



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 01:42 PM JST

PDB ID : 5XB7
Title : GH42 alpha-L-arabinopyranosidase from Bifidobacterium animalis subsp. lactis BI-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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

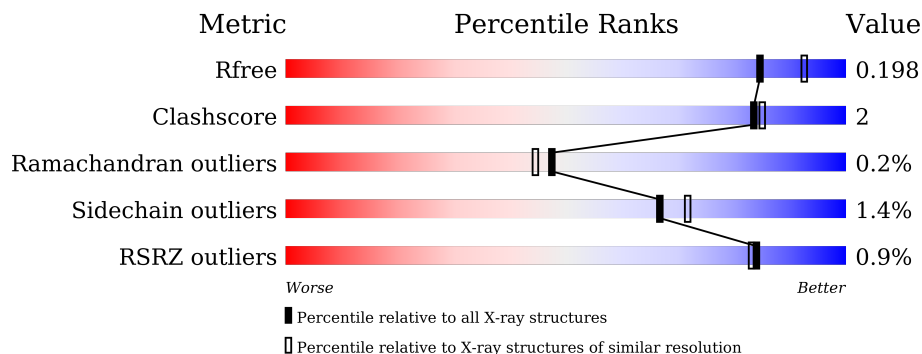
1 Overall quality at a glance

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 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 $\leq 5\%$. 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	 88% 8% . .
1	B	712	 86% 9% . .
1	C	712	 2% 88% 7% . .
1	D	712	 % 88% 7% . .
1	E	712	 % 89% 7% . .
1	F	712	 % 90% 7% . .

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 [i](#)

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

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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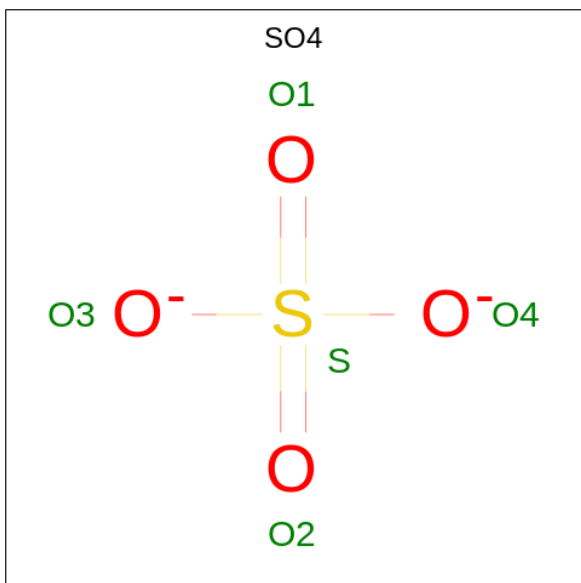
Chain	Residue	Modelled	Actual	Comment	Reference
B	708	HIS	-	expression tag	UNP A0A1M2TTS0
B	709	HIS	-	expression tag	UNP A0A1M2TTS0
B	710	HIS	-	expression tag	UNP A0A1M2TTS0
B	711	HIS	-	expression tag	UNP A0A1M2TTS0
B	712	HIS	-	expression tag	UNP A0A1M2TTS0
C	702	ALA	-	expression tag	UNP A0A1M2TTS0
C	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).



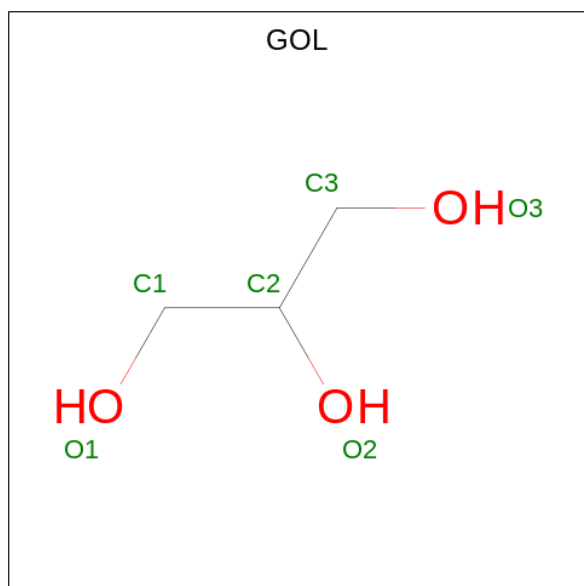
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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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		

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

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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 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

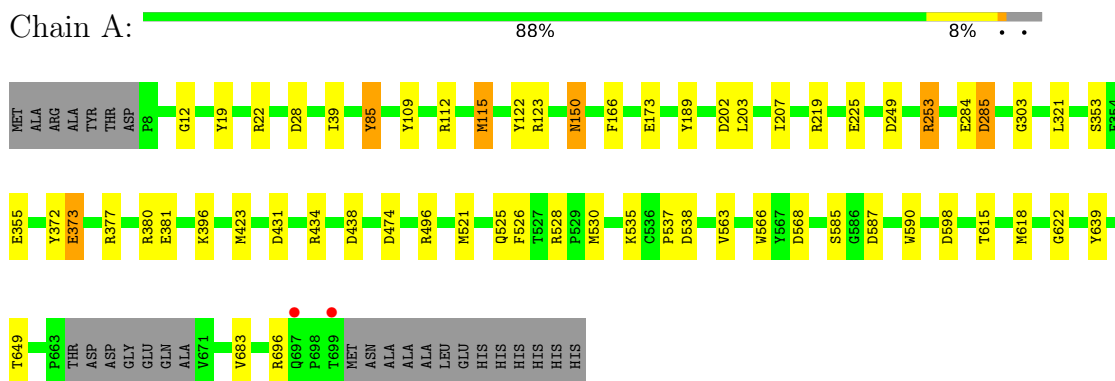
- Molecule 4 is water.

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

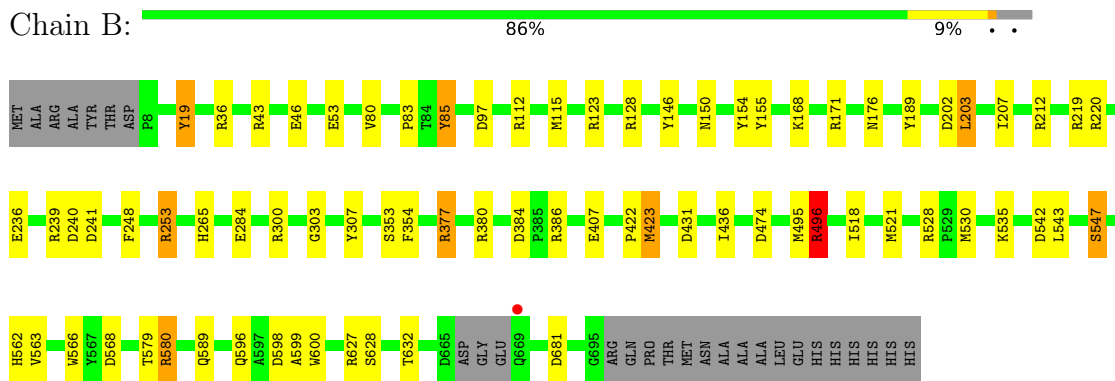
3 Residue-property plots

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.

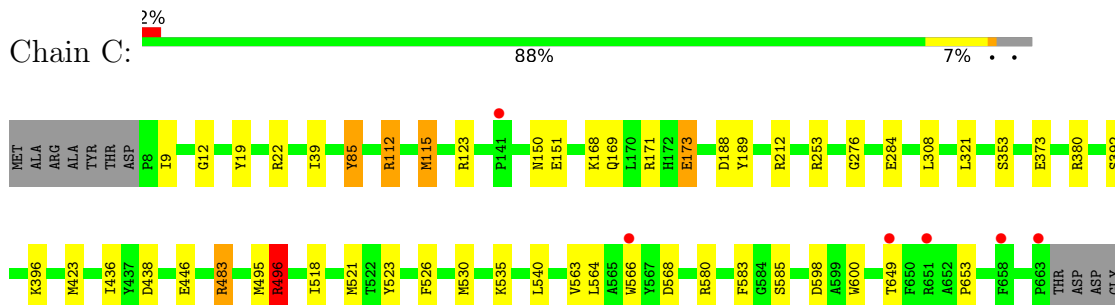
- Molecule 1: Beta-galactosidase



- Molecule 1: Beta-galactosidase

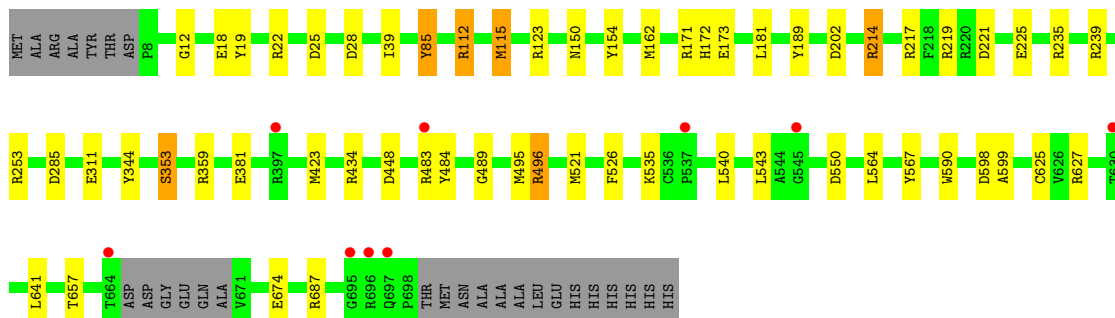
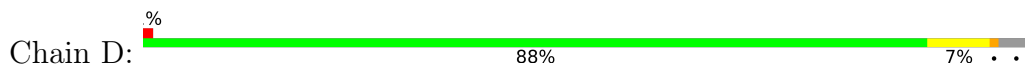


- Molecule 1: Beta-galactosidase

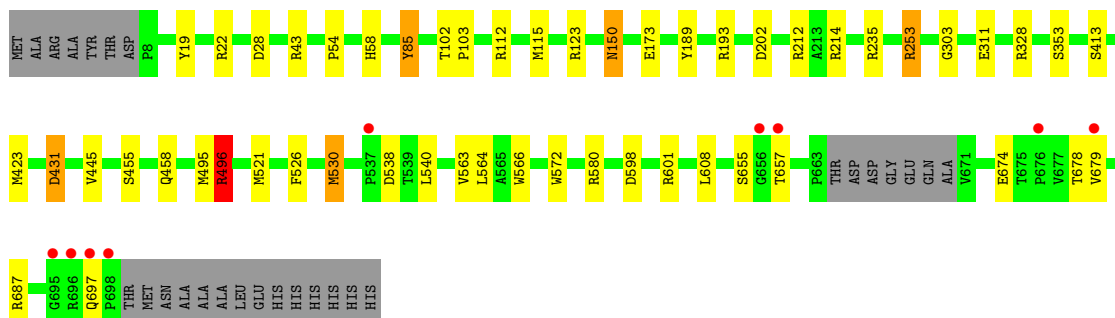
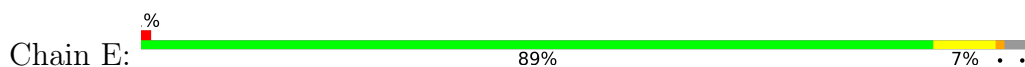




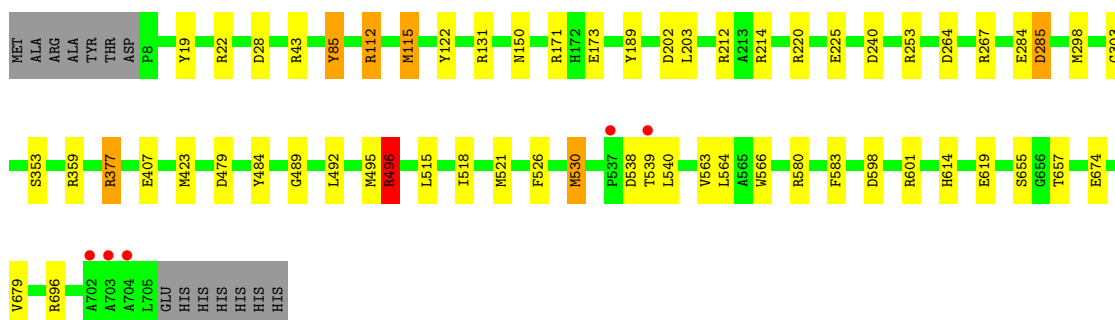
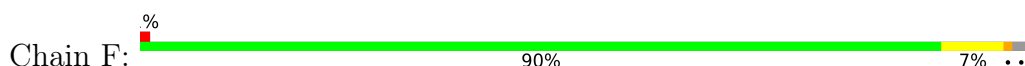
• Molecule 1: Beta-galactosidase



• 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)	Xtrriage
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	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: SO4, GOL

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%)

All (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
1	D	590	TRP	CB-CG	6.37	1.61	1.50
1	D	381	GLU	CD-OE2	6.26	1.32	1.25
1	A	372	TYR	CE1-CZ	6.07	1.46	1.38
1	B	307	TYR	CE1-CZ	-6.07	1.30	1.38
1	A	109	TYR	CE1-CZ	5.95	1.46	1.38
1	A	22	ARG	CZ-NH1	5.95	1.40	1.33
1	A	585	SER	CB-OG	-5.76	1.34	1.42
1	D	171	ARG	CZ-NH2	5.72	1.40	1.33
1	E	572	TRP	CB-CG	5.66	1.60	1.50
1	A	373	GLU	CD-OE2	5.60	1.31	1.25
1	E	413	SER	CB-OG	5.59	1.49	1.42
1	F	22	ARG	CZ-NH1	5.56	1.40	1.33
1	B	236	GLU	CD-OE1	-5.55	1.19	1.25
1	B	547	SER	CB-OG	5.55	1.49	1.42
1	C	585	SER	CB-OG	-5.48	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	GLU	CD-OE1	5.45	1.31	1.25
1	F	225	GLU	CG-CD	5.39	1.60	1.51
1	B	253	ARG	CZ-NH1	5.37	1.40	1.33
1	B	19	TYR	CE1-CZ	-5.37	1.31	1.38
1	D	253	ARG	CZ-NH1	5.34	1.40	1.33
1	A	253	ARG	CZ-NH1	5.33	1.40	1.33
1	C	253	ARG	CZ-NH1	5.32	1.40	1.33
1	F	253	ARG	CZ-NH1	5.32	1.40	1.33
1	B	628	SER	CB-OG	-5.30	1.35	1.42
1	E	253	ARG	CZ-NH1	5.28	1.40	1.33
1	A	355	GLU	CD-OE2	5.24	1.31	1.25
1	A	590	TRP	CB-CG	5.21	1.59	1.50
1	D	344	TYR	CE1-CZ	5.11	1.45	1.38
1	F	530	MET	CG-SD	5.08	1.94	1.81
1	D	567	TYR	CE1-CZ	-5.08	1.31	1.38
1	A	525	GLN	CD-NE2	5.06	1.45	1.32
1	A	639	TYR	CG-CD1	-5.05	1.32	1.39
1	D	311	GLU	CD-OE1	5.01	1.31	1.25

All (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
1	C	483	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	F	359	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	E	123	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	D	123	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	123	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	F	28	ASP	CB-CG-OD1	8.70	126.13	118.30
1	B	598	ASP	CB-CG-OD1	8.69	126.12	118.30
1	D	253	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	E	253	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	C	253	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	253	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	386	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	B	253	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	F	598	ASP	CB-CG-OD1	8.41	125.87	118.30
1	E	22	ARG	NE-CZ-NH2	-8.41	116.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	131	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	F	253	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	D	253	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	E	253	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	C	123	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	C	253	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	253	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	E	580	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	528	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	F	580	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	F	253	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	B	253	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	F	580	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	B	36	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	C	580	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	377	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	123	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	E	328	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	E	580	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	22	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	496	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	F	696	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	F	264	ASP	CB-CG-OD1	7.54	125.09	118.30
1	F	264	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	E	214	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	F	530	MET	CA-CB-CG	7.51	126.07	113.30
1	B	212	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	434	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	538	ASP	CB-CG-OD1	7.41	124.96	118.30
1	A	598	ASP	CB-CG-OD1	7.37	124.93	118.30
1	F	212	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	F	285	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	F	43	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	F	202	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	F	598	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	F	202	ASP	CB-CG-OD1	7.18	124.76	118.30
1	B	241	ASP	CB-CG-OD1	7.15	124.73	118.30
1	D	112	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	300	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	598	ASP	CB-CG-OD1	7.04	124.63	118.30
1	F	601	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	168	LYS	CD-CE-NZ	-6.96	95.69	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	43	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	F	479	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	377	ARG	CG-CD-NE	-6.80	97.53	111.80
1	A	219	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	300	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	627	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	D	235	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	D	359	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	496	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	434	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	168	LYS	CD-CE-NZ	-6.64	96.42	111.70
1	A	28	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	225	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	C	598	ASP	CB-CG-OD1	6.62	124.25	118.30
1	F	220	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	483	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	E	601	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	202	ASP	CB-CG-OD1	6.49	124.14	118.30
1	F	214	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	220	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	E	193	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	214	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	E	202	ASP	CB-CG-OD1	6.34	124.00	118.30
1	C	173	GLU	OE1-CD-OE2	6.32	130.89	123.30
1	E	212	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	D	239	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	F	22	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	580	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	E	598	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	448	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	22	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	E	28	ASP	CB-CG-OD1	6.14	123.83	118.30
1	E	123	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	E	22	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	530	MET	CA-CB-CG	6.08	123.63	113.30
1	D	239	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	202	ASP	CB-CG-OD1	6.01	123.71	118.30
1	F	407	GLU	OE1-CD-OE2	-5.99	116.12	123.30
1	D	225	GLU	OE1-CD-OE2	-5.98	116.12	123.30
1	A	202	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	188	ASP	CB-CG-OD1	-5.97	112.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	193	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	162	MET	CG-SD-CE	-5.93	90.71	100.20
1	A	123	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	25	ASP	CB-CG-OD1	5.93	123.63	118.30
1	D	112	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	530	MET	CG-SD-CE	-5.88	90.79	100.20
1	A	438	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	F	112	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	377	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	474	ASP	CB-CG-OD1	5.81	123.53	118.30
1	E	235	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	C	691	ASP	CB-CG-OD1	5.74	123.47	118.30
1	F	298	MET	CG-SD-CE	-5.74	91.02	100.20
1	A	285	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	681	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	438	ASP	CB-CG-OD1	5.68	123.42	118.30
1	F	28	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	112	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	696	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	E	328	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	203	LEU	CA-CB-CG	-5.54	102.55	115.30
1	A	528	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	407	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	C	380	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	377	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	580	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	97	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	587	ASP	CB-CG-OD1	5.47	123.22	118.30
1	E	431	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	380	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	F	131	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	E	202	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	F	285	ASP	CB-CG-OD1	5.30	123.07	118.30
1	E	43	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	285	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	D	221	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	530	MET	CA-CB-CG	5.26	122.25	113.30
1	D	285	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	496	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	A	538	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	97	ASP	CB-CG-OD1	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	D	550	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	171	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	F	173	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	D	217	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	627	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	474	ASP	CB-CG-OD1	5.04	122.83	118.30
1	D	28	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	212	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	F	496	ARG	NE-CZ-NH1	-5.00	117.80	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
1:B:284:GLU:HB3	1:F:530:MET:HE1	1.63	0.78
1:A:380:ARG:HH21	3:A:806:GOL:H32	1.47	0.77
1:E:655:SER:OG	1:E:679:VAL:HG23	1.86	0.76
1:A:622:GLY:H	3:A:803:GOL:C1	1.99	0.74
3:C:803:GOL:H11	4:C:1041:HOH:O	1.86	0.74
1:A:615:THR:N	1:A:618:MET:HE3	2.02	0.74
1:B:155:TYR:HA	3:B:806:GOL:C3	2.18	0.73
1:B:171:ARG:HH11	1:B:176:ASN:ND2	1.90	0.69
1:E:311:GLU:OE1	3:E:803:GOL:H11	1.94	0.68
1:B:436:ILE:HD11	1:B:600:TRP:CH2	2.28	0.67
1:E:173:GLU:HB2	4:E:905:HOH:O	1.95	0.67
1:C:373:GLU:HG2	4:C:1276:HOH:O	1.92	0.67
1:B:303:GLY:HA3	4:B:1079:HOH:O	1.96	0.64
1:D:540:LEU:HD12	1:D:564:LEU:HB3	1.78	0.64
1:E:540:LEU:HD12	1:E:564:LEU:HB3	1.79	0.63
1:F:115:MET:CE	4:F:1261:HOH:O	2.48	0.62
1:F:240:ASP:H	3:F:805:GOL:H2	1.63	0.62
1:A:563:VAL:HG11	1:A:566:TRP:CE2	2.37	0.60
1:F:518:ILE:CD1	1:F:583:PHE:CE2	2.84	0.59
1:B:436:ILE:HD11	1:B:600:TRP:CZ2	2.37	0.59
1:E:530:MET:HE1	1:F:285:ASP:H	1.67	0.58
1:F:563:VAL:HG11	1:F:566:TRP:CE2	2.37	0.58
1:F:377:ARG:HG2	3:F:806:GOL:H12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:809:GOL:O1	3:C:810:GOL:C1	2.52	0.58
1:F:115:MET:HE3	4:F:1261:HOH:O	2.03	0.58
1:F:303:GLY:HA3	4:F:1012:HOH:O	2.05	0.56
1:D:173:GLU:OE2	1:D:214:ARG:NH2	2.32	0.55
1:B:189:TYR:HA	1:E:19:TYR:CE1	2.41	0.55
3:F:809:GOL:C3	4:F:1006:HOH:O	2.53	0.55
1:B:377:ARG:NH2	4:B:903:HOH:O	2.40	0.55
1:C:151:GLU:OE1	3:C:806:GOL:H2	2.06	0.55
1:E:303:GLY:HA3	4:E:1113:HOH:O	2.06	0.55
1:E:530:MET:HE1	1:F:284:GLU:HB3	1.89	0.54
1:C:169:GLN:O	1:C:173:GLU:HG3	2.08	0.54
1:A:615:THR:HG22	1:A:618:MET:HE2	1.89	0.54
1:F:614:HIS:NE2	1:F:619:GLU:OE2	2.36	0.53
1:C:396:LYS:NZ	1:C:446:GLU:OE1	2.39	0.53
1:C:483:ARG:HD2	4:C:954:HOH:O	2.07	0.53
3:C:803:GOL:C3	4:C:1041:HOH:O	2.43	0.53
1:D:484:TYR:CZ	1:D:489:GLY:HA3	2.44	0.53
1:C:19:TYR:CE1	1:D:189:TYR:HA	2.44	0.52
1:C:518:ILE:HD12	1:C:583:PHE:CE2	2.45	0.52
1:A:615:THR:H	1:A:618:MET:HE3	1.72	0.52
1:B:562:HIS:ND1	3:B:807:GOL:H12	2.24	0.52
1:B:155:TYR:CA	3:B:806:GOL:H32	2.35	0.52
1:B:239:ARG:HB3	3:B:809:GOL:H2	1.92	0.52
1:A:85:TYR:CD2	1:A:150:ASN:HB3	2.45	0.52
1:D:657:THR:CG2	1:D:674:GLU:HA	2.39	0.52
1:A:284:GLU:OE2	1:A:321:LEU:O	2.28	0.51
1:A:615:THR:HG22	1:A:618:MET:CE	2.40	0.51
1:D:115:MET:HE3	4:D:1159:HOH:O	2.10	0.51
1:C:540:LEU:HD12	1:C:564:LEU:HB3	1.93	0.51
1:F:85:TYR:CD2	1:F:150:ASN:HB3	2.45	0.51
1:A:189:TYR:HA	1:D:19:TYR:CE1	2.46	0.51
1:B:563:VAL:HG11	1:B:566:TRP:CE2	2.47	0.50
1:B:171:ARG:HH11	1:B:176:ASN:HD22	1.60	0.50
1:E:85:TYR:CD2	1:E:150:ASN:HB3	2.46	0.49
1:F:655:SER:OG	1:F:679:VAL:HG23	2.12	0.49
1:D:173:GLU:OE1	3:D:809:GOL:O1	2.29	0.49
1:D:115:MET:CE	4:D:1159:HOH:O	2.60	0.49
1:B:53:GLU:OE2	1:B:128:ARG:NH2	2.45	0.49
1:B:240:ASP:HB2	3:B:809:GOL:H11	1.94	0.49
1:D:12:GLY:HA2	1:D:39:ILE:HG12	1.95	0.49
1:B:580:ARG:HE	3:B:807:GOL:H11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:CD2	1:D:150:ASN:HB3	2.48	0.48
1:B:284:GLU:CB	1:F:530:MET:HE1	2.37	0.48
1:C:12:GLY:HA2	1:C:39:ILE:HG23	1.96	0.48
1:B:547:SER:OG	1:B:596:GLN:OE1	2.29	0.47
1:E:697:GLN:H	1:E:697:GLN:CD	2.16	0.47
1:B:85:TYR:CE2	1:B:112:ARG:HD2	2.50	0.47
1:A:19:TYR:CE1	1:C:189:TYR:HA	2.50	0.47
1:C:436:ILE:HD11	1:C:600:TRP:CZ2	2.49	0.47
1:B:85:TYR:CD2	1:B:150:ASN:HB3	2.49	0.47
1:C:535:LYS:HG3	1:C:568:ASP:HB2	1.95	0.47
3:C:809:GOL:O1	3:C:810:GOL:H11	2.14	0.47
1:C:563:VAL:HG11	1:C:566:TRP:CE2	2.50	0.47
1:E:657:THR:CG2	1:E:674:GLU:HA	2.45	0.47
1:E:85:TYR:CE2	1:E:112:ARG:HD2	2.50	0.46
1:A:85:TYR:CE2	1:A:112:ARG:HD2	2.51	0.45
3:C:803:GOL:C2	4:C:1041:HOH:O	2.64	0.45
1:B:19:TYR:CE1	1:F:189:TYR:HA	2.51	0.45
1:A:535:LYS:HG3	1:A:568:ASP:HB2	1.99	0.45
1:E:253:ARG:NH2	1:E:431:ASP:OD1	2.50	0.45
1:A:12:GLY:HA2	1:A:39:ILE:HG23	1.99	0.45
1:D:85:TYR:CE2	1:D:112:ARG:HD2	2.52	0.45
1:D:543:LEU:HD11	1:D:599:ALA:HB1	1.99	0.45
1:F:492:LEU:C	1:F:492:LEU:HD23	2.37	0.45
1:F:495:MET:O	1:F:496:ARG:HB2	2.17	0.45
1:F:657:THR:CG2	1:F:674:GLU:HA	2.47	0.45
1:A:285:ASP:HB2	1:C:530:MET:CE	2.46	0.44
1:C:284:GLU:OE2	1:C:321:LEU:O	2.34	0.44
1:C:678:THR:O	1:C:679:VAL:C	2.56	0.44
1:B:354:PHE:CZ	3:B:808:GOL:H31	2.53	0.44
1:F:540:LEU:HD12	1:F:564:LEU:HB3	1.98	0.44
1:B:543:LEU:HD11	1:B:599:ALA:HB1	2.00	0.44
1:D:687:ARG:HG2	4:D:1189:HOH:O	2.18	0.44
1:E:189:TYR:HA	1:F:19:TYR:CE1	2.52	0.44
1:A:207:ILE:HD12	1:A:207:ILE:C	2.38	0.44
1:D:172:HIS:ND1	4:D:902:HOH:O	2.37	0.43
1:C:85:TYR:CD1	1:C:85:TYR:C	2.92	0.43
1:A:537:PRO:HD2	4:A:1181:HOH:O	2.19	0.43
1:C:649:THR:HA	1:C:683:VAL:O	2.17	0.43
1:C:85:TYR:CD2	1:C:150:ASN:HB3	2.53	0.43
1:D:154:TYR:CG	1:D:219:ARG:HB3	2.53	0.43
1:F:267:ARG:HH11	1:F:267:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:THR:O	1:B:589:GLN:HA	2.19	0.43
1:B:46:GLU:O	1:B:83:PRO:HA	2.19	0.43
1:E:54:PRO:HD2	1:E:58:HIS:O	2.18	0.43
1:E:455:SER:OG	1:E:458:GLN:HG3	2.19	0.43
1:B:422:PRO:HG2	1:B:423:MET:CE	2.48	0.43
1:E:102:THR:HB	1:E:103:PRO:CD	2.48	0.43
1:B:535:LYS:HG3	1:B:568:ASP:HB2	2.00	0.42
1:F:518:ILE:HD13	1:F:583:PHE:CE2	2.53	0.42
1:A:166:PHE:CD2	1:A:203:LEU:HD11	2.55	0.42
1:C:115:MET:CE	4:C:1106:HOH:O	2.66	0.42
1:E:563:VAL:HG11	1:E:566:TRP:CE2	2.53	0.42
1:C:495:MET:O	1:C:496:ARG:HB2	2.19	0.42
1:B:240:ASP:H	3:B:809:GOL:H2	1.84	0.42
1:D:181:LEU:C	1:D:181:LEU:HD23	2.40	0.42
1:D:535:LYS:HE3	1:D:535:LYS:HB2	1.88	0.42
1:E:495:MET:O	1:E:496:ARG:HB2	2.19	0.42
1:B:253:ARG:NH2	1:B:431:ASP:OD1	2.52	0.42
1:B:632:THR:HG23	4:B:981:HOH:O	2.19	0.42
1:F:115:MET:HG3	1:F:122:TYR:CZ	2.55	0.42
1:A:649:THR:HA	1:A:683:VAL:O	2.19	0.42
1:B:248:PHE:HB3	1:B:265:HIS:CE1	2.55	0.42
1:B:422:PRO:HG2	1:B:423:MET:HE3	2.02	0.42
1:F:564:LEU:N	1:F:564:LEU:HD12	2.34	0.42
1:B:580:ARG:HG2	3:B:807:GOL:H2	2.02	0.41
1:D:495:MET:O	1:D:496:ARG:HB2	2.20	0.41
1:F:484:TYR:CZ	1:F:489:GLY:HA3	2.55	0.41
1:A:303:GLY:HA3	4:A:971:HOH:O	2.19	0.41
1:C:85:TYR:CE2	1:C:112:ARG:HD2	2.54	0.41
1:F:515:LEU:HD23	1:F:518:ILE:HG13	2.02	0.41
1:E:678:THR:O	1:E:679:VAL:C	2.59	0.41
1:C:276:GLY:HA2	1:C:308:LEU:O	2.20	0.41
1:B:154:TYR:CG	1:B:219:ARG:HB3	2.55	0.41
1:D:625:CYS:HB3	1:D:641:LEU:HB2	2.02	0.41
1:B:518:ILE:HD12	1:B:518:ILE:N	2.36	0.41
1:A:115:MET:HG3	1:A:122:TYR:CZ	2.55	0.41
1:B:495:MET:O	1:B:496:ARG:HB2	2.21	0.41
1:B:207:ILE:C	1:B:207:ILE:HD12	2.41	0.41
1:B:80:VAL:O	1:B:146:TYR:HA	2.20	0.40
1:E:445:VAL:HG21	1:E:608:LEU:HD13	2.03	0.40
1:F:85:TYR:CE2	1:F:112:ARG:HD2	2.56	0.40
1:A:253:ARG:NH2	1:A:431:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:HG13	1:C:392:SER:HB3	2.03	0.40
1:F:518:ILE:HD13	1:F:583:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

All (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
1	D	353	SER
1	E	353	SER
1	F	538	ASP

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

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	115	MET
1	A	150	ASN
1	A	396	LYS
1	A	423	MET
1	A	496	ARG
1	A	521	MET
1	A	526	PHE
1	A	530	MET
1	B	85	TYR
1	B	115	MET
1	B	203	LEU
1	B	423	MET
1	B	496	ARG
1	B	521	MET
1	B	542	ASP
1	C	22	ARG
1	C	85	TYR
1	C	115	MET
1	C	423	MET
1	C	496	ARG
1	C	521	MET

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Mol	Chain	Res	Type
1	C	526	PHE
1	C	653	PRO
1	C	684	THR
1	D	85	TYR
1	D	115	MET
1	D	353	SER
1	D	423	MET
1	D	496	ARG
1	D	521	MET
1	D	526	PHE
1	E	85	TYR
1	E	115	MET
1	E	150	ASN
1	E	423	MET
1	E	496	ARG
1	E	521	MET
1	E	526	PHE
1	F	85	TYR
1	F	115	MET
1	F	203	LEU
1	F	423	MET
1	F	496	ARG
1	F	521	MET
1	F	526	PHE
1	F	539	THR

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	804	-	5,5,5	0.99	0	5,5,5	0.98	0
2	SO4	B	803	-	4,4,4	0.34	0	6,6,6	0.78	0
3	GOL	A	804	-	5,5,5	0.94	0	5,5,5	1.14	1 (20%)
3	GOL	B	815	-	5,5,5	0.70	0	5,5,5	1.30	0
3	GOL	F	809	-	5,5,5	0.29	0	5,5,5	1.33	1 (20%)
3	GOL	C	810	-	5,5,5	0.64	0	5,5,5	1.46	1 (20%)
2	SO4	B	802	-	4,4,4	0.45	0	6,6,6	0.42	0
3	GOL	B	808	-	5,5,5	0.64	0	5,5,5	1.22	0
3	GOL	D	805	-	5,5,5	0.48	0	5,5,5	1.41	1 (20%)
3	GOL	F	807	-	5,5,5	0.61	0	5,5,5	2.08	2 (40%)
3	GOL	C	804	-	5,5,5	0.63	0	5,5,5	1.56	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	801	-	4,4,4	0.16	0	6,6,6	1.46	1 (16%)
3	GOL	E	806	-	5,5,5	1.03	1 (20%)	5,5,5	2.15	2 (40%)
3	GOL	B	814	-	5,5,5	0.52	0	5,5,5	1.39	1 (20%)
3	GOL	A	806	-	5,5,5	0.53	0	5,5,5	1.14	0
3	GOL	B	806	-	5,5,5	0.67	0	5,5,5	1.37	1 (20%)
3	GOL	F	804	-	5,5,5	0.60	0	5,5,5	2.01	1 (20%)
3	GOL	E	804	-	5,5,5	0.33	0	5,5,5	1.45	1 (20%)
3	GOL	F	803	-	5,5,5	1.36	1 (20%)	5,5,5	1.17	1 (20%)
2	SO4	F	801	-	4,4,4	0.57	0	6,6,6	1.45	2 (33%)
2	SO4	E	801	-	4,4,4	0.18	0	6,6,6	1.43	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	804	-	5,5,5	0.40	0	5,5,5	0.57	0
3	GOL	A	807	-	5,5,5	0.30	0	5,5,5	0.49	0
3	GOL	A	809	-	5,5,5	0.63	0	5,5,5	0.46	0
2	SO4	D	801	-	4,4,4	0.14	0	6,6,6	1.21	1 (16%)
2	SO4	A	801	-	4,4,4	0.38	0	6,6,6	1.15	1 (16%)
3	GOL	B	809	-	5,5,5	0.28	0	5,5,5	1.58	1 (20%)
2	SO4	B	816	-	4,4,4	0.39	0	6,6,6	0.86	0
3	GOL	D	803	-	5,5,5	1.05	0	5,5,5	1.69	1 (20%)
3	GOL	D	807	-	5,5,5	0.34	0	5,5,5	0.45	0
3	GOL	E	803	-	5,5,5	1.39	1 (20%)	5,5,5	3.10	3 (60%)
3	GOL	E	809	-	5,5,5	0.32	0	5,5,5	0.41	0
3	GOL	B	811	-	5,5,5	0.69	0	5,5,5	0.90	0
3	GOL	F	810	-	5,5,5	0.73	0	5,5,5	0.90	0
2	SO4	A	810	-	4,4,4	0.46	0	6,6,6	0.48	0
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
3	GOL	B	813	-	5,5,5	0.88	0	5,5,5	2.08	2 (40%)
2	SO4	E	811	-	4,4,4	0.41	0	6,6,6	0.44	0
3	GOL	F	812	-	5,5,5	0.43	0	5,5,5	0.80	0
3	GOL	F	808	-	5,5,5	0.64	0	5,5,5	1.05	0
3	GOL	B	805	-	5,5,5	0.75	0	5,5,5	1.57	1 (20%)
3	GOL	A	803	-	5,5,5	0.85	0	5,5,5	2.78	3 (60%)
2	SO4	D	802	-	4,4,4	0.42	0	6,6,6	0.67	0
2	SO4	C	802	-	4,4,4	0.40	0	6,6,6	0.70	0
3	GOL	A	802	-	5,5,5	1.29	1 (20%)	5,5,5	0.89	0
3	GOL	E	805	-	5,5,5	0.81	0	5,5,5	1.37	0
3	GOL	A	808	-	5,5,5	0.34	0	5,5,5	0.63	0
3	GOL	C	807	-	5,5,5	0.71	0	5,5,5	1.64	1 (20%)
2	SO4	E	802	-	4,4,4	0.42	0	6,6,6	1.27	1 (16%)
3	GOL	C	806	-	5,5,5	1.21	1 (20%)	5,5,5	1.31	1 (20%)
3	GOL	E	808	-	5,5,5	0.40	0	5,5,5	0.60	0
3	GOL	F	806	-	5,5,5	0.67	0	5,5,5	1.24	1 (20%)
2	SO4	B	801	-	4,4,4	0.61	0	6,6,6	1.44	1 (16%)
3	GOL	D	808	-	5,5,5	0.43	0	5,5,5	0.82	0
3	GOL	F	813	-	5,5,5	0.58	0	5,5,5	0.84	0
3	GOL	B	807	-	5,5,5	0.41	0	5,5,5	0.94	0
3	GOL	D	806	-	5,5,5	0.56	0	5,5,5	1.82	2 (40%)
3	GOL	B	810	-	5,5,5	0.76	0	5,5,5	1.33	1 (20%)
3	GOL	C	811	-	5,5,5	0.50	0	5,5,5	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	811	-	5,5,5	1.05	1 (20%)	5,5,5	2.44	2 (40%)
2	SO4	F	802	-	4,4,4	0.34	0	6,6,6	0.33	0
3	GOL	E	807	-	5,5,5	0.52	0	5,5,5	1.94	2 (40%)
2	SO4	F	814	-	4,4,4	0.44	0	6,6,6	0.57	0
3	GOL	C	805	-	5,5,5	0.81	0	5,5,5	0.91	0
3	GOL	D	809	-	5,5,5	0.45	0	5,5,5	0.70	0
3	GOL	C	809	-	5,5,5	0.46	0	5,5,5	1.39	1 (20%)
3	GOL	B	812	-	5,5,5	0.39	0	5,5,5	0.88	0
3	GOL	A	805	-	5,5,5	0.72	0	5,5,5	2.17	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	B	804	-	-	0/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-
3	GOL	B	815	-	-	2/4/4/4	-
3	GOL	F	809	-	-	4/4/4/4	-
3	GOL	C	810	-	-	3/4/4/4	-
3	GOL	D	805	-	-	2/4/4/4	-
3	GOL	B	808	-	-	2/4/4/4	-
3	GOL	C	804	-	-	0/4/4/4	-
3	GOL	C	808	-	-	2/4/4/4	-
3	GOL	C	803	-	-	0/4/4/4	-
3	GOL	E	806	-	-	1/4/4/4	-
3	GOL	B	814	-	-	2/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	B	806	-	-	4/4/4/4	-
3	GOL	F	804	-	-	2/4/4/4	-
3	GOL	E	804	-	-	2/4/4/4	-
3	GOL	F	803	-	-	0/4/4/4	-
3	GOL	E	803	-	-	3/4/4/4	-
3	GOL	F	807	-	-	2/4/4/4	-
3	GOL	D	804	-	-	1/4/4/4	-
3	GOL	B	809	-	-	1/4/4/4	-
3	GOL	A	809	-	-	0/4/4/4	-
3	GOL	A	807	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	803	-	-	0/4/4/4	-
3	GOL	D	807	-	-	0/4/4/4	-
3	GOL	E	809	-	-	0/4/4/4	-
3	GOL	B	811	-	-	4/4/4/4	-
3	GOL	F	810	-	-	0/4/4/4	-
3	GOL	E	810	-	-	4/4/4/4	-
3	GOL	F	805	-	-	2/4/4/4	-
3	GOL	B	813	-	-	3/4/4/4	-
3	GOL	F	812	-	-	2/4/4/4	-
3	GOL	F	808	-	-	2/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	E	805	-	-	0/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	C	807	-	-	2/4/4/4	-
3	GOL	C	806	-	-	2/4/4/4	-
3	GOL	E	808	-	-	2/4/4/4	-
3	GOL	F	806	-	-	4/4/4/4	-
3	GOL	D	808	-	-	3/4/4/4	-
3	GOL	F	813	-	-	0/4/4/4	-
3	GOL	B	807	-	-	3/4/4/4	-
3	GOL	D	806	-	-	2/4/4/4	-
3	GOL	B	810	-	-	4/4/4/4	-
3	GOL	C	811	-	-	2/4/4/4	-
3	GOL	F	811	-	-	2/4/4/4	-
3	GOL	E	807	-	-	2/4/4/4	-
3	GOL	C	805	-	-	2/4/4/4	-
3	GOL	D	809	-	-	4/4/4/4	-
3	GOL	C	809	-	-	2/4/4/4	-
3	GOL	B	812	-	-	2/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
3	F	811	GOL	O2-C2	-2.05	1.37	1.43
3	C	806	GOL	O1-C1	2.03	1.51	1.42

All (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
3	E	806	GOL	O2-C2-C1	-3.34	94.42	109.12
3	D	803	GOL	O1-C1-C2	3.30	126.01	110.20
3	F	804	GOL	O3-C3-C2	-3.24	94.69	110.20
3	E	807	GOL	O1-C1-C2	-3.23	94.73	110.20
3	E	803	GOL	O1-C1-C2	3.11	125.10	110.20
3	B	813	GOL	C3-C2-C1	3.10	123.78	111.70
3	F	811	GOL	O2-C2-C1	-3.10	95.47	109.12
3	C	804	GOL	O3-C3-C2	-3.07	95.50	110.20
3	B	805	GOL	C3-C2-C1	-3.04	99.87	111.70
2	B	801	SO4	O4-S-O1	-2.98	93.78	109.31
3	A	803	GOL	O2-C2-C1	-2.97	96.02	109.12
3	A	803	GOL	O2-C2-C3	2.95	122.09	109.12
3	E	806	GOL	C3-C2-C1	2.89	122.95	111.70
3	E	803	GOL	O3-C3-C2	-2.85	96.53	110.20
3	E	807	GOL	O3-C3-C2	-2.82	96.69	110.20
3	F	806	GOL	O2-C2-C1	-2.65	97.46	109.12
3	D	806	GOL	C3-C2-C1	2.64	121.97	111.70
2	C	801	SO4	O2-S-O1	-2.60	90.20	109.43
3	A	805	GOL	C3-C2-C1	2.49	121.40	111.70
2	E	802	SO4	O4-S-O1	2.48	122.24	109.31
2	A	801	SO4	O3-S-O1	-2.46	96.45	109.31
3	B	806	GOL	O3-C3-C2	2.46	121.99	110.20
3	B	810	GOL	C3-C2-C1	2.42	121.13	111.70
3	B	813	GOL	O2-C2-C3	-2.42	98.44	109.12
3	C	808	GOL	O2-C2-C1	-2.41	98.49	109.12
2	F	801	SO4	O3-S-O1	-2.35	97.06	109.31
3	F	807	GOL	O1-C1-C2	-2.33	99.03	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	810	GOL	O1-C1-C2	2.32	121.34	110.20
3	C	809	GOL	O1-C1-C2	-2.27	99.30	110.20
3	E	804	GOL	C3-C2-C1	-2.24	102.98	111.70
2	F	801	SO4	O3-S-O2	2.24	120.99	109.31
3	C	806	GOL	O1-C1-C2	2.24	120.93	110.20
3	B	814	GOL	O1-C1-C2	-2.21	99.62	110.20
3	B	809	GOL	O1-C1-C2	-2.17	99.78	110.20
3	D	805	GOL	C3-C2-C1	-2.15	103.34	111.70
3	F	809	GOL	O1-C1-C2	-2.15	99.89	110.20
3	D	806	GOL	O2-C2-C3	-2.12	99.78	109.12
2	E	801	SO4	O4-S-O2	-2.11	98.31	109.31
2	E	801	SO4	O4-S-O3	2.07	117.91	109.06
3	F	803	GOL	O1-C1-C2	2.05	120.04	110.20
3	C	808	GOL	O1-C1-C2	-2.05	100.38	110.20
3	A	804	GOL	O1-C1-C2	2.02	119.89	110.20
2	D	801	SO4	O3-S-O2	-2.01	98.81	109.31
3	C	807	GOL	O2-C2-C3	-2.00	100.29	109.12

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	A	805	GOL	O1-C1-C2-C3
3	A	807	GOL	O1-C1-C2-C3
3	A	807	GOL	C1-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	B	806	GOL	O1-C1-C2-C3
3	B	810	GOL	O1-C1-C2-C3
3	B	810	GOL	C1-C2-C3-O3
3	B	811	GOL	O1-C1-C2-C3
3	B	811	GOL	C1-C2-C3-O3
3	B	811	GOL	O2-C2-C3-O3
3	B	812	GOL	C1-C2-C3-O3
3	B	813	GOL	C1-C2-C3-O3
3	B	814	GOL	C1-C2-C3-O3
3	B	814	GOL	O2-C2-C3-O3
3	B	815	GOL	C1-C2-C3-O3
3	C	805	GOL	O1-C1-C2-C3
3	C	806	GOL	C1-C2-C3-O3
3	C	807	GOL	C1-C2-C3-O3
3	C	808	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	808	GOL	O2-C2-C3-O3
3	C	810	GOL	O1-C1-C2-C3
3	C	811	GOL	O1-C1-C2-C3
3	D	805	GOL	O1-C1-C2-C3
3	D	806	GOL	C1-C2-C3-O3
3	D	809	GOL	C1-C2-C3-O3
3	E	804	GOL	O1-C1-C2-C3
3	E	807	GOL	O1-C1-C2-C3
3	E	808	GOL	O1-C1-C2-O2
3	E	808	GOL	O1-C1-C2-C3
3	E	810	GOL	O1-C1-C2-C3
3	F	804	GOL	O1-C1-C2-C3
3	F	807	GOL	C1-C2-C3-O3
3	F	809	GOL	C1-C2-C3-O3
3	F	809	GOL	O2-C2-C3-O3
3	F	811	GOL	O1-C1-C2-C3
3	B	806	GOL	O1-C1-C2-O2
3	B	806	GOL	O2-C2-C3-O3
3	B	812	GOL	O2-C2-C3-O3
3	B	815	GOL	O2-C2-C3-O3
3	C	805	GOL	O1-C1-C2-O2
3	D	806	GOL	O2-C2-C3-O3
3	E	803	GOL	O2-C2-C3-O3
3	F	807	GOL	O2-C2-C3-O3
3	A	806	GOL	O1-C1-C2-C3
3	B	806	GOL	C1-C2-C3-O3
3	B	807	GOL	O1-C1-C2-C3
3	D	808	GOL	C1-C2-C3-O3
3	D	809	GOL	O1-C1-C2-C3
3	E	803	GOL	C1-C2-C3-O3
3	F	806	GOL	O1-C1-C2-C3
3	F	806	GOL	C1-C2-C3-O3
3	F	808	GOL	O1-C1-C2-C3
3	F	809	GOL	O1-C1-C2-C3
3	F	812	GOL	O1-C1-C2-C3
3	A	803	GOL	O2-C2-C3-O3
3	B	805	GOL	O2-C2-C3-O3
3	B	810	GOL	O1-C1-C2-O2
3	B	810	GOL	O2-C2-C3-O3
3	B	811	GOL	O1-C1-C2-O2
3	B	813	GOL	O2-C2-C3-O3
3	C	810	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	811	GOL	O1-C1-C2-O2
3	D	805	GOL	O1-C1-C2-O2
3	E	804	GOL	O1-C1-C2-O2
3	E	810	GOL	O1-C1-C2-O2
3	F	804	GOL	O1-C1-C2-O2
3	F	808	GOL	O1-C1-C2-O2
3	A	806	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-O2
3	A	807	GOL	O2-C2-C3-O3
3	C	806	GOL	O2-C2-C3-O3
3	C	807	GOL	O2-C2-C3-O3
3	D	808	GOL	O2-C2-C3-O3
3	D	809	GOL	O2-C2-C3-O3
3	E	803	GOL	O1-C1-C2-O2
3	F	806	GOL	O1-C1-C2-O2
3	F	811	GOL	O1-C1-C2-O2
3	B	807	GOL	O2-C2-C3-O3
3	A	805	GOL	O1-C1-C2-O2
3	A	808	GOL	O2-C2-C3-O3
3	D	804	GOL	O1-C1-C2-O2
3	D	808	GOL	O1-C1-C2-O2
3	F	809	GOL	O1-C1-C2-O2
3	F	812	GOL	O1-C1-C2-O2
3	F	806	GOL	O2-C2-C3-O3
3	B	808	GOL	O1-C1-C2-O2
3	D	809	GOL	O1-C1-C2-O2
3	E	810	GOL	O2-C2-C3-O3
3	B	809	GOL	O1-C1-C2-C3
3	B	813	GOL	O1-C1-C2-C3
3	F	805	GOL	O1-C1-C2-C3
3	E	807	GOL	O1-C1-C2-O2
3	F	805	GOL	O1-C1-C2-O2
3	A	808	GOL	C1-C2-C3-O3
3	B	807	GOL	C1-C2-C3-O3
3	B	808	GOL	O1-C1-C2-C3
3	C	809	GOL	C1-C2-C3-O3
3	C	810	GOL	C1-C2-C3-O3
3	E	806	GOL	C1-C2-C3-O3
3	E	810	GOL	C1-C2-C3-O3
3	C	809	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 24 short contacts:

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

6.1 Protein, DNA and RNA chains

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

All (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
1	E	537	PRO	3.1
1	F	537	PRO	3.1
1	E	695	GLY	3.0
1	F	703	ALA	3.0
1	C	678	THR	2.9
1	C	658	PHE	2.8
1	C	676	PRO	2.8
1	C	683	VAL	2.7
1	D	630	THR	2.6
1	F	702	ALA	2.6
1	D	696	ARG	2.6
1	A	699	THR	2.5
1	C	672	THR	2.5
1	C	682	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	141	PRO	2.4
1	E	696	ARG	2.4
1	C	675	THR	2.3
1	E	656	GLY	2.3
1	B	669	GLN	2.3
1	D	695	GLY	2.3
1	C	649	THR	2.2
1	E	698	PRO	2.2
1	D	397	ARG	2.2
1	E	657	THR	2.2
1	F	539	THR	2.2
1	C	673	ALA	2.2
1	F	704	ALA	2.2
1	C	566	TRP	2.1
1	C	663	PRO	2.1
1	E	676	PRO	2.1
1	D	537	PRO	2.1
1	E	679	VAL	2.1
1	D	545	GLY	2.1
1	D	483	ARG	2.0

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(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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	811	6/6	0.77	0.23	48,54,57,62	0
3	GOL	B	809	6/6	0.78	0.28	41,46,52,55	0
3	GOL	C	806	6/6	0.78	0.27	38,47,53,56	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	F	810	6/6	0.83	0.32	49,54,58,60	0
3	GOL	E	809	6/6	0.83	0.23	56,62,63,69	0
3	GOL	D	809	6/6	0.84	0.15	45,57,59,67	0
3	GOL	C	810	6/6	0.84	0.22	40,57,60,63	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	808	6/6	0.84	0.20	48,49,52,55	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	A	808	6/6	0.85	0.13	52,58,60,66	0
3	GOL	E	808	6/6	0.85	0.15	48,52,60,62	0
3	GOL	B	807	6/6	0.86	0.17	43,56,61,62	0
3	GOL	E	810	6/6	0.86	0.19	45,47,52,63	0
3	GOL	B	810	6/6	0.86	0.30	50,54,61,65	0
3	GOL	A	805	6/6	0.86	0.17	39,58,62,62	0
3	GOL	B	814	6/6	0.86	0.21	50,54,57,64	0
3	GOL	F	808	6/6	0.87	0.15	36,50,51,53	0
3	GOL	A	806	6/6	0.87	0.20	47,56,59,60	0
3	GOL	D	806	6/6	0.87	0.18	34,50,54,55	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	B	812	6/6	0.91	0.27	36,42,52,56	0
3	GOL	F	806	6/6	0.91	0.12	35,46,56,57	0
3	GOL	D	808	6/6	0.91	0.16	32,37,47,55	0
3	GOL	F	807	6/6	0.92	0.17	42,51,52,53	0
3	GOL	C	809	6/6	0.92	0.14	36,47,53,55	0
3	GOL	C	807	6/6	0.92	0.17	32,50,53,55	0
3	GOL	E	805	6/6	0.92	0.20	35,42,46,50	0
3	GOL	F	812	6/6	0.92	0.18	33,38,49,67	0
3	GOL	A	803	6/6	0.92	0.20	34,47,49,54	0
3	GOL	D	803	6/6	0.93	0.15	22,22,23,29	0
2	SO4	A	810	5/5	0.93	0.27	56,60,73,75	0
3	GOL	D	805	6/6	0.93	0.15	37,42,46,54	0
3	GOL	F	804	6/6	0.93	0.14	29,35,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	F	811	6/6	0.93	0.15	32,49,56,56	0
2	SO4	D	802	5/5	0.93	0.30	60,61,65,77	0
3	GOL	E	807	6/6	0.93	0.19	35,45,50,51	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
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	803	5/5	0.94	0.22	48,55,62,69	0
3	GOL	E	804	6/6	0.94	0.13	34,41,44,48	0
3	GOL	B	813	6/6	0.94	0.14	32,48,52,59	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
2	SO4	B	816	5/5	0.95	0.20	54,57,66,71	0
3	GOL	C	803	6/6	0.96	0.12	23,27,29,34	0
3	GOL	E	803	6/6	0.96	0.11	21,23,25,26	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
2	SO4	E	811	5/5	0.97	0.15	51,53,62,68	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	801	5/5	0.98	0.11	33,36,38,39	0
2	SO4	D	801	5/5	0.98	0.08	35,42,49,51	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
2	SO4	B	801	5/5	0.99	0.07	30,38,42,43	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.