

wwPDB X-ray Structure Validation Summary Report (i)

Jul 3, 2024 – 05:28 PM EDT

PDB ID	:	30SR
Title	:	Maltose-bound maltose sensor engineered by insertion of circularly permuted
		green fluorescent protein into E. coli maltose binding protein at position 311
Authors	:	Echevarria, I.M.; Marvin, J.S.; Looger, L.L.; Schreiter, E.R.
Deposited on		
Resolution	:	2.00 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 (1)) were used in the production of this report:

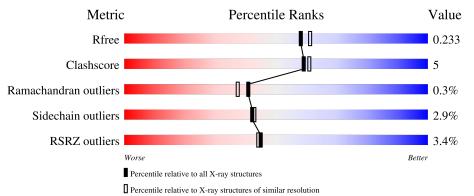
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
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	А	653	84%	7%	8%
1	В	653	4% 82% 9	% •	8%
2	С	2	100%		
2	D	2	100%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10100 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 Maltose-binding periplasmic protein, Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	A 604	Total	С	Ν	0	\mathbf{S}	0	1	0
			4752	3046	787	907	12			
1	В	601	Total	С	Ν	0	S	0	2	0
	I B	001	4743	3040	785	906	12	0	3	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-35	MET	-	expression tag	UNP P0AEY0
А	-34	ARG	-	expression tag	UNP P0AEY0
А	-33	GLY	-	expression tag	UNP P0AEY0
А	-32	SER	-	expression tag	UNP P0AEY0
А	-31	HIS	-	expression tag	UNP P0AEY0
А	-30	HIS	-	expression tag	UNP P0AEY0
А	-29	HIS	-	expression tag	UNP P0AEY0
А	-28	HIS	-	expression tag	UNP P0AEY0
А	-27	HIS	-	expression tag	UNP P0AEY0
А	-26	HIS	-	expression tag	UNP P0AEY0
А	-25	GLY	-	expression tag	UNP P0AEY0
А	-24	MET	-	expression tag	UNP P0AEY0
А	-23	ALA	-	expression tag	UNP P0AEY0
А	-22	SER	-	expression tag	UNP P0AEY0
А	-21	MET	-	expression tag	UNP P0AEY0
А	-20	THR	-	expression tag	UNP P0AEY0
А	-19	GLY	-	expression tag	UNP P0AEY0
А	-18	GLY	-	expression tag	UNP P0AEY0
А	-17	GLN	-	expression tag	UNP P0AEY0
А	-16	GLN	-	expression tag	UNP P0AEY0
А	-15	MET	-	expression tag	UNP P0AEY0
А	-14	GLY	-	expression tag	UNP P0AEY0
А	-13	ARG	-	expression tag	UNP P0AEY0
А	-12	ASP	-	expression tag	UNP P0AEY0
А	-11	LEU	-	expression tag	UNP P0AEY0

There are 122 discrepancies between the modelled and reference sequences:



		vious page	Actual	Comment	Reference
Chain	Residue	Modelled	Actual	Comment	
A	-10	TYR	-	expression tag	UNP POAEY0
A	-9	ASP	-	expression tag	UNP POAEYO
A	-8	ASP	-	expression tag	UNP POAEY0
A	-7	ASP	-	expression tag	UNP POAEY0
A	-6	ASP	-	expression tag	UNP POAEY0
A	-5	LYS	-	expression tag	UNP POAEY0
A	-4	ASP	-	expression tag	UNP P0AEY0
A	-3	ARG	-	expression tag	UNP P0AEY0
A	-2	TRP	-	expression tag	UNP POAEY0
А	-1	GLY	-	expression tag	UNP P0AEY0
А	0	SER	-	expression tag	UNP P0AEY0
A	312	GLY	-	linker	UNP P0AEY0
A	313	GLY	-	linker	UNP P0AEY0
А	325	ARG	LYS	conflict	UNP P42212
A	330	ALA	VAL	conflict	UNP P42212
А	342	GLY	SER	conflict	UNP P42212
А	347	TYR	ASP	conflict	UNP P42212
А	373	LYS	ALA	conflict	UNP P42212
А	398	LEU	HIS	conflict	UNP P42212
А	406	GLY	-	linker	UNP P42212
А	407	GLY	-	linker	UNP P42212
А	408	THR	-	linker	UNP P42212
А	409	GLY	-	linker	UNP P42212
А	410	GLY	-	linker	UNP P42212
А	411	SER	-	linker	UNP P42212
А	412	MET	-	linker	UNP P42212
А	413	VAL	-	linker	UNP P42212
А	476	LEU	PHE	conflict	UNP P42212
А	478	C12	SER	chromophore	UNP P42212
А	478	C12	TYR	chromophore	UNP P42212
А	478	C12	GLY	chromophore	UNP P42212
А	505	ILE	VAL	conflict	UNP P42212
А	557	PHE	TYR	conflict	UNP P42212
А	559	ASN	-	linker	UNP P42212
А	560	PRO	-	linker	UNP P42212
А	609	ASP	ALA	conflict	UNP POAEY0
В	-35	MET	-	expression tag	UNP POAEY0
В	-34	ARG	-	expression tag	UNP POAEY0
В	-33	GLY	-	expression tag	UNP POAEY0
В	-32	SER	-	expression tag	UNP POAEY0
В	-31	HIS	-	expression tag	UNP POAEY0
В	-30	HIS	-	expression tag	UNP POAEY0
L	I	1	1	· · · · · · · · · · · · · · · · · · ·	I

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Chain	Residue	Modelled	Actual	Comment	Reference			
В	-29	HIS	-	expression tag	UNP P0AEY0			
В	-28	HIS	-	expression tag	UNP P0AEY0			
В	-27	HIS	-	expression tag	UNP P0AEY0			
В	-26	HIS	-	expression tag	UNP P0AEY0			
В	-25	GLY	-	expression tag	UNP P0AEY0			
В	-24	MET	-	expression tag	UNP P0AEY0			
В	-23	ALA	-	expression tag	UNP P0AEY0			
В	-22	SER	-	expression tag	UNP P0AEY0			
В	-21	MET	-	expression tag	UNP P0AEY0			
В	-20	THR	-	expression tag	UNP P0AEY0			
В	-19	GLY	-	expression tag	UNP POAEY0			
В	-18	GLY	-	expression tag	UNP POAEY0			
В	-17	GLN	-	expression tag	UNP P0AEY0			
В	-16	GLN	-	expression tag	UNP P0AEY0			
В	-15	MET	-	expression tag	UNP P0AEY0			
В	-14	GLY	-	expression tag	UNP P0AEY0			
В	-13	ARG	-	expression tag	UNP POAEY0			
В	-12	ASP	-	expression tag	UNP P0AEY0			
В	-11	LEU	-	expression tag	UNP POAEY0			
В	-10	TYR	-	expression tag	UNP P0AEY0			
В	-9	ASP	-	expression tag	UNP POAEY0			
В	-8	ASP	-	expression tag	UNP POAEY0			
В	-7	ASP	-	expression tag	UNP POAEY0			
В	-6	ASP	-	expression tag	UNP POAEY0			
В	-5	LYS	-	expression tag	UNP POAEY0			
В	-4	ASP	-	expression tag	UNP POAEY0			
В	-3	ARG	-	expression tag	UNP P0AEY0			
В	-2	TRP	-	expression tag	UNP P0AEY0			
В	-1	GLY	-	expression tag	UNP P0AEY0			
В	0	SER	-	expression tag	UNP P0AEY0			
В	312	GLY	-	linker	UNP P0AEY0			
В	313	GLY	-	linker	UNP P0AEY0			
В	325	ARG	LYS	conflict	UNP P42212			
В	330	ALA	VAL	conflict	UNP P42212			
В	342	GLY	SER	conflict	UNP P42212			
В	347	TYR	ASP	conflict	UNP P42212			
В	373	LYS	ALA	conflict	UNP P42212			
В	398	LEU	HIS	conflict	UNP P42212			
В	406	GLY	-	linker	UNP P42212			
В	407	GLY	-	linker	UNP P42212			
В	408	THR	-	linker	UNP P42212			
D								
B B B B B B	342 347 373 398 406 407	GLY TYR LYS LEU GLY GLY	SER ASP ALA HIS -	conflict conflict conflict conflict linker linker	UNP P42212 UNP P42212 UNP P42212 UNP P42212 UNP P42212 UNP P42212 UNP P42212			

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Chain	Residue	Modelled	Actual	Comment	Reference
В	410	GLY	-	linker	UNP P42212
В	411	SER	-	linker	UNP P42212
В	412	MET	-	linker	UNP P42212
В	413	VAL	-	linker	UNP P42212
В	476	LEU	PHE	conflict	UNP P42212
В	478	C12	SER	chromophore	UNP P42212
В	478	C12	TYR	chromophore	UNP P42212
В	478	C12	GLY	chromophore	UNP P42212
В	505	ILE	VAL	conflict	UNP P42212
В	557	PHE	TYR	conflict	UNP P42212
В	559	ASN	-	linker	UNP P42212
В	560	PRO	-	linker	UNP P42212
В	609	ASP	ALA	conflict	UNP POAEY0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	2	Total C O 23 12 11	0	0	0
2	D	2	Total C O 23 12 11	0	0	0

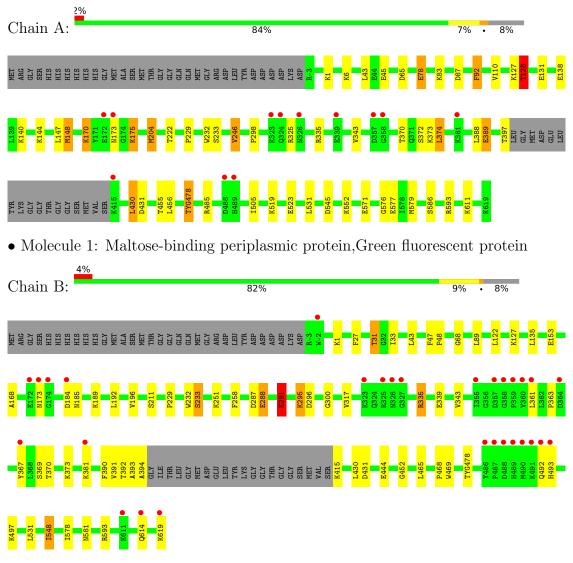
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	302	Total O 302 302	0	0
3	В	257	Total O 257 257	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,Green fluorescent protein

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

Chain C:

100%



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

Chain D:

100%

GLC1 GLC2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness (in resolution range)	$99.9 (34.24-2.00) \\100.0 (32.65-2.00)$	Depositor EDS
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.33 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	4825 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.6	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 47.5	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: C12, 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		Boi	nd lengths	Bond angles		
	Moi Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.08	3/4846~(0.1%)	0.93	8/6563~(0.1%)	
1	В	1.01	5/4843~(0.1%)	0.87	5/6559~(0.1%)	
All	All	1.04	8/9689~(0.1%)	0.90	13/13122~(0.1%)	

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	233	SER	CB-OG	-6.63	1.33	1.42
1	А	246	VAL	CB-CG2	-5.66	1.41	1.52
1	А	389	GLU	CG-CD	5.48	1.60	1.51
1	В	288	GLU	CB-CG	5.35	1.62	1.52
1	В	288	GLU	CG-CD	5.19	1.59	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	335	ARG	NE-CZ-NH2	12.38	126.49	120.30
1	А	335	ARG	NE-CZ-NH1	-11.87	114.37	120.30
1	А	148	MET	CG-SD-CE	-7.47	88.24	100.20
1	В	287	ASP	CB-CG-OD1	6.79	124.41	118.30
1	А	128	THR	N-CA-CB	-5.85	99.18	110.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4752	0	4670	45	0
1	В	4743	0	4659	43	0
2	С	23	0	20	0	0
2	D	23	0	20	0	0
3	А	302	0	0	18	0
3	В	257	0	0	9	0
All	All	10100	0	9369	88	0

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.

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 5.

The worst 5 of 88 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:295:LYS:HD2	3:B:760:HOH:O	1.29	1.25
1:B:300:GLY:HA3	3:B:750:HOH:O	1.69	0.92
1:B:335:ARG:HB3	1:B:343:VAL:HG21	1.54	0.86
1:A:577:GLU:CB	3:A:762:HOH:O	2.25	0.85
1:A:128:THR:HG21	3:A:918:HOH:O	1.77	0.83

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	А	598/653~(92%)	584 (98%)	13~(2%)	1 (0%)	47 44
1	В	597/653~(91%)	588 (98%)	7 (1%)	2(0%)	41 37
All	All	1195/1306~(92%)	1172 (98%)	20 (2%)	3~(0%)	41 37



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	173	ASN
1	А	173	ASN
1	В	168	ALA

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	А	499/537~(93%)	481 (96%)	18 (4%)	35 34	
1	В	499/537~(93%)	488~(98%)	11 (2%)	52 55	
All	All	998/1074 (93%)	969~(97%)	29 (3%)	42 43	

5 of 29 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	519	LYS
1	В	444	GLU
1	А	611	LYS
1	В	369	SER
1	А	593	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	315	HIS
1	В	315	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

2 non-standard protein/DNA/RNA residues 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	Trune	Chain	Res Link		Bo	ond leng	\mathbf{ths}	B	ond ang	les		
IVIOI	Type	Chain	res	nes	res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	C12	А	478	-	20,23,24	1.33	2 (10%)	21,32,34	2.03	4 (19%)		
1	C12	В	478	-	20,23,24	1.69	5 (25%)	21,32,34	1.96	4 (19%)		

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
1	C12	А	478	-	-	3/8/15/16	0/2/2/2
1	C12	В	478	-	-	4/8/15/16	0/2/2/2

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	478	C12	CB2-CA2	-4.82	1.47	1.51
1	А	478	C12	CB2-CA2	-3.77	1.48	1.51
1	В	478	C12	C2-N3	-3.07	1.31	1.36
1	В	478	C12	CA3-N3	-2.53	1.44	1.49
1	А	478	C12	C2-N3	-2.44	1.32	1.36

The worst 5 of 7 bond length outliers are listed below:

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	478	C12	CG2-CB2-CA2	6.87	130.04	112.40
1	В	478	C12	CG2-CB2-CA2	5.77	127.20	112.40
1	В	478	C12	CB2-CA2-C2	-4.33	118.66	131.20
1	А	478	C12	O3-C3-CA3	-3.18	117.29	126.32
1	В	478	C12	C3-CA3-N3	2.75	116.10	111.92



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
1	В	478	C12	N2-CA2-CB2-CG2
1	А	478	C12	C2-CA2-CB2-CG2
1	В	478	C12	C2-CA2-CB2-CG2
1	А	478	C12	CA2-CB2-CG2-CD1
1	В	478	C12	CA2-CB2-CG2-CD1

5 of 7 torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	478	C12	1	0

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	Trune	Chain	Dec	Link	Bo	ond leng	ths	Bond angles			
	Type	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	GLC	С	1	2	12,12,12	1.05	1 (8%)	$17,\!17,\!17$	1.41	3 (17%)	
2	GLC	С	2	2	11,11,12	0.89	0	$15,\!15,\!17$	1.35	2 (13%)	
2	GLC	D	1	2	12,12,12	1.00	0	$17,\!17,\!17$	1.54	4 (23%)	
2	GLC	D	2	2	11,11,12	0.68	0	$15,\!15,\!17$	1.74	3 (20%)	

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	С	1	2	-	0/2/22/22	0/1/1/1
2	GLC	С	2	2	-	0/2/19/22	0/1/1/1



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	1	GLC	O5-C5	-2.50	1.38	1.44

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	D	2	GLC	O5-C5-C6	-3.79	101.27	107.20
2	С	1	GLC	O5-C1-C2	3.61	116.72	110.28
2	D	1	GLC	O1-C1-O5	-3.46	100.00	110.38
2	D	2	GLC	C2-C3-C4	-3.38	105.05	110.89
2	D	2	GLC	O5-C1-C2	-3.30	105.67	110.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

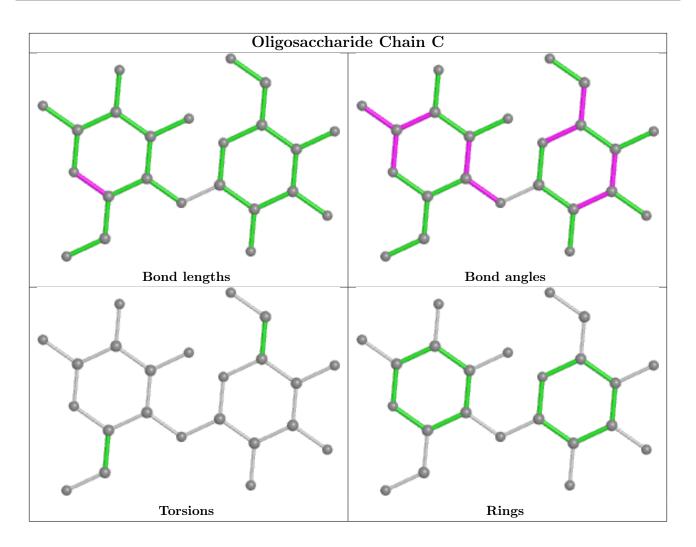
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6

There are no ring outliers.

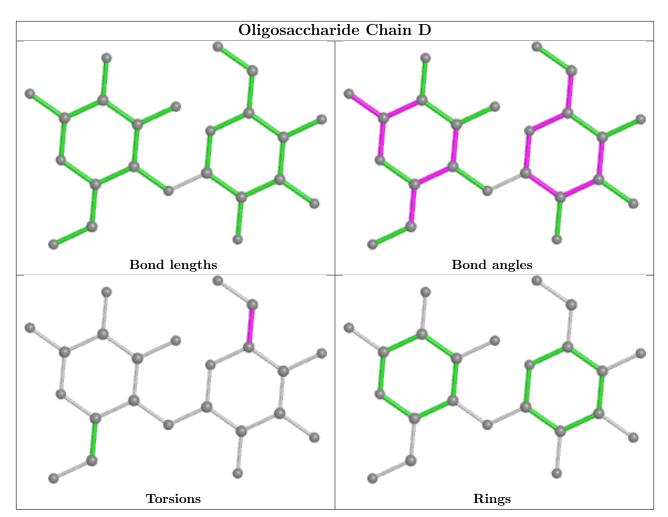
No monomer is involved in short contacts.

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)

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, 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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	603/653~(92%)	-0.15	12 (1%) 65	63	8, 19, 39, 55	0
1	В	600/653~(91%)	0.03	29 (4%) 30	29	11, 23, 51, 72	0
All	All	1203/1306~(92%)	-0.06	41 (3%) 45	44	8, 21, 44, 72	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	489	HIS	5.7
1	В	359	PRO	5.0
1	В	173	ASN	4.9
1	В	360	VAL	4.7
1	В	358	GLY	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	C12	А	478	22/23	0.95	0.17	7,16,20,21	0
1	C12	В	478	22/23	0.95	0.15	14,20,21,24	0

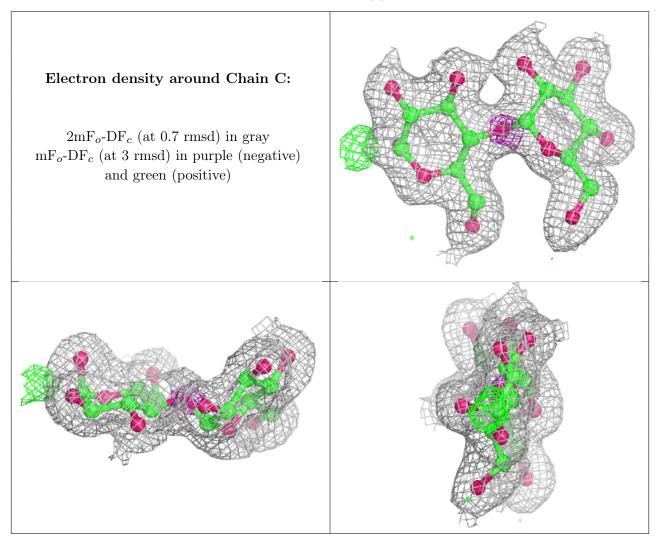
6.3 Carbohydrates (i)

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, 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.

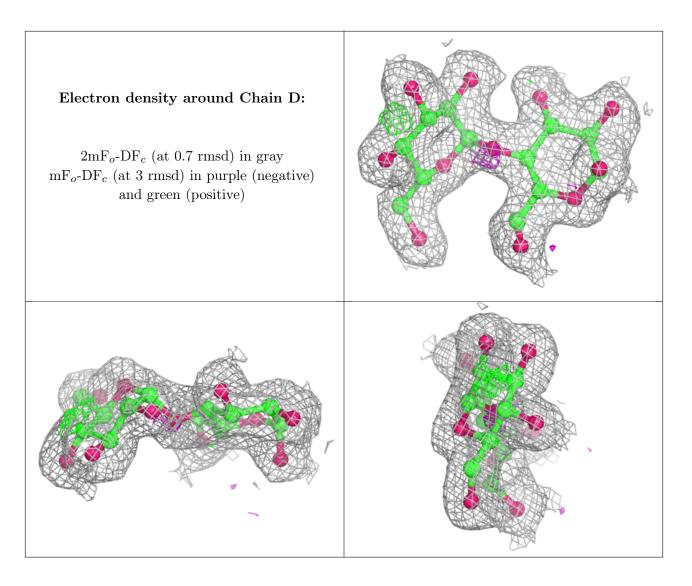


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	GLC	С	1	12/12	0.96	0.15	$2,\!11,\!14,\!15$	0
2	GLC	D	1	12/12	0.96	0.15	$5,\!14,\!20,\!25$	0
2	GLC	D	2	11/12	0.96	0.14	9,11,13,13	0
2	GLC	С	2	11/12	0.97	0.14	6,8,9,10	0

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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

