



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 02:28 am GMT

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 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

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

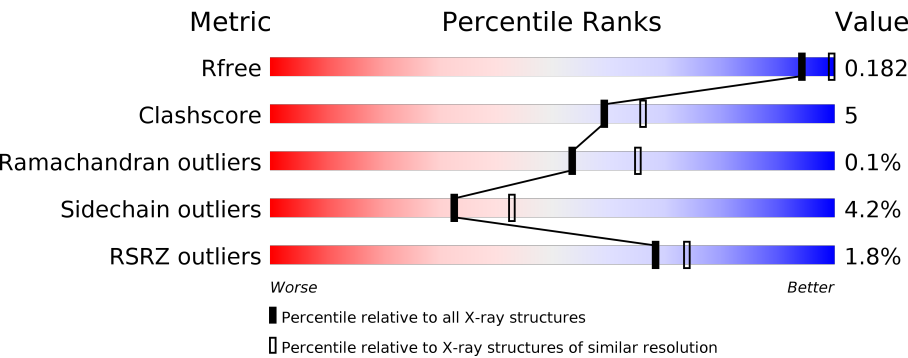
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

# 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 2.28 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 <sub>free</sub>	111664	6121 (2.30-2.26)
Clashscore	122126	6842 (2.30-2.26)
Ramachandran outliers	120053	6755 (2.30-2.26)
Sidechain outliers	120020	6755 (2.30-2.26)
RSRZ outliers	108989	5992 (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  $\geq 3$ , 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>%</div><div><div></div><div>85%</div><div>9%</div><div></div></div><div></div></div>
1	B	448	<div><div></div><div>85%</div><div>9%</div><div></div></div> <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	GOL	B	509	-	-	-	X
2	GOL	C	505	-	-	X	-
2	GOL	D	502	-	-	X	-
2	GOL	D	505	-	-	X	-
2	GOL	E	505	-	-	X	-
2	GOL	F	502	-	-	X	-
2	GOL	G	502	-	-	-	X
3	SO4	E	516	-	-	-	X
3	SO4	G	508	-	-	-	X
3	SO4	H	505	-	-	-	X
3	SO4	H	514	-	-	-	X
4	CIT	A	515	-	-	X	-
4	CIT	B	520	-	-	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 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	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: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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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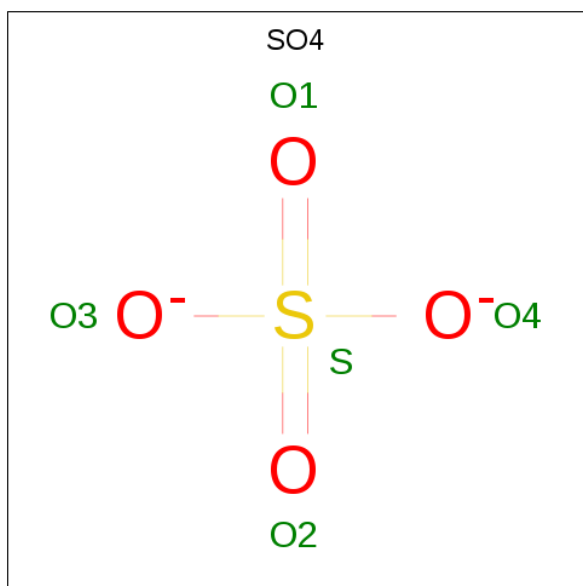
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	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: O<sub>4</sub>S).



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		
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: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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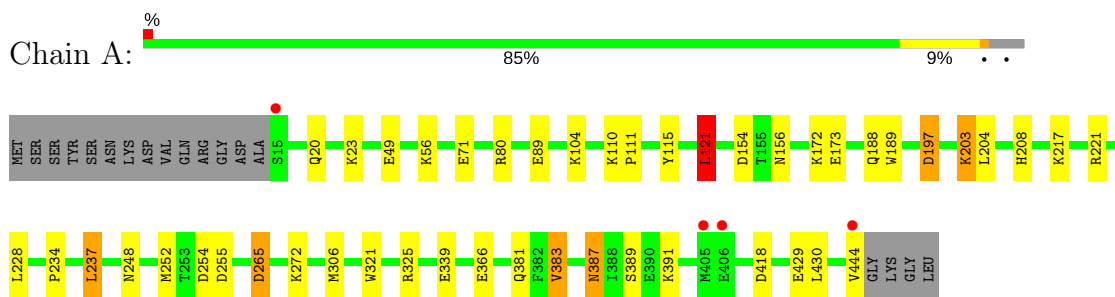
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	368	Total 368	O 368	0	0

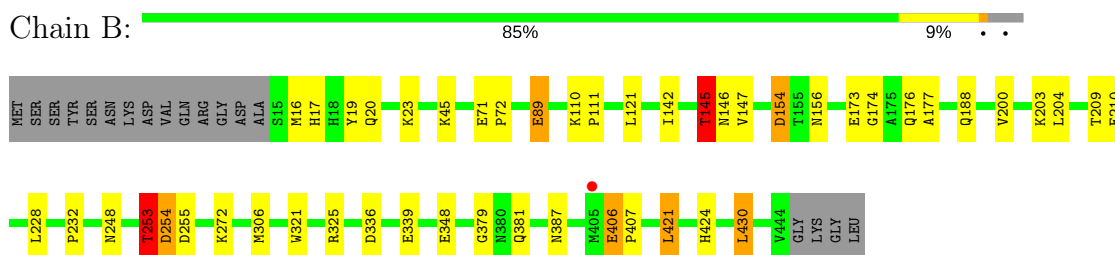
### 3 Residue-property plots [i](#)

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.

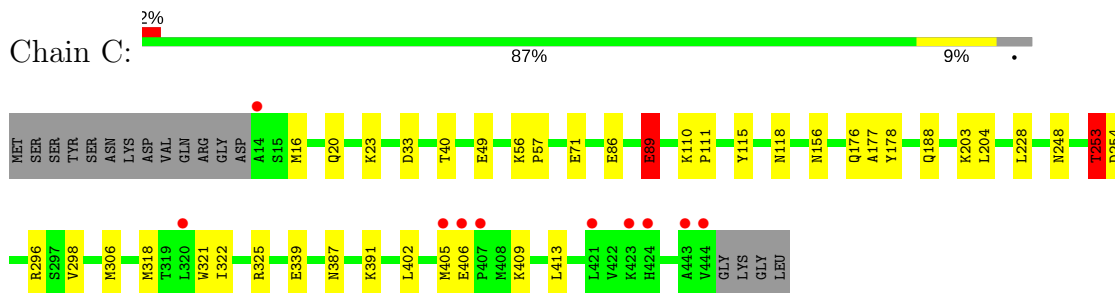
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



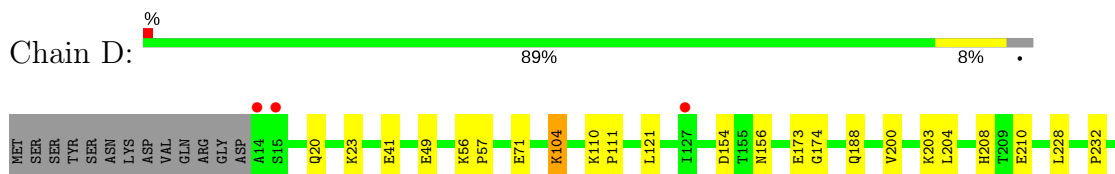
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

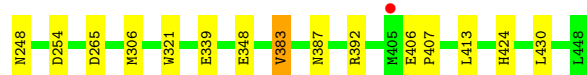


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

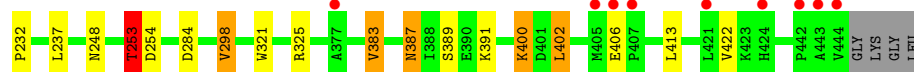
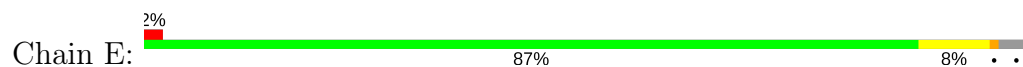


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

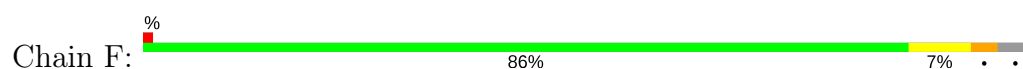




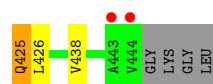
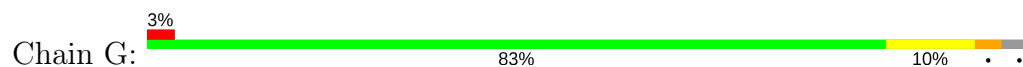
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



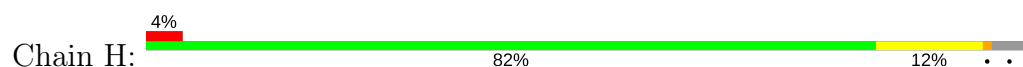
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

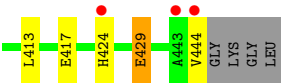


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



- 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, $\alpha$ , $\beta$ , $\gamma$	107.71Å 202.16Å 287.29Å 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) 96.9 (29.88-2.28)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.146 , 0.177 0.155 , 0.182	Depositor DCC
$R_{free}$ test set	13898 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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	1.02	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 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	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
5	G	439	0	0	17	0
5	H	368	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32820	0	27255	283	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 5.

The worst 5 of 283 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)
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 [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	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%)	49	60
1	G	430/448 (96%)	415 (96%)	15 (4%)	0	100	100
1	H	428/448 (96%)	410 (96%)	17 (4%)	1 (0%)	49	60
All	All	3446/3584 (96%)	3320 (96%)	124 (4%)	2 (0%)	53	65

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%)	48	63
1	B	373/383 (97%)	361 (97%)	12 (3%)	42	56
1	C	371/383 (97%)	358 (96%)	13 (4%)	39	52
1	D	372/383 (97%)	363 (98%)	9 (2%)	52	67
1	E	372/383 (97%)	356 (96%)	16 (4%)	32	41
1	F	369/383 (96%)	348 (94%)	21 (6%)	23	29
1	G	371/383 (97%)	349 (94%)	22 (6%)	21	27
1	H	369/383 (96%)	348 (94%)	21 (6%)	23	29
All	All	2970/3064 (97%)	2846 (96%)	124 (4%)	32	43

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

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Mol	Chain	Res	Type
1	D	387	ASN
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 ⓘ

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	0.64	0	5,5,5	0.50	0
2	GOL	A	502	-	5,5,5	0.59	0	5,5,5	0.38	0
2	GOL	A	503	-	5,5,5	0.85	0	5,5,5	2.14	2 (40%)
2	GOL	A	504	-	5,5,5	0.45	0	5,5,5	0.59	0
3	SO4	A	505	-	4,4,4	1.32	1 (25%)	6,6,6	1.05	0
3	SO4	A	506	-	4,4,4	0.56	0	6,6,6	0.50	0
3	SO4	A	507	-	4,4,4	0.75	0	6,6,6	0.76	0
3	SO4	A	508	-	4,4,4	0.64	0	6,6,6	0.47	0
3	SO4	A	509	-	4,4,4	0.56	0	6,6,6	1.08	1 (16%)
3	SO4	A	510	-	4,4,4	0.75	0	6,6,6	0.83	0
3	SO4	A	511	-	4,4,4	0.77	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	512	-	4,4,4	1.17	1 (25%)	6,6,6	1.34	1 (16%)
3	SO4	A	513	-	4,4,4	0.53	0	6,6,6	0.69	0
3	SO4	A	514	-	4,4,4	0.91	0	6,6,6	0.73	0
4	CIT	A	515	-	3,12,12	1.96	2 (66%)	3,17,17	1.98	1 (33%)
2	GOL	B	501	-	5,5,5	0.60	0	5,5,5	1.15	0
2	GOL	B	502	-	5,5,5	0.52	0	5,5,5	0.67	0
2	GOL	B	503	-	5,5,5	0.95	0	5,5,5	1.39	1 (20%)
2	GOL	B	504	-	5,5,5	0.71	0	5,5,5	1.16	0
2	GOL	B	505	-	5,5,5	1.11	0	5,5,5	0.75	0
2	GOL	B	506	-	5,5,5	0.70	0	5,5,5	0.54	0
2	GOL	B	507	-	5,5,5	0.36	0	5,5,5	1.44	1 (20%)
2	GOL	B	508	-	5,5,5	0.72	0	5,5,5	0.88	0
2	GOL	B	509	-	5,5,5	0.64	0	5,5,5	0.79	0
3	SO4	B	510	-	4,4,4	0.56	0	6,6,6	0.70	0
3	SO4	B	511	-	4,4,4	0.81	0	6,6,6	0.54	0
3	SO4	B	512	-	4,4,4	0.80	0	6,6,6	1.16	0
3	SO4	B	513	-	4,4,4	0.47	0	6,6,6	0.53	0
3	SO4	B	514	-	4,4,4	0.59	0	6,6,6	0.56	0
3	SO4	B	515	-	4,4,4	0.84	0	6,6,6	0.78	0
3	SO4	B	516	-	4,4,4	0.84	0	6,6,6	1.24	0
3	SO4	B	517	-	4,4,4	0.97	0	6,6,6	1.18	0
3	SO4	B	518	-	4,4,4	0.58	0	6,6,6	0.16	0
3	SO4	B	519	-	4,4,4	0.66	0	6,6,6	0.64	0
4	CIT	B	520	-	3,12,12	4.11	2 (66%)	3,17,17	4.54	2 (66%)
2	GOL	C	501	-	5,5,5	0.24	0	5,5,5	0.66	0
2	GOL	C	502	-	5,5,5	0.59	0	5,5,5	0.55	0
2	GOL	C	503	-	5,5,5	2.28	3 (60%)	5,5,5	2.16	2 (40%)
2	GOL	C	504	-	5,5,5	0.64	0	5,5,5	0.89	0
2	GOL	C	505	-	5,5,5	2.75	1 (20%)	5,5,5	1.66	1 (20%)
3	SO4	C	506	-	4,4,4	0.54	0	6,6,6	0.46	0
3	SO4	C	507	-	4,4,4	0.82	0	6,6,6	0.63	0
3	SO4	C	508	-	4,4,4	0.60	0	6,6,6	0.52	0
3	SO4	C	509	-	4,4,4	0.51	0	6,6,6	0.19	0
3	SO4	C	510	-	4,4,4	0.90	0	6,6,6	0.43	0
3	SO4	C	511	-	4,4,4	0.56	0	6,6,6	0.66	0
3	SO4	C	512	-	4,4,4	0.64	0	6,6,6	0.67	0
3	SO4	C	513	-	4,4,4	0.83	0	6,6,6	1.27	1 (16%)
3	SO4	C	514	-	4,4,4	0.56	0	6,6,6	0.40	0
3	SO4	C	515	-	4,4,4	0.82	0	6,6,6	1.29	1 (16%)
3	SO4	C	516	-	4,4,4	0.69	0	6,6,6	0.82	0
3	SO4	C	517	-	4,4,4	0.78	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	518	-	4,4,4	0.58	0	6,6,6	0.35	0
4	CIT	C	519	-	3,12,12	4.04	3 (100%)	3,17,17	4.65	2 (66%)
2	GOL	D	501	-	5,5,5	0.81	0	5,5,5	0.50	0
2	GOL	D	502	-	5,5,5	0.94	0	5,5,5	1.57	2 (40%)
2	GOL	D	503	-	5,5,5	0.56	0	5,5,5	1.73	2 (40%)
2	GOL	D	504	-	5,5,5	0.69	0	5,5,5	1.27	1 (20%)
2	GOL	D	505	-	5,5,5	0.97	0	5,5,5	1.42	1 (20%)
3	SO4	D	506	-	4,4,4	0.53	0	6,6,6	0.65	0
3	SO4	D	507	-	4,4,4	0.64	0	6,6,6	0.38	0
3	SO4	D	508	-	4,4,4	1.25	0	6,6,6	0.63	0
3	SO4	D	509	-	4,4,4	0.93	0	6,6,6	1.59	2 (33%)
3	SO4	D	510	-	4,4,4	0.67	0	6,6,6	0.55	0
3	SO4	D	511	-	4,4,4	0.77	0	6,6,6	1.92	2 (33%)
3	SO4	D	512	-	4,4,4	0.63	0	6,6,6	1.21	1 (16%)
3	SO4	D	513	-	4,4,4	0.71	0	6,6,6	0.77	0
3	SO4	D	514	-	4,4,4	0.63	0	6,6,6	0.39	0
3	SO4	D	515	-	4,4,4	0.63	0	6,6,6	0.42	0
3	SO4	D	516	-	4,4,4	0.65	0	6,6,6	0.79	0
3	SO4	D	517	-	4,4,4	0.58	0	6,6,6	0.67	0
2	GOL	E	501	-	5,5,5	0.51	0	5,5,5	0.25	0
2	GOL	E	502	-	5,5,5	0.59	0	5,5,5	0.45	0
2	GOL	E	503	-	5,5,5	0.70	0	5,5,5	1.68	1 (20%)
2	GOL	E	504	-	5,5,5	0.75	0	5,5,5	0.81	0
2	GOL	E	505	-	5,5,5	1.49	0	5,5,5	2.51	4 (80%)
2	GOL	E	506	-	5,5,5	0.36	0	5,5,5	0.28	0
3	SO4	E	507	-	4,4,4	0.58	0	6,6,6	0.63	0
3	SO4	E	508	-	4,4,4	0.85	0	6,6,6	1.02	0
3	SO4	E	509	-	4,4,4	0.77	0	6,6,6	1.32	1 (16%)
3	SO4	E	510	-	4,4,4	0.68	0	6,6,6	0.33	0
3	SO4	E	511	-	4,4,4	0.65	0	6,6,6	1.42	1 (16%)
3	SO4	E	512	-	4,4,4	0.68	0	6,6,6	0.75	0
3	SO4	E	513	-	4,4,4	0.68	0	6,6,6	0.94	0
3	SO4	E	514	-	4,4,4	1.20	0	6,6,6	1.16	0
3	SO4	E	515	-	4,4,4	0.88	0	6,6,6	0.80	0
3	SO4	E	516	-	4,4,4	0.63	0	6,6,6	0.37	0
4	CIT	E	517	-	3,12,12	0.84	0	3,17,17	3.07	2 (66%)
2	GOL	F	501	-	5,5,5	0.82	0	5,5,5	0.33	0
2	GOL	F	502	-	5,5,5	0.49	0	5,5,5	0.61	0
2	GOL	F	503	-	5,5,5	0.68	0	5,5,5	0.35	0
2	GOL	F	504	-	5,5,5	0.23	0	5,5,5	0.49	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	0.67	0	6,6,6	0.54	0
3	SO4	F	506	-	4,4,4	0.63	0	6,6,6	0.22	0
3	SO4	F	507	-	4,4,4	0.64	0	6,6,6	0.30	0
3	SO4	F	508	-	4,4,4	1.05	0	6,6,6	0.85	0
3	SO4	F	509	-	4,4,4	0.63	0	6,6,6	0.79	0
3	SO4	F	510	-	4,4,4	0.71	0	6,6,6	0.54	0
3	SO4	F	511	-	4,4,4	0.79	0	6,6,6	0.77	0
3	SO4	F	512	-	4,4,4	0.70	0	6,6,6	0.83	0
3	SO4	F	513	-	4,4,4	0.77	0	6,6,6	1.34	1 (16%)
3	SO4	F	514	-	4,4,4	0.84	0	6,6,6	0.46	0
3	SO4	F	515	-	4,4,4	0.59	0	6,6,6	0.44	0
2	GOL	G	501	-	5,5,5	0.61	0	5,5,5	0.86	0
2	GOL	G	502	-	5,5,5	0.36	0	5,5,5	0.49	0
2	GOL	G	503	-	5,5,5	0.53	0	5,5,5	1.10	1 (20%)
2	GOL	G	504	-	5,5,5	0.49	0	5,5,5	0.86	0
3	SO4	G	505	-	4,4,4	0.45	0	6,6,6	0.71	0
3	SO4	G	506	-	4,4,4	0.81	0	6,6,6	0.93	0
3	SO4	G	507	-	4,4,4	0.78	0	6,6,6	0.48	0
3	SO4	G	508	-	4,4,4	0.22	0	6,6,6	0.30	0
3	SO4	G	509	-	4,4,4	0.52	0	6,6,6	0.59	0
3	SO4	G	510	-	4,4,4	0.60	0	6,6,6	0.30	0
3	SO4	G	511	-	4,4,4	0.17	0	6,6,6	0.65	0
3	SO4	G	512	-	4,4,4	0.60	0	6,6,6	0.41	0
4	CIT	G	513	-	3,12,12	2.36	3 (100%)	3,17,17	2.33	2 (66%)
2	GOL	H	501	-	5,5,5	0.62	0	5,5,5	0.55	0
2	GOL	H	502	-	5,5,5	0.40	0	5,5,5	0.90	0
2	GOL	H	503	-	5,5,5	0.83	0	5,5,5	0.89	0
3	SO4	H	504	-	4,4,4	0.62	0	6,6,6	0.57	0
3	SO4	H	505	-	4,4,4	0.51	0	6,6,6	0.47	0
3	SO4	H	506	-	4,4,4	0.80	0	6,6,6	0.82	0
3	SO4	H	507	-	4,4,4	0.23	0	6,6,6	0.36	0
3	SO4	H	508	-	4,4,4	0.60	0	6,6,6	0.45	0
3	SO4	H	509	-	4,4,4	0.78	0	6,6,6	0.84	0
3	SO4	H	510	-	4,4,4	0.62	0	6,6,6	0.43	0
3	SO4	H	511	-	4,4,4	0.50	0	6,6,6	0.42	0
3	SO4	H	512	-	4,4,4	0.52	0	6,6,6	0.73	0
3	SO4	H	513	-	4,4,4	0.50	0	6,6,6	0.73	0
3	SO4	H	514	-	4,4,4	0.22	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	-	-	0/6/16/16	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	-	-	0/6/16/16	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
3	SO4	C	507	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/6/16/16	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
3	SO4	E	513	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/6/16/16	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	-	-	0/6/16/16	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
3	SO4	H	510	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	519	CIT	C2-C3	-2.44	1.51	1.54
3	A	512	SO4	O1-S	2.02	1.56	1.45
4	G	513	CIT	C4-C3	2.05	1.57	1.54
3	A	505	SO4	O2-S	2.09	1.56	1.45
4	A	515	CIT	O7-C3	2.15	1.46	1.43

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	519	CIT	C3-C2-C1	-6.88	104.63	114.95
4	C	519	CIT	C4-C3-C2	-4.19	99.32	109.70
2	A	503	GOL	C3-C2-C1	-3.38	98.60	111.63
4	A	515	CIT	C4-C3-C2	-2.96	102.38	109.70
3	D	509	SO4	O4-S-O1	-2.91	93.52	109.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

37 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	3	0
2	A	502	GOL	2	0
2	A	503	GOL	1	0
3	A	510	SO4	1	0
4	A	515	CIT	6	0
2	B	502	GOL	1	0
2	B	503	GOL	3	0
2	B	504	GOL	3	0
2	B	505	GOL	2	0
3	B	511	SO4	1	0
3	B	513	SO4	1	0
3	B	514	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	520	CIT	8	0
2	C	503	GOL	3	0
2	C	504	GOL	2	0
2	C	505	GOL	4	0
3	C	508	SO4	1	0
4	C	519	CIT	4	0
2	D	502	GOL	5	0
2	D	503	GOL	2	0
2	D	505	GOL	4	0
3	D	512	SO4	1	0
2	E	504	GOL	1	0
2	E	505	GOL	5	0
4	E	517	CIT	2	0
2	F	502	GOL	5	0
2	F	504	GOL	2	0
3	F	506	SO4	1	0
2	G	502	GOL	1	0
3	G	510	SO4	1	0
4	G	513	CIT	7	0
2	H	501	GOL	1	0
2	H	502	GOL	2	0
2	H	503	GOL	1	0
3	H	505	SO4	1	0
3	H	508	SO4	1	0
3	H	509	SO4	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 [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	430/448 (95%)	-0.68	4 (0%) 84 87	8, 13, 35, 96	0
1	B	430/448 (95%)	-0.70	1 (0%) 94 96	9, 17, 36, 91	0
1	C	431/448 (96%)	-0.51	10 (2%) 60 66	9, 18, 50, 107	0
1	D	435/448 (97%)	-0.50	4 (0%) 84 87	14, 22, 45, 88	0
1	E	430/448 (95%)	-0.39	10 (2%) 60 66	14, 23, 56, 114	0
1	F	430/448 (95%)	-0.38	6 (1%) 75 79	16, 27, 53, 116	0
1	G	430/448 (95%)	-0.14	12 (2%) 53 59	15, 32, 61, 111	1 (0%)
1	H	430/448 (95%)	0.08	16 (3%) 41 47	22, 37, 61, 115	0
All	All	3446/3584 (96%)	-0.40	63 (1%) 68 74	8, 23, 53, 116	1 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	9.2
1	E	444	VAL	8.5
1	F	405	MET	8.3
1	C	444	VAL	7.1
1	F	444	VAL	6.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	G	508	5/5	0.68	0.48	96,103,128,136	0
3	SO4	E	516	5/5	0.69	0.47	91,102,118,122	0
3	SO4	C	507	5/5	0.71	0.32	72,81,101,102	0
3	SO4	E	509	5/5	0.71	0.30	46,60,77,91	5
3	SO4	H	514	5/5	0.72	0.43	101,112,123,125	0
2	GOL	G	502	6/6	0.72	0.49	56,68,77,82	0
2	GOL	G	504	6/6	0.74	0.31	52,58,67,71	0
2	GOL	F	503	6/6	0.77	0.32	59,67,71,72	0
3	SO4	E	507	5/5	0.78	0.31	78,97,117,120	0
2	GOL	B	509	6/6	0.78	0.40	50,58,65,66	0
3	SO4	H	505	5/5	0.79	0.41	75,97,102,103	0
3	SO4	H	509	5/5	0.80	0.34	43,46,66,74	5
2	GOL	B	508	6/6	0.80	0.18	63,65,68,70	0
3	SO4	B	514	5/5	0.80	0.31	61,66,79,82	5
3	SO4	D	513	5/5	0.80	0.32	71,82,108,108	0
3	SO4	G	506	5/5	0.81	0.20	45,80,86,98	0
2	GOL	E	505	6/6	0.81	0.30	32,45,48,49	0
2	GOL	F	504	6/6	0.82	0.20	50,57,62,66	0
3	SO4	F	507	5/5	0.83	0.37	71,88,91,99	5
2	GOL	E	506	6/6	0.83	0.18	58,72,74,75	0
2	GOL	D	503	6/6	0.83	0.14	43,49,54,62	0
3	SO4	D	516	5/5	0.83	0.33	75,76,93,95	0
2	GOL	B	505	6/6	0.83	0.23	43,54,65,67	0
3	SO4	F	511	5/5	0.84	0.20	54,74,86,91	0
2	GOL	C	505	6/6	0.84	0.27	21,27,34,43	0
2	GOL	C	503	6/6	0.84	0.29	18,24,28,33	6
3	SO4	E	515	5/5	0.85	0.27	52,70,82,84	0
2	GOL	H	502	6/6	0.85	0.18	52,62,74,81	0
3	SO4	C	518	5/5	0.86	0.34	83,92,120,127	0
3	SO4	D	511	5/5	0.86	0.24	49,62,78,78	0
3	SO4	B	518	5/5	0.86	0.36	102,103,116,122	0
3	SO4	F	505	5/5	0.86	0.32	72,75,85,96	0
3	SO4	D	515	5/5	0.87	0.38	76,91,101,105	0
3	SO4	H	507	5/5	0.87	0.42	104,110,115,123	0
3	SO4	G	505	5/5	0.87	0.28	71,98,113,117	0
3	SO4	G	512	5/5	0.87	0.33	80,91,99,104	0
2	GOL	B	506	6/6	0.88	0.44	56,67,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CIT	E	517	13/13	0.88	0.21	35,64,73,87	0
2	GOL	E	504	6/6	0.88	0.25	37,56,61,63	0
4	CIT	C	519	13/13	0.88	0.21	26,45,62,62	0
3	SO4	B	513	5/5	0.89	0.32	79,94,112,117	0
4	CIT	B	520	13/13	0.89	0.24	31,46,59,64	0
3	SO4	F	513	5/5	0.89	0.27	56,60,79,90	0
3	SO4	D	514	5/5	0.89	0.29	62,91,99,102	0
3	SO4	H	512	5/5	0.89	0.33	81,83,96,96	0
2	GOL	H	501	6/6	0.89	0.21	32,43,45,48	0
3	SO4	E	510	5/5	0.89	0.43	84,91,94,107	0
2	GOL	B	507	6/6	0.89	0.18	54,64,72,76	0
2	GOL	H	503	6/6	0.89	0.12	38,42,49,53	0
2	GOL	A	504	6/6	0.89	0.14	38,45,53,54	0
3	SO4	G	510	5/5	0.89	0.41	90,99,107,116	0
3	SO4	G	511	5/5	0.90	0.42	82,101,104,113	0
2	GOL	A	502	6/6	0.90	0.15	54,66,71,72	0
3	SO4	B	511	5/5	0.90	0.34	45,58,66,67	5
3	SO4	C	515	5/5	0.90	0.24	49,58,72,74	0
3	SO4	H	506	5/5	0.90	0.31	59,63,68,77	0
3	SO4	C	514	5/5	0.91	0.30	65,79,88,91	0
3	SO4	F	509	5/5	0.91	0.33	56,75,85,85	0
2	GOL	A	501	6/6	0.91	0.15	28,38,48,60	0
3	SO4	B	517	5/5	0.91	0.23	39,41,60,63	0
3	SO4	B	516	5/5	0.91	0.25	51,67,68,72	0
3	SO4	E	513	5/5	0.91	0.32	75,76,88,92	0
4	CIT	G	513	13/13	0.91	0.18	35,44,66,66	0
3	SO4	H	504	5/5	0.91	0.34	73,79,92,107	0
3	SO4	E	508	5/5	0.91	0.27	39,43,56,60	5
3	SO4	F	510	5/5	0.91	0.27	62,74,79,88	0
3	SO4	H	508	5/5	0.91	0.37	69,71,88,94	0
3	SO4	F	508	5/5	0.91	0.32	54,67,89,95	0
3	SO4	F	514	5/5	0.91	0.27	59,70,77,89	0
3	SO4	A	514	5/5	0.92	0.23	48,62,67,83	0
2	GOL	C	504	6/6	0.92	0.14	36,38,44,56	0
2	GOL	B	503	6/6	0.92	0.21	29,31,43,48	0
3	SO4	E	512	5/5	0.92	0.23	50,66,84,88	0
3	SO4	A	507	5/5	0.92	0.35	39,52,60,70	5
3	SO4	F	512	5/5	0.92	0.22	64,69,90,96	0
3	SO4	D	507	5/5	0.92	0.40	78,96,97,105	0
3	SO4	A	506	5/5	0.92	0.30	66,66,86,88	0
2	GOL	D	505	6/6	0.92	0.15	32,36,39,50	0
3	SO4	B	519	5/5	0.92	0.34	56,73,88,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	504	6/6	0.92	0.15	31,37,44,54	0
4	CIT	A	515	13/13	0.92	0.17	15,29,39,49	13
3	SO4	E	514	5/5	0.92	0.30	41,52,66,79	0
3	SO4	D	508	5/5	0.92	0.24	48,59,67,81	0
3	SO4	A	513	5/5	0.92	0.33	74,76,86,93	0
3	SO4	H	510	5/5	0.92	0.30	78,82,95,96	0
2	GOL	E	501	6/6	0.92	0.13	35,49,58,64	0
3	SO4	F	515	5/5	0.93	0.34	90,102,112,113	0
3	SO4	C	509	5/5	0.93	0.32	104,108,116,118	0
2	GOL	B	502	6/6	0.93	0.13	32,37,45,57	0
3	SO4	C	506	5/5	0.93	0.43	76,77,94,94	0
3	SO4	F	506	5/5	0.93	0.40	86,87,108,111	0
3	SO4	A	512	5/5	0.93	0.26	41,41,58,59	0
2	GOL	F	502	6/6	0.93	0.13	40,47,49,56	0
3	SO4	C	510	5/5	0.93	0.33	51,60,76,78	0
3	SO4	D	517	5/5	0.93	0.21	34,35,49,51	5
3	SO4	D	512	5/5	0.93	0.25	60,73,82,87	0
2	GOL	F	501	6/6	0.94	0.19	25,32,35,37	0
2	GOL	G	501	6/6	0.94	0.14	40,49,64,65	0
3	SO4	A	508	5/5	0.94	0.36	62,73,75,86	0
3	SO4	C	508	5/5	0.94	0.30	74,75,79,82	0
2	GOL	G	503	6/6	0.94	0.23	29,36,38,44	0
3	SO4	G	507	5/5	0.94	0.22	40,46,60,61	5
3	SO4	H	511	5/5	0.94	0.33	70,92,95,103	0
3	SO4	D	510	5/5	0.94	0.25	66,78,95,97	0
3	SO4	C	517	5/5	0.94	0.24	56,64,78,90	0
3	SO4	D	506	5/5	0.94	0.32	72,74,85,96	0
2	GOL	E	503	6/6	0.94	0.21	50,57,62,65	0
2	GOL	C	502	6/6	0.94	0.10	31,38,49,63	0
3	SO4	B	512	5/5	0.94	0.32	44,48,51,65	5
3	SO4	D	509	5/5	0.95	0.16	45,56,68,71	0
3	SO4	A	511	5/5	0.95	0.18	39,53,58,69	0
2	GOL	A	503	6/6	0.95	0.14	14,18,19,24	0
3	SO4	C	516	5/5	0.96	0.21	40,58,64,72	0
3	SO4	C	511	5/5	0.96	0.19	67,67,82,88	0
2	GOL	D	502	6/6	0.96	0.20	31,35,39,41	0
3	SO4	A	505	5/5	0.96	0.20	32,35,47,64	0
3	SO4	A	509	5/5	0.96	0.19	55,62,69,75	0
2	GOL	B	504	6/6	0.96	0.14	30,35,38,40	0
2	GOL	D	501	6/6	0.97	0.16	18,22,23,24	0
2	GOL	E	502	6/6	0.97	0.17	22,26,27,32	0
2	GOL	C	501	6/6	0.97	0.13	18,20,21,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	501	6/6	0.97	0.14	18,25,27,34	0
3	SO4	C	513	5/5	0.97	0.20	43,45,49,62	0
3	SO4	B	510	5/5	0.97	0.25	68,70,76,86	0
3	SO4	C	512	5/5	0.98	0.19	40,46,54,54	0
3	SO4	E	511	5/5	0.98	0.15	39,41,44,55	0
3	SO4	H	513	5/5	0.99	0.19	53,53,57,60	0
3	SO4	B	515	5/5	0.99	0.12	23,35,38,39	0
3	SO4	A	510	5/5	0.99	0.08	23,24,26,37	0
3	SO4	G	509	5/5	1.00	0.07	24,25,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.