



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:32 am GMT

PDB ID : 4NXK  
Title : Crystal structure of Abp-D197A, a catalytic mutant of a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*  
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.  
Deposited on : 2013-12-09  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

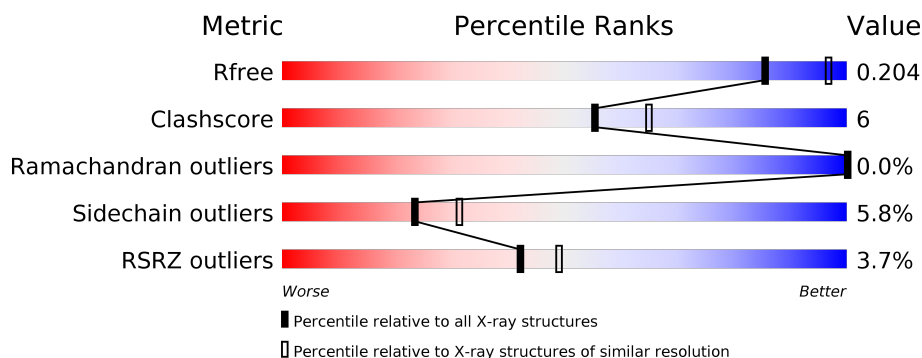
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 88%, yellow 88%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>88%</span> <span>8%</span> <span>• •</span> </div> </div>
1	B	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 85%, yellow 85%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>9%</span> <span>• •</span> </div> </div>
1	C	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 83%, yellow 83%, yellow 93%, green 93%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>83%</span> <span>10%</span> <span>• •</span> </div> </div>
1	D	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 86%, yellow 86%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>10%</span> <span>• •</span> </div> </div>
1	E	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 86%, yellow 86%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>86%</span> <span>9%</span> <span>• •</span> </div> </div>
1	F	448	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 85%, yellow 85%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>10%</span> <span>• •</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	448	
1	H	448	

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
2	SO4	A	504	-	-	-	X
2	SO4	A	507	-	-	-	X
2	SO4	A	508	-	-	-	X
2	SO4	B	501	-	-	-	X
2	SO4	B	502	-	-	-	X
2	SO4	B	506	-	-	-	X
2	SO4	C	502	-	-	-	X
2	SO4	C	503	-	-	-	X
2	SO4	C	507	-	-	-	X
2	SO4	C	509	-	-	-	X
2	SO4	D	503	-	-	-	X
2	SO4	D	504	-	-	-	X
2	SO4	D	507	-	-	-	X
2	SO4	D	508	-	-	-	X
2	SO4	E	501	-	-	-	X
2	SO4	E	502	-	-	-	X
2	SO4	E	503	-	-	-	X
2	SO4	E	506	-	-	-	X
2	SO4	E	508	-	-	-	X
2	SO4	F	502	-	-	-	X
2	SO4	F	504	-	-	-	X
2	SO4	F	505	-	-	-	X
2	SO4	F	506	-	-	-	X
2	SO4	G	503	-	-	-	X
2	SO4	G	505	-	-	-	X
2	SO4	G	506	-	-	-	X
2	SO4	H	502	-	-	X	-
2	SO4	H	504	-	-	-	X
2	SO4	H	505	-	-	-	X
3	GOL	A	511	-	-	-	X
3	GOL	B	511	-	-	-	X
3	GOL	B	513	-	-	-	X
3	GOL	C	514	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	513	-	-	-	X
3	GOL	E	510	-	-	-	X
3	GOL	E	511	-	-	-	X
3	GOL	E	513	-	-	-	X
3	GOL	H	509	-	-	X	-
4	CIT	A	513	-	-	X	X
4	CIT	B	514	-	-	X	X
4	CIT	C	515	-	-	X	X
4	CIT	D	516	-	-	X	X
4	CIT	E	514	-	-	X	X
4	CIT	G	509	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31524 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 Abp, a GH27 beta-L-arabinopyranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	4	0
			3494	2235	599	635	25			
1	B	430	Total	C	N	O	S	0	2	0
			3482	2227	598	632	25			
1	C	430	Total	C	N	O	S	0	2	0
			3479	2226	597	631	25			
1	D	435	Total	C	N	O	S	0	2	0
			3509	2247	604	633	25			
1	E	431	Total	C	N	O	S	0	2	0
			3481	2227	598	631	25			
1	F	430	Total	C	N	O	S	0	0	0
			3467	2218	596	628	25			
1	G	430	Total	C	N	O	S	0	2	0
			3479	2226	597	631	25			
1	H	430	Total	C	N	O	S	0	3	0
			3483	2230	597	629	27			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
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	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
2	C	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		
2	C	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		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	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	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	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		
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		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

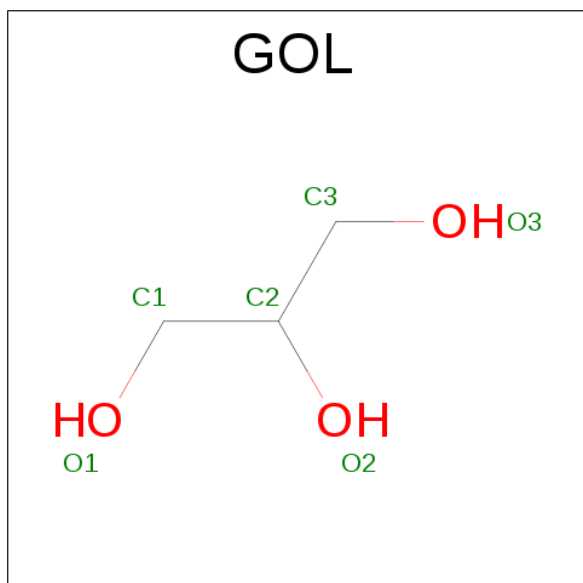
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0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

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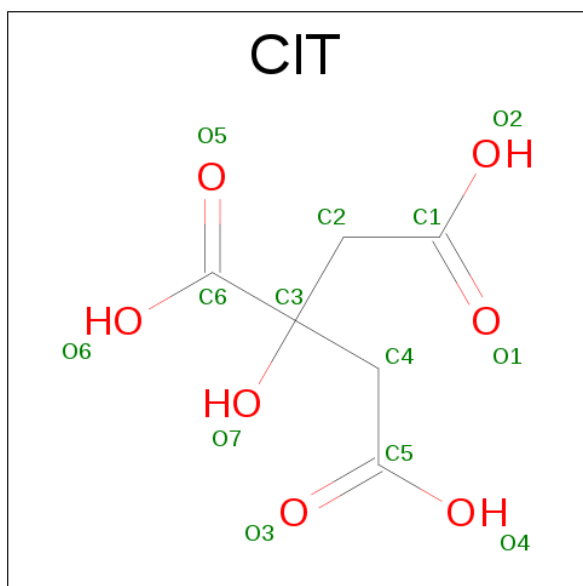
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	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		

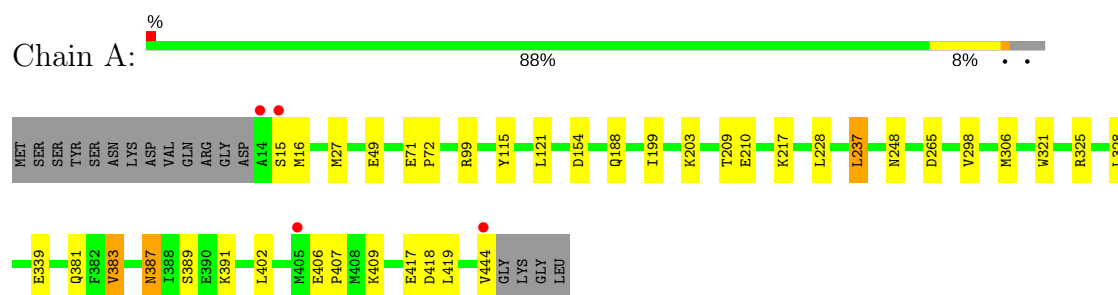
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	574	Total	O	0	0
			574	574		
5	B	491	Total	O	0	0
			491	491		
5	C	433	Total	O	0	0
			433	433		
5	D	402	Total	O	0	0
			402	402		
5	E	377	Total	O	0	0
			377	377		
5	F	299	Total	O	0	0
			299	299		
5	G	295	Total	O	0	0
			295	295		
5	H	191	Total	O	0	0
			191	191		

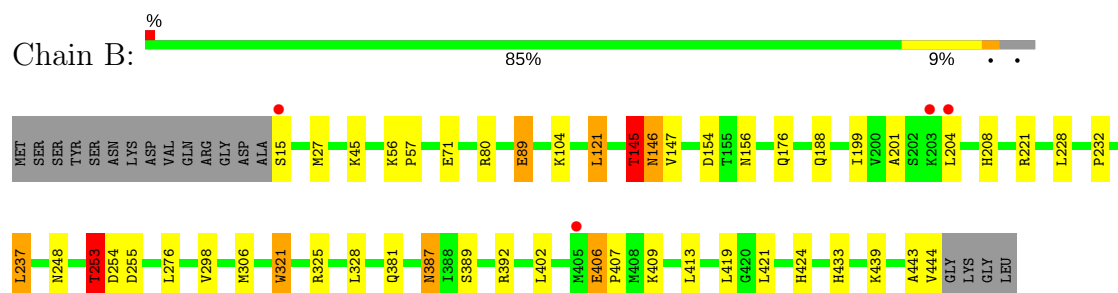
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

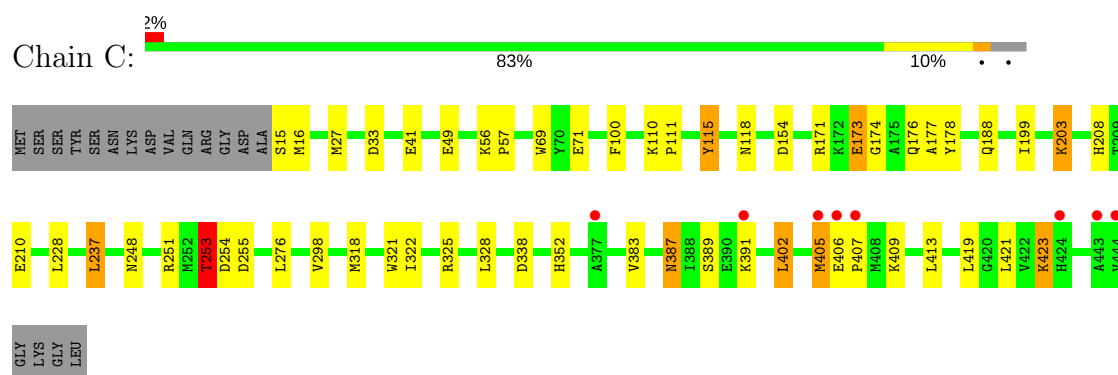
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



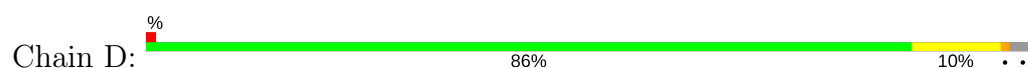
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

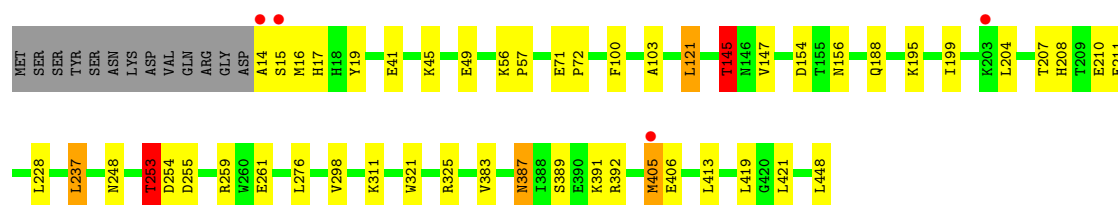


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

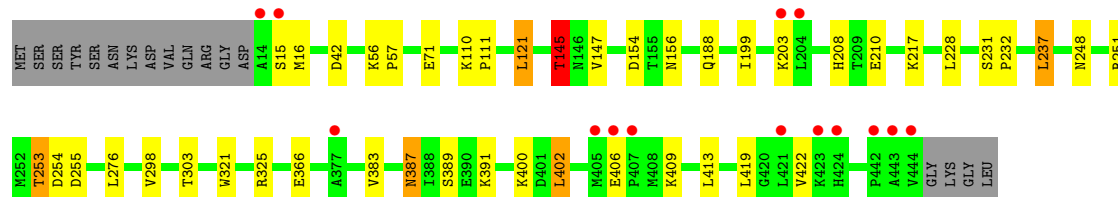
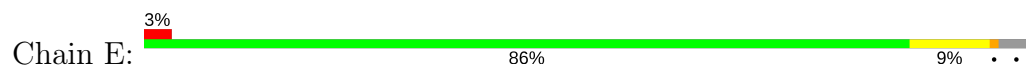


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

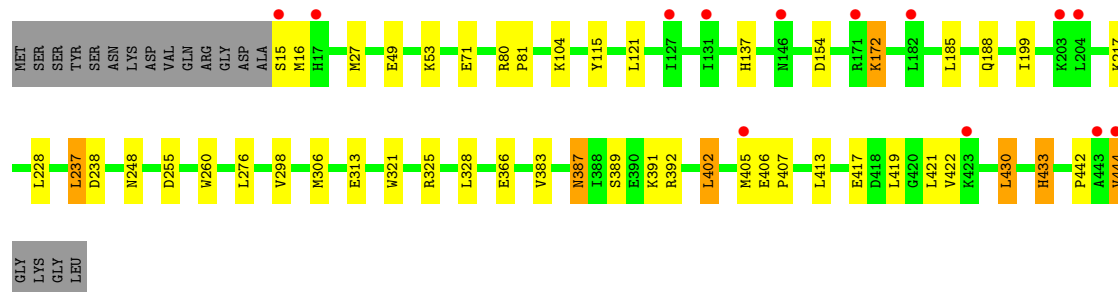
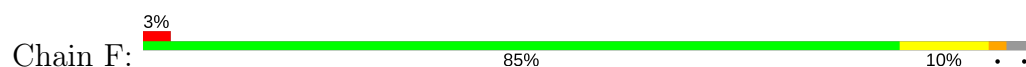




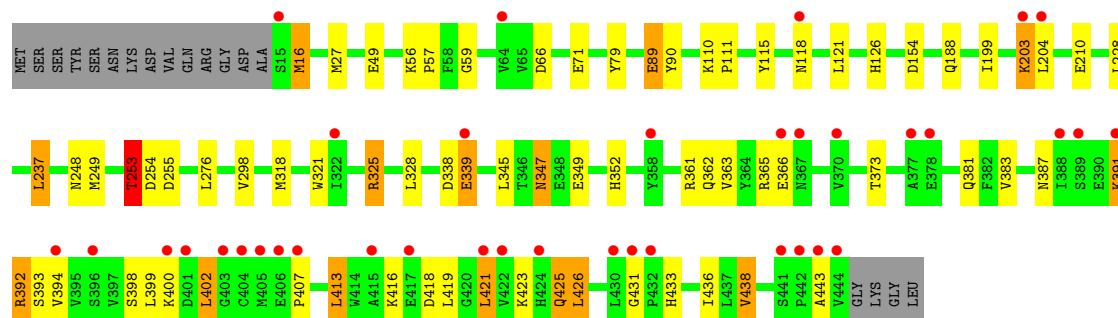
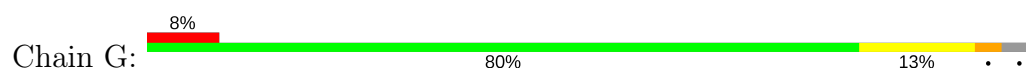
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



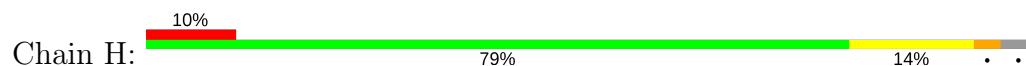
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

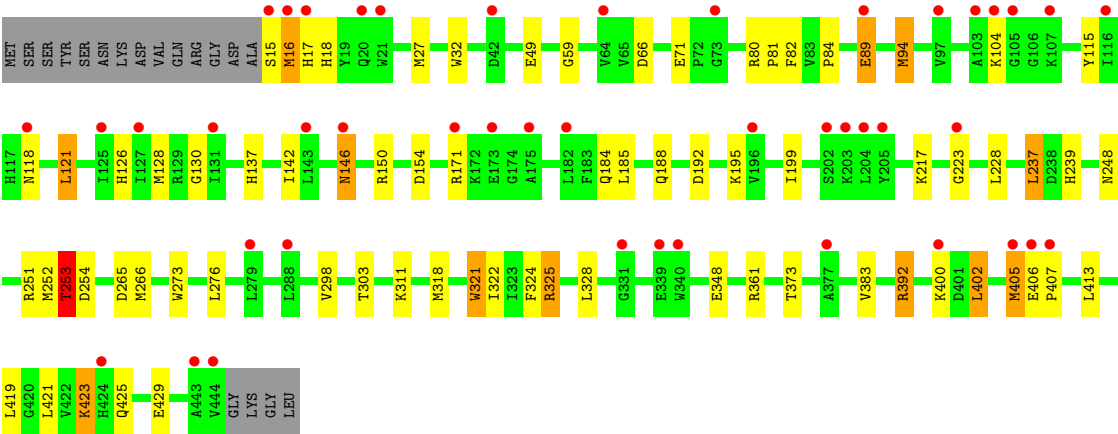


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.70Å 203.53Å 286.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.30 24.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (24.86-2.30) 96.4 (24.84-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.170 , 0.201 0.175 , 0.204	Depositor DCC
$R_{free}$ test set	13610 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.972	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	1.07	0/3608	0.92	7/4898 (0.1%)
1	B	1.03	1/3587 (0.0%)	0.91	9/4869 (0.2%)
1	C	0.99	4/3587 (0.1%)	0.89	8/4869 (0.2%)
1	D	0.95	1/3617 (0.0%)	0.90	9/4906 (0.2%)
1	E	0.88	0/3589	0.86	6/4873 (0.1%)
1	F	0.87	1/3569 (0.0%)	0.88	8/4845 (0.2%)
1	G	0.86	0/3587	0.90	6/4869 (0.1%)
1	H	0.81	0/3594	0.87	10/4877 (0.2%)
All	All	0.94	7/28738 (0.0%)	0.89	63/39006 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	TYR	CG-CD1	-5.57	1.31	1.39
1	D	325	ARG	CZ-NH1	5.39	1.40	1.33
1	C	173	GLU	CD-OE1	5.30	1.31	1.25
1	C	115	TYR	CG-CD2	-5.23	1.32	1.39
1	B	321	TRP	CG-CD1	-5.20	1.29	1.36

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	C	154	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	C	171	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	E	154	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	D	405	MET	CG-SD-CE	8.29	113.46	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3376	35	0
1	B	3482	0	3360	28	0
1	C	3479	0	3361	46	0
1	D	3509	0	3408	36	0
1	E	3481	0	3365	21	0
1	F	3467	0	3347	18	0
1	G	3479	0	3361	56	0
1	H	3483	0	3373	73	0
2	A	45	0	0	0	0
2	B	40	0	0	0	0
2	C	45	0	0	1	0
2	D	55	0	0	3	0
2	E	45	0	0	0	0
2	F	35	0	0	0	0
2	G	30	0	0	0	0
2	H	35	0	0	3	0
3	A	18	0	24	3	0
3	B	30	0	40	3	0
3	C	30	0	37	9	0
3	D	24	0	31	6	0
3	E	24	0	31	5	0
3	F	24	0	32	3	0
3	G	12	0	16	3	0
3	H	18	0	24	11	0
4	A	13	0	5	15	0
4	B	13	0	5	6	0
4	C	13	0	5	8	0
4	D	13	0	5	9	0
4	E	13	0	5	7	0
4	G	13	0	5	3	0
5	A	574	0	0	14	0
5	B	491	0	0	8	0
5	C	433	0	0	13	0
5	D	402	0	0	6	0
5	E	377	0	0	5	0
5	F	299	0	0	5	0
5	G	295	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	191	0	0	25	0
All	All	31524	0	27216	331	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 6.

The worst 5 of 331 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)
3:E:510:GOL:O3	3:E:510:GOL:C3	1.65	1.45
1:G:352:HIS:HB2	5:G:864:HOH:O	1.32	1.26
1:H:16:MET:CE	1:H:16:MET:HA	1.67	1.24
4:D:516:CIT:C6	4:D:516:CIT:O2	1.85	1.15
1:H:16:MET:HE3	1:H:16:MET:HA	1.12	1.09

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	433/448 (97%)	419 (97%)	14 (3%)	0	100	100
1	B	430/448 (96%)	414 (96%)	16 (4%)	0	100	100
1	C	430/448 (96%)	419 (97%)	11 (3%)	0	100	100
1	D	435/448 (97%)	422 (97%)	13 (3%)	0	100	100
1	E	431/448 (96%)	419 (97%)	12 (3%)	0	100	100
1	F	428/448 (96%)	416 (97%)	12 (3%)	0	100	100
1	G	430/448 (96%)	416 (97%)	14 (3%)	0	100	100
1	H	431/448 (96%)	418 (97%)	12 (3%)	1 (0%)	51	63
All	All	3448/3584 (96%)	3343 (97%)	104 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	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	372/382 (97%)	359 (96%)	13 (4%)	41	56
1	B	370/382 (97%)	348 (94%)	22 (6%)	23	30
1	C	370/382 (97%)	351 (95%)	19 (5%)	28	37
1	D	372/382 (97%)	354 (95%)	18 (5%)	30	40
1	E	370/382 (97%)	348 (94%)	22 (6%)	23	30
1	F	368/382 (96%)	344 (94%)	24 (6%)	20	26
1	G	370/382 (97%)	339 (92%)	31 (8%)	13	15
1	H	371/382 (97%)	348 (94%)	23 (6%)	21	28
All	All	2963/3056 (97%)	2791 (94%)	172 (6%)	23	31

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	203	LYS
1	F	71	GLU
1	H	253	THR
1	E	276	LEU
1	E	400	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	156	ASN
1	H	18	HIS
1	D	387	ASN

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Mol	Chain	Res	Type
1	E	20	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

102 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	SO4	A	501	-	4,4,4	0.82	0	6,6,6	0.47	0
2	SO4	A	502	-	4,4,4	0.50	0	6,6,6	0.65	0
2	SO4	A	503	-	4,4,4	0.61	0	6,6,6	0.53	0
2	SO4	A	504	-	4,4,4	1.00	0	6,6,6	1.68	1 (16%)
2	SO4	A	505	-	4,4,4	0.56	0	6,6,6	0.56	0
2	SO4	A	506	-	4,4,4	0.67	0	6,6,6	1.05	0
2	SO4	A	507	-	4,4,4	1.07	0	6,6,6	1.11	0
2	SO4	A	508	-	4,4,4	0.86	0	6,6,6	1.07	0
2	SO4	A	509	-	4,4,4	0.53	0	6,6,6	0.55	0
3	GOL	A	510	-	5,5,5	0.75	0	5,5,5	0.93	0
3	GOL	A	511	-	5,5,5	0.37	0	5,5,5	0.46	0
3	GOL	A	512	-	5,5,5	0.58	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CIT	A	513	-	3,12,12	3.66	1 (33%)	3,17,17	3.35	1 (33%)
2	SO4	B	501	-	4,4,4	1.03	0	6,6,6	1.16	1 (16%)
2	SO4	B	502	-	4,4,4	0.72	0	6,6,6	0.86	0
2	SO4	B	503	-	4,4,4	0.67	0	6,6,6	0.37	0
2	SO4	B	504	-	4,4,4	0.54	0	6,6,6	0.60	0
2	SO4	B	505	-	4,4,4	0.87	0	6,6,6	1.22	0
2	SO4	B	506	-	4,4,4	1.17	0	6,6,6	0.86	0
2	SO4	B	507	-	4,4,4	0.69	0	6,6,6	0.56	0
2	SO4	B	508	-	4,4,4	0.70	0	6,6,6	0.70	0
3	GOL	B	509	-	5,5,5	0.77	0	5,5,5	0.60	0
3	GOL	B	510	-	5,5,5	0.71	0	5,5,5	0.63	0
3	GOL	B	511	-	5,5,5	0.44	0	5,5,5	1.61	1 (20%)
3	GOL	B	512	-	5,5,5	0.22	0	5,5,5	1.22	1 (20%)
3	GOL	B	513	-	5,5,5	0.69	0	5,5,5	1.10	1 (20%)
4	CIT	B	514	-	3,12,12	2.59	2 (66%)	3,17,17	4.78	1 (33%)
2	SO4	C	501	-	4,4,4	0.77	0	6,6,6	0.48	0
2	SO4	C	502	-	4,4,4	0.86	0	6,6,6	0.62	0
2	SO4	C	503	-	4,4,4	0.78	0	6,6,6	0.90	0
2	SO4	C	504	-	4,4,4	0.59	0	6,6,6	0.91	0
2	SO4	C	505	-	4,4,4	0.81	0	6,6,6	0.57	0
2	SO4	C	506	-	4,4,4	0.88	0	6,6,6	0.44	0
2	SO4	C	507	-	4,4,4	0.86	0	6,6,6	1.66	2 (33%)
2	SO4	C	508	-	4,4,4	0.54	0	6,6,6	0.44	0
2	SO4	C	509	-	4,4,4	1.03	0	6,6,6	0.66	0
3	GOL	C	510	-	5,5,5	1.35	0	5,5,5	2.36	2 (40%)
3	GOL	C	511	-	5,5,5	0.66	0	5,5,5	1.16	0
3	GOL	C	512	-	5,5,5	0.36	0	5,5,5	1.82	1 (20%)
3	GOL	C	513	-	5,5,5	1.30	1 (20%)	5,5,5	1.77	2 (40%)
3	GOL	C	514	-	5,5,5	1.17	1 (20%)	5,5,5	0.89	0
4	CIT	C	515	-	3,12,12	2.93	2 (66%)	3,17,17	7.14	2 (66%)
2	SO4	D	501	-	4,4,4	0.61	0	6,6,6	0.42	0
2	SO4	D	502	-	4,4,4	0.79	0	6,6,6	0.78	0
2	SO4	D	503	-	4,4,4	0.59	0	6,6,6	0.58	0
2	SO4	D	504	-	4,4,4	0.43	0	6,6,6	0.60	0
2	SO4	D	505	-	4,4,4	0.56	0	6,6,6	0.53	0
2	SO4	D	506	-	4,4,4	0.68	0	6,6,6	0.55	0
2	SO4	D	507	-	4,4,4	0.70	0	6,6,6	1.40	2 (33%)
2	SO4	D	508	-	4,4,4	0.86	0	6,6,6	0.56	0
2	SO4	D	509	-	4,4,4	0.66	0	6,6,6	0.40	0
2	SO4	D	510	-	4,4,4	0.72	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	511	-	4,4,4	0.63	0	6,6,6	0.17	0
3	GOL	D	512	-	5,5,5	1.08	1 (20%)	5,5,5	1.03	0
3	GOL	D	513	-	5,5,5	0.79	0	5,5,5	1.38	1 (20%)
3	GOL	D	514	-	5,5,5	0.24	0	5,5,5	0.26	0
3	GOL	D	515	-	5,5,5	0.50	0	5,5,5	0.87	0
4	CIT	D	516	-	3,12,12	2.44	1 (33%)	3,17,17	4.16	3 (100%)
2	SO4	E	501	-	4,4,4	0.86	0	6,6,6	1.05	0
2	SO4	E	502	-	4,4,4	0.49	0	6,6,6	0.35	0
2	SO4	E	503	-	4,4,4	0.60	0	6,6,6	0.92	0
2	SO4	E	504	-	4,4,4	0.75	0	6,6,6	0.70	0
2	SO4	E	505	-	4,4,4	0.65	0	6,6,6	0.36	0
2	SO4	E	506	-	4,4,4	0.81	0	6,6,6	0.41	0
2	SO4	E	507	-	4,4,4	0.63	0	6,6,6	0.90	0
2	SO4	E	508	-	4,4,4	0.88	0	6,6,6	0.67	0
2	SO4	E	509	-	4,4,4	0.71	0	6,6,6	0.89	0
3	GOL	E	510	-	5,5,5	2.79	2 (40%)	5,5,5	2.82	3 (60%)
3	GOL	E	511	-	5,5,5	0.38	0	5,5,5	0.48	0
3	GOL	E	512	-	5,5,5	0.60	0	5,5,5	0.83	0
3	GOL	E	513	-	5,5,5	0.78	0	5,5,5	1.33	1 (20%)
4	CIT	E	514	-	3,12,12	1.44	0	3,17,17	3.34	1 (33%)
2	SO4	F	501	-	4,4,4	0.55	0	6,6,6	0.35	0
2	SO4	F	502	-	4,4,4	0.73	0	6,6,6	0.26	0
2	SO4	F	503	-	4,4,4	0.55	0	6,6,6	0.75	0
2	SO4	F	504	-	4,4,4	0.67	0	6,6,6	0.29	0
2	SO4	F	505	-	4,4,4	0.66	0	6,6,6	0.36	0
2	SO4	F	506	-	4,4,4	0.68	0	6,6,6	0.64	0
2	SO4	F	507	-	4,4,4	0.65	0	6,6,6	0.44	0
3	GOL	F	508	-	5,5,5	0.33	0	5,5,5	1.29	0
3	GOL	F	509	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	F	510	-	5,5,5	0.40	0	5,5,5	0.46	0
3	GOL	F	511	-	5,5,5	0.64	0	5,5,5	0.50	0
2	SO4	G	501	-	4,4,4	0.58	0	6,6,6	0.82	0
2	SO4	G	502	-	4,4,4	0.56	0	6,6,6	0.51	0
2	SO4	G	503	-	4,4,4	0.79	0	6,6,6	0.86	0
2	SO4	G	504	-	4,4,4	0.58	0	6,6,6	0.50	0
2	SO4	G	505	-	4,4,4	0.75	0	6,6,6	0.69	0
2	SO4	G	506	-	4,4,4	0.64	0	6,6,6	0.46	0
3	GOL	G	507	-	5,5,5	1.15	0	5,5,5	0.95	0
3	GOL	G	508	-	5,5,5	0.66	0	5,5,5	1.17	1 (20%)
4	CIT	G	509	-	3,12,12	2.21	1 (33%)	3,17,17	6.13	3 (100%)
2	SO4	H	501	-	4,4,4	0.86	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	502	-	4,4,4	0.69	0	6,6,6	0.41	0
2	SO4	H	503	-	4,4,4	0.55	0	6,6,6	0.34	0
2	SO4	H	504	-	4,4,4	0.88	0	6,6,6	0.35	0
2	SO4	H	505	-	4,4,4	0.58	0	6,6,6	0.46	0
2	SO4	H	506	-	4,4,4	0.67	0	6,6,6	0.34	0
2	SO4	H	507	-	4,4,4	0.63	0	6,6,6	0.61	0
3	GOL	H	508	-	5,5,5	0.46	0	5,5,5	0.62	0
3	GOL	H	509	-	5,5,5	0.60	0	5,5,5	0.88	0
3	GOL	H	510	-	5,5,5	0.20	0	5,5,5	0.34	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	SO4	A	508	-	-	0/0/0/0	0/0/0/0
2	SO4	A	509	-	-	0/0/0/0	0/0/0/0
3	GOL	A	510	-	-	0/4/4/4	0/0/0/0
3	GOL	A	511	-	-	0/4/4/4	0/0/0/0
3	GOL	A	512	-	-	0/4/4/4	0/0/0/0
4	CIT	A	513	-	-	0/6/16/16	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	SO4	B	507	-	-	0/0/0/0	0/0/0/0
2	SO4	B	508	-	-	0/0/0/0	0/0/0/0
3	GOL	B	509	-	-	0/4/4/4	0/0/0/0
3	GOL	B	510	-	-	0/4/4/4	0/0/0/0
3	GOL	B	511	-	-	0/4/4/4	0/0/0/0
3	GOL	B	512	-	-	0/4/4/4	0/0/0/0
3	GOL	B	513	-	-	0/4/4/4	0/0/0/0
4	CIT	B	514	-	-	0/6/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	SO4	C	505	-	-	0/0/0/0	0/0/0/0
2	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	SO4	C	508	-	-	0/0/0/0	0/0/0/0
2	SO4	C	509	-	-	0/0/0/0	0/0/0/0
3	GOL	C	510	-	-	0/4/4/4	0/0/0/0
3	GOL	C	511	-	-	0/4/4/4	0/0/0/0
3	GOL	C	512	-	-	0/4/4/4	0/0/0/0
3	GOL	C	513	-	-	0/4/4/4	0/0/0/0
3	GOL	C	514	-	-	0/4/4/4	0/0/0/0
4	CIT	C	515	-	-	0/6/16/16	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
2	SO4	D	505	-	-	0/0/0/0	0/0/0/0
2	SO4	D	506	-	-	0/0/0/0	0/0/0/0
2	SO4	D	507	-	-	0/0/0/0	0/0/0/0
2	SO4	D	508	-	-	0/0/0/0	0/0/0/0
2	SO4	D	509	-	-	0/0/0/0	0/0/0/0
2	SO4	D	510	-	-	0/0/0/0	0/0/0/0
2	SO4	D	511	-	-	0/0/0/0	0/0/0/0
3	GOL	D	512	-	-	0/4/4/4	0/0/0/0
3	GOL	D	513	-	-	0/4/4/4	0/0/0/0
3	GOL	D	514	-	-	0/4/4/4	0/0/0/0
3	GOL	D	515	-	-	0/4/4/4	0/0/0/0
4	CIT	D	516	-	-	0/6/16/16	0/0/0/0
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
2	SO4	E	502	-	-	0/0/0/0	0/0/0/0
2	SO4	E	503	-	-	0/0/0/0	0/0/0/0
2	SO4	E	504	-	-	0/0/0/0	0/0/0/0
2	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	SO4	E	506	-	-	0/0/0/0	0/0/0/0
2	SO4	E	507	-	-	0/0/0/0	0/0/0/0
2	SO4	E	508	-	-	0/0/0/0	0/0/0/0
2	SO4	E	509	-	-	0/0/0/0	0/0/0/0
3	GOL	E	510	-	-	0/4/4/4	0/0/0/0
3	GOL	E	511	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	512	-	-	0/4/4/4	0/0/0/0
3	GOL	E	513	-	-	0/4/4/4	0/0/0/0
4	CIT	E	514	-	-	0/6/16/16	0/0/0/0
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	SO4	F	503	-	-	0/0/0/0	0/0/0/0
2	SO4	F	504	-	-	0/0/0/0	0/0/0/0
2	SO4	F	505	-	-	0/0/0/0	0/0/0/0
2	SO4	F	506	-	-	0/0/0/0	0/0/0/0
2	SO4	F	507	-	-	0/0/0/0	0/0/0/0
3	GOL	F	508	-	-	0/4/4/4	0/0/0/0
3	GOL	F	509	-	-	0/4/4/4	0/0/0/0
3	GOL	F	510	-	-	0/4/4/4	0/0/0/0
3	GOL	F	511	-	-	0/4/4/4	0/0/0/0
2	SO4	G	501	-	-	0/0/0/0	0/0/0/0
2	SO4	G	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	503	-	-	0/0/0/0	0/0/0/0
2	SO4	G	504	-	-	0/0/0/0	0/0/0/0
2	SO4	G	505	-	-	0/0/0/0	0/0/0/0
2	SO4	G	506	-	-	0/0/0/0	0/0/0/0
3	GOL	G	507	-	-	0/4/4/4	0/0/0/0
3	GOL	G	508	-	-	0/4/4/4	0/0/0/0
4	CIT	G	509	-	-	0/6/16/16	0/0/0/0
2	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	502	-	-	0/0/0/0	0/0/0/0
2	SO4	H	503	-	-	0/0/0/0	0/0/0/0
2	SO4	H	504	-	-	0/0/0/0	0/0/0/0
2	SO4	H	505	-	-	0/0/0/0	0/0/0/0
2	SO4	H	506	-	-	0/0/0/0	0/0/0/0
2	SO4	H	507	-	-	0/0/0/0	0/0/0/0
3	GOL	H	508	-	-	0/4/4/4	0/0/0/0
3	GOL	H	509	-	-	0/4/4/4	0/0/0/0
3	GOL	H	510	-	-	0/4/4/4	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	CIT	C4-C3	-5.91	1.45	1.54
4	C	515	CIT	C2-C3	-4.25	1.48	1.54
4	D	516	CIT	C2-C3	-4.08	1.48	1.54
4	B	514	CIT	C4-C3	-3.72	1.49	1.54
4	C	515	CIT	C4-C3	-2.70	1.50	1.54

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	515	CIT	C3-C2-C1	-11.81	96.50	114.95
4	B	514	CIT	C3-C4-C5	-8.06	102.37	114.95
4	E	514	CIT	C3-C2-C1	-5.74	105.98	114.95
4	A	513	CIT	C3-C4-C5	-5.45	106.43	114.95
4	D	516	CIT	C3-C2-C1	-4.61	107.75	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	512	GOL	3	0
4	A	513	CIT	15	0
3	B	512	GOL	1	0
3	B	513	GOL	2	0
4	B	514	CIT	6	0
2	C	505	SO4	1	0
3	C	510	GOL	3	0
3	C	511	GOL	2	0
3	C	514	GOL	4	0
4	C	515	CIT	8	0
2	D	501	SO4	1	0
2	D	504	SO4	1	0
2	D	510	SO4	1	0
3	D	512	GOL	3	0
3	D	513	GOL	3	0
4	D	516	CIT	9	0
3	E	510	GOL	2	0
3	E	511	GOL	2	0
3	E	512	GOL	1	0
4	E	514	CIT	7	0
3	F	509	GOL	2	0
3	F	510	GOL	1	0
3	G	507	GOL	1	0
3	G	508	GOL	2	0
4	G	509	CIT	3	0
2	H	502	SO4	2	0
2	H	506	SO4	1	0
3	H	509	GOL	11	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	431/448 (96%)	-0.65	4 (0%) 84 87	11, 17, 38, 100	0
1	B	430/448 (95%)	-0.61	4 (0%) 84 87	13, 23, 44, 96	0
1	C	430/448 (95%)	-0.48	8 (1%) 67 73	12, 24, 58, 108	0
1	D	435/448 (97%)	-0.46	4 (0%) 84 87	20, 28, 52, 109	0
1	E	431/448 (96%)	-0.31	14 (3%) 48 55	18, 29, 68, 123	0
1	F	430/448 (95%)	-0.10	13 (3%) 51 58	22, 37, 68, 113	0
1	G	430/448 (95%)	0.36	37 (8%) 11 16	20, 45, 79, 130	1 (0%)
1	H	430/448 (95%)	0.68	44 (10%) 7 10	29, 54, 82, 124	0
All	All	3447/3584 (96%)	-0.20	128 (3%) 42 49	11, 31, 70, 130	1 (0%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	10.6
1	C	444	VAL	8.6
1	G	405	MET	8.2
1	F	444	VAL	8.0
1	E	444	VAL	7.5

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	504	5/5	0.89	0.23	13.78	57,72,75,83	0
2	SO4	F	505	5/5	0.86	0.35	11.57	105,112,128,128	0
2	SO4	C	507	5/5	0.85	0.23	9.12	39,40,70,80	5
2	SO4	B	506	5/5	0.93	0.21	8.47	34,44,50,60	5
4	CIT	C	515	13/13	0.87	0.31	8.32	42,60,81,81	0
2	SO4	A	507	5/5	0.96	0.21	8.00	36,40,45,59	0
2	SO4	D	508	5/5	0.93	0.28	7.73	47,60,76,84	0
2	SO4	B	502	5/5	0.92	0.29	7.30	52,84,94,99	0
2	SO4	D	504	5/5	0.91	0.28	6.94	72,91,106,117	0
3	GOL	C	514	6/6	0.88	0.27	6.82	27,35,47,54	0
2	SO4	E	502	5/5	0.79	0.33	6.80	87,116,121,127	0
4	CIT	D	516	13/13	0.87	0.29	6.61	54,71,79,84	0
4	CIT	A	513	13/13	0.85	0.23	6.47	34,51,69,69	0
2	SO4	E	506	5/5	0.92	0.29	6.46	46,73,80,81	0
2	SO4	E	508	5/5	0.90	0.20	6.35	74,79,114,125	0
3	GOL	D	513	6/6	0.89	0.20	6.11	35,44,47,48	0
2	SO4	C	503	5/5	0.86	0.29	6.06	76,89,97,100	0
3	GOL	E	511	6/6	0.94	0.15	5.90	36,42,48,58	0
2	SO4	C	502	5/5	0.91	0.24	5.70	64,90,94,99	0
3	GOL	A	511	6/6	0.94	0.13	5.52	26,31,41,48	0
2	SO4	B	501	5/5	0.89	0.25	5.52	54,65,82,90	0
3	GOL	E	513	6/6	0.87	0.26	5.47	47,51,57,59	0
2	SO4	E	501	5/5	0.77	0.22	5.25	67,77,81,109	0
2	SO4	D	503	5/5	0.89	0.22	5.16	60,83,94,104	0
2	SO4	C	509	5/5	0.85	0.28	5.07	66,67,83,102	0
3	GOL	E	510	6/6	0.86	0.24	4.87	28,29,34,35	0
2	SO4	G	505	5/5	0.90	0.36	4.53	69,70,91,107	0
2	SO4	F	506	5/5	0.93	0.28	4.39	63,72,80,93	0
2	SO4	G	506	5/5	0.82	0.27	4.29	76,103,107,111	0
4	CIT	E	514	13/13	0.86	0.25	4.12	51,79,91,96	0
2	SO4	G	503	5/5	0.92	0.21	3.78	67,75,77,82	0
4	CIT	B	514	13/13	0.79	0.28	3.74	41,70,87,88	0
2	SO4	E	503	5/5	0.95	0.25	3.64	66,66,80,81	0
4	CIT	G	509	13/13	0.84	0.23	3.63	49,64,81,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	507	5/5	0.84	0.24	3.59	61,65,78,83	0
2	SO4	F	504	5/5	0.81	0.32	3.11	73,79,109,111	0
2	SO4	H	504	5/5	0.79	0.37	2.77	61,88,101,103	0
2	SO4	H	505	5/5	0.92	0.34	2.72	80,95,101,106	0
3	GOL	B	513	6/6	0.95	0.20	2.32	35,40,51,59	0
2	SO4	F	502	5/5	0.78	0.21	2.22	77,81,98,115	0
2	SO4	A	508	5/5	0.95	0.20	2.19	50,57,67,68	0
3	GOL	B	511	6/6	0.96	0.17	2.15	24,28,34,35	0
2	SO4	A	503	5/5	0.97	0.13	1.27	39,54,55,58	0
3	GOL	F	511	6/6	0.76	0.20	1.19	60,71,75,82	0
3	GOL	H	510	6/6	0.83	0.27	1.16	73,83,87,104	0
3	GOL	C	510	6/6	0.96	0.14	1.05	22,25,27,27	0
3	GOL	B	510	6/6	0.96	0.08	0.92	28,36,38,43	0
3	GOL	F	508	6/6	0.95	0.16	0.76	34,37,41,44	0
3	GOL	C	513	6/6	0.95	0.14	0.69	33,43,47,47	0
2	SO4	A	502	5/5	0.99	0.09	0.67	27,28,30,38	0
3	GOL	F	509	6/6	0.87	0.24	0.51	45,58,75,79	0
3	GOL	D	512	6/6	0.96	0.13	0.40	25,28,32,35	0
3	GOL	H	509	6/6	0.89	0.19	0.29	48,55,68,71	0
3	GOL	A	510	6/6	0.97	0.10	0.15	16,17,22,23	0
2	SO4	G	501	5/5	0.99	0.09	-0.01	29,29,34,36	0
2	SO4	H	501	5/5	0.89	0.16	-0.02	63,66,76,97	0
3	GOL	G	508	6/6	0.91	0.10	-0.60	34,41,46,52	0
3	GOL	G	507	6/6	0.95	0.12	-0.87	29,34,37,45	0
2	SO4	G	502	5/5	0.83	0.35	-	66,88,106,106	0
2	SO4	D	505	5/5	0.91	0.27	-	69,94,98,107	0
2	SO4	B	505	5/5	0.92	0.27	-	50,75,78,80	0
2	SO4	C	508	5/5	0.93	0.33	-	82,83,86,94	0
2	SO4	F	501	5/5	0.92	0.30	-	81,92,101,104	0
3	GOL	C	511	6/6	0.92	0.16	-	31,44,47,47	0
2	SO4	B	503	5/5	0.90	0.37	-	80,90,94,100	0
2	SO4	B	504	5/5	0.97	0.28	-	68,78,86,89	0
3	GOL	H	508	6/6	0.87	0.22	-	54,60,76,80	0
2	SO4	C	505	5/5	0.93	0.27	-	65,81,89,90	0
2	SO4	H	503	5/5	0.87	0.34	-	96,103,112,116	0
3	GOL	B	512	6/6	0.84	0.17	-	55,64,67,72	0
2	SO4	B	507	5/5	0.91	0.33	-	66,91,99,113	0
2	SO4	D	506	5/5	0.93	0.28	-	66,80,90,95	0
2	SO4	D	502	5/5	0.88	0.28	-	61,64,83,85	0
2	SO4	B	508	5/5	0.93	0.33	-	57,68,75,92	0
2	SO4	E	507	5/5	0.98	0.13	-	51,52,54,61	0
3	GOL	F	510	6/6	0.79	0.32	-	69,76,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	E	512	6/6	0.84	0.31	-	60,66,69,73	0
2	SO4	E	504	5/5	0.90	0.30	-	65,82,90,91	0
2	SO4	E	509	5/5	0.90	0.33	-	73,74,89,98	0
2	SO4	H	502	5/5	0.88	0.37	-	81,87,105,106	0
2	SO4	A	509	5/5	0.94	0.34	-	74,74,92,98	0
3	GOL	D	514	6/6	0.91	0.25	-	60,74,80,81	0
2	SO4	D	509	5/5	0.88	0.33	-	71,93,95,105	0
2	SO4	F	507	5/5	0.87	0.34	-	68,80,81,99	0
2	SO4	G	504	5/5	0.86	0.35	-	73,84,103,105	0
2	SO4	H	507	5/5	0.87	0.44	-	84,88,103,114	0
2	SO4	A	506	5/5	0.95	0.21	-	60,66,69,78	0
2	SO4	A	501	5/5	0.90	0.38	-	59,75,87,105	0
2	SO4	D	511	5/5	0.89	0.27	-	71,96,107,107	0
3	GOL	D	515	6/6	0.85	0.13	-	48,58,67,71	0
2	SO4	A	505	5/5	0.86	0.25	-	71,72,98,101	0
2	SO4	C	501	5/5	0.90	0.29	-	65,83,86,90	0
3	GOL	B	509	6/6	0.72	0.55	-	58,68,77,80	0
2	SO4	E	505	5/5	0.87	0.32	-	80,89,103,103	0
2	SO4	D	510	5/5	0.93	0.25	-	79,82,92,95	0
3	GOL	C	512	6/6	0.89	0.17	-	45,52,69,72	0
2	SO4	C	506	5/5	0.92	0.28	-	60,66,76,86	0
2	SO4	C	504	5/5	0.98	0.15	-	50,51,61,65	0
3	GOL	A	512	6/6	0.86	0.21	-	61,65,69,72	0
2	SO4	H	506	5/5	0.83	0.44	-	98,99,112,117	0
2	SO4	D	501	5/5	0.85	0.34	-	96,99,111,124	0
2	SO4	F	503	5/5	0.81	0.34	-	72,77,104,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.