Full wwPDB X-ray Structure Validation Report ⓘ

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 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:

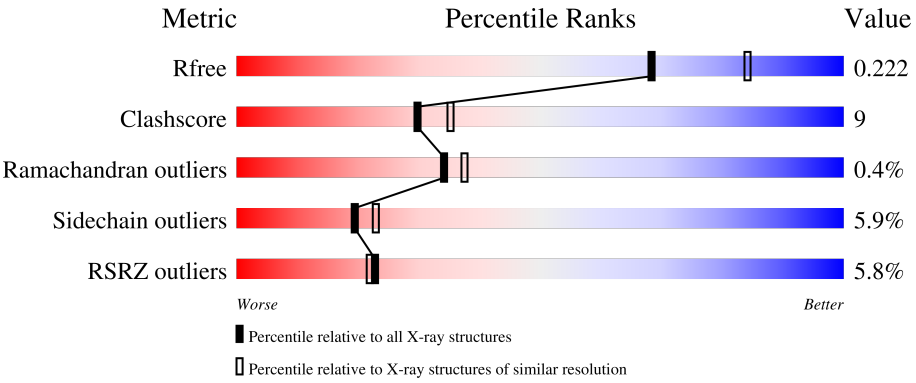
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

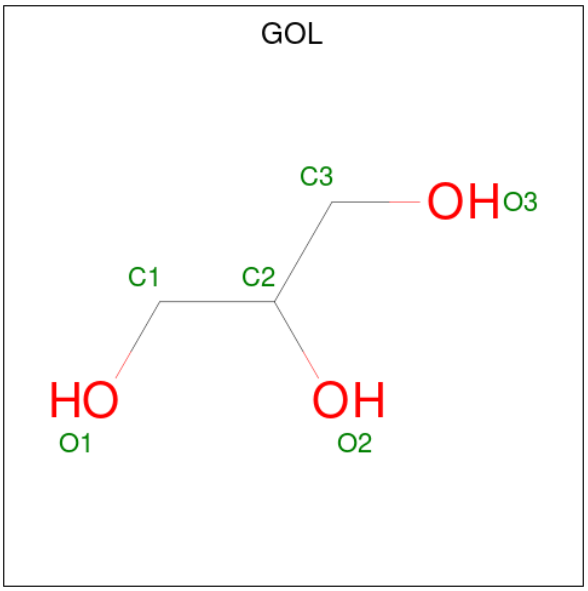
There are 6 unique types of molecules in this entry. The entry contains 31507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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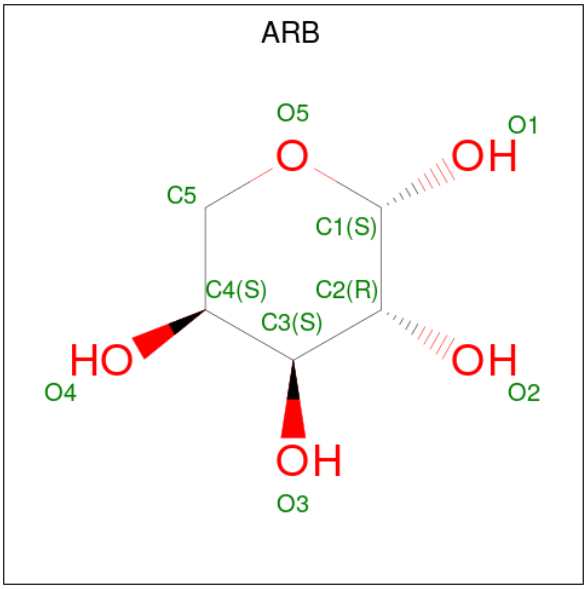
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

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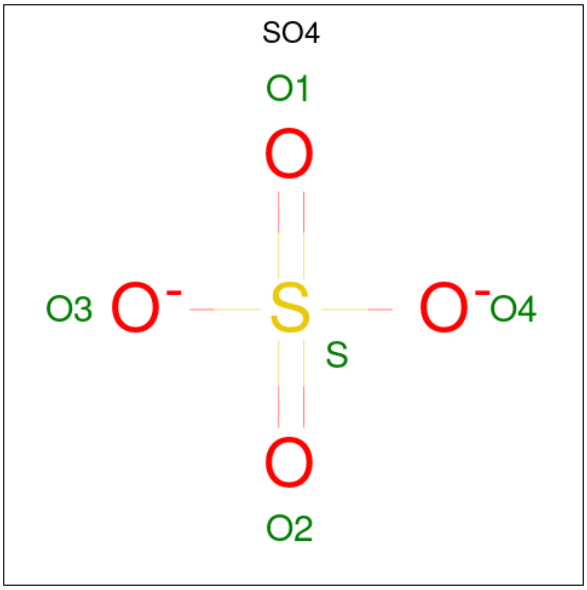
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 10 5 5	0	0
3	G	1	Total C O 10 5 5	0	0
3	H	1	Total C O 10 5 5	0	0

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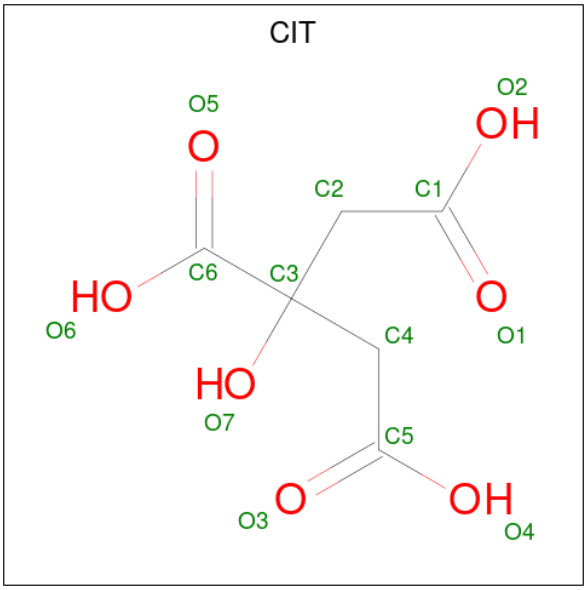
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0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

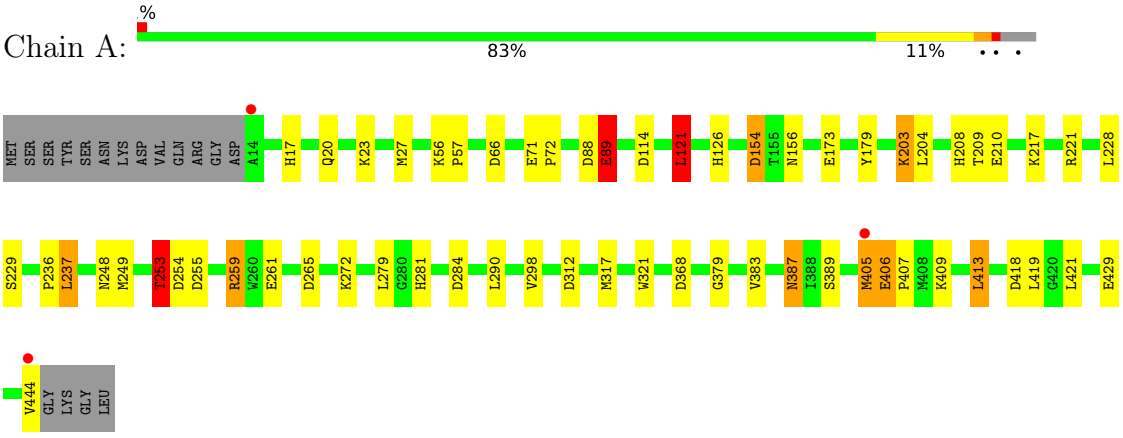
- Molecule 6 is water.

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

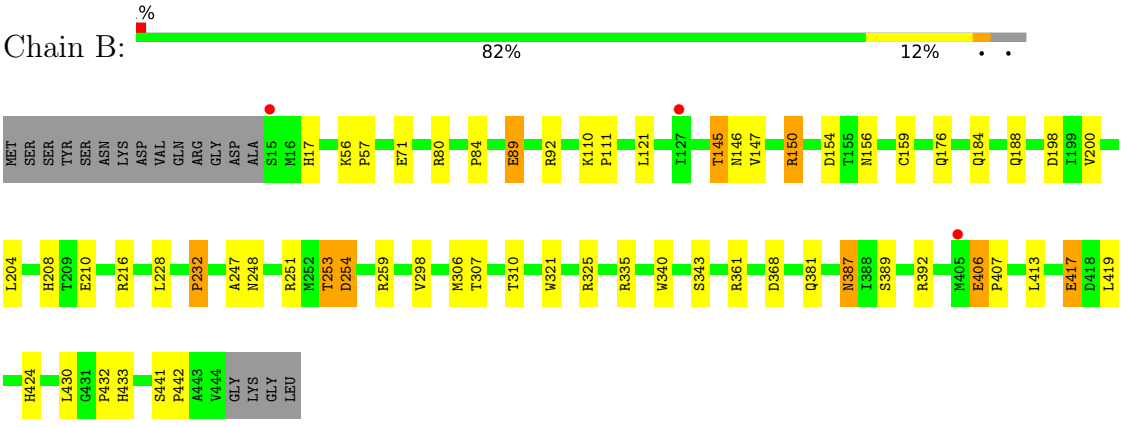
3 Residue-property plots (i)

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.

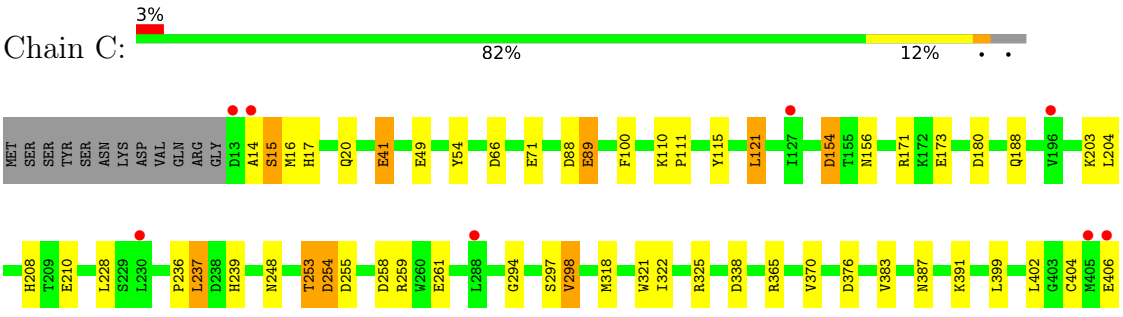
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

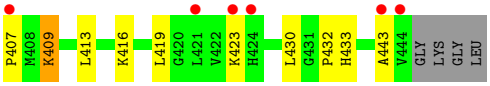


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

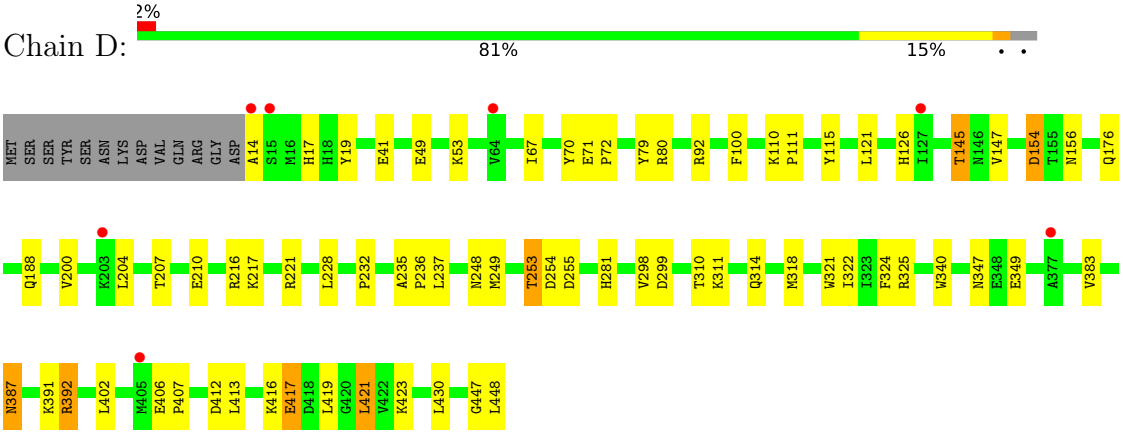


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

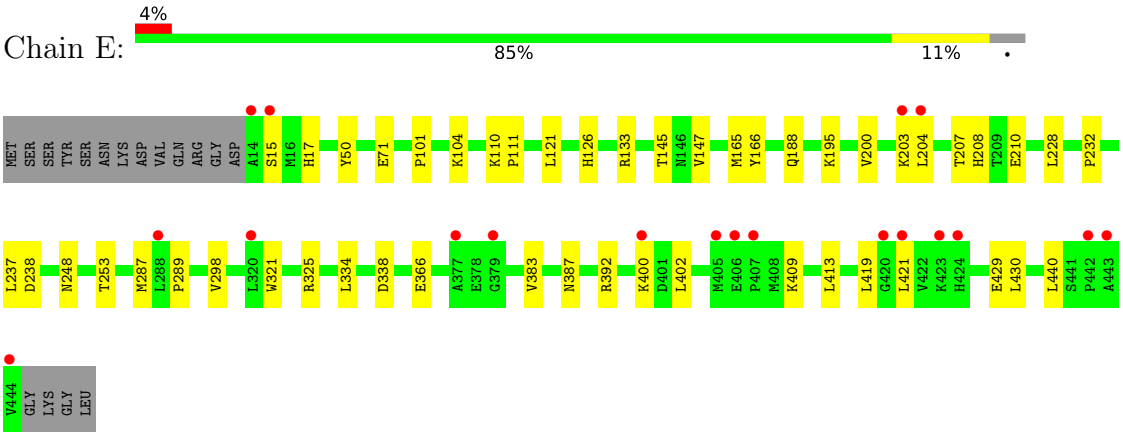




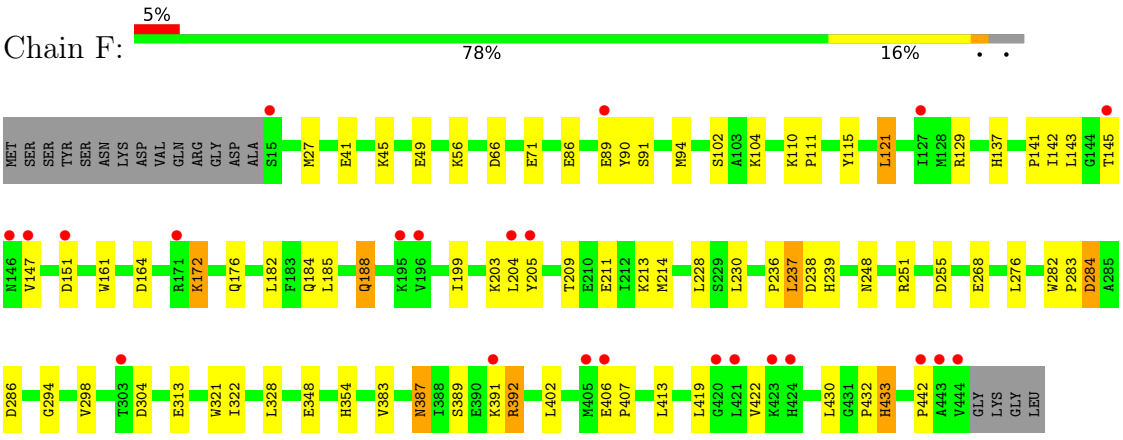
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



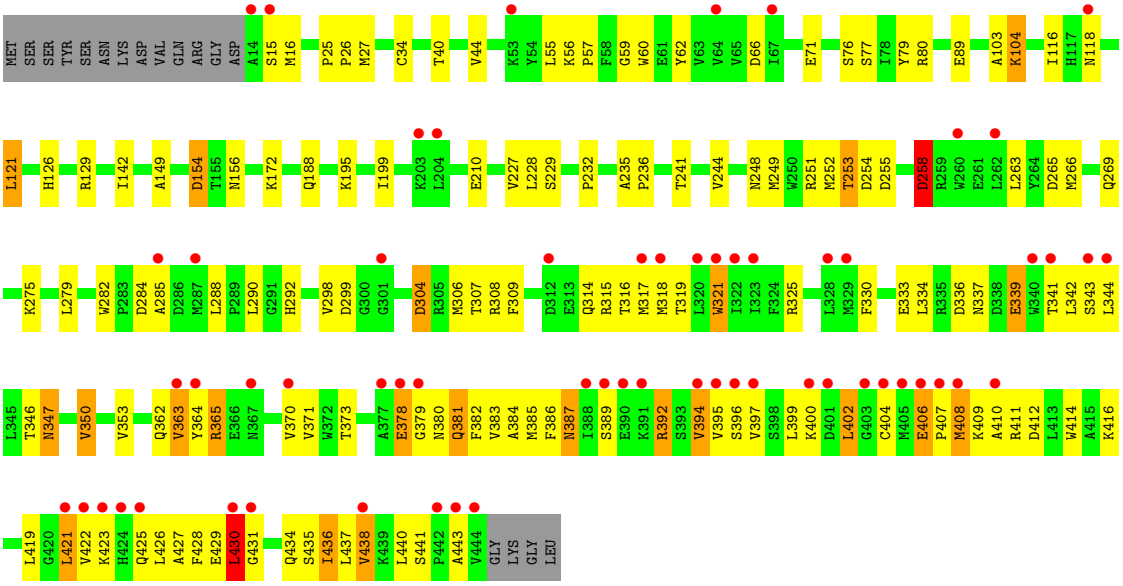
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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

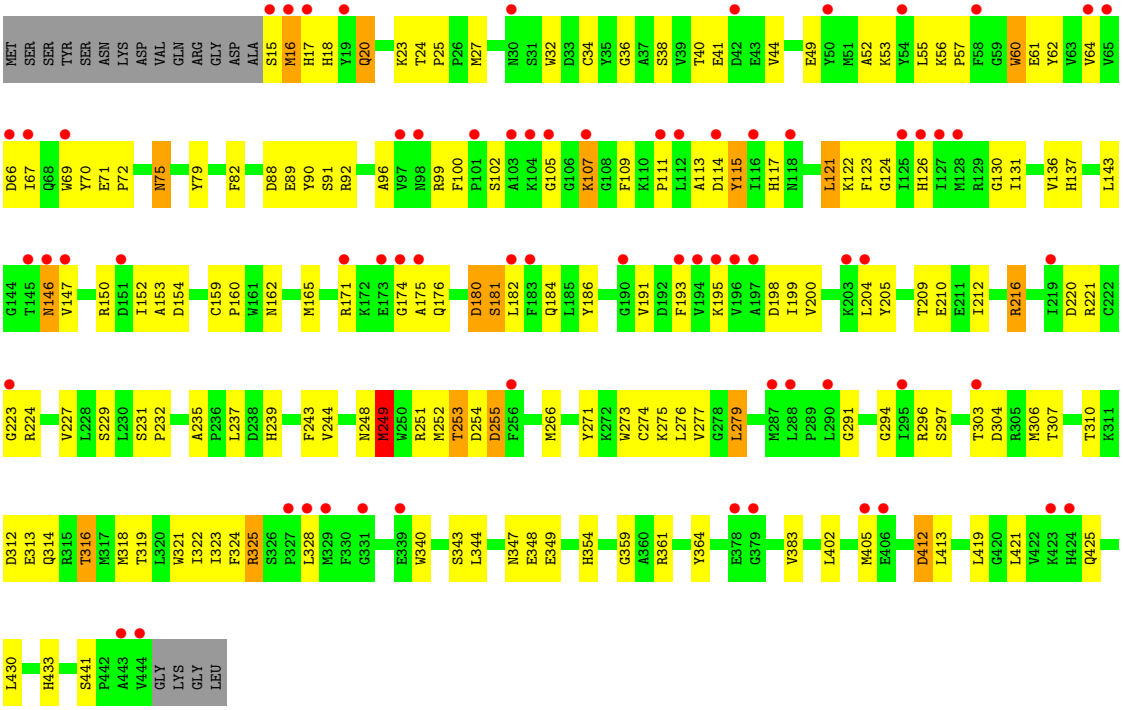


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



• 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

All (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
1	A	89	GLU	CG-CD	5.01	1.59	1.51

All (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
1	A	368	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	259	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	G	430	LEU	CA-CB-CG	7.24	131.94	115.30
1	H	180	ASP	CB-CG-OD2	7.24	124.81	118.30
1	A	154	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	237	LEU	CA-CB-CG	-7.05	99.08	115.30
1	A	121	LEU	CB-CG-CD1	6.97	122.84	111.00
1	G	80	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	88	ASP	CB-CG-OD1	6.88	124.50	118.30
1	G	154[A]	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	G	154[B]	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	80	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	G	251	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	216	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	H	249	MET	CG-SD-CE	6.53	110.64	100.20
1	C	338	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	H	88	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	A	284	ASP	CB-CG-OD1	6.34	124.01	118.30
1	G	80	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	92	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	H	216	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	C	171	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	B	80	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	89	GLU	CB-CA-C	-6.04	98.31	110.40
1	C	180	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	284	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	418	ASP	CB-CG-OD1	5.96	123.66	118.30
1	H	255	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	376	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	92	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	325	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	D	421	LEU	CA-CB-CG	5.80	128.64	115.30
1	C	41	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	C	325	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	251	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	237	LEU	CA-CB-CG	-5.74	102.10	115.30
1	F	284	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	254	ASP	CB-CG-OD1	5.54	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	412	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	88	ASP	CB-CG-OD1	5.53	123.28	118.30
1	F	237	LEU	CA-CB-CG	-5.50	102.65	115.30
1	C	121	LEU	CB-CG-CD1	5.48	120.32	111.00
1	C	298	VAL	N-CA-CB	-5.44	99.53	111.50
1	D	299	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	221	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	312	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	150	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	G	304	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	368	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	27	MET	CG-SD-CE	5.30	108.68	100.20
1	B	361	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	B	150	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	H	180	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	D	80	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	405	MET	CG-SD-CE	5.21	108.53	100.20
1	C	171	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	259	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	253	THR	N-CA-CB	-5.14	100.53	110.30
1	C	254	ASP	CB-CG-OD1	5.14	122.92	118.30
1	F	164	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	129	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	114	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	88	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	G	392	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	238	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	413	LEU	CB-CG-CD1	5.07	119.62	111.00
1	D	154	ASP	OD1-CG-OD2	5.06	132.91	123.30
1	F	286	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	C	255	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	298	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	B	335	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	C	15	SER	N-CA-C	5.00	124.51	111.00

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:G:346:THR:HG21	6:G:846:HOH:O	1.73	0.87
1:H:324:PHE:O	6:H:761:HOH:O	1.93	0.85
1:H:82:PHE:HA	6:H:658:HOH:O	1.76	0.85
1:G:431:GLY:HA3	6:G:666:HOH:O	1.77	0.84
1:B:228:LEU:H	1:B:248:ASN:HD22	1.22	0.83
1:F:228:LEU:H	1:F:248:ASN:HD22	1.22	0.83
1:G:292:HIS:ND1	1:G:336:ASP:OD2	2.10	0.83
1:H:425[B]:GLN:NE2	6:H:766:HOH:O	2.08	0.82
1:D:210:GLU:H	5:D:515:CIT:H22	1.44	0.82
1:E:145:THR:HG23	6:E:841:HOH:O	1.81	0.81
1:G:318:MET:HB3	6:G:835:HOH:O	1.80	0.80
1:H:56:LYS:HB2	6:H:742:HOH:O	1.82	0.80
1:A:228:LEU:H	1:A:248:ASN:HD22	1.31	0.79
1:B:210:GLU:H	5:B:519:CIT:H41	1.47	0.78
1:G:77:SER:OG	1:G:299:ASP:OD1	2.01	0.77
1:A:154:ASP:HB2	6:A:744:HOH:O	1.85	0.77
1:C:228:LEU:H	1:C:248:ASN:HD22	1.32	0.77
1:E:208:HIS:HA	5:E:517:CIT:O5	1.85	0.76
1:C:14:ALA:HB3	6:C:958:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:GLU:CB	6:D:810:HOH:O	2.34	0.75
1:H:340:TRP:O	1:H:343:SER:OG	2.04	0.75
1:H:70:TYR:CE2	6:H:649:HOH:O	2.40	0.75
1:H:92:ARG:HD3	1:H:181:SER:OG	1.87	0.73
1:E:228:LEU:H	1:E:248:ASN:HD22	1.34	0.73
1:H:56:LYS:CB	6:H:742:HOH:O	2.35	0.73
1:H:159:CYS:SG	1:H:198:ASP:OD1	2.45	0.73
1:H:184:GLN:HA	6:H:646:HOH:O	1.89	0.73
1:H:223:GLY:N	6:H:760:HOH:O	2.17	0.72
1:D:17:HIS:CE1	6:D:782:HOH:O	2.41	0.72
1:B:406:GLU:HB2	1:B:407:PRO:CD	2.20	0.71
1:G:363:VAL:CG1	1:G:371:VAL:HG23	2.20	0.71
1:A:89:GLU:H	1:A:89:GLU:CD	1.94	0.71
1:A:406:GLU:HB2	1:A:407:PRO:CD	2.21	0.70
1:H:318:MET:O	1:H:322:ILE:HG12	1.91	0.70
1:C:188[B]:GLN:CD	6:C:830:HOH:O	2.30	0.70
1:C:253:THR:HG23	1:C:254:ASP:O	1.91	0.70
1:F:41:GLU:OE2	1:F:102:SER:OG	2.07	0.70
1:H:114:ASP:HA	6:H:746:HOH:O	1.92	0.69
1:G:342:LEU:HD12	1:G:342:LEU:O	1.93	0.69
1:D:417:GLU:HB2	6:D:810:HOH:O	1.93	0.68
1:B:210:GLU:HG2	5:B:519:CIT:H42	1.76	0.68
1:G:378:GLU:N	1:G:378:GLU:OE1	2.27	0.67
1:G:304:ASP:OD1	1:G:304:ASP:C	2.31	0.67
2:A:501:GOL:C1	6:A:1086:HOH:O	2.42	0.67
1:F:129:ARG:NH1	1:F:211:GLU:OE2	2.22	0.67
1:D:228:LEU:H	1:D:248:ASN:HD22	1.43	0.66
1:G:362:GLN:NE2	6:G:837:HOH:O	2.28	0.65
1:G:275:LYS:HE3	1:H:244:VAL:HG11	1.78	0.65
1:G:412:ASP:OD2	1:G:436:ILE:HD11	1.95	0.65
1:C:14:ALA:CB	6:C:958:HOH:O	2.41	0.65
1:C:210:GLU:HB2	5:C:519:CIT:H41	1.76	0.65
1:B:145:THR:HG23	6:B:945:HOH:O	1.96	0.65
4:D:510:SO4:O2	6:D:961:HOH:O	2.13	0.65
1:H:75:ASN:N	1:H:75:ASN:HD22	1.94	0.65
1:H:182:LEU:O	1:H:186:TYR:CD2	2.50	0.65
1:A:210:GLU:HB2	5:A:515:CIT:H22	1.79	0.64
1:A:265:ASP:HB3	6:A:975:HOH:O	1.96	0.64
1:H:20:GLN:HE21	1:H:20:GLN:N	1.95	0.64
1:A:173:GLU:OE2	4:A:506:SO4:O4	2.14	0.64
1:D:448:LEU:C	6:D:824:HOH:O	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ASP:OD1	2:G:501:GOL:H11	1.98	0.64
1:G:266:MET:HE3	1:G:321:TRP:CH2	2.33	0.64
2:A:501:GOL:C2	6:A:1086:HOH:O	2.45	0.64
1:G:334:LEU:O	1:G:337:ASN:ND2	2.30	0.64
1:D:210:GLU:HB2	5:D:515:CIT:H41	1.80	0.64
5:B:519:CIT:O1	6:B:1049:HOH:O	2.16	0.63
5:G:510:CIT:H22	5:G:510:CIT:O3	1.97	0.63
1:H:210:GLU:OE1	1:H:210:GLU:HA	1.99	0.63
1:B:253:THR:HG23	1:B:254:ASP:O	1.98	0.62
1:H:66:ASP:HA	1:H:126:HIS:HB2	1.82	0.62
1:D:255:ASP:OD2	2:D:501:GOL:H31	2.00	0.62
1:G:394:VAL:HA	1:G:429:GLU:HA	1.82	0.62
4:B:507:SO4:O3	6:B:1031:HOH:O	2.15	0.62
1:G:342:LEU:HD12	1:G:342:LEU:C	2.20	0.62
1:G:347:ASN:HD22	1:G:350:VAL:H	1.47	0.62
1:D:188:GLN:NE2	6:D:820:HOH:O	2.32	0.61
1:F:110:LYS:HB3	1:F:111:PRO:HD3	1.82	0.61
1:A:208:HIS:HA	5:A:515:CIT:O6	2.00	0.61
1:G:428:PHE:O	1:G:430:LEU:HD22	2.00	0.61
1:H:130:GLY:C	6:H:634:HOH:O	2.38	0.61
1:C:49:GLU:OE2	1:C:115:TYR:OH	2.17	0.61
1:C:210:GLU:H	5:C:519:CIT:H22	1.65	0.61
1:G:210:GLU:H	5:G:510:CIT:H42	1.65	0.61
1:A:89:GLU:CG	6:A:856:HOH:O	2.49	0.60
1:B:253:THR:CG2	1:B:254:ASP:O	2.49	0.60
1:A:203:LYS:HE3	6:A:1127:HOH:O	2.02	0.60
1:A:208:HIS:C	5:A:515:CIT:O6	2.39	0.60
1:E:325:ARG:HD2	6:E:984:HOH:O	2.01	0.60
1:F:45:LYS:NZ	6:F:838:HOH:O	2.23	0.60
1:G:346:THR:CG2	6:G:846:HOH:O	2.38	0.60
1:G:350:VAL:HG22	1:G:437:LEU:HD23	1.84	0.60
1:H:175:ALA:N	2:H:502:GOL:H32	2.16	0.60
1:G:66:ASP:OD2	1:G:195:LYS:NZ	2.35	0.60
1:A:208:HIS:CA	5:A:515:CIT:O6	2.50	0.60
1:G:350:VAL:HG22	1:G:437:LEU:CD2	2.32	0.60
1:A:154:ASP:CB	6:A:744:HOH:O	2.43	0.60
1:G:172:LYS:NZ	6:G:677:HOH:O	2.34	0.60
1:G:154[B]:ASP:OD2	6:G:653:HOH:O	2.16	0.59
1:B:156:ASN:HD21	1:D:204:LEU:HD11	1.67	0.59
1:G:378:GLU:CD	1:G:378:GLU:H	2.05	0.59
1:A:255:ASP:OD2	2:A:501:GOL:C1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:THR:CG2	1:D:254:ASP:O	2.50	0.59
1:E:188:GLN:HG2	6:E:831:HOH:O	2.02	0.59
1:G:365:ARG:HB2	1:G:370:VAL:HG22	1.85	0.59
1:B:176:GLN:HB3	2:B:503:GOL:H31	1.84	0.59
1:G:347:ASN:HB3	1:G:350:VAL:HB	1.83	0.59
1:G:344:LEU:HD21	6:G:804:HOH:O	2.02	0.59
1:H:252[A]:MET:HG2	1:H:273:TRP:CD1	2.37	0.59
1:H:136:VAL:HG21	1:H:153:ALA:HB2	1.85	0.59
1:G:228:LEU:H	1:G:248:ASN:HD22	1.51	0.59
1:F:161:TRP:O	6:F:674:HOH:O	2.17	0.58
1:H:254:ASP:O	1:H:255:ASP:C	2.42	0.58
1:B:210:GLU:CG	5:B:519:CIT:H42	2.33	0.58
1:G:252:MET:O	6:G:842:HOH:O	2.17	0.58
1:H:102:SER:OG	1:H:111:PRO:HB2	2.04	0.58
1:A:156:ASN:HD21	1:C:204:LEU:HD11	1.69	0.58
1:G:330:PHE:CE2	1:G:334:LEU:HD23	2.39	0.58
1:H:159:CYS:CB	1:H:198:ASP:OD1	2.52	0.58
1:G:308:ARG:CB	6:G:830:HOH:O	2.52	0.58
1:G:315:ARG:N	6:G:804:HOH:O	2.37	0.58
1:D:176:GLN:HB3	2:D:503:GOL:H32	1.86	0.57
1:F:184:GLN:O	1:F:188:GLN:HG2	2.04	0.57
1:G:314:GLN:HB3	6:G:804:HOH:O	2.03	0.57
1:H:17:HIS:HB2	6:H:670:HOH:O	2.04	0.57
2:C:505:GOL:H2	4:C:510:SO4:O3	2.05	0.57
1:G:339:GLU:OE2	1:G:339:GLU:N	2.37	0.57
1:G:421:LEU:HD12	1:G:422:VAL:N	2.18	0.57
1:H:107:LYS:O	6:H:659:HOH:O	2.17	0.57
1:H:107:LYS:HA	1:H:107:LYS:CE	2.34	0.57
2:A:501:GOL:H11	6:A:1086:HOH:O	2.05	0.57
1:H:70:TYR:HE2	6:H:649:HOH:O	1.81	0.57
1:H:105:GLY:O	6:H:710:HOH:O	2.18	0.57
1:G:306:MET:O	1:G:307:THR:C	2.40	0.57
1:D:49:GLU:OE1	1:D:115:TYR:OH	2.21	0.57
1:D:255:ASP:CG	2:D:501:GOL:H31	2.25	0.57
6:A:845:HOH:O	2:E:504:GOL:H12	2.05	0.57
1:B:204:LEU:HD11	1:D:156:ASN:HD21	1.69	0.57
1:G:266:MET:O	1:G:269:GLN:N	2.37	0.57
1:A:253:THR:HG23	1:A:254:ASP:O	2.04	0.56
2:A:501:GOL:O2	6:A:1086:HOH:O	2.18	0.56
1:E:366:GLU:HB2	6:E:953:HOH:O	2.04	0.56
1:G:253:THR:HG23	1:G:254:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:380:ASN:ND2	6:G:730:HOH:O	2.19	0.56
1:C:208:HIS:ND1	5:C:519:CIT:O5	2.31	0.56
1:H:38:SER:O	1:H:296:ARG:NH2	2.33	0.56
1:H:49:GLU:OE2	1:H:115:TYR:OH	2.24	0.56
1:H:252[B]:MET:SD	1:H:266[B]:MET:CE	2.93	0.56
1:D:253:THR:HG22	1:D:254:ASP:O	2.06	0.55
1:F:188:GLN:HG3	6:F:791:HOH:O	2.05	0.55
1:H:313:GLU:OE2	6:H:667:HOH:O	2.18	0.55
1:H:252[B]:MET:HE1	1:H:273:TRP:HB2	1.87	0.55
1:D:67:ILE:HD13	1:D:79:TYR:CE1	2.41	0.55
1:F:392:ARG:NH1	6:F:640:HOH:O	2.39	0.55
1:H:248:ASN:ND2	6:H:739:HOH:O	2.39	0.55
1:H:113:ALA:O	1:H:117:HIS:ND1	2.40	0.55
1:H:239:HIS:HA	6:H:664:HOH:O	2.06	0.55
1:C:253:THR:CG2	1:C:254:ASP:O	2.55	0.55
1:H:67:ILE:CG1	1:H:126:HIS:CE1	2.89	0.55
1:H:200:VAL:HB	1:H:232:PRO:O	2.07	0.54
1:F:151:ASP:O	1:F:172:LYS:HG2	2.08	0.54
1:H:130:GLY:O	1:H:165:MET:CE	2.56	0.54
1:G:279:LEU:C	1:G:279:LEU:HD23	2.28	0.54
1:G:396:SER:CB	1:G:427:ALA:HB2	2.37	0.54
1:G:395:VAL:HB	1:G:430:LEU:HD23	1.90	0.54
1:H:67:ILE:HG13	1:H:126:HIS:CE1	2.42	0.54
1:H:312:ASP:O	1:H:316:THR:HG23	2.08	0.54
1:B:154:ASP:OD2	6:B:782:HOH:O	2.18	0.54
5:E:517:CIT:H22	6:E:670:HOH:O	2.08	0.54
1:H:198:ASP:O	1:H:198:ASP:OD2	2.26	0.54
1:G:421:LEU:HD11	1:G:423:LYS:HE3	1.90	0.54
1:H:27:MET:HA	1:H:328:LEU:O	2.07	0.53
1:H:56:LYS:N	1:H:57:PRO:CD	2.71	0.53
1:H:150:ARG:HD2	6:H:627:HOH:O	2.08	0.53
1:H:253:THR:HB	6:H:606:HOH:O	2.08	0.53
1:B:150:ARG:HD2	6:B:725:HOH:O	2.07	0.53
5:C:519:CIT:O1	5:C:519:CIT:C6	2.57	0.53
1:F:49:GLU:OE2	1:F:115:TYR:OH	2.23	0.53
1:F:387:ASN:ND2	1:F:389:SER:H	2.07	0.53
1:H:131:ILE:CD1	1:H:152:ILE:HD11	2.39	0.53
1:G:341:THR:O	1:G:344:LEU:HB2	2.09	0.53
1:G:381:GLN:NE2	1:G:404:CYS:SG	2.82	0.53
1:G:266:MET:HE3	1:G:285:ALA:HB1	1.90	0.53
1:H:115:TYR:O	1:H:115:TYR:CG	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLU:H	5:B:519:CIT:C4	2.20	0.52
1:D:325:ARG:HD2	6:D:979:HOH:O	2.07	0.52
1:D:176:GLN:H	2:D:503:GOL:C3	2.22	0.52
1:B:406:GLU:HB2	1:B:407:PRO:HD2	1.90	0.52
1:E:101:PRO:O	1:E:104:LYS:HB2	2.09	0.52
1:G:346:THR:CB	6:G:846:HOH:O	2.57	0.52
1:H:297:SER:CB	6:H:615:HOH:O	2.57	0.52
1:H:123:PHE:CD2	1:H:191:VAL:HG22	2.45	0.52
1:H:70:TYR:O	1:H:72:PRO:HD3	2.09	0.52
1:C:17:HIS:CE1	6:C:779:HOH:O	2.62	0.52
4:C:508:SO4:O3	6:C:1007:HOH:O	2.18	0.52
1:H:273:TRP:CE3	1:H:276:LEU:HD23	2.45	0.52
1:E:210:GLU:HB2	5:E:517:CIT:H22	1.91	0.52
1:F:406:GLU:HB2	1:F:407:PRO:HD2	1.92	0.52
1:H:324:PHE:O	1:H:325:ARG:HB2	2.10	0.52
1:A:387:ASN:HD22	1:A:389:SER:H	1.58	0.52
1:C:318:MET:O	1:C:322:ILE:HG12	2.10	0.52
1:G:103:ALA:O	1:G:104:LYS:C	2.47	0.52
6:A:1140:HOH:O	2:E:504:GOL:H32	2.11	0.51
1:F:204:LEU:HB2	1:F:205:TYR:CD2	2.44	0.51
1:G:406:GLU:HG3	1:G:407:PRO:O	2.10	0.51
1:G:337:ASN:CG	6:G:843:HOH:O	2.48	0.51
1:G:363:VAL:HG13	1:G:371:VAL:O	2.10	0.51
1:G:410:ALA:HB2	1:G:440:LEU:HD23	1.92	0.51
1:H:316:THR:HG21	1:H:433:HIS:O	2.10	0.51
1:D:281:HIS:O	1:D:281:HIS:ND1	2.43	0.51
1:G:318:MET:CB	6:G:835:HOH:O	2.48	0.51
1:G:319:THR:OG1	1:G:414:TRP:NE1	2.34	0.51
1:H:412:ASP:C	1:H:412:ASP:OD1	2.49	0.51
1:D:417:GLU:HB3	6:D:810:HOH:O	2.06	0.51
1:G:290:LEU:HD21	1:G:317:MET:HE1	1.92	0.51
1:D:392:ARG:NH1	4:D:512:SO4:O4	2.44	0.51
1:D:423:LYS:HE3	2:D:502:GOL:H2	1.93	0.51
1:H:23:LYS:HA	1:H:279:LEU:CD2	2.40	0.51
1:B:306:MET:CE	6:B:674:HOH:O	2.58	0.51
1:D:318:MET:O	1:D:322:ILE:HG12	2.11	0.51
1:G:353:VAL:O	1:G:353:VAL:HG12	2.10	0.51
1:B:306:MET:HE1	6:B:674:HOH:O	2.11	0.51
1:D:406:GLU:HB2	1:D:407:PRO:CD	2.41	0.51
1:G:27:MET:HE2	1:G:59:GLY:C	2.31	0.51
1:G:308:ARG:HB2	6:G:830:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:LYS:HA	1:H:107:LYS:HE2	1.93	0.51
1:A:259:ARG:NH2	1:A:261:GLU:OE2	2.44	0.51
1:H:52:ALA:HA	6:H:742:HOH:O	2.09	0.51
1:H:64:VAL:HG22	1:H:124:GLY:HA3	1.93	0.51
1:G:314:GLN:CB	6:G:804:HOH:O	2.59	0.50
1:H:90:TYR:CE1	1:H:143:LEU:HD12	2.45	0.50
1:A:154:ASP:OD1	6:A:1101:HOH:O	2.18	0.50
1:A:279:LEU:HD23	1:A:279:LEU:C	2.31	0.50
1:D:210:GLU:CG	5:D:515:CIT:H21	2.41	0.50
1:H:89:GLU:HB3	1:H:90:TYR:CE2	2.47	0.50
1:B:145:THR:HG21	1:B:147:VAL:HG22	1.93	0.50
1:F:176:GLN:OE1	1:F:214:MET:HG2	2.12	0.50
1:A:89:GLU:HG3	6:A:856:HOH:O	2.11	0.50
1:D:412:ASP:C	1:D:412:ASP:OD1	2.49	0.50
1:G:275:LYS:CE	1:H:244:VAL:HG11	2.41	0.50
1:H:100:PHE:CD1	1:H:109:PHE:HE1	2.30	0.50
1:H:252[B]:MET:HE3	1:H:324:PHE:CE2	2.46	0.50
1:H:297:SER:HB2	6:H:615:HOH:O	2.11	0.50
1:E:204:LEU:HD11	1:G:156:ASN:HD21	1.75	0.50
1:G:290:LEU:HD21	1:G:317:MET:CE	2.41	0.50
1:D:200:VAL:HB	1:D:232:PRO:O	2.12	0.50
1:D:67:ILE:HG13	1:D:126:HIS:CE1	2.47	0.49
1:G:373:THR:OG1	1:G:382:PHE:O	2.18	0.49
1:G:421:LEU:HD12	1:G:422:VAL:CA	2.42	0.49
1:C:416:LYS:HD2	6:C:948:HOH:O	2.12	0.49
1:F:56:LYS:HD3	1:F:121:LEU:HD13	1.93	0.49
1:H:310:THR:O	1:H:314:GLN:HG3	2.12	0.49
1:D:207:THR:N	4:D:506:SO4:O1	2.45	0.49
1:G:333:GLU:OE2	1:G:334:LEU:N	2.45	0.49
1:H:319:THR:O	1:H:323:ILE:HG22	2.13	0.49
1:A:387:ASN:ND2	1:A:389:SER:H	2.11	0.49
1:G:25:PRO:HG3	1:G:282:TRP:CE3	2.48	0.49
1:H:253:THR:HG22	1:H:254:ASP:O	2.12	0.49
1:B:146:ASN:CB	6:B:801:HOH:O	2.60	0.48
1:F:145:THR:O	6:F:881:HOH:O	2.19	0.48
1:G:364:TYR:O	1:G:370:VAL:HA	2.12	0.48
1:H:62:TYR:N	6:H:744:HOH:O	2.46	0.48
1:H:231:SER:HB2	1:H:232:PRO:HA	1.95	0.48
1:D:210:GLU:H	5:D:515:CIT:C2	2.19	0.48
1:D:387:ASN:C	1:D:387:ASN:HD22	2.15	0.48
1:E:145:THR:HG22	1:E:147:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:GLU:HG2	6:F:647:HOH:O	2.13	0.48
1:H:124:GLY:HA2	1:H:193:PHE:O	2.12	0.48
1:H:252[B]:MET:CE	1:H:273:TRP:HB2	2.43	0.48
5:D:515:CIT:H41	6:D:634:HOH:O	2.13	0.48
1:F:387:ASN:HD22	1:F:389:SER:H	1.62	0.48
1:G:56:LYS:HB3	1:G:57:PRO:HD3	1.94	0.48
1:G:284:ASP:OD1	6:G:777:HOH:O	2.20	0.48
1:B:432:PRO:O	1:B:433:HIS:HB2	2.14	0.48
1:G:347:ASN:CG	6:G:785:HOH:O	2.52	0.48
1:G:384:ALA:HA	1:G:436:ILE:O	2.13	0.48
1:H:67:ILE:HB	1:H:126:HIS:CE1	2.48	0.48
1:H:291:GLY:O	1:H:306:MET:HA	2.13	0.48
1:E:208:HIS:HE1	6:E:610:HOH:O	1.96	0.47
1:H:159:CYS:HB3	1:H:162:ASN:O	2.14	0.47
1:H:229:SER:HA	1:H:249:MET:O	2.14	0.47
1:C:423:LYS:N	4:C:516:SO4:O3	2.32	0.47
1:D:176:GLN:CB	2:D:503:GOL:H32	2.44	0.47
1:G:142:ILE:HD11	1:G:149:ALA:HA	1.95	0.47
1:H:75:ASN:N	1:H:75:ASN:ND2	2.61	0.47
1:G:76:SER:OG	1:G:77:SER:N	2.47	0.47
1:G:66:ASP:HA	1:G:126:HIS:HB2	1.96	0.47
1:H:131:ILE:HD13	1:H:152:ILE:HD11	1.96	0.47
1:D:310:THR:O	1:D:314:GLN:HG3	2.14	0.47
1:E:210:GLU:HG2	5:E:517:CIT:H41	1.94	0.47
1:F:86:GLU:HB3	1:F:94:MET:O	2.14	0.47
1:F:209:THR:O	1:F:213:LYS:HG3	2.15	0.47
1:G:241:THR:HG21	1:H:271:TYR:CE1	2.50	0.47
1:G:434:GLN:NE2	6:G:784:HOH:O	2.48	0.47
1:G:387:ASN:ND2	1:G:389:SER:OG	2.46	0.47
1:A:255:ASP:OD1	2:A:501:GOL:H12	2.14	0.47
1:C:399:LEU:HB3	1:C:404:CYS:HB2	1.97	0.47
1:D:110:LYS:HB3	1:D:111:PRO:HD3	1.97	0.47
1:E:210:GLU:CG	5:E:517:CIT:H41	2.45	0.47
1:G:399:LEU:HA	1:G:402:LEU:HB2	1.95	0.47
1:H:67:ILE:HD12	1:H:126:HIS:CE1	2.50	0.47
1:H:69:TRP:HA	1:H:99:ARG:HH22	1.79	0.47
1:E:133:ARG:HD3	1:E:166:TYR:CZ	2.50	0.47
1:G:253:THR:N	6:G:828:HOH:O	2.45	0.47
1:A:56:LYS:HD3	1:A:121:LEU:HD13	1.97	0.47
1:A:253:THR:CG2	1:A:254:ASP:O	2.63	0.47
1:B:310:THR:HB	4:B:516:SO4:O3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:SER:OG	1:F:141:PRO:O	2.22	0.47
1:C:41:GLU:HB2	1:C:100:PHE:HA	1.96	0.47
1:F:182:LEU:O	1:F:185:LEU:HB3	2.15	0.47
1:H:306:MET:O	1:H:307:THR:C	2.53	0.47
1:A:281:HIS:O	1:A:281:HIS:ND1	2.49	0.46
1:B:208:HIS:ND1	5:B:519:CIT:O5	2.46	0.46
1:H:24:THR:O	1:H:25:PRO:C	2.49	0.46
1:H:41:GLU:OE2	1:H:102:SER:HB3	2.15	0.46
1:C:239:HIS:ND1	4:C:512:SO4:O4	2.32	0.46
1:D:253:THR:HG23	1:D:254:ASP:O	2.15	0.46
1:F:129:ARG:HD2	1:F:211:GLU:OE2	2.14	0.46
1:H:224:ARG:HG3	1:H:224:ARG:HH11	1.80	0.46
1:H:274:CYS:SG	1:H:275:LYS:HE2	2.56	0.46
1:B:387:ASN:HD22	1:B:389:SER:H	1.62	0.46
1:G:342:LEU:HG	6:G:737:HOH:O	2.15	0.46
1:F:322:ILE:HG23	1:F:354:HIS:HB2	1.98	0.46
1:H:67:ILE:HD13	1:H:79:TYR:OH	2.16	0.46
1:F:282:TRP:O	1:F:283:PRO:C	2.54	0.46
1:G:288:LEU:HD21	1:G:321:TRP:CD1	2.50	0.46
1:B:110:LYS:HB3	1:B:111:PRO:HD3	1.98	0.46
1:D:253:THR:HB	6:D:610:HOH:O	2.16	0.46
1:G:318:MET:CA	6:G:835:HOH:O	2.64	0.46
1:A:72:PRO:HG2	6:A:1054:HOH:O	2.16	0.46
1:B:387:ASN:ND2	1:B:389:SER:H	2.14	0.46
1:B:247:ALA:O	6:B:697:HOH:O	2.21	0.45
1:G:232:PRO:HB3	3:G:502:ARB:O2	2.16	0.45
1:H:146:ASN:OD1	1:H:146:ASN:N	2.43	0.45
1:H:221:ARG:HA	6:H:637:HOH:O	2.16	0.45
5:D:515:CIT:C1	5:D:515:CIT:O5	2.64	0.45
1:G:40:THR:O	1:G:44:VAL:HG23	2.16	0.45
1:H:130:GLY:CA	6:H:634:HOH:O	2.64	0.45
1:C:294:GLY:HA2	1:C:297:SER:HB3	1.97	0.45
1:G:26:PRO:HB3	1:G:62:TYR:CE2	2.51	0.45
1:G:392:ARG:HB2	1:G:431:GLY:HA2	1.98	0.45
1:H:32:TRP:CE3	1:H:36:GLY:HA2	2.51	0.45
1:H:55:LEU:HB3	1:H:60:TRP:HB2	1.98	0.45
1:H:322:ILE:HG23	1:H:354:HIS:HB2	1.99	0.45
1:H:224:ARG:HG3	1:H:224:ARG:NH1	2.31	0.45
1:B:441:SER:HB2	1:B:442:PRO:HD2	1.98	0.45
2:D:503:GOL:O2	4:D:513:SO4:O1	2.23	0.45
1:H:16:MET:HB3	1:H:18:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:LEU:O	6:H:724:HOH:O	2.21	0.45
2:A:501:GOL:C3	6:A:1086:HOH:O	2.63	0.45
1:A:255:ASP:CG	2:A:501:GOL:H12	2.36	0.45
1:C:259:ARG:NH2	1:C:261:GLU:OE2	2.50	0.45
1:H:126:HIS:CD2	6:H:737:HOH:O	2.69	0.45
1:B:424:HIS:HB2	6:B:764:HOH:O	2.16	0.45
1:B:146:ASN:OD1	1:B:146:ASN:N	2.37	0.45
1:C:110:LYS:HB3	1:C:111:PRO:HD3	1.99	0.45
1:F:27:MET:HA	1:F:328:LEU:O	2.16	0.45
1:E:200:VAL:O	1:E:207:THR:HA	2.17	0.45
1:B:406:GLU:CB	1:B:407:PRO:CD	2.91	0.44
1:D:349:GLU:OE2	1:D:416:LYS:HG2	2.16	0.44
1:F:255:ASP:OD1	3:F:502:ARB:O2	2.26	0.44
1:F:137:HIS:CE1	1:H:137:HIS:CE1	3.05	0.44
1:G:244:VAL:HG11	1:H:275:LYS:HD2	1.99	0.44
1:G:378:GLU:O	1:G:380:ASN:N	2.51	0.44
1:A:208:HIS:HE1	6:A:611:HOH:O	2.00	0.44
1:H:220:ASP:C	6:H:776:HOH:O	2.56	0.44
1:A:379:GLY:N	6:A:1021:HOH:O	2.37	0.44
1:H:16:MET:HB3	1:H:18:HIS:HD2	1.82	0.44
1:H:61:GLU:C	6:H:744:HOH:O	2.56	0.44
1:H:193:PHE:CD1	1:H:227:VAL:CG1	3.01	0.44
1:C:236:PRO:HG2	1:C:239:HIS:HD2	1.83	0.44
1:D:221:ARG:NH2	4:D:514:SO4:O3	2.42	0.44
1:H:195:LYS:NZ	6:H:737:HOH:O	2.51	0.44
1:H:160:PRO:HG3	1:H:204:LEU:HG	1.98	0.44
1:H:239:HIS:O	1:H:243:PHE:CD2	2.70	0.44
1:A:290:LEU:HD21	1:A:317:MET:CE	2.48	0.44
1:A:409:LYS:HD2	1:A:444:VAL:HG23	2.00	0.44
1:B:306:MET:O	1:B:307:THR:C	2.56	0.44
1:B:392:ARG:HE	1:E:338:ASP:HA	1.83	0.44
1:A:89:GLU:CD	1:A:89:GLU:N	2.68	0.43
6:A:1139:HOH:O	2:E:504:GOL:H31	2.18	0.43
1:G:66:ASP:OD1	3:G:502:ARB:O4	2.33	0.43
1:H:253:THR:CG2	1:H:254:ASP:O	2.65	0.43
1:E:17:HIS:NE2	4:E:506:SO4:O4	2.50	0.43
1:G:55:LEU:HB3	1:G:60:TRP:CD1	2.53	0.43
1:G:258:ASP:OD1	1:G:258:ASP:N	2.50	0.43
1:A:379:GLY:CA	6:A:1021:HOH:O	2.66	0.43
1:C:365:ARG:HG3	1:C:370:VAL:HG22	1.99	0.43
5:C:519:CIT:H41	6:C:666:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:519:CIT:O1	5:C:519:CIT:O6	2.37	0.43
1:D:145:THR:HB	1:D:147:VAL:H	1.83	0.43
1:F:432:PRO:O	1:F:433:HIS:HB2	2.17	0.43
1:G:426:LEU:HD12	6:G:714:HOH:O	2.17	0.43
1:A:209:THR:N	5:A:515:CIT:O6	2.50	0.43
1:F:294:GLY:O	1:F:304:ASP:HA	2.19	0.43
1:F:313:GLU:OE2	1:F:433:HIS:HD2	2.00	0.43
1:H:348:GLU:O	1:H:348:GLU:CD	2.56	0.43
1:B:56:LYS:N	1:B:57:PRO:CD	2.82	0.43
1:B:340:TRP:O	1:B:343:SER:OG	2.26	0.43
1:E:126:HIS:HA	1:E:195:LYS:O	2.19	0.43
1:H:55:LEU:C	1:H:57:PRO:HD2	2.39	0.43
1:H:180:ASP:OD2	1:H:221:ARG:NH1	2.42	0.43
1:H:193:PHE:CD1	1:H:227:VAL:HG12	2.54	0.43
1:B:17:HIS:HE1	4:B:505:SO4:O2	2.01	0.43
1:C:432:PRO:O	1:C:433:HIS:HB2	2.19	0.43
1:E:110:LYS:HB3	1:E:111:PRO:HD3	2.01	0.43
1:E:145:THR:CG2	1:E:147:VAL:HG13	2.48	0.43
1:E:210:GLU:HB2	5:E:517:CIT:H41	2.00	0.43
1:E:248:ASN:ND2	6:E:733:HOH:O	2.51	0.43
1:H:235:ALA:HB2	1:H:251:ARG:O	2.17	0.43
1:F:199:ILE:HG21	1:F:230:LEU:HD22	2.00	0.43
1:H:23:LYS:HA	1:H:279:LEU:HD23	2.00	0.43
1:A:210:GLU:H	5:A:515:CIT:H41	1.84	0.43
1:H:113:ALA:O	1:H:117:HIS:CE1	2.72	0.43
1:H:294:GLY:O	1:H:304:ASP:HA	2.18	0.43
1:A:56:LYS:N	1:A:57:PRO:CD	2.82	0.43
1:F:142:ILE:HG22	1:F:143:LEU:O	2.18	0.43
1:G:118:ASN:HB3	6:G:779:HOH:O	2.19	0.43
1:H:89:GLU:OE2	1:H:89:GLU:HA	2.19	0.43
1:H:216:ARG:NE	6:H:743:HOH:O	2.51	0.43
1:A:290:LEU:HD21	1:A:317:MET:HE2	2.00	0.42
1:C:406:GLU:HB2	1:C:407:PRO:HD2	2.01	0.42
1:C:409:LYS:HD2	1:C:443:ALA:HA	2.00	0.42
1:B:417[B]:GLU:CD	6:B:860:HOH:O	2.57	0.42
1:C:258:ASP:OD1	1:C:258:ASP:N	2.52	0.42
1:D:14:ALA:HA	1:D:19:TYR:HD2	1.83	0.42
1:F:89:GLU:C	6:F:690:HOH:O	2.57	0.42
1:F:442:PRO:HA	6:F:714:HOH:O	2.19	0.42
1:H:67:ILE:HA	1:H:126:HIS:ND1	2.34	0.42
1:H:92:ARG:CD	1:H:181:SER:OG	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HB2	1:C:407:PRO:CD	2.49	0.42
1:F:387:ASN:HD22	1:F:387:ASN:C	2.22	0.42
1:H:174:GLY:N	2:H:502:GOL:C3	2.83	0.42
1:B:89:GLU:HG3	6:B:892:HOH:O	2.19	0.42
1:B:200:VAL:HB	1:B:232:PRO:O	2.20	0.42
1:D:70:TYR:O	1:D:72:PRO:HD3	2.20	0.42
1:H:277:VAL:HG21	1:H:324:PHE:CZ	2.55	0.42
1:G:266:MET:CE	1:G:285:ALA:HB1	2.50	0.42
1:D:311:LYS:HG2	1:D:340:TRP:CE2	2.55	0.42
1:E:409:LYS:O	1:E:440:LEU:HA	2.20	0.42
1:B:159:CYS:HB2	1:B:198:ASP:CG	2.40	0.42
1:E:200:VAL:HB	1:E:232:PRO:O	2.19	0.42
5:E:517:CIT:C2	6:E:670:HOH:O	2.66	0.42
1:G:396:SER:HB3	1:G:427:ALA:HB2	2.01	0.42
1:G:411:ARG:O	1:G:438:VAL:HA	2.20	0.42
1:D:324:PHE:O	1:D:325:ARG:HB2	2.20	0.42
1:E:210:GLU:CB	5:E:517:CIT:H41	2.49	0.42
1:G:409:LYS:HG2	6:G:648:HOH:O	2.20	0.42
1:A:66:ASP:HA	1:A:126:HIS:HB2	2.01	0.42
1:C:54:TYR:OH	2:C:504:GOL:H2	2.19	0.42
1:C:173:GLU:HG3	6:C:970:HOH:O	2.19	0.42
1:G:79:TYR:O	6:G:762:HOH:O	2.22	0.42
1:H:216:ARG:CD	6:H:743:HOH:O	2.67	0.42
1:D:210:GLU:HG2	5:D:515:CIT:H21	2.02	0.41
1:F:251:ARG:HA	1:F:284:ASP:HB3	2.02	0.41
1:G:253:THR:C	1:G:254:ASP:O	2.57	0.41
1:G:347:ASN:ND2	1:G:350:VAL:H	2.13	0.41
1:H:180:ASP:N	1:H:180:ASP:OD1	2.51	0.41
1:H:277:VAL:HG11	6:H:761:HOH:O	2.20	0.41
1:H:347:ASN:OD1	1:H:349:GLU:N	2.52	0.41
1:C:16:MET:HE2	6:C:892:HOH:O	2.19	0.41
1:C:208:HIS:HD1	5:C:519:CIT:C6	2.30	0.41
1:E:50:TYR:CD2	1:E:334:LEU:HB3	2.55	0.41
1:E:237:LEU:HD13	1:F:238:ASP:HA	2.02	0.41
1:F:268:GLU:HG3	6:F:852:HOH:O	2.21	0.41
1:H:159:CYS:HA	1:H:160:PRO:HD3	1.86	0.41
1:D:347:ASN:C	1:D:347:ASN:OD1	2.58	0.41
1:E:287:MET:O	1:E:289:PRO:HD3	2.19	0.41
1:G:55:LEU:HB3	1:G:60:TRP:HB2	2.01	0.41
1:H:122:LYS:HB2	6:H:744:HOH:O	2.20	0.41
1:H:364:TYR:CD1	1:H:364:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD11	1:C:156:ASN:HD21	1.85	0.41
1:B:184:GLN:O	1:B:188[A]:GLN:HG3	2.21	0.41
1:E:210:GLU:HG2	5:E:517:CIT:C4	2.51	0.41
1:G:318:MET:HG3	1:G:344:LEU:HD22	2.02	0.41
1:G:330:PHE:CD2	1:G:334:LEU:CD2	3.03	0.41
1:G:343:SER:N	6:G:737:HOH:O	2.52	0.41
1:H:252[B]:MET:SD	1:H:266[B]:MET:HE2	2.59	0.41
1:C:210:GLU:HG2	5:C:519:CIT:H21	2.02	0.41
1:D:416:LYS:HE2	6:D:935:HOH:O	2.20	0.41
1:G:378:GLU:N	1:G:378:GLU:CD	2.70	0.41
1:G:406:GLU:CG	1:G:407:PRO:O	2.68	0.41
1:H:199:ILE:HD11	1:H:212:ILE:HG13	2.03	0.41
1:A:387:ASN:HD22	1:A:387:ASN:C	2.23	0.41
1:F:236:PRO:HG2	1:F:239:HIS:HD2	1.86	0.41
1:G:195:LYS:HA	1:G:229:SER:HB3	2.02	0.41
1:G:385:MET:O	1:G:435:SER:HA	2.20	0.41
1:A:229:SER:HB2	1:A:249:MET:HG3	2.01	0.41
2:B:503:GOL:H2	4:B:514:SO4:O2	2.20	0.41
1:G:116:ILE:O	1:G:121:LEU:HB2	2.20	0.41
1:G:408:MET:CA	6:G:713:HOH:O	2.67	0.41
1:H:40:THR:O	1:H:44:VAL:HG23	2.21	0.41
1:A:20:GLN:HE21	1:A:23:LYS:HE3	1.85	0.41
1:G:227:VAL:HA	1:G:248:ASN:HD22	1.86	0.41
1:G:265:ASP:HB3	6:G:765:HOH:O	2.21	0.41
1:D:235:ALA:HA	1:D:236:PRO:HD3	1.92	0.41
1:G:253:THR:HB	6:G:828:HOH:O	2.20	0.41
1:G:325:ARG:HD3	6:G:824:HOH:O	2.20	0.41
5:G:510:CIT:O3	5:G:510:CIT:C2	2.65	0.41
1:A:217:LYS:HE3	6:A:1106:HOH:O	2.21	0.41
5:C:519:CIT:O6	5:C:519:CIT:C1	2.69	0.41
1:G:315:ARG:O	1:G:316:THR:C	2.58	0.41
1:G:386:PHE:CE1	1:G:435:SER:HB2	2.56	0.41
1:H:204:LEU:HB2	1:H:205:TYR:CD2	2.56	0.41
1:H:174:GLY:N	2:H:502:GOL:H31	2.36	0.40
1:H:273:TRP:HE3	1:H:276:LEU:HD23	1.86	0.40
1:A:272:LYS:CD	6:B:774:HOH:O	2.70	0.40
1:G:387:ASN:HB3	1:G:431:GLY:O	2.21	0.40
1:H:176:GLN:HB3	2:H:502:GOL:H2	2.02	0.40
1:G:235:ALA:HA	1:G:236:PRO:HD3	1.93	0.40
1:H:61:GLU:HB2	6:H:744:HOH:O	2.21	0.40
1:H:359:GLY:O	6:H:764:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLU:HB2	1:D:100:PHE:HA	2.03	0.40
1:F:90:TYR:N	6:F:690:HOH:O	2.53	0.40
1:F:276:LEU:HD22	1:F:276:LEU:N	2.37	0.40
1:C:20:GLN:HG3	6:C:779:HOH:O	2.21	0.40
1:E:392:ARG:HD3	1:E:429:GLU:OE1	2.21	0.40

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

All (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
1	G	443	ALA
1	H	53	LYS
1	H	96	ALA
1	H	60	TRP
1	H	115	TYR
1	F	66	ASP
1	D	447	GLY
1	G	397	VAL

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

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	89	GLU
1	A	121	LEU

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Mol	Chain	Res	Type
1	A	203	LYS
1	A	236	PRO
1	A	237	LEU
1	A	253	THR
1	A	298	VAL
1	A	321	TRP
1	A	383	VAL
1	A	387	ASN
1	A	405	MET
1	A	406	GLU
1	A	413	LEU
1	A	419	LEU
1	A	421	LEU
1	A	429	GLU
1	B	71	GLU
1	B	84	PRO
1	B	89	GLU
1	B	121	LEU
1	B	145	THR
1	B	232	PRO
1	B	253	THR
1	B	298	VAL
1	B	321	TRP
1	B	381	GLN
1	B	387	ASN
1	B	406	GLU
1	B	413	LEU
1	B	417[A]	GLU
1	B	417[B]	GLU
1	B	419	LEU
1	B	430	LEU
1	C	15	SER
1	C	66	ASP
1	C	71	GLU
1	C	89	GLU
1	C	121	LEU
1	C	154	ASP
1	C	203	LYS
1	C	237	LEU
1	C	253	THR
1	C	298	VAL
1	C	321	TRP

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Mol	Chain	Res	Type
1	C	383	VAL
1	C	387	ASN
1	C	391	LYS
1	C	402	LEU
1	C	409	LYS
1	C	413	LEU
1	C	419	LEU
1	C	430	LEU
1	D	53	LYS
1	D	71	GLU
1	D	121	LEU
1	D	145	THR
1	D	154	ASP
1	D	216	ARG
1	D	217	LYS
1	D	237	LEU
1	D	249	MET
1	D	253	THR
1	D	298	VAL
1	D	321	TRP
1	D	383	VAL
1	D	387	ASN
1	D	391	LYS
1	D	392	ARG
1	D	402	LEU
1	D	413	LEU
1	D	417	GLU
1	D	419	LEU
1	D	421	LEU
1	D	430	LEU
1	E	15	SER
1	E	71	GLU
1	E	121	LEU
1	E	203	LYS
1	E	253	THR
1	E	298	VAL
1	E	321	TRP
1	E	383	VAL
1	E	387	ASN
1	E	400	LYS
1	E	402	LEU
1	E	413	LEU

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Mol	Chain	Res	Type
1	E	419	LEU
1	E	421	LEU
1	E	430	LEU
1	F	71	GLU
1	F	104	LYS
1	F	121	LEU
1	F	147	VAL
1	F	172	LYS
1	F	188	GLN
1	F	203	LYS
1	F	237	LEU
1	F	298	VAL
1	F	321	TRP
1	F	383	VAL
1	F	387	ASN
1	F	391	LYS
1	F	392	ARG
1	F	402	LEU
1	F	413	LEU
1	F	419	LEU
1	F	422	VAL
1	F	430	LEU
1	F	433	HIS
1	G	15	SER
1	G	16	MET
1	G	34	CYS
1	G	71	GLU
1	G	121	LEU
1	G	199	ILE
1	G	249	MET
1	G	253	THR
1	G	258	ASP
1	G	263	LEU
1	G	298	VAL
1	G	309	PHE
1	G	321	TRP
1	G	339	GLU
1	G	347	ASN
1	G	350	VAL
1	G	363	VAL
1	G	365	ARG
1	G	378	GLU

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Mol	Chain	Res	Type
1	G	381	GLN
1	G	383	VAL
1	G	387	ASN
1	G	394	VAL
1	G	400	LYS
1	G	402	LEU
1	G	406	GLU
1	G	408	MET
1	G	416	LYS
1	G	419	LEU
1	G	421	LEU
1	G	425	GLN
1	G	430	LEU
1	G	436	ILE
1	G	438	VAL
1	G	441	SER
1	H	15	SER
1	H	16	MET
1	H	20	GLN
1	H	34	CYS
1	H	71	GLU
1	H	75	ASN
1	H	91	SER
1	H	107	LYS
1	H	121	LEU
1	H	146	ASN
1	H	147	VAL
1	H	154	ASP
1	H	171	ARG
1	H	181	SER
1	H	209	THR
1	H	237	LEU
1	H	249	MET
1	H	253	THR
1	H	279	LEU
1	H	303	THR
1	H	316	THR
1	H	321	TRP
1	H	361	ARG
1	H	383	VAL
1	H	402	LEU
1	H	405	MET

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Mol	Chain	Res	Type
1	H	413	LEU
1	H	419	LEU
1	H	421	LEU
1	H	430	LEU
1	H	441	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	156	ASN
1	A	208	HIS
1	A	248	ASN
1	A	381	GLN
1	A	387	ASN
1	B	17	HIS
1	B	20	GLN
1	B	156	ASN
1	B	248	ASN
1	B	356	ASN
1	B	387	ASN
1	C	156	ASN
1	C	248	ASN
1	C	356	ASN
1	C	387	ASN
1	D	156	ASN
1	D	248	ASN
1	D	356	ASN
1	D	387	ASN
1	E	18	HIS
1	E	156	ASN
1	E	208	HIS
1	E	248	ASN
1	E	356	ASN
1	E	387	ASN
1	F	134	GLN
1	F	137	HIS
1	F	248	ASN
1	F	356	ASN
1	F	387	ASN
1	F	433	HIS
1	G	118	ASN

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Mol	Chain	Res	Type
1	G	156	ASN
1	G	208	HIS
1	G	248	ASN
1	G	314	GLN
1	G	337	ASN
1	G	347	ASN
1	G	356	ASN
1	G	387	ASN
1	H	17	HIS
1	H	18	HIS
1	H	20	GLN
1	H	75	ASN
1	H	126	HIS
1	H	137	HIS
1	H	246	ASN
1	H	248	ASN
1	H	356	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
5	G	510	CIT	C2-C3	5.02	1.60	1.53
5	D	515	CIT	C3-C6	-4.63	1.48	1.53
5	C	519	CIT	C2-C3	-3.99	1.48	1.53
5	D	515	CIT	C2-C3	-3.94	1.48	1.53
5	G	510	CIT	C4-C3	-3.86	1.49	1.53
5	A	515	CIT	O6-C6	-3.37	1.17	1.30
5	C	519	CIT	O3-C5	3.22	1.32	1.22
3	A	502	ARB	O1-C1	2.45	1.47	1.39
3	G	502	ARB	O1-C1	2.42	1.47	1.39
5	A	515	CIT	O1-C1	2.40	1.30	1.22
3	B	504	ARB	O5-C5	-2.40	1.39	1.43
5	C	519	CIT	O4-C5	-2.34	1.22	1.30
5	C	519	CIT	C3-C6	-2.33	1.51	1.53
3	A	502	ARB	O5-C1	2.30	1.46	1.43
5	A	515	CIT	C4-C3	-2.28	1.51	1.53
3	H	503	ARB	C4-C3	2.25	1.55	1.52
5	A	515	CIT	C2-C3	2.23	1.56	1.53
3	C	506	ARB	C3-C2	-2.19	1.46	1.52
5	A	515	CIT	O3-C5	2.17	1.29	1.22
3	D	504	ARB	C1-C2	2.17	1.57	1.52
5	G	510	CIT	O6-C6	-2.12	1.22	1.30

All (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
5	B	519	CIT	O6-C6-C3	7.47	126.02	113.05
5	C	519	CIT	C3-C4-C5	7.31	131.52	113.81
5	G	510	CIT	O7-C3-C6	-6.50	99.73	108.86
3	A	502	ARB	O5-C1-C2	6.24	118.71	109.43
3	E	505	ARB	O5-C1-C2	6.13	118.54	109.43
5	G	510	CIT	O7-C3-C2	5.91	123.22	109.40
3	F	502	ARB	O5-C1-C2	5.91	118.21	109.43
5	G	510	CIT	C3-C2-C1	5.76	127.77	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	510	CIT	O5-C6-C3	-5.58	114.35	122.25
3	C	506	ARB	O5-C1-C2	5.35	117.38	109.43
3	E	505	ARB	O4-C4-C3	5.12	120.39	110.14
3	D	504	ARB	O5-C1-C2	5.03	116.90	109.43
3	C	506	ARB	C5-C4-C3	4.85	115.62	109.67
5	D	515	CIT	C3-C2-C1	4.67	125.12	113.81
5	E	517	CIT	C4-C3-C6	-4.65	100.12	110.11
2	C	504	GOL	O2-C2-C3	-4.59	88.89	109.12
3	B	504	ARB	C5-O5-C1	4.50	120.27	112.71
3	G	502	ARB	O3-C3-C4	-4.42	101.54	109.99
3	D	504	ARB	C5-O5-C1	4.41	120.13	112.71
3	B	504	ARB	O5-C1-C2	4.38	115.94	109.43
3	F	502	ARB	O3-C3-C4	4.30	118.23	109.99
5	B	519	CIT	C4-C3-C2	4.28	120.33	109.16
5	C	519	CIT	C4-C3-C6	-4.22	101.05	110.11
3	B	504	ARB	O4-C4-C5	-4.19	100.58	109.15
5	G	510	CIT	C4-C3-C6	-4.12	101.25	110.11
5	G	510	CIT	O6-C6-C3	4.10	120.17	113.05
3	H	503	ARB	C5-C4-C3	4.10	114.71	109.67
5	A	515	CIT	O5-C6-C3	4.10	128.06	122.25
5	E	517	CIT	C3-C4-C5	3.98	123.45	113.81
5	B	519	CIT	C3-C2-C1	3.91	123.29	113.81
3	F	502	ARB	O2-C2-C1	3.87	118.14	109.16
3	E	505	ARB	C5-O5-C1	3.84	119.17	112.71
3	G	502	ARB	C4-C3-C2	3.70	117.29	110.89
3	A	502	ARB	O5-C5-C4	3.63	116.37	110.77
5	E	517	CIT	O7-C3-C6	-3.62	103.79	108.86
5	C	519	CIT	O6-C6-C3	3.45	119.05	113.05
5	A	515	CIT	C3-C2-C1	3.38	122.00	113.81
5	E	517	CIT	C2-C3-C6	3.36	117.32	110.11
3	E	505	ARB	O3-C3-C4	3.32	116.35	109.99
3	F	502	ARB	C5-O5-C1	3.27	118.21	112.71
3	H	503	ARB	C4-C3-C2	3.27	116.55	110.89
5	C	519	CIT	C2-C3-C6	3.25	117.10	110.11
3	A	502	ARB	O4-C4-C3	3.13	116.41	110.14
5	D	515	CIT	O4-C5-C4	3.11	124.35	114.35
2	C	504	GOL	O3-C3-C2	-3.09	95.37	110.20
5	B	519	CIT	O2-C1-C2	3.02	124.05	114.35
3	F	502	ARB	O3-C3-C2	-3.02	103.38	110.35
5	C	519	CIT	O7-C3-C2	-3.00	102.38	109.40
3	F	502	ARB	O4-C4-C3	2.99	116.12	110.14
3	E	505	ARB	C5-C4-C3	-2.96	106.03	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	503	GOL	C3-C2-C1	-2.92	100.34	111.70
3	C	506	ARB	O2-C2-C3	2.89	117.03	110.35
5	C	519	CIT	C4-C3-C2	2.88	116.68	109.16
3	B	504	ARB	O2-C2-C1	2.88	115.83	109.16
3	B	504	ARB	O4-C4-C3	2.87	115.89	110.14
3	E	505	ARB	O4-C4-C5	-2.86	103.30	109.15
3	D	504	ARB	O3-C3-C4	-2.84	104.56	109.99
3	C	506	ARB	O3-C3-C2	-2.83	103.80	110.35
3	F	502	ARB	C5-C4-C3	-2.83	106.19	109.67
3	G	502	ARB	O4-C4-C5	-2.82	103.38	109.15
5	C	519	CIT	O7-C3-C6	2.79	112.78	108.86
3	C	506	ARB	O4-C4-C5	-2.77	103.48	109.15
3	A	502	ARB	C5-C4-C3	-2.75	106.28	109.67
5	D	515	CIT	O6-C6-C3	2.70	117.74	113.05
5	G	510	CIT	C2-C3-C6	2.70	115.90	110.11
3	A	502	ARB	O2-C2-C1	2.68	115.39	109.16
3	A	502	ARB	O3-C3-C2	-2.67	104.17	110.35
3	G	502	ARB	C5-C4-C3	2.67	112.95	109.67
3	A	502	ARB	C5-O5-C1	2.66	117.18	112.71
3	A	502	ARB	O4-C4-C5	-2.65	103.73	109.15
5	D	515	CIT	O7-C3-C6	-2.63	105.18	108.86
3	G	502	ARB	O4-C4-C3	2.54	115.22	110.14
5	A	515	CIT	O7-C3-C2	2.53	115.33	109.40
3	A	502	ARB	C1-C2-C3	2.52	115.55	110.31
4	C	509	SO4	O2-S-O1	-2.47	91.20	109.43
5	D	515	CIT	C3-C4-C5	2.45	119.75	113.81
5	D	515	CIT	O4-C5-O3	-2.45	117.19	123.30
3	B	504	ARB	O3-C3-C2	-2.43	104.72	110.35
3	D	504	ARB	O1-C1-C2	2.43	115.88	109.03
4	C	509	SO4	O4-S-O1	2.43	121.98	109.31
3	G	502	ARB	O1-C1-C2	2.42	115.83	109.03
5	E	517	CIT	O3-C5-C4	-2.40	115.92	122.94
2	H	501	GOL	C3-C2-C1	-2.39	102.40	111.70
3	E	505	ARB	O5-C5-C4	2.31	114.34	110.77
3	H	503	ARB	C1-C2-C3	2.27	115.03	110.31
3	E	505	ARB	C1-C2-C3	2.27	115.02	110.31
3	D	504	ARB	O5-C5-C4	2.19	114.15	110.77
3	B	504	ARB	C5-C4-C3	2.14	112.29	109.67
5	A	515	CIT	O6-C6-O5	-2.12	117.06	123.82
4	A	513	SO4	O4-S-O3	2.12	118.13	109.06
3	D	504	ARB	O2-C2-C3	2.12	115.25	110.35
3	G	502	ARB	O3-C3-C2	-2.08	105.54	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	503	GOL	O1-C1-C2	-2.07	100.28	110.20
3	G	502	ARB	O2-C2-C3	2.07	115.13	110.35
3	C	506	ARB	O2-C2-C1	2.05	113.92	109.16
5	G	510	CIT	O7-C3-C4	-2.05	104.60	109.40
4	G	503	SO4	O4-S-O3	2.03	117.72	109.06
3	G	502	ARB	C5-O5-C1	2.02	116.10	112.71
2	B	501	GOL	O2-C2-C3	-2.02	100.25	109.12

There are no chirality outliers.

All (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
2	D	501	GOL	O1-C1-C2-C3
2	E	501	GOL	O1-C1-C2-C3
2	E	502	GOL	O1-C1-C2-C3
2	E	504	GOL	O1-C1-C2-O2
2	E	504	GOL	O1-C1-C2-C3
2	F	501	GOL	C1-C2-C3-O3
2	H	502	GOL	O1-C1-C2-C3
2	H	502	GOL	C1-C2-C3-O3
5	A	515	CIT	O7-C3-C4-C5
5	A	515	CIT	C2-C3-C6-O5
5	A	515	CIT	C2-C3-C6-O6
5	A	515	CIT	O7-C3-C6-O5
5	A	515	CIT	O7-C3-C6-O6
5	B	519	CIT	C2-C3-C4-C5
5	B	519	CIT	C6-C3-C4-C5
5	C	519	CIT	C1-C2-C3-O7
5	C	519	CIT	C1-C2-C3-C4
5	C	519	CIT	C1-C2-C3-C6
5	D	515	CIT	C1-C2-C3-O7
5	D	515	CIT	C1-C2-C3-C4
5	D	515	CIT	C2-C3-C6-O5
5	D	515	CIT	C2-C3-C6-O6
5	D	515	CIT	O7-C3-C6-O5
5	D	515	CIT	O7-C3-C6-O6
5	E	517	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
5	E	517	CIT	C2-C3-C6-O6
5	E	517	CIT	O7-C3-C6-O5
5	E	517	CIT	O7-C3-C6-O6
5	G	510	CIT	O7-C3-C6-O5
5	G	510	CIT	O7-C3-C6-O6
5	B	519	CIT	C1-C2-C3-O7
5	D	515	CIT	C1-C2-C3-C6
2	A	501	GOL	O2-C2-C3-O3
2	F	501	GOL	O2-C2-C3-O3
5	B	519	CIT	O7-C3-C4-C5
2	A	501	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3
2	C	505	GOL	C1-C2-C3-O3
2	D	503	GOL	O1-C1-C2-C3
2	E	501	GOL	C1-C2-C3-O3
2	G	501	GOL	O1-C1-C2-C3
5	B	519	CIT	C2-C3-C6-O6
5	G	510	CIT	C4-C3-C6-O5
5	G	510	CIT	C4-C3-C6-O6
2	A	501	GOL	O1-C1-C2-O2
2	B	502	GOL	O2-C2-C3-O3
2	B	503	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
2	C	504	GOL	O1-C1-C2-O2
2	D	501	GOL	O1-C1-C2-O2
2	D	503	GOL	O1-C1-C2-O2
2	E	502	GOL	O1-C1-C2-O2
2	H	502	GOL	O1-C1-C2-O2
2	H	502	GOL	O2-C2-C3-O3
5	B	519	CIT	C1-C2-C3-C4
2	B	501	GOL	O1-C1-C2-O2
2	C	504	GOL	O2-C2-C3-O3
2	E	501	GOL	O1-C1-C2-O2
5	E	517	CIT	O7-C3-C4-C5
5	E	517	CIT	C4-C3-C6-O5
5	E	517	CIT	C4-C3-C6-O6
2	C	501	GOL	O2-C2-C3-O3
2	E	501	GOL	O2-C2-C3-O3
5	A	515	CIT	C6-C3-C4-C5
2	B	502	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	503	GOL	O2-C2-C3-O3
5	C	519	CIT	O7-C3-C4-C5
5	B	519	CIT	O2-C1-C2-C3
2	D	502	GOL	O1-C1-C2-O2
5	B	519	CIT	O1-C1-C2-C3
2	G	501	GOL	O1-C1-C2-O2
5	A	515	CIT	C2-C3-C4-C5
5	D	515	CIT	O7-C3-C4-C5
2	E	503	GOL	C1-C2-C3-O3
5	B	519	CIT	C2-C3-C6-O5
5	G	510	CIT	C2-C3-C6-O6
2	G	501	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 (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, 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%)

All (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
1	C	444	VAL	8.7
1	G	405	MET	7.2
1	H	127	ILE	7.1
1	H	405	MET	6.3
1	F	15	SER	6.0
1	C	405	MET	5.8
1	G	391	LYS	5.7
1	A	14	ALA	5.5
1	H	443	ALA	5.4
1	E	406	GLU	5.3
1	E	405	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	H	288	LEU	5.2
1	F	405	MET	5.2
1	C	14	ALA	5.1
1	H	15	SER	5.1
1	A	444	VAL	5.0
1	G	15	SER	4.8
1	H	146	ASN	4.5
1	H	104	LYS	4.4
1	H	103	ALA	4.4
1	E	14	ALA	4.4
1	H	406	GLU	4.4
1	G	403	GLY	4.4
1	H	196	VAL	4.3
1	G	404	CYS	4.3
1	G	442	PRO	4.3
1	F	443	ALA	4.2
1	B	405	MET	4.2
1	H	118	ASN	4.0
1	G	430	LEU	4.0
1	D	14	ALA	4.0
1	G	377	ALA	4.0
1	H	64	VAL	3.9
1	G	443	ALA	3.9
1	G	328	LEU	3.9
1	E	421	LEU	3.8
1	H	101	PRO	3.8
1	B	15	SER	3.7
1	H	125	ILE	3.7
1	G	341	THR	3.7
1	G	321	TRP	3.7
1	H	107	LYS	3.7
1	H	328	LEU	3.6
1	G	388	ILE	3.6
1	F	127	ILE	3.6
1	G	401	ASP	3.5
1	H	190	GLY	3.4
1	E	424	HIS	3.4
1	H	204	LEU	3.4
1	G	389	SER	3.3
1	F	146	ASN	3.3
1	H	126	HIS	3.3
1	H	287	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	171	ARG	3.3
1	H	183	PHE	3.3
1	H	331	GLY	3.2
1	G	424	HIS	3.2
1	G	379	GLY	3.2
1	G	406	GLU	3.1
1	H	424	HIS	3.1
1	G	203	LYS	3.1
1	E	442	PRO	3.1
1	E	443	ALA	3.1
1	H	173	GLU	3.1
1	H	329	MET	3.1
1	F	196	VAL	3.1
1	C	423	LYS	3.1
1	G	363	VAL	3.1
1	E	420	GLY	3.0
1	F	406	GLU	3.0
1	G	410	ALA	3.0
1	H	203	LYS	3.0
1	H	50	TYR	3.0
1	E	204	LEU	2.9
1	F	303	THR	2.9
1	G	322	ILE	2.8
1	C	443	ALA	2.8
1	C	424	HIS	2.8
1	H	147	VAL	2.8
1	G	287	MET	2.8
1	F	442	PRO	2.8
1	H	66	ASP	2.8
1	H	114	ASP	2.8
1	B	127	ILE	2.8
1	G	407	PRO	2.8
1	H	145	THR	2.8
1	E	400	LYS	2.8
1	H	195	LYS	2.8
1	H	112	LEU	2.8
1	G	370	VAL	2.7
1	H	128	MET	2.7
1	G	378	GLU	2.7
1	G	438	VAL	2.7
1	C	127	ILE	2.7
1	E	423	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	98	ASN	2.7
1	E	203	LYS	2.7
1	H	379	GLY	2.7
1	H	378	GLU	2.6
1	H	54	TYR	2.6
1	G	431	GLY	2.6
1	D	377	ALA	2.6
1	H	197	ALA	2.6
1	F	145	THR	2.6
1	F	424	HIS	2.6
1	C	421	LEU	2.6
1	E	407	PRO	2.6
1	C	406	GLU	2.6
1	H	16	MET	2.6
1	H	30	ASN	2.6
1	E	377	ALA	2.5
1	G	204	LEU	2.5
1	H	175	ALA	2.5
1	F	423	LYS	2.5
1	H	105	GLY	2.5
1	G	422	VAL	2.5
1	H	303	THR	2.5
1	H	42	ASP	2.5
1	G	367	ASN	2.4
1	E	379	GLY	2.4
1	G	323	ILE	2.4
1	F	195	LYS	2.4
1	A	405	MET	2.4
1	D	127	ILE	2.4
1	C	288	LEU	2.4
1	C	196	VAL	2.4
1	F	421	LEU	2.3
1	C	407	PRO	2.3
1	H	17	HIS	2.3
1	G	400	LYS	2.3
1	G	64	VAL	2.3
1	G	301	GLY	2.3
1	H	423	LYS	2.3
1	G	395	VAL	2.3
1	H	97	VAL	2.3
1	G	262	LEU	2.3
1	G	343	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	288	LEU	2.3
1	H	327	PRO	2.3
1	E	15	SER	2.2
1	D	203	LYS	2.2
1	D	405	MET	2.2
1	H	193	PHE	2.2
1	H	256	PHE	2.2
1	G	396	SER	2.2
1	H	174	GLY	2.2
1	G	340	TRP	2.2
1	F	89	GLU	2.2
1	H	295	ILE	2.2
1	H	171	ARG	2.2
1	F	391	LYS	2.2
1	H	219	ILE	2.2
1	G	421	LEU	2.2
1	F	147	VAL	2.2
1	G	318	MET	2.2
1	C	13	ASP	2.2
1	G	320	LEU	2.2
1	H	182	LEU	2.2
1	G	397	VAL	2.2
1	G	394	VAL	2.1
1	H	65	VAL	2.1
1	F	151	ASP	2.1
1	G	408	MET	2.1
1	H	111	PRO	2.1
1	H	339	GLU	2.1
1	G	317	MET	2.1
1	H	116	ILE	2.1
1	G	344	LEU	2.1
1	H	290	LEU	2.1
1	D	64	VAL	2.1
1	H	19	TYR	2.1
1	G	312	ASP	2.1
1	G	425	GLN	2.1
1	G	423	LYS	2.1
1	H	194	VAL	2.1
1	C	230	LEU	2.1
1	F	204	LEU	2.1
1	G	390	GLU	2.1
1	F	205	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	260	TRP	2.1
1	H	223	GLY	2.1
1	D	15	SER	2.0
1	E	320	LEU	2.0
1	G	67	ILE	2.0
1	H	67	ILE	2.0
1	G	118	ASN	2.0
1	H	69	TRP	2.0
1	H	151	ASP	2.0
1	G	329	MET	2.0
1	F	420	GLY	2.0
1	H	58	PHE	2.0
1	G	364	TYR	2.0
1	G	285	ALA	2.0
1	G	53	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 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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

There are no such residues in this entry.