



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:12 AM UTC

PDB ID : 5XB7 / pdb_00005xb7
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.

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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:

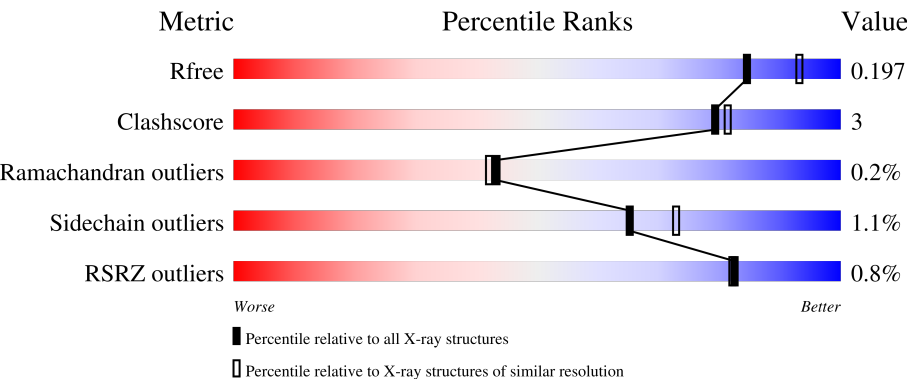
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	84%12%..
1	B	712	87%9%..
1	C	712	% 87%8%..
1	D	712	% 87%9%.
1	E	712	% 88%8%..

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Mol	Chain	Length	Quality of chain
1	F	712	% 89% 8% ..

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	-	-
3	GOL	F	809	-	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
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 (CCD ID: SO4) (formula: O₄S).



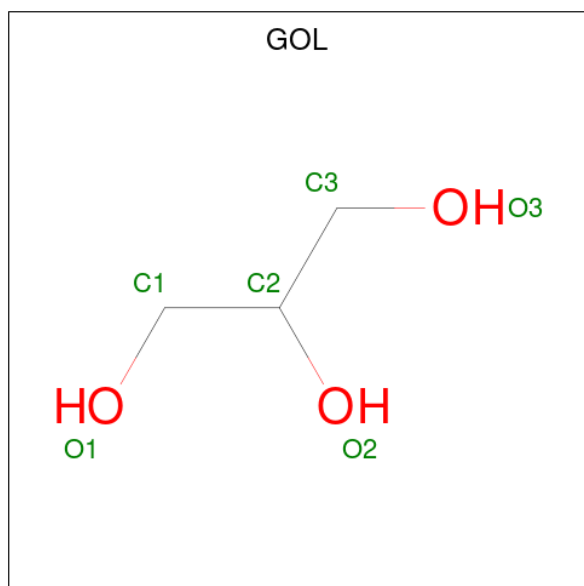
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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	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	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		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

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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		

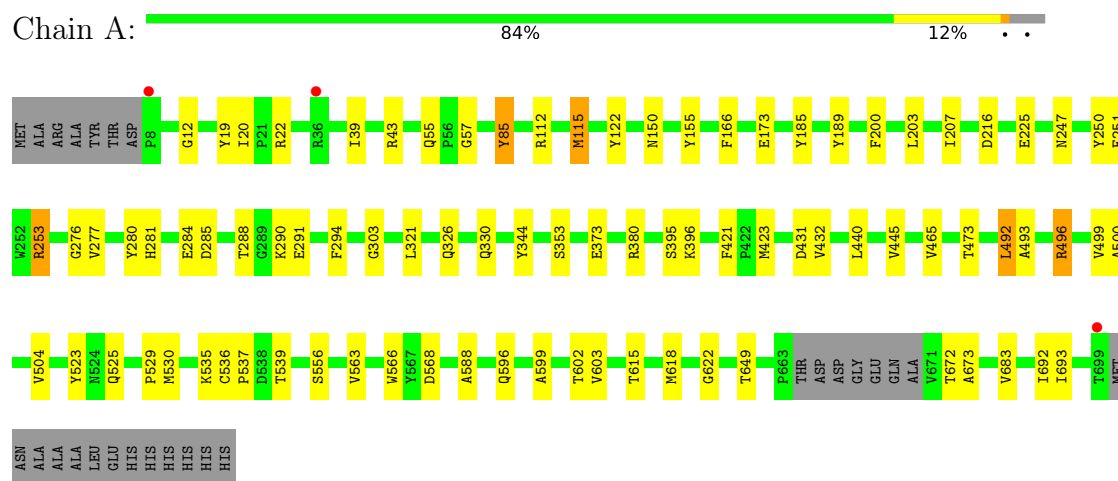
- Molecule 4 is water.

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		

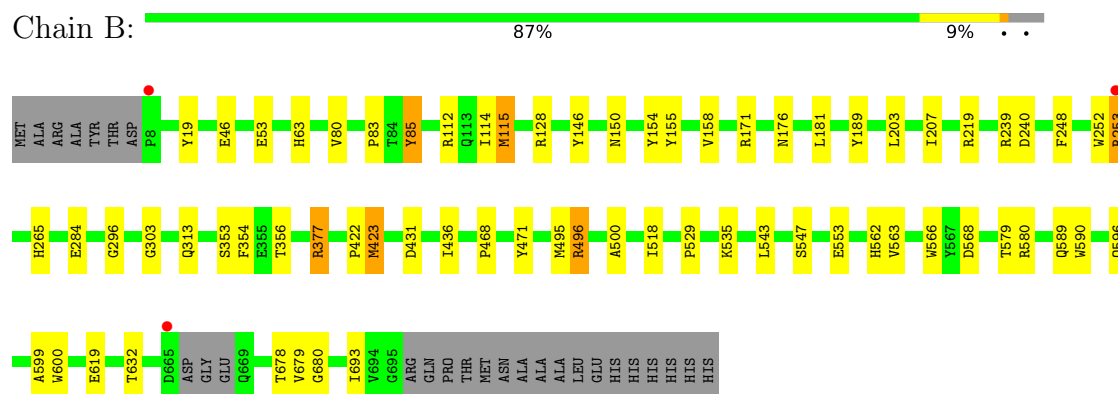
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

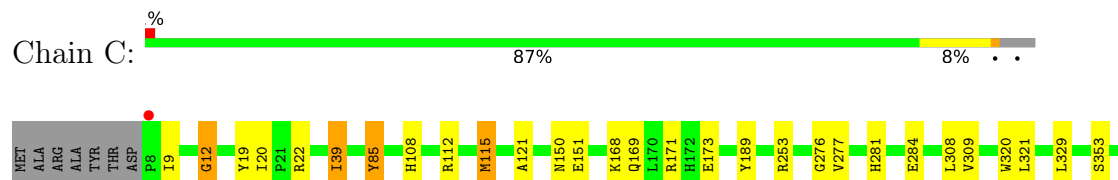
• Molecule 1: Beta-galactosidase

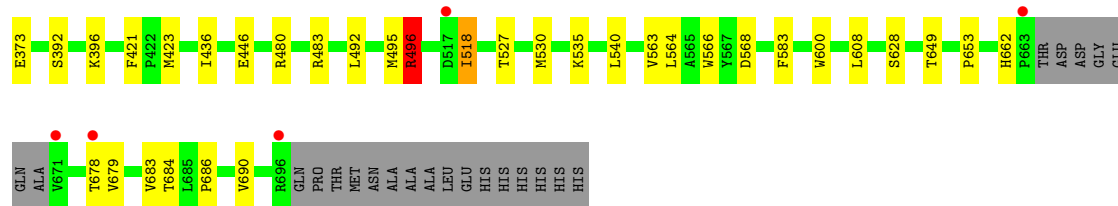


• Molecule 1: Beta-galactosidase

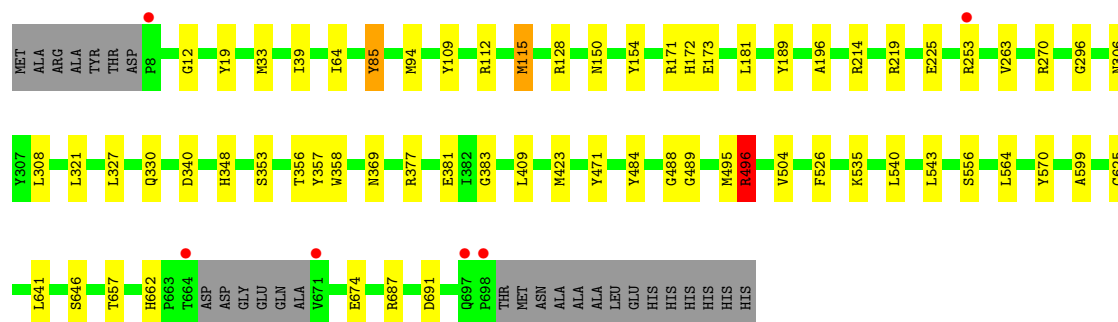
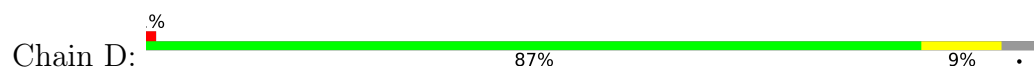


• Molecule 1: Beta-galactosidase

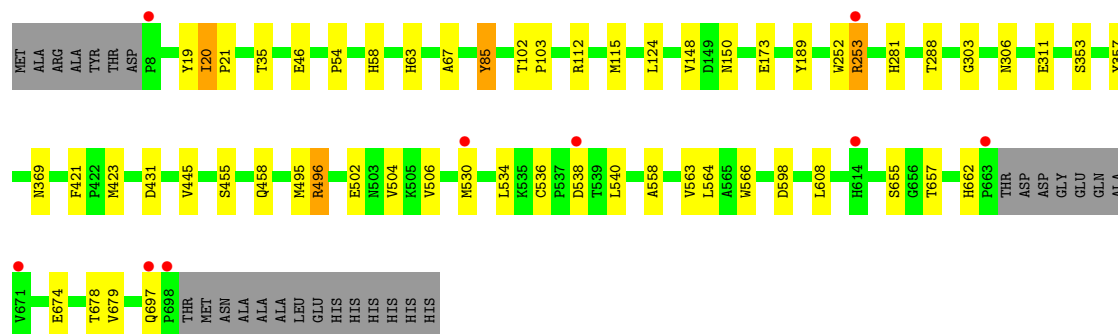
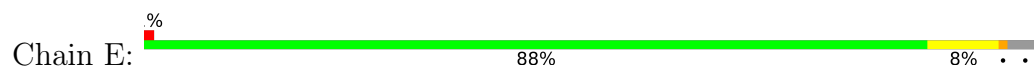




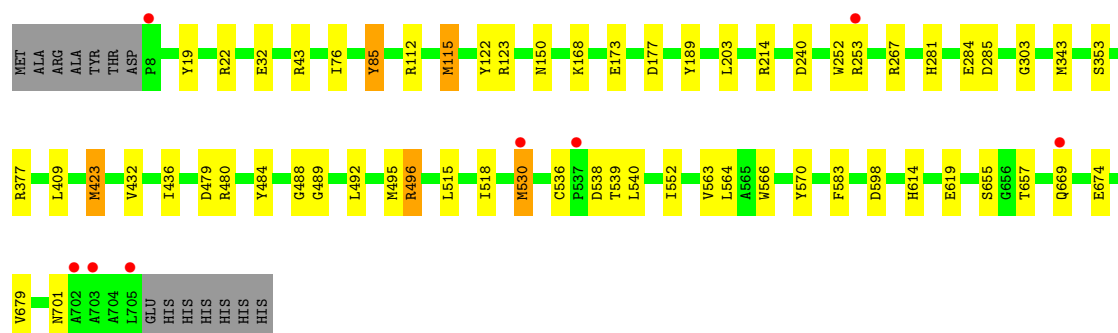
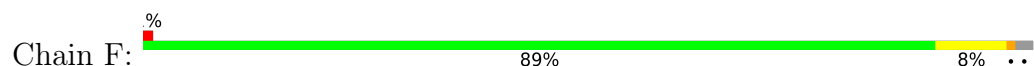
• Molecule 1: Beta-galactosidase



• 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)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.155 , 0.191 0.165 , 0.197	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)	0.37 , 37.7	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 ⓘ

5.1 Standard geometry ⓘ

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	1.54	36/5558 (0.6%)	1.18	11/7588 (0.1%)
1	B	1.38	11/5552 (0.2%)	1.14	9/7580 (0.1%)
1	C	1.37	12/5534 (0.2%)	1.13	11/7554 (0.1%)
1	D	1.47	23/5558 (0.4%)	1.16	14/7588 (0.2%)
1	E	1.37	16/5551 (0.3%)	1.15	8/7578 (0.1%)
1	F	1.34	13/5648 (0.2%)	1.15	10/7712 (0.1%)
All	All	1.41	111/33401 (0.3%)	1.15	63/45600 (0.1%)

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	ARG	CZ-NH2	7.66	1.43	1.33
1	F	479	ASP	C-N	7.32	1.43	1.33
1	F	480	ARG	C-N	7.07	1.44	1.33
1	B	553	GLU	CA-C	7.00	1.61	1.52
1	B	468	PRO	C-O	6.94	1.29	1.24
1	A	276	GLY	CA-C	-6.78	1.46	1.52
1	A	602	THR	N-CA	6.77	1.54	1.46
1	A	330	GLN	N-CA	6.61	1.54	1.46
1	D	263	VAL	C-O	6.46	1.30	1.23
1	A	556	SER	CA-C	-6.42	1.44	1.52
1	B	590	TRP	C-O	6.42	1.31	1.24
1	E	534	LEU	CA-C	6.36	1.60	1.52
1	D	94	MET	CA-C	-6.35	1.44	1.52
1	A	280	TYR	N-CA	-6.21	1.38	1.45
1	D	296	GLY	CA-C	-6.16	1.45	1.52
1	D	348	HIS	CA-C	6.15	1.61	1.52
1	A	294	PHE	N-CA	6.10	1.53	1.46
1	D	33	MET	CA-C	-6.06	1.44	1.52
1	D	381	GLU	N-CA	-6.06	1.39	1.46
1	E	558	ALA	CA-C	6.05	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	377	ARG	CA-C	-6.02	1.45	1.52
1	A	493	ALA	CA-C	-6.01	1.45	1.52
1	A	20	ILE	C-O	-6.00	1.16	1.24
1	A	692	ILE	N-CA	-5.98	1.39	1.46
1	D	306	ASN	C-O	-5.97	1.16	1.23
1	E	67	ALA	N-CA	-5.97	1.39	1.46
1	B	296	GLY	C-O	5.96	1.31	1.23
1	A	440	LEU	N-CA	-5.94	1.39	1.46
1	F	177	ASP	C-O	5.93	1.30	1.23
1	A	291	GLU	N-CA	5.93	1.53	1.46
1	A	473	THR	N-CA	-5.92	1.38	1.45
1	F	570	TYR	C-O	-5.87	1.16	1.24
1	A	525	GLN	CD-NE2	5.83	1.45	1.33
1	A	22	ARG	CZ-NH1	5.73	1.40	1.32
1	D	64	ILE	CA-C	5.70	1.59	1.52
1	B	500	ALA	CA-C	-5.69	1.45	1.52
1	C	686	PRO	CA-C	5.68	1.59	1.52
1	E	252	TRP	C-N	-5.67	1.25	1.33
1	B	619	GLU	CA-C	-5.67	1.45	1.52
1	D	358	TRP	CA-C	5.66	1.59	1.53
1	E	357	TYR	CA-C	-5.64	1.45	1.52
1	A	277	VAL	N-CA	-5.57	1.39	1.46
1	E	502	GLU	C-O	-5.53	1.16	1.24
1	E	35	THR	N-CA	5.52	1.53	1.46
1	C	39	ILE	CA-C	-5.52	1.46	1.52
1	D	691	ASP	CA-C	-5.51	1.46	1.52
1	F	123	ARG	C-O	-5.50	1.17	1.24
1	A	344	TYR	N-CA	-5.50	1.38	1.45
1	A	155	TYR	C-O	5.49	1.30	1.23
1	B	590	TRP	CA-C	-5.49	1.46	1.52
1	F	530	MET	CG-SD	5.45	1.94	1.80
1	B	114	ILE	N-CA	5.44	1.51	1.46
1	A	523	TYR	N-CA	-5.43	1.39	1.45
1	F	488	GLY	C-O	-5.43	1.18	1.24
1	D	171	ARG	CZ-NH2	5.41	1.40	1.33
1	A	603	VAL	CA-C	-5.39	1.46	1.52
1	C	608	LEU	CA-C	5.39	1.59	1.52
1	F	22	ARG	CZ-NH1	5.38	1.40	1.32
1	F	598	ASP	C-O	-5.38	1.17	1.24
1	D	308	LEU	N-CA	-5.36	1.39	1.46
1	F	32	GLU	C-O	-5.35	1.17	1.24
1	A	693	ILE	CA-C	-5.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	LEU	N-CA	-5.35	1.40	1.46
1	A	43	ARG	N-CA	5.34	1.52	1.46
1	E	46	GLU	CA-C	5.33	1.59	1.52
1	E	421	PHE	N-CA	-5.33	1.41	1.45
1	D	327	LEU	N-CA	5.32	1.52	1.46
1	F	76	ILE	N-CA	5.32	1.53	1.46
1	A	57	GLY	C-O	-5.32	1.16	1.24
1	D	488	GLY	C-O	-5.29	1.18	1.24
1	A	185	TYR	CA-C	-5.28	1.45	1.52
1	A	290	LYS	N-CA	5.28	1.52	1.46
1	F	669	GLN	CD-OE1	5.26	1.33	1.23
1	C	108	HIS	CA-C	-5.25	1.46	1.52
1	E	288	THR	C-O	-5.25	1.17	1.24
1	B	529	PRO	CA-C	-5.25	1.46	1.52
1	E	598	ASP	N-CA	5.25	1.52	1.46
1	D	409	LEU	N-CA	-5.24	1.40	1.46
1	A	588	ALA	CA-C	-5.22	1.46	1.52
1	D	357	TYR	N-CA	-5.21	1.40	1.46
1	E	369	ASN	N-CA	-5.21	1.41	1.46
1	A	395	SER	CA-C	-5.21	1.46	1.52
1	D	196	ALA	C-O	5.21	1.30	1.23
1	E	148	VAL	C-O	-5.21	1.18	1.23
1	A	288	THR	CA-C	-5.20	1.45	1.52
1	B	253	ARG	CZ-NH1	5.20	1.40	1.32
1	A	465	VAL	N-CA	5.20	1.53	1.46
1	E	306	ASN	C-O	-5.19	1.17	1.23
1	D	253	ARG	CZ-NH1	5.17	1.40	1.32
1	A	253	ARG	CZ-NH1	5.17	1.40	1.32
1	D	340	ASP	CA-C	-5.16	1.45	1.52
1	C	253	ARG	CZ-NH1	5.16	1.40	1.32
1	F	253	ARG	CZ-NH1	5.15	1.40	1.32
1	C	277	VAL	N-CA	-5.15	1.40	1.46
1	D	109	TYR	C-O	5.14	1.29	1.23
1	A	529	PRO	C-O	-5.13	1.18	1.23
1	A	599	ALA	N-CA	5.13	1.52	1.46
1	A	55	GLN	C-O	5.12	1.28	1.24
1	E	253	ARG	CZ-NH1	5.12	1.40	1.32
1	D	356	THR	N-CA	-5.10	1.39	1.46
1	D	369	ASN	CA-C	-5.09	1.46	1.52
1	C	329	LEU	CA-C	5.08	1.59	1.52
1	A	500	ALA	N-CA	5.07	1.52	1.45
1	E	506	VAL	N-CA	5.06	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	527	THR	CA-C	-5.05	1.46	1.52
1	A	499	VAL	C-O	5.04	1.30	1.24
1	C	309	VAL	C-O	5.04	1.30	1.23
1	C	421	PHE	N-CA	5.03	1.50	1.45
1	B	693	ILE	C-O	-5.02	1.18	1.24
1	C	121	ALA	C-O	-5.01	1.18	1.24
1	A	216	ASP	CA-C	-5.01	1.46	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	536	CYS	CA-C-N	-7.49	112.46	120.47
1	F	536	CYS	C-N-CA	-7.49	112.46	120.47
1	C	628	SER	N-CA-C	7.24	118.73	108.74
1	E	281	HIS	N-CA-C	7.24	114.74	108.22
1	B	377	ARG	CG-CD-NE	-6.58	97.53	112.00
1	D	321	LEU	CA-C-N	-6.44	113.31	120.14
1	D	321	LEU	C-N-CA	-6.44	113.31	120.14
1	A	281	HIS	N-CA-C	6.42	114.00	108.22
1	F	252	TRP	CA-C-N	-6.24	114.59	123.20
1	F	252	TRP	C-N-CA	-6.24	114.59	123.20
1	A	536	CYS	CA-C-N	-6.09	112.23	119.84
1	A	536	CYS	C-N-CA	-6.09	112.23	119.84
1	B	356	THR	N-CA-C	-6.00	104.81	111.71
1	F	530	MET	CA-CB-CG	5.99	126.07	114.10
1	E	536	CYS	CA-C-N	-5.99	113.65	120.89
1	E	536	CYS	C-N-CA	-5.99	113.65	120.89
1	F	552	ILE	N-CA-C	5.97	116.71	108.12
1	C	281	HIS	N-CA-C	5.96	113.58	108.22
1	D	570	TYR	N-CA-C	5.89	119.29	111.75
1	C	496	ARG	NE-CZ-NH1	-5.79	115.72	121.50
1	E	20	ILE	CA-C-N	-5.78	114.00	119.90
1	E	20	ILE	C-N-CA	-5.78	114.00	119.90
1	D	556	SER	CB-CA-C	-5.73	105.28	110.44
1	B	313	GLN	N-CA-C	5.71	118.55	110.50
1	B	63	HIS	N-CA-C	5.61	117.47	111.36
1	E	662	HIS	N-CA-C	5.56	113.22	108.22
1	D	369	ASN	N-CA-C	-5.52	103.16	108.07
1	A	496	ARG	CB-CG-CD	5.49	123.93	111.30
1	D	225	GLU	CB-CG-CD	5.45	121.87	112.60
1	C	496	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	D	496	ARG	CB-CG-CD	5.42	123.77	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	690	VAL	N-CA-C	5.38	115.64	108.27
1	B	158	VAL	N-CA-C	-5.38	106.18	111.88
1	A	200	PHE	CA-C-N	-5.37	115.20	120.52
1	A	200	PHE	C-N-CA	-5.37	115.20	120.52
1	D	128	ARG	N-CA-C	5.34	116.79	111.07
1	A	225	GLU	CB-CG-CD	5.34	121.68	112.60
1	D	646	SER	CB-CA-C	-5.33	100.79	108.84
1	C	12	GLY	N-CA-C	5.31	120.25	111.59
1	C	171	ARG	N-CA-C	-5.30	105.50	111.28
1	A	395	SER	CB-CA-C	-5.29	101.03	109.75
1	D	662	HIS	N-CA-C	5.26	112.96	108.22
1	B	471	TYR	N-CA-C	5.22	116.97	111.28
1	C	662	HIS	N-CA-C	5.21	112.81	108.13
1	F	168	LYS	CA-CB-CG	-5.20	103.69	114.10
1	D	330	GLN	N-CA-C	-5.19	105.70	111.36
1	C	20	ILE	CB-CA-C	-5.19	104.71	110.68
1	D	471	TYR	N-CA-C	5.18	117.60	111.33
1	B	252	TRP	CA-C-N	-5.17	116.07	123.20
1	B	252	TRP	C-N-CA	-5.17	116.07	123.20
1	D	270	ARG	N-CA-C	5.16	117.64	111.71
1	A	326	GLN	N-CA-C	5.16	116.90	111.28
1	F	281	HIS	N-CA-C	5.11	112.82	108.22
1	C	480	ARG	O-C-N	5.09	127.95	122.15
1	D	383	GLY	N-CA-C	-5.09	108.66	115.32
1	F	432	VAL	N-CA-CB	5.08	116.49	110.55
1	C	168	LYS	CD-CE-NZ	-5.07	95.69	111.90
1	E	124	LEU	N-CA-C	5.06	116.48	111.07
1	B	680	GLY	N-CA-C	5.06	120.83	114.25
1	A	247	ASN	N-CA-C	5.06	117.38	107.57
1	A	432	VAL	N-CA-C	-5.04	105.79	110.53
1	F	436	ILE	N-CA-C	5.03	115.26	110.53
1	E	63	HIS	N-CA-C	5.02	116.83	111.36

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	29	0
1	B	5399	0	5106	41	0
1	C	5381	0	5095	26	0
1	D	5404	0	5117	22	0
1	E	5397	0	5110	22	0
1	F	5493	0	5196	34	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	11	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	6	0
All	All	35416	0	31180	171	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 3.

All (171) 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: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:B:155:TYR:HA	3:B:806:GOL:C3	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:HH11	1:B:176:ASN:ND2	1.90	0.69
1:B:284:GLU:HB3	1:F:530:MET:HE1	1.75	0.68
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:A:615:THR:HG22	1:A:618:MET:HE3	1.74	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:A:615:THR:N	1:A:618:MET:HE3	2.13	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:A:421:PHE:HB3	1:A:423:MET:HE3	1.85	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
3:C:809:GOL:O1	3:C:810:GOL:C1	2.52	0.58
1:F:303:GLY:HA3	4:F:1012:HOH:O	2.05	0.56
1:E:530:MET:HE1	1:F:284:GLU:HB3	1.87	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
1:A:445:VAL:HG22	1:A:618:MET:HE2	1.87	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:C:169:GLN:O	1:C:173:GLU:HG3	2.08	0.54
3:B:808:GOL:O1	1:F:423:MET:HE1	2.08	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:E:697:GLN:H	1:E:697:GLN:CD	2.16	0.52
1:C:518:ILE:HD12	1:C:583:PHE:CE2	2.45	0.52
1:B:562:HIS:ND1	3:B:807:GOL:H12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:492:LEU:C	1:F:492:LEU:HD23	2.37	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:F:115:MET:HE1	4:F:1261:HOH:O	2.10	0.49
1:A:615:THR:HG22	1:A:618:MET:CE	2.40	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:C:678:THR:O	1:C:679:VAL:C	2.56	0.49
1:A:207:ILE:HD12	1:A:207:ILE:C	2.38	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
1:D:85:TYR:CD2	1:D:150:ASN:HB3	2.48	0.48
1:C:85:TYR:CD1	1:C:85:TYR:C	2.92	0.48
1:A:615:THR:H	1:A:618:MET:HE3	1.78	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: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:D:181:LEU:C	1:D:181:LEU:HD23	2.40	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:E:678:THR:O	1:E:679:VAL:C	2.59	0.46
1:B:207:ILE:C	1:B:207:ILE:HD12	2.41	0.46
1:F:115:MET:HE3	4:F:1261:HOH:O	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:GLU:CD	1:F:214:ARG:HH21	2.24	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:492:LEU:C	1:C:492:LEU:HD23	2.42	0.44
1:A:672:THR:O	1:A:673:ALA:C	2.60	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:B:115:MET:HE2	1:B:115:MET:HB2	1.65	0.43
1:D:115:MET:HE3	4:D:1159:HOH:O	2.17	0.43
1:D:172:HIS:ND1	4:D:902:HOH:O	2.37	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:B:181:LEU:C	1:B:181:LEU:HD23	2.43	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
1:B:579:THR:O	1:B:589:GLN:HA	2.19	0.43
1:F:701:ASN:OD1	1:F:701:ASN:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:678:THR:O	1:B:679:VAL:C	2.62	0.42
1:A:492:LEU:C	1:A:492:LEU:HD23	2.45	0.42
1:B:248:PHE:HB3	1:B:265:HIS:CE1	2.55	0.42
1:D:85:TYR:C	1:D:85:TYR:CD1	2.96	0.42
1:F:564:LEU:N	1:F:564:LEU:HD12	2.34	0.42
1:A:250:TYR:O	1:A:251:GLU:C	2.62	0.41
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:43:ARG:HB2	1:F:343:MET:HE1	2.02	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:B:422:PRO:HG2	1:B:423:MET:HE3	2.02	0.41
1:E:20:ILE:O	1:E:21:PRO: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:173:GLU:CD	1:D:214:ARG:HH21	2.23	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:C:320:TRP:O	1:C:321:LEU:C	2.61	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:F:409:LEU:C	1:F:409:LEU:HD23	2.46	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
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%)	48	46
1	B	681/712 (96%)	654 (96%)	26 (4%)	1 (0%)	48	46
1	C	678/712 (95%)	652 (96%)	25 (4%)	1 (0%)	48	46
1	D	681/712 (96%)	652 (96%)	28 (4%)	1 (0%)	48	46
1	E	680/712 (96%)	654 (96%)	24 (4%)	2 (0%)	36	35
1	F	696/712 (98%)	668 (96%)	26 (4%)	2 (0%)	36	35
All	All	4097/4272 (96%)	3931 (96%)	158 (4%)	8 (0%)	43	42

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/580 (97%)	552 (99%)	8 (1%)	59	66
1	B	559/580 (96%)	554 (99%)	5 (1%)	70	78
1	C	557/580 (96%)	549 (99%)	8 (1%)	59	66
1	D	560/580 (97%)	554 (99%)	6 (1%)	65	73
1	E	559/580 (96%)	554 (99%)	5 (1%)	70	78
1	F	568/580 (98%)	562 (99%)	6 (1%)	65	73
All	All	3363/3480 (97%)	3325 (99%)	38 (1%)	65	73

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	115	MET
1	A	396	LYS
1	A	496	ARG
1	A	504	VAL
1	A	530	MET
1	A	539	THR
1	A	596	GLN
1	B	85	TYR
1	B	115	MET
1	B	203	LEU
1	B	423	MET
1	B	496	ARG
1	C	22	ARG
1	C	85	TYR
1	C	115	MET
1	C	423	MET
1	C	496	ARG
1	C	518	ILE
1	C	653	PRO
1	C	684	THR
1	D	85	TYR
1	D	115	MET
1	D	423	MET
1	D	496	ARG
1	D	504	VAL
1	D	526	PHE

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Mol	Chain	Res	Type
1	E	85	TYR
1	E	115	MET
1	E	423	MET
1	E	496	ARG
1	E	504	VAL
1	F	85	TYR
1	F	115	MET
1	F	203	LEU
1	F	423	MET
1	F	496	ARG
1	F	539	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	406	ASN
1	A	475	GLN
1	A	525	GLN
1	A	549	ASN
1	A	596	GLN
1	B	58	HIS
1	B	176	ASN
1	B	330	GLN
1	B	503	ASN
1	C	192	ASN
1	C	475	GLN
1	C	549	ASN
1	D	315	GLN
1	D	406	ASN
1	D	596	GLN
1	E	58	HIS
1	E	77	ASN
1	E	192	ASN
1	E	549	ASN
1	E	697	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	C	804	-	5,5,5	0.66	0	5,5,5	1.68	1 (20%)
2	SO4	D	802	-	4,4,4	0.49	0	6,6,6	0.66	0
3	GOL	B	814	-	5,5,5	0.53	0	5,5,5	1.49	1 (20%)
2	SO4	C	801	-	4,4,4	0.16	0	6,6,6	1.44	1 (16%)
3	GOL	F	805	-	5,5,5	0.62	0	5,5,5	0.52	0
3	GOL	E	803	-	5,5,5	1.42	1 (20%)	5,5,5	3.30	3 (60%)
2	SO4	B	803	-	4,4,4	0.44	0	6,6,6	0.78	0
3	GOL	B	807	-	5,5,5	0.44	0	5,5,5	1.02	0
2	SO4	F	814	-	4,4,4	0.52	0	6,6,6	0.62	0
3	GOL	E	809	-	5,5,5	0.33	0	5,5,5	0.45	0
3	GOL	C	810	-	5,5,5	0.67	0	5,5,5	1.54	1 (20%)
3	GOL	F	810	-	5,5,5	0.74	0	5,5,5	0.95	0
3	GOL	A	808	-	5,5,5	0.35	0	5,5,5	0.66	0
3	GOL	C	805	-	5,5,5	0.84	0	5,5,5	0.96	0
3	GOL	A	805	-	5,5,5	0.74	0	5,5,5	2.31	2 (40%)
3	GOL	E	804	-	5,5,5	0.36	0	5,5,5	1.56	1 (20%)
3	GOL	B	805	-	5,5,5	0.78	0	5,5,5	1.67	1 (20%)
3	GOL	F	813	-	5,5,5	0.60	0	5,5,5	0.89	0
3	GOL	C	808	-	5,5,5	0.86	0	5,5,5	1.68	2 (40%)
3	GOL	D	803	-	5,5,5	1.06	0	5,5,5	1.79	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	808	-	5,5,5	0.64	0	5,5,5	1.12	0
3	GOL	D	806	-	5,5,5	0.57	0	5,5,5	1.94	2 (40%)
3	GOL	B	810	-	5,5,5	0.78	0	5,5,5	1.40	1 (20%)
3	GOL	F	812	-	5,5,5	0.46	0	5,5,5	0.88	0
3	GOL	E	806	-	5,5,5	1.05	1 (20%)	5,5,5	2.29	3 (60%)
3	GOL	B	809	-	5,5,5	0.31	0	5,5,5	1.70	1 (20%)
3	GOL	F	803	-	5,5,5	1.40	2 (40%)	5,5,5	1.23	1 (20%)
3	GOL	F	804	-	5,5,5	0.63	0	5,5,5	2.14	2 (40%)
3	GOL	B	808	-	5,5,5	0.65	0	5,5,5	1.29	0
3	GOL	B	815	-	5,5,5	0.72	0	5,5,5	1.37	1 (20%)
2	SO4	E	801	-	4,4,4	0.18	0	6,6,6	1.35	1 (16%)
3	GOL	D	808	-	5,5,5	0.45	0	5,5,5	0.89	0
3	GOL	B	812	-	5,5,5	0.39	0	5,5,5	0.95	0
3	GOL	F	809	-	5,5,5	0.31	0	5,5,5	1.43	2 (40%)
3	GOL	A	809	-	5,5,5	0.66	0	5,5,5	0.48	0
3	GOL	A	802	-	5,5,5	1.36	1 (20%)	5,5,5	0.94	0
2	SO4	A	810	-	4,4,4	0.54	0	6,6,6	0.42	0
2	SO4	E	811	-	4,4,4	0.50	0	6,6,6	0.44	0
3	GOL	B	813	-	5,5,5	0.89	0	5,5,5	2.21	3 (60%)
3	GOL	F	811	-	5,5,5	1.07	1 (20%)	5,5,5	2.60	2 (40%)
3	GOL	D	805	-	5,5,5	0.51	0	5,5,5	1.51	1 (20%)
2	SO4	F	802	-	4,4,4	0.44	0	6,6,6	0.31	0
3	GOL	A	803	-	5,5,5	0.91	0	5,5,5	2.98	3 (60%)
3	GOL	A	804	-	5,5,5	0.97	0	5,5,5	1.19	1 (20%)
2	SO4	B	801	-	4,4,4	0.63	0	6,6,6	1.43	1 (16%)
3	GOL	C	803	-	5,5,5	1.43	1 (20%)	5,5,5	1.15	0
3	GOL	C	806	-	5,5,5	1.24	1 (20%)	5,5,5	1.37	1 (20%)
3	GOL	C	809	-	5,5,5	0.48	0	5,5,5	1.50	1 (20%)
3	GOL	D	807	-	5,5,5	0.35	0	5,5,5	0.49	0
3	GOL	F	806	-	5,5,5	0.69	0	5,5,5	1.32	1 (20%)
3	GOL	A	806	-	5,5,5	0.56	0	5,5,5	1.21	1 (20%)
3	GOL	E	807	-	5,5,5	0.54	0	5,5,5	2.09	2 (40%)
3	GOL	A	807	-	5,5,5	0.31	0	5,5,5	0.53	0
3	GOL	C	811	-	5,5,5	0.51	0	5,5,5	0.92	0
3	GOL	B	804	-	5,5,5	1.04	0	5,5,5	1.03	0
3	GOL	B	806	-	5,5,5	0.69	0	5,5,5	1.44	1 (20%)
2	SO4	E	802	-	4,4,4	0.49	0	6,6,6	1.24	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	802	-	4,4,4	0.49	0	6,6,6	0.69	0
3	GOL	E	808	-	5,5,5	0.41	0	5,5,5	0.66	0
2	SO4	D	801	-	4,4,4	0.25	0	6,6,6	1.18	1 (16%)
3	GOL	E	805	-	5,5,5	0.83	0	5,5,5	1.48	0
3	GOL	D	804	-	5,5,5	0.40	0	5,5,5	0.61	0
2	SO4	F	801	-	4,4,4	0.61	0	6,6,6	1.44	2 (33%)
3	GOL	C	807	-	5,5,5	0.73	0	5,5,5	1.76	1 (20%)
3	GOL	F	807	-	5,5,5	0.64	0	5,5,5	2.22	2 (40%)
2	SO4	B	802	-	4,4,4	0.51	0	6,6,6	0.42	0
2	SO4	A	801	-	4,4,4	0.27	0	6,6,6	1.17	1 (16%)
3	GOL	B	811	-	5,5,5	0.71	0	5,5,5	0.94	0
3	GOL	D	809	-	5,5,5	0.45	0	5,5,5	0.73	0
2	SO4	B	816	-	4,4,4	0.47	0	6,6,6	0.83	0
3	GOL	E	810	-	5,5,5	0.55	0	5,5,5	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	810	-	-	4/4/4/4	-
3	GOL	F	812	-	-	2/4/4/4	-
3	GOL	E	806	-	-	0/4/4/4	-
3	GOL	B	809	-	-	0/4/4/4	-
3	GOL	F	803	-	-	0/4/4/4	-
3	GOL	F	804	-	-	2/4/4/4	-
3	GOL	B	808	-	-	1/4/4/4	-
3	GOL	B	815	-	-	2/4/4/4	-
3	GOL	B	812	-	-	2/4/4/4	-
3	GOL	F	809	-	-	4/4/4/4	-
3	GOL	A	809	-	-	0/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	F	811	-	-	2/4/4/4	-
3	GOL	B	813	-	-	2/4/4/4	-
3	GOL	D	805	-	-	2/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-
3	GOL	C	803	-	-	0/4/4/4	-
3	GOL	C	806	-	-	2/4/4/4	-
3	GOL	C	809	-	-	1/4/4/4	-
3	GOL	D	807	-	-	0/4/4/4	-
3	GOL	F	806	-	-	4/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	E	807	-	-	2/4/4/4	-
3	GOL	A	807	-	-	4/4/4/4	-
3	GOL	C	811	-	-	2/4/4/4	-
3	GOL	B	804	-	-	0/4/4/4	-
3	GOL	B	806	-	-	4/4/4/4	-
3	GOL	E	808	-	-	2/4/4/4	-
3	GOL	E	805	-	-	0/4/4/4	-
3	GOL	D	804	-	-	1/4/4/4	-
3	GOL	C	807	-	-	2/4/4/4	-
3	GOL	F	807	-	-	2/4/4/4	-
3	GOL	B	811	-	-	4/4/4/4	-
3	GOL	D	809	-	-	4/4/4/4	-
3	GOL	D	808	-	-	3/4/4/4	-
3	GOL	E	810	-	-	3/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	GOL	C1-C2	2.67	1.62	1.51
3	F	803	GOL	O1-C1	2.35	1.52	1.42
3	C	803	GOL	C1-C2	2.34	1.60	1.51
3	E	803	GOL	O3-C3	2.27	1.52	1.42
3	E	806	GOL	O2-C2	-2.15	1.37	1.43
3	F	811	GOL	O2-C2	-2.10	1.37	1.43
3	C	806	GOL	O1-C1	2.04	1.51	1.42
3	F	803	GOL	C1-C2	2.00	1.59	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	803	GOL	O2-C2-C1	5.79	133.15	109.18
3	A	803	GOL	O1-C1-C2	-4.71	89.19	110.38
3	A	805	GOL	O2-C2-C1	-4.05	92.40	109.18
3	F	807	GOL	O2-C2-C1	-4.03	92.47	109.18
3	F	811	GOL	C3-C2-C1	3.75	125.56	111.80
3	E	806	GOL	O2-C2-C1	-3.56	94.42	109.18
3	F	804	GOL	O3-C3-C2	-3.49	94.69	110.38
3	E	807	GOL	O1-C1-C2	-3.48	94.73	110.38
3	D	803	GOL	O1-C1-C2	3.47	126.01	110.38
3	F	811	GOL	O2-C2-C1	-3.31	95.47	109.18
3	C	804	GOL	O3-C3-C2	-3.31	95.50	110.38
3	E	803	GOL	O1-C1-C2	3.27	125.10	110.38
3	B	813	GOL	C3-C2-C1	3.27	123.78	111.80
3	B	805	GOL	C3-C2-C1	-3.25	99.87	111.80
3	A	803	GOL	O2-C2-C1	-3.18	96.02	109.18
3	A	803	GOL	O2-C2-C3	3.12	122.09	109.18
3	E	803	GOL	O3-C3-C2	-3.08	96.53	110.38
3	E	806	GOL	C3-C2-C1	3.04	122.95	111.80
3	E	807	GOL	O3-C3-C2	-3.04	96.69	110.38
2	B	801	SO4	O4-S-O1	-3.02	93.78	109.56
3	F	806	GOL	O2-C2-C1	-2.83	97.46	109.18
3	D	806	GOL	C3-C2-C1	2.78	121.97	111.80
2	C	801	SO4	O2-S-O1	-2.68	90.20	109.06
3	A	805	GOL	C3-C2-C1	2.62	121.40	111.80
3	B	813	GOL	O2-C2-C3	-2.59	98.44	109.18
3	C	808	GOL	O2-C2-C1	-2.58	98.49	109.18
3	B	806	GOL	O3-C3-C2	2.58	121.99	110.38
3	B	810	GOL	C3-C2-C1	2.55	121.13	111.80
3	F	807	GOL	O1-C1-C2	-2.52	99.03	110.38
2	A	801	SO4	O3-S-O1	-2.51	96.45	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	809	GOL	O1-C1-C2	-2.46	99.30	110.38
3	C	810	GOL	O1-C1-C2	2.43	121.34	110.38
2	E	802	SO4	O4-S-O1	2.43	122.24	109.56
3	E	804	GOL	C3-C2-C1	-2.40	102.98	111.80
2	F	801	SO4	O3-S-O1	-2.39	97.06	109.56
3	B	814	GOL	O1-C1-C2	-2.39	99.62	110.38
3	B	809	GOL	O1-C1-C2	-2.35	99.78	110.38
3	C	806	GOL	O1-C1-C2	2.34	120.93	110.38
3	F	809	GOL	O1-C1-C2	-2.33	99.89	110.38
3	D	805	GOL	C3-C2-C1	-2.31	103.34	111.80
3	D	806	GOL	O2-C2-C3	-2.27	99.78	109.18
3	C	808	GOL	O1-C1-C2	-2.22	100.38	110.38
2	F	801	SO4	O3-S-O2	2.19	120.99	109.56
2	E	801	SO4	O4-S-O2	-2.15	98.31	109.56
3	F	803	GOL	O1-C1-C2	2.15	120.04	110.38
3	C	807	GOL	O2-C2-C3	-2.15	100.29	109.18
3	A	804	GOL	O1-C1-C2	2.11	119.89	110.38
3	F	804	GOL	C3-C2-C1	2.08	119.43	111.80
3	B	813	GOL	O2-C2-C1	-2.07	100.59	109.18
3	F	809	GOL	C3-C2-C1	-2.07	104.20	111.80
2	D	801	SO4	O3-S-O2	-2.06	98.81	109.56
3	B	815	GOL	O1-C1-C2	2.05	119.59	110.38
3	A	806	GOL	O3-C3-C2	2.01	119.41	110.38
3	E	806	GOL	O1-C1-C2	-2.00	101.36	110.38

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
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

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Mol	Chain	Res	Type	Atoms
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
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	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	805	GOL	O1-C1-C2-C3
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	E	810	GOL	O1-C1-C2-C3
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

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Mol	Chain	Res	Type	Atoms
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
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	E	807	GOL	O1-C1-C2-O2
3	F	805	GOL	O1-C1-C2-O2
3	C	809	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 25 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.30	3 (0%) 88 88	17, 25, 38, 61	0
1	B	685/712 (96%)	-0.51	3 (0%) 88 88	17, 23, 36, 58	0
1	C	682/712 (95%)	-0.24	6 (0%) 81 80	16, 27, 43, 65	0
1	D	685/712 (96%)	-0.18	6 (0%) 81 80	17, 27, 44, 68	0
1	E	684/712 (96%)	-0.28	9 (1%) 75 74	17, 26, 41, 64	0
1	F	698/712 (98%)	-0.47	8 (1%) 78 77	16, 23, 39, 58	0
All	All	4119/4272 (96%)	-0.33	35 (0%) 82 82	16, 25, 41, 68	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	8	PRO	5.4
1	C	8	PRO	5.2
1	E	8	PRO	5.0
1	A	8	PRO	3.6
1	B	8	PRO	3.6
1	D	8	PRO	3.6
1	F	705	LEU	3.3
1	F	703	ALA	3.1
1	D	698	PRO	3.0
1	D	664	THR	2.8
1	A	699	THR	2.8
1	C	671	VAL	2.8
1	E	697	GLN	2.6
1	C	696	ARG	2.5
1	B	253	ARG	2.5
1	F	253	ARG	2.4
1	F	702	ALA	2.4
1	C	663	PRO	2.3
1	C	517	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	669	GLN	2.3
1	B	665	ASP	2.3
1	F	530	MET	2.3
1	D	253	ARG	2.2
1	F	537	PRO	2.2
1	E	698	PRO	2.2
1	E	671	VAL	2.2
1	A	36	ARG	2.1
1	E	530	MET	2.1
1	E	538	ASP	2.1
1	C	678	THR	2.1
1	E	614	HIS	2.1
1	D	697	GLN	2.0
1	E	253	ARG	2.0
1	D	671	VAL	2.0
1	E	663	PRO	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 oligosaccharides 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	B	809	6/6	0.79	0.17	41,46,52,55	0
3	GOL	B	810	6/6	0.80	0.22	50,54,61,65	0
3	GOL	A	806	6/6	0.81	0.17	47,56,59,60	0
3	GOL	C	810	6/6	0.81	0.17	40,57,60,63	0
3	GOL	C	811	6/6	0.81	0.16	52,56,58,59	0
3	GOL	D	804	6/6	0.81	0.19	53,57,59,62	0
3	GOL	A	809	6/6	0.83	0.20	55,59,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	F	805	6/6	0.83	0.16	45,53,56,63	0
3	GOL	A	804	6/6	0.84	0.17	49,54,55,56	0
3	GOL	F	808	6/6	0.84	0.15	36,50,51,53	0
3	GOL	B	806	6/6	0.85	0.17	42,50,53,60	0
3	GOL	F	809	6/6	0.85	0.15	38,53,59,59	0
3	GOL	F	810	6/6	0.85	0.18	49,54,58,60	0
3	GOL	B	808	6/6	0.86	0.19	52,55,66,70	0
3	GOL	E	807	6/6	0.86	0.14	35,45,50,51	0
3	GOL	A	803	6/6	0.87	0.15	34,47,49,54	0
3	GOL	F	806	6/6	0.87	0.13	35,46,56,57	0
3	GOL	D	807	6/6	0.87	0.17	52,57,61,63	0
3	GOL	D	809	6/6	0.87	0.14	45,57,59,67	0
3	GOL	C	808	6/6	0.87	0.17	48,49,52,55	0
3	GOL	B	814	6/6	0.88	0.17	50,54,57,64	0
3	GOL	E	808	6/6	0.88	0.12	48,52,60,62	0
3	GOL	E	810	6/6	0.88	0.18	45,47,52,63	0
3	GOL	C	804	6/6	0.88	0.12	38,41,45,47	0
3	GOL	F	813	6/6	0.88	0.19	51,65,66,67	0
3	GOL	A	805	6/6	0.89	0.16	39,58,62,62	0
2	SO4	D	802	5/5	0.89	0.08	60,61,65,77	0
3	GOL	E	809	6/6	0.89	0.18	56,62,63,69	0
3	GOL	B	807	6/6	0.89	0.14	43,56,61,62	0
3	GOL	B	811	6/6	0.89	0.14	48,54,57,62	0
3	GOL	C	809	6/6	0.90	0.14	36,47,53,55	0
3	GOL	C	805	6/6	0.90	0.16	38,61,62,62	0
2	SO4	B	802	5/5	0.91	0.11	48,54,55,63	0
3	GOL	B	813	6/6	0.91	0.15	32,48,52,59	0
3	GOL	C	806	6/6	0.91	0.14	38,47,53,56	0
3	GOL	A	808	6/6	0.91	0.12	52,58,60,66	0
3	GOL	D	805	6/6	0.91	0.12	37,42,46,54	0
3	GOL	D	806	6/6	0.91	0.15	34,50,54,55	0
3	GOL	C	807	6/6	0.92	0.13	32,50,53,55	0
3	GOL	A	802	6/6	0.92	0.10	21,27,28,29	0
3	GOL	B	815	6/6	0.92	0.12	32,53,57,65	0
2	SO4	B	816	5/5	0.92	0.08	54,57,66,71	0
3	GOL	E	804	6/6	0.92	0.11	34,41,44,48	0
3	GOL	E	805	6/6	0.92	0.10	35,42,46,50	0
3	GOL	A	807	6/6	0.92	0.14	48,51,54,73	0
3	GOL	F	811	6/6	0.92	0.14	32,49,56,56	0
2	SO4	A	810	5/5	0.92	0.08	56,60,73,75	0
2	SO4	E	802	5/5	0.93	0.13	36,42,48,52	0
3	GOL	B	805	6/6	0.93	0.11	29,37,41,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	812	6/6	0.93	0.11	36,42,52,56	0
2	SO4	F	802	5/5	0.93	0.07	54,62,66,71	0
3	GOL	D	808	6/6	0.93	0.11	32,37,47,55	0
3	GOL	F	807	6/6	0.93	0.12	42,51,52,53	0
2	SO4	F	814	5/5	0.93	0.08	51,54,60,69	0
2	SO4	C	802	5/5	0.93	0.07	52,56,61,65	0
2	SO4	B	803	5/5	0.93	0.07	48,55,62,69	0
3	GOL	E	806	6/6	0.93	0.12	35,49,57,59	0
3	GOL	F	812	6/6	0.93	0.14	33,38,49,67	0
3	GOL	D	803	6/6	0.93	0.09	22,22,23,29	0
2	SO4	E	811	5/5	0.94	0.07	51,53,62,68	0
3	GOL	F	803	6/6	0.94	0.09	20,24,24,29	0
3	GOL	F	804	6/6	0.94	0.10	29,35,41,45	0
3	GOL	C	803	6/6	0.95	0.08	23,27,29,34	0
3	GOL	E	803	6/6	0.95	0.07	21,23,25,26	0
2	SO4	E	801	5/5	0.96	0.13	33,36,38,39	0
3	GOL	B	804	6/6	0.96	0.07	20,24,25,28	0
2	SO4	D	801	5/5	0.96	0.11	35,42,49,51	0
2	SO4	A	801	5/5	0.97	0.08	36,37,41,45	0
2	SO4	C	801	5/5	0.97	0.08	31,37,41,44	0
2	SO4	F	801	5/5	0.97	0.08	31,36,39,40	0
2	SO4	B	801	5/5	0.97	0.08	30,38,42,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.