



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 02:21 PM BST

PDB ID : 4UNI
Title : beta-(1,6)-galactosidase from Bifidobacterium animalis subsp. lactis BI-04 in complex with galactose
Authors : Viborg, A.H.; Fredslund, F.; Katayama, T.; Nielsen, S.K.; Svensson, B.; Kitaoka, M.; Lo Leggio, L.; Abou Hachem, M.
Deposited on : 2014-05-28
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

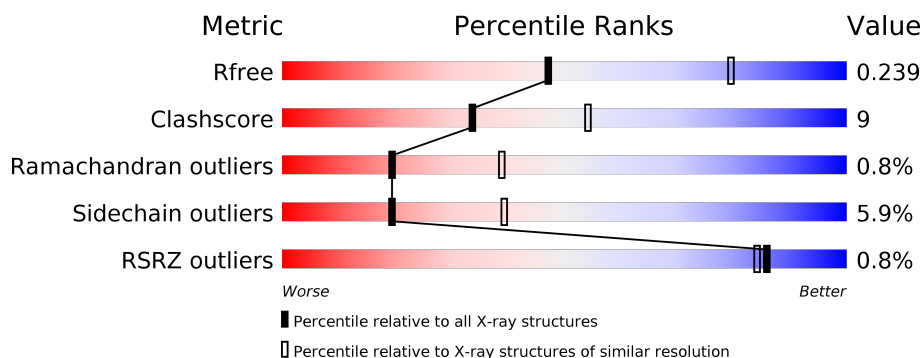
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	695	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% 17% .. </div> </div>
1	B	695	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 77%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 77% 19% .. </div> </div>
1	C	695	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 79%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 18% .. </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	1700	-	-	X	-

2 Entry composition [i](#)

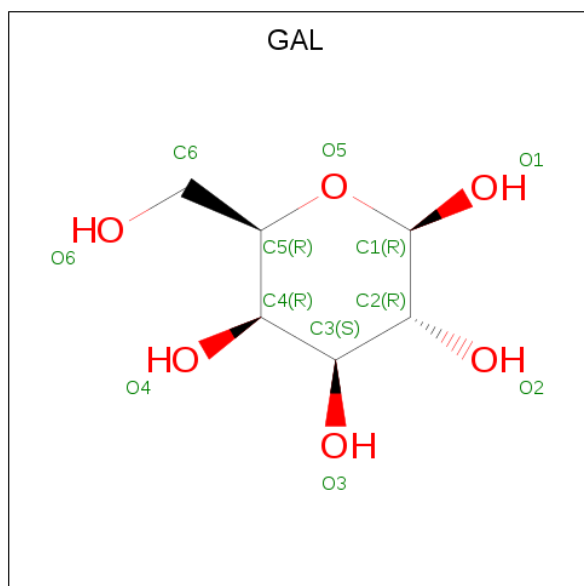
There are 7 unique types of molecules in this entry. The entry contains 32465 atoms, of which 15567 are hydrogens and 0 are deuteriums.

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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	689	Total	C	H	N	O	S	0	0	0
			10600	3462	5123	954	1038	23			
1	B	688	Total	C	H	N	O	S	0	0	0
			10588	3456	5121	951	1037	23			
1	C	687	Total	C	H	N	O	S	0	0	0
			10597	3453	5135	950	1036	23			

- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	12	6		
2	B	1	Total	C	H	O	0	0
			24	6	12	6		
2	C	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



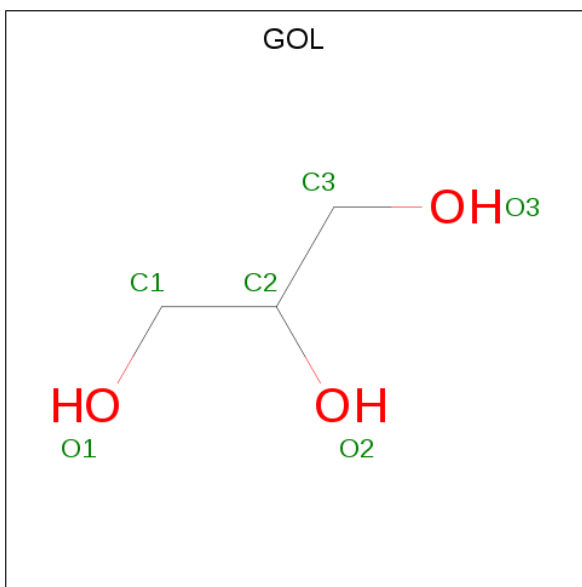
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	A	1	Total	C	H	O	0	0
			24	6	14	4		
3	B	1	Total	C	H	O	0	0
			24	6	14	4		
3	C	1	Total	C	H	O	0	0
			24	6	14	4		
3	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Zn	0	0
			1	1		

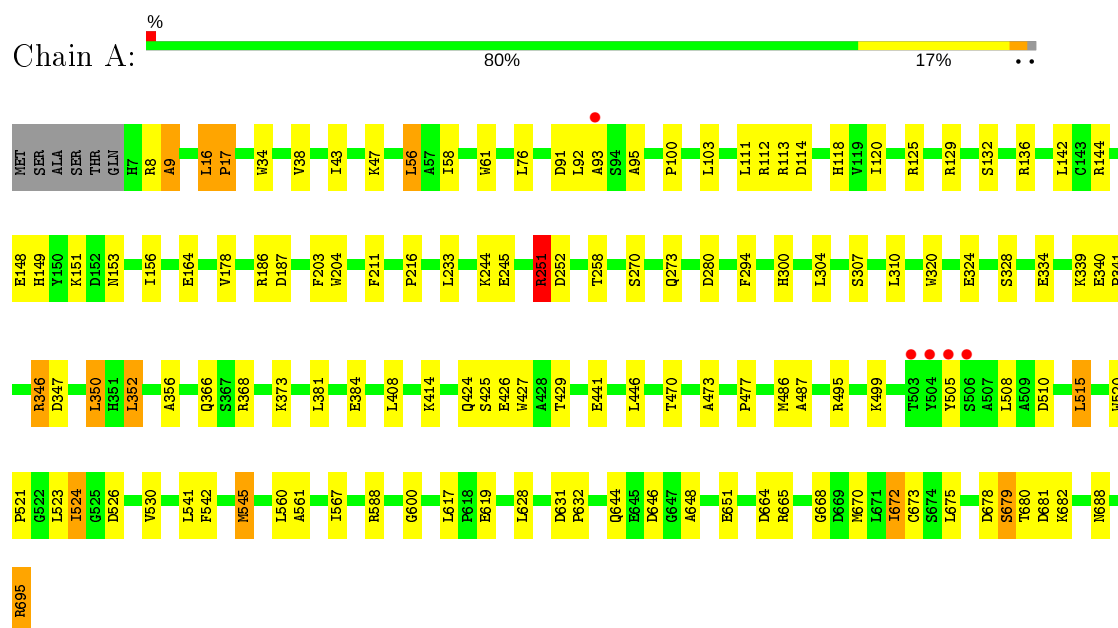
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	155	Total	O	0	0
			155	155		
7	B	95	Total	O	0	0
			95	95		
7	C	97	Total	O	0	0
			97	97		

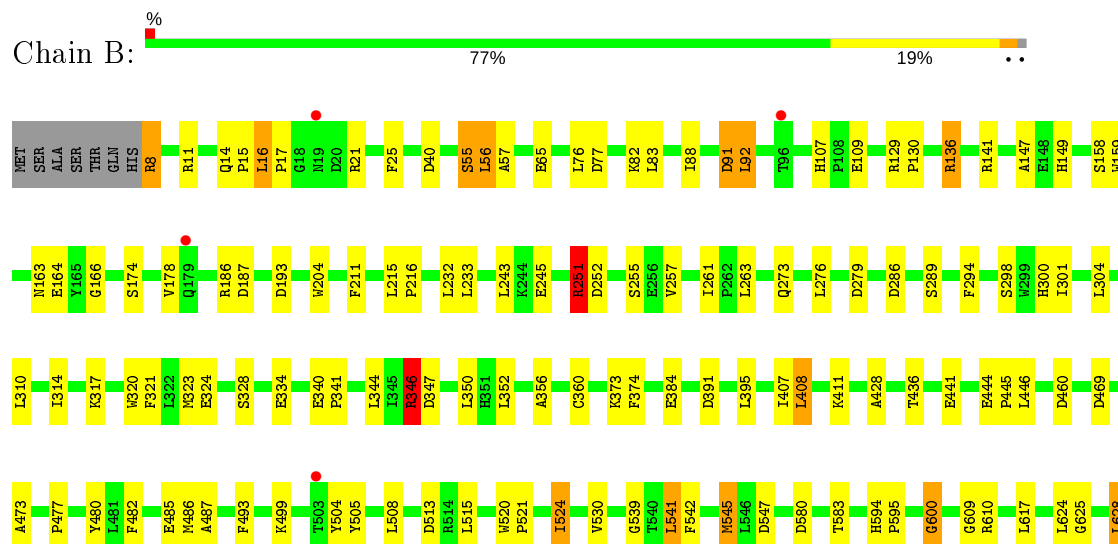
3 Residue-property plots

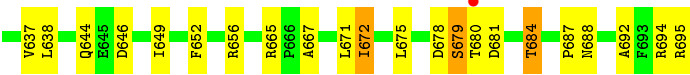
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BETA-GALACTOSIDASE

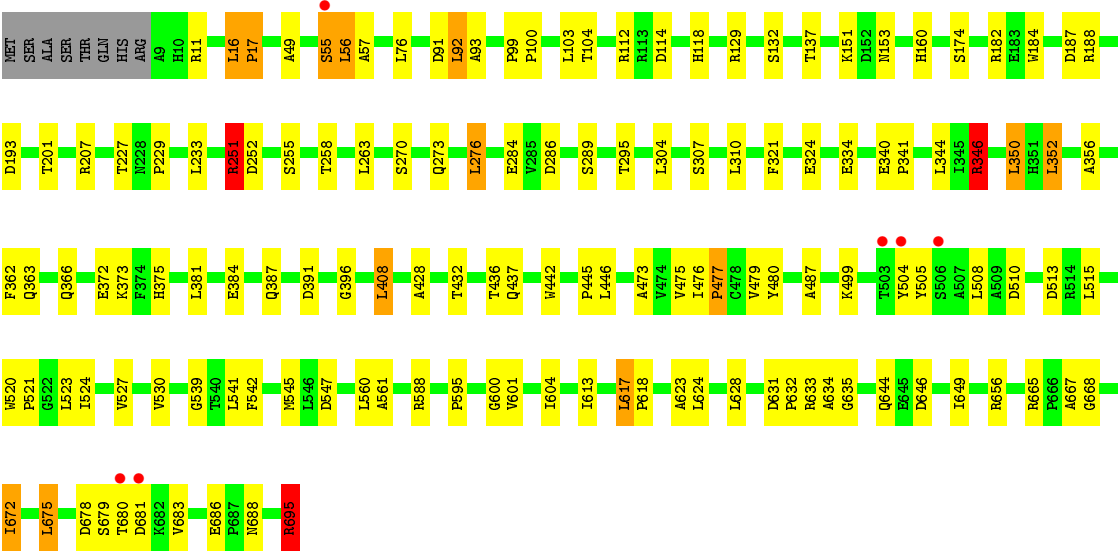
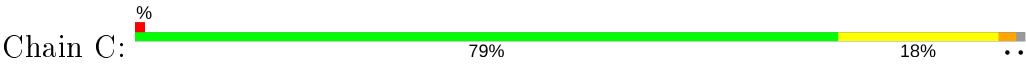


• Molecule 1: BETA-GALACTOSIDASE





● Molecule 1: BETA-GALACTOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.52Å 199.44Å 217.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.60 29.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.73-2.60) 99.6 (29.73-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.175 , 0.234 0.179 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32465	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, 0.333 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: PEG, GOL, ZN, PGE, GAL

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	0.70	0/5632	0.81	4/7679 (0.1%)
1	B	0.73	0/5621	0.84	8/7664 (0.1%)
1	C	0.70	0/5616	0.82	4/7657 (0.1%)
All	All	0.71	0/16869	0.82	16/23000 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	C	695	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	346	ARG	CG-CD-NE	-6.91	97.29	111.80
1	A	346	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	251	ARG	NE-CZ-NH1	6.77	123.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	LEU	Peptide

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	5477	5123	5172	90	0
1	B	5467	5121	5165	99	0
1	C	5462	5135	5163	88	0
2	A	12	12	12	2	0
2	B	12	12	12	3	0
2	C	12	12	12	3	0
3	A	30	42	42	1	0
3	B	10	14	14	0	0
3	C	20	28	28	4	0
4	A	14	20	20	5	0
4	B	7	10	10	0	0
4	C	21	30	30	2	0
5	A	6	8	8	2	0
6	C	1	0	0	0	0
7	A	155	0	0	4	0
7	B	95	0	0	2	0
7	C	97	0	0	5	0
All	All	16898	15567	15688	275	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 9.

The worst 5 of 275 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:14:GLN:OE1	1:B:21:ARG:NH1	2.00	0.94
1:A:8:ARG:O	1:A:9:ALA:HB3	1.81	0.80
1:C:324:GLU:OE1	2:C:1696:GAL:H1	1.84	0.78
1:B:82:LYS:O	7:B:2008:HOH:O	2.01	0.78
1:A:665:ARG:NH2	1:A:668:GLY:O	2.21	0.74

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	687/695 (99%)	657 (96%)	25 (4%)	5 (1%)	22	43
1	B	686/695 (99%)	650 (95%)	30 (4%)	6 (1%)	17	35
1	C	685/695 (99%)	653 (95%)	27 (4%)	5 (1%)	22	43
All	All	2058/2085 (99%)	1960 (95%)	82 (4%)	16 (1%)	19	39

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	GLY
1	B	600	GLY
1	A	477	PRO
1	A	510	ASP
1	B	477	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	A	575/581 (99%)	544 (95%)	31 (5%)	22	44
1	B	574/581 (99%)	539 (94%)	35 (6%)	18	38
1	C	574/581 (99%)	539 (94%)	35 (6%)	18	38
All	All	1723/1743 (99%)	1622 (94%)	101 (6%)	19	39

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	384	GLU
1	B	541	LEU
1	C	646	ASP
1	B	436	THR
1	B	505	TYR

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

Mol	Chain	Res	Type
1	A	535	HIS
1	C	300	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	1700	-	6,6,6	0.61	0	5,5,5	0.55	0
2	GAL	C	1696	-	12,12,12	0.65	0	17,17,17	1.93	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	1696	-	12,12,12	0.64	0	17,17,17	1.70	4 (23%)
5	GOL	A	1702	-	5,5,5	1.27	0	5,5,5	1.20	0
3	PGE	C	1699	-	9,9,9	0.66	0	8,8,8	0.74	0
3	PGE	A	1699	-	9,9,9	0.59	0	8,8,8	0.59	0
2	GAL	A	1696	-	12,12,12	0.78	0	17,17,17	1.79	5 (29%)
3	PGE	A	1697	-	9,9,9	0.70	0	8,8,8	0.41	0
4	PEG	C	1698	-	6,6,6	0.54	0	5,5,5	0.59	0
3	PGE	A	1698	-	9,9,9	0.65	0	8,8,8	0.40	0
4	PEG	A	1701	-	6,6,6	0.63	0	5,5,5	0.42	0
4	PEG	C	1701	-	6,6,6	0.45	0	5,5,5	0.81	0
4	PEG	B	1698	-	6,6,6	0.72	0	5,5,5	1.15	0
4	PEG	C	1700	-	6,6,6	0.57	0	5,5,5	0.58	0
3	PGE	C	1702	-	9,9,9	0.83	0	8,8,8	0.65	0
3	PGE	B	1697	-	9,9,9	0.77	0	8,8,8	0.64	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
4	PEG	A	1700	-	-	3/4/4/4	-
2	GAL	C	1696	-	-	0/2/22/22	0/1/1/1
2	GAL	B	1696	-	-	0/2/22/22	0/1/1/1
5	GOL	A	1702	-	-	4/4/4/4	-
3	PGE	C	1699	-	-	4/7/7/7	-
3	PGE	A	1699	-	-	5/7/7/7	-
2	GAL	A	1696	-	-	0/2/22/22	0/1/1/1
3	PGE	A	1697	-	-	2/7/7/7	-
4	PEG	C	1698	-	-	2/4/4/4	-
3	PGE	A	1698	-	-	0/7/7/7	-
4	PEG	A	1701	-	-	1/4/4/4	-
4	PEG	C	1701	-	-	3/4/4/4	-
4	PEG	B	1698	-	-	1/4/4/4	-
4	PEG	C	1700	-	-	1/4/4/4	-
3	PGE	C	1702	-	-	5/7/7/7	-
3	PGE	B	1697	-	-	3/7/7/7	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1696	GAL	C1-O5-C5	-3.86	106.38	113.66
2	B	1696	GAL	C1-O5-C5	-3.82	106.45	113.66
2	C	1696	GAL	O3-C3-C2	3.45	118.32	110.35
2	A	1696	GAL	O1-C1-O5	-3.43	100.07	110.38
2	B	1696	GAL	C1-C2-C3	-3.30	103.46	110.31

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1702	GOL	C1-C2-C3-O3
5	A	1702	GOL	O2-C2-C3-O3
3	C	1702	PGE	C1-C2-O2-C3
4	C	1698	PEG	O1-C1-C2-O2
3	C	1702	PGE	C3-C4-O3-C5

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1700	PEG	5	0
2	C	1696	GAL	3	0
2	B	1696	GAL	3	0
5	A	1702	GOL	2	0
3	C	1699	PGE	1	0
3	A	1699	PGE	1	0
2	A	1696	GAL	2	0
4	C	1701	PEG	1	0
4	C	1700	PEG	1	0
3	C	1702	PGE	3	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	689/695 (99%)	-0.36	5 (0%) 87 86	31, 44, 62, 94	0
1	B	688/695 (98%)	-0.33	5 (0%) 87 86	31, 47, 67, 95	0
1	C	687/695 (98%)	-0.31	6 (0%) 84 82	32, 46, 64, 95	0
All	All	2064/2085 (98%)	-0.33	16 (0%) 86 84	31, 46, 65, 95	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	THR	3.7
1	A	504	TYR	3.0
1	A	505	TYR	2.8
1	C	504	TYR	2.7
1	C	503	THR	2.7

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](#)

There are no monosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
3	PGE	C	1702	10/10	0.87	0.31	42,52,61,62	0
3	PGE	A	1699	10/10	0.89	0.26	44,55,61,67	0
5	GOL	A	1702	6/6	0.90	0.22	27,33,40,45	0
4	PEG	C	1701	7/7	0.91	0.23	43,51,61,67	0
3	PGE	C	1699	10/10	0.91	0.18	30,47,57,60	0
4	PEG	C	1700	7/7	0.92	0.24	41,50,63,64	0
3	PGE	A	1697	10/10	0.92	0.18	23,44,53,59	0
4	PEG	B	1698	7/7	0.93	0.15	39,49,59,70	0
4	PEG	A	1700	7/7	0.94	0.20	38,48,57,59	0
2	GAL	B	1696	12/12	0.94	0.15	45,58,72,86	0
3	PGE	B	1697	10/10	0.94	0.20	33,44,54,60	0
4	PEG	A	1701	7/7	0.95	0.28	45,54,63,63	0
2	GAL	A	1696	12/12	0.95	0.15	37,49,62,74	0
4	PEG	C	1698	7/7	0.95	0.22	42,50,59,63	0
2	GAL	C	1696	12/12	0.96	0.15	40,49,61,69	0
3	PGE	A	1698	10/10	0.96	0.26	43,54,63,68	0
6	ZN	C	1697	1/1	0.99	0.03	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.