



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:18 AM UTC

PDB ID : 4NXK / pdb_00004nxk
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 Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

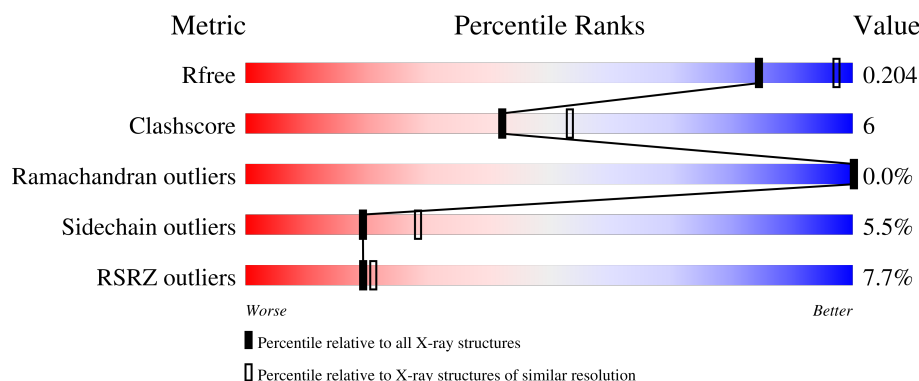
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	% 87% 8% ...
1	B	448	2% 84% 10% ...
1	C	448	2% 83% 12% ...
1	D	448	% 85% 10% ...
1	E	448	3% 85% 10% ...

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Mol	Chain	Length	Quality of chain
1	F	448	
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	H	502	-	-	X	-
3	GOL	C	510	-	X	X	-
3	GOL	C	513	-	X	-	-
3	GOL	C	514	-	-	X	-
3	GOL	D	513	-	-	X	-
3	GOL	E	510	-	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	-
4	CIT	E	514	-	-	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 (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	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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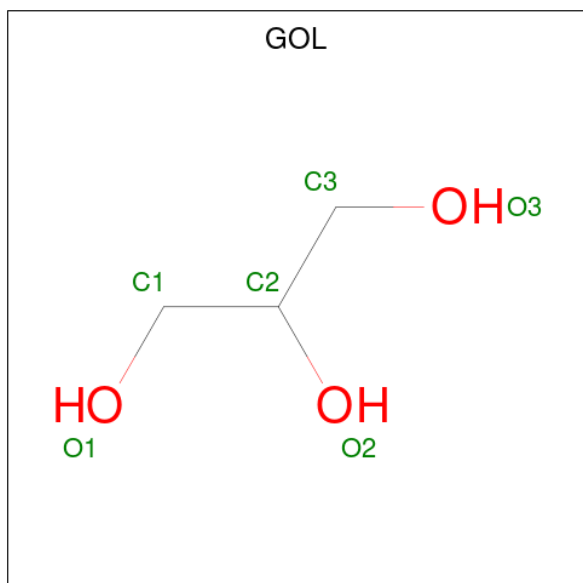
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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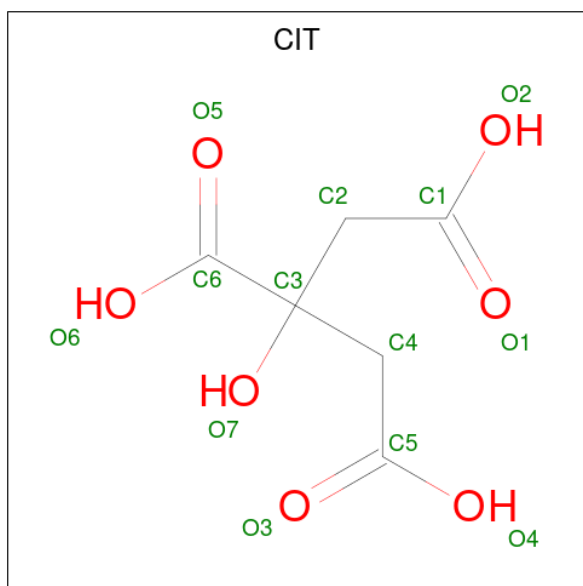
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	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 (CCD ID: 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		

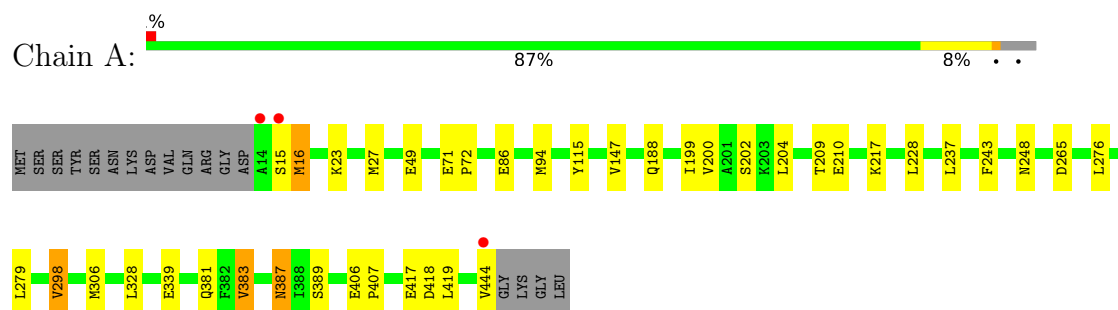
- Molecule 5 is water.

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		

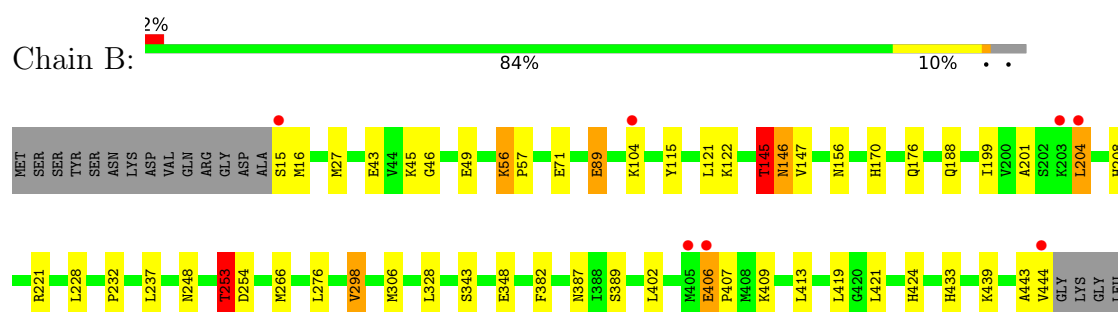
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

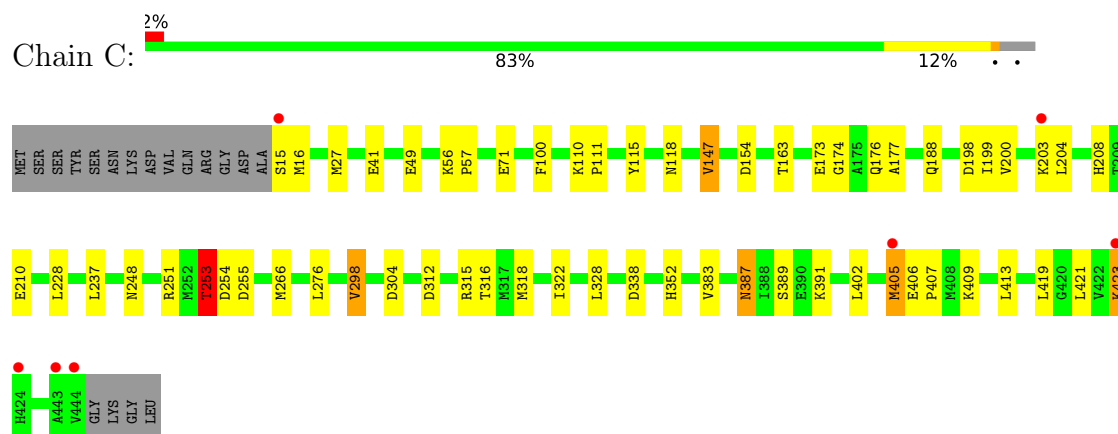
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



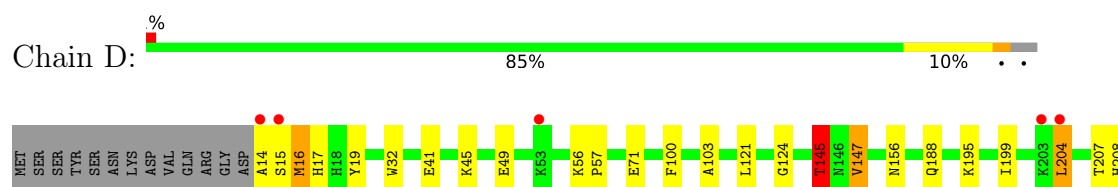
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



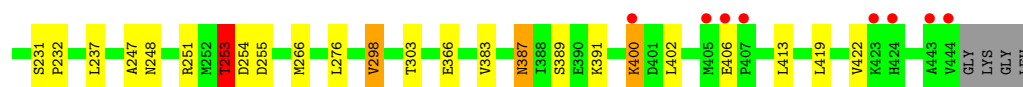
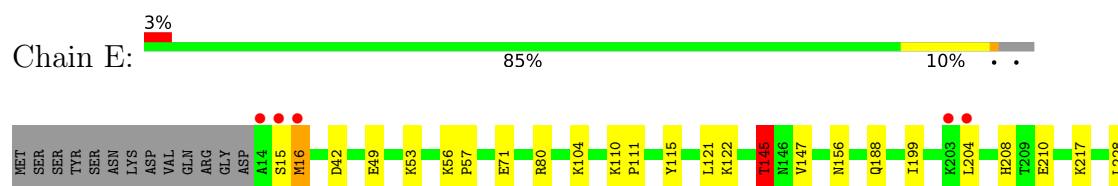
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



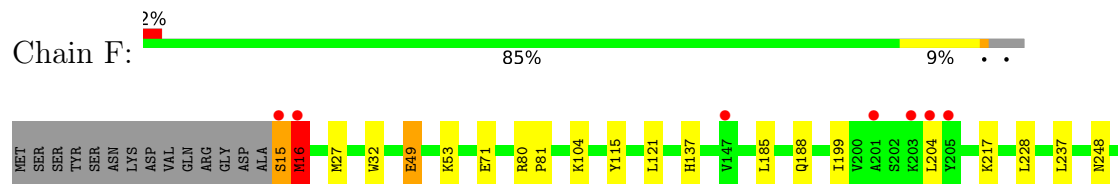
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



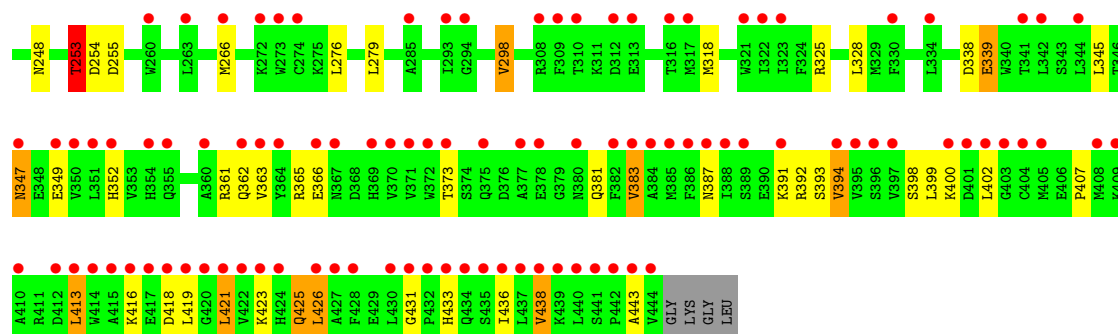
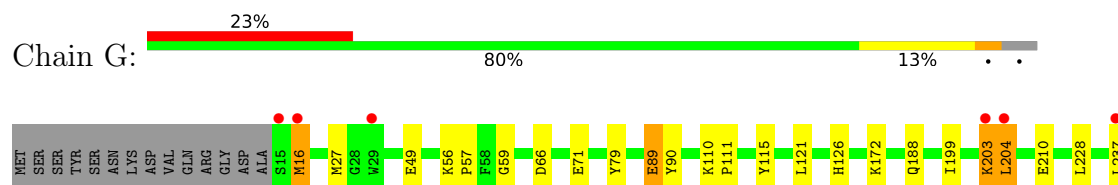
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



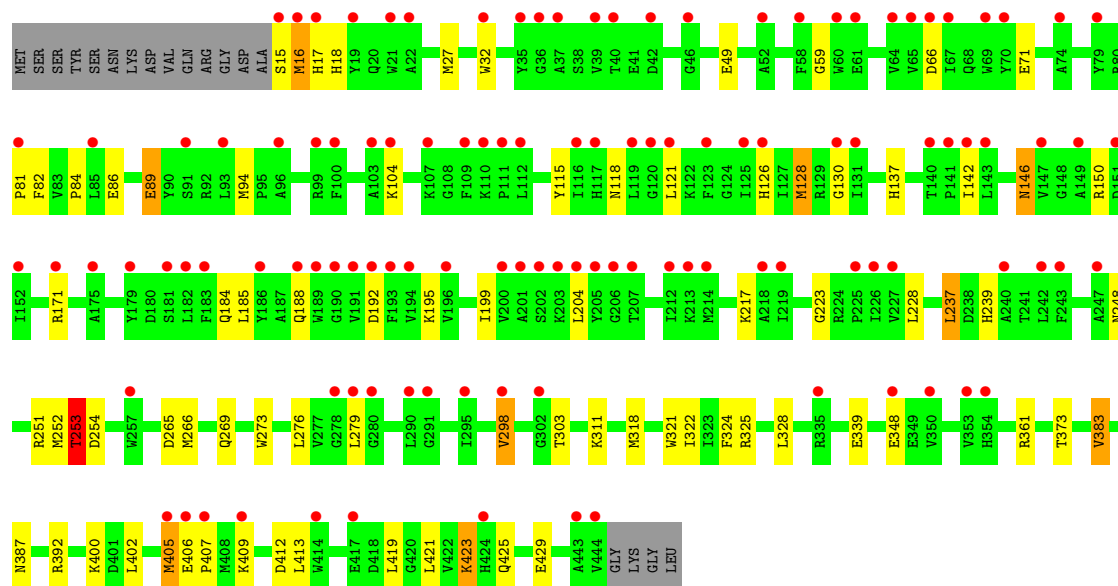
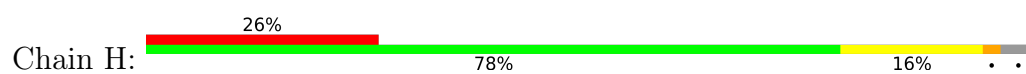
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.70Å 203.53Å 286.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.30 24.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (24.86-2.30) 96.5 (24.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.170 , 0.201 0.176 , 0.204	Depositor DCC
R_{free} test set	13611 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.972	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.37	4/3608 (0.1%)	1.02	5/4898 (0.1%)
1	B	1.33	8/3587 (0.2%)	1.01	5/4869 (0.1%)
1	C	1.27	6/3587 (0.2%)	0.98	4/4869 (0.1%)
1	D	1.25	4/3617 (0.1%)	1.01	8/4906 (0.2%)
1	E	1.13	4/3589 (0.1%)	0.98	6/4873 (0.1%)
1	F	1.15	1/3569 (0.0%)	1.01	8/4845 (0.2%)
1	G	1.15	0/3587	1.02	7/4869 (0.1%)
1	H	1.11	2/3594 (0.1%)	0.99	8/4877 (0.2%)
All	All	1.22	29/28738 (0.1%)	1.00	51/39006 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	HIS	CD2-NE2	-7.73	1.29	1.37
1	B	170	HIS	CG-ND1	-6.93	1.30	1.38
1	D	124	GLY	N-CA	6.54	1.52	1.45
1	C	163	THR	N-CA	6.05	1.53	1.46
1	B	382	PHE	C-O	-5.95	1.16	1.24
1	E	400	LYS	CA-CB	5.81	1.62	1.53
1	F	383	VAL	N-CA	-5.79	1.39	1.46
1	C	315	ARG	C-O	-5.76	1.17	1.24
1	E	80	ARG	C-O	-5.75	1.17	1.24
1	D	289	PRO	CA-C	-5.71	1.47	1.53
1	B	122	LYS	CA-C	-5.65	1.46	1.52
1	C	154	ASP	CG-OD1	5.58	1.35	1.25
1	C	312	ASP	C-O	-5.58	1.17	1.24
1	E	104	LYS	CA-CB	5.55	1.62	1.53
1	A	202	SER	C-O	5.53	1.30	1.23
1	B	46	GLY	C-O	-5.48	1.17	1.23
1	A	23	LYS	N-CA	-5.47	1.39	1.46
1	C	147	VAL	CA-C	-5.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	C-O	-5.31	1.18	1.24
1	H	387	ASN	N-CA	-5.29	1.39	1.46
1	B	56	LYS	N-CA	-5.25	1.41	1.46
1	A	94	MET	CA-C	5.24	1.57	1.52
1	A	243	PHE	N-CA	-5.22	1.40	1.46
1	D	325	ARG	CZ-NH1	5.22	1.40	1.32
1	B	343	SER	N-CA	-5.21	1.39	1.46
1	H	237	LEU	CA-C	-5.15	1.45	1.52
1	E	247	ALA	N-CA	-5.08	1.39	1.45
1	C	304	ASP	C-O	-5.04	1.17	1.23
1	D	325	ARG	CD-NE	-5.02	1.39	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	LEU	N-CA-C	8.36	120.02	111.07
1	E	298	VAL	CB-CA-C	8.26	118.87	110.70
1	C	204	LEU	N-CA-C	8.16	119.95	111.14
1	A	204	LEU	N-CA-C	7.84	119.46	111.07
1	D	204	LEU	N-CA-C	7.77	119.53	111.14
1	E	298	VAL	N-CA-CB	-7.61	101.03	112.67
1	B	348	GLU	CB-CG-CD	7.58	125.49	112.60
1	G	298	VAL	CB-CA-C	7.54	118.17	110.70
1	G	204	LEU	N-CA-C	7.38	118.96	111.07
1	C	253	THR	N-CA-CB	-7.22	99.12	111.69
1	F	298	VAL	CB-CA-C	7.18	117.81	110.70
1	G	253	THR	N-CA-CB	-7.17	99.22	111.69
1	E	204	LEU	N-CA-C	7.01	118.57	111.07
1	D	298	VAL	N-CA-CB	-6.96	102.03	112.67
1	F	204	LEU	N-CA-C	6.89	118.45	111.07
1	F	348	GLU	CB-CG-CD	6.80	124.16	112.60
1	D	298	VAL	CB-CA-C	6.74	117.37	110.70
1	F	53	LYS	CB-CA-C	-6.74	99.47	110.79
1	H	204	LEU	N-CA-C	6.71	118.25	111.07
1	F	298	VAL	N-CA-CB	-6.62	102.54	112.67
1	D	253	THR	N-CA-CB	-6.51	99.42	111.53
1	B	253	THR	N-CA-CB	-6.41	100.55	111.69
1	D	145	THR	CB-CA-C	-6.41	96.55	111.09
1	H	298	VAL	N-CA-C	-6.29	107.16	113.20
1	D	32	TRP	N-CA-C	6.27	117.78	111.07
1	G	298	VAL	N-CA-CB	-6.17	103.23	112.67
1	A	200	VAL	CB-CA-C	-6.15	105.60	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	THR	CB-CA-C	-6.11	97.23	111.09
1	H	298	VAL	CB-CA-C	6.11	116.74	110.70
1	D	363	VAL	N-CA-C	-6.06	104.94	110.82
1	G	383	VAL	CB-CA-C	5.92	118.41	110.42
1	H	253	THR	N-CA-CB	-5.91	100.54	111.53
1	F	16	MET	CA-C-O	5.86	126.92	120.71
1	G	298	VAL	N-CA-C	-5.85	107.59	113.20
1	A	298	VAL	N-CA-CB	-5.78	101.69	111.23
1	C	298	VAL	N-CA-CB	-5.74	101.76	111.23
1	G	394	VAL	N-CA-CB	5.74	116.97	110.72
1	E	253	THR	N-CA-CB	-5.73	100.87	111.53
1	D	405	MET	CG-SD-CE	5.71	113.46	100.90
1	H	383	VAL	CB-CA-C	5.71	117.89	110.12
1	B	145	THR	CB-CA-C	-5.65	98.08	110.67
1	A	86	GLU	CB-CA-C	-5.61	100.91	109.89
1	B	298	VAL	N-CA-CB	-5.55	102.08	111.23
1	H	298	VAL	N-CA-CB	-5.48	104.28	112.67
1	F	49	GLU	CA-CB-CG	-5.41	103.27	114.10
1	C	200	VAL	CB-CA-C	-5.28	106.43	111.44
1	A	383	VAL	CA-CB-CG2	5.20	119.24	110.40
1	E	104	LYS	CB-CG-CD	5.20	123.25	111.30
1	H	86	GLU	CB-CA-C	-5.16	101.64	109.89
1	H	405	MET	CB-CG-SD	5.02	127.77	112.70
1	F	32	TRP	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3376	36	0
1	B	3482	0	3360	31	0
1	C	3479	0	3361	49	0
1	D	3509	0	3408	38	0
1	E	3481	0	3365	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3467	0	3347	19	0
1	G	3479	0	3361	59	0
1	H	3483	0	3373	75	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	1	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	10	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	10	0
4	A	13	0	5	14	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	12	0
5	D	402	0	0	6	0
5	E	377	0	0	6	0
5	F	299	0	0	5	0
5	G	295	0	0	23	0
5	H	191	0	0	25	0
All	All	31524	0	27216	350	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.

All (350) 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:O2	4:D:516:CIT:C6	1.85	1.15
1:H:16:MET:HE3	1:H:16:MET:CA	1.74	1.13
1:G:203:LYS:H	1:G:203:LYS:HD3	1.17	1.08
4:D:516:CIT:O2	4:D:516:CIT:O6	1.78	1.02
1:D:16:MET:HE3	5:D:782:HOH:O	1.61	1.01
1:C:210:GLU:HB2	4:C:515:CIT:H21	1.43	1.00
1:C:405:MET:HA	1:C:405:MET:HE2	1.42	0.99
1:B:89:GLU:HG2	5:B:916:HOH:O	1.66	0.96
1:H:217:LYS:HA	5:H:670:HOH:O	1.68	0.94
1:C:118:ASN:HB3	5:C:1001:HOH:O	1.68	0.93
1:H:16:MET:HA	1:H:16:MET:HE3	0.94	0.93
1:G:188[B]:GLN:HG3	5:G:683:HOH:O	1.68	0.92
1:E:188[A]:GLN:HG2	5:E:787:HOH:O	1.72	0.90
1:H:252[B]:MET:CE	1:H:273:TRP:HB2	2.03	0.89
1:G:203:LYS:H	1:G:203:LYS:CD	1.82	0.89
1:G:203:LYS:HD3	1:G:203:LYS:N	1.90	0.86
1:H:128:MET:HE3	1:H:128:MET:HA	1.59	0.85
1:H:146:ASN:HB3	5:H:720:HOH:O	1.76	0.85
1:G:443:ALA:CB	5:G:754:HOH:O	2.23	0.83
1:A:210:GLU:H	4:A:513:CIT:H42	1.44	0.82
1:F:228:LEU:H	1:F:248:ASN:HD22	1.28	0.81
1:F:306:MET:HE3	5:F:646:HOH:O	1.81	0.80
1:H:252[B]:MET:HE2	1:H:273:TRP:HB2	1.62	0.80
4:B:514:CIT:O4	4:B:514:CIT:C1	2.29	0.80
4:D:516:CIT:O6	4:D:516:CIT:C1	2.30	0.79
1:G:443:ALA:HB2	5:G:754:HOH:O	1.82	0.78
1:A:228:LEU:H	1:A:248:ASN:HD22	1.31	0.78
1:E:208:HIS:HA	4:E:514:CIT:O1	1.84	0.78
1:A:210:GLU:H	4:A:513:CIT:C4	1.97	0.77
1:C:210:GLU:HB2	4:C:515:CIT:C2	2.15	0.77
1:B:443:ALA:O	1:B:444:VAL:HB	1.85	0.77
1:C:405:MET:HA	1:C:405:MET:CE	2.13	0.77
1:B:228:LEU:H	1:B:248:ASN:HD22	1.32	0.76
3:C:511:GOL:H11	5:C:681:HOH:O	1.85	0.76
1:H:228:LEU:H	1:H:248:ASN:HD22	1.34	0.75
4:C:515:CIT:O1	4:C:515:CIT:C6	2.29	0.75
1:A:210:GLU:HB2	4:A:513:CIT:H22	1.69	0.74
1:C:228:LEU:H	1:C:248:ASN:HD22	1.36	0.71
1:E:228:LEU:H	1:E:248:ASN:HD22	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:514:CIT:O4	4:B:514:CIT:C6	2.30	0.71
1:B:253:THR:HG23	1:B:254:ASP:O	1.89	0.71
1:G:210:GLU:HB2	4:G:509:CIT:H22	1.73	0.70
1:C:352:HIS:HB2	5:C:923:HOH:O	1.92	0.70
1:C:253:THR:HG23	1:C:254:ASP:O	1.91	0.70
1:G:228:LEU:H	1:G:248:ASN:HD22	1.40	0.69
1:A:210:GLU:HG2	4:A:513:CIT:H42	1.75	0.69
1:C:423:LYS:HD2	5:C:816:HOH:O	1.91	0.69
1:D:228:LEU:H	1:D:248:ASN:HD22	1.39	0.69
1:G:253:THR:HG23	1:G:254:ASP:O	1.93	0.68
1:H:32:TRP:CD2	3:H:509:GOL:H31	2.28	0.68
1:H:188:GLN:HG3	5:H:672:HOH:O	1.93	0.68
4:E:514:CIT:O1	4:E:514:CIT:O7	2.09	0.68
1:H:32:TRP:CG	3:H:509:GOL:H31	2.29	0.68
1:H:16:MET:CE	1:H:16:MET:CA	2.51	0.67
1:H:195:LYS:HZ3	3:H:509:GOL:H2	1.59	0.67
1:B:176:GLN:HB3	3:B:513:GOL:H31	1.75	0.67
4:B:514:CIT:O4	4:B:514:CIT:C2	2.38	0.67
1:G:349:GLU:HB3	1:G:413:LEU:CD1	2.25	0.67
1:H:82:PHE:HA	5:H:682:HOH:O	1.93	0.67
1:E:253:THR:HG23	1:E:254:ASP:O	1.94	0.66
1:H:142:ILE:HG12	5:H:777:HOH:O	1.93	0.66
1:D:208:HIS:HA	4:D:516:CIT:O2	1.95	0.66
1:A:210:GLU:CG	4:A:513:CIT:H22	2.26	0.66
1:C:177:ALA:H	3:C:514:GOL:H31	1.59	0.66
1:G:398:SER:HA	1:G:425:GLN:HB3	1.77	0.66
1:D:195:LYS:NZ	3:D:512:GOL:H32	2.11	0.65
1:A:210:GLU:HB2	4:A:513:CIT:C2	2.26	0.65
1:F:137:HIS:CE1	1:H:137:HIS:CE1	2.84	0.65
1:H:253:THR:HG23	1:H:254:ASP:O	1.97	0.65
1:G:433:HIS:HB2	5:G:698:HOH:O	1.96	0.65
1:A:417:GLU:HG3	5:A:1115:HOH:O	1.95	0.65
1:D:45:LYS:O	1:D:49:GLU:HG3	1.97	0.65
1:B:221:ARG:HH21	3:B:512:GOL:H2	1.62	0.64
4:E:514:CIT:C2	4:E:514:CIT:O3	2.46	0.64
1:C:118:ASN:HB3	5:C:1012:HOH:O	1.97	0.64
1:D:17:HIS:NE2	2:D:501:SO4:O3	2.30	0.64
1:C:423:LYS:HD2	1:C:423:LYS:H	1.63	0.64
1:H:192:ASP:OD1	5:H:617:HOH:O	2.15	0.64
4:A:513:CIT:H21	5:A:1173:HOH:O	1.99	0.63
1:H:252[B]:MET:HE2	1:H:273:TRP:CD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:LYS:HZ3	3:D:512:GOL:H32	1.62	0.63
1:H:252[B]:MET:CE	1:H:273:TRP:CB	2.74	0.63
1:H:195:LYS:NZ	3:H:509:GOL:H2	2.13	0.63
1:D:253:THR:HG23	1:D:254:ASP:O	1.98	0.62
1:G:421:LEU:HD21	5:G:754:HOH:O	1.99	0.62
1:C:16:MET:HE2	5:C:922:HOH:O	1.99	0.62
1:H:16:MET:HE3	1:H:16:MET:C	2.24	0.62
1:H:252[B]:MET:HE2	1:H:273:TRP:CB	2.30	0.62
1:A:210:GLU:CB	4:A:513:CIT:H22	2.29	0.61
1:C:176:GLN:HB3	3:C:514:GOL:H2	1.82	0.61
1:G:347:ASN:HD22	1:G:347:ASN:C	2.08	0.61
1:H:130:GLY:C	5:H:621:HOH:O	2.44	0.60
1:C:208:HIS:HA	4:C:515:CIT:O1	2.01	0.60
1:C:208:HIS:CA	4:C:515:CIT:O1	2.50	0.60
1:A:444:VAL:HG13	5:A:1092:HOH:O	2.02	0.60
1:G:407:PRO:HB2	5:G:754:HOH:O	2.02	0.60
1:D:207:THR:N	2:D:504:SO4:O1	2.36	0.59
1:H:251:ARG:HH12	3:H:509:GOL:H11	1.66	0.59
1:H:248:ASN:ND2	5:H:748:HOH:O	2.34	0.59
1:G:391:LYS:HD2	5:G:765:HOH:O	2.02	0.59
1:C:188[B]:GLN:HG2	5:C:946:HOH:O	2.01	0.59
1:C:253:THR:CG2	1:C:254:ASP:O	2.51	0.58
1:C:423:LYS:H	1:C:423:LYS:CD	2.15	0.58
3:E:510:GOL:C3	3:E:510:GOL:HO3	2.08	0.58
1:B:406:GLU:HB2	1:B:407:PRO:HD2	1.85	0.58
1:A:265:ASP:HB3	5:A:822:HOH:O	2.03	0.58
1:B:208:HIS:ND1	4:B:514:CIT:H41	2.18	0.58
1:E:210:GLU:HB2	4:E:514:CIT:H21	1.84	0.58
1:D:259:ARG:NH2	1:D:261:GLU:OE1	2.37	0.57
1:G:349:GLU:HB3	1:G:413:LEU:HD12	1.86	0.57
1:H:81:PRO:O	5:H:743:HOH:O	2.17	0.57
1:A:188[B]:GLN:HG2	5:A:857:HOH:O	2.03	0.57
1:B:146:ASN:HB3	5:B:924:HOH:O	2.03	0.57
1:G:79:TYR:O	5:G:764:HOH:O	2.17	0.57
1:E:253:THR:CG2	1:E:254:ASP:O	2.52	0.57
1:G:59:GLY:C	5:G:814:HOH:O	2.46	0.57
1:H:130:GLY:O	5:H:621:HOH:O	2.18	0.57
1:B:188[B]:GLN:HG3	5:B:961:HOH:O	2.03	0.57
1:D:211:GLU:N	4:D:516:CIT:O1	2.32	0.57
1:B:253:THR:CG2	1:B:254:ASP:O	2.53	0.57
1:A:306:MET:HE2	5:A:788:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LYS:HD2	5:E:890:HOH:O	2.05	0.56
1:G:254:ASP:OD1	3:G:508:GOL:C1	2.53	0.56
1:H:253:THR:CG2	1:H:254:ASP:O	2.54	0.56
1:G:387:ASN:ND2	1:G:431:GLY:O	2.37	0.56
1:A:16:MET:HE1	5:A:1055:HOH:O	2.05	0.55
1:A:210:GLU:HG3	4:A:513:CIT:H22	1.89	0.55
1:C:405:MET:CE	1:C:405:MET:CA	2.84	0.55
4:E:514:CIT:O3	4:E:514:CIT:H21	2.06	0.55
1:C:208:HIS:C	4:C:515:CIT:O1	2.49	0.55
1:F:49:GLU:OE2	1:F:115:TYR:OH	2.22	0.55
1:A:49[A]:GLU:OE2	1:A:115:TYR:OH	2.24	0.55
1:H:425[B]:GLN:NE2	5:H:622:HOH:O	2.38	0.55
1:H:84:PRO:HG2	2:H:502:SO4:O3	2.07	0.55
1:E:42:ASP:OD1	5:E:963:HOH:O	2.18	0.54
1:H:146:ASN:OD1	1:H:146:ASN:N	2.32	0.54
1:G:49[A]:GLU:OE2	1:G:115:TYR:OH	2.25	0.54
1:H:59:GLY:O	5:H:765:HOH:O	2.19	0.54
1:G:338:ASP:C	5:G:699:HOH:O	2.50	0.54
1:G:399:LEU:HD23	5:G:692:HOH:O	2.07	0.54
1:H:49:GLU:OE2	1:H:115:TYR:OH	2.25	0.54
1:H:266[B]:MET:HE3	1:H:269:GLN:HB2	1.89	0.54
1:G:253:THR:CG2	1:G:254:ASP:O	2.54	0.54
1:G:210:GLU:HG2	4:G:509:CIT:H42	1.90	0.54
1:C:49:GLU:OE2	1:C:115:TYR:OH	2.25	0.54
1:C:255:ASP:OD1	3:C:510:GOL:H12	2.07	0.54
1:G:210:GLU:H	4:G:509:CIT:H42	1.73	0.54
1:D:208:HIS:CA	4:D:516:CIT:O2	2.55	0.54
1:G:254:ASP:OD1	3:G:508:GOL:H11	2.07	0.54
1:F:366:GLU:HG3	5:F:802:HOH:O	2.06	0.53
1:G:362:GLN:NE2	5:G:861:HOH:O	2.27	0.53
1:H:84:PRO:CG	2:H:502:SO4:O3	2.57	0.53
1:H:223:GLY:N	5:H:759:HOH:O	2.41	0.53
1:G:349:GLU:HB3	1:G:413:LEU:HD11	1.90	0.53
1:D:253:THR:CG2	1:D:254:ASP:O	2.56	0.53
1:G:443:ALA:HB3	5:G:754:HOH:O	1.98	0.53
1:E:122:LYS:NZ	5:E:932:HOH:O	2.39	0.53
1:B:146:ASN:OD1	1:B:146:ASN:N	2.34	0.52
1:C:251:ARG:HH12	3:C:510:GOL:H11	1.73	0.52
1:H:324:PHE:O	5:H:776:HOH:O	2.19	0.52
1:A:210:GLU:CG	4:A:513:CIT:H42	2.38	0.52
1:D:311:LYS:N	2:D:510:SO4:O4	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252[B]:MET:HE2	1:H:273:TRP:CG	2.44	0.52
1:A:406:GLU:HB2	1:A:407:PRO:HD2	1.91	0.52
1:G:426:LEU:HD21	1:G:438:VAL:HG21	1.91	0.52
4:B:514:CIT:O4	4:B:514:CIT:O1	2.28	0.51
1:A:188[A]:GLN:OE1	5:A:774:HOH:O	2.19	0.51
1:B:443:ALA:O	1:B:444:VAL:CB	2.58	0.51
1:A:306:MET:CE	5:A:788:HOH:O	2.59	0.51
1:H:223:GLY:HA2	5:H:759:HOH:O	2.11	0.51
1:H:142:ILE:CG1	5:H:777:HOH:O	2.55	0.51
1:B:232:PRO:HD2	5:B:1073:HOH:O	2.11	0.51
1:H:94:MET:CE	1:H:185:LEU:HD21	2.41	0.51
1:D:145:THR:CG2	5:D:999:HOH:O	2.59	0.51
1:F:260:TRP:CD2	1:F:433:HIS:CD2	3.00	0.50
1:D:208:HIS:C	4:D:516:CIT:O2	2.54	0.50
1:F:442:PRO:HB2	1:F:444:VAL:HG12	1.94	0.50
2:C:505:SO4:O3	5:C:705:HOH:O	2.18	0.50
1:D:210:GLU:HB2	4:D:516:CIT:H41	1.93	0.50
1:H:184:GLN:HA	5:H:779:HOH:O	2.11	0.50
1:C:210:GLU:CB	4:C:515:CIT:H21	2.27	0.50
1:H:311:LYS:N	2:H:506:SO4:O3	2.30	0.50
4:C:515:CIT:H22	5:C:630:HOH:O	2.11	0.49
1:C:188[B]:GLN:OE1	5:C:811:HOH:O	2.19	0.49
1:D:14:ALA:HA	1:D:19:TYR:CD2	2.47	0.49
1:D:255:ASP:OD2	3:D:513:GOL:H31	2.11	0.49
1:A:210:GLU:N	4:A:513:CIT:H42	2.21	0.49
4:B:514:CIT:O2	4:B:514:CIT:O5	2.31	0.49
1:D:14:ALA:HA	1:D:19:TYR:HD2	1.77	0.49
1:A:209:THR:N	4:A:513:CIT:H41	2.28	0.49
1:A:387:ASN:HD22	1:A:389:SER:H	1.61	0.48
1:F:406:GLU:HB2	1:F:407:PRO:HD2	1.95	0.48
1:G:325:ARG:HD3	5:G:731:HOH:O	2.13	0.48
1:G:361:ARG:NH1	1:G:373:THR:CG2	2.77	0.48
1:G:392:ARG:HB2	1:G:392:ARG:HH21	1.78	0.48
1:H:251:ARG:HH12	3:H:509:GOL:C1	2.26	0.48
1:C:254:ASP:OD1	3:C:511:GOL:H31	2.13	0.48
4:E:514:CIT:O1	4:E:514:CIT:O6	2.30	0.48
1:G:255:ASP:OD1	3:G:507:GOL:H32	2.14	0.48
1:F:387:ASN:C	1:F:387:ASN:HD22	2.21	0.47
1:G:16:MET:N	1:G:16:MET:HE2	2.29	0.47
1:D:448:LEU:C	5:D:780:HOH:O	2.56	0.47
1:H:32:TRP:CD1	3:H:509:GOL:H31	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HB2	1:C:407:PRO:HD2	1.95	0.47
1:H:32:TRP:CE2	3:H:509:GOL:C3	2.98	0.47
1:G:416:LYS:HB2	1:G:416:LYS:HE2	1.41	0.47
1:H:406:GLU:HB2	1:H:407:PRO:HD2	1.96	0.47
1:G:339:GLU:N	5:G:699:HOH:O	2.48	0.47
1:A:210:GLU:H	4:A:513:CIT:H41	1.75	0.47
1:H:171:ARG:HB2	1:H:171:ARG:NH1	2.30	0.47
1:C:338:ASP:HA	1:H:392:ARG:HE	1.80	0.47
1:H:361:ARG:NH1	1:H:373:THR:CG2	2.78	0.47
1:D:254:ASP:OD1	3:D:513:GOL:C1	2.63	0.46
1:G:203:LYS:CD	1:G:203:LYS:N	2.55	0.46
1:B:253:THR:HG21	1:B:266:MET:HE1	1.97	0.46
1:C:173:GLU:HG3	5:C:667:HOH:O	2.15	0.46
1:D:253:THR:HG21	1:D:266:MET:HE1	1.97	0.46
1:C:41:GLU:CD	5:C:933:HOH:O	2.57	0.46
1:H:266[B]:MET:HG2	1:H:321:TRP:CH2	2.50	0.46
1:H:89:GLU:HB2	5:H:629:HOH:O	2.14	0.46
1:E:145:THR:HB	1:E:147:VAL:H	1.81	0.46
1:E:254:ASP:OD1	3:E:511:GOL:O2	2.34	0.46
1:F:255:ASP:OD2	3:F:509:GOL:H12	2.16	0.45
1:G:172:LYS:NZ	5:G:859:HOH:O	2.49	0.45
1:G:253:THR:HG21	1:G:266:MET:HE1	1.98	0.45
1:H:239:HIS:HA	5:H:605:HOH:O	2.16	0.45
1:B:145:THR:HB	1:B:147:VAL:H	1.81	0.45
1:E:231[A]:SER:OG	1:E:251:ARG:NH1	2.50	0.45
1:A:217:LYS:HE3	3:A:512:GOL:C3	2.47	0.45
1:B:204:LEU:HD11	1:D:156:ASN:HD21	1.81	0.45
1:B:387:ASN:HD22	1:B:389:SER:H	1.63	0.45
1:E:253:THR:HG21	1:E:266:MET:HE1	1.98	0.45
1:A:387:ASN:HD22	1:A:387:ASN:C	2.23	0.45
1:H:406:GLU:OE1	1:H:406:GLU:N	2.50	0.45
1:A:49[B]:GLU:OE2	1:A:115:TYR:OH	2.28	0.45
1:D:387:ASN:C	1:D:387:ASN:HD22	2.24	0.45
1:H:223:GLY:CA	5:H:759:HOH:O	2.64	0.45
1:H:265:ASP:HB3	5:H:769:HOH:O	2.17	0.45
1:B:439:LYS:NZ	5:B:895:HOH:O	2.40	0.45
1:G:393:SER:HB3	5:G:732:HOH:O	2.16	0.45
1:H:146:ASN:CB	5:H:720:HOH:O	2.51	0.44
1:E:16:MET:HA	5:E:696:HOH:O	2.16	0.44
1:H:253:THR:HG21	1:H:266[A]:MET:HE1	1.99	0.44
1:H:412:ASP:C	1:H:412:ASP:OD1	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:OE2	1:B:115:TYR:OH	2.32	0.44
1:D:103:ALA:O	5:D:833:HOH:O	2.21	0.44
1:H:392:ARG:NH1	1:H:429:GLU:HB3	2.31	0.44
1:A:418[A]:ASP:OD1	5:A:1147:HOH:O	2.21	0.44
3:A:512:GOL:H32	5:A:1157:HOH:O	2.17	0.44
1:A:210:GLU:CB	4:A:513:CIT:H42	2.48	0.44
1:F:80:ARG:HA	1:F:81:PRO:HD3	1.85	0.44
1:H:16:MET:HE3	1:H:17:HIS:N	2.33	0.44
1:D:145:THR:HB	1:D:147:VAL:H	1.83	0.43
1:E:156:ASN:HD21	1:G:204:LEU:HD11	1.83	0.43
1:E:255:ASP:OD1	3:E:511:GOL:H11	2.18	0.43
1:E:49:GLU:OE2	1:E:115:TYR:OH	2.29	0.43
1:H:318:MET:O	1:H:322:ILE:HG12	2.19	0.43
1:C:406:GLU:OE1	1:C:406:GLU:N	2.50	0.43
3:F:509:GOL:H11	5:F:770:HOH:O	2.18	0.43
1:C:405:MET:HE2	1:C:405:MET:CA	2.24	0.43
1:D:211:GLU:HB2	4:D:516:CIT:O1	2.17	0.43
1:E:56:LYS:N	1:E:57:PRO:CD	2.81	0.43
1:F:185:LEU:O	1:F:188:GLN:HG2	2.18	0.43
1:A:72:PRO:HG2	5:A:882:HOH:O	2.18	0.43
1:B:176:GLN:CB	3:B:513:GOL:H31	2.46	0.43
1:G:425:GLN:HA	5:G:692:HOH:O	2.18	0.43
1:F:217:LYS:CE	3:F:510:GOL:O2	2.67	0.43
1:H:252[B]:MET:HE1	1:H:324:PHE:CZ	2.53	0.43
1:A:406:GLU:N	1:A:406:GLU:OE1	2.52	0.42
1:B:387:ASN:HD22	1:B:387:ASN:C	2.26	0.42
1:B:387:ASN:ND2	1:B:389:SER:H	2.17	0.42
1:H:16:MET:HB3	1:H:18:HIS:CD2	2.54	0.42
1:B:433:HIS:N	1:B:433:HIS:CD2	2.87	0.42
1:D:254:ASP:OD1	3:D:513:GOL:H11	2.18	0.42
1:F:81:PRO:HD2	5:F:803:HOH:O	2.18	0.42
1:H:66:ASP:HA	1:H:126:HIS:HB2	2.01	0.42
1:C:255:ASP:CG	3:C:510:GOL:H12	2.45	0.42
1:D:279:LEU:C	1:D:279:LEU:HD23	2.43	0.42
1:E:303:THR:HB	5:E:811:HOH:O	2.20	0.42
1:H:104:LYS:O	1:H:104:LYS:HG3	2.19	0.42
1:A:279:LEU:HD23	1:A:279:LEU:C	2.44	0.42
1:A:339:GLU:HG3	5:A:922:HOH:O	2.19	0.42
1:E:231[A]:SER:OG	1:E:232:PRO:HA	2.19	0.42
1:A:387:ASN:ND2	1:A:389:SER:H	2.18	0.42
1:B:424:HIS:HB2	5:B:831:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:MET:O	1:C:322:ILE:HG12	2.20	0.42
1:F:15:SER:OG	1:F:16:MET:HE2	2.19	0.42
1:H:32:TRP:CE2	3:H:509:GOL:H31	2.53	0.42
1:C:41:GLU:HB2	1:C:100:PHE:HA	2.01	0.42
1:D:188:GLN:HB3	5:D:854:HOH:O	2.20	0.42
1:E:387:ASN:HD22	1:E:389:SER:H	1.67	0.42
1:F:313:GLU:OE2	1:F:433:HIS:HD2	2.02	0.42
1:G:436:ILE:HA	5:G:680:HOH:O	2.18	0.42
1:A:27:MET:HA	1:A:328:LEU:O	2.19	0.42
1:E:387:ASN:ND2	1:E:389:SER:H	2.17	0.42
1:B:201:ALA:N	5:B:1073:HOH:O	2.31	0.42
1:C:255:ASP:OD1	3:C:510:GOL:C1	2.67	0.42
1:D:56:LYS:N	1:D:57:PRO:CD	2.82	0.42
1:G:89:GLU:HG2	1:G:90:TYR:CD2	2.55	0.42
1:H:150:ARG:HD2	5:H:638:HOH:O	2.20	0.42
1:A:217:LYS:HE3	3:A:512:GOL:O3	2.20	0.41
1:C:387:ASN:C	1:C:387:ASN:HD22	2.27	0.41
1:B:27:MET:HA	1:B:328:LEU:O	2.20	0.41
1:B:406:GLU:HB2	1:B:407:PRO:CD	2.50	0.41
1:F:387:ASN:ND2	1:F:389:SER:H	2.19	0.41
1:B:156:ASN:HD21	1:D:204:LEU:HD11	1.85	0.41
1:C:56:LYS:N	1:C:57:PRO:CD	2.83	0.41
1:H:27:MET:HA	1:H:328:LEU:O	2.20	0.41
1:F:27:MET:HA	1:F:328:LEU:O	2.20	0.41
1:G:66:ASP:HA	1:G:126:HIS:HB2	2.03	0.41
1:C:27:MET:HA	1:C:328:LEU:O	2.20	0.41
1:D:387:ASN:HD22	1:D:389:SER:H	1.69	0.41
4:E:514:CIT:O1	4:E:514:CIT:C6	2.65	0.41
1:G:110:LYS:HB3	1:G:111:PRO:HD3	2.01	0.41
1:G:318:MET:CE	1:G:345:LEU:HD23	2.50	0.41
1:B:306:MET:HE1	5:B:764:HOH:O	2.20	0.41
1:C:110:LYS:HB3	1:C:111:PRO:HD3	2.02	0.41
1:D:255:ASP:CG	3:D:513:GOL:H31	2.45	0.41
1:G:279:LEU:C	1:G:279:LEU:HD23	2.45	0.41
1:C:387:ASN:ND2	1:C:389:SER:H	2.18	0.41
1:G:347:ASN:HD22	1:G:349:GLU:H	1.69	0.41
1:C:174:GLY:H	3:C:514:GOL:H32	1.85	0.41
1:C:253:THR:HG21	1:C:266:MET:HE1	2.03	0.41
1:C:423:LYS:CD	1:C:423:LYS:N	2.84	0.41
1:D:41:GLU:HB2	1:D:100:PHE:HA	2.03	0.41
1:D:387:ASN:ND2	1:D:389:SER:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:LYS:HE2	3:E:512:GOL:H2	2.02	0.41
1:G:56:LYS:N	1:G:57:PRO:CD	2.83	0.41
1:G:253:THR:HB	5:G:603:HOH:O	2.20	0.41
1:G:423:LYS:N	5:G:852:HOH:O	2.52	0.41
1:H:251:ARG:NH1	3:H:509:GOL:H11	2.34	0.41
1:H:423:LYS:HG2	5:H:643:HOH:O	2.20	0.41
5:A:997:HOH:O	1:C:203:LYS:HG2	2.21	0.41
1:B:56:LYS:N	1:B:57:PRO:CD	2.84	0.40
1:E:110:LYS:HB3	1:E:111:PRO:HD3	2.03	0.40
1:G:16:MET:HE3	1:G:16:MET:HB2	1.86	0.40
1:H:279:LEU:HD23	1:H:279:LEU:C	2.46	0.40
1:C:198:ASP:O	1:C:198:ASP:CG	2.64	0.40
1:D:406:GLU:HG3	5:D:634:HOH:O	2.21	0.40
1:F:417:GLU:HG3	5:F:846:HOH:O	2.21	0.40
1:G:27:MET:HA	1:G:328:LEU:O	2.21	0.40
1:H:130:GLY:CA	5:H:621:HOH:O	2.69	0.40
1:C:177:ALA:H	3:C:514:GOL:C3	2.28	0.40
1:E:387:ASN:HD22	1:E:387:ASN:C	2.29	0.40
1:C:387:ASN:HD22	1:C:389:SER:H	1.68	0.40
1:E:53:LYS:NZ	2:E:507:SO4:O3	2.45	0.40
1:G:16:MET:HB3	5:G:811:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	55
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%)	360 (97%)	12 (3%)	34	51
1	B	370/382 (97%)	350 (95%)	20 (5%)	20	29
1	C	370/382 (97%)	351 (95%)	19 (5%)	21	32
1	D	372/382 (97%)	353 (95%)	19 (5%)	21	32
1	E	370/382 (97%)	350 (95%)	20 (5%)	20	29
1	F	368/382 (96%)	349 (95%)	19 (5%)	21	31
1	G	370/382 (97%)	343 (93%)	27 (7%)	13	18
1	H	371/382 (97%)	346 (93%)	25 (7%)	15	21
All	All	2963/3056 (97%)	2802 (95%)	161 (5%)	19	29

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	16	MET
1	A	71	GLU

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Mol	Chain	Res	Type
1	A	147	VAL
1	A	199	ILE
1	A	237	LEU
1	A	276	LEU
1	A	298	VAL
1	A	381	GLN
1	A	383	VAL
1	A	387	ASN
1	A	419	LEU
1	B	15	SER
1	B	16	MET
1	B	45	LYS
1	B	71	GLU
1	B	89	GLU
1	B	104	LYS
1	B	121	LEU
1	B	145	THR
1	B	146	ASN
1	B	199	ILE
1	B	237	LEU
1	B	253	THR
1	B	276	LEU
1	B	298	VAL
1	B	402	LEU
1	B	406	GLU
1	B	409	LYS
1	B	413	LEU
1	B	419	LEU
1	B	421	LEU
1	C	15	SER
1	C	71	GLU
1	C	147	VAL
1	C	199	ILE
1	C	237	LEU
1	C	253	THR
1	C	276	LEU
1	C	298	VAL
1	C	316	THR
1	C	383	VAL
1	C	387	ASN
1	C	391	LYS
1	C	402	LEU

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Mol	Chain	Res	Type
1	C	405	MET
1	C	409	LYS
1	C	413	LEU
1	C	419	LEU
1	C	421	LEU
1	C	423	LYS
1	D	15	SER
1	D	16	MET
1	D	71	GLU
1	D	121	LEU
1	D	145	THR
1	D	147	VAL
1	D	199	ILE
1	D	237	LEU
1	D	253	THR
1	D	276	LEU
1	D	298	VAL
1	D	339	GLU
1	D	383	VAL
1	D	387	ASN
1	D	405	MET
1	D	406	GLU
1	D	413	LEU
1	D	419	LEU
1	D	421	LEU
1	E	15	SER
1	E	16	MET
1	E	71	GLU
1	E	121	LEU
1	E	145	THR
1	E	199	ILE
1	E	237	LEU
1	E	253	THR
1	E	276	LEU
1	E	298	VAL
1	E	366	GLU
1	E	383	VAL
1	E	387	ASN
1	E	391	LYS
1	E	400	LYS
1	E	402	LEU
1	E	406	GLU

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Mol	Chain	Res	Type
1	E	413	LEU
1	E	419	LEU
1	E	422	VAL
1	F	15	SER
1	F	16	MET
1	F	71	GLU
1	F	104	LYS
1	F	121	LEU
1	F	199	ILE
1	F	237	LEU
1	F	276	LEU
1	F	298	VAL
1	F	383	VAL
1	F	392	ARG
1	F	402	LEU
1	F	405	MET
1	F	413	LEU
1	F	419	LEU
1	F	421	LEU
1	F	422	VAL
1	F	430	LEU
1	F	444	VAL
1	G	16	MET
1	G	71	GLU
1	G	89	GLU
1	G	121	LEU
1	G	199	ILE
1	G	203	LYS
1	G	237	LEU
1	G	253	THR
1	G	276	LEU
1	G	298	VAL
1	G	339	GLU
1	G	347	ASN
1	G	363	VAL
1	G	365	ARG
1	G	366	GLU
1	G	381	GLN
1	G	383	VAL
1	G	394	VAL
1	G	400	LYS
1	G	402	LEU

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Mol	Chain	Res	Type
1	G	413	LEU
1	G	418	ASP
1	G	419	LEU
1	G	421	LEU
1	G	425	GLN
1	G	426	LEU
1	G	438	VAL
1	H	15	SER
1	H	16	MET
1	H	71	GLU
1	H	89	GLU
1	H	118	ASN
1	H	121	LEU
1	H	128	MET
1	H	146	ASN
1	H	199	ILE
1	H	237	LEU
1	H	253	THR
1	H	276	LEU
1	H	298	VAL
1	H	303	THR
1	H	339	GLU
1	H	348	GLU
1	H	383	VAL
1	H	400	LYS
1	H	402	LEU
1	H	405	MET
1	H	409	LYS
1	H	413	LEU
1	H	419	LEU
1	H	421	LEU
1	H	423	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	156	ASN
1	A	208	HIS
1	A	246	ASN
1	A	248	ASN
1	A	355	GLN

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Mol	Chain	Res	Type
1	A	356	ASN
1	A	387	ASN
1	B	17	HIS
1	B	20	GLN
1	B	156	ASN
1	B	246	ASN
1	B	248	ASN
1	B	381	GLN
1	B	387	ASN
1	C	18	HIS
1	C	20	GLN
1	C	68	GLN
1	C	138	GLN
1	C	156	ASN
1	C	246	ASN
1	C	248	ASN
1	C	355	GLN
1	C	387	ASN
1	C	424	HIS
1	D	18	HIS
1	D	20	GLN
1	D	156	ASN
1	D	246	ASN
1	D	248	ASN
1	D	387	ASN
1	D	424	HIS
1	E	18	HIS
1	E	20	GLN
1	E	138	GLN
1	E	146	ASN
1	E	156	ASN
1	E	208	HIS
1	E	246	ASN
1	E	248	ASN
1	E	369	HIS
1	E	387	ASN
1	F	18	HIS
1	F	20	GLN
1	F	75	ASN
1	F	137	HIS
1	F	246	ASN
1	F	248	ASN

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Mol	Chain	Res	Type
1	F	369	HIS
1	F	387	ASN
1	F	433	HIS
1	G	156	ASN
1	G	208	HIS
1	G	248	ASN
1	G	347	ASN
1	G	362	GLN
1	G	369	HIS
1	G	381	GLN
1	H	18	HIS
1	H	68	GLN
1	H	137	HIS
1	H	170	HIS
1	H	239	HIS
1	H	246	ASN
1	H	248	ASN
1	H	355	GLN
1	H	424	HIS

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 oligosaccharides 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	C	501	-	4,4,4	0.76	0	6,6,6	0.50	0
2	SO4	F	507	-	4,4,4	0.64	0	6,6,6	0.45	0
2	SO4	G	503	-	4,4,4	0.78	0	6,6,6	0.85	0
2	SO4	C	506	-	4,4,4	0.85	0	6,6,6	0.42	0
4	CIT	G	509	-	12,12,12	2.42	4 (33%)	17,17,17	2.96	7 (41%)
2	SO4	E	506	-	4,4,4	0.79	0	6,6,6	0.41	0
2	SO4	D	504	-	4,4,4	0.43	0	6,6,6	0.58	0
4	CIT	D	516	-	12,12,12	2.18	4 (33%)	17,17,17	2.05	6 (35%)
3	GOL	B	512	-	5,5,5	0.27	0	5,5,5	1.39	1 (20%)
2	SO4	C	504	-	4,4,4	0.60	0	6,6,6	0.95	0
3	GOL	F	511	-	5,5,5	0.69	0	5,5,5	0.50	0
2	SO4	B	506	-	4,4,4	1.15	0	6,6,6	0.80	0
2	SO4	A	505	-	4,4,4	0.54	0	6,6,6	0.56	0
2	SO4	D	509	-	4,4,4	0.66	0	6,6,6	0.36	0
2	SO4	A	506	-	4,4,4	0.67	0	6,6,6	0.92	0
2	SO4	H	501	-	4,4,4	0.85	0	6,6,6	0.66	0
2	SO4	B	508	-	4,4,4	0.69	0	6,6,6	0.66	0
2	SO4	H	507	-	4,4,4	0.63	0	6,6,6	0.66	0
2	SO4	F	506	-	4,4,4	0.67	0	6,6,6	0.63	0
2	SO4	C	509	-	4,4,4	1.00	0	6,6,6	0.59	0
3	GOL	H	510	-	5,5,5	0.27	0	5,5,5	0.38	0
2	SO4	A	502	-	4,4,4	0.57	0	6,6,6	0.65	0
2	SO4	A	509	-	4,4,4	0.53	0	6,6,6	0.56	0
2	SO4	C	503	-	4,4,4	0.78	0	6,6,6	0.97	0
3	GOL	F	508	-	5,5,5	0.33	0	5,5,5	1.45	1 (20%)
2	SO4	D	506	-	4,4,4	0.68	0	6,6,6	0.50	0
2	SO4	A	508	-	4,4,4	0.83	0	6,6,6	1.08	0
2	SO4	F	503	-	4,4,4	0.54	0	6,6,6	0.73	0
3	GOL	C	513	-	5,5,5	1.26	1 (20%)	5,5,5	2.05	2 (40%)
2	SO4	E	504	-	4,4,4	0.74	0	6,6,6	0.75	0
2	SO4	F	504	-	4,4,4	0.66	0	6,6,6	0.28	0
3	GOL	A	511	-	5,5,5	0.40	0	5,5,5	0.53	0
4	CIT	B	514	-	12,12,12	1.90	4 (33%)	17,17,17	2.46	7 (41%)
2	SO4	E	502	-	4,4,4	0.49	0	6,6,6	0.31	0
3	GOL	G	507	-	5,5,5	1.11	0	5,5,5	1.05	0
2	SO4	G	504	-	4,4,4	0.58	0	6,6,6	0.52	0
2	SO4	G	506	-	4,4,4	0.64	0	6,6,6	0.44	0
2	SO4	B	504	-	4,4,4	0.54	0	6,6,6	0.59	0
3	GOL	B	509	-	5,5,5	0.83	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	513	-	5,5,5	0.74	0	5,5,5	1.50	1 (20%)
2	SO4	D	501	-	4,4,4	0.62	0	6,6,6	0.48	0
2	SO4	H	505	-	4,4,4	0.57	0	6,6,6	0.45	0
3	GOL	G	508	-	5,5,5	0.68	0	5,5,5	1.29	1 (20%)
2	SO4	E	507	-	4,4,4	0.61	0	6,6,6	0.91	0
2	SO4	C	505	-	4,4,4	0.80	0	6,6,6	0.61	0
3	GOL	E	512	-	5,5,5	0.65	0	5,5,5	0.91	0
2	SO4	E	505	-	4,4,4	0.65	0	6,6,6	0.33	0
3	GOL	C	514	-	5,5,5	1.19	1 (20%)	5,5,5	0.97	0
2	SO4	A	501	-	4,4,4	0.81	0	6,6,6	0.51	0
3	GOL	E	510	-	5,5,5	2.83	2 (40%)	5,5,5	3.07	3 (60%)
2	SO4	B	507	-	4,4,4	0.70	0	6,6,6	0.50	0
2	SO4	B	502	-	4,4,4	0.71	0	6,6,6	0.80	0
2	SO4	H	502	-	4,4,4	0.69	0	6,6,6	0.45	0
3	GOL	C	512	-	5,5,5	0.33	0	5,5,5	2.06	1 (20%)
3	GOL	A	512	-	5,5,5	0.63	0	5,5,5	0.57	0
3	GOL	H	509	-	5,5,5	0.62	0	5,5,5	0.95	0
2	SO4	D	508	-	4,4,4	0.84	0	6,6,6	0.58	0
2	SO4	C	508	-	4,4,4	0.54	0	6,6,6	0.45	0
2	SO4	H	504	-	4,4,4	0.86	0	6,6,6	0.33	0
2	SO4	D	511	-	4,4,4	0.64	0	6,6,6	0.21	0
3	GOL	A	510	-	5,5,5	0.76	0	5,5,5	1.05	0
2	SO4	A	504	-	4,4,4	0.98	0	6,6,6	1.51	1 (16%)
3	GOL	D	515	-	5,5,5	0.55	0	5,5,5	0.99	0
2	SO4	B	505	-	4,4,4	0.85	0	6,6,6	1.17	0
2	SO4	B	503	-	4,4,4	0.66	0	6,6,6	0.34	0
2	SO4	A	507	-	4,4,4	1.04	0	6,6,6	1.10	0
2	SO4	G	501	-	4,4,4	0.51	0	6,6,6	0.86	0
4	CIT	E	514	-	12,12,12	1.33	1 (8%)	17,17,17	2.01	6 (35%)
2	SO4	B	501	-	4,4,4	1.00	0	6,6,6	1.03	0
2	SO4	E	509	-	4,4,4	0.71	0	6,6,6	0.94	0
3	GOL	C	511	-	5,5,5	0.61	0	5,5,5	1.33	0
3	GOL	B	510	-	5,5,5	0.75	0	5,5,5	0.68	0
3	GOL	E	511	-	5,5,5	0.40	0	5,5,5	0.52	0
2	SO4	H	503	-	4,4,4	0.56	0	6,6,6	0.38	0
4	CIT	C	515	-	12,12,12	2.60	6 (50%)	17,17,17	2.54	5 (29%)
2	SO4	C	502	-	4,4,4	0.86	0	6,6,6	0.68	0
3	GOL	D	512	-	5,5,5	1.05	1 (20%)	5,5,5	1.19	0
2	SO4	F	502	-	4,4,4	0.72	0	6,6,6	0.22	0
2	SO4	D	507	-	4,4,4	0.68	0	6,6,6	1.38	2 (33%)
2	SO4	H	506	-	4,4,4	0.68	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	A	513	-	12,12,12	3.40	4 (33%)	17,17,17	1.57	2 (11%)
3	GOL	B	511	-	5,5,5	0.49	0	5,5,5	1.75	1 (20%)
2	SO4	A	503	-	4,4,4	0.59	0	6,6,6	0.56	0
2	SO4	C	507	-	4,4,4	0.83	0	6,6,6	1.64	2 (33%)
3	GOL	H	508	-	5,5,5	0.52	0	5,5,5	0.70	0
2	SO4	G	502	-	4,4,4	0.55	0	6,6,6	0.45	0
2	SO4	D	510	-	4,4,4	0.72	0	6,6,6	0.69	0
3	GOL	D	513	-	5,5,5	0.73	0	5,5,5	1.54	1 (20%)
3	GOL	F	510	-	5,5,5	0.44	0	5,5,5	0.50	0
3	GOL	C	510	-	5,5,5	1.29	0	5,5,5	2.67	2 (40%)
2	SO4	D	502	-	4,4,4	0.79	0	6,6,6	0.82	0
2	SO4	G	505	-	4,4,4	0.74	0	6,6,6	0.63	0
2	SO4	E	501	-	4,4,4	0.84	0	6,6,6	1.11	0
3	GOL	B	513	-	5,5,5	0.64	0	5,5,5	1.25	1 (20%)
2	SO4	D	505	-	4,4,4	0.55	0	6,6,6	0.50	0
3	GOL	F	509	-	5,5,5	0.41	0	5,5,5	0.33	0
2	SO4	D	503	-	4,4,4	0.59	0	6,6,6	0.60	0
2	SO4	F	505	-	4,4,4	0.67	0	6,6,6	0.35	0
2	SO4	F	501	-	4,4,4	0.54	0	6,6,6	0.32	0
2	SO4	E	503	-	4,4,4	0.57	0	6,6,6	0.88	0
2	SO4	E	508	-	4,4,4	0.87	0	6,6,6	0.72	0
3	GOL	D	514	-	5,5,5	0.27	0	5,5,5	0.32	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
4	CIT	C	515	-	-	8/16/16/16	-
3	GOL	C	512	-	-	1/4/4/4	-
3	GOL	D	512	-	-	3/4/4/4	-
3	GOL	A	512	-	-	2/4/4/4	-
3	GOL	H	509	-	-	4/4/4/4	-
3	GOL	H	510	-	-	4/4/4/4	-
4	CIT	A	513	-	-	12/16/16/16	-
3	GOL	B	511	-	-	2/4/4/4	-
3	GOL	F	508	-	-	2/4/4/4	-
3	GOL	H	508	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	510	-	-	0/4/4/4	-
3	GOL	C	513	-	-	4/4/4/4	-
3	GOL	D	515	-	-	0/4/4/4	-
4	CIT	G	509	-	-	10/16/16/16	-
3	GOL	D	513	-	-	2/4/4/4	-
3	GOL	F	510	-	-	4/4/4/4	-
3	GOL	C	510	-	-	4/4/4/4	-
4	CIT	D	516	-	-	5/16/16/16	-
3	GOL	E	511	-	-	2/4/4/4	-
3	GOL	A	511	-	-	0/4/4/4	-
3	GOL	B	512	-	-	0/4/4/4	-
3	GOL	F	511	-	-	4/4/4/4	-
4	CIT	B	514	-	-	10/16/16/16	-
3	GOL	G	507	-	-	4/4/4/4	-
3	GOL	B	509	-	-	2/4/4/4	-
3	GOL	E	513	-	-	2/4/4/4	-
3	GOL	G	508	-	-	4/4/4/4	-
3	GOL	B	513	-	-	2/4/4/4	-
4	CIT	E	514	-	-	7/16/16/16	-
3	GOL	C	511	-	-	0/4/4/4	-
3	GOL	F	509	-	-	2/4/4/4	-
3	GOL	B	510	-	-	1/4/4/4	-
3	GOL	E	512	-	-	2/4/4/4	-
3	GOL	C	514	-	-	2/4/4/4	-
3	GOL	E	510	-	-	2/4/4/4	-
3	GOL	D	514	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	CIT	C3-C6	-8.79	1.44	1.53
4	A	513	CIT	C4-C3	-6.48	1.45	1.54
4	G	509	CIT	C3-C6	-5.47	1.47	1.53
3	E	510	GOL	O3-C3	5.38	1.65	1.42
4	C	515	CIT	C3-C6	-4.74	1.48	1.53
4	C	515	CIT	C2-C3	-4.49	1.48	1.54
4	G	509	CIT	C2-C3	4.41	1.59	1.54
4	D	516	CIT	C2-C3	-4.28	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	514	CIT	C4-C3	-3.84	1.49	1.54
4	D	516	CIT	C3-C6	-3.65	1.49	1.53
4	C	515	CIT	O2-C1	-3.46	1.19	1.30
4	B	514	CIT	O4-C5	-3.19	1.20	1.30
4	D	516	CIT	O6-C6	-3.09	1.19	1.30
4	D	516	CIT	O2-C1	-3.07	1.20	1.30
4	C	515	CIT	O4-C5	-2.90	1.21	1.30
3	E	510	GOL	O2-C2	2.82	1.51	1.43
4	C	515	CIT	C4-C3	-2.62	1.50	1.54
4	A	513	CIT	O4-C5	-2.54	1.22	1.30
3	C	513	GOL	O2-C2	-2.45	1.36	1.43
4	G	509	CIT	O1-C1	2.45	1.30	1.22
4	G	509	CIT	O6-C6	-2.44	1.21	1.30
3	C	514	GOL	O3-C3	2.34	1.52	1.42
4	E	514	CIT	C4-C3	2.30	1.56	1.54
4	A	513	CIT	O2-C1	-2.23	1.23	1.30
4	C	515	CIT	O6-C6	-2.10	1.22	1.30
3	D	512	GOL	O3-C3	-2.08	1.33	1.42
4	B	514	CIT	C2-C3	-2.06	1.51	1.54
4	B	514	CIT	O6-C6	-2.04	1.23	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	515	CIT	C3-C2-C1	-6.37	96.50	113.92
4	G	509	CIT	C3-C2-C1	5.95	130.20	113.92
4	G	509	CIT	O6-C6-C3	5.50	123.69	113.14
4	B	514	CIT	O7-C3-C6	5.21	116.34	108.96
3	C	510	GOL	O2-C2-C1	-4.82	89.20	109.18
4	B	514	CIT	O7-C3-C4	-4.76	98.53	109.38
4	G	509	CIT	O7-C3-C6	-4.44	102.66	108.96
4	B	514	CIT	C3-C4-C5	-4.23	102.37	113.92
4	C	515	CIT	O2-C1-C2	4.16	127.52	114.35
3	E	510	GOL	O1-C1-C2	4.13	128.96	110.38
3	E	510	GOL	C3-C2-C1	4.12	126.89	111.80
4	G	509	CIT	C2-C3-C6	-4.02	101.14	110.03
4	D	516	CIT	O7-C3-C4	3.87	118.20	109.38
4	A	513	CIT	O7-C3-C6	-3.65	103.79	108.96
3	C	513	GOL	O2-C2-C1	-3.64	94.09	109.18
4	E	514	CIT	O6-C6-C3	3.64	120.12	113.14
4	C	515	CIT	O5-C6-C3	-3.50	115.32	122.09
4	G	509	CIT	C4-C3-C2	3.49	118.28	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	512	GOL	O3-C3-C2	-3.40	95.09	110.38
4	G	509	CIT	O7-C3-C2	3.35	117.02	109.38
4	C	515	CIT	O1-C1-C2	-3.28	113.67	122.95
4	D	516	CIT	C4-C3-C2	-3.18	101.15	109.31
4	E	514	CIT	O4-C5-C4	3.13	124.27	114.35
4	G	509	CIT	O5-C6-C3	-3.10	116.08	122.09
4	E	514	CIT	O1-C1-C2	-3.10	114.17	122.95
4	B	514	CIT	O6-C6-C3	2.96	118.81	113.14
4	D	516	CIT	O7-C3-C2	-2.95	102.65	109.38
4	B	514	CIT	O6-C6-O5	-2.91	114.55	123.86
4	E	514	CIT	C3-C2-C1	-2.90	105.98	113.92
3	C	510	GOL	O2-C2-C3	2.90	121.18	109.18
3	B	512	GOL	O3-C3-C2	-2.85	97.53	110.38
4	D	516	CIT	C3-C4-C5	2.85	121.72	113.92
4	C	515	CIT	O6-C6-C3	2.84	118.59	113.14
3	B	511	GOL	O1-C1-C2	2.79	122.92	110.38
3	E	510	GOL	O3-C3-C2	2.75	122.75	110.38
4	A	513	CIT	C3-C4-C5	-2.74	106.43	113.92
2	C	507	SO4	O4-S-O1	2.70	123.70	109.56
3	C	513	GOL	O1-C1-C2	-2.66	98.39	110.38
4	D	516	CIT	O7-C3-C6	2.63	112.69	108.96
3	G	508	GOL	O2-C2-C3	2.59	119.89	109.18
3	B	513	GOL	C3-C2-C1	-2.51	102.60	111.80
2	A	504	SO4	O4-S-O3	-2.44	95.09	108.54
3	E	513	GOL	O1-C1-C2	-2.43	99.43	110.38
4	B	514	CIT	O5-C6-C3	2.35	126.64	122.09
3	D	513	GOL	C3-C2-C1	-2.34	103.22	111.80
2	D	507	SO4	O2-S-O1	-2.31	92.80	109.06
2	C	507	SO4	O2-S-O1	-2.28	92.99	109.06
3	F	508	GOL	O1-C1-C2	-2.28	100.13	110.38
4	D	516	CIT	C3-C2-C1	-2.26	107.75	113.92
2	D	507	SO4	O3-S-O2	2.21	121.11	109.56
4	B	514	CIT	C2-C3-C6	2.19	114.87	110.03
4	E	514	CIT	O2-C1-C2	2.16	121.19	114.35
4	E	514	CIT	O7-C3-C2	-2.14	104.49	109.38

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	509	GOL	O1-C1-C2-C3
3	B	511	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	513	GOL	O1-C1-C2-O2
3	B	513	GOL	O1-C1-C2-C3
3	C	510	GOL	C1-C2-C3-O3
3	C	513	GOL	O1-C1-C2-C3
3	C	513	GOL	C1-C2-C3-O3
3	C	513	GOL	O2-C2-C3-O3
3	D	513	GOL	C1-C2-C3-O3
3	E	510	GOL	O1-C1-C2-C3
3	E	511	GOL	O1-C1-C2-C3
3	E	512	GOL	O1-C1-C2-C3
3	F	509	GOL	C1-C2-C3-O3
3	F	509	GOL	O2-C2-C3-O3
3	F	510	GOL	O1-C1-C2-O2
3	F	510	GOL	O1-C1-C2-C3
3	F	510	GOL	C1-C2-C3-O3
3	F	511	GOL	C1-C2-C3-O3
3	G	507	GOL	O1-C1-C2-C3
3	G	507	GOL	C1-C2-C3-O3
3	G	508	GOL	O1-C1-C2-C3
3	G	508	GOL	C1-C2-C3-O3
3	H	508	GOL	O1-C1-C2-C3
3	H	508	GOL	C1-C2-C3-O3
3	H	509	GOL	C1-C2-C3-O3
4	A	513	CIT	C1-C2-C3-O7
4	A	513	CIT	C1-C2-C3-C6
4	A	513	CIT	C2-C3-C4-C5
4	A	513	CIT	C6-C3-C4-C5
4	B	514	CIT	C1-C2-C3-O7
4	B	514	CIT	C1-C2-C3-C4
4	B	514	CIT	O7-C3-C6-O5
4	B	514	CIT	O7-C3-C6-O6
4	B	514	CIT	C4-C3-C6-O5
4	B	514	CIT	C4-C3-C6-O6
4	D	516	CIT	C1-C2-C3-O7
4	D	516	CIT	C1-C2-C3-C4
4	E	514	CIT	C2-C3-C4-C5
4	E	514	CIT	O7-C3-C4-C5
4	E	514	CIT	C6-C3-C4-C5
4	E	514	CIT	O7-C3-C6-O5
4	E	514	CIT	O7-C3-C6-O6
4	E	514	CIT	C4-C3-C6-O5
4	E	514	CIT	C4-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	513	CIT	C1-C2-C3-C4
4	B	514	CIT	C1-C2-C3-C6
4	C	515	CIT	O7-C3-C4-C5
4	D	516	CIT	C1-C2-C3-C6
3	B	509	GOL	O1-C1-C2-O2
3	B	511	GOL	O1-C1-C2-O2
3	G	507	GOL	O2-C2-C3-O3
4	C	515	CIT	C2-C3-C4-C5
4	G	509	CIT	C2-C3-C4-C5
3	A	512	GOL	C1-C2-C3-O3
3	C	510	GOL	O1-C1-C2-C3
3	C	514	GOL	O1-C1-C2-C3
3	D	512	GOL	O1-C1-C2-C3
3	D	512	GOL	C1-C2-C3-O3
3	E	513	GOL	O1-C1-C2-C3
3	F	508	GOL	O1-C1-C2-C3
3	F	511	GOL	O1-C1-C2-C3
3	H	509	GOL	O1-C1-C2-C3
3	H	510	GOL	O1-C1-C2-C3
3	H	510	GOL	C1-C2-C3-O3
4	A	513	CIT	C2-C3-C6-O6
3	C	510	GOL	O1-C1-C2-O2
3	C	510	GOL	O2-C2-C3-O3
3	C	513	GOL	O1-C1-C2-O2
3	C	514	GOL	O1-C1-C2-O2
3	D	513	GOL	O2-C2-C3-O3
3	E	510	GOL	O1-C1-C2-O2
3	E	511	GOL	O1-C1-C2-O2
3	E	512	GOL	O1-C1-C2-O2
3	F	508	GOL	O1-C1-C2-O2
3	F	511	GOL	O1-C1-C2-O2
3	F	511	GOL	O2-C2-C3-O3
3	G	507	GOL	O1-C1-C2-O2
3	G	508	GOL	O1-C1-C2-O2
3	H	509	GOL	O2-C2-C3-O3
3	H	510	GOL	O1-C1-C2-O2
4	A	513	CIT	O7-C3-C4-C5
3	D	512	GOL	O1-C1-C2-O2
3	G	508	GOL	O2-C2-C3-O3
3	H	508	GOL	O1-C1-C2-O2
4	A	513	CIT	O7-C3-C6-O5
4	A	513	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	515	CIT	O7-C3-C6-O6
4	G	509	CIT	O7-C3-C6-O6
4	C	515	CIT	C2-C3-C6-O6
4	C	515	CIT	C4-C3-C6-O6
3	D	514	GOL	O1-C1-C2-O2
3	F	510	GOL	O2-C2-C3-O3
3	H	508	GOL	O2-C2-C3-O3
3	A	512	GOL	O1-C1-C2-O2
3	B	510	GOL	O1-C1-C2-O2
3	C	512	GOL	O2-C2-C3-O3
3	H	509	GOL	O1-C1-C2-O2
4	B	514	CIT	C3-C4-C5-O3
4	B	514	CIT	C3-C4-C5-O4
4	A	513	CIT	C4-C3-C6-O5
4	A	513	CIT	C4-C3-C6-O6
4	G	509	CIT	C2-C3-C6-O5
4	G	509	CIT	C2-C3-C6-O6
3	H	510	GOL	O2-C2-C3-O3
4	B	514	CIT	O7-C3-C4-C5
4	G	509	CIT	C1-C2-C3-C4
4	G	509	CIT	C6-C3-C4-C5
4	G	509	CIT	O7-C3-C6-O5
4	A	513	CIT	C2-C3-C6-O5
4	C	515	CIT	C4-C3-C6-O5
4	G	509	CIT	C4-C3-C6-O5
3	D	514	GOL	O2-C2-C3-O3
4	G	509	CIT	C4-C3-C6-O6
4	D	516	CIT	O2-C1-C2-C3
4	C	515	CIT	O7-C3-C6-O5
4	G	509	CIT	C1-C2-C3-C6
3	E	513	GOL	O1-C1-C2-O2
4	D	516	CIT	O1-C1-C2-C3
4	C	515	CIT	C6-C3-C4-C5

There are no ring outliers.

29 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	509	CIT	3	0
2	D	504	SO4	1	0
4	D	516	CIT	9	0
3	B	512	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	514	CIT	6	0
3	G	507	GOL	1	0
2	D	501	SO4	1	0
3	G	508	GOL	2	0
2	E	507	SO4	1	0
2	C	505	SO4	1	0
3	E	512	GOL	1	0
3	C	514	GOL	4	0
3	E	510	GOL	2	0
2	H	502	SO4	2	0
3	A	512	GOL	3	0
3	H	509	GOL	10	0
4	E	514	CIT	7	0
3	C	511	GOL	2	0
3	E	511	GOL	2	0
4	C	515	CIT	8	0
3	D	512	GOL	2	0
2	H	506	SO4	1	0
4	A	513	CIT	14	0
2	D	510	SO4	1	0
3	D	513	GOL	4	0
3	F	510	GOL	1	0
3	C	510	GOL	4	0
3	B	513	GOL	2	0
3	F	509	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	431/448 (96%)	-0.74	3 (0%)	84 85	10, 17, 38, 100	4 (0%)
1	B	430/448 (95%)	-0.50	7 (1%)	70 72	13, 23, 44, 96	2 (0%)
1	C	430/448 (95%)	-0.46	7 (1%)	70 72	12, 24, 58, 108	2 (0%)
1	D	435/448 (97%)	-0.32	5 (1%)	78 79	14, 28, 52, 109	2 (0%)
1	E	431/448 (96%)	-0.20	13 (3%)	52 54	17, 29, 68, 123	2 (0%)
1	F	430/448 (95%)	0.14	9 (2%)	63 65	22, 37, 68, 113	0
1	G	430/448 (95%)	1.03	105 (24%)	2 2	20, 45, 79, 130	3 (0%)
1	H	430/448 (95%)	1.44	116 (26%)	1 1	23, 54, 82, 124	3 (0%)
All	All	3447/3584 (96%)	0.05	265 (7%)	19 21	10, 31, 70, 130	18 (0%)

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	444	VAL	6.8
1	C	444	VAL	6.4
1	H	444	VAL	6.4
1	A	444	VAL	6.1
1	E	444	VAL	6.1
1	A	14	ALA	5.9
1	D	14	ALA	5.9
1	G	444	VAL	5.9
1	G	370	VAL	5.7
1	B	15	SER	5.7
1	G	15	SER	5.7
1	H	15	SER	5.4
1	H	16	MET	5.3
1	E	14	ALA	5.3
1	H	204	LEU	5.2
1	E	15	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	204	LEU	4.6
1	F	204	LEU	4.5
1	G	430	LEU	4.5
1	G	415	ALA	4.5
1	E	204	LEU	4.3
1	E	405	MET	4.3
1	H	203	LYS	4.2
1	G	405	MET	4.2
1	H	201	ALA	4.2
1	G	428	PHE	4.2
1	G	421	LEU	4.1
1	D	203	LYS	4.0
1	H	149	ALA	4.0
1	G	388	ILE	4.0
1	G	441	SER	4.0
1	H	17	HIS	3.9
1	F	203	LYS	3.9
1	G	371	VAL	3.8
1	G	432	PRO	3.8
1	G	372	TRP	3.7
1	G	383	VAL	3.7
1	G	404	CYS	3.6
1	G	426	LEU	3.6
1	H	143	LEU	3.6
1	H	183	PHE	3.6
1	F	405	MET	3.6
1	G	420	GLY	3.6
1	G	350	VAL	3.6
1	H	179	TYR	3.6
1	G	413	LEU	3.6
1	H	189	TRP	3.6
1	G	416	LYS	3.5
1	H	125	ILE	3.5
1	G	442	PRO	3.5
1	H	147	VAL	3.5
1	H	200	VAL	3.5
1	H	175	ALA	3.5
1	E	400	LYS	3.5
1	H	202	SER	3.4
1	G	364	TYR	3.4
1	H	37	ALA	3.4
1	H	111	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	109	PHE	3.3
1	G	422	VAL	3.3
1	G	366	GLU	3.3
1	D	15	SER	3.3
1	G	377	ALA	3.3
1	H	116	ILE	3.3
1	G	378	GLU	3.3
1	G	260	TRP	3.3
1	C	405	MET	3.2
1	H	91	SER	3.2
1	G	427	ALA	3.2
1	H	120	GLY	3.2
1	A	15	SER	3.1
1	G	435	SER	3.1
1	H	193	PHE	3.1
1	H	103	ALA	3.1
1	G	312	ASP	3.1
1	G	397	VAL	3.1
1	G	293	ILE	3.1
1	G	436	ILE	3.1
1	H	190	GLY	3.1
1	B	444	VAL	3.1
1	F	205	TYR	3.1
1	H	104	LYS	3.1
1	H	100	PHE	3.1
1	H	194	VAL	3.1
1	H	121	LEU	3.1
1	H	60	TRP	3.0
1	H	52	ALA	3.0
1	H	227	VAL	3.0
1	G	417	GLU	3.0
1	H	32	TRP	3.0
1	G	387	ASN	3.0
1	G	403	GLY	3.0
1	H	96	ALA	3.0
1	H	67	ILE	3.0
1	F	15	SER	3.0
1	G	385	MET	3.0
1	H	61	GLU	3.0
1	H	218	ALA	2.9
1	G	402	LEU	2.9
1	G	424	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	395	VAL	2.9
1	G	389	SER	2.9
1	G	386	PHE	2.9
1	G	438	VAL	2.9
1	H	40	THR	2.9
1	H	405	MET	2.9
1	G	419	LEU	2.9
1	G	354	HIS	2.8
1	G	313	GLU	2.8
1	G	431	GLY	2.8
1	H	21	TRP	2.8
1	G	382	PHE	2.8
1	H	409	LYS	2.8
1	G	401	ASP	2.8
1	H	205	TYR	2.8
1	H	298	VAL	2.8
1	H	219	ILE	2.7
1	G	440	LEU	2.7
1	H	117	HIS	2.7
1	G	321	TRP	2.7
1	E	16	MET	2.7
1	B	104	LYS	2.7
1	E	203	LYS	2.7
1	G	309	PHE	2.7
1	G	322	ILE	2.7
1	C	15	SER	2.7
1	H	182	LEU	2.7
1	G	434	GLN	2.6
1	G	391	LYS	2.6
1	H	191	VAL	2.6
1	G	396	SER	2.6
1	G	342	LEU	2.6
1	C	443	ALA	2.6
1	G	418	ASP	2.6
1	G	363	VAL	2.6
1	H	107	LYS	2.6
1	H	171	ARG	2.6
1	G	316	THR	2.6
1	G	341	THR	2.6
1	G	317	MET	2.6
1	H	64	VAL	2.6
1	G	369	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	351	LEU	2.5
1	H	112	LEU	2.5
1	H	207	THR	2.5
1	H	280	GLY	2.5
1	H	58	PHE	2.5
1	H	126	HIS	2.5
1	H	350	VAL	2.5
1	H	35	TYR	2.5
1	G	443	ALA	2.5
1	H	65	VAL	2.5
1	H	131	ILE	2.5
1	G	16	MET	2.5
1	G	384	ALA	2.5
1	G	373	THR	2.5
1	H	196	VAL	2.5
1	G	344	LEU	2.5
1	G	437	LEU	2.5
1	G	408	MET	2.5
1	G	380	ASN	2.5
1	H	407	PRO	2.5
1	B	203	LYS	2.4
1	D	53	LYS	2.4
1	H	22	ALA	2.4
1	G	310	THR	2.4
1	G	273	TRP	2.4
1	H	69	TRP	2.4
1	H	242	LEU	2.4
1	H	81	PRO	2.4
1	G	263	LEU	2.4
1	H	279	LEU	2.4
1	H	414	TRP	2.4
1	G	433	HIS	2.4
1	G	308	ARG	2.4
1	H	42	ASP	2.4
1	G	285	ALA	2.4
1	H	243	PHE	2.4
1	H	93	LEU	2.4
1	E	406	GLU	2.4
1	G	412	ASP	2.3
1	H	46	GLY	2.3
1	H	130	GLY	2.3
1	G	360	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	240	ALA	2.3
1	C	424	HIS	2.3
1	G	237	LEU	2.3
1	G	347	ASN	2.3
1	H	36	GLY	2.3
1	F	16	MET	2.3
1	H	226	ILE	2.3
1	G	349	GLU	2.3
1	G	400	LYS	2.3
1	G	294	GLY	2.3
1	G	355	GLN	2.3
1	H	123	PHE	2.3
1	G	203	LYS	2.3
1	H	290	LEU	2.3
1	H	278	GLY	2.3
1	H	214	MET	2.3
1	H	79	TYR	2.3
1	H	140	THR	2.3
1	C	423	LYS	2.3
1	H	348	GLU	2.2
1	G	29	TRP	2.2
1	G	330	PHE	2.2
1	G	394	VAL	2.2
1	H	85	LEU	2.2
1	H	335	ARG	2.2
1	H	354	HIS	2.2
1	H	424	HIS	2.2
1	H	188	GLN	2.2
1	E	443	ALA	2.2
1	H	19	TYR	2.2
1	G	414	TRP	2.2
1	H	152	ILE	2.2
1	D	204	LEU	2.2
1	H	39	VAL	2.2
1	B	405	MET	2.2
1	G	272	LYS	2.2
1	G	352	HIS	2.2
1	H	406	GLU	2.2
1	H	181	SER	2.2
1	H	70	TYR	2.2
1	B	204	LEU	2.2
1	G	266	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	423	LYS	2.2
1	H	206	GLY	2.2
1	G	274	CYS	2.2
1	H	247	ALA	2.2
1	G	334	LEU	2.1
1	H	142	ILE	2.1
1	B	406	GLU	2.1
1	G	423	LYS	2.1
1	H	110	LYS	2.1
1	E	407	PRO	2.1
1	H	302	GLY	2.1
1	G	410	ALA	2.1
1	H	186	TYR	2.1
1	G	409	LYS	2.1
1	H	212	ILE	2.1
1	H	141	PRO	2.1
1	H	257	TRP	2.1
1	H	99	ARG	2.1
1	C	203	LYS	2.1
1	H	66	ASP	2.1
1	H	151	ASP	2.1
1	E	424	HIS	2.1
1	H	291	GLY	2.1
1	H	74	ALA	2.1
1	H	443	ALA	2.1
1	G	323	ILE	2.1
1	G	375	GLN	2.1
1	H	119	LEU	2.1
1	F	147	VAL	2.1
1	H	353	VAL	2.1
1	H	213	LYS	2.0
1	H	417	GLU	2.0
1	G	367	ASN	2.0
1	H	192	ASP	2.0
1	H	295	ILE	2.0
1	H	225	PRO	2.0
1	F	201	ALA	2.0
1	G	362	GLN	2.0
1	G	439	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	H	504	5/5	0.50	0.19	61,88,101,103	0
2	SO4	H	503	5/5	0.64	0.14	96,103,112,116	0
2	SO4	H	506	5/5	0.64	0.14	98,99,112,117	0
2	SO4	H	507	5/5	0.69	0.13	84,88,103,114	0
2	SO4	F	502	5/5	0.70	0.19	77,81,98,115	0
3	GOL	B	512	6/6	0.71	0.19	55,64,67,72	0
2	SO4	F	505	5/5	0.73	0.21	105,112,128,128	0
2	SO4	F	503	5/5	0.73	0.12	72,77,104,107	0
4	CIT	B	514	13/13	0.73	0.21	41,70,87,88	0
4	CIT	D	516	13/13	0.73	0.18	54,71,79,84	0
2	SO4	G	506	5/5	0.74	0.14	76,103,107,111	0
2	SO4	E	501	5/5	0.75	0.20	67,77,81,109	0
2	SO4	D	509	5/5	0.75	0.12	71,93,95,105	0
2	SO4	H	502	5/5	0.76	0.10	81,87,105,106	0
3	GOL	E	512	6/6	0.77	0.14	60,66,69,73	0
3	GOL	B	509	6/6	0.77	0.23	58,68,77,80	0
2	SO4	G	504	5/5	0.77	0.13	73,84,103,105	0
2	SO4	H	505	5/5	0.78	0.17	80,95,101,106	0
2	SO4	C	503	5/5	0.78	0.17	76,89,97,100	0
2	SO4	E	502	5/5	0.78	0.17	87,116,121,127	0
2	SO4	F	504	5/5	0.78	0.13	73,79,109,111	0
2	SO4	D	507	5/5	0.79	0.18	61,65,78,83	0
2	SO4	G	505	5/5	0.79	0.17	69,70,91,107	0
3	GOL	F	510	6/6	0.80	0.18	69,76,87,91	0
2	SO4	C	509	5/5	0.80	0.24	66,67,83,102	0
2	SO4	E	505	5/5	0.80	0.15	80,89,103,103	0
4	CIT	E	514	13/13	0.80	0.16	51,79,91,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	515	6/6	0.81	0.19	48,58,67,71	0
4	CIT	C	515	13/13	0.81	0.17	42,60,81,81	0
2	SO4	F	507	5/5	0.81	0.20	68,80,81,99	0
2	SO4	A	504	5/5	0.81	0.18	57,72,75,83	0
2	SO4	G	502	5/5	0.82	0.13	66,88,106,106	0
2	SO4	C	508	5/5	0.82	0.12	82,83,86,94	0
2	SO4	D	504	5/5	0.82	0.16	72,91,106,117	0
3	GOL	F	511	6/6	0.82	0.18	60,71,75,82	0
2	SO4	B	503	5/5	0.83	0.13	80,90,94,100	0
3	GOL	E	510	6/6	0.83	0.15	28,29,34,35	0
2	SO4	D	505	5/5	0.83	0.13	69,94,98,107	0
4	CIT	G	509	13/13	0.83	0.16	49,64,81,91	0
2	SO4	B	507	5/5	0.84	0.15	66,91,99,113	0
2	SO4	C	501	5/5	0.84	0.18	65,83,86,90	0
3	GOL	C	514	6/6	0.84	0.20	27,35,47,54	0
2	SO4	E	509	5/5	0.84	0.18	73,74,89,98	0
4	CIT	A	513	13/13	0.84	0.15	34,51,69,69	0
2	SO4	C	502	5/5	0.85	0.17	64,90,94,99	0
3	GOL	H	510	6/6	0.85	0.15	73,83,87,104	0
2	SO4	H	501	5/5	0.85	0.13	63,66,76,97	0
2	SO4	D	501	5/5	0.85	0.12	96,99,111,124	0
3	GOL	H	508	6/6	0.86	0.15	54,60,76,80	0
3	GOL	C	512	6/6	0.86	0.18	45,52,69,72	0
2	SO4	D	511	5/5	0.86	0.11	71,96,107,107	0
2	SO4	B	501	5/5	0.86	0.22	54,65,82,90	0
2	SO4	B	508	5/5	0.86	0.21	57,68,75,92	0
2	SO4	E	504	5/5	0.86	0.15	65,82,90,91	0
2	SO4	D	502	5/5	0.86	0.15	61,64,83,85	0
2	SO4	D	503	5/5	0.86	0.15	60,83,94,104	0
2	SO4	D	510	5/5	0.87	0.16	79,82,92,95	0
2	SO4	A	505	5/5	0.87	0.17	71,72,98,101	0
3	GOL	H	509	6/6	0.87	0.14	48,55,68,71	0
2	SO4	F	501	5/5	0.87	0.10	81,92,101,104	0
2	SO4	G	503	5/5	0.87	0.18	67,75,77,82	0
2	SO4	B	505	5/5	0.87	0.17	50,75,78,80	0
2	SO4	A	509	5/5	0.87	0.16	74,74,92,98	0
2	SO4	A	501	5/5	0.87	0.17	59,75,87,105	0
3	GOL	E	513	6/6	0.87	0.14	47,51,57,59	0
3	GOL	A	512	6/6	0.87	0.13	61,65,69,72	0
3	GOL	F	509	6/6	0.88	0.15	45,58,75,79	0
2	SO4	E	503	5/5	0.88	0.17	66,66,80,81	0
3	GOL	D	514	6/6	0.88	0.18	60,74,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	506	5/5	0.88	0.20	60,66,76,86	0
2	SO4	B	502	5/5	0.89	0.15	52,84,94,99	0
3	GOL	C	511	6/6	0.90	0.12	31,44,47,47	0
2	SO4	D	506	5/5	0.90	0.15	66,80,90,95	0
2	SO4	C	505	5/5	0.90	0.21	65,81,89,90	0
2	SO4	E	506	5/5	0.90	0.20	46,73,80,81	0
2	SO4	F	506	5/5	0.90	0.20	63,72,80,93	0
2	SO4	D	508	5/5	0.91	0.23	47,60,76,84	0
3	GOL	B	513	6/6	0.91	0.13	35,40,51,59	0
2	SO4	A	506	5/5	0.91	0.15	60,66,69,78	0
2	SO4	B	504	5/5	0.91	0.18	68,78,86,89	0
2	SO4	C	507	5/5	0.91	0.17	39,40,70,80	5
3	GOL	F	508	6/6	0.91	0.11	34,37,41,44	0
3	GOL	G	508	6/6	0.92	0.09	34,41,46,52	0
2	SO4	A	508	5/5	0.92	0.15	50,57,67,68	0
2	SO4	E	508	5/5	0.92	0.15	74,79,114,125	0
3	GOL	D	513	6/6	0.92	0.14	35,44,47,48	0
2	SO4	B	506	5/5	0.92	0.13	34,44,50,60	5
3	GOL	E	511	6/6	0.93	0.10	36,42,48,58	0
3	GOL	G	507	6/6	0.93	0.10	29,34,37,45	0
2	SO4	A	507	5/5	0.93	0.16	36,40,45,59	0
3	GOL	D	512	6/6	0.94	0.07	25,28,32,35	0
3	GOL	C	513	6/6	0.95	0.09	33,43,47,47	0
3	GOL	B	510	6/6	0.95	0.07	28,36,38,43	0
3	GOL	C	510	6/6	0.95	0.08	22,25,27,27	0
3	GOL	B	511	6/6	0.95	0.09	24,28,34,35	0
3	GOL	A	511	6/6	0.95	0.09	26,31,41,48	0
2	SO4	E	507	5/5	0.96	0.13	51,52,54,61	0
3	GOL	A	510	6/6	0.97	0.06	16,17,22,23	0
2	SO4	A	503	5/5	0.97	0.11	39,54,55,58	0
2	SO4	C	504	5/5	0.97	0.09	50,51,61,65	0
2	SO4	A	502	5/5	0.99	0.04	27,28,30,38	0
2	SO4	G	501	5/5	0.99	0.05	29,29,34,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.