wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 09:24 PM EDT

PDB ID	:	4NZF
Title	:	Crystal structure of Abp-D197A (a GH27-b-L-arabinopyranosidase from Geobacillus stearothermophilus), in complex with arabinose
Authors	:	Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on	:	2013-12-12
Resolution	:	2.19 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

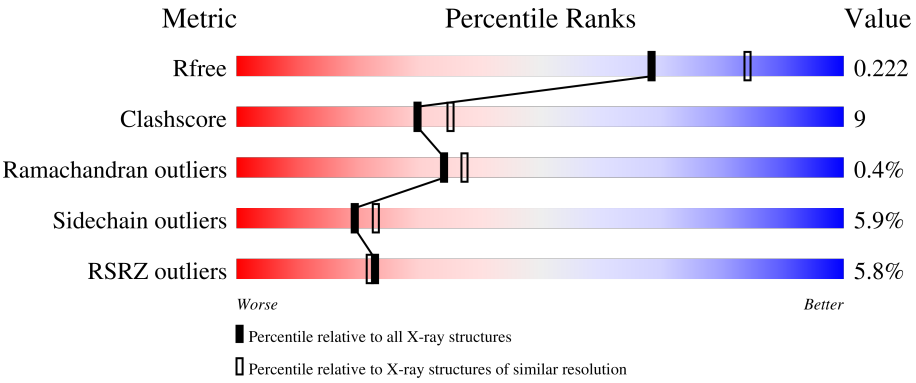
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	83% 11%
1	B	448	82% 12%
1	C	448	3% 82% 12%
1	D	448	2% 81% 15%
1	E	448	4% 85% 11%

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Mol	Chain	Length	Quality of chain
1	F	448	5% 78% 16%
1	G	448	14% 63% 28% 5%
1	H	448	15% 60% 32%

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	A	501	-	-	X	-
2	GOL	D	503	-	-	X	-
2	GOL	H	502	-	-	X	-
4	SO4	F	507	-	-	-	X
5	CIT	A	515	-	X	X	-
5	CIT	B	519	-	-	X	-
5	CIT	C	519	-	-	X	-
5	CIT	D	515	-	-	X	-
5	CIT	E	517	-	-	X	-

2 Entry composition (i)

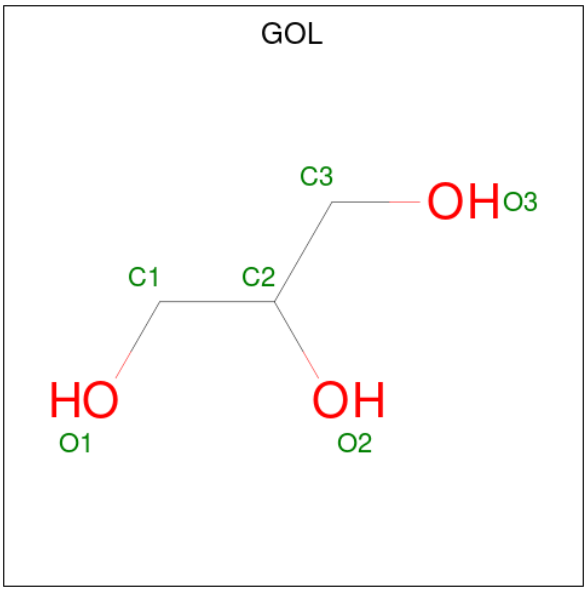
There are 6 unique types of molecules in this entry. The entry contains 31507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	0
			3489	2232	599	633	25			
1	B	430	Total	C	N	O	S	0	2	0
			3482	2227	598	632	25			
1	C	432	Total	C	N	O	S	0	2	0
			3492	2233	599	635	25			
1	D	435	Total	C	N	O	S	0	1	0
			3503	2242	603	633	25			
1	E	431	Total	C	N	O	S	0	1	0
			3477	2224	597	631	25			
1	F	430	Total	C	N	O	S	0	0	0
			3467	2218	596	628	25			
1	G	431	Total	C	N	O	S	0	4	0
			3494	2235	599	635	25			
1	H	430	Total	C	N	O	S	0	3	0
			3483	2230	597	629	27			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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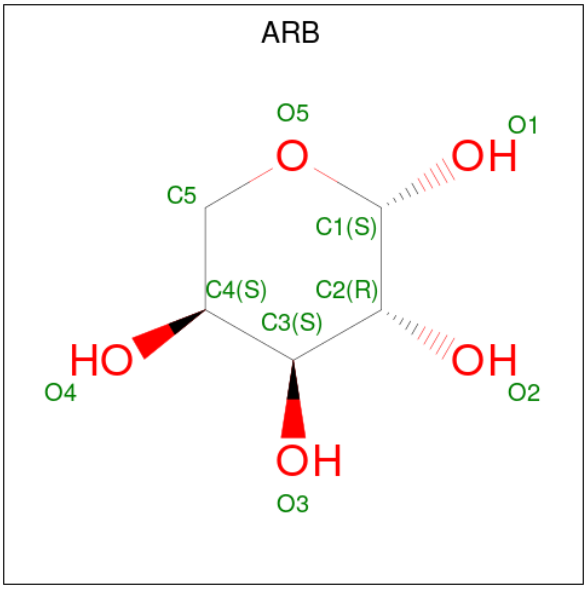
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

- Molecule 3 is beta-L-arabinopyranose (three-letter code: ARB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0
3	E	1	Total C O 10 5 5	0	0

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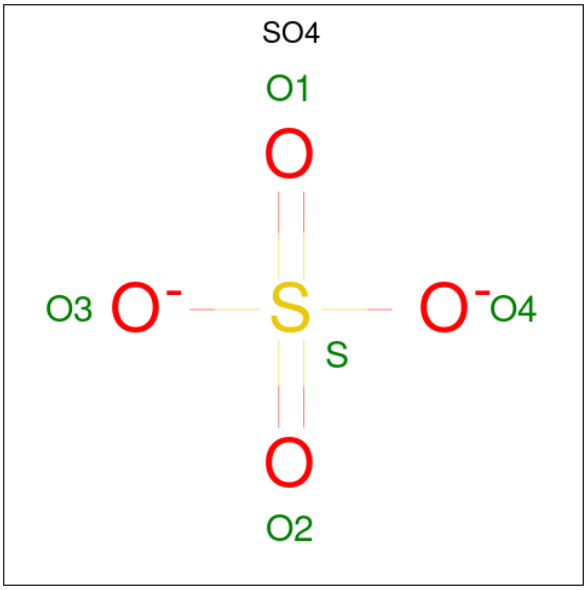
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 10 5 5	0	0
3	G	1	Total C O 10 5 5	0	0
3	H	1	Total C O 10 5 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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

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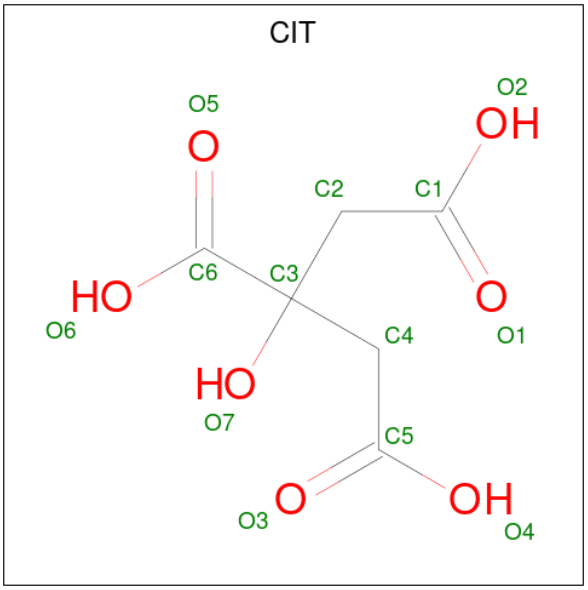
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

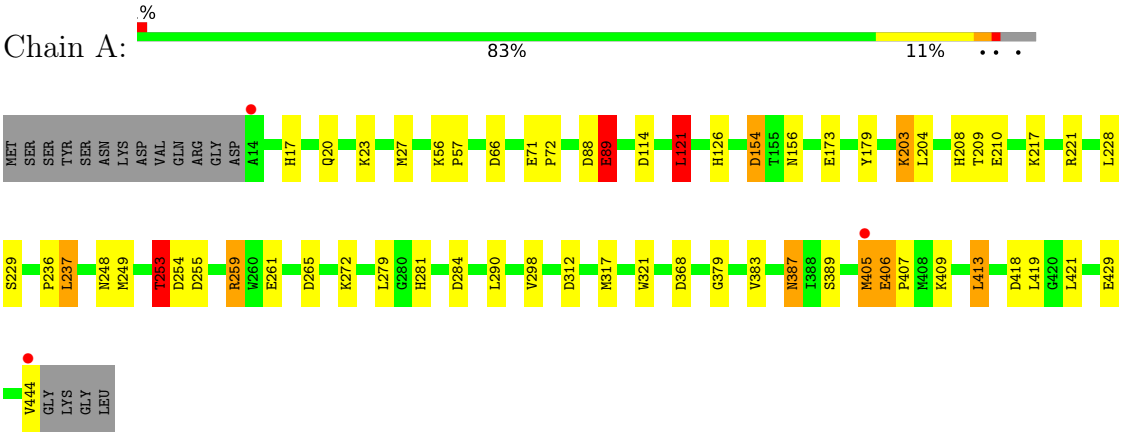
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	540	Total O 540 540	0	0
6	B	465	Total O 465 465	0	0
6	C	421	Total O 421 421	0	0
6	D	380	Total O 380 380	0	0
6	E	388	Total O 388 388	0	0
6	F	298	Total O 298 298	0	0
6	G	264	Total O 264 264	0	0
6	H	176	Total O 176 176	0	0

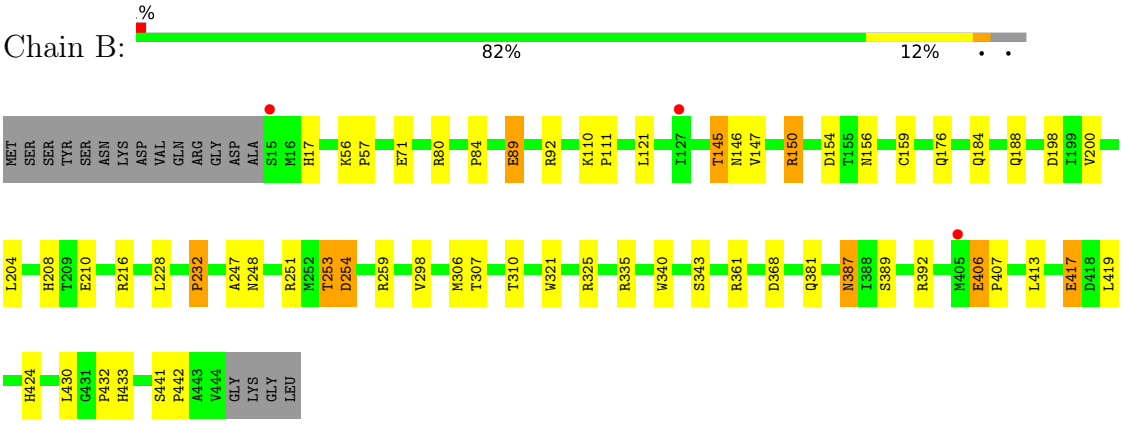
3 Residue-property plots (i)

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

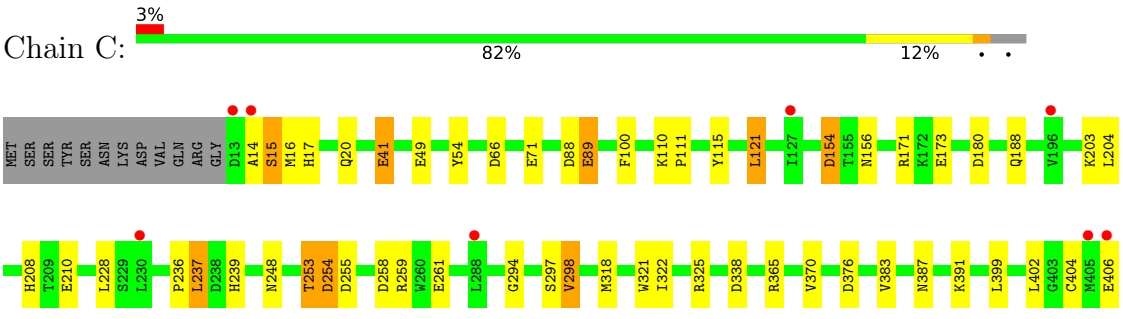
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

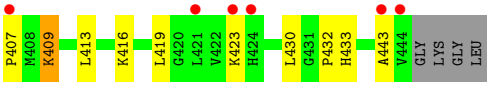


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

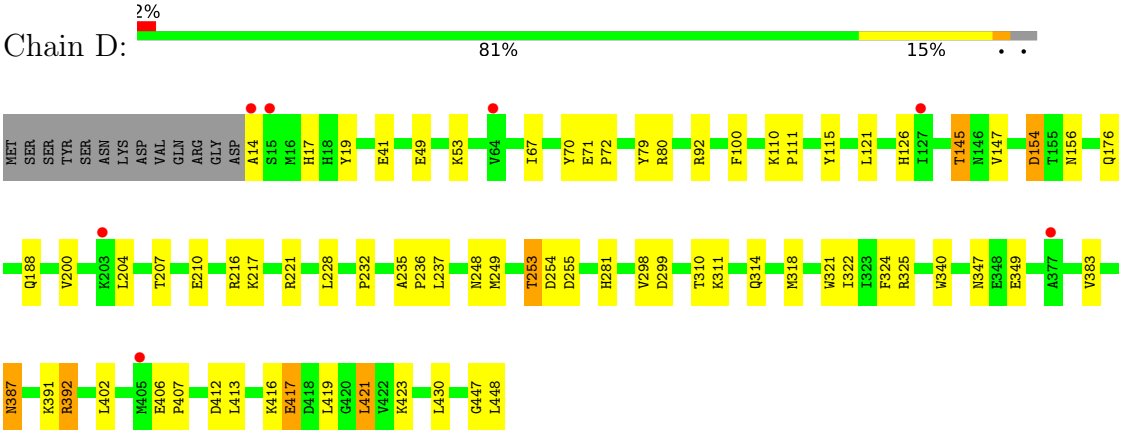


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

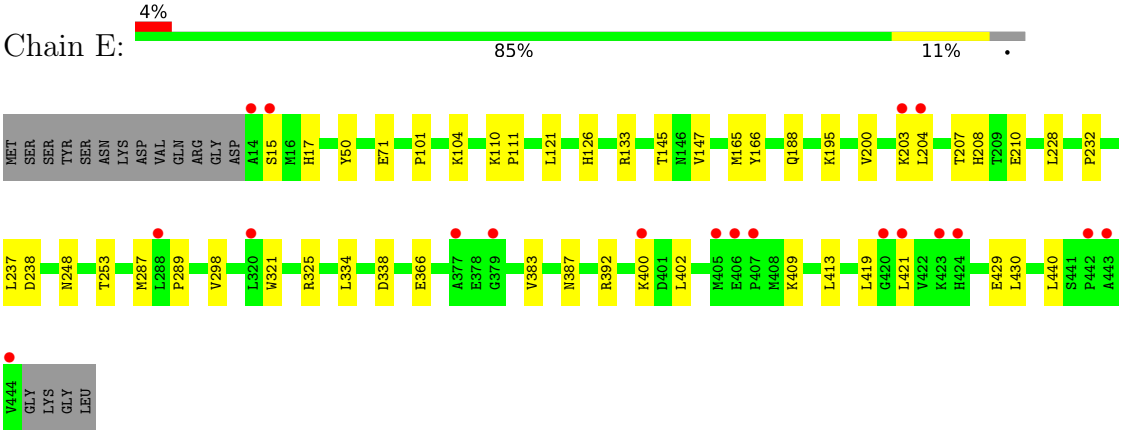




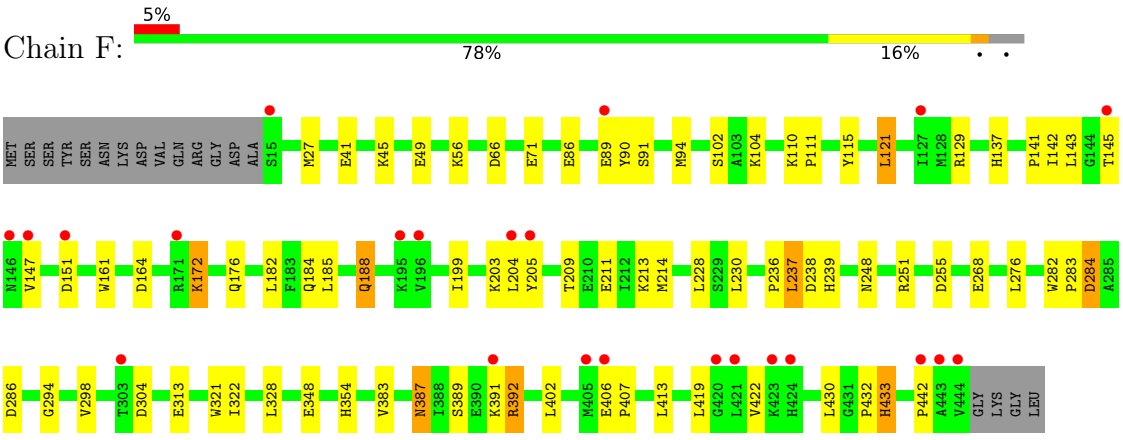
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



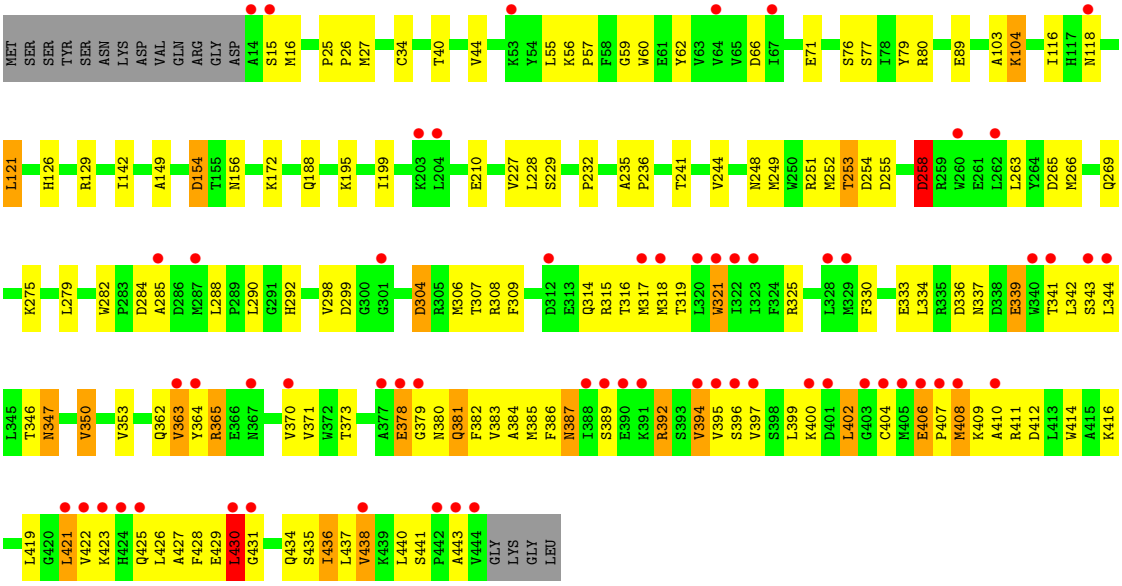
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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

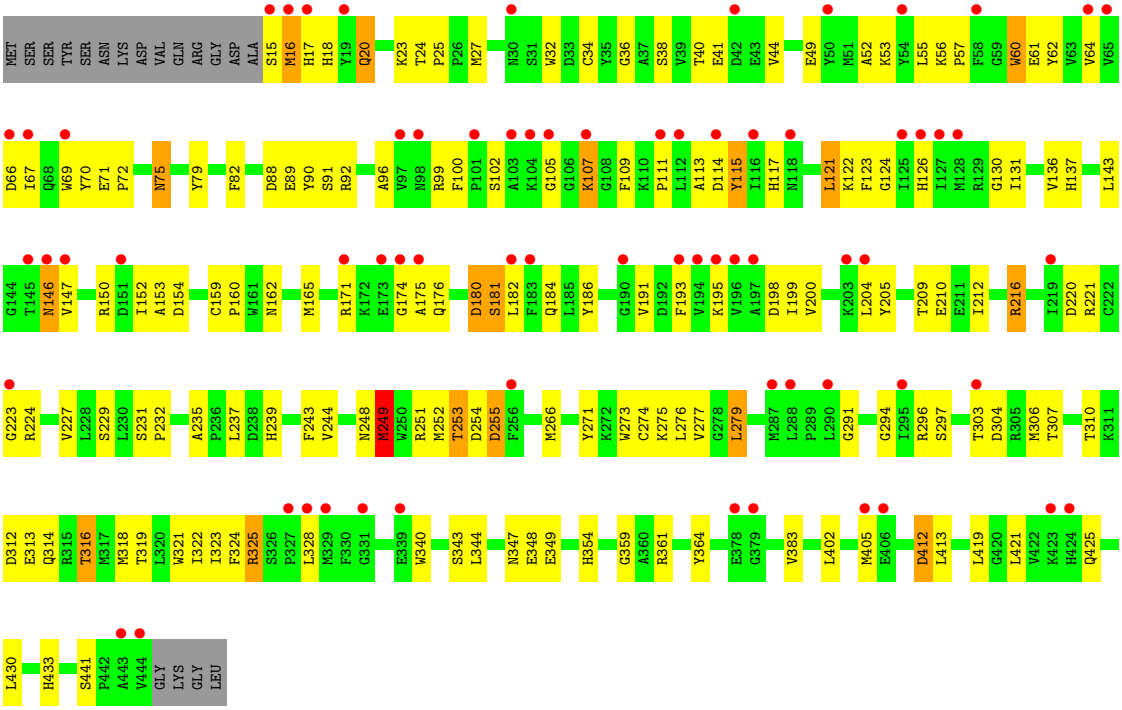


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.60Å 201.50Å 286.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.71 – 2.19 34.68 – 2.19	Depositor EDS
% Data completeness (in resolution range)	89.0 (34.71-2.19) 89.1 (34.68-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.168 , 0.219 0.176 , 0.222	Depositor DCC
R_{free} test set	14318 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31507	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARB, CIT, GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.10	3/3600 (0.1%)	1.06	17/4887 (0.3%)
1	B	1.02	1/3587 (0.0%)	1.00	12/4869 (0.2%)
1	C	0.93	1/3600 (0.0%)	0.99	19/4887 (0.4%)
1	D	0.98	0/3608	0.99	7/4895 (0.1%)
1	E	0.87	0/3582	0.92	1/4863 (0.0%)
1	F	0.85	0/3569	0.91	4/4845 (0.1%)
1	G	0.96	1/3608 (0.0%)	1.06	10/4898 (0.2%)
1	H	0.86	0/3594	1.00	7/4877 (0.1%)
All	All	0.95	6/28748 (0.0%)	0.99	77/39021 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	THR	CB-CG2	-7.02	1.29	1.52
1	G	89	GLU	CG-CD	5.74	1.60	1.51
1	A	179	TYR	CE1-CZ	-5.29	1.31	1.38
1	C	154	ASP	CB-CG	-5.24	1.40	1.51
1	B	325	ARG	CZ-NH2	5.02	1.39	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	C	154	ASP	CB-CG-OD2	-9.64	109.63	118.30
1	C	338	ASP	CB-CG-OD1	8.30	125.78	118.30
1	G	251	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	368	ASP	CB-CG-OD1	8.02	125.52	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	165	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3489	0	3372	47	0
1	B	3482	0	3360	40	0
1	C	3492	0	3370	35	0
1	D	3503	0	3395	49	0
1	E	3477	0	3356	30	0
1	F	3467	0	3347	43	0
1	G	3494	0	3376	124	0
1	H	3483	0	3373	140	0
2	A	6	0	8	8	0
2	B	18	0	24	2	0
2	C	30	0	40	2	0
2	D	18	0	24	7	0
2	E	24	0	32	3	0
2	F	6	0	8	0	0
2	G	6	0	8	1	0
2	H	12	0	16	4	0
3	A	10	0	10	0	0
3	B	10	0	10	0	0
3	C	10	0	10	0	0
3	D	10	0	10	0	0
3	E	10	0	10	0	0
3	F	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	10	0	10	2	0
3	H	10	0	10	0	0
4	A	60	0	0	1	0
4	B	70	0	0	4	0
4	C	60	0	0	4	0
4	D	50	0	0	5	0
4	E	55	0	0	1	0
4	F	55	0	0	0	0
4	G	35	0	0	0	0
4	H	25	0	0	0	0
5	A	13	0	5	6	0
5	B	13	0	5	6	0
5	C	13	0	5	9	0
5	D	13	0	5	7	0
5	E	13	0	5	9	0
5	G	13	0	5	3	0
6	A	540	0	0	21	1
6	B	465	0	0	13	1
6	C	421	0	0	10	0
6	D	380	0	0	11	0
6	E	388	0	0	8	0
6	F	298	0	0	10	0
6	G	264	0	0	35	0
6	H	176	0	0	37	0
All	All	31507	0	27219	522	1

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 9.

The worst 5 of 522 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:347:ASN:HA	6:G:785:HOH:O	1.48	1.10
1:A:17:HIS:CE1	6:A:1094:HOH:O	2.18	0.96
1:G:363:VAL:HG13	1:G:371:VAL:HG23	1.47	0.93
1:A:406:GLU:HB2	1:A:407:PRO:HD2	1.49	0.92
1:G:188[B]:GLN:HG3	6:G:731:HOH:O	1.70	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:836:HOH:O	6:B:1011:HOH:O[4_445]	2.02	0.18

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%)	417 (96%)	15 (4%)	0	100 100
1	B	430/448 (96%)	412 (96%)	18 (4%)	0	100 100
1	C	432/448 (96%)	419 (97%)	13 (3%)	0	100 100
1	D	434/448 (97%)	415 (96%)	18 (4%)	1 (0%)	47 55
1	E	430/448 (96%)	411 (96%)	19 (4%)	0	100 100
1	F	428/448 (96%)	406 (95%)	21 (5%)	1 (0%)	47 55
1	G	433/448 (97%)	393 (91%)	35 (8%)	5 (1%)	13 10
1	H	431/448 (96%)	384 (89%)	41 (10%)	6 (1%)	11 8
All	All	3450/3584 (96%)	3257 (94%)	180 (5%)	13 (0%)	34 37

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	379	GLY
1	H	121	LEU
1	H	325	ARG
1	G	104	LYS
1	G	258	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/382 (97%)	354 (95%)	17 (5%)	27	34
1	B	370/382 (97%)	353 (95%)	17 (5%)	27	34
1	C	371/382 (97%)	352 (95%)	19 (5%)	24	29
1	D	371/382 (97%)	349 (94%)	22 (6%)	19	23
1	E	369/382 (97%)	354 (96%)	15 (4%)	30	39
1	F	368/382 (96%)	348 (95%)	20 (5%)	22	26
1	G	372/382 (97%)	337 (91%)	35 (9%)	8	8
1	H	371/382 (97%)	340 (92%)	31 (8%)	11	11
All	All	2963/3056 (97%)	2787 (94%)	176 (6%)	19	23

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	199	ILE
1	G	438	VAL
1	G	263	LEU
1	G	383	VAL
1	H	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	248	ASN
1	G	248	ASN
1	H	356	ASN
1	F	356	ASN
1	G	118	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

116 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	$\#\|Z\| > 2$
4	SO4	C	509	-	4,4,4	0.63	0	6,6,6	1.63	2 (33%)
4	SO4	F	506	-	4,4,4	0.52	0	6,6,6	0.34	0
4	SO4	C	507	-	4,4,4	0.62	0	6,6,6	0.63	0
3	ARB	A	502	-	10,10,10	1.31	2 (20%)	14,14,14	2.81	9 (64%)
4	SO4	H	506	-	4,4,4	0.54	0	6,6,6	0.58	0
4	SO4	H	505	-	4,4,4	0.42	0	6,6,6	0.50	0
4	SO4	A	508	-	4,4,4	0.49	0	6,6,6	0.14	0
4	SO4	D	510	-	4,4,4	0.45	0	6,6,6	0.76	0
5	CIT	D	515	-	12,12,12	2.05	2 (16%)	17,17,17	2.05	6 (35%)
2	GOL	E	503	-	5,5,5	0.42	0	5,5,5	1.10	0
2	GOL	H	502	-	5,5,5	0.27	0	5,5,5	0.98	0
4	SO4	B	505	-	4,4,4	0.49	0	6,6,6	0.48	0
2	GOL	C	502	-	5,5,5	0.39	0	5,5,5	0.43	0
3	ARB	C	506	-	10,10,10	1.00	1 (10%)	14,14,14	2.53	6 (42%)
5	CIT	G	510	-	12,12,12	3.73	4 (33%)	17,17,17	3.37	8 (47%)
3	ARB	B	504	-	10,10,10	1.10	1 (10%)	14,14,14	2.53	7 (50%)
4	SO4	F	505	-	4,4,4	0.41	0	6,6,6	0.67	0
4	SO4	F	512	-	4,4,4	0.45	0	6,6,6	0.38	0
4	SO4	G	503	-	4,4,4	0.35	0	6,6,6	1.18	1 (16%)
4	SO4	G	506	-	4,4,4	0.41	0	6,6,6	0.30	0
4	SO4	G	508	-	4,4,4	0.46	0	6,6,6	0.50	0
2	GOL	C	504	-	5,5,5	0.69	0	5,5,5	2.58	2 (40%)
4	SO4	A	513	-	4,4,4	0.92	0	6,6,6	1.18	1 (16%)
4	SO4	E	506	-	4,4,4	0.43	0	6,6,6	0.26	0
4	SO4	H	504	-	4,4,4	0.39	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	G	504	-	4,4,4	0.57	0	6,6,6	0.31	0
4	SO4	E	512	-	4,4,4	0.50	0	6,6,6	0.91	0
4	SO4	B	514	-	4,4,4	0.45	0	6,6,6	0.41	0
4	SO4	A	503	-	4,4,4	0.72	0	6,6,6	0.45	0
4	SO4	E	509	-	4,4,4	0.62	0	6,6,6	0.47	0
4	SO4	C	512	-	4,4,4	0.64	0	6,6,6	1.17	0
4	SO4	H	507	-	4,4,4	0.38	0	6,6,6	0.36	0
4	SO4	B	511	-	4,4,4	0.46	0	6,6,6	0.47	0
4	SO4	F	513	-	4,4,4	0.49	0	6,6,6	0.68	0
2	GOL	D	502	-	5,5,5	0.41	0	5,5,5	0.53	0
4	SO4	B	516	-	4,4,4	0.62	0	6,6,6	0.68	0
4	SO4	D	514	-	4,4,4	0.42	0	6,6,6	0.63	0
4	SO4	B	509	-	4,4,4	0.74	0	6,6,6	0.67	0
2	GOL	C	505	-	5,5,5	1.13	0	5,5,5	1.25	0
4	SO4	A	507	-	4,4,4	0.45	0	6,6,6	0.79	0
4	SO4	E	516	-	4,4,4	0.43	0	6,6,6	0.32	0
4	SO4	C	516	-	4,4,4	0.38	0	6,6,6	0.48	0
4	SO4	F	511	-	4,4,4	0.34	0	6,6,6	0.26	0
4	SO4	B	507	-	4,4,4	0.40	0	6,6,6	0.43	0
4	SO4	E	514	-	4,4,4	0.38	0	6,6,6	0.43	0
4	SO4	A	504	-	4,4,4	0.43	0	6,6,6	1.06	0
4	SO4	B	515	-	4,4,4	0.55	0	6,6,6	0.44	0
4	SO4	C	514	-	4,4,4	0.47	0	6,6,6	0.52	0
2	GOL	A	501	-	5,5,5	0.39	0	5,5,5	0.61	0
4	SO4	D	513	-	4,4,4	0.39	0	6,6,6	0.48	0
4	SO4	B	513	-	4,4,4	0.53	0	6,6,6	0.42	0
4	SO4	F	503	-	4,4,4	0.44	0	6,6,6	0.23	0
4	SO4	A	509	-	4,4,4	0.58	0	6,6,6	0.61	0
4	SO4	F	507	-	4,4,4	0.39	0	6,6,6	0.18	0
5	CIT	A	515	-	12,12,12	3.38	6 (50%)	17,17,17	2.64	5 (29%)
4	SO4	D	507	-	4,4,4	0.58	0	6,6,6	0.43	0
2	GOL	D	503	-	5,5,5	0.39	0	5,5,5	1.75	2 (40%)
2	GOL	G	501	-	5,5,5	0.43	0	5,5,5	1.15	0
4	SO4	A	506	-	4,4,4	0.63	0	6,6,6	0.60	0
4	SO4	A	505	-	4,4,4	0.39	0	6,6,6	0.54	0
4	SO4	E	515	-	4,4,4	0.52	0	6,6,6	0.57	0
4	SO4	D	505	-	4,4,4	0.48	0	6,6,6	0.61	0
3	ARB	E	505	-	10,10,10	0.61	0	14,14,14	2.96	8 (57%)
4	SO4	E	511	-	4,4,4	0.49	0	6,6,6	0.46	0
4	SO4	F	504	-	4,4,4	0.56	0	6,6,6	0.63	0
4	SO4	G	509	-	4,4,4	0.49	0	6,6,6	0.53	0
2	GOL	B	502	-	5,5,5	0.58	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	C	515	-	4,4,4	0.43	0	6,6,6	0.30	0
4	SO4	G	505	-	4,4,4	0.37	0	6,6,6	0.19	0
3	ARB	G	502	-	10,10,10	1.25	1 (10%)	14,14,14	2.33	9 (64%)
4	SO4	D	506	-	4,4,4	0.50	0	6,6,6	0.71	0
4	SO4	H	508	-	4,4,4	0.40	0	6,6,6	0.50	0
5	CIT	B	519	-	12,12,12	3.82	2 (16%)	17,17,17	4.94	6 (35%)
4	SO4	C	513	-	4,4,4	0.68	0	6,6,6	0.67	0
4	SO4	D	508	-	4,4,4	0.43	0	6,6,6	0.44	0
2	GOL	H	501	-	5,5,5	0.32	0	5,5,5	1.37	1 (20%)
4	SO4	B	518	-	4,4,4	0.33	0	6,6,6	0.30	0
2	GOL	D	501	-	5,5,5	0.32	0	5,5,5	1.00	0
4	SO4	E	507	-	4,4,4	0.32	0	6,6,6	0.73	0
2	GOL	B	501	-	5,5,5	0.61	0	5,5,5	1.43	1 (20%)
5	CIT	C	519	-	12,12,12	2.04	4 (33%)	17,17,17	2.72	7 (41%)
4	SO4	G	507	-	4,4,4	0.44	0	6,6,6	0.36	0
3	ARB	F	502	-	10,10,10	0.96	0	14,14,14	2.81	7 (50%)
4	SO4	F	510	-	4,4,4	0.50	0	6,6,6	0.64	0
4	SO4	D	511	-	4,4,4	0.45	0	6,6,6	0.56	0
4	SO4	B	508	-	4,4,4	0.44	0	6,6,6	0.97	0
4	SO4	E	513	-	4,4,4	0.64	0	6,6,6	0.47	0
4	SO4	B	510	-	4,4,4	0.56	0	6,6,6	0.43	0
4	SO4	A	514	-	4,4,4	0.56	0	6,6,6	0.48	0
3	ARB	D	504	-	10,10,10	1.11	1 (10%)	14,14,14	2.35	6 (42%)
2	GOL	F	501	-	5,5,5	0.34	0	5,5,5	0.65	0
4	SO4	E	510	-	4,4,4	0.78	0	6,6,6	0.75	0
4	SO4	A	510	-	4,4,4	0.79	0	6,6,6	1.06	0
4	SO4	D	509	-	4,4,4	0.46	0	6,6,6	0.54	0
4	SO4	C	511	-	4,4,4	0.43	0	6,6,6	0.69	0
4	SO4	C	510	-	4,4,4	0.41	0	6,6,6	0.62	0
3	ARB	H	503	-	10,10,10	1.12	1 (10%)	14,14,14	1.61	3 (21%)
4	SO4	C	518	-	4,4,4	0.35	0	6,6,6	0.31	0
2	GOL	E	501	-	5,5,5	0.30	0	5,5,5	0.59	0
4	SO4	D	512	-	4,4,4	0.42	0	6,6,6	0.35	0
4	SO4	F	508	-	4,4,4	0.51	0	6,6,6	0.46	0
2	GOL	C	501	-	5,5,5	0.39	0	5,5,5	0.87	0
4	SO4	B	506	-	4,4,4	0.68	0	6,6,6	0.84	0
2	GOL	E	502	-	5,5,5	0.42	0	5,5,5	0.19	0
5	CIT	E	517	-	12,12,12	1.92	1 (8%)	17,17,17	4.06	7 (41%)
2	GOL	E	504	-	5,5,5	0.31	0	5,5,5	0.70	0
4	SO4	F	509	-	4,4,4	0.45	0	6,6,6	0.21	0
4	SO4	A	512	-	4,4,4	0.62	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	B	503	-	5,5,5	0.70	0	5,5,5	1.13	0
4	SO4	E	508	-	4,4,4	0.60	0	6,6,6	0.51	0
4	SO4	A	511	-	4,4,4	0.30	0	6,6,6	0.41	0
4	SO4	C	508	-	4,4,4	0.50	0	6,6,6	0.22	0
4	SO4	B	517	-	4,4,4	0.55	0	6,6,6	0.42	0
2	GOL	C	503	-	5,5,5	0.41	0	5,5,5	0.59	0
4	SO4	C	517	-	4,4,4	0.55	0	6,6,6	0.39	0
4	SO4	B	512	-	4,4,4	0.44	0	6,6,6	0.53	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
5	CIT	A	515	-	-	7/16/16/16	-
3	ARB	D	504	-	-	-	0/1/1/1
2	GOL	F	501	-	-	2/4/4/4	-
2	GOL	D	503	-	-	2/4/4/4	-
2	GOL	G	501	-	-	3/4/4/4	-
3	ARB	A	502	-	-	-	0/1/1/1
3	ARB	H	503	-	-	-	0/1/1/1
3	ARB	E	505	-	-	-	0/1/1/1
2	GOL	E	501	-	-	4/4/4/4	-
5	CIT	D	515	-	-	8/16/16/16	-
2	GOL	E	503	-	-	2/4/4/4	-
2	GOL	D	502	-	-	1/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
2	GOL	H	502	-	-	4/4/4/4	-
2	GOL	C	505	-	-	1/4/4/4	-
2	GOL	E	502	-	-	2/4/4/4	-
5	CIT	E	517	-	-	7/16/16/16	-
3	ARB	G	502	-	-	-	0/1/1/1
5	CIT	B	519	-	-	9/16/16/16	-
2	GOL	E	504	-	-	2/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	H	501	-	-	0/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ARB	C	506	-	-	-	0/1/1/1
2	GOL	B	503	-	-	2/4/4/4	-
5	CIT	G	510	-	-	5/16/16/16	-
2	GOL	B	501	-	-	2/4/4/4	-
3	ARB	B	504	-	-	-	0/1/1/1
2	GOL	A	501	-	-	4/4/4/4	-
5	CIT	C	519	-	-	4/16/16/16	-
2	GOL	C	503	-	-	0/4/4/4	-
3	ARB	F	502	-	-	-	0/1/1/1
2	GOL	C	504	-	-	3/4/4/4	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	519	CIT	C3-C6	-11.69	1.41	1.53
5	G	510	CIT	C3-C6	-10.63	1.42	1.53
5	A	515	CIT	C3-C6	-9.66	1.43	1.53
5	E	517	CIT	C3-C6	-5.60	1.47	1.53
5	B	519	CIT	C4-C3	-5.06	1.47	1.53

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	519	CIT	O5-C6-C3	-12.24	104.92	122.25
5	B	519	CIT	O7-C3-C6	-12.03	91.98	108.86
5	E	517	CIT	O5-C6-C3	-10.79	106.97	122.25
5	E	517	CIT	O6-C6-C3	8.97	128.63	113.05
5	A	515	CIT	O7-C3-C6	-8.20	97.35	108.86

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	C	501	GOL	C1-C2-C3-O3
2	C	502	GOL	C1-C2-C3-O3
2	C	504	GOL	C1-C2-C3-O3

There are no ring outliers.

33 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	510	SO4	1	0
5	D	515	CIT	7	0
2	H	502	GOL	4	0
4	B	505	SO4	1	0
5	G	510	CIT	3	0
2	C	504	GOL	1	0
4	E	506	SO4	1	0
4	B	514	SO4	1	0
4	C	512	SO4	1	0
2	D	502	GOL	1	0
4	B	516	SO4	1	0
4	D	514	SO4	1	0
2	C	505	GOL	1	0
4	C	516	SO4	1	0
4	B	507	SO4	1	0
2	A	501	GOL	8	0
4	D	513	SO4	1	0
5	A	515	CIT	6	0
2	D	503	GOL	4	0
2	G	501	GOL	1	0
4	A	506	SO4	1	0
3	G	502	ARB	2	0
4	D	506	SO4	1	0
5	B	519	CIT	6	0
2	D	501	GOL	2	0
5	C	519	CIT	9	0
3	F	502	ARB	1	0
4	C	510	SO4	1	0
4	D	512	SO4	1	0
5	E	517	CIT	9	0
2	E	504	GOL	3	0
2	B	503	GOL	2	0
4	C	508	SO4	1	0

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, 95^{th} 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	431/448 (96%)	-0.43	3 (0%)	87	86	11, 17, 35, 83	0
1	B	430/448 (95%)	-0.41	3 (0%)	87	86	14, 23, 38, 74	0
1	C	432/448 (96%)	-0.22	14 (3%)	47	45	12, 24, 55, 99	0
1	D	435/448 (97%)	-0.33	7 (1%)	72	70	18, 26, 47, 97	0
1	E	431/448 (96%)	-0.09	19 (4%)	34	32	18, 29, 63, 110	0
1	F	430/448 (95%)	0.09	23 (5%)	26	25	19, 37, 61, 98	0
1	G	431/448 (96%)	0.58	61 (14%)	2	2	19, 43, 76, 134	1 (0%)
1	H	430/448 (95%)	0.91	69 (16%)	1	1	32, 55, 77, 116	0
All	All	3450/3584 (96%)	0.01	199 (5%)	23	22	11, 29, 66, 134	1 (0%)

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	14	ALA	14.3
1	E	444	VAL	13.4
1	F	444	VAL	10.1
1	G	444	VAL	9.7
1	H	444	VAL	9.5

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	507	5/5	0.65	0.45	122,124,130,137	0
4	SO4	H	505	5/5	0.65	0.37	92,113,123,129	0
4	SO4	E	515	5/5	0.66	0.34	86,91,115,116	0
4	SO4	B	518	5/5	0.75	0.40	99,101,110,114	0
2	GOL	E	502	6/6	0.77	0.20	63,67,70,78	0
4	SO4	F	503	5/5	0.78	0.28	97,105,115,117	0
2	GOL	B	502	6/6	0.78	0.19	65,74,76,81	0
4	SO4	B	512	5/5	0.78	0.26	94,106,111,116	0
2	GOL	H	501	6/6	0.80	0.20	55,57,63,68	0
4	SO4	G	509	5/5	0.80	0.27	75,83,99,102	0
4	SO4	A	512	5/5	0.80	0.25	71,78,105,108	0
4	SO4	C	514	5/5	0.81	0.26	73,86,97,108	0
4	SO4	A	514	5/5	0.81	0.27	76,91,105,108	0
4	SO4	H	507	5/5	0.81	0.33	86,101,114,127	0
4	SO4	B	510	5/5	0.82	0.31	75,91,105,106	0
4	SO4	E	511	5/5	0.82	0.28	63,86,95,95	0
4	SO4	C	516	5/5	0.83	0.30	111,116,121,126	0
2	GOL	F	501	6/6	0.84	0.21	51,61,68,74	0
4	SO4	D	514	5/5	0.84	0.26	73,86,96,103	0
4	SO4	C	515	5/5	0.84	0.32	97,102,106,109	0
4	SO4	C	517	5/5	0.85	0.31	68,76,103,106	0
4	SO4	B	515	5/5	0.85	0.43	89,95,97,102	0
4	SO4	F	512	5/5	0.85	0.36	82,88,100,103	0
5	CIT	E	517	13/13	0.85	0.24	39,62,77,81	0
4	SO4	H	504	5/5	0.86	0.31	86,96,99,111	0
4	SO4	F	506	5/5	0.87	0.17	70,70,87,88	0
5	CIT	G	510	13/13	0.87	0.23	36,59,73,76	0
4	SO4	G	507	5/5	0.88	0.25	75,84,96,105	0
4	SO4	D	512	5/5	0.88	0.36	94,95,103,107	0
4	SO4	F	505	5/5	0.88	0.28	79,91,98,108	0
2	GOL	H	502	6/6	0.88	0.18	54,56,62,63	0
4	SO4	C	509	5/5	0.88	0.18	41,46,57,63	5
4	SO4	H	508	5/5	0.88	0.28	90,96,107,110	0
4	SO4	F	509	5/5	0.88	0.28	94,96,105,113	0
4	SO4	B	516	5/5	0.88	0.33	67,73,74,94	0
4	SO4	E	506	5/5	0.89	0.33	80,86,91,93	0
2	GOL	E	503	6/6	0.89	0.24	49,57,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	507	5/5	0.89	0.30	58,59,70,75	0
4	SO4	D	513	5/5	0.89	0.28	75,91,102,109	0
5	CIT	A	515	13/13	0.89	0.20	31,43,56,58	0
5	CIT	C	519	13/13	0.89	0.20	26,43,64,66	0
5	CIT	D	515	13/13	0.89	0.26	32,55,69,86	0
4	SO4	F	504	5/5	0.89	0.29	87,90,100,100	0
2	GOL	C	503	6/6	0.89	0.15	50,60,63,66	0
4	SO4	F	513	5/5	0.90	0.29	74,77,87,96	0
4	SO4	E	513	5/5	0.90	0.23	73,95,101,108	0
5	CIT	B	519	13/13	0.90	0.24	41,53,72,75	0
4	SO4	D	509	5/5	0.90	0.30	63,82,90,102	0
4	SO4	E	516	5/5	0.90	0.30	92,99,110,113	0
4	SO4	B	513	5/5	0.90	0.20	68,71,82,83	0
4	SO4	A	503	5/5	0.90	0.31	44,57,70,74	0
4	SO4	C	511	5/5	0.91	0.27	63,77,82,89	0
4	SO4	G	506	5/5	0.91	0.37	85,87,103,110	0
4	SO4	E	512	5/5	0.91	0.24	77,78,87,92	0
2	GOL	D	501	6/6	0.91	0.17	33,35,37,39	0
3	ARB	H	503	10/10	0.91	0.21	52,62,67,67	0
4	SO4	B	514	5/5	0.91	0.28	68,74,85,99	0
2	GOL	D	502	6/6	0.91	0.10	42,57,59,59	0
4	SO4	D	506	5/5	0.92	0.24	54,69,81,86	0
4	SO4	B	505	5/5	0.92	0.32	67,83,85,87	0
4	SO4	D	510	5/5	0.92	0.20	62,64,72,76	0
4	SO4	C	513	5/5	0.92	0.35	55,62,71,72	0
4	SO4	G	504	5/5	0.92	0.30	66,80,88,90	0
2	GOL	G	501	6/6	0.92	0.12	40,47,52,54	0
2	GOL	E	501	6/6	0.92	0.14	37,45,50,61	0
2	GOL	B	501	6/6	0.92	0.15	29,35,40,43	0
3	ARB	G	502	10/10	0.92	0.21	32,39,44,50	0
2	GOL	E	504	6/6	0.93	0.16	49,51,55,64	0
4	SO4	C	518	5/5	0.93	0.31	86,87,96,100	0
2	GOL	B	503	6/6	0.93	0.13	32,35,41,47	0
4	SO4	F	508	5/5	0.93	0.30	66,73,90,92	0
4	SO4	D	507	5/5	0.93	0.22	46,55,60,71	0
4	SO4	B	506	5/5	0.93	0.19	35,44,51,56	5
4	SO4	A	511	5/5	0.93	0.31	65,73,84,89	0
4	SO4	D	511	5/5	0.93	0.27	70,75,87,97	0
4	SO4	G	505	5/5	0.93	0.32	73,73,76,76	5
4	SO4	B	511	5/5	0.93	0.34	73,76,88,99	0
2	GOL	C	502	6/6	0.93	0.11	48,53,54,57	0
4	SO4	A	508	5/5	0.94	0.28	75,77,84,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	508	5/5	0.94	0.28	59,67,76,91	0
4	SO4	E	508	5/5	0.94	0.21	53,63,76,84	0
4	SO4	E	509	5/5	0.94	0.23	59,61,73,74	0
4	SO4	H	506	5/5	0.94	0.11	59,72,79,80	0
4	SO4	D	508	5/5	0.94	0.23	67,84,93,94	0
2	GOL	D	503	6/6	0.94	0.17	37,41,42,48	0
4	SO4	F	510	5/5	0.94	0.20	60,61,72,86	0
4	SO4	B	517	5/5	0.94	0.34	65,76,82,86	0
4	SO4	E	514	5/5	0.94	0.25	77,82,93,94	0
2	GOL	A	501	6/6	0.94	0.12	25,32,38,41	0
2	GOL	C	505	6/6	0.94	0.16	23,31,37,43	0
4	SO4	A	505	5/5	0.94	0.35	71,72,81,82	0
4	SO4	E	510	5/5	0.95	0.24	52,58,73,73	0
4	SO4	B	509	5/5	0.95	0.20	50,60,63,75	0
4	SO4	C	512	5/5	0.95	0.16	55,58,63,71	0
4	SO4	G	508	5/5	0.95	0.15	59,72,82,86	0
4	SO4	F	511	5/5	0.95	0.28	89,98,104,104	0
3	ARB	F	502	10/10	0.95	0.17	32,43,48,55	0
2	GOL	C	501	6/6	0.95	0.14	28,33,40,44	0
4	SO4	A	509	5/5	0.95	0.29	53,59,70,74	0
3	ARB	B	504	10/10	0.96	0.17	19,22,30,32	0
4	SO4	D	505	5/5	0.96	0.14	49,60,66,67	0
3	ARB	D	504	10/10	0.96	0.14	19,25,28,32	0
4	SO4	A	513	5/5	0.96	0.20	43,47,49,55	0
4	SO4	C	508	5/5	0.96	0.16	45,56,57,70	0
2	GOL	C	504	6/6	0.96	0.13	34,42,47,47	0
4	SO4	A	510	5/5	0.96	0.14	31,37,42,62	0
3	ARB	E	505	10/10	0.97	0.14	24,28,36,40	0
4	SO4	B	507	5/5	0.97	0.26	62,68,74,82	0
3	ARB	C	506	10/10	0.97	0.17	19,25,35,36	0
3	ARB	A	502	10/10	0.98	0.17	15,20,26,29	0
4	SO4	A	507	5/5	0.98	0.13	34,43,45,47	0
4	SO4	E	507	5/5	0.98	0.11	45,47,54,58	0
4	SO4	C	510	5/5	0.98	0.17	44,52,62,68	0
4	SO4	A	504	5/5	0.98	0.17	42,49,59,62	0
4	SO4	G	503	5/5	1.00	0.07	28,29,36,39	0
4	SO4	A	506	5/5	1.00	0.07	24,27,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.