Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 06:07 PM EDT

PDB ID	:	2EBH
Title	:	Crystal structures reveal a thiol-protease like catalytic triad in the C-terminal region of Pasteurella multocida toxin
Authors	:	Kitadokoro, K.; Horiguchi, Y.; Kamitani, S.
Deposited on	:	2007-02-08
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 (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:

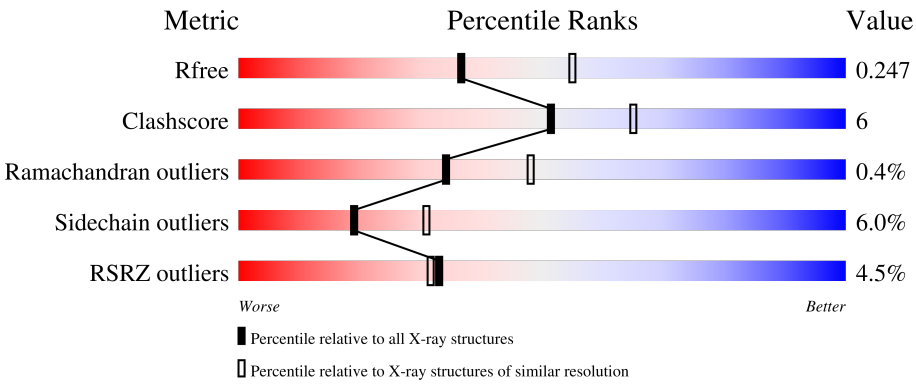
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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 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	X	746	4%, 79%, 15%, • 5%
2	A	2	50%, 50%
2	B	2	50%, 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6060 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 Dermonecrotic toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	711	5643	3603	939	1075	26	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	540	MET	-	cloning artifact	UNP P17452
X	541	GLY	-	cloning artifact	UNP P17452
X	542	HIS	-	expression tag	UNP P17452
X	543	HIS	-	expression tag	UNP P17452
X	544	HIS	-	expression tag	UNP P17452
X	545	HIS	-	expression tag	UNP P17452
X	546	HIS	-	expression tag	UNP P17452
X	547	HIS	-	expression tag	UNP P17452
X	548	ASP	-	cloning artifact	UNP P17452
X	549	TYR	-	cloning artifact	UNP P17452
X	550	ASP	-	cloning artifact	UNP P17452
X	551	ILE	-	cloning artifact	UNP P17452
X	552	PRO	-	cloning artifact	UNP P17452
X	553	THR	-	cloning artifact	UNP P17452
X	554	THR	-	cloning artifact	UNP P17452
X	555	GLU	-	cloning artifact	UNP P17452
X	556	ASN	-	cloning artifact	UNP P17452
X	557	LEU	-	cloning artifact	UNP P17452
X	558	TYR	-	cloning artifact	UNP P17452
X	559	PHE	-	cloning artifact	UNP P17452
X	560	GLN	-	cloning artifact	UNP P17452
X	561	GLY	-	cloning artifact	UNP P17452
X	562	ALA	-	cloning artifact	UNP P17452
X	563	HIS	-	cloning artifact	UNP P17452
X	564	MET	-	cloning artifact	UNP P17452
X	565	GLY	-	cloning artifact	UNP P17452
X	566	ILE	-	cloning artifact	UNP P17452

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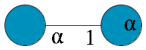
Chain	Residue	Modelled	Actual	Comment	Reference
X	567	GLN	-	cloning artifact	UNP P17452
X	568	ARG	-	cloning artifact	UNP P17452
X	1165	SER	CYS	engineered mutation	UNP P17452

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	A	2	23	12	11	0	0	0
			Total	C	O			
2	B	2	23	12	11	0	0	0

- Molecule 3 is water.

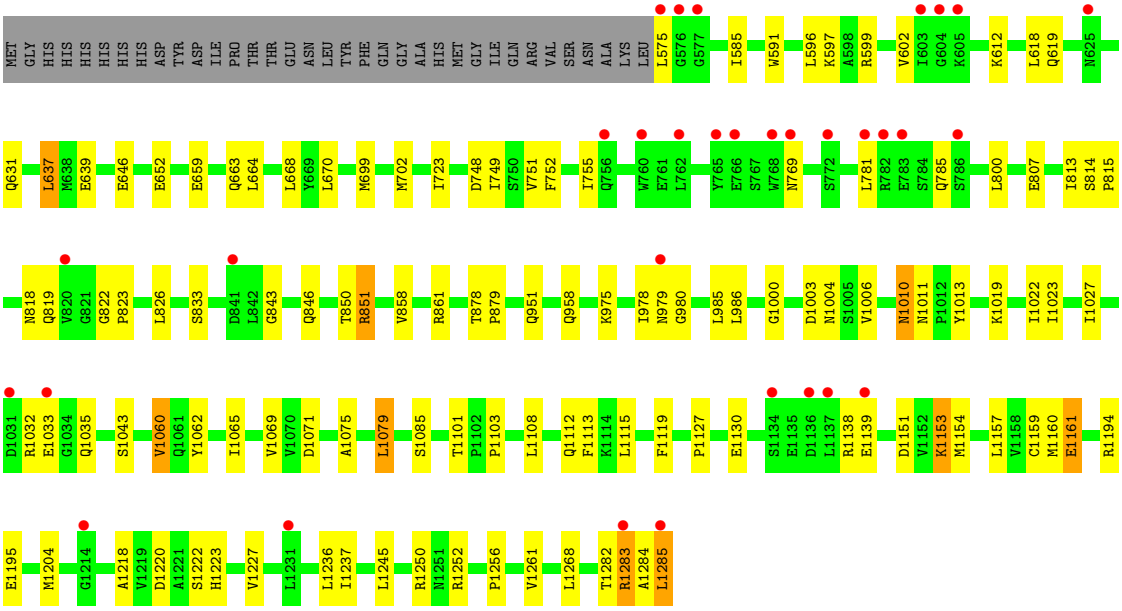
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	X	371	371	371	0	0

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: Dermonecrotic toxin

Chain X:



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

Chain A:

• Molecule 2: alpha-D-glucopyranose-(1-1)-alpha-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	110.75Å 150.56Å 77.91Å 90.00° 104.54° 90.00°	Depositor
Resolution (Å)	43.69 – 2.40 43.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.69-2.40) 98.9 (43.67-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.249 0.211 , 0.247	Depositor DCC
R_{free} test set	2412 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: 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	X	0.39	0/5769	0.53	0/7811

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 (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	X	5643	0	5575	63	0
2	A	23	0	21	0	0
2	B	23	0	21	0	0
3	X	371	0	0	4	0
All	All	6060	0	5617	63	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 6.

All (63) 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:X:1283:ARG:HA	1:X:1284:ALA:HB3	1.59	0.83
1:X:1223:HIS:HD2	1:X:1250:ARG:HH12	1.30	0.80
1:X:1027:ILE:HD11	1:X:1062:TYR:HB3	1.63	0.79
1:X:1283:ARG:HA	1:X:1284:ALA:CB	2.22	0.69
1:X:1119:PHE:HE2	1:X:1227:VAL:CG1	2.08	0.67
1:X:843:GLY:H	1:X:846:GLN:HE21	1.43	0.66
1:X:1119:PHE:HE2	1:X:1227:VAL:HG13	1.59	0.66
1:X:602:VAL:HG21	1:X:652:GLU:HG2	1.79	0.64
1:X:752:PHE:O	1:X:755:ILE:HG12	1.98	0.63
1:X:1060:VAL:HG13	1:X:1065:ILE:O	1.97	0.63
1:X:1119:PHE:CE2	1:X:1227:VAL:HG13	2.32	0.63
1:X:1060:VAL:HG22	1:X:1065:ILE:HG13	1.80	0.63
1:X:1010:ASN:HD22	1:X:1010:ASN:H	1.47	0.60
1:X:1113:PHE:O	1:X:1252:ARG:HA	2.02	0.59
1:X:1069:VAL:HG13	1:X:1079:LEU:HG	1.82	0.59
1:X:1283:ARG:CA	1:X:1284:ALA:HB3	2.31	0.59
1:X:819:GLN:HE21	1:X:822:GLY:HA3	1.67	0.59
1:X:1010:ASN:HD22	1:X:1010:ASN:N	2.01	0.59
1:X:637:LEU:HD13	1:X:664:LEU:HD11	1.85	0.59
1:X:585:ILE:O	1:X:585:ILE:HG22	2.02	0.58
1:X:814:SER:HB2	1:X:815:PRO:HD2	1.87	0.55
1:X:1019:LYS:HG2	1:X:1023:ILE:HD13	1.90	0.54
1:X:1223:HIS:CD2	1:X:1250:ARG:HH12	2.18	0.54
1:X:1032:ARG:HE	1:X:1035:GLN:NE2	2.07	0.53
1:X:1194:ARG:NH1	1:X:1195:GLU:O	2.42	0.52
1:X:807:GLU:HG3	1:X:1006:VAL:HG23	1.91	0.52
1:X:781:LEU:O	1:X:785:GLN:HB2	2.09	0.51
1:X:1010:ASN:H	1:X:1010:ASN:ND2	2.09	0.50
1:X:585:ILE:HD13	3:X:365:HOH:O	2.11	0.49
1:X:749:ILE:HD11	1:X:800:LEU:HB2	1.95	0.49
1:X:1011:ASN:ND2	1:X:1013:TYR:H	2.10	0.49
1:X:619:GLN:HG2	3:X:183:HOH:O	2.13	0.48
1:X:1027:ILE:CD1	1:X:1062:TYR:HB3	2.38	0.48
1:X:1108:LEU:HB2	1:X:1256:PRO:HG2	1.95	0.48
1:X:1127:PRO:HA	1:X:1130:GLU:HG2	1.94	0.48
1:X:639:GLU:OE2	1:X:851:ARG:NH2	2.47	0.48
1:X:878:THR:HB	1:X:879:PRO:HD3	1.96	0.47
1:X:1204:MET:HG3	1:X:1268:LEU:O	2.15	0.47
1:X:1023:ILE:O	1:X:1027:ILE:HG12	2.14	0.47
1:X:1000:GLY:HA2	1:X:1022:ILE:HG12	1.97	0.47
1:X:1282:THR:HG22	1:X:1283:ARG:HD3	1.97	0.47
1:X:843:GLY:H	1:X:846:GLN:NE2	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1284:ALA:HA	1:X:1285:LEU:C	2.37	0.45
1:X:861:ARG:HD3	1:X:1003:ASP:OD1	2.16	0.44
1:X:1223:HIS:HD2	1:X:1250:ARG:NH1	2.06	0.43
1:X:1159:CYS:O	1:X:1222:SER:HA	2.17	0.43
1:X:1159:CYS:SG	1:X:1161:GLU:HB2	2.59	0.43
1:X:1153:LYS:O	1:X:1157:LEU:HG	2.19	0.42
1:X:1101:THR:HG22	3:X:75:HOH:O	2.20	0.42
1:X:1151:ASP:HB3	1:X:1154:MET:HB2	2.02	0.42
1:X:813:ILE:HA	1:X:818:ASN:ND2	2.35	0.41
1:X:1218:ALA:O	1:X:1237:ILE:HA	2.20	0.41
1:X:850:THR:HG21	3:X:171:HOH:O	2.20	0.41
1:X:575:LEU:HD22	1:X:1112:GLN:H	1.86	0.41
1:X:1220:ASP:HB3	1:X:1236:LEU:HB3	2.02	0.41
1:X:699:MET:HA	1:X:702:MET:HE3	2.03	0.41
1:X:748:ASP:O	1:X:751:VAL:HG22	2.21	0.41
1:X:1283:ARG:CA	1:X:1284:ALA:CB	2.93	0.41
1:X:819:GLN:NE2	1:X:823:PRO:HD2	2.36	0.41
1:X:723:ILE:HG12	1:X:858:VAL:HG13	2.03	0.40
1:X:599:ARG:HA	1:X:599:ARG:HD2	1.91	0.40
1:X:591:TRP:H	1:X:663:GLN:NE2	2.20	0.40
1:X:1071:ASP:HB2	1:X:1075:ALA:HB3	2.02	0.40

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	X	709/746 (95%)	685 (97%)	21 (3%)	3 (0%)	34 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	980	GLY
1	X	979	ASN
1	X	1103	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	616/646 (95%)	579 (94%)	37 (6%)	19 31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	596	LEU
1	X	597	LYS
1	X	612	LYS
1	X	618	LEU
1	X	631	GLN
1	X	637	LEU
1	X	646	GLU
1	X	659	GLU
1	X	668	LEU
1	X	670	LEU
1	X	769	ASN
1	X	826	LEU
1	X	833	SER
1	X	851	ARG
1	X	951	GLN
1	X	958	GLN
1	X	975	LYS
1	X	978	ILE
1	X	985	LEU
1	X	986	LEU
1	X	1004	ASN
1	X	1010	ASN
1	X	1033	GLU
1	X	1043	SER

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Mol	Chain	Res	Type
1	X	1060	VAL
1	X	1079	LEU
1	X	1085	SER
1	X	1115	LEU
1	X	1138	ARG
1	X	1139	GLU
1	X	1153	LYS
1	X	1160	MET
1	X	1161	GLU
1	X	1245	LEU
1	X	1261	VAL
1	X	1283	ARG
1	X	1285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	619	GLN
1	X	631	GLN
1	X	663	GLN
1	X	818	ASN
1	X	819	GLN
1	X	839	GLN
1	X	846	GLN
1	X	867	ASN
1	X	907	ASN
1	X	926	ASN
1	X	934	ASN
1	X	950	GLN
1	X	972	ASN
1	X	993	ASN
1	X	1001	HIS
1	X	1004	ASN
1	X	1010	ASN
1	X	1011	ASN
1	X	1021	ASN
1	X	1035	GLN
1	X	1112	GLN
1	X	1131	ASN
1	X	1203	GLN
1	X	1223	HIS
1	X	1266	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)

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	A	1	2	11,11,12	0.42	0	15,15,17	1.12	2 (13%)
2	GLC	A	2	2	12,12,12	0.53	0	17,17,17	0.59	0
2	GLC	B	1	2	11,11,12	0.42	0	15,15,17	1.08	1 (6%)
2	GLC	B	2	2	12,12,12	0.55	0	17,17,17	0.70	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	A	1	2	-	0/2/19/22	0/1/1/1
2	GLC	A	2	2	-	0/2/22/22	0/1/1/1
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	GLC	B	2	2	-	0/2/22/22	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})
2	B	1	GLC	C1-O5-C5	3.19	116.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	GLC	C1-O5-C5	2.65	115.78	112.19
2	A	1	GLC	C1-C2-C3	2.47	112.70	109.67

There are no chirality outliers.

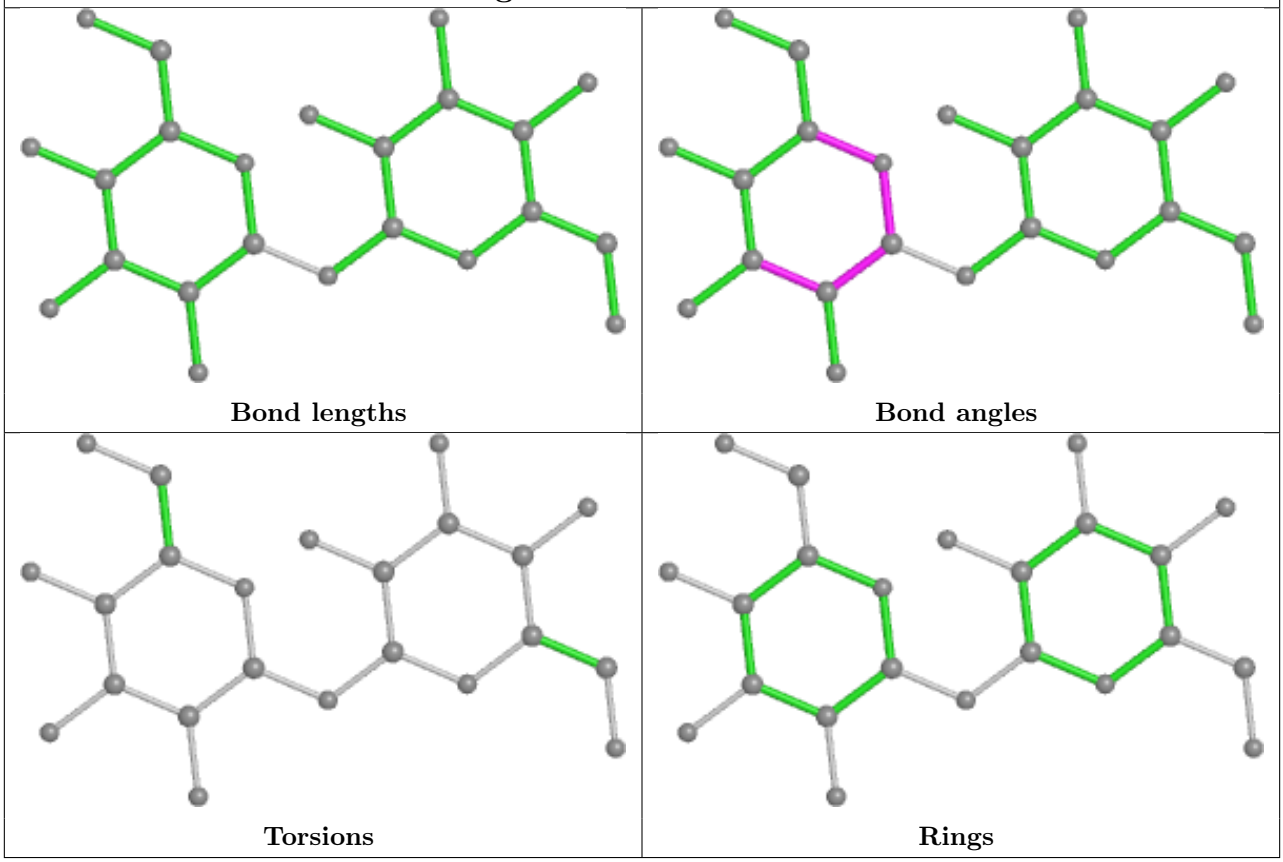
There are no torsion outliers.

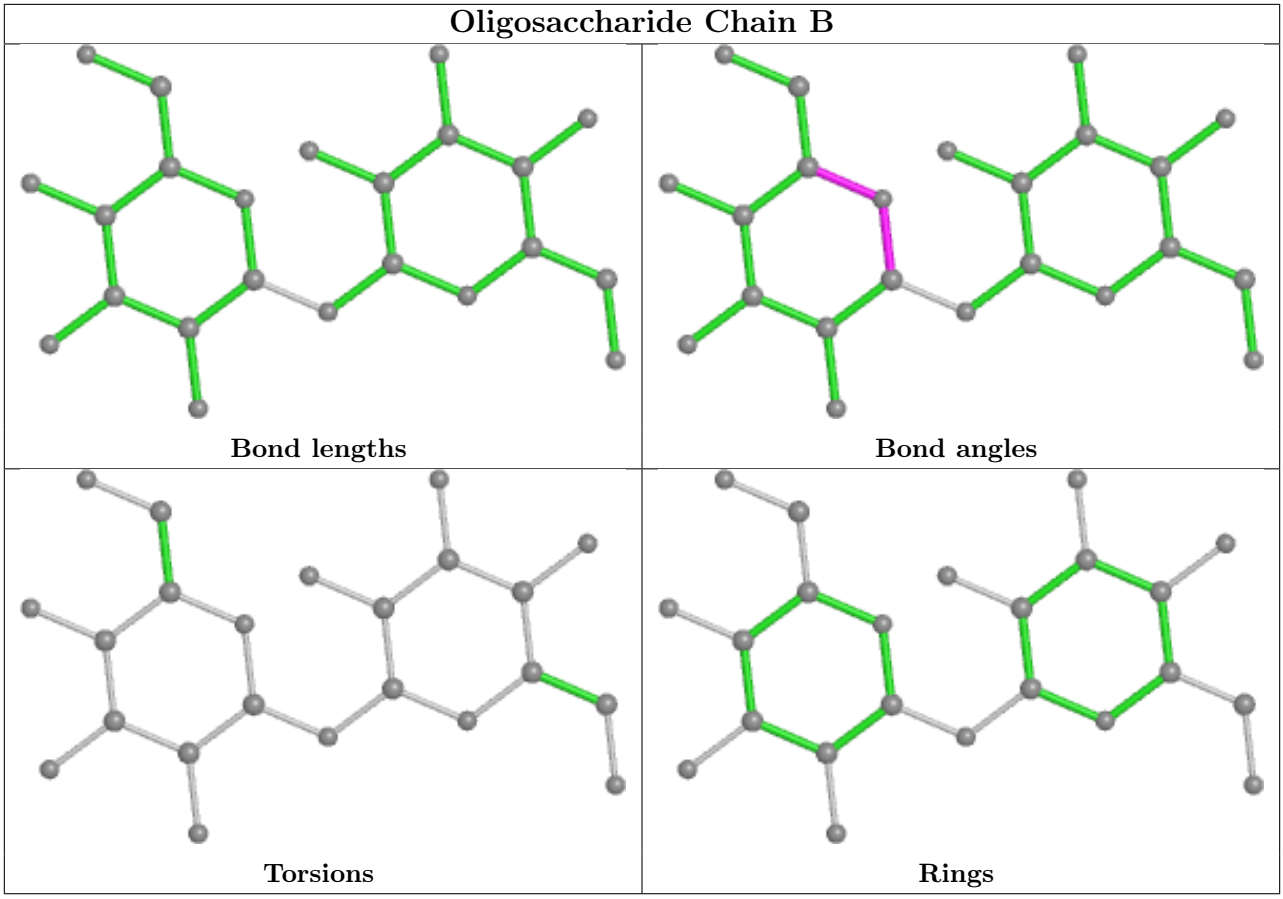
There are no ring outliers.

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.

Oligosaccharide Chain A





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	X	711/746 (95%)	0.14	32 (4%) 33 31	20, 40, 68, 77	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	575	LEU	7.2
1	X	576	GLY	5.2
1	X	768	TRP	4.1
1	X	769	ASN	3.8
1	X	760	TRP	3.8
1	X	820	VAL	3.6
1	X	1033	GLU	3.5
1	X	1031	ASP	3.4
1	X	1136	ASP	3.2
1	X	762	LEU	2.9
1	X	1134	SER	2.8
1	X	1231	LEU	2.7
1	X	604	GLY	2.7
1	X	1283	ARG	2.7
1	X	772	SER	2.7
1	X	577	GLY	2.7
1	X	1214	GLY	2.5
1	X	1139	GLU	2.5
1	X	783	GLU	2.4
1	X	625	ASN	2.4
1	X	765	TYR	2.4
1	X	756	GLN	2.4
1	X	1137	LEU	2.3
1	X	786	SER	2.3
1	X	782	ARG	2.3
1	X	1285	LEU	2.2
1	X	605	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	841	ASP	2.1
1	X	766	GLU	2.1
1	X	979	ASN	2.1
1	X	603	ILE	2.1
1	X	781	LEU	2.1

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)

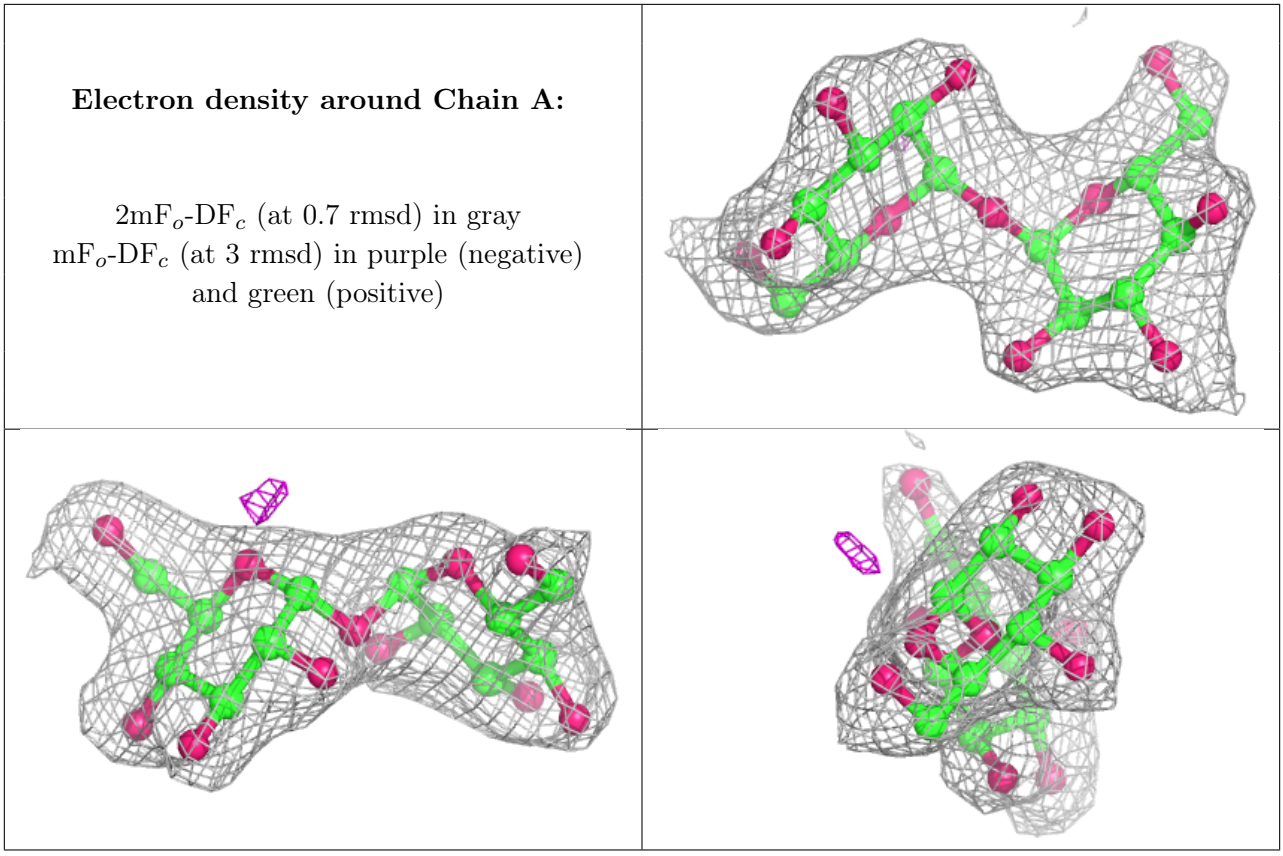
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	B	2	12/12	0.76	0.26	120,121,121,121	0
2	GLC	B	1	11/12	0.81	0.21	120,120,120,120	0
2	GLC	A	2	12/12	0.93	0.16	53,55,56,56	0
2	GLC	A	1	11/12	0.94	0.17	56,56,57,57	0

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

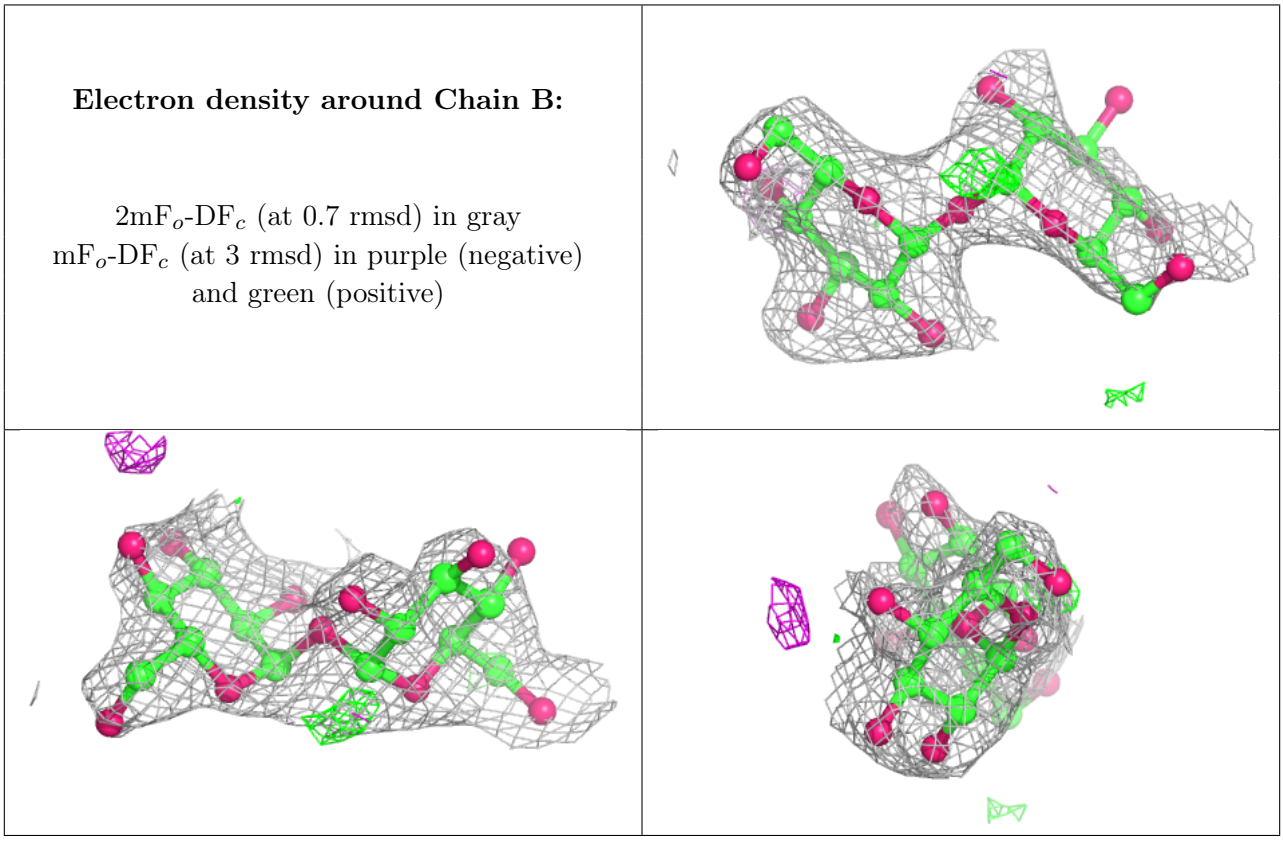
Electron density around Chain A:

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



Electron density around Chain B:

$2mF_o$-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.