



wwPDB X-ray Structure Validation Summary Report

Nov 25, 2014 – 06:23 PM EST

PDB ID : 4NX0
Title : Crystal structure of Abp-WT, a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on : 2013-12-08
Resolution : 2.28 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

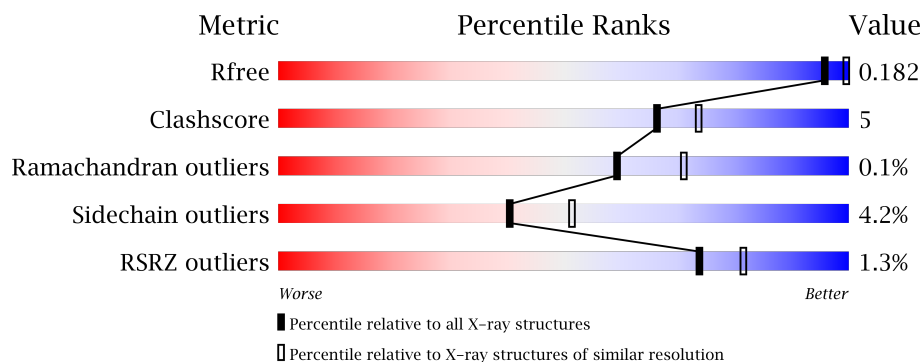
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 2.28 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}	66092	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	
1	F	448	
1	G	448	
1	H	448	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	501	-	X
2	GOL	A	502	-	X
2	GOL	A	504	-	X
2	GOL	B	503	-	X
2	GOL	B	504	-	X
2	GOL	B	505	-	X
2	GOL	B	506	-	X
2	GOL	B	508	-	X
2	GOL	B	509	-	X
2	GOL	C	502	-	X
2	GOL	C	503	-	X
2	GOL	C	504	-	X
2	GOL	C	505	-	X
2	GOL	D	502	-	X
2	GOL	D	505	-	X
2	GOL	E	503	-	X
2	GOL	E	504	-	X
2	GOL	E	505	-	X
2	GOL	E	506	-	X
2	GOL	F	503	-	X
2	GOL	F	504	-	X
2	GOL	G	502	-	X
2	GOL	G	504	-	X
2	GOL	H	502	-	X
3	SO4	A	505	-	X
3	SO4	A	506	-	X
3	SO4	A	507	-	X
3	SO4	A	508	-	X
3	SO4	A	509	-	X
3	SO4	A	511	-	X
3	SO4	A	512	-	X
3	SO4	A	513	-	X
3	SO4	B	510	-	X
3	SO4	B	511	-	X
3	SO4	B	512	-	X
3	SO4	B	513	-	X
3	SO4	B	514	-	X
3	SO4	B	516	-	X
3	SO4	B	517	-	X
3	SO4	B	518	-	X
3	SO4	B	519	-	X
3	SO4	C	506	-	X
3	SO4	C	507	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	C	508	-	X
3	SO4	C	509	-	X
3	SO4	C	510	-	X
3	SO4	C	511	-	X
3	SO4	C	512	-	X
3	SO4	C	513	-	X
3	SO4	C	514	-	X
3	SO4	C	515	-	X
3	SO4	C	516	-	X
3	SO4	C	517	-	X
3	SO4	D	506	-	X
3	SO4	D	507	-	X
3	SO4	D	508	-	X
3	SO4	D	509	-	X
3	SO4	D	510	-	X
3	SO4	D	511	-	X
3	SO4	D	512	-	X
3	SO4	D	513	-	X
3	SO4	D	514	-	X
3	SO4	D	515	-	X
3	SO4	D	516	-	X
3	SO4	D	517	-	X
3	SO4	E	507	-	X
3	SO4	E	508	-	X
3	SO4	E	509	-	X
3	SO4	E	510	-	X
3	SO4	E	511	-	X
3	SO4	E	512	-	X
3	SO4	E	513	-	X
3	SO4	E	514	-	X
3	SO4	E	515	-	X
3	SO4	E	516	-	X
3	SO4	F	505	-	X
3	SO4	F	506	-	X
3	SO4	F	507	-	X
3	SO4	F	508	-	X
3	SO4	F	509	-	X
3	SO4	F	510	-	X
3	SO4	F	511	-	X
3	SO4	F	512	-	X
3	SO4	F	513	-	X
3	SO4	F	514	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	F	515	-	X
3	SO4	G	505	-	X
3	SO4	G	506	-	X
3	SO4	G	507	-	X
3	SO4	G	508	-	X
3	SO4	G	510	-	X
3	SO4	G	511	-	X
3	SO4	G	512	-	X
3	SO4	H	504	-	X
3	SO4	H	505	-	X
3	SO4	H	506	-	X
3	SO4	H	507	-	X
3	SO4	H	508	-	X
3	SO4	H	509	-	X
3	SO4	H	510	-	X
3	SO4	H	511	-	X
3	SO4	H	512	-	X
3	SO4	H	513	-	X
3	SO4	H	514	-	X
4	CIT	A	515	-	X
4	CIT	B	520	-	X
4	CIT	C	519	-	X
4	CIT	E	517	-	X
4	CIT	G	513	-	X

2 Entry composition

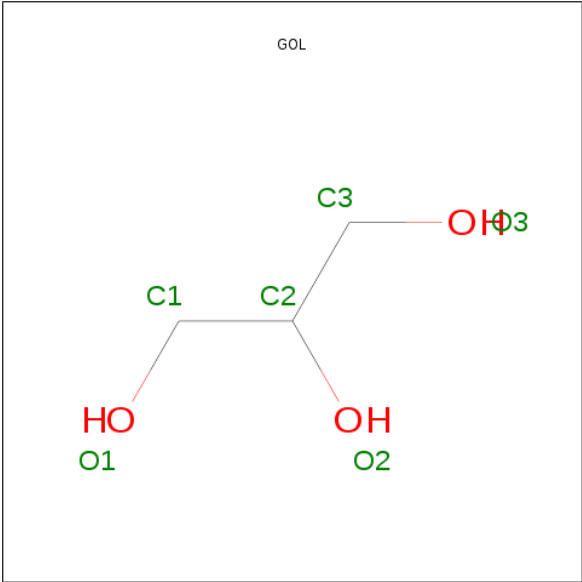
There are 5 unique types of molecules in this entry. The entry contains 32820 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Abp, a GH27 beta-L-arabinopyranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	4	0
			3492	2233	598	636	25			
1	B	430	Total	C	N	O	S	0	4	0
			3496	2235	598	638	25			
1	C	431	Total	C	N	O	S	0	2	0
			3487	2230	598	634	25			
1	D	435	Total	C	N	O	S	0	1	0
			3506	2243	603	635	25			
1	E	430	Total	C	N	O	S	0	3	0
			3484	2228	597	634	25			
1	F	430	Total	C	N	O	S	0	0	0
			3470	2219	596	630	25			
1	G	430	Total	C	N	O	S	0	2	0
			3481	2226	596	634	25			
1	H	430	Total	C	N	O	S	0	0	0
			3470	2219	596	630	25			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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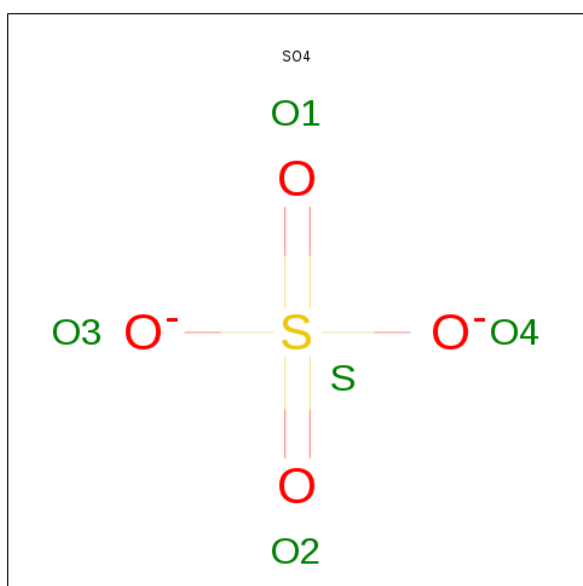
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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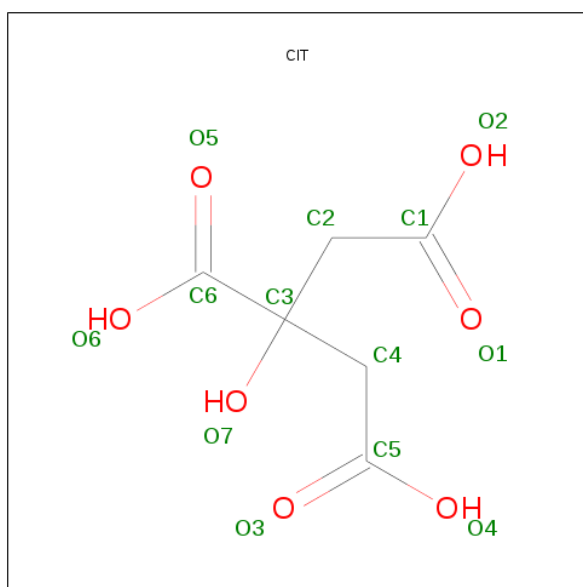
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	E	1	Total	C	O	0	0
			13	6	7		
4	G	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	662	Total	O	0	0
			662	662		
5	B	625	Total	O	0	0
			625	625		
5	C	579	Total	O	0	0
			579	579		
5	D	536	Total	O	0	0
			536	536		
5	E	500	Total	O	0	0
			500	500		
5	F	495	Total	O	0	0
			495	495		
5	G	439	Total	O	0	0
			439	439		

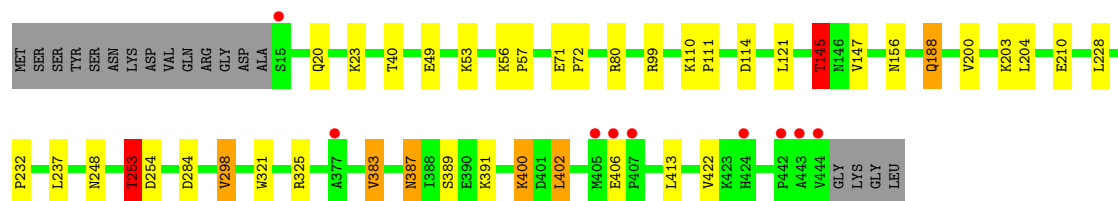
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	368	Total 368	O 368	0	0

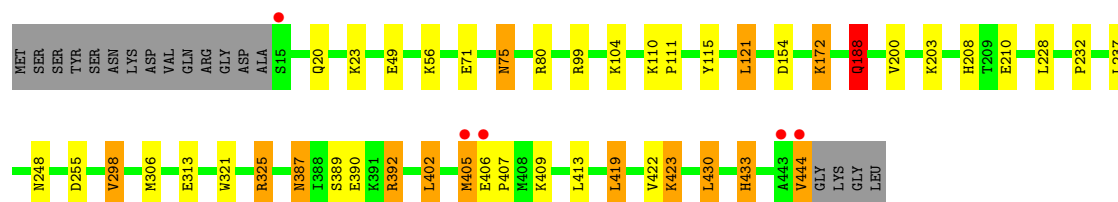
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain E:



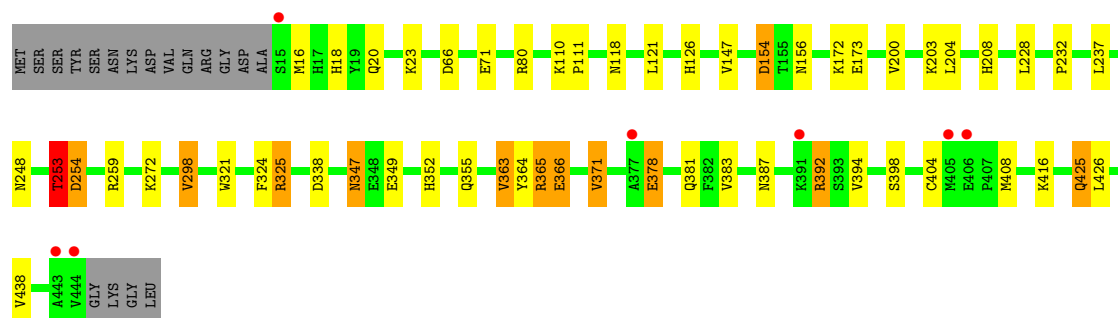
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain F:



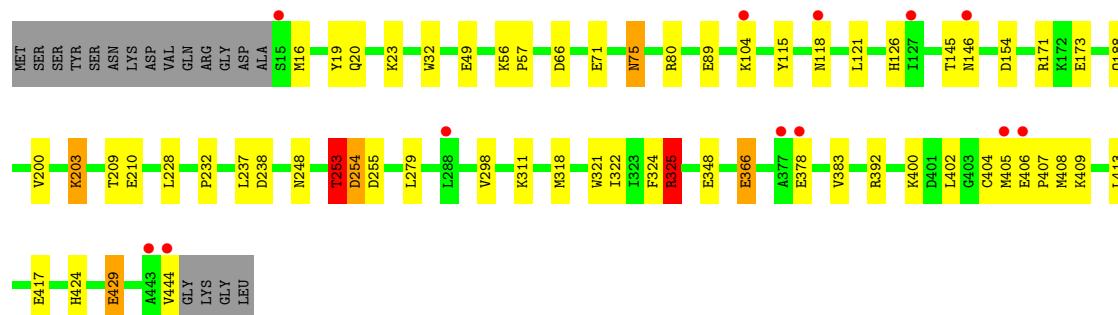
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain G:



- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.71 Å 202.16 Å 287.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.28 29.88 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.90-2.28) 96.8 (29.88-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.146 , 0.177 0.154 , 0.182	Depositor DCC
R_{free} test set	13898 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 275069 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32820	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CIT

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	1.02	4/3606 (0.1%)	0.93	9/4895 (0.2%)
1	B	1.01	0/3607	0.94	12/4896 (0.2%)
1	C	0.96	1/3595 (0.0%)	0.91	6/4880 (0.1%)
1	D	0.95	2/3611 (0.1%)	0.89	5/4899 (0.1%)
1	E	0.88	2/3595 (0.1%)	0.89	12/4881 (0.2%)
1	F	0.85	0/3572	0.90	12/4849 (0.2%)
1	G	0.84	0/3589	0.94	11/4872 (0.2%)
1	H	0.84	1/3572 (0.0%)	0.93	11/4849 (0.2%)
All	All	0.92	10/28747 (0.0%)	0.92	78/39021 (0.2%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	TYR	CG-CD1	-5.97	1.31	1.39
1	D	49	GLU	CG-CD	5.70	1.60	1.51
1	A	366	GLU	CD-OE2	5.59	1.31	1.25
1	E	188[A]	GLN	CG-CD	5.58	1.63	1.51
1	E	188[B]	GLN	CG-CD	5.58	1.63	1.51

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	325	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	H	325	ARG	NE-CZ-NH2	-10.71	114.95	120.30
1	C	325	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	H	80	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	F	80	ARG	NE-CZ-NH2	-7.78	116.41	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3492	0	3370	36	0
1	B	3496	0	3369	38	0
1	C	3487	0	3365	27	0
1	D	3506	0	3394	27	0
1	E	3484	0	3363	27	0
1	F	3470	0	3346	29	0
1	G	3481	0	3356	39	0
1	H	3470	0	3346	33	0
2	A	24	0	32	6	0
2	B	54	0	72	9	0
2	C	30	0	40	9	0
2	D	30	0	40	11	0
2	E	36	0	48	6	0
2	F	24	0	32	7	0
2	G	24	0	32	1	0
2	H	18	0	24	4	0
3	A	50	0	0	1	0
3	B	50	0	0	3	0
3	C	65	0	0	1	0
3	D	60	0	0	1	0
3	E	50	0	0	0	0
3	F	55	0	0	1	0
3	G	40	0	0	1	0
3	H	55	0	0	3	0
4	A	13	0	6	6	0
4	B	13	0	5	8	0
4	C	13	0	5	4	0
4	E	13	0	5	2	0
4	G	13	0	5	7	0
5	A	662	0	0	18	0
5	B	625	0	0	17	0
5	C	579	0	0	13	0
5	D	536	0	0	8	0
5	E	500	0	0	4	0
5	F	495	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	439	0	0	17	0
5	H	368	0	0	10	0
All	All	32820	0	27255	283	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:505:GOL:O3	2:C:505:GOL:C3	1.67	1.40
4:A:515:CIT:O5	4:A:515:CIT:C5	1.75	1.20
1:H:146:ASN:HB3	5:H:917:HOH:O	1.40	1.18
4:C:519:CIT:O4	4:C:519:CIT:H21	1.47	1.11
1:C:49:GLU:HG2	5:C:1111:HOH:O	1.53	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/448 (96%)	418 (97%)	14 (3%)	0	100	100
1	B	432/448 (96%)	413 (96%)	19 (4%)	0	100	100
1	C	431/448 (96%)	416 (96%)	15 (4%)	0	100	100
1	D	434/448 (97%)	419 (96%)	15 (4%)	0	100	100
1	E	431/448 (96%)	416 (96%)	15 (4%)	0	100	100
1	F	428/448 (96%)	413 (96%)	14 (3%)	1 (0%)	56	67
1	G	430/448 (96%)	415 (96%)	15 (4%)	0	100	100
1	H	428/448 (96%)	410 (96%)	17 (4%)	1 (0%)	56	67
All	All	3446/3584 (96%)	3320 (96%)	124 (4%)	2 (0%)	59	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	325	ARG
1	F	325	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/383 (97%)	363 (97%)	10 (3%)	57	72
1	B	373/383 (97%)	361 (97%)	12 (3%)	51	66
1	C	371/383 (97%)	358 (96%)	13 (4%)	48	61
1	D	372/383 (97%)	363 (98%)	9 (2%)	61	77
1	E	372/383 (97%)	356 (96%)	16 (4%)	40	50
1	F	369/383 (96%)	348 (94%)	21 (6%)	29	35
1	G	371/383 (97%)	349 (94%)	22 (6%)	28	33
1	H	369/383 (96%)	348 (94%)	21 (6%)	29	35
All	All	2970/3064 (97%)	2846 (96%)	124 (4%)	40	51

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	402	LEU
1	F	321	TRP
1	H	321	TRP
1	E	406	GLU
1	F	104	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	356	ASN
1	E	248	ASN
1	H	75	ASN
1	D	387	ASN

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Mol	Chain	Res	Type
1	E	20	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

130 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	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.65	0	5,5,5	0.54	0
2	GOL	A	502	-	5,5,5	0.54	0	5,5,5	0.44	0
2	GOL	A	503	-	5,5,5	0.84	0	5,5,5	2.12	2 (40%)
2	GOL	A	504	-	5,5,5	0.43	0	5,5,5	0.65	0
3	SO4	A	505	-	4,4,4	2.02	2 (50%)	6,6,6	0.76	0
3	SO4	A	506	-	4,4,4	0.75	0	6,6,6	0.35	0
3	SO4	A	507	-	4,4,4	0.91	0	6,6,6	1.00	1 (16%)
3	SO4	A	508	-	4,4,4	0.86	0	6,6,6	0.42	0
3	SO4	A	509	-	4,4,4	0.53	0	6,6,6	0.79	0
3	SO4	A	510	-	4,4,4	1.27	0	6,6,6	0.50	0
3	SO4	A	511	-	4,4,4	1.07	0	6,6,6	0.72	0
3	SO4	A	512	-	4,4,4	1.56	1 (25%)	6,6,6	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	513	-	4,4,4	0.72	0	6,6,6	0.68	0
3	SO4	A	514	-	4,4,4	1.33	0	6,6,6	0.64	0
4	CIT	A	515	-	12,12,12	1.73	5 (41%)	17,17,17	5.57	13 (76%)
2	GOL	B	501	-	5,5,5	0.54	0	5,5,5	1.11	0
2	GOL	B	502	-	5,5,5	0.49	0	5,5,5	0.69	0
2	GOL	B	503	-	5,5,5	0.96	0	5,5,5	1.47	1 (20%)
2	GOL	B	504	-	5,5,5	0.73	0	5,5,5	1.12	0
2	GOL	B	505	-	5,5,5	1.03	0	5,5,5	0.81	0
2	GOL	B	506	-	5,5,5	0.63	0	5,5,5	0.59	0
2	GOL	B	507	-	5,5,5	0.36	0	5,5,5	1.57	1 (20%)
2	GOL	B	508	-	5,5,5	0.64	0	5,5,5	0.86	0
2	GOL	B	509	-	5,5,5	0.57	0	5,5,5	0.83	0
3	SO4	B	510	-	4,4,4	0.76	0	6,6,6	0.63	0
3	SO4	B	511	-	4,4,4	1.13	0	6,6,6	0.77	0
3	SO4	B	512	-	4,4,4	1.07	0	6,6,6	0.96	0
3	SO4	B	513	-	4,4,4	0.48	0	6,6,6	0.38	0
3	SO4	B	514	-	4,4,4	0.74	0	6,6,6	0.43	0
3	SO4	B	515	-	4,4,4	1.05	0	6,6,6	0.65	0
3	SO4	B	516	-	4,4,4	1.14	0	6,6,6	0.91	0
3	SO4	B	517	-	4,4,4	1.63	1 (25%)	6,6,6	1.33	1 (16%)
3	SO4	B	518	-	4,4,4	0.62	0	6,6,6	0.31	0
3	SO4	B	519	-	4,4,4	0.84	0	6,6,6	0.52	0
4	CIT	B	520	-	12,12,12	2.07	3 (25%)	17,17,17	1.87	4 (23%)
2	GOL	C	501	-	5,5,5	0.21	0	5,5,5	0.70	0
2	GOL	C	502	-	5,5,5	0.58	0	5,5,5	0.60	0
2	GOL	C	503	-	5,5,5	2.18	3 (60%)	5,5,5	2.32	2 (40%)
2	GOL	C	504	-	5,5,5	0.60	0	5,5,5	0.96	1 (20%)
2	GOL	C	505	-	5,5,5	2.68	1 (20%)	5,5,5	1.65	1 (20%)
3	SO4	C	506	-	4,4,4	0.67	0	6,6,6	0.29	0
3	SO4	C	507	-	4,4,4	1.09	0	6,6,6	0.56	0
3	SO4	C	508	-	4,4,4	0.73	0	6,6,6	0.34	0
3	SO4	C	509	-	4,4,4	0.58	0	6,6,6	0.23	0
3	SO4	C	510	-	4,4,4	1.14	0	6,6,6	0.35	0
3	SO4	C	511	-	4,4,4	0.86	0	6,6,6	0.56	0
3	SO4	C	512	-	4,4,4	0.73	0	6,6,6	0.73	0
3	SO4	C	513	-	4,4,4	1.23	0	6,6,6	0.91	0
3	SO4	C	514	-	4,4,4	0.74	0	6,6,6	0.43	0
3	SO4	C	515	-	4,4,4	1.03	0	6,6,6	0.94	0
3	SO4	C	516	-	4,4,4	1.02	0	6,6,6	0.92	0
3	SO4	C	517	-	4,4,4	1.24	0	6,6,6	0.42	0
3	SO4	C	518	-	4,4,4	0.68	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	C	519	-	12,12,12	2.86	6 (50%)	17,17,17	3.83	9 (52%)
2	GOL	D	501	-	5,5,5	0.76	0	5,5,5	0.44	0
2	GOL	D	502	-	5,5,5	0.93	0	5,5,5	1.55	2 (40%)
2	GOL	D	503	-	5,5,5	0.53	0	5,5,5	1.80	2 (40%)
2	GOL	D	504	-	5,5,5	0.71	0	5,5,5	1.37	1 (20%)
2	GOL	D	505	-	5,5,5	0.94	0	5,5,5	1.39	1 (20%)
3	SO4	D	506	-	4,4,4	0.73	0	6,6,6	0.50	0
3	SO4	D	507	-	4,4,4	0.76	0	6,6,6	0.34	0
3	SO4	D	508	-	4,4,4	1.65	2 (50%)	6,6,6	0.78	0
3	SO4	D	509	-	4,4,4	1.16	0	6,6,6	1.45	2 (33%)
3	SO4	D	510	-	4,4,4	0.86	0	6,6,6	0.46	0
3	SO4	D	511	-	4,4,4	1.11	0	6,6,6	1.65	2 (33%)
3	SO4	D	512	-	4,4,4	0.79	0	6,6,6	1.51	2 (33%)
3	SO4	D	513	-	4,4,4	0.91	0	6,6,6	0.46	0
3	SO4	D	514	-	4,4,4	0.82	0	6,6,6	0.34	0
3	SO4	D	515	-	4,4,4	0.73	0	6,6,6	0.53	0
3	SO4	D	516	-	4,4,4	0.80	0	6,6,6	0.48	0
3	SO4	D	517	-	4,4,4	1.15	1 (25%)	6,6,6	0.73	0
2	GOL	E	501	-	5,5,5	0.46	0	5,5,5	0.26	0
2	GOL	E	502	-	5,5,5	0.52	0	5,5,5	0.44	0
2	GOL	E	503	-	5,5,5	0.70	0	5,5,5	1.72	2 (40%)
2	GOL	E	504	-	5,5,5	0.74	0	5,5,5	0.83	0
2	GOL	E	505	-	5,5,5	1.39	0	5,5,5	2.54	4 (80%)
2	GOL	E	506	-	5,5,5	0.31	0	5,5,5	0.31	0
3	SO4	E	507	-	4,4,4	0.67	0	6,6,6	0.62	0
3	SO4	E	508	-	4,4,4	1.18	0	6,6,6	0.62	0
3	SO4	E	509	-	4,4,4	1.20	0	6,6,6	0.97	0
3	SO4	E	510	-	4,4,4	0.85	0	6,6,6	0.22	0
3	SO4	E	511	-	4,4,4	1.29	1 (25%)	6,6,6	1.37	1 (16%)
3	SO4	E	512	-	4,4,4	0.89	0	6,6,6	0.68	0
3	SO4	E	513	-	4,4,4	0.84	0	6,6,6	1.18	1 (16%)
3	SO4	E	514	-	4,4,4	2.03	1 (25%)	6,6,6	1.19	1 (16%)
3	SO4	E	515	-	4,4,4	1.14	0	6,6,6	0.93	0
3	SO4	E	516	-	4,4,4	0.78	0	6,6,6	0.26	0
4	CIT	E	517	-	12,12,12	1.38	1 (8%)	17,17,17	2.08	5 (29%)
2	GOL	F	501	-	5,5,5	0.75	0	5,5,5	0.31	0
2	GOL	F	502	-	5,5,5	0.45	0	5,5,5	0.62	0
2	GOL	F	503	-	5,5,5	0.62	0	5,5,5	0.43	0
2	GOL	F	504	-	5,5,5	0.20	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	505	-	4,4,4	0.94	0	6,6,6	0.49	0
3	SO4	F	506	-	4,4,4	0.75	0	6,6,6	0.30	0
3	SO4	F	507	-	4,4,4	0.73	0	6,6,6	0.36	0
3	SO4	F	508	-	4,4,4	1.43	1 (25%)	6,6,6	1.02	1 (16%)
3	SO4	F	509	-	4,4,4	0.83	0	6,6,6	0.58	0
3	SO4	F	510	-	4,4,4	0.98	0	6,6,6	0.41	0
3	SO4	F	511	-	4,4,4	1.13	0	6,6,6	0.46	0
3	SO4	F	512	-	4,4,4	0.86	0	6,6,6	0.84	0
3	SO4	F	513	-	4,4,4	0.89	0	6,6,6	1.31	1 (16%)
3	SO4	F	514	-	4,4,4	1.21	0	6,6,6	0.42	0
3	SO4	F	515	-	4,4,4	0.68	0	6,6,6	0.33	0
2	GOL	G	501	-	5,5,5	0.58	0	5,5,5	0.87	0
2	GOL	G	502	-	5,5,5	0.36	0	5,5,5	0.53	0
2	GOL	G	503	-	5,5,5	0.52	0	5,5,5	1.23	1 (20%)
2	GOL	G	504	-	5,5,5	0.48	0	5,5,5	0.93	0
3	SO4	G	505	-	4,4,4	0.54	0	6,6,6	0.70	0
3	SO4	G	506	-	4,4,4	1.34	1 (25%)	6,6,6	0.99	1 (16%)
3	SO4	G	507	-	4,4,4	0.97	0	6,6,6	0.38	0
3	SO4	G	508	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	G	509	-	4,4,4	1.10	1 (25%)	6,6,6	0.58	0
3	SO4	G	510	-	4,4,4	0.64	0	6,6,6	0.28	0
3	SO4	G	511	-	4,4,4	0.47	0	6,6,6	0.72	0
3	SO4	G	512	-	4,4,4	0.65	0	6,6,6	0.46	0
4	CIT	G	513	-	12,12,12	1.98	4 (33%)	17,17,17	4.94	10 (58%)
2	GOL	H	501	-	5,5,5	0.56	0	5,5,5	0.60	0
2	GOL	H	502	-	5,5,5	0.35	0	5,5,5	0.97	0
2	GOL	H	503	-	5,5,5	0.78	0	5,5,5	0.90	0
3	SO4	H	504	-	4,4,4	0.66	0	6,6,6	0.45	0
3	SO4	H	505	-	4,4,4	0.60	0	6,6,6	0.57	0
3	SO4	H	506	-	4,4,4	1.04	0	6,6,6	0.80	0
3	SO4	H	507	-	4,4,4	0.13	0	6,6,6	0.42	0
3	SO4	H	508	-	4,4,4	0.65	0	6,6,6	0.31	0
3	SO4	H	509	-	4,4,4	1.49	1 (25%)	6,6,6	0.73	0
3	SO4	H	510	-	4,4,4	0.79	0	6,6,6	0.35	0
3	SO4	H	511	-	4,4,4	0.54	0	6,6,6	0.43	0
3	SO4	H	512	-	4,4,4	0.74	0	6,6,6	0.73	0
3	SO4	H	513	-	4,4,4	0.56	0	6,6,6	0.88	0
3	SO4	H	514	-	4,4,4	0.24	0	6,6,6	0.46	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
2	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	A	504	-	-	0/4/4/4	0/0/0/0
3	SO4	A	505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	506	-	-	0/0/0/0	0/0/0/0
3	SO4	A	507	-	-	0/0/0/0	0/0/0/0
3	SO4	A	508	-	-	0/0/0/0	0/0/0/0
3	SO4	A	509	-	-	0/0/0/0	0/0/0/0
3	SO4	A	510	-	-	0/0/0/0	0/0/0/0
3	SO4	A	511	-	-	0/0/0/0	0/0/0/0
3	SO4	A	512	-	-	0/0/0/0	0/0/0/0
3	SO4	A	513	-	-	0/0/0/0	0/0/0/0
3	SO4	A	514	-	-	0/0/0/0	0/0/0/0
4	CIT	A	515	-	-	0/16/16/16	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	505	-	-	0/4/4/4	0/0/0/0
2	GOL	B	506	-	-	0/4/4/4	0/0/0/0
2	GOL	B	507	-	-	0/4/4/4	0/0/0/0
2	GOL	B	508	-	-	0/4/4/4	0/0/0/0
2	GOL	B	509	-	-	0/4/4/4	0/0/0/0
3	SO4	B	510	-	-	0/0/0/0	0/0/0/0
3	SO4	B	511	-	-	0/0/0/0	0/0/0/0
3	SO4	B	512	-	-	0/0/0/0	0/0/0/0
3	SO4	B	513	-	-	0/0/0/0	0/0/0/0
3	SO4	B	514	-	-	0/0/0/0	0/0/0/0
3	SO4	B	515	-	-	0/0/0/0	0/0/0/0
3	SO4	B	516	-	-	0/0/0/0	0/0/0/0
3	SO4	B	517	-	-	0/0/0/0	0/0/0/0
3	SO4	B	518	-	-	0/0/0/0	0/0/0/0
3	SO4	B	519	-	-	0/0/0/0	0/0/0/0
4	CIT	B	520	-	-	0/16/16/16	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	GOL	C	505	-	-	0/4/4/4	0/0/0/0
3	SO4	C	506	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	507	-	-	0/0/0/0	0/0/0/0
3	SO4	C	508	-	-	0/0/0/0	0/0/0/0
3	SO4	C	509	-	-	0/0/0/0	0/0/0/0
3	SO4	C	510	-	-	0/0/0/0	0/0/0/0
3	SO4	C	511	-	-	0/0/0/0	0/0/0/0
3	SO4	C	512	-	-	0/0/0/0	0/0/0/0
3	SO4	C	513	-	-	0/0/0/0	0/0/0/0
3	SO4	C	514	-	-	0/0/0/0	0/0/0/0
3	SO4	C	515	-	-	0/0/0/0	0/0/0/0
3	SO4	C	516	-	-	0/0/0/0	0/0/0/0
3	SO4	C	517	-	-	0/0/0/0	0/0/0/0
3	SO4	C	518	-	-	0/0/0/0	0/0/0/0
4	CIT	C	519	-	-	0/16/16/16	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	GOL	D	503	-	-	0/4/4/4	0/0/0/0
2	GOL	D	504	-	-	0/4/4/4	0/0/0/0
2	GOL	D	505	-	-	0/4/4/4	0/0/0/0
3	SO4	D	506	-	-	0/0/0/0	0/0/0/0
3	SO4	D	507	-	-	0/0/0/0	0/0/0/0
3	SO4	D	508	-	-	0/0/0/0	0/0/0/0
3	SO4	D	509	-	-	0/0/0/0	0/0/0/0
3	SO4	D	510	-	-	0/0/0/0	0/0/0/0
3	SO4	D	511	-	-	0/0/0/0	0/0/0/0
3	SO4	D	512	-	-	0/0/0/0	0/0/0/0
3	SO4	D	513	-	-	0/0/0/0	0/0/0/0
3	SO4	D	514	-	-	0/0/0/0	0/0/0/0
3	SO4	D	515	-	-	0/0/0/0	0/0/0/0
3	SO4	D	516	-	-	0/0/0/0	0/0/0/0
3	SO4	D	517	-	-	0/0/0/0	0/0/0/0
2	GOL	E	501	-	-	0/4/4/4	0/0/0/0
2	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	GOL	E	503	-	-	0/4/4/4	0/0/0/0
2	GOL	E	504	-	-	0/4/4/4	0/0/0/0
2	GOL	E	505	-	-	0/4/4/4	0/0/0/0
2	GOL	E	506	-	-	0/4/4/4	0/0/0/0
3	SO4	E	507	-	-	0/0/0/0	0/0/0/0
3	SO4	E	508	-	-	0/0/0/0	0/0/0/0
3	SO4	E	509	-	-	0/0/0/0	0/0/0/0
3	SO4	E	510	-	-	0/0/0/0	0/0/0/0
3	SO4	E	511	-	-	0/0/0/0	0/0/0/0
3	SO4	E	512	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	E	513	-	-	0/0/0/0	0/0/0/0
3	SO4	E	514	-	-	0/0/0/0	0/0/0/0
3	SO4	E	515	-	-	0/0/0/0	0/0/0/0
3	SO4	E	516	-	-	0/0/0/0	0/0/0/0
4	CIT	E	517	-	-	0/16/16/16	0/0/0/0
2	GOL	F	501	-	-	0/4/4/4	0/0/0/0
2	GOL	F	502	-	-	0/4/4/4	0/0/0/0
2	GOL	F	503	-	-	0/4/4/4	0/0/0/0
2	GOL	F	504	-	-	0/4/4/4	0/0/0/0
3	SO4	F	505	-	-	0/0/0/0	0/0/0/0
3	SO4	F	506	-	-	0/0/0/0	0/0/0/0
3	SO4	F	507	-	-	0/0/0/0	0/0/0/0
3	SO4	F	508	-	-	0/0/0/0	0/0/0/0
3	SO4	F	509	-	-	0/0/0/0	0/0/0/0
3	SO4	F	510	-	-	0/0/0/0	0/0/0/0
3	SO4	F	511	-	-	0/0/0/0	0/0/0/0
3	SO4	F	512	-	-	0/0/0/0	0/0/0/0
3	SO4	F	513	-	-	0/0/0/0	0/0/0/0
3	SO4	F	514	-	-	0/0/0/0	0/0/0/0
3	SO4	F	515	-	-	0/0/0/0	0/0/0/0
2	GOL	G	501	-	-	0/4/4/4	0/0/0/0
2	GOL	G	502	-	-	0/4/4/4	0/0/0/0
2	GOL	G	503	-	-	0/4/4/4	0/0/0/0
2	GOL	G	504	-	-	0/4/4/4	0/0/0/0
3	SO4	G	505	-	-	0/0/0/0	0/0/0/0
3	SO4	G	506	-	-	0/0/0/0	0/0/0/0
3	SO4	G	507	-	-	0/0/0/0	0/0/0/0
3	SO4	G	508	-	-	0/0/0/0	0/0/0/0
3	SO4	G	509	-	-	0/0/0/0	0/0/0/0
3	SO4	G	510	-	-	0/0/0/0	0/0/0/0
3	SO4	G	511	-	-	0/0/0/0	0/0/0/0
3	SO4	G	512	-	-	0/0/0/0	0/0/0/0
4	CIT	G	513	-	-	0/16/16/16	0/0/0/0
2	GOL	H	501	-	-	0/4/4/4	0/0/0/0
2	GOL	H	502	-	-	0/4/4/4	0/0/0/0
2	GOL	H	503	-	-	0/4/4/4	0/0/0/0
3	SO4	H	504	-	-	0/0/0/0	0/0/0/0
3	SO4	H	505	-	-	0/0/0/0	0/0/0/0
3	SO4	H	506	-	-	0/0/0/0	0/0/0/0
3	SO4	H	507	-	-	0/0/0/0	0/0/0/0
3	SO4	H	508	-	-	0/0/0/0	0/0/0/0
3	SO4	H	509	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	H	510	-	-	0/0/0/0	0/0/0/0
3	SO4	H	511	-	-	0/0/0/0	0/0/0/0
3	SO4	H	512	-	-	0/0/0/0	0/0/0/0
3	SO4	H	513	-	-	0/0/0/0	0/0/0/0
3	SO4	H	514	-	-	0/0/0/0	0/0/0/0

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	519	CIT	C3-C6	6.18	1.60	1.53
2	C	505	GOL	O3-C3	5.84	1.67	1.42
4	B	520	CIT	O7-C3	4.72	1.53	1.43
4	C	519	CIT	O7-C3	4.26	1.52	1.43
4	C	519	CIT	C4-C3	3.58	1.58	1.53

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	515	CIT	O5-C6-C3	-16.22	99.83	122.20
4	G	513	CIT	O5-C6-C3	-14.48	102.24	122.20
4	A	515	CIT	O6-C6-C3	10.85	128.67	112.89
4	G	513	CIT	O6-C6-C3	10.73	128.50	112.89
4	C	519	CIT	O2-C1-O1	7.54	142.34	123.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	430/448 (95%)	-0.75	3 (0%) 84 91	8, 13, 35, 96	0
1	B	430/448 (95%)	-0.75	1 (0%) 93 97	9, 17, 36, 91	0
1	C	431/448 (96%)	-0.59	6 (1%) 72 80	9, 18, 50, 107	0
1	D	435/448 (97%)	-0.58	3 (0%) 84 91	14, 22, 45, 88	0
1	E	430/448 (95%)	-0.50	9 (2%) 60 69	14, 23, 56, 114	0
1	F	430/448 (95%)	-0.47	5 (1%) 75 83	16, 27, 53, 116	0
1	G	430/448 (95%)	-0.26	7 (1%) 68 77	15, 32, 61, 111	1 (0%)
1	H	430/448 (95%)	-0.04	12 (2%) 50 60	22, 37, 61, 115	0
All	All	3446/3584 (96%)	-0.49	46 (1%) 74 81	8, 23, 53, 116	1 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	9.7
1	E	444	VAL	9.0
1	F	405	MET	8.0
1	G	444	VAL	7.1
1	C	444	VAL	7.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	F	510	5/5	0.24	106.88	62,74,79,88	0
3	SO4	D	506	5/5	0.27	48.85	72,74,85,96	0
3	SO4	D	510	5/5	0.21	41.09	66,78,95,97	0
3	SO4	H	505	5/5	0.37	39.82	75,97,102,103	0
3	SO4	D	511	5/5	0.22	34.00	49,62,78,78	0
3	SO4	B	512	5/5	0.29	29.53	44,48,51,65	5
3	SO4	B	514	5/5	0.28	27.95	61,66,79,82	5
3	SO4	E	509	5/5	0.29	27.57	46,60,77,91	5
3	SO4	A	506	5/5	0.26	27.47	66,66,86,88	0
2	GOL	B	506	6/6	0.46	26.32	56,67,71,71	0
3	SO4	H	504	5/5	0.31	25.60	73,79,92,107	0
3	SO4	F	515	5/5	0.35	24.56	90,102,112,113	0
3	SO4	C	510	5/5	0.28	24.17	51,60,76,78	0
3	SO4	G	507	5/5	0.23	23.55	40,46,60,61	5
3	SO4	B	510	5/5	0.23	23.22	68,70,76,86	0
2	GOL	E	503	6/6	0.22	22.42	50,57,62,65	0
2	GOL	E	506	6/6	0.19	22.33	58,72,74,75	0
2	GOL	B	509	6/6	0.39	21.81	50,58,65,66	0
3	SO4	H	508	5/5	0.33	20.42	69,71,88,94	0
3	SO4	B	517	5/5	0.21	19.42	39,41,60,63	0
3	SO4	A	512	5/5	0.22	18.80	41,41,58,59	0
3	SO4	D	516	5/5	0.29	17.87	75,76,93,95	0
3	SO4	E	513	5/5	0.31	15.93	75,76,88,92	0
3	SO4	G	512	5/5	0.30	14.86	80,91,99,104	0
3	SO4	G	508	5/5	0.45	14.11	96,103,128,136	0
3	SO4	C	508	5/5	0.29	13.87	74,75,79,82	0
2	GOL	G	502	6/6	0.49	13.59	56,68,77,82	0
2	GOL	E	505	6/6	0.27	13.50	32,45,48,49	0
3	SO4	B	519	5/5	0.30	13.32	56,73,88,106	0
2	GOL	C	503	6/6	0.29	13.13	18,24,28,33	6
3	SO4	E	508	5/5	0.23	12.81	39,43,56,60	5
3	SO4	D	512	5/5	0.25	12.61	60,73,82,87	0
3	SO4	B	513	5/5	0.30	12.31	79,94,112,117	0
3	SO4	F	513	5/5	0.24	11.92	56,60,79,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	G	510	5/5	0.36	11.78	90,99,107,116	0
2	GOL	G	504	6/6	0.30	11.77	52,58,67,71	0
3	SO4	B	516	5/5	0.23	11.44	51,67,68,72	0
3	SO4	G	505	5/5	0.30	11.01	71,98,113,117	0
2	GOL	B	505	6/6	0.22	11.00	43,54,65,67	0
3	SO4	H	507	5/5	0.40	10.54	104,110,115,123	0
3	SO4	H	514	5/5	0.38	10.34	101,112,123,125	0
3	SO4	E	512	5/5	0.23	10.10	50,66,84,88	0
3	SO4	A	509	5/5	0.19	9.95	55,62,69,75	0
3	SO4	H	512	5/5	0.30	9.86	81,83,96,96	0
3	SO4	C	507	5/5	0.30	9.68	72,81,101,102	0
3	SO4	H	506	5/5	0.27	9.13	59,63,68,77	0
3	SO4	F	509	5/5	0.30	8.90	56,75,85,85	0
3	SO4	C	515	5/5	0.22	8.85	49,58,72,74	0
3	SO4	E	511	5/5	0.13	8.80	39,41,44,55	0
3	SO4	F	505	5/5	0.28	8.60	72,75,85,96	0
3	SO4	E	515	5/5	0.24	8.58	52,70,82,84	0
2	GOL	D	505	6/6	0.14	8.35	32,36,39,50	0
3	SO4	A	507	5/5	0.32	8.30	39,52,60,70	5
3	SO4	D	507	5/5	0.35	7.93	78,96,97,105	0
3	SO4	F	512	5/5	0.22	7.32	64,69,90,96	0
3	SO4	B	511	5/5	0.31	7.11	45,58,66,67	5
3	SO4	H	511	5/5	0.29	6.89	70,92,95,103	0
3	SO4	D	517	5/5	0.21	6.72	34,35,49,51	5
3	SO4	E	510	5/5	0.38	6.66	84,91,94,107	0
3	SO4	G	511	5/5	0.37	6.51	82,101,104,113	0
3	SO4	E	516	5/5	0.45	6.36	91,102,118,122	0
3	SO4	D	509	5/5	0.16	6.33	45,56,68,71	0
3	SO4	C	516	5/5	0.19	6.32	40,58,64,72	0
3	SO4	C	511	5/5	0.17	6.15	67,67,82,88	0
2	GOL	C	505	6/6	0.25	5.70	21,27,34,43	0
2	GOL	H	502	6/6	0.17	5.67	52,62,74,81	0
3	SO4	D	515	5/5	0.34	5.65	76,91,101,105	0
3	SO4	C	506	5/5	0.36	5.41	76,77,94,94	0
3	SO4	C	514	5/5	0.28	5.24	65,79,88,91	0
2	GOL	F	503	6/6	0.34	5.17	59,67,71,72	0
3	SO4	G	506	5/5	0.18	5.14	45,80,86,98	0
3	SO4	H	513	5/5	0.16	5.10	53,53,57,60	0
3	SO4	D	513	5/5	0.30	5.10	71,82,108,108	0
3	SO4	A	508	5/5	0.32	5.04	62,73,75,86	0
3	SO4	C	512	5/5	0.16	5.02	40,46,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	F	514	5/5	0.25	4.64	59,70,77,89	0
3	SO4	F	511	5/5	0.19	4.44	54,74,86,91	0
3	SO4	H	510	5/5	0.28	4.44	78,82,95,96	0
4	CIT	C	519	13/13	0.18	4.32	26,45,62,62	0
4	CIT	A	515	13/13	0.15	4.32	15,29,39,49	13
3	SO4	A	513	5/5	0.30	4.25	74,76,86,93	0
3	SO4	D	508	5/5	0.23	4.22	48,59,67,81	0
3	SO4	C	517	5/5	0.24	4.16	56,64,78,90	0
3	SO4	A	505	5/5	0.17	4.03	32,35,47,64	0
2	GOL	B	508	6/6	0.16	3.92	63,65,68,70	0
2	GOL	A	504	6/6	0.15	3.87	38,45,53,54	0
3	SO4	E	514	5/5	0.26	3.78	41,52,66,79	0
3	SO4	C	509	5/5	0.29	3.72	104,108,116,118	0
4	CIT	B	520	13/13	0.21	3.71	31,46,59,64	0
2	GOL	E	504	6/6	0.25	3.65	37,56,61,63	0
3	SO4	A	511	5/5	0.17	3.58	39,53,58,69	0
3	SO4	E	507	5/5	0.28	3.42	78,97,117,120	0
2	GOL	A	501	6/6	0.14	3.33	28,38,48,60	0
3	SO4	F	507	5/5	0.33	3.27	71,88,91,99	5
3	SO4	F	506	5/5	0.37	3.25	86,87,108,111	0
3	SO4	B	518	5/5	0.34	3.13	102,103,116,122	0
4	CIT	G	513	13/13	0.15	3.04	35,44,66,66	0
2	GOL	F	504	6/6	0.17	3.04	50,57,62,66	0
4	CIT	E	517	13/13	0.19	2.85	35,64,73,87	0
2	GOL	B	503	6/6	0.19	2.82	29,31,43,48	0
2	GOL	B	504	6/6	0.14	2.71	30,35,38,40	0
2	GOL	A	502	6/6	0.15	2.63	54,66,71,72	0
3	SO4	F	508	5/5	0.27	2.54	54,67,89,95	0
2	GOL	D	502	6/6	0.18	2.47	31,35,39,41	0
2	GOL	C	502	6/6	0.10	2.44	31,38,49,63	0
3	SO4	C	513	5/5	0.17	2.36	43,45,49,62	0
2	GOL	C	504	6/6	0.14	2.35	36,38,44,56	0
3	SO4	H	509	5/5	0.28	2.21	43,46,66,74	5
3	SO4	D	514	5/5	0.26	2.14	62,91,99,102	0
2	GOL	F	502	6/6	0.12	1.57	40,47,49,56	0
2	GOL	E	501	6/6	0.12	1.52	35,49,58,64	0
2	GOL	B	502	6/6	0.12	1.36	32,37,45,57	0
2	GOL	D	504	6/6	0.14	1.31	31,37,44,54	0
3	SO4	B	515	5/5	0.10	1.26	23,35,38,39	0
2	GOL	F	501	6/6	0.17	1.14	25,32,35,37	0
2	GOL	H	501	6/6	0.19	1.09	32,43,45,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	G	501	6/6	0.13	1.07	40,49,64,65	0
2	GOL	G	503	6/6	0.20	0.93	29,36,38,44	0
3	SO4	A	514	5/5	0.19	0.90	48,62,67,83	0
2	GOL	E	502	6/6	0.14	0.84	22,26,27,32	0
3	SO4	C	518	5/5	0.29	0.83	83,92,120,127	0
2	GOL	H	503	6/6	0.12	0.22	38,42,49,53	0
2	GOL	C	501	6/6	0.12	0.20	18,20,21,22	0
2	GOL	D	501	6/6	0.14	0.17	18,22,23,24	0
2	GOL	D	503	6/6	0.12	-0.03	43,49,54,62	0
2	GOL	A	503	6/6	0.11	-0.14	14,18,19,24	0
2	GOL	B	501	6/6	0.12	-0.14	18,25,27,34	0
3	SO4	G	509	5/5	0.06	-0.53	24,25,28,29	0
3	SO4	A	510	5/5	0.07	-0.56	23,24,26,37	0
2	GOL	B	507	6/6	0.20	-	54,64,72,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.