



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:58 pm BST

PDB ID : 5XB7
Title : GH42 alpha-L-arabinopyranosidase from Bifidobacterium animalis subsp. lactis Bl-04
Authors : Viborg, A.H.; Katayama, T.; Arakawa, T.; Abou Hachem, M.; Lo Leggio, L.; Kitaoka, M.; Svensson, B.; Fushinobu, S.
Deposited on : 2017-03-16
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 ⓘ 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	:	2.11
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)	:	2.11

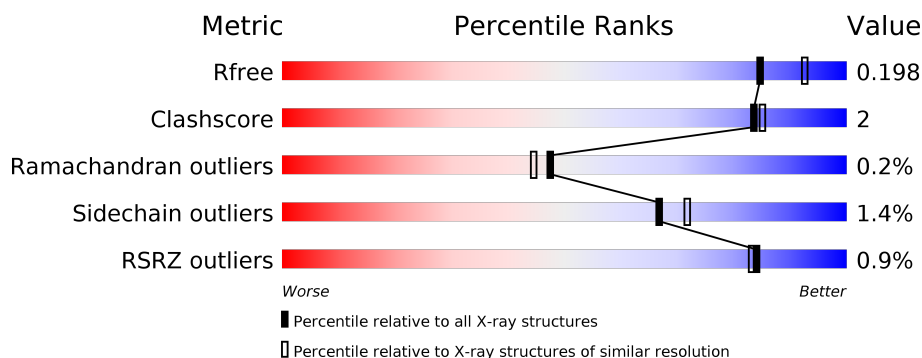
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 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	712	<div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	B	712	<div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	C	712	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	D	712	<div> <div>%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	E	712	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>• •</div> </div>
1	F	712	<div> <div>%</div> <div>90%</div> <div>7%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	803	-	-	X	-
3	GOL	E	803	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35416 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	0	0
			5404	3429	933	1021	21			
1	B	685	Total	C	N	O	S	0	0	0
			5399	3425	930	1023	21			
1	C	682	Total	C	N	O	S	0	0	0
			5381	3415	929	1016	21			
1	D	685	Total	C	N	O	S	0	0	0
			5404	3429	933	1021	21			
1	E	684	Total	C	N	O	S	0	0	0
			5397	3425	932	1019	21			
1	F	698	Total	C	N	O	S	0	0	0
			5493	3480	948	1043	22			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	702	ALA	-	expression tag	UNP A0A1M2TTS0
A	703	ALA	-	expression tag	UNP A0A1M2TTS0
A	704	ALA	-	expression tag	UNP A0A1M2TTS0
A	705	LEU	-	expression tag	UNP A0A1M2TTS0
A	706	GLU	-	expression tag	UNP A0A1M2TTS0
A	707	HIS	-	expression tag	UNP A0A1M2TTS0
A	708	HIS	-	expression tag	UNP A0A1M2TTS0
A	709	HIS	-	expression tag	UNP A0A1M2TTS0
A	710	HIS	-	expression tag	UNP A0A1M2TTS0
A	711	HIS	-	expression tag	UNP A0A1M2TTS0
A	712	HIS	-	expression tag	UNP A0A1M2TTS0
B	702	ALA	-	expression tag	UNP A0A1M2TTS0
B	703	ALA	-	expression tag	UNP A0A1M2TTS0
B	704	ALA	-	expression tag	UNP A0A1M2TTS0
B	705	LEU	-	expression tag	UNP A0A1M2TTS0
B	706	GLU	-	expression tag	UNP A0A1M2TTS0
B	707	HIS	-	expression tag	UNP A0A1M2TTS0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	708	HIS	-	expression tag	UNP A0A1M2TTS0
B	709	HIS	-	expression tag	UNP A0A1M2TTS0
B	710	HIS	-	expression tag	UNP A0A1M2TTS0
B	711	HIS	-	expression tag	UNP A0A1M2TTS0
B	712	HIS	-	expression tag	UNP A0A1M2TTS0
C	702	ALA	-	expression tag	UNP A0A1M2TTS0
C	703	ALA	-	expression tag	UNP A0A1M2TTS0
C	704	ALA	-	expression tag	UNP A0A1M2TTS0
C	705	LEU	-	expression tag	UNP A0A1M2TTS0
C	706	GLU	-	expression tag	UNP A0A1M2TTS0
C	707	HIS	-	expression tag	UNP A0A1M2TTS0
C	708	HIS	-	expression tag	UNP A0A1M2TTS0
C	709	HIS	-	expression tag	UNP A0A1M2TTS0
C	710	HIS	-	expression tag	UNP A0A1M2TTS0
C	711	HIS	-	expression tag	UNP A0A1M2TTS0
C	712	HIS	-	expression tag	UNP A0A1M2TTS0
D	702	ALA	-	expression tag	UNP A0A1M2TTS0
D	703	ALA	-	expression tag	UNP A0A1M2TTS0
D	704	ALA	-	expression tag	UNP A0A1M2TTS0
D	705	LEU	-	expression tag	UNP A0A1M2TTS0
D	706	GLU	-	expression tag	UNP A0A1M2TTS0
D	707	HIS	-	expression tag	UNP A0A1M2TTS0
D	708	HIS	-	expression tag	UNP A0A1M2TTS0
D	709	HIS	-	expression tag	UNP A0A1M2TTS0
D	710	HIS	-	expression tag	UNP A0A1M2TTS0
D	711	HIS	-	expression tag	UNP A0A1M2TTS0
D	712	HIS	-	expression tag	UNP A0A1M2TTS0
E	702	ALA	-	expression tag	UNP A0A1M2TTS0
E	703	ALA	-	expression tag	UNP A0A1M2TTS0
E	704	ALA	-	expression tag	UNP A0A1M2TTS0
E	705	LEU	-	expression tag	UNP A0A1M2TTS0
E	706	GLU	-	expression tag	UNP A0A1M2TTS0
E	707	HIS	-	expression tag	UNP A0A1M2TTS0
E	708	HIS	-	expression tag	UNP A0A1M2TTS0
E	709	HIS	-	expression tag	UNP A0A1M2TTS0
E	710	HIS	-	expression tag	UNP A0A1M2TTS0
E	711	HIS	-	expression tag	UNP A0A1M2TTS0
E	712	HIS	-	expression tag	UNP A0A1M2TTS0
F	702	ALA	-	expression tag	UNP A0A1M2TTS0
F	703	ALA	-	expression tag	UNP A0A1M2TTS0
F	704	ALA	-	expression tag	UNP A0A1M2TTS0
F	705	LEU	-	expression tag	UNP A0A1M2TTS0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	706	GLU	-	expression tag	UNP A0A1M2TTS0
F	707	HIS	-	expression tag	UNP A0A1M2TTS0
F	708	HIS	-	expression tag	UNP A0A1M2TTS0
F	709	HIS	-	expression tag	UNP A0A1M2TTS0
F	710	HIS	-	expression tag	UNP A0A1M2TTS0
F	711	HIS	-	expression tag	UNP A0A1M2TTS0
F	712	HIS	-	expression tag	UNP A0A1M2TTS0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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		

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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	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	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	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

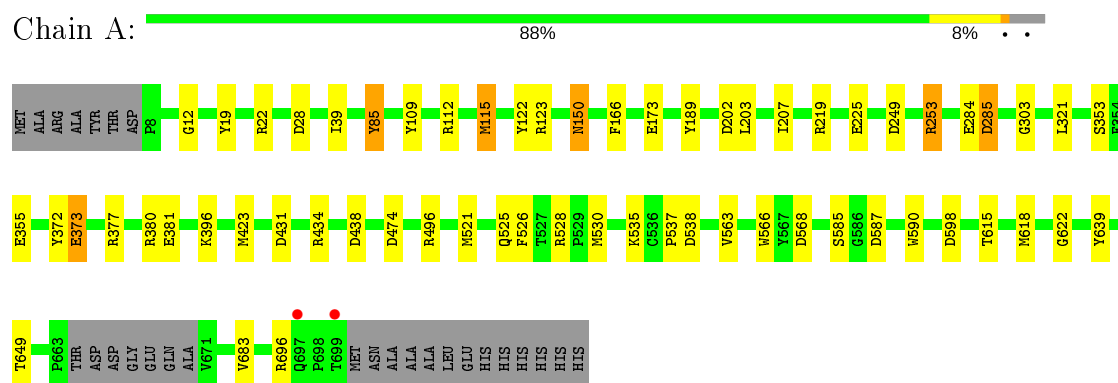
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	435	Total	O	0	0
			435	435		
4	B	459	Total	O	0	0
			459	459		
4	C	388	Total	O	0	0
			388	388		
4	D	383	Total	O	0	0
			383	383		
4	E	386	Total	O	0	0
			386	386		
4	F	477	Total	O	0	0
			477	477		

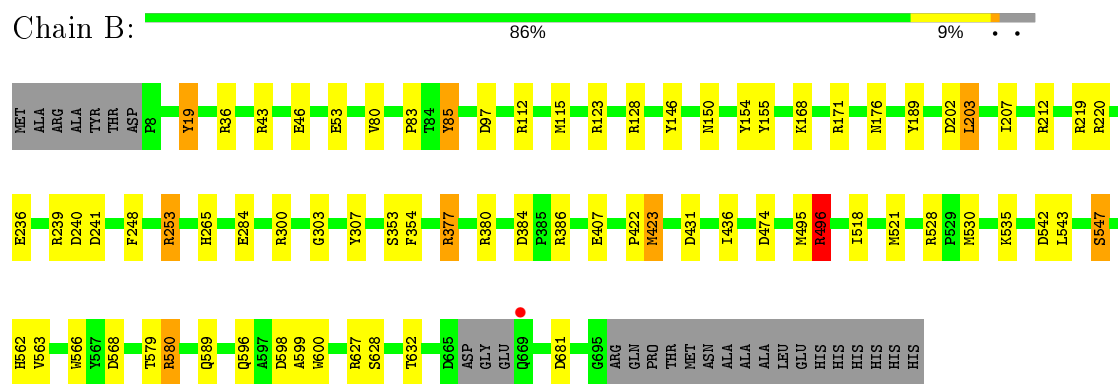
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

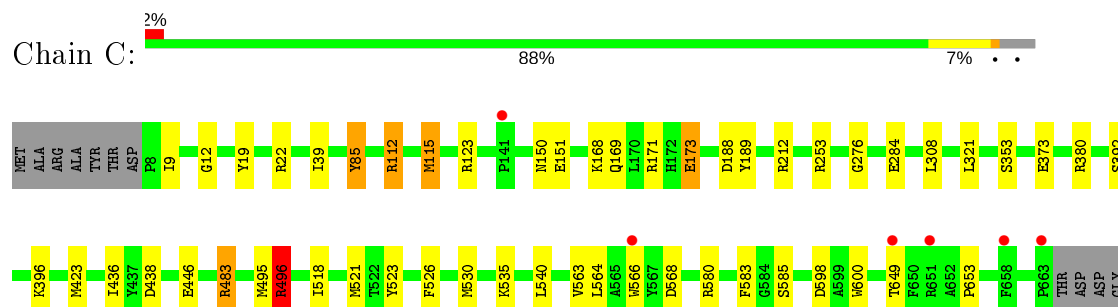
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase

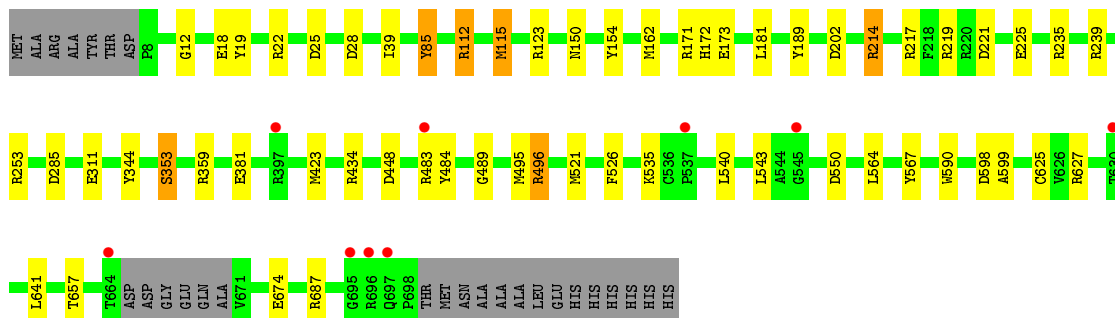
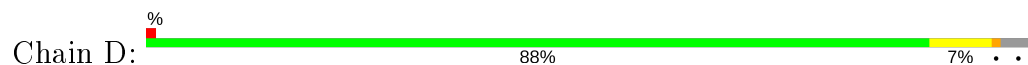


• Molecule 1: Beta-galactosidase

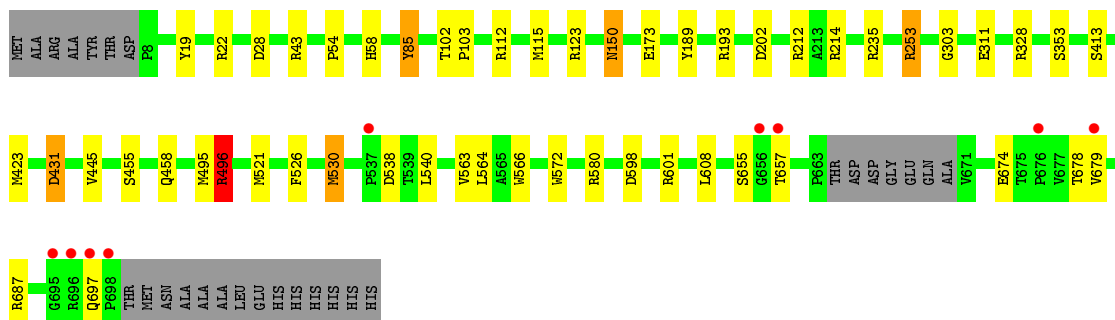
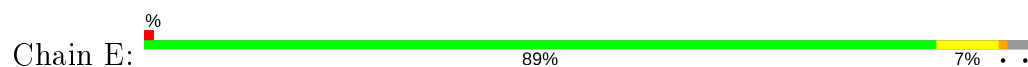




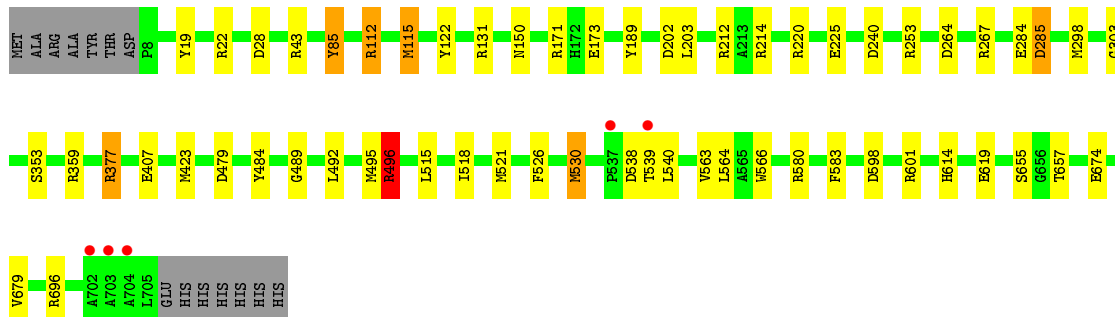
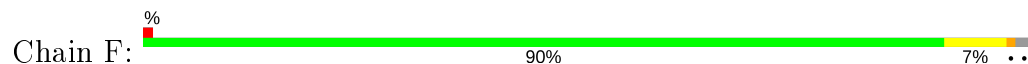
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.95Å 177.95Å 375.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.00 49.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.37-2.00) 100.0 (49.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.155 , 0.191 0.166 , 0.198	Depositor DCC
R_{free} test set	20004 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35416	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: GOL, SO4

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	1.19	12/5558 (0.2%)	1.06	21/7588 (0.3%)
1	B	1.10	6/5552 (0.1%)	1.05	30/7580 (0.4%)
1	C	1.08	4/5534 (0.1%)	1.02	18/7554 (0.2%)
1	D	1.13	9/5558 (0.2%)	1.05	28/7588 (0.4%)
1	E	1.07	3/5551 (0.1%)	1.02	26/7578 (0.3%)
1	F	1.05	4/5648 (0.1%)	1.08	33/7712 (0.4%)
All	All	1.10	38/33401 (0.1%)	1.05	156/45600 (0.3%)

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	ARG	CZ-NH2	7.97	1.43	1.33
1	C	523	TYR	CE1-CZ	7.14	1.47	1.38
1	D	225	GLU	CG-CD	7.07	1.62	1.51
1	A	381	GLU	CD-OE2	-6.72	1.18	1.25
1	A	225	GLU	CG-CD	6.66	1.61	1.51

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	C	123	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	C	496	ARG	NE-CZ-NH1	-9.17	115.72	120.30
1	D	123	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	E	687	ARG	NE-CZ-NH2	-8.97	115.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5404	0	5117	24	0
1	B	5399	0	5106	39	0
1	C	5381	0	5095	24	0
1	D	5404	0	5117	20	0
1	E	5397	0	5110	21	0
1	F	5493	0	5196	29	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	15	0	0	0	0
3	A	48	0	64	2	0
3	B	72	0	96	10	0
3	C	54	0	72	7	0
3	D	42	0	56	1	0
3	E	48	0	63	1	0
3	F	66	0	88	3	0
4	A	435	0	0	4	0
4	B	459	0	0	3	0
4	C	388	0	0	7	0
4	D	383	0	0	4	0
4	E	386	0	0	2	0
4	F	477	0	0	5	0
All	All	35416	0	31180	153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 153 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:F:614:HIS:HB3	4:F:1289:HOH:O	1.57	1.02
1:B:155:TYR:HA	3:B:806:GOL:H32	1.55	0.88
3:C:803:GOL:H32	4:C:1041:HOH:O	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:HG2	4:A:1286:HOH:O	1.81	0.79
1:A:173:GLU:HB2	4:A:908:HOH:O	1.82	0.78

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	681/712 (96%)	651 (96%)	29 (4%)	1 (0%)	51	49
1	B	681/712 (96%)	654 (96%)	26 (4%)	1 (0%)	51	49
1	C	678/712 (95%)	652 (96%)	25 (4%)	1 (0%)	51	49
1	D	681/712 (96%)	652 (96%)	28 (4%)	1 (0%)	51	49
1	E	680/712 (96%)	654 (96%)	24 (4%)	2 (0%)	41	37
1	F	696/712 (98%)	668 (96%)	26 (4%)	2 (0%)	41	37
All	All	4097/4272 (96%)	3931 (96%)	158 (4%)	8 (0%)	47	44

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	353	SER
1	B	353	SER
1	E	538	ASP
1	F	353	SER
1	A	353	SER

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	560/580 (97%)	551 (98%)	9 (2%)	62	67
1	B	559/580 (96%)	552 (99%)	7 (1%)	69	74
1	C	557/580 (96%)	548 (98%)	9 (2%)	62	67
1	D	560/580 (97%)	553 (99%)	7 (1%)	69	74
1	E	559/580 (96%)	552 (99%)	7 (1%)	69	74
1	F	568/580 (98%)	560 (99%)	8 (1%)	67	72
All	All	3363/3480 (97%)	3316 (99%)	47 (1%)	67	72

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	521	MET
1	D	115	MET
1	F	496	ARG
1	C	653	PRO
1	D	353	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

71 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	D	805	-	5,5,5	0.48	0	5,5,5	1.41	1 (20%)
3	GOL	C	808	-	5,5,5	0.84	0	5,5,5	1.57	2 (40%)
3	GOL	C	803	-	5,5,5	1.36	1 (20%)	5,5,5	1.10	0
2	SO4	C	802	-	4,4,4	0.40	0	6,6,6	0.70	0
3	GOL	A	803	-	5,5,5	0.85	0	5,5,5	2.78	3 (60%)
3	GOL	B	809	-	5,5,5	0.28	0	5,5,5	1.58	1 (20%)
3	GOL	F	813	-	5,5,5	0.58	0	5,5,5	0.84	0
3	GOL	F	810	-	5,5,5	0.73	0	5,5,5	0.90	0
3	GOL	B	810	-	5,5,5	0.76	0	5,5,5	1.33	1 (20%)
3	GOL	F	808	-	5,5,5	0.64	0	5,5,5	1.05	0
2	SO4	F	801	-	4,4,4	0.57	0	6,6,6	1.45	2 (33%)
3	GOL	C	806	-	5,5,5	1.21	1 (20%)	5,5,5	1.31	1 (20%)
3	GOL	B	806	-	5,5,5	0.67	0	5,5,5	1.37	1 (20%)
3	GOL	F	812	-	5,5,5	0.43	0	5,5,5	0.80	0
3	GOL	D	803	-	5,5,5	1.05	0	5,5,5	1.69	1 (20%)
3	GOL	E	810	-	5,5,5	0.54	0	5,5,5	0.87	0
3	GOL	F	805	-	5,5,5	0.60	0	5,5,5	0.51	0
2	SO4	E	801	-	4,4,4	0.18	0	6,6,6	1.43	2 (33%)
2	SO4	D	802	-	4,4,4	0.42	0	6,6,6	0.67	0
3	GOL	C	804	-	5,5,5	0.63	0	5,5,5	1.56	1 (20%)
3	GOL	B	804	-	5,5,5	0.99	0	5,5,5	0.98	0
2	SO4	E	802	-	4,4,4	0.42	0	6,6,6	1.27	1 (16%)
3	GOL	A	809	-	5,5,5	0.63	0	5,5,5	0.46	0
3	GOL	B	807	-	5,5,5	0.41	0	5,5,5	0.94	0
3	GOL	C	809	-	5,5,5	0.46	0	5,5,5	1.39	1 (20%)
3	GOL	A	805	-	5,5,5	0.72	0	5,5,5	2.17	2 (40%)
2	SO4	B	816	-	4,4,4	0.39	0	6,6,6	0.86	0
3	GOL	E	808	-	5,5,5	0.40	0	5,5,5	0.60	0
3	GOL	E	809	-	5,5,5	0.32	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	810	-	4,4,4	0.46	0	6,6,6	0.48	0
3	GOL	A	802	-	5,5,5	1.29	1 (20%)	5,5,5	0.89	0
3	GOL	F	806	-	5,5,5	0.67	0	5,5,5	1.24	1 (20%)
2	SO4	F	814	-	4,4,4	0.44	0	6,6,6	0.57	0
3	GOL	B	805	-	5,5,5	0.75	0	5,5,5	1.57	1 (20%)
3	GOL	A	807	-	5,5,5	0.30	0	5,5,5	0.49	0
3	GOL	B	812	-	5,5,5	0.39	0	5,5,5	0.88	0
3	GOL	C	810	-	5,5,5	0.64	0	5,5,5	1.46	1 (20%)
3	GOL	C	807	-	5,5,5	0.71	0	5,5,5	1.64	1 (20%)
3	GOL	F	809	-	5,5,5	0.29	0	5,5,5	1.33	1 (20%)
3	GOL	E	804	-	5,5,5	0.33	0	5,5,5	1.45	1 (20%)
2	SO4	C	801	-	4,4,4	0.16	0	6,6,6	1.46	1 (16%)
2	SO4	F	802	-	4,4,4	0.34	0	6,6,6	0.33	0
3	GOL	D	809	-	5,5,5	0.45	0	5,5,5	0.70	0
3	GOL	D	804	-	5,5,5	0.40	0	5,5,5	0.57	0
3	GOL	D	808	-	5,5,5	0.43	0	5,5,5	0.82	0
2	SO4	D	801	-	4,4,4	0.14	0	6,6,6	1.21	1 (16%)
3	GOL	F	803	-	5,5,5	1.36	1 (20%)	5,5,5	1.17	1 (20%)
3	GOL	B	815	-	5,5,5	0.70	0	5,5,5	1.30	0
3	GOL	C	811	-	5,5,5	0.50	0	5,5,5	0.84	0
3	GOL	F	804	-	5,5,5	0.60	0	5,5,5	2.01	1 (20%)
3	GOL	E	806	-	5,5,5	1.03	1 (20%)	5,5,5	2.15	2 (40%)
3	GOL	B	811	-	5,5,5	0.69	0	5,5,5	0.90	0
2	SO4	B	803	-	4,4,4	0.34	0	6,6,6	0.78	0
3	GOL	D	806	-	5,5,5	0.56	0	5,5,5	1.82	2 (40%)
2	SO4	A	801	-	4,4,4	0.38	0	6,6,6	1.15	1 (16%)
3	GOL	A	808	-	5,5,5	0.34	0	5,5,5	0.63	0
3	GOL	E	803	-	5,5,5	1.39	1 (20%)	5,5,5	3.10	3 (60%)
3	GOL	A	804	-	5,5,5	0.94	0	5,5,5	1.14	1 (20%)
2	SO4	B	802	-	4,4,4	0.45	0	6,6,6	0.42	0
3	GOL	E	807	-	5,5,5	0.52	0	5,5,5	1.94	2 (40%)
2	SO4	E	811	-	4,4,4	0.41	0	6,6,6	0.44	0
3	GOL	B	814	-	5,5,5	0.52	0	5,5,5	1.39	1 (20%)
3	GOL	B	813	-	5,5,5	0.88	0	5,5,5	2.08	2 (40%)
2	SO4	B	801	-	4,4,4	0.61	0	6,6,6	1.44	1 (16%)
3	GOL	F	807	-	5,5,5	0.61	0	5,5,5	2.08	2 (40%)
3	GOL	C	805	-	5,5,5	0.81	0	5,5,5	0.91	0
3	GOL	D	807	-	5,5,5	0.34	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	805	-	5,5,5	0.81	0	5,5,5	1.37	0
3	GOL	B	808	-	5,5,5	0.64	0	5,5,5	1.22	0
3	GOL	A	806	-	5,5,5	0.53	0	5,5,5	1.14	0
3	GOL	F	811	-	5,5,5	1.05	1 (20%)	5,5,5	2.44	2 (40%)

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	D	805	-	-	2/4/4/4	-
3	GOL	C	808	-	-	2/4/4/4	-
3	GOL	C	803	-	-	0/4/4/4	-
3	GOL	D	809	-	-	4/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	E	809	-	-	0/4/4/4	-
3	GOL	F	813	-	-	0/4/4/4	-
3	GOL	F	810	-	-	0/4/4/4	-
3	GOL	B	810	-	-	4/4/4/4	-
3	GOL	F	808	-	-	2/4/4/4	-
3	GOL	C	806	-	-	2/4/4/4	-
3	GOL	B	806	-	-	4/4/4/4	-
3	GOL	F	812	-	-	2/4/4/4	-
3	GOL	E	810	-	-	4/4/4/4	-
3	GOL	F	805	-	-	2/4/4/4	-
3	GOL	E	807	-	-	2/4/4/4	-
3	GOL	C	804	-	-	0/4/4/4	-
3	GOL	B	804	-	-	0/4/4/4	-
3	GOL	B	809	-	-	1/4/4/4	-
3	GOL	A	809	-	-	0/4/4/4	-
3	GOL	B	807	-	-	3/4/4/4	-
3	GOL	C	809	-	-	2/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	F	806	-	-	4/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	A	807	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	812	-	-	2/4/4/4	-
3	GOL	C	810	-	-	3/4/4/4	-
3	GOL	F	809	-	-	4/4/4/4	-
3	GOL	E	804	-	-	2/4/4/4	-
3	GOL	D	804	-	-	1/4/4/4	-
3	GOL	F	803	-	-	0/4/4/4	-
3	GOL	F	804	-	-	2/4/4/4	-
3	GOL	D	808	-	-	3/4/4/4	-
3	GOL	B	815	-	-	2/4/4/4	-
3	GOL	C	811	-	-	2/4/4/4	-
3	GOL	E	806	-	-	1/4/4/4	-
3	GOL	B	811	-	-	4/4/4/4	-
3	GOL	E	808	-	-	2/4/4/4	-
3	GOL	D	806	-	-	2/4/4/4	-
3	GOL	C	807	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	E	803	-	-	3/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-
3	GOL	B	814	-	-	2/4/4/4	-
3	GOL	B	813	-	-	3/4/4/4	-
3	GOL	D	803	-	-	0/4/4/4	-
3	GOL	F	807	-	-	2/4/4/4	-
3	GOL	C	805	-	-	2/4/4/4	-
3	GOL	D	807	-	-	0/4/4/4	-
3	GOL	E	805	-	-	0/4/4/4	-
3	GOL	B	808	-	-	2/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	F	811	-	-	2/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	GOL	C1-C2	2.49	1.62	1.51
3	F	803	GOL	O1-C1	2.34	1.52	1.42
3	E	803	GOL	O3-C3	2.26	1.52	1.42
3	C	803	GOL	C1-C2	2.19	1.60	1.51
3	E	806	GOL	O2-C2	-2.10	1.37	1.43

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	803	GOL	O2-C2-C1	5.45	133.15	109.12
3	A	803	GOL	O1-C1-C2	-4.38	89.19	110.20
3	A	805	GOL	O2-C2-C1	-3.80	92.40	109.12
3	F	807	GOL	O2-C2-C1	-3.78	92.47	109.12
3	F	811	GOL	C3-C2-C1	3.56	125.56	111.70

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	805	GOL	O1-C1-C2-C3
3	C	808	GOL	C1-C2-C3-O3
3	C	808	GOL	O2-C2-C3-O3
3	A	803	GOL	C1-C2-C3-O3
3	B	810	GOL	O1-C1-C2-C3

There are no ring outliers.

15 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	803	GOL	4	0
3	A	803	GOL	1	0
3	B	809	GOL	3	0
3	C	806	GOL	1	0
3	B	806	GOL	3	0
3	F	805	GOL	1	0
3	B	807	GOL	3	0
3	C	809	GOL	2	0
3	F	806	GOL	1	0
3	C	810	GOL	2	0
3	F	809	GOL	1	0
3	D	809	GOL	1	0
3	E	803	GOL	1	0
3	B	808	GOL	1	0
3	A	806	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	685/712 (96%)	-0.46	2 (0%) 94 93	17, 25, 38, 61	0
1	B	685/712 (96%)	-0.48	1 (0%) 95 95	17, 23, 36, 58	0
1	C	682/712 (95%)	-0.28	13 (1%) 66 65	16, 27, 43, 65	0
1	D	685/712 (96%)	-0.21	9 (1%) 77 76	17, 27, 44, 68	0
1	E	684/712 (96%)	-0.38	9 (1%) 77 76	17, 26, 41, 64	0
1	F	698/712 (98%)	-0.51	5 (0%) 87 87	16, 23, 39, 58	0
All	All	4119/4272 (96%)	-0.39	39 (0%) 84 83	16, 25, 41, 68	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	697	GLN	4.6
1	A	697	GLN	3.4
1	C	651	ARG	3.3
1	E	697	GLN	3.3
1	D	664	THR	3.2

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](#)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	GOL	F	813	6/6	0.60	0.24	51,65,66,67	0
3	GOL	B	808	6/6	0.74	0.31	52,55,66,70	0
3	GOL	D	804	6/6	0.76	0.25	53,57,59,62	0
3	GOL	B	811	6/6	0.77	0.23	48,54,57,62	0
3	GOL	C	806	6/6	0.78	0.27	38,47,53,56	0
3	GOL	B	809	6/6	0.78	0.28	41,46,52,55	0
3	GOL	C	805	6/6	0.81	0.18	38,61,62,62	0
3	GOL	A	809	6/6	0.81	0.20	55,59,63,65	0
3	GOL	D	807	6/6	0.82	0.21	52,57,61,63	0
3	GOL	E	809	6/6	0.83	0.23	56,62,63,69	0
3	GOL	F	810	6/6	0.83	0.32	49,54,58,60	0
3	GOL	C	808	6/6	0.84	0.20	48,49,52,55	0
3	GOL	F	805	6/6	0.84	0.31	45,53,56,63	0
3	GOL	A	807	6/6	0.84	0.22	48,51,54,73	0
3	GOL	C	810	6/6	0.84	0.22	40,57,60,63	0
3	GOL	D	809	6/6	0.84	0.15	45,57,59,67	0
3	GOL	A	804	6/6	0.85	0.17	49,54,55,56	0
3	GOL	B	806	6/6	0.85	0.25	42,50,53,60	0
3	GOL	E	808	6/6	0.85	0.15	48,52,60,62	0
3	GOL	A	808	6/6	0.85	0.13	52,58,60,66	0
3	GOL	B	810	6/6	0.86	0.30	50,54,61,65	0
3	GOL	B	814	6/6	0.86	0.21	50,54,57,64	0
3	GOL	E	810	6/6	0.86	0.19	45,47,52,63	0
3	GOL	B	807	6/6	0.86	0.17	43,56,61,62	0
3	GOL	A	805	6/6	0.86	0.17	39,58,62,62	0
3	GOL	F	808	6/6	0.87	0.15	36,50,51,53	0
3	GOL	D	806	6/6	0.87	0.18	34,50,54,55	0
3	GOL	A	806	6/6	0.87	0.20	47,56,59,60	0
3	GOL	C	811	6/6	0.89	0.18	52,56,58,59	0
3	GOL	F	809	6/6	0.90	0.27	38,53,59,59	0
3	GOL	B	815	6/6	0.90	0.26	32,53,57,65	0
3	GOL	C	804	6/6	0.90	0.15	38,41,45,47	0
3	GOL	D	808	6/6	0.91	0.16	32,37,47,55	0
3	GOL	F	806	6/6	0.91	0.12	35,46,56,57	0
3	GOL	B	812	6/6	0.91	0.27	36,42,52,56	0
3	GOL	F	807	6/6	0.92	0.17	42,51,52,53	0
3	GOL	C	807	6/6	0.92	0.17	32,50,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	803	6/6	0.92	0.20	34,47,49,54	0
3	GOL	E	805	6/6	0.92	0.20	35,42,46,50	0
3	GOL	C	809	6/6	0.92	0.14	36,47,53,55	0
3	GOL	F	812	6/6	0.92	0.18	33,38,49,67	0
2	SO4	A	810	5/5	0.93	0.27	56,60,73,75	0
3	GOL	D	803	6/6	0.93	0.15	22,22,23,29	0
2	SO4	D	802	5/5	0.93	0.30	60,61,65,77	0
3	GOL	D	805	6/6	0.93	0.15	37,42,46,54	0
3	GOL	E	807	6/6	0.93	0.19	35,45,50,51	0
3	GOL	F	804	6/6	0.93	0.14	29,35,41,45	0
3	GOL	F	811	6/6	0.93	0.15	32,49,56,56	0
3	GOL	E	804	6/6	0.94	0.13	34,41,44,48	0
3	GOL	B	805	6/6	0.94	0.14	29,37,41,49	0
3	GOL	A	802	6/6	0.94	0.14	21,27,28,29	0
2	SO4	B	802	5/5	0.94	0.30	48,54,55,63	0
2	SO4	F	814	5/5	0.94	0.24	51,54,60,69	0
2	SO4	B	803	5/5	0.94	0.22	48,55,62,69	0
3	GOL	B	813	6/6	0.94	0.14	32,48,52,59	0
2	SO4	B	816	5/5	0.95	0.20	54,57,66,71	0
3	GOL	E	806	6/6	0.95	0.14	35,49,57,59	0
3	GOL	F	803	6/6	0.95	0.14	20,24,24,29	0
3	GOL	C	803	6/6	0.96	0.12	23,27,29,34	0
2	SO4	C	802	5/5	0.96	0.16	52,56,61,65	0
2	SO4	E	802	5/5	0.96	0.15	36,42,48,52	0
3	GOL	E	803	6/6	0.96	0.11	21,23,25,26	0
3	GOL	B	804	6/6	0.97	0.15	20,24,25,28	0
2	SO4	F	802	5/5	0.97	0.23	54,62,66,71	0
2	SO4	E	811	5/5	0.97	0.15	51,53,62,68	0
2	SO4	D	801	5/5	0.98	0.08	35,42,49,51	0
2	SO4	E	801	5/5	0.98	0.11	33,36,38,39	0
2	SO4	B	801	5/5	0.99	0.07	30,38,42,43	0
2	SO4	A	801	5/5	0.99	0.08	36,37,41,45	0
2	SO4	C	801	5/5	0.99	0.08	31,37,41,44	0
2	SO4	F	801	5/5	0.99	0.08	31,36,39,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.