5-C5	2.71	115.87	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4503	NAG	O5-C5-C6-O6
3	B	4503	NAG	C4-C5-C6-O6
3	A	4503	NAG	O5-C5-C6-O6
3	A	4503	NAG	C4-C5-C6-O6
3	A	4503	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	472/496 (95%)	0.39	13 (2%)	53	49	37, 72, 112, 140	0
1	B	467/496 (94%)	0.52	34 (7%)	15	11	42, 77, 121, 164	0
All	All	939/992 (94%)	0.45	47 (5%)	28	25	37, 74, 118, 164	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4383	GLN	5.2
1	B	4395	THR	4.2
1	B	4086	TYR	4.2
1	B	4429	LEU	4.0
1	B	4090	LEU	3.9

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

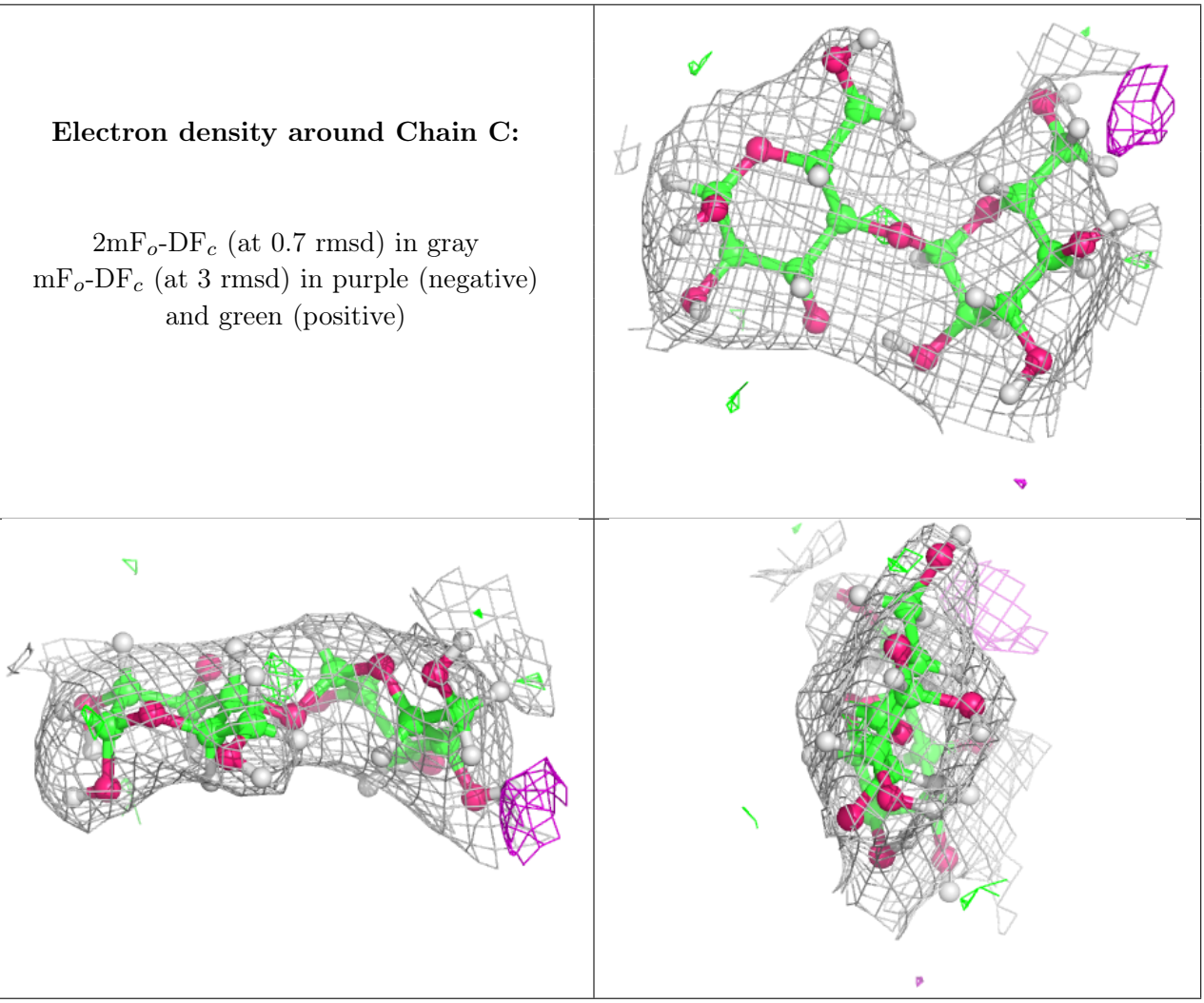
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GLC	D	2	11/12	0.86	0.23	41,51,62,63	0
2	GLC	D	1	12/12	0.93	0.23	46,61,75,77	0
2	GLC	C	1	12/12	0.93	0.18	35,42,50,56	0
2	GLC	C	2	11/12	0.95	0.22	35,52,67,70	0

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

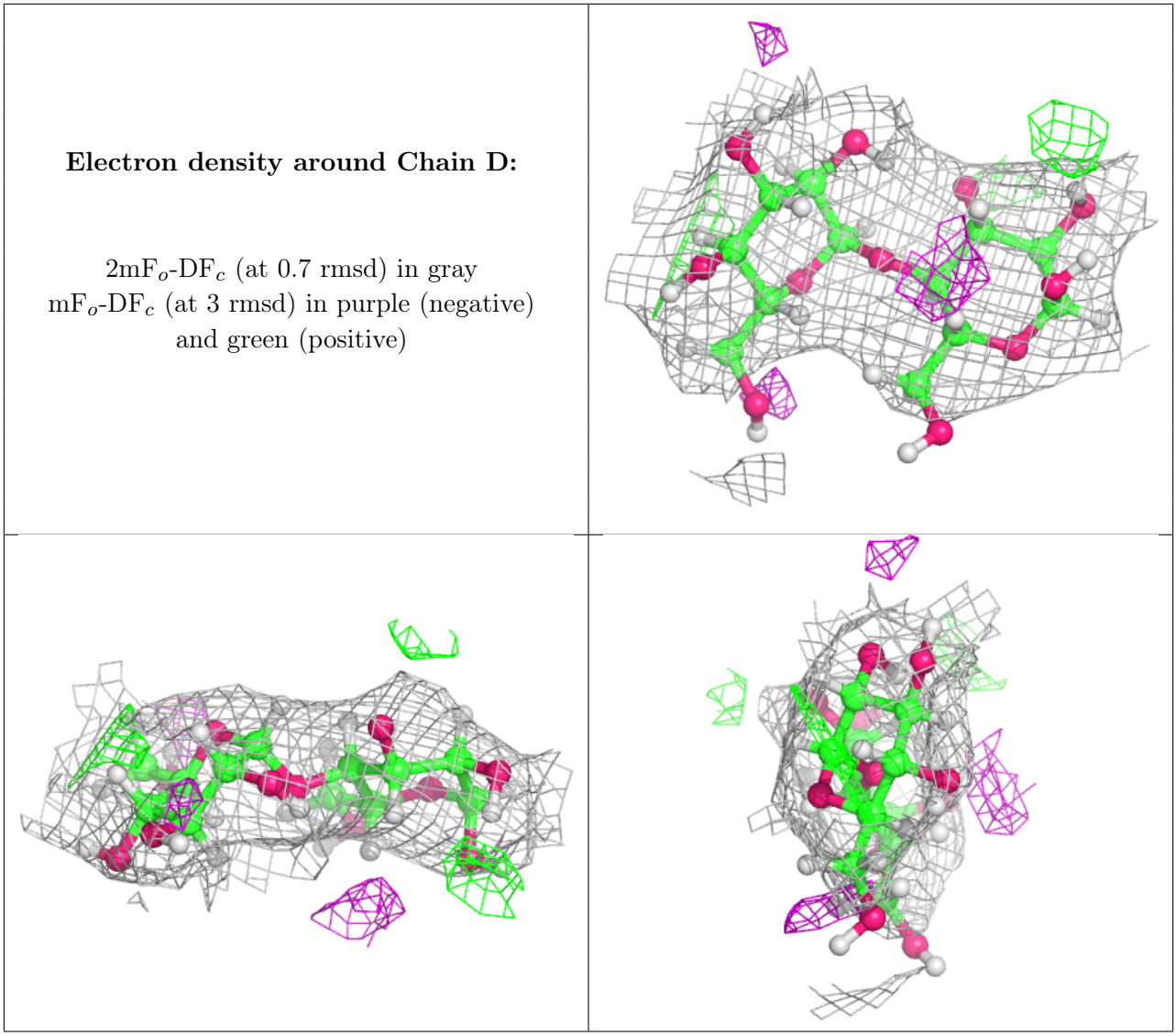
Electron density around Chain C:

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



Electron density around Chain D:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	4503	14/15	0.69	0.32	111,135,170,173	0
3	NAG	A	4502	14/15	0.84	0.17	84,101,117,123	0
3	NAG	B	4503	14/15	0.86	0.25	74,81,96,97	0
3	NAG	B	4502	14/15	0.87	0.24	65,84,101,104	28

6.5 Other polymers (i)

There are no such residues in this entry.