



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2016 – 02:37 PM EDT

PDB ID : 4LPC
Title : Crystal Structure of E.Coli Branching Enzyme in complex with maltoheptaose
Authors : Feng, L.; Geiger, J.H.
Deposited on : 2013-07-16
Resolution : 2.39 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

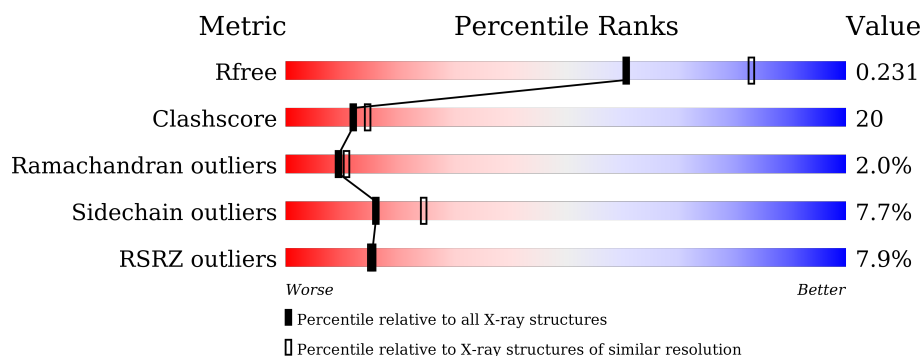
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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 $\leq 5\%$. 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	612	<div> <div>9%</div> <div>60%</div> <div>30%</div> <div>5%</div> <div>.</div> </div>
1	B	612	<div> <div>2%</div> <div>67%</div> <div>24%</div> <div>6%</div> <div>..</div> </div>
1	C	612	<div> <div>17%</div> <div>62%</div> <div>29%</div> <div>.</div> <div>5%</div> </div>
1	D	612	<div> <div>2%</div> <div>68%</div> <div>23%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	801	-	-	-	X
2	GLC	A	803	-	-	-	X
2	GLC	D	806	-	-	-	X
3	GOL	A	805	-	-	-	X
3	GOL	A	807	-	-	X	X
3	GOL	B	813	-	-	-	X
3	GOL	B	815	-	-	X	-
4	GLC	A	808	-	-	-	X
4	GLC	A	809	-	-	-	X
5	BGC	B	801	-	-	-	X
5	BGC	B	816	-	-	-	X
5	BGC	D	810	-	-	X	X
5	BGC	D	812	-	-	-	X
5	GLC	D	813	-	-	-	X
6	BGC	B	803	-	-	-	X
6	GLC	B	804	-	-	-	X
6	GLC	B	808	-	-	-	X
7	BGC	B	810	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20728 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	5	0
			4870	3109	867	878	16			
1	B	598	Total	C	N	O	S	0	2	0
			4935	3149	880	890	16			
1	C	582	Total	C	N	O	S	0	1	0
			4795	3068	850	861	16			
1	D	588	Total	C	N	O	S	0	4	0
			4867	3108	865	877	17			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	3	Total	C	O	0	0
			34	18	16		

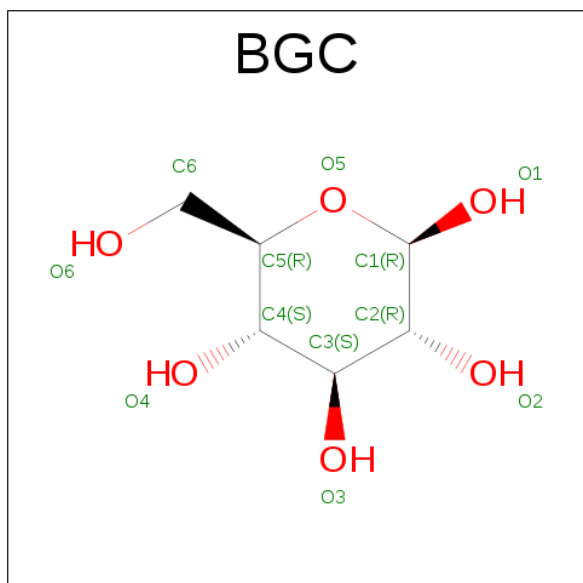
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	2	Total	C	O	0	0
			23	12	11		
5	B	2	Total	C	O	0	0
			23	12	11		
5	D	2	Total	C	O	0	0
			23	12	11		
5	D	2	Total	C	O	0	0
			23	12	11		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	7	Total	C	O	0	0
			78	42	36		

- Molecule 7 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	4	Total	C	O	0	0
			45	24	21		

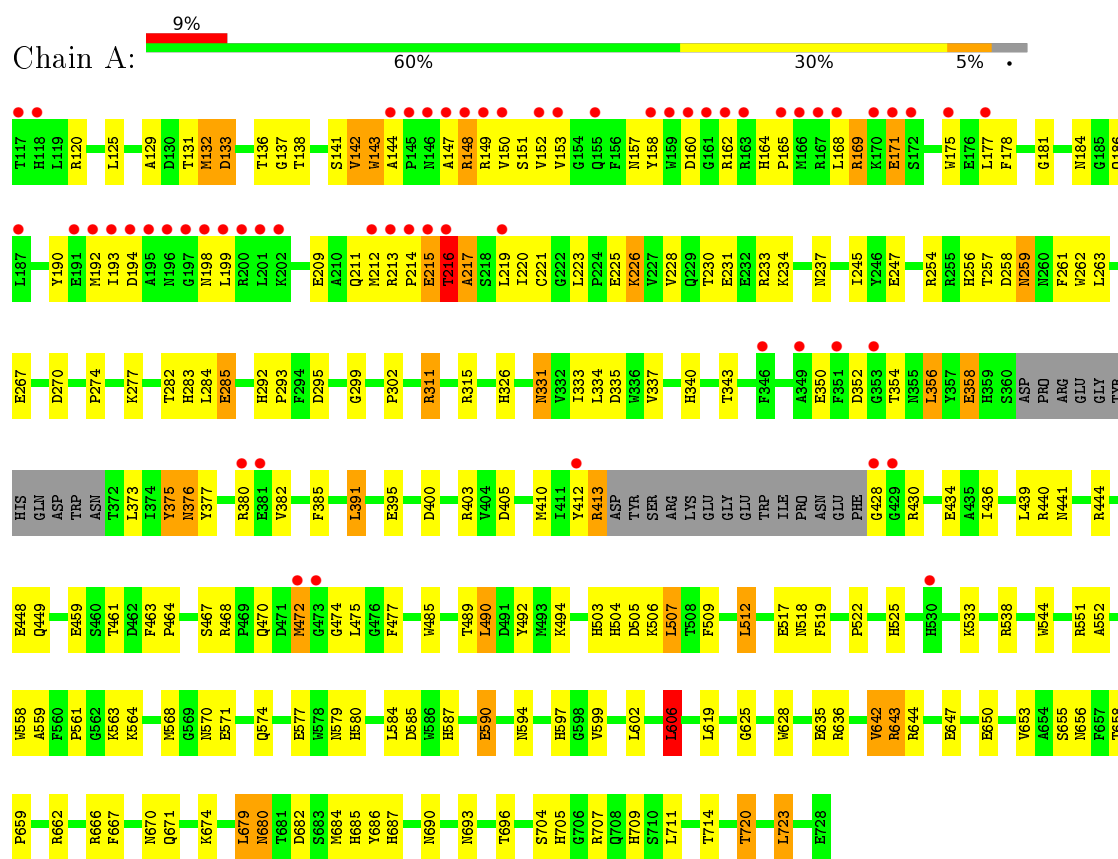
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	220	Total	O	0	0
			220	220		
9	B	329	Total	O	0	0
			329	329		
9	C	72	Total	O	0	0
			72	72		
9	D	221	Total	O	0	0
			221	221		

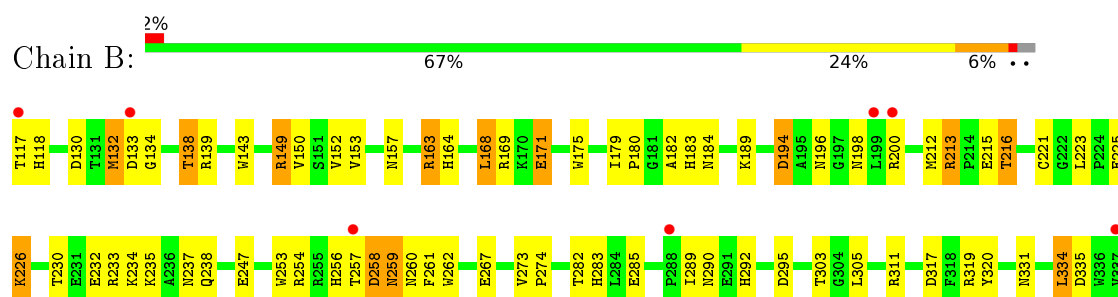
3 Residue-property plots

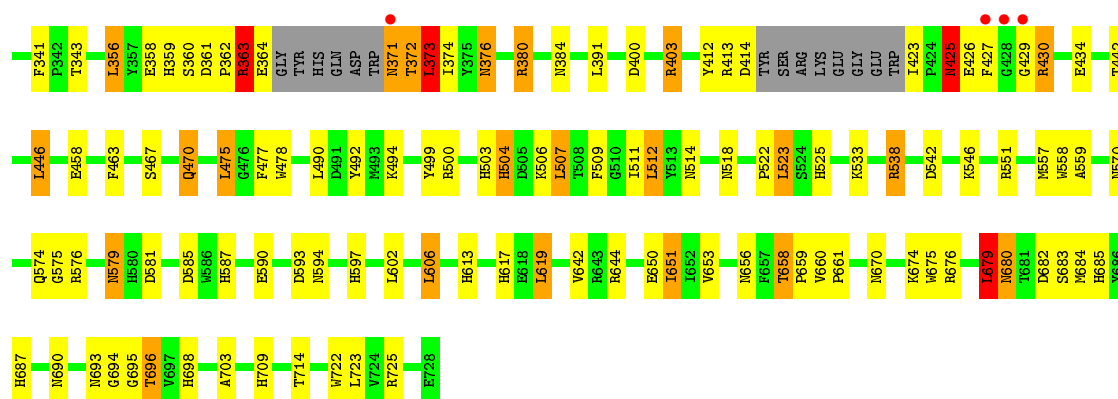
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: 1,4-alpha-glucan branching enzyme GlgB

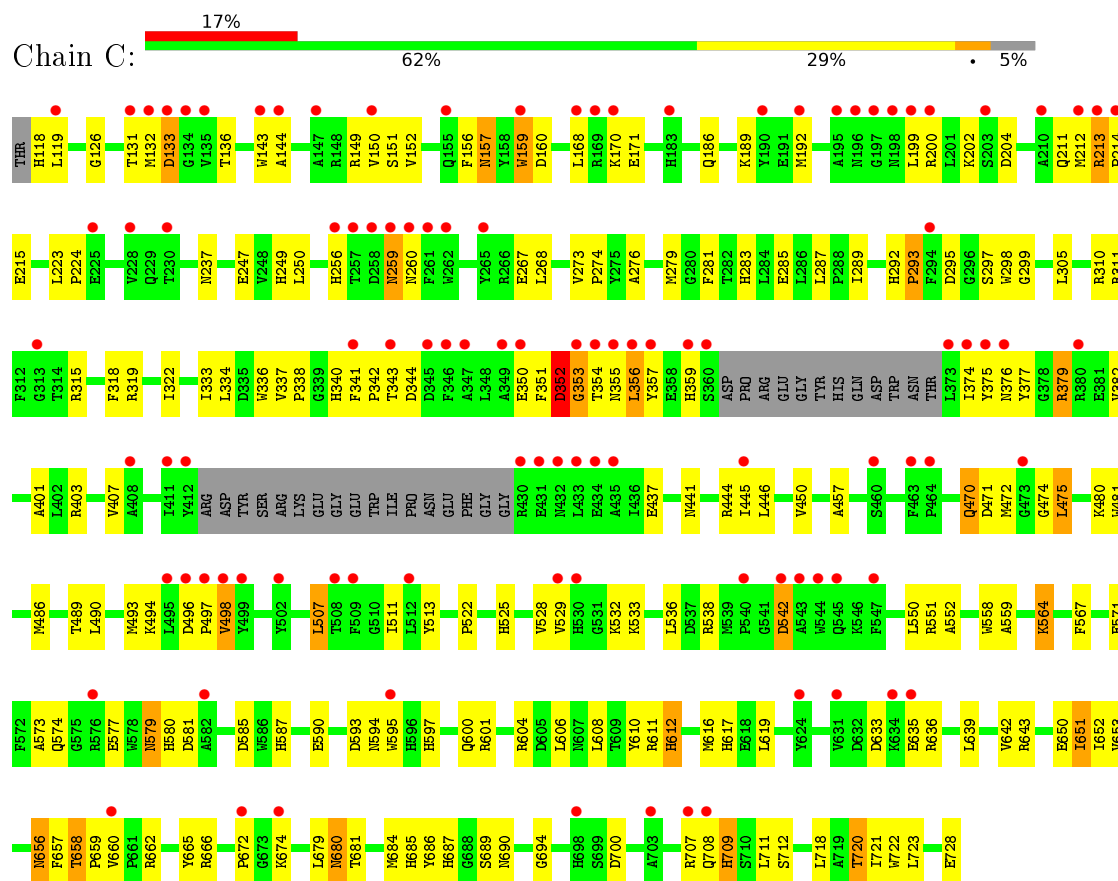


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

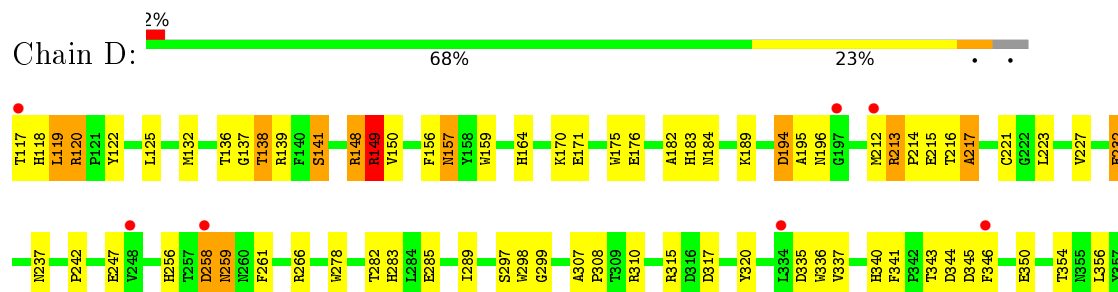


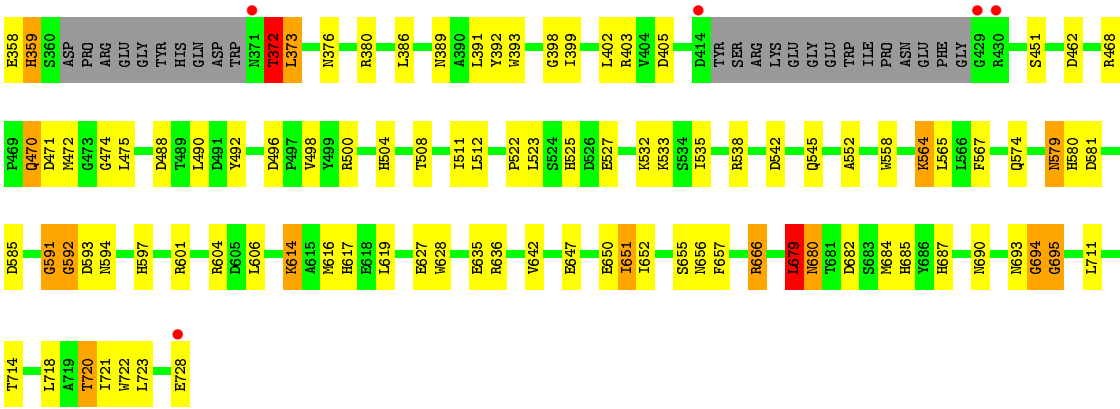


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.19Å 103.42Å 185.94Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 41.27 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.39) 90.4 (41.27-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.183 , 0.234 0.182 , 0.231	Depositor DCC
R_{free} test set	6287 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 124846 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20728	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, GOL, BGC

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	0.57	0/5024	0.66	5/6820 (0.1%)
1	B	0.72	1/5092 (0.0%)	0.77	5/6914 (0.1%)
1	C	0.37	0/4948	0.48	0/6719
1	D	0.56	0/5021	0.67	3/6817 (0.0%)
All	All	0.57	1/20085 (0.0%)	0.66	13/27270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	TRP	CB-CG	5.21	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	B	373	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	606	LEU	CA-CB-CG	6.50	130.26	115.30
1	B	723	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	643	ARG	NE-CZ-NH2	-6.12	117.24	120.30

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 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	4870	0	4590	218	0
1	B	4935	0	4647	207	0
1	C	4795	0	4527	158	0
1	D	4867	0	4586	180	0
2	A	46	0	42	6	0
2	C	23	0	21	0	0
2	D	23	0	21	1	0
3	A	18	0	24	6	0
3	B	30	0	40	12	0
3	D	18	0	24	2	0
4	A	34	0	30	6	0
5	B	46	0	42	11	0
5	D	46	0	42	7	0
6	B	78	0	66	7	0
7	B	12	0	12	0	0
8	D	45	0	39	1	0
9	A	220	0	0	29	0
9	B	329	0	0	49	0
9	C	72	0	0	14	0
9	D	221	0	0	17	0
All	All	20728	0	18753	768	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 20.

The worst 5 of 768 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:D:212[A]:MET:CE	1:D:213:ARG:HH12	1.14	1.58
1:D:212[A]:MET:CE	1:D:213:ARG:NH1	1.91	1.29
1:D:470:GLN:N	1:D:470:GLN:HE21	1.33	1.26
1:D:212[A]:MET:HG3	1:D:213:ARG:NH1	1.50	1.25
1:B:434:GLU:HG2	9:B:1114:HOH:O	1.35	1.24

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	586/612 (96%)	546 (93%)	31 (5%)	9 (2%)	13	17
1	B	594/612 (97%)	566 (95%)	18 (3%)	10 (2%)	11	14
1	C	577/612 (94%)	512 (89%)	49 (8%)	16 (3%)	6	5
1	D	586/612 (96%)	545 (93%)	29 (5%)	12 (2%)	9	11
All	All	2343/2448 (96%)	2169 (93%)	127 (5%)	47 (2%)	9	11

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	TRP
1	A	148	ARG
1	A	215	GLU
1	A	226	LYS
1	B	194	ASP

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	503/521 (96%)	465 (92%)	38 (8%)	16	25
1	B	510/521 (98%)	464 (91%)	46 (9%)	12	17
1	C	495/521 (95%)	460 (93%)	35 (7%)	18	28
1	D	503/521 (96%)	467 (93%)	36 (7%)	18	28
All	All	2011/2084 (96%)	1856 (92%)	155 (8%)	16	24

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	504	HIS
1	C	157	ASN
1	D	523	LEU
1	B	511	ILE
1	B	619	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	617	HIS
1	C	237	ASN
1	D	597	HIS
1	B	656	ASN
1	B	705	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 carbohydrates 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	801	2	12,12,12	0.49	0	17,17,17	0.80	0
2	GLC	A	802	2	11,11,12	0.49	0	15,15,17	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	803	2	12,12,12	0.70	0	17,17,17	1.21	2 (11%)
2	GLC	A	804	2	11,11,12	0.47	0	15,15,17	2.22	2 (13%)
4	GLC	A	808	4	12,12,12	0.47	0	17,17,17	1.63	4 (23%)
4	GLC	A	809	4	11,11,12	0.76	0	15,15,17	0.92	0
4	GLC	A	810	4	11,11,12	0.60	0	15,15,17	1.58	5 (33%)
5	BGC	B	801	5	12,12,12	0.75	0	17,17,17	1.60	3 (17%)
5	GLC	B	802	5	11,11,12	0.39	0	15,15,17	2.21	4 (26%)
6	BGC	B	803	6	12,12,12	0.42	0	17,17,17	1.92	6 (35%)
6	GLC	B	804	6	11,11,12	0.48	0	15,15,17	1.59	3 (20%)
6	GLC	B	805	6	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
6	GLC	B	806	6	11,11,12	0.56	0	15,15,17	1.33	2 (13%)
6	GLC	B	807	6	11,11,12	0.63	0	15,15,17	2.15	6 (40%)
6	GLC	B	808	6	11,11,12	0.59	0	15,15,17	1.33	2 (13%)
6	GLC	B	809	6	11,11,12	0.65	0	15,15,17	1.25	2 (13%)
5	BGC	B	816	5	12,12,12	0.56	0	17,17,17	1.21	2 (11%)
5	GLC	B	817	5	11,11,12	0.80	0	15,15,17	1.12	1 (6%)
2	GLC	C	801	2	12,12,12	0.54	0	17,17,17	0.53	0
2	GLC	C	802	2	11,11,12	0.67	0	15,15,17	0.96	1 (6%)
8	GLC	D	801	8	12,12,12	0.62	0	17,17,17	1.45	3 (17%)
8	GLC	D	802	8	11,11,12	0.76	0	15,15,17	1.89	2 (13%)
8	GLC	D	803	8	11,11,12	0.57	0	15,15,17	1.17	1 (6%)
8	GLC	D	804	8	11,11,12	0.77	0	15,15,17	1.38	2 (13%)
2	GLC	D	805	2	12,12,12	0.48	0	17,17,17	0.78	0
2	GLC	D	806	2	11,11,12	0.55	0	15,15,17	1.40	2 (13%)
5	BGC	D	810	5	12,12,12	0.67	0	17,17,17	2.14	6 (35%)
5	GLC	D	811	5	11,11,12	0.56	0	15,15,17	1.89	3 (20%)
5	BGC	D	812	5	12,12,12	0.50	0	17,17,17	1.55	4 (23%)
5	GLC	D	813	5	11,11,12	0.51	0	15,15,17	1.59	2 (13%)

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	801	2	-	0/2/22/22	0/1/1/1
2	GLC	A	802	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	803	2	-	0/2/22/22	0/1/1/1
2	GLC	A	804	2	-	0/2/19/22	0/1/1/1
4	GLC	A	808	4	-	0/2/22/22	0/1/1/1
4	GLC	A	809	4	-	0/2/19/22	0/1/1/1
4	GLC	A	810	4	-	0/2/19/22	0/1/1/1
5	BGC	B	801	5	-	0/2/22/22	0/1/1/1
5	GLC	B	802	5	-	0/2/19/22	0/1/1/1
6	BGC	B	803	6	-	0/2/22/22	0/1/1/1
6	GLC	B	804	6	-	0/2/19/22	0/1/1/1
6	GLC	B	805	6	-	0/2/19/22	0/1/1/1
6	GLC	B	806	6	-	0/2/19/22	0/1/1/1
6	GLC	B	807	6	-	0/2/19/22	0/1/1/1
6	GLC	B	808	6	-	0/2/19/22	0/1/1/1
6	GLC	B	809	6	-	0/2/19/22	0/1/1/1
5	BGC	B	816	5	-	0/2/22/22	0/1/1/1
5	GLC	B	817	5	-	0/2/19/22	0/1/1/1
2	GLC	C	801	2	-	0/2/22/22	0/1/1/1
2	GLC	C	802	2	-	0/2/19/22	0/1/1/1
8	GLC	D	801	8	-	0/2/22/22	0/1/1/1
8	GLC	D	802	8	-	0/2/19/22	0/1/1/1
8	GLC	D	803	8	-	0/2/19/22	0/1/1/1
8	GLC	D	804	8	-	0/2/19/22	0/1/1/1
2	GLC	D	805	2	-	0/2/22/22	0/1/1/1
2	GLC	D	806	2	-	0/2/19/22	0/1/1/1
5	BGC	D	810	5	-	0/2/22/22	0/1/1/1
5	GLC	D	811	5	-	0/2/19/22	0/1/1/1
5	BGC	D	812	5	-	0/2/22/22	0/1/1/1
5	GLC	D	813	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	810	BGC	C1-C2-C3	-4.65	103.06	110.68
5	B	801	BGC	O5-C1-C2	-4.27	102.52	110.00
6	B	803	BGC	C4-C3-C2	-4.20	103.04	110.79
6	B	808	GLC	O5-C1-C2	-3.67	105.02	110.89
4	A	810	GLC	O5-C1-C2	-3.42	105.43	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	GLC	2	0
2	A	804	GLC	4	0
4	A	808	GLC	5	0
4	A	809	GLC	1	0
5	B	801	BGC	2	0
5	B	802	GLC	2	0
6	B	803	BGC	1	0
6	B	804	GLC	4	0
6	B	805	GLC	3	0
6	B	806	GLC	1	0
6	B	807	GLC	2	0
6	B	808	GLC	1	0
5	B	816	BGC	4	0
5	B	817	GLC	3	0
8	D	804	GLC	1	0
2	D	805	GLC	1	0
5	D	810	BGC	7	0

5.6 Ligand geometry [i](#)

12 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	GOL	A	805	-	5,5,5	0.48	0	5,5,5	0.28	0
3	GOL	A	806	-	5,5,5	0.25	0	5,5,5	0.40	0
3	GOL	A	807	-	5,5,5	0.44	0	5,5,5	0.76	0
7	BGC	B	810	-	12,12,12	0.48	0	17,17,17	0.88	0
3	GOL	B	811	-	5,5,5	0.45	0	5,5,5	0.18	0
3	GOL	B	812	-	5,5,5	0.40	0	5,5,5	0.62	0
3	GOL	B	813	-	5,5,5	0.51	0	5,5,5	0.83	0
3	GOL	B	814	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	B	815	-	5,5,5	0.40	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	807	-	5,5,5	0.31	0	5,5,5	0.26	0
3	GOL	D	808	-	5,5,5	0.29	0	5,5,5	0.39	0
3	GOL	D	809	-	5,5,5	0.32	0	5,5,5	0.44	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
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
3	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	GOL	A	807	-	-	0/4/4/4	0/0/0/0
7	BGC	B	810	-	-	0/2/22/22	0/1/1/1
3	GOL	B	811	-	-	0/4/4/4	0/0/0/0
3	GOL	B	812	-	-	0/4/4/4	0/0/0/0
3	GOL	B	813	-	-	0/4/4/4	0/0/0/0
3	GOL	B	814	-	-	0/4/4/4	0/0/0/0
3	GOL	B	815	-	-	0/4/4/4	0/0/0/0
3	GOL	D	807	-	-	0/4/4/4	0/0/0/0
3	GOL	D	808	-	-	0/4/4/4	0/0/0/0
3	GOL	D	809	-	-	0/4/4/4	0/0/0/0

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.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	807	GOL	6	0
3	B	812	GOL	2	0
3	B	813	GOL	3	0
3	B	815	GOL	7	0
3	D	808	GOL	1	0
3	D	809	GOL	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 [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	587/612 (95%)	0.28	58 (9%) 9 9	25, 48, 124, 144	1 (0%)
1	B	598/612 (97%)	-0.11	11 (1%) 71 71	21, 38, 63, 77	5 (0%)
1	C	582/612 (95%)	0.86	106 (18%) 2 2	57, 88, 123, 143	2 (0%)
1	D	588/612 (96%)	0.06	12 (2%) 68 68	35, 49, 70, 86	3 (0%)
All	All	2355/2448 (96%)	0.27	187 (7%) 15 15	21, 51, 114, 144	11 (0%)

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	SER	8.3
1	A	201	LEU	7.1
1	C	213	ARG	7.0
1	A	159	TRP	6.6
1	A	195	ALA	6.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	GLC	B	804	11/12	0.83	0.34	10.13	90,91,93,93	1
5	BGC	B	801	12/12	0.84	0.23	9.31	82,84,86,89	0
5	GLC	D	813	11/12	0.68	0.39	8.32	106,107,108,109	1
6	GLC	B	808	11/12	0.90	0.24	7.50	74,76,78,79	0
5	BGC	D	812	12/12	0.64	0.31	7.26	104,106,106,106	0
5	BGC	D	810	12/12	0.86	0.27	5.93	65,69,71,73	0
6	BGC	B	803	12/12	0.85	0.20	4.64	82,86,87,88	0
4	GLC	A	809	11/12	0.86	0.23	3.51	75,78,81,85	0
5	BGC	B	816	12/12	0.90	0.22	3.42	59,69,70,71	0
2	GLC	A	801	12/12	0.96	0.21	3.34	66,68,69,70	0
4	GLC	A	808	12/12	0.89	0.21	3.26	72,76,77,79	0
2	GLC	D	806	11/12	0.83	0.30	3.02	83,84,85,86	0
2	GLC	A	803	12/12	0.83	0.20	2.97	91,92,92,93	0
2	GLC	A	802	11/12	0.95	0.21	1.93	64,69,70,71	0
2	GLC	C	802	11/12	0.89	0.28	1.40	83,84,85,85	0
8	GLC	D	803	11/12	0.94	0.17	1.06	72,74,76,78	0
6	GLC	B	809	11/12	0.89	0.16	0.44	62,69,72,72	0
8	GLC	D	804	11/12	0.92	0.16	-0.04	64,70,71,73	0
2	GLC	D	805	12/12	0.91	0.14	-0.81	77,79,81,81	0
6	GLC	B	805	11/12	0.22	0.68	-	95,96,97,97	11
8	GLC	D	801	12/12	0.80	0.43	-	95,98,98,99	0
5	GLC	D	811	11/12	0.86	0.32	-	68,70,71,73	0
4	GLC	A	810	11/12	0.82	0.30	-	88,90,91,92	0
5	GLC	B	802	11/12	0.72	0.31	-	86,87,88,89	0
6	GLC	B	806	11/12	0.55	0.57	-	92,94,95,95	10
8	GLC	D	802	11/12	0.87	0.35	-	83,91,92,93	0
5	GLC	B	817	11/12	0.85	0.32	-	69,71,73,74	0
2	GLC	A	804	11/12	0.84	0.23	-	90,90,91,92	0
6	GLC	B	807	11/12	0.64	0.34	-	83,87,89,89	4
2	GLC	C	801	12/12	0.91	0.28	-	84,85,86,86	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	A	807	6/6	0.92	0.24	6.48	62,63,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	813	6/6	0.89	0.21	5.34	47,51,53,55	0
7	BGC	B	810	12/12	0.80	0.28	3.22	85,87,89,89	0
3	GOL	A	805	6/6	0.97	0.14	2.29	53,57,59,60	0
3	GOL	B	815	6/6	0.87	0.21	1.93	49,53,53,54	0
3	GOL	A	806	6/6	0.95	0.13	0.93	36,38,40,41	0
3	GOL	B	812	6/6	0.96	0.15	0.50	45,48,49,50	0
3	GOL	B	814	6/6	0.92	0.12	-0.33	72,72,73,74	0
3	GOL	D	808	6/6	0.92	0.12	-0.83	55,59,59,60	0
3	GOL	D	807	6/6	0.95	0.09	-1.65	50,51,52,53	0
3	GOL	B	811	6/6	0.96	0.12	-	47,49,53,55	0
3	GOL	D	809	6/6	0.58	0.27	-	85,86,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.