Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 PM GMT

PDB ID	:	4NX0
Title	:	Crystal structure of Abp-WT, a GH27-b-L-arabinopyranosidase from Geobacillus stearothermophilus
Authors	:	Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on	:	2013-12-08
Resolution	:	2.28 Å(reported)

This is a 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

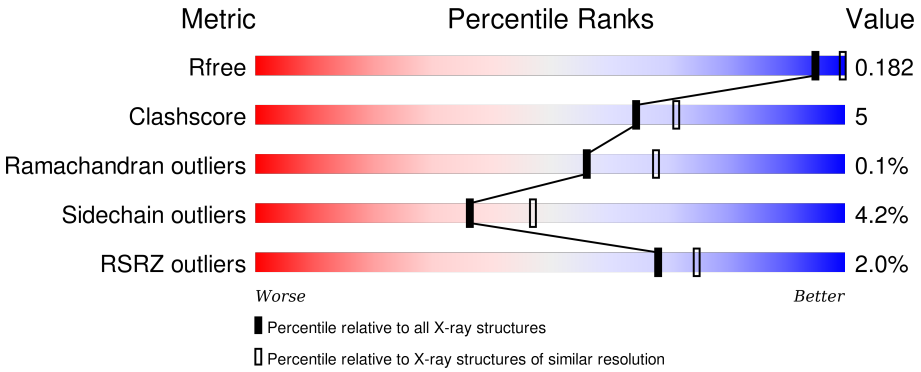
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.28 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	85% 9%
1	B	448	85% 9%
1	C	448	2% 87% 9%
1	D	448	89% 8%
1	E	448	3% 87% 8%

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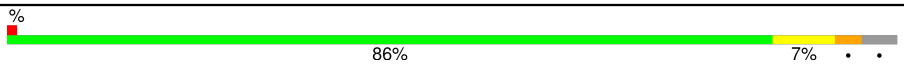
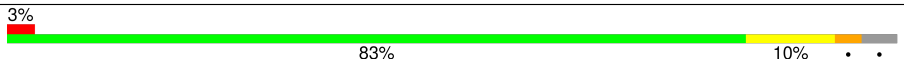
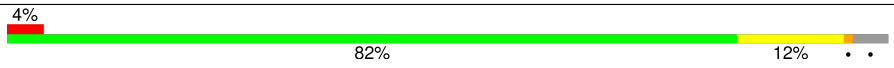
Mol	Chain	Length	Quality of chain
1	F	448	
1	G	448	
1	H	448	

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	GOL	A	501	-	-	-	X
2	GOL	A	504	-	-	-	X
2	GOL	B	503	-	-	-	X
2	GOL	B	504	-	-	-	X
2	GOL	B	505	-	-	-	X
2	GOL	B	508	-	-	-	X
2	GOL	C	503	-	-	-	X
2	GOL	C	505	-	-	X	X
2	GOL	D	502	-	-	X	X
2	GOL	D	505	-	-	X	X
2	GOL	E	504	-	-	-	X
2	GOL	E	505	-	-	X	X
2	GOL	F	502	-	-	X	-
2	GOL	F	504	-	-	-	X
2	GOL	H	502	-	-	-	X
3	SO4	A	505	-	-	-	X
3	SO4	A	511	-	-	-	X
3	SO4	B	515	-	-	-	X
3	SO4	C	507	-	-	-	X
3	SO4	C	515	-	-	-	X
3	SO4	C	516	-	-	-	X
3	SO4	C	517	-	-	-	X
3	SO4	D	508	-	-	-	X
3	SO4	D	509	-	-	-	X
3	SO4	D	517	-	-	-	X
3	SO4	E	509	-	-	-	X
3	SO4	E	514	-	-	-	X
3	SO4	E	515	-	-	-	X
3	SO4	F	508	-	-	-	X
3	SO4	F	511	-	-	-	X
3	SO4	F	512	-	-	-	X
3	SO4	F	513	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	F	514	-	-	-	X
3	SO4	G	505	-	-	-	X
3	SO4	G	506	-	-	-	X
3	SO4	G	507	-	-	-	X
3	SO4	H	506	-	-	-	X
3	SO4	H	509	-	-	-	X
3	SO4	H	510	-	-	-	X
3	SO4	H	513	-	-	-	X
4	CIT	A	515	-	-	X	X
4	CIT	B	520	-	-	X	X
4	CIT	C	519	-	-	-	X
4	CIT	E	517	-	-	-	X
4	CIT	G	513	-	-	X	X

2 Entry composition (i)

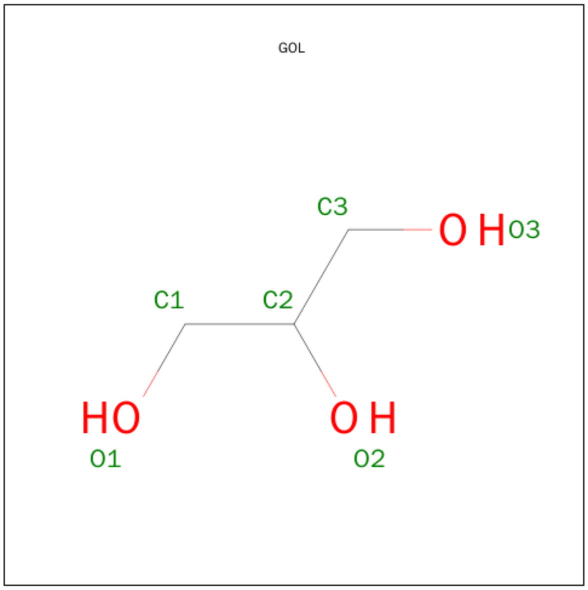
There are 5 unique types of molecules in this entry. The entry contains 32820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Abp, a GH27 beta-L-arabinopyranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	4	0
			3492	2233	598	636	25			
1	B	430	Total	C	N	O	S	0	4	0
			3496	2235	598	638	25			
1	C	431	Total	C	N	O	S	0	2	0
			3487	2230	598	634	25			
1	D	435	Total	C	N	O	S	0	1	0
			3506	2243	603	635	25			
1	E	430	Total	C	N	O	S	0	3	0
			3484	2228	597	634	25			
1	F	430	Total	C	N	O	S	0	0	0
			3470	2219	596	630	25			
1	G	430	Total	C	N	O	S	0	2	0
			3481	2226	596	634	25			
1	H	430	Total	C	N	O	S	0	0	0
			3470	2219	596	630	25			

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



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

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

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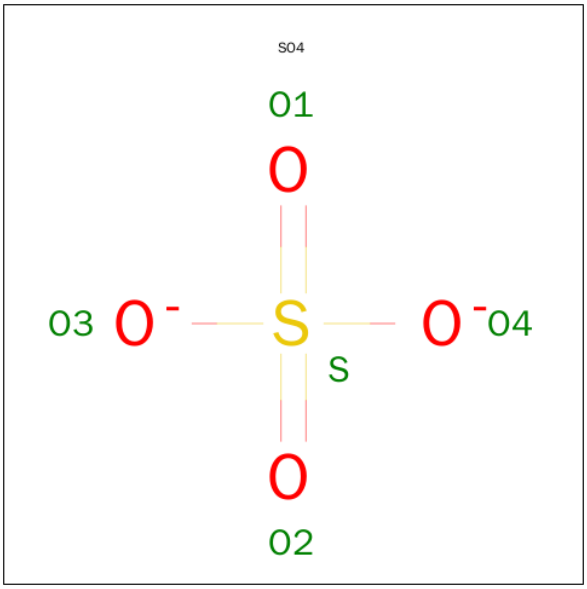
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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

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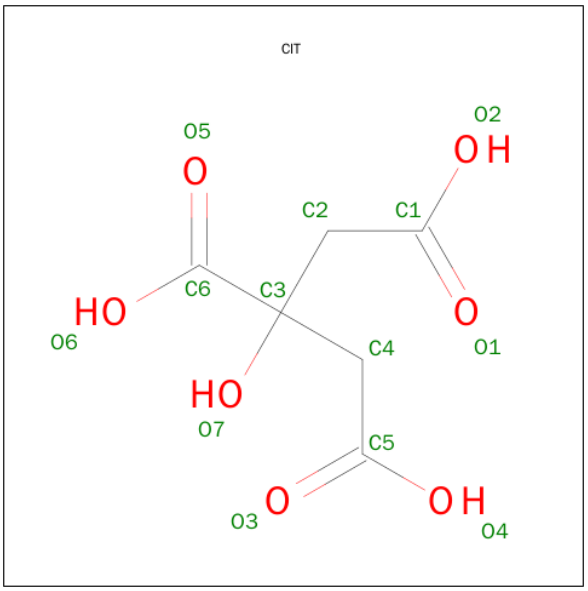
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	662	Total O 662 662	0	0
5	B	625	Total O 625 625	0	0
5	C	579	Total O 579 579	0	0
5	D	536	Total O 536 536	0	0
5	E	500	Total O 500 500	0	0
5	F	495	Total O 495 495	0	0
5	G	439	Total O 439 439	0	0

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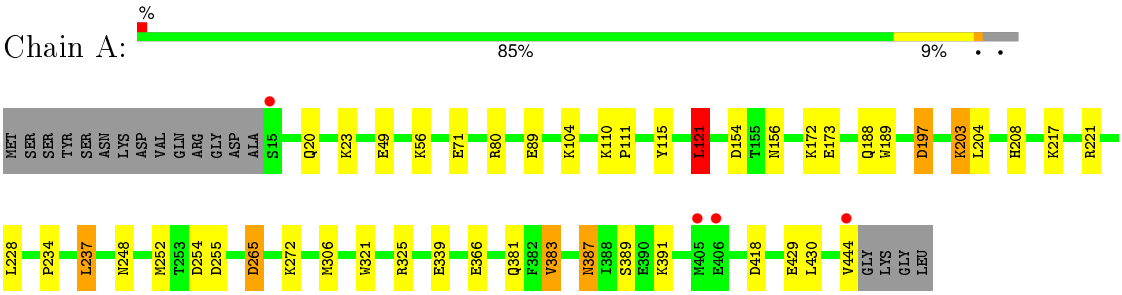
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	368	Total	O	0	0
			368	368		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

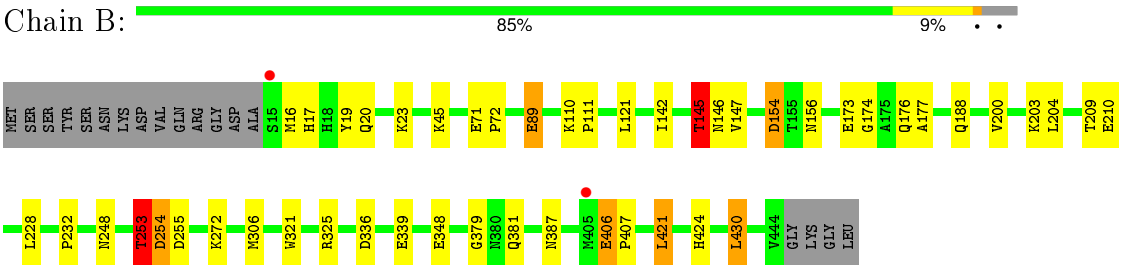
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain A:



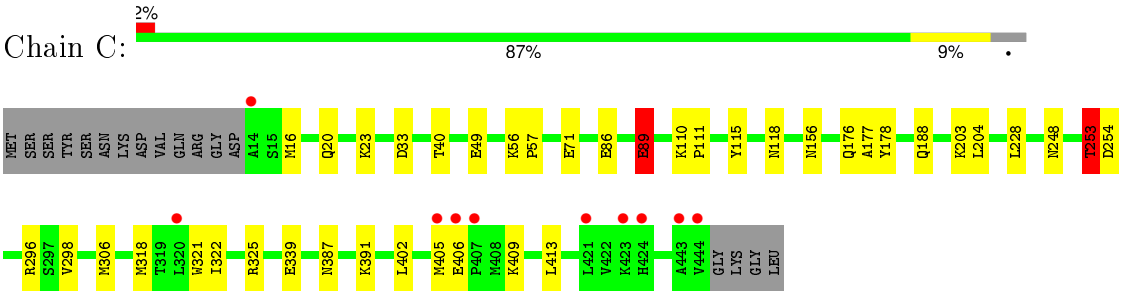
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain B:



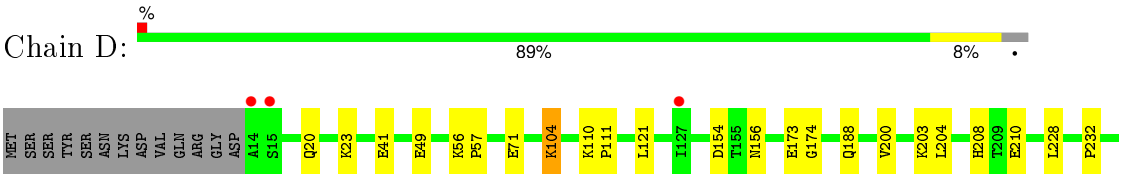
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain C:

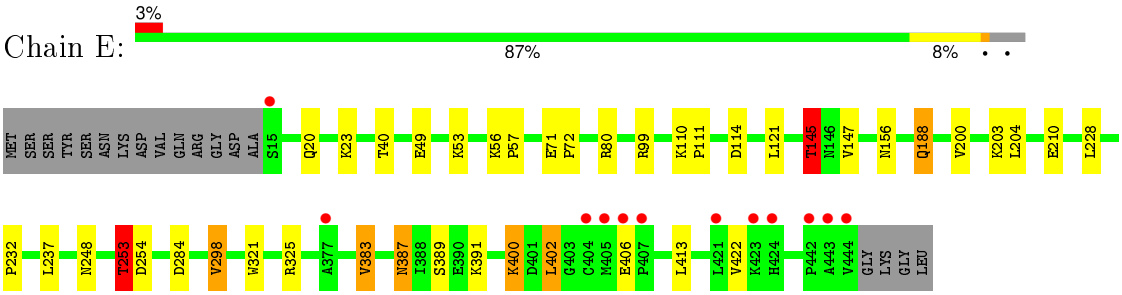


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

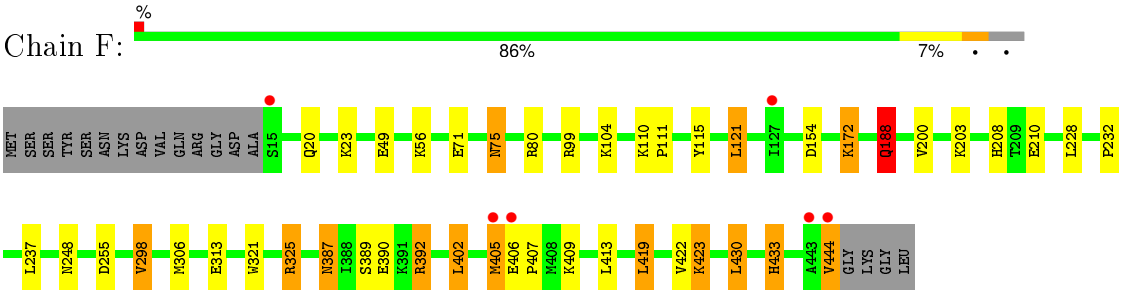
Chain D:



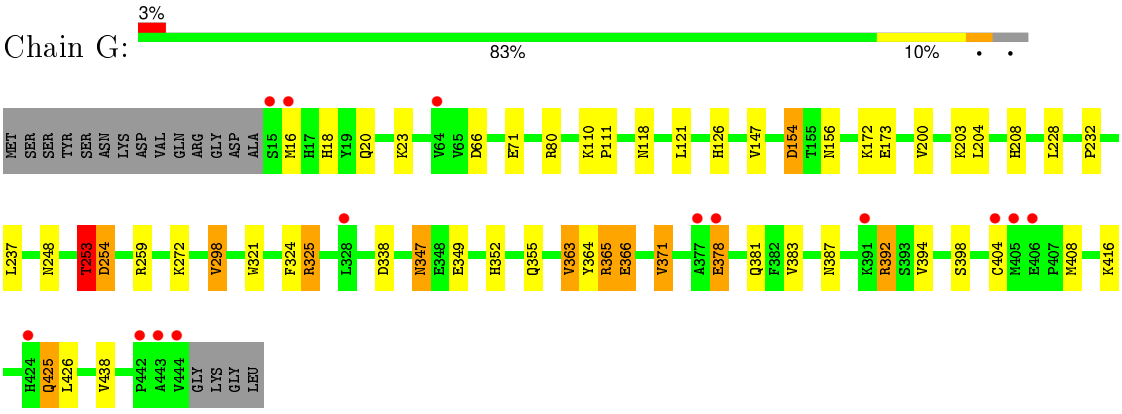
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



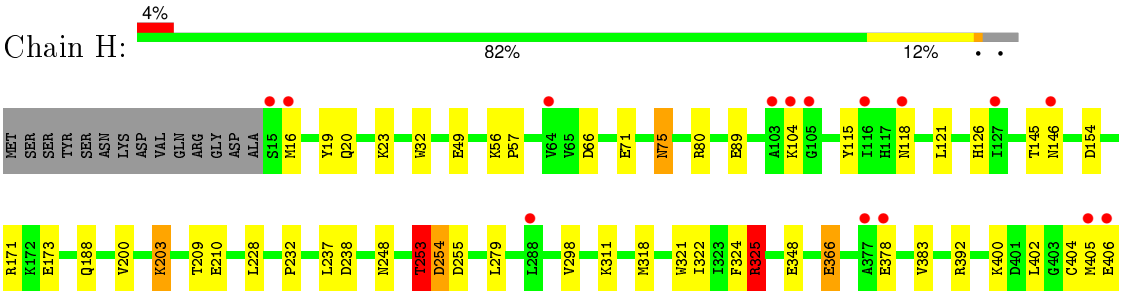
• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

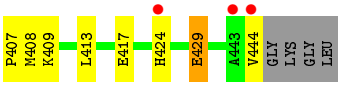


• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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




P407
M408
K409
L413
E417
H424
E429
A443
V444
GLY
LYS
GLY
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.71Å 202.16Å 287.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.28 29.88 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.90-2.28) 96.9 (29.88-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.146 , 0.177 0.155 , 0.182	Depositor DCC
R_{free} test set	13899 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 275069 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32820	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, SO4, CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.02	4/3606 (0.1%)	0.93	9/4895 (0.2%)
1	B	1.01	0/3607	0.94	12/4896 (0.2%)
1	C	0.96	1/3595 (0.0%)	0.91	6/4880 (0.1%)
1	D	0.95	2/3611 (0.1%)	0.89	5/4899 (0.1%)
1	E	0.88	2/3595 (0.1%)	0.89	12/4881 (0.2%)
1	F	0.85	0/3572	0.90	12/4849 (0.2%)
1	G	0.84	0/3589	0.94	11/4872 (0.2%)
1	H	0.84	1/3572 (0.0%)	0.93	11/4849 (0.2%)
All	All	0.92	10/28747 (0.0%)	0.92	78/39021 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	TYR	CG-CD1	-5.97	1.31	1.39
1	D	49	GLU	CG-CD	5.70	1.60	1.51
1	A	366	GLU	CD-OE2	5.59	1.31	1.25
1	E	188[A]	GLN	CG-CD	5.58	1.63	1.51
1	E	188[B]	GLN	CG-CD	5.58	1.63	1.51
1	A	265	ASP	CB-CG	5.53	1.63	1.51
1	D	265	ASP	CB-CG	5.46	1.63	1.51
1	H	325	ARG	CZ-NH1	5.11	1.39	1.33
1	A	189	TRP	CB-CG	-5.05	1.41	1.50
1	A	89	GLU	CG-CD	5.03	1.59	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	325	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	H	325	ARG	NE-CZ-NH2	-10.71	114.95	120.30
1	C	325	ARG	NE-CZ-NH1	-7.94	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	80	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	F	80	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	F	80	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	E	80	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	F	325	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	G	80	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	325	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	H	80	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	99	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	325	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	G	154[A]	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	G	154[B]	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	H	253	THR	N-CA-CB	-5.97	98.95	110.30
1	E	253	THR	N-CA-CB	-5.96	98.98	110.30
1	A	254	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	430	LEU	CB-CG-CD1	5.87	120.98	111.00
1	B	253	THR	N-CA-CB	-5.86	99.17	110.30
1	C	253	THR	N-CA-CB	-5.86	99.17	110.30
1	G	253	THR	N-CA-CB	-5.85	99.18	110.30
1	F	430	LEU	CB-CG-CD1	5.81	120.88	111.00
1	E	80	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	D	154	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	G	154[A]	ASP	CB-CG-OD1	5.74	123.47	118.30
1	G	154[B]	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	237	LEU	CA-CB-CG	-5.73	102.11	115.30
1	A	154	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	383	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	D	154	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	121	LEU	CB-CG-CD1	5.69	120.68	111.00
1	E	284	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	F	298	VAL	N-CA-CB	-5.69	98.97	111.50
1	B	421	LEU	CA-CB-CG	5.68	128.37	115.30
1	E	298	VAL	N-CA-CB	-5.67	99.03	111.50
1	D	430	LEU	CB-CG-CD2	5.63	120.57	111.00
1	B	121	LEU	CB-CG-CD1	5.62	120.56	111.00
1	C	89	GLU	CB-CA-C	-5.61	99.18	110.40
1	B	145	THR	CB-CA-C	-5.60	96.47	111.60
1	B	255	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	154[A]	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	154[B]	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	E	145	THR	CB-CA-C	-5.52	96.69	111.60
1	G	254	ASP	CB-CG-OD1	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	383	VAL	CG1-CB-CG2	5.49	119.68	110.90
1	F	419	LEU	CA-CB-CG	5.47	127.87	115.30
1	E	114	ASP	CB-CG-OD1	5.41	123.17	118.30
1	H	254	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	33	ASP	CB-CG-OD1	5.38	123.14	118.30
1	H	154	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	383	VAL	CG1-CB-CG2	5.32	119.40	110.90
1	F	154	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	339[A]	GLU	CB-CA-C	5.27	120.94	110.40
1	C	339[B]	GLU	CB-CA-C	5.27	120.94	110.40
1	B	339[A]	GLU	CB-CA-C	5.27	120.94	110.40
1	B	339[B]	GLU	CB-CA-C	5.27	120.94	110.40
1	H	209	THR	N-CA-CB	-5.26	100.30	110.30
1	A	80	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	80	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	99	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	298	VAL	N-CA-CB	-5.20	100.06	111.50
1	H	405	MET	CA-CB-CG	5.19	122.13	113.30
1	F	188	GLN	N-CA-CB	5.18	119.93	110.60
1	H	325	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	H	366	GLU	CG-CD-OE2	5.16	128.62	118.30
1	F	405	MET	CG-SD-CE	5.12	108.39	100.20
1	E	298	VAL	CG1-CB-CG2	5.12	119.08	110.90
1	D	254	ASP	CB-CG-OD1	5.08	122.88	118.30
1	G	366	GLU	CB-CA-C	5.08	120.55	110.40
1	A	121	LEU	CB-CG-CD1	5.07	119.61	111.00
1	A	430	LEU	CB-CG-CD2	5.03	119.55	111.00
1	B	254	ASP	CB-CG-OD1	5.03	122.83	118.30
1	H	171	ARG	CG-CD-NE	5.02	122.34	111.80
1	E	402	LEU	CB-CG-CD1	5.01	119.52	111.00
1	F	298	VAL	CG1-CB-CG2	5.01	118.92	110.90
1	F	402	LEU	CB-CG-CD1	5.01	119.51	111.00
1	A	197	ASP	CB-CG-OD1	5.00	122.81	118.30

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	3492	0	3370	36	0
1	B	3496	0	3369	38	0
1	C	3487	0	3365	27	0
1	D	3506	0	3394	27	0
1	E	3484	0	3363	27	0
1	F	3470	0	3346	29	0
1	G	3481	0	3356	39	0
1	H	3470	0	3346	33	0
2	A	24	0	32	6	0
2	B	54	0	72	9	0
2	C	30	0	40	9	0
2	D	30	0	40	11	0
2	E	36	0	48	6	0
2	F	24	0	32	7	0
2	G	24	0	32	1	0
2	H	18	0	24	4	0
3	A	50	0	0	1	0
3	B	50	0	0	3	0
3	C	65	0	0	1	0
3	D	60	0	0	1	0
3	E	50	0	0	0	0
3	F	55	0	0	1	0
3	G	40	0	0	1	0
3	H	55	0	0	3	0
4	A	13	0	6	6	0
4	B	13	0	5	8	0
4	C	13	0	5	4	0
4	E	13	0	5	2	0
4	G	13	0	5	7	0
5	A	662	0	0	18	0
5	B	625	0	0	17	0
5	C	579	0	0	13	0
5	D	536	0	0	8	0
5	E	500	0	0	4	0
5	F	495	0	0	11	0
5	G	439	0	0	17	0
5	H	368	0	0	10	0
All	All	32820	0	27255	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:505:GOL:O3	2:C:505:GOL:C3	1.67	1.40
4:A:515:CIT:O5	4:A:515:CIT:C5	1.75	1.20
1:H:146:ASN:HB3	5:H:917:HOH:O	1.40	1.18
4:C:519:CIT:O4	4:C:519:CIT:H21	1.47	1.11
1:C:49:GLU:HG2	5:C:1111:HOH:O	1.53	1.09
4:C:519:CIT:O2	4:C:519:CIT:O6	1.69	1.08
4:G:513:CIT:C5	4:G:513:CIT:O5	1.94	1.06
1:C:118:ASN:HB3	5:C:1124:HOH:O	1.55	1.04
4:C:519:CIT:C6	4:C:519:CIT:O2	2.06	1.02
4:A:515:CIT:H42	5:A:975:HOH:O	1.66	0.95
1:B:348:GLU:HB2	5:B:1067:HOH:O	1.66	0.93
1:D:174:GLY:H	2:D:502:GOL:H31	1.36	0.91
1:G:352:HIS:HB2	5:G:942:HOH:O	1.71	0.90
1:D:210:GLU:HB2	2:D:505:GOL:H11	1.55	0.88
1:E:210:GLU:HB2	4:E:517:CIT:H21	1.56	0.86
1:A:188[B]:GLN:HG2	5:A:875:HOH:O	1.77	0.83
4:C:519:CIT:C2	4:C:519:CIT:O4	2.26	0.83
1:E:40:THR:HG21	2:E:505:GOL:H11	1.61	0.82
1:B:210:GLU:H	4:B:520:CIT:H22	1.44	0.81
1:C:176:GLN:HB3	2:C:505:GOL:H2	1.61	0.81
1:C:177:ALA:H	2:C:505:GOL:H31	1.44	0.80
1:G:398:SER:HA	1:G:425:GLN:HB2	1.60	0.80
1:F:228:LEU:H	1:F:248:ASN:HD22	1.29	0.80
1:F:210:GLU:HB2	2:F:502:GOL:H11	1.67	0.76
1:B:228:LEU:H	1:B:248:ASN:HD22	1.32	0.76
4:G:513:CIT:H41	5:G:834:HOH:O	1.85	0.76
1:E:228:LEU:H	1:E:248:ASN:HD22	1.32	0.76
1:A:228:LEU:H	1:A:248:ASN:HD22	1.32	0.75
1:H:228:LEU:H	1:H:248:ASN:HD22	1.34	0.75
4:G:513:CIT:C4	5:G:834:HOH:O	2.35	0.74
1:E:188[A]:GLN:HG2	5:E:783:HOH:O	1.87	0.74
1:B:210:GLU:HB2	4:B:520:CIT:H41	1.69	0.74
1:A:418[A]:ASP:OD1	5:A:988:HOH:O	2.05	0.73
1:G:228:LEU:H	1:G:248:ASN:HD22	1.36	0.73
1:C:118:ASN:CB	5:C:1124:HOH:O	2.25	0.73
1:H:238:ASP:OD2	5:H:850:HOH:O	2.07	0.73
1:A:418[A]:ASP:OD2	5:A:1255:HOH:O	2.08	0.72
1:B:89:GLU:HG2	5:B:1197:HOH:O	1.88	0.72
1:D:228:LEU:H	1:D:248:ASN:HD22	1.37	0.72
1:E:40:THR:CG2	2:E:505:GOL:H11	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:H	1:C:248:ASN:HD22	1.37	0.71
4:A:515:CIT:O4	4:A:515:CIT:O5	2.07	0.71
1:C:188[B]:GLN:HG2	5:C:834:HOH:O	1.89	0.71
1:H:311:LYS:N	3:H:508:SO4:O3	2.19	0.71
1:A:381:GLN:NE2	5:A:1230:HOH:O	2.22	0.71
1:C:253:THR:HG23	1:C:254:ASP:O	1.92	0.70
1:G:154[B]:ASP:OD2	5:G:691:HOH:O	2.09	0.70
1:H:145:THR:OG1	5:H:846:HOH:O	2.10	0.70
1:G:365:ARG:HD2	5:G:798:HOH:O	1.91	0.70
1:A:381:GLN:CD	5:A:1230:HOH:O	2.30	0.70
1:G:416:LYS:HD3	5:G:969:HOH:O	1.92	0.70
1:B:253:THR:HG23	1:B:254:ASP:O	1.92	0.69
1:D:306:MET:HE1	5:D:726:HOH:O	1.93	0.68
1:C:118:ASN:HB3	5:C:1114:HOH:O	1.91	0.68
1:E:49:GLU:HG3	5:E:974:HOH:O	1.93	0.68
4:A:515:CIT:C4	5:A:975:HOH:O	2.33	0.68
1:H:424:HIS:ND1	5:H:957:HOH:O	2.27	0.68
1:B:154[B]:ASP:OD2	5:B:805:HOH:O	2.12	0.67
1:G:253:THR:HG23	1:G:254:ASP:O	1.95	0.67
1:G:364:TYR:CE2	1:G:371:VAL:HG13	2.30	0.67
1:E:253:THR:HG23	1:E:254:ASP:O	1.95	0.66
1:F:423:LYS:HB3	1:F:423:LYS:NZ	2.10	0.66
3:B:513:SO4:O1	5:B:1225:HOH:O	2.13	0.65
1:C:306:MET:HE1	5:C:731:HOH:O	1.96	0.65
1:G:416:LYS:CD	5:G:969:HOH:O	2.45	0.65
1:G:208:HIS:HD2	4:G:513:CIT:O7	1.79	0.65
1:F:313:GLU:OE2	1:F:433:HIS:HD2	1.78	0.65
1:E:145:THR:CG2	5:E:971:HOH:O	2.45	0.65
1:A:172:LYS:NZ	5:A:1164:HOH:O	2.24	0.63
1:C:40:THR:CG2	2:C:503:GOL:H2	2.29	0.62
1:E:40:THR:OG1	2:E:505:GOL:H31	1.99	0.62
1:H:253:THR:HG23	1:H:254:ASP:O	2.00	0.62
5:F:1055:HOH:O	1:H:203:LYS:HE3	1.99	0.61
1:F:306:MET:HE2	5:F:848:HOH:O	1.99	0.61
4:G:513:CIT:C1	5:G:784:HOH:O	2.48	0.60
1:A:306:MET:HE2	5:A:993:HOH:O	2.00	0.60
1:H:255:ASP:OD2	2:H:502:GOL:H12	2.01	0.60
1:G:18:HIS:HE1	5:G:952:HOH:O	1.83	0.59
1:B:177:ALA:H	2:B:503:GOL:H31	1.67	0.59
1:H:188:GLN:HG3	5:H:752:HOH:O	2.00	0.59
1:F:409:LYS:CD	5:F:1092:HOH:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ARG:HH22	2:E:504:GOL:H2	1.68	0.59
1:G:364:TYR:CE2	1:G:371:VAL:CG1	2.86	0.59
1:B:210:GLU:H	4:B:520:CIT:C2	2.14	0.59
1:B:145:THR:CG2	5:B:969:HOH:O	2.51	0.59
3:H:505:SO4:O4	5:H:799:HOH:O	2.17	0.58
1:A:265:ASP:HB3	5:A:768:HOH:O	2.02	0.58
1:F:409:LYS:HD3	5:F:1092:HOH:O	2.04	0.58
1:H:404:CYS:HB3	1:H:408:MET:HE2	1.86	0.58
1:D:174:GLY:N	2:D:502:GOL:H31	2.12	0.57
1:A:173:GLU:OE2	3:A:510:SO4:O3	2.23	0.57
1:F:56:LYS:NZ	5:F:906:HOH:O	2.37	0.57
1:B:306:MET:HE1	5:B:733:HOH:O	2.05	0.57
1:A:255:ASP:OD2	2:A:501:GOL:C3	2.53	0.57
4:E:517:CIT:O2	4:E:517:CIT:O6	2.23	0.56
1:D:41:GLU:CD	5:D:1046:HOH:O	2.42	0.56
1:G:347:ASN:HD22	1:G:347:ASN:C	2.09	0.56
1:E:40:THR:CG2	2:E:505:GOL:C1	2.83	0.56
1:D:208:HIS:HA	2:D:505:GOL:H2	1.88	0.55
4:G:513:CIT:O5	4:G:513:CIT:O3	2.23	0.55
1:G:404:CYS:HB3	1:G:408:MET:HE2	1.88	0.55
1:H:392:ARG:CZ	1:H:429:GLU:HG2	2.36	0.55
4:A:515:CIT:O1	4:A:515:CIT:C6	2.54	0.55
2:F:502:GOL:H32	5:F:861:HOH:O	2.07	0.55
1:G:392:ARG:NH1	3:G:510:SO4:O3	2.40	0.55
1:B:17:HIS:HE1	3:B:511:SO4:O2	1.90	0.55
4:B:520:CIT:O2	4:B:520:CIT:O6	2.25	0.54
1:A:221:ARG:HH21	2:A:502:GOL:H2	1.72	0.54
1:G:363:VAL:HG13	1:G:371:VAL:HG22	1.89	0.54
1:B:174:GLY:H	2:B:503:GOL:H32	1.73	0.54
1:A:208:HIS:HD2	4:A:515:CIT:O7	1.91	0.53
1:H:210:GLU:HB2	2:H:503:GOL:H2	1.90	0.53
4:B:520:CIT:C1	4:B:520:CIT:O6	2.56	0.53
1:D:424:HIS:H	2:D:503:GOL:H32	1.74	0.53
4:G:513:CIT:H42	5:G:834:HOH:O	2.05	0.53
1:C:253:THR:CG2	1:C:254:ASP:O	2.57	0.53
1:E:145:THR:HG22	5:E:971:HOH:O	2.07	0.53
1:A:49[B]:GLU:OE2	1:A:115:TYR:OH	2.27	0.53
1:B:406:GLU:HB2	1:B:407:PRO:CD	2.39	0.52
1:B:253:THR:CG2	1:B:254:ASP:O	2.58	0.52
1:F:390:GLU:OE2	1:F:433:HIS:HE1	1.91	0.52
1:B:176:GLN:HB3	2:B:503:GOL:H2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:HIS:HA	2:F:502:GOL:H2	1.91	0.52
1:A:49[A]:GLU:OE2	1:A:115:TYR:OH	2.26	0.52
1:F:392:ARG:NH1	3:F:506:SO4:O1	2.43	0.52
1:E:40:THR:HG21	2:E:505:GOL:C1	2.33	0.52
1:G:147:VAL:O	5:G:790:HOH:O	2.18	0.52
1:C:40:THR:HG21	2:C:503:GOL:H2	1.91	0.52
1:D:104:LYS:HD3	5:D:1097:HOH:O	2.10	0.52
2:B:505:GOL:H31	1:E:53:LYS:HZ2	1.74	0.52
1:H:32:TRP:CD1	2:H:501:GOL:H32	2.46	0.51
1:H:16:MET:HG2	1:H:19:TYR:CZ	2.45	0.51
1:H:75:ASN:H	1:H:75:ASN:HD22	1.59	0.51
2:B:504:GOL:C1	5:B:1104:HOH:O	2.58	0.51
1:B:204:LEU:HD11	1:D:156:ASN:HD21	1.76	0.51
3:C:508:SO4:O3	5:C:792:HOH:O	2.19	0.51
1:B:156:ASN:HD21	1:D:204:LEU:HD11	1.75	0.51
1:G:378:GLU:CD	1:G:378:GLU:N	2.64	0.51
1:G:259:ARG:NH1	2:G:502:GOL:O2	2.37	0.51
1:B:336:ASP:OD1	3:B:514:SO4:O3	2.27	0.50
1:B:173:GLU:HG3	5:B:1204:HOH:O	2.10	0.50
1:H:253:THR:CG2	1:H:254:ASP:O	2.60	0.50
1:B:142:ILE:HD12	1:B:147:VAL:HG23	1.92	0.50
2:B:504:GOL:H11	5:B:1104:HOH:O	2.11	0.50
1:F:49:GLU:OE2	1:F:115:TYR:OH	2.27	0.50
1:A:306:MET:CE	5:A:993:HOH:O	2.58	0.49
1:B:210:GLU:HG2	4:B:520:CIT:H21	1.95	0.49
1:E:253:THR:CG2	1:E:254:ASP:O	2.59	0.49
1:D:188:GLN:NE2	5:D:683:HOH:O	2.44	0.49
1:F:188:GLN:HG3	5:F:950:HOH:O	2.11	0.49
1:G:253:THR:CG2	1:G:254:ASP:O	2.59	0.49
1:B:20:GLN:NE2	1:B:23:LYS:HE3	2.28	0.49
2:C:505:GOL:HO3	2:C:505:GOL:C3	2.11	0.49
1:D:20:GLN:NE2	1:D:23:LYS:HE3	2.27	0.49
1:H:146:ASN:OD1	1:H:146:ASN:N	2.38	0.49
1:A:272:LYS:CD	5:B:1041:HOH:O	2.60	0.49
1:H:75:ASN:HD22	1:H:75:ASN:N	2.09	0.48
1:C:16:MET:HE1	5:C:926:HOH:O	2.13	0.48
1:H:406:GLU:HB2	1:H:407:PRO:CD	2.44	0.48
1:F:208:HIS:HB3	2:F:502:GOL:O1	2.14	0.48
1:A:265:ASP:HB3	5:A:837:HOH:O	2.11	0.48
1:B:20:GLN:HE21	1:B:23:LYS:HE3	1.78	0.48
1:D:174:GLY:H	2:D:502:GOL:C3	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:GLN:OE1	1:G:23:LYS:HE3	2.13	0.48
1:D:424:HIS:HB3	2:D:503:GOL:H11	1.95	0.48
1:B:406:GLU:HB2	1:B:407:PRO:HD2	1.96	0.48
2:B:504:GOL:O3	5:B:1187:HOH:O	2.20	0.47
1:B:146:ASN:OD1	1:B:146:ASN:N	2.38	0.47
1:C:49:GLU:OE2	1:C:115:TYR:OH	2.26	0.47
1:D:20:GLN:HE21	1:D:23:LYS:HE3	1.79	0.47
1:H:23:LYS:HG3	1:H:279:LEU:HD21	1.96	0.47
1:H:173:GLU:HA	3:H:509:SO4:O3	2.15	0.47
1:A:110:LYS:HB3	1:A:111:PRO:HD3	1.97	0.47
1:A:255:ASP:CG	2:A:501:GOL:H31	2.35	0.47
1:B:16:MET:HG2	1:B:19:TYR:CZ	2.49	0.47
1:A:203:LYS:HD3	5:A:1249:HOH:O	2.13	0.47
1:G:16:MET:HB3	1:G:16:MET:HE2	1.80	0.47
1:B:145:THR:HB	1:B:147:VAL:H	1.80	0.47
1:F:255:ASP:OD2	2:F:504:GOL:H31	2.13	0.47
2:F:502:GOL:C3	5:F:861:HOH:O	2.60	0.47
1:E:20:GLN:NE2	1:E:23:LYS:HE3	2.29	0.47
1:C:296:ARG:NH1	2:C:503:GOL:H31	2.30	0.47
1:G:355:GLN:HB3	5:G:799:HOH:O	2.14	0.47
1:D:406:GLU:HB2	1:D:407:PRO:CD	2.46	0.46
1:F:406:GLU:HB2	1:F:407:PRO:CD	2.45	0.46
1:A:49[A]:GLU:OE1	5:A:1111:HOH:O	2.21	0.46
1:A:387:ASN:ND2	1:A:389:SER:H	2.14	0.46
2:D:502:GOL:O2	3:D:512:SO4:O3	2.33	0.46
1:A:387:ASN:HD22	1:A:389:SER:H	1.64	0.46
1:A:444:VAL:HG12	5:A:1183:HOH:O	2.15	0.46
1:H:75:ASN:ND2	1:H:75:ASN:N	2.64	0.46
1:G:172:LYS:NZ	5:G:874:HOH:O	2.48	0.46
1:D:424:HIS:HB2	5:D:1128:HOH:O	2.15	0.45
1:D:188:GLN:HB3	5:D:1066:HOH:O	2.15	0.45
1:D:210:GLU:HG2	2:D:505:GOL:H31	1.98	0.45
1:H:49:GLU:OE2	1:H:115:TYR:OH	2.28	0.45
1:F:20:GLN:NE2	1:F:23:LYS:HE3	2.31	0.45
1:B:200:VAL:HB	1:B:232:PRO:O	2.17	0.45
1:E:145:THR:HB	1:E:147:VAL:H	1.80	0.45
1:A:172:LYS:HE3	5:A:1092:HOH:O	2.16	0.45
1:G:154[A]:ASP:OD1	5:G:715:HOH:O	2.21	0.45
1:B:379:GLY:HA3	5:B:965:HOH:O	2.16	0.45
1:F:423:LYS:HZ2	1:F:423:LYS:HB3	1.78	0.45
2:B:505:GOL:H31	1:E:53:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:416:LYS:HE2	1:G:416:LYS:HB2	1.54	0.45
1:H:200:VAL:HB	1:H:232:PRO:O	2.17	0.44
1:E:110:LYS:HB3	1:E:111:PRO:HD3	1.99	0.44
1:E:400:LYS:HB2	1:E:400:LYS:HE3	1.71	0.44
1:G:338:ASP:HA	5:G:1035:HOH:O	2.17	0.44
1:A:217:LYS:HE3	2:A:502:GOL:O3	2.18	0.44
1:H:417:GLU:HG3	5:H:816:HOH:O	2.15	0.44
1:F:444:VAL:HA	5:F:863:HOH:O	2.18	0.44
1:F:444:VAL:HG13	1:F:444:VAL:O	2.17	0.44
1:C:16:MET:CE	5:C:926:HOH:O	2.66	0.44
1:D:339:GLU:HG3	5:D:930:HOH:O	2.17	0.44
1:B:145:THR:HG22	5:B:969:HOH:O	2.15	0.44
1:F:75:ASN:N	1:F:75:ASN:HD22	2.16	0.44
1:C:110:LYS:HB3	1:C:111:PRO:HD3	2.00	0.44
1:B:424:HIS:HB2	5:B:1219:HOH:O	2.18	0.44
1:H:378:GLU:OE2	5:H:875:HOH:O	2.21	0.44
2:F:504:GOL:H32	5:F:755:HOH:O	2.17	0.43
1:B:110:LYS:HB3	1:B:111:PRO:HD3	2.00	0.43
1:C:20:GLN:NE2	1:C:23:LYS:HE3	2.33	0.43
1:G:16:MET:HA	1:G:16:MET:HE3	2.00	0.43
1:A:56:LYS:HD3	1:A:121:LEU:HD13	2.00	0.43
1:H:66:ASP:HA	1:H:126:HIS:HB2	2.01	0.43
1:D:173:GLU:HA	2:D:502:GOL:H11	1.99	0.43
1:E:204:LEU:HD11	1:G:156:ASN:HD21	1.84	0.43
1:D:110:LYS:HB3	1:D:111:PRO:HD3	2.01	0.43
2:C:504:GOL:H31	5:G:685:HOH:O	2.18	0.43
1:G:66:ASP:HA	1:G:126:HIS:HB2	2.01	0.43
1:D:56:LYS:N	1:D:57:PRO:CD	2.81	0.43
1:F:423:LYS:HZ3	1:F:423:LYS:HB3	1.84	0.43
2:H:502:GOL:H11	5:H:677:HOH:O	2.19	0.42
1:A:204:LEU:HD11	1:C:156:ASN:HD21	1.83	0.42
2:B:502:GOL:H11	5:B:1071:HOH:O	2.19	0.42
1:A:255:ASP:OD2	2:A:501:GOL:H31	2.18	0.42
1:G:110:LYS:HB3	1:G:111:PRO:HD3	2.00	0.42
1:E:387:ASN:HD22	1:E:389:SER:H	1.67	0.42
1:C:89:GLU:CG	5:C:1025:HOH:O	2.66	0.42
5:A:1104:HOH:O	1:B:272:LYS:CD	2.67	0.42
1:C:86:GLU:OE1	2:C:504:GOL:C1	2.68	0.42
1:C:118:ASN:CG	5:C:1124:HOH:O	2.56	0.42
1:A:387:ASN:HD22	1:A:387:ASN:C	2.22	0.42
1:B:45:LYS:NZ	5:B:1167:HOH:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ASN:HD21	1:G:204:LEU:HD11	1.84	0.42
1:H:56:LYS:N	1:H:57:PRO:CD	2.83	0.42
1:C:56:LYS:N	1:C:57:PRO:CD	2.83	0.42
1:C:318:MET:O	1:C:322:ILE:HG12	2.20	0.42
1:G:378:GLU:OE1	1:G:378:GLU:N	2.52	0.42
1:F:56:LYS:HD3	1:F:121:LEU:HD13	2.02	0.42
1:H:406:GLU:HB2	1:H:407:PRO:HD2	2.01	0.42
1:A:339:GLU:HG3	5:A:904:HOH:O	2.19	0.42
1:E:56:LYS:N	1:E:57:PRO:CD	2.82	0.42
1:G:272:LYS:CD	5:H:850:HOH:O	2.68	0.41
1:B:188[B]:GLN:NE2	5:B:1195:HOH:O	2.54	0.41
1:B:209:THR:N	4:B:520:CIT:H22	2.36	0.41
1:F:110:LYS:HB3	1:F:111:PRO:HD3	2.03	0.41
1:E:200:VAL:HB	1:E:232:PRO:O	2.19	0.41
1:H:318:MET:O	1:H:322:ILE:HG12	2.20	0.41
1:E:387:ASN:ND2	1:E:389:SER:H	2.18	0.41
1:A:20:GLN:NE2	1:A:23:LYS:HE3	2.33	0.41
1:G:324:PHE:O	1:G:325:ARG:HB2	2.20	0.41
1:B:210:GLU:CG	4:B:520:CIT:H21	2.50	0.41
1:E:20:GLN:HE21	1:E:23:LYS:HE3	1.84	0.41
1:D:200:VAL:HB	1:D:232:PRO:O	2.19	0.41
1:G:347:ASN:HD22	1:G:349:GLU:H	1.68	0.41
1:D:348:GLU:HG2	5:D:1123:HOH:O	2.20	0.41
1:A:197:ASP:OD2	2:A:503:GOL:H11	2.21	0.41
1:F:406:GLU:HB2	1:F:407:PRO:HD2	2.03	0.41
1:A:156:ASN:HD21	1:C:204:LEU:HD11	1.85	0.41
5:C:1158:HOH:O	1:G:173:GLU:HB2	2.20	0.41
1:D:210:GLU:CB	2:D:505:GOL:H11	2.38	0.41
1:G:200:VAL:HB	1:G:232:PRO:O	2.20	0.41
1:F:200:VAL:HB	1:F:232:PRO:O	2.20	0.41
1:F:387:ASN:ND2	1:F:389:SER:H	2.20	0.40
1:A:234:PRO:HA	1:A:252:MET:O	2.20	0.40
1:H:203:LYS:HB2	1:H:203:LYS:HE2	1.78	0.40
1:C:89:GLU:HG2	5:C:1025:HOH:O	2.21	0.40
1:G:172:LYS:HE3	5:G:704:HOH:O	2.20	0.40
1:F:20:GLN:HE21	1:F:23:LYS:HE3	1.86	0.40
1:F:172:LYS:HD3	5:F:692:HOH:O	2.21	0.40
1:H:324:PHE:O	1:H:325:ARG:HB2	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	432/448 (96%)	418 (97%)	14 (3%)	0	100	100
1	B	432/448 (96%)	413 (96%)	19 (4%)	0	100	100
1	C	431/448 (96%)	416 (96%)	15 (4%)	0	100	100
1	D	434/448 (97%)	419 (96%)	15 (4%)	0	100	100
1	E	431/448 (96%)	416 (96%)	15 (4%)	0	100	100
1	F	428/448 (96%)	413 (96%)	14 (3%)	1 (0%)	52	63
1	G	430/448 (96%)	415 (96%)	15 (4%)	0	100	100
1	H	428/448 (96%)	410 (96%)	17 (4%)	1 (0%)	52	63
All	All	3446/3584 (96%)	3320 (96%)	124 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	325	ARG
1	F	325	ARG

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	373/383 (97%)	363 (97%)	10 (3%)	52	68
1	B	373/383 (97%)	361 (97%)	12 (3%)	46	61
1	C	371/383 (97%)	358 (96%)	13 (4%)	43	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	372/383 (97%)	363 (98%)	9 (2%)	57 72
1	E	372/383 (97%)	356 (96%)	16 (4%)	35 46
1	F	369/383 (96%)	348 (94%)	21 (6%)	25 32
1	G	371/383 (97%)	349 (94%)	22 (6%)	24 30
1	H	369/383 (96%)	348 (94%)	21 (6%)	25 32
All	All	2970/3064 (97%)	2846 (96%)	124 (4%)	36 47

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	104	LYS
1	A	121	LEU
1	A	203	LYS
1	A	237	LEU
1	A	321	TRP
1	A	383	VAL
1	A	387	ASN
1	A	391	LYS
1	A	429	GLU
1	B	71	GLU
1	B	72	PRO
1	B	89	GLU
1	B	145	THR
1	B	203	LYS
1	B	253	THR
1	B	321	TRP
1	B	381	GLN
1	B	387	ASN
1	B	406	GLU
1	B	421	LEU
1	B	430	LEU
1	C	71	GLU
1	C	89	GLU
1	C	203	LYS
1	C	253	THR
1	C	298	VAL
1	C	321	TRP
1	C	387	ASN
1	C	391	LYS

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Mol	Chain	Res	Type
1	C	402	LEU
1	C	405	MET
1	C	406	GLU
1	C	409	LYS
1	C	413	LEU
1	D	71	GLU
1	D	104	LYS
1	D	121	LEU
1	D	203	LYS
1	D	321	TRP
1	D	383	VAL
1	D	387	ASN
1	D	392	ARG
1	D	413	LEU
1	E	71	GLU
1	E	72	PRO
1	E	145	THR
1	E	203	LYS
1	E	237	LEU
1	E	253	THR
1	E	298	VAL
1	E	321	TRP
1	E	383	VAL
1	E	387	ASN
1	E	391	LYS
1	E	400	LYS
1	E	402	LEU
1	E	406	GLU
1	E	413	LEU
1	E	422	VAL
1	F	71	GLU
1	F	75	ASN
1	F	104	LYS
1	F	121	LEU
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	387	ASN
1	F	392	ARG

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Mol	Chain	Res	Type
1	F	402	LEU
1	F	405	MET
1	F	413	LEU
1	F	419	LEU
1	F	422	VAL
1	F	423	LYS
1	F	430	LEU
1	F	433	HIS
1	F	444	VAL
1	G	71	GLU
1	G	118	ASN
1	G	121	LEU
1	G	203	LYS
1	G	237	LEU
1	G	253	THR
1	G	298	VAL
1	G	321	TRP
1	G	347	ASN
1	G	363	VAL
1	G	365	ARG
1	G	366	GLU
1	G	371	VAL
1	G	378	GLU
1	G	381	GLN
1	G	383	VAL
1	G	387	ASN
1	G	392	ARG
1	G	394	VAL
1	G	425	GLN
1	G	426	LEU
1	G	438	VAL
1	H	20	GLN
1	H	71	GLU
1	H	75	ASN
1	H	89	GLU
1	H	104	LYS
1	H	118	ASN
1	H	121	LEU
1	H	203	LYS
1	H	237	LEU
1	H	253	THR
1	H	298	VAL

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Mol	Chain	Res	Type
1	H	321	TRP
1	H	348	GLU
1	H	366	GLU
1	H	383	VAL
1	H	400	LYS
1	H	402	LEU
1	H	409	LYS
1	H	413	LEU
1	H	429	GLU
1	H	444	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) 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	387	ASN
1	C	20	GLN
1	C	156	ASN
1	C	248	ASN
1	C	356	ASN
1	C	387	ASN
1	D	18	HIS
1	D	20	GLN
1	D	156	ASN
1	D	188	GLN
1	D	248	ASN
1	D	356	ASN
1	D	387	ASN
1	E	18	HIS
1	E	20	GLN
1	E	156	ASN
1	E	248	ASN
1	E	356	ASN

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Mol	Chain	Res	Type
1	E	387	ASN
1	F	18	HIS
1	F	20	GLN
1	F	75	ASN
1	F	137	HIS
1	F	248	ASN
1	F	356	ASN
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	356	ASN
1	G	387	ASN
1	H	20	GLN
1	H	75	ASN
1	H	137	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry

130 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	501	-	5,5,5	0.65	0	5,5,5	0.51	0
2	GOL	A	502	-	5,5,5	0.56	0	5,5,5	0.43	0
2	GOL	A	503	-	5,5,5	0.85	0	5,5,5	2.09	2 (40%)
2	GOL	A	504	-	5,5,5	0.44	0	5,5,5	0.61	0
3	SO4	A	505	-	4,4,4	2.02	2 (50%)	6,6,6	0.78	0
3	SO4	A	506	-	4,4,4	0.75	0	6,6,6	0.35	0
3	SO4	A	507	-	4,4,4	0.90	0	6,6,6	1.01	1 (16%)
3	SO4	A	508	-	4,4,4	0.85	0	6,6,6	0.43	0
3	SO4	A	509	-	4,4,4	0.52	0	6,6,6	0.80	0
3	SO4	A	510	-	4,4,4	1.27	0	6,6,6	0.50	0
3	SO4	A	511	-	4,4,4	1.07	0	6,6,6	0.73	0
3	SO4	A	512	-	4,4,4	1.56	1 (25%)	6,6,6	0.96	0
3	SO4	A	513	-	4,4,4	0.72	0	6,6,6	0.70	0
3	SO4	A	514	-	4,4,4	1.32	0	6,6,6	0.66	0
4	CIT	A	515	-	3,12,12	1.90	2 (66%)	3,17,17	2.02	1 (33%)
2	GOL	B	501	-	5,5,5	0.57	0	5,5,5	1.10	0
2	GOL	B	502	-	5,5,5	0.50	0	5,5,5	0.66	0
2	GOL	B	503	-	5,5,5	0.98	0	5,5,5	1.39	1 (20%)
2	GOL	B	504	-	5,5,5	0.74	0	5,5,5	1.12	0
2	GOL	B	505	-	5,5,5	1.07	0	5,5,5	0.79	0
2	GOL	B	506	-	5,5,5	0.66	0	5,5,5	0.57	0
2	GOL	B	507	-	5,5,5	0.37	0	5,5,5	1.46	1 (20%)
2	GOL	B	508	-	5,5,5	0.68	0	5,5,5	0.86	0
2	GOL	B	509	-	5,5,5	0.60	0	5,5,5	0.80	0
3	SO4	B	510	-	4,4,4	0.76	0	6,6,6	0.65	0
3	SO4	B	511	-	4,4,4	1.12	0	6,6,6	0.78	0
3	SO4	B	512	-	4,4,4	1.06	0	6,6,6	0.98	0
3	SO4	B	513	-	4,4,4	0.47	0	6,6,6	0.38	0
3	SO4	B	514	-	4,4,4	0.74	0	6,6,6	0.44	0
3	SO4	B	515	-	4,4,4	1.04	0	6,6,6	0.66	0
3	SO4	B	516	-	4,4,4	1.13	0	6,6,6	0.92	0
3	SO4	B	517	-	4,4,4	1.63	1 (25%)	6,6,6	1.35	1 (16%)
3	SO4	B	518	-	4,4,4	0.61	0	6,6,6	0.31	0
3	SO4	B	519	-	4,4,4	0.83	0	6,6,6	0.54	0
4	CIT	B	520	-	3,12,12	3.97	2 (66%)	3,17,17	4.26	2 (66%)
2	GOL	C	501	-	5,5,5	0.22	0	5,5,5	0.65	0
2	GOL	C	502	-	5,5,5	0.58	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	C	503	-	5,5,5	2.23	3 (60%)	5,5,5	2.18	2 (40%)
2	GOL	C	504	-	5,5,5	0.62	0	5,5,5	0.88	0
2	GOL	C	505	-	5,5,5	2.70	1 (20%)	5,5,5	1.68	1 (20%)
3	SO4	C	506	-	4,4,4	0.66	0	6,6,6	0.30	0
3	SO4	C	507	-	4,4,4	1.08	0	6,6,6	0.57	0
3	SO4	C	508	-	4,4,4	0.73	0	6,6,6	0.35	0
3	SO4	C	509	-	4,4,4	0.57	0	6,6,6	0.23	0
3	SO4	C	510	-	4,4,4	1.13	0	6,6,6	0.35	0
3	SO4	C	511	-	4,4,4	0.85	0	6,6,6	0.58	0
3	SO4	C	512	-	4,4,4	0.72	0	6,6,6	0.75	0
3	SO4	C	513	-	4,4,4	1.23	0	6,6,6	0.93	0
3	SO4	C	514	-	4,4,4	0.74	0	6,6,6	0.43	0
3	SO4	C	515	-	4,4,4	1.03	0	6,6,6	0.96	0
3	SO4	C	516	-	4,4,4	1.02	0	6,6,6	0.93	0
3	SO4	C	517	-	4,4,4	1.24	0	6,6,6	0.43	0
3	SO4	C	518	-	4,4,4	0.67	0	6,6,6	0.29	0
4	CIT	C	519	-	3,12,12	3.89	3 (100%)	3,17,17	4.51	2 (66%)
2	GOL	D	501	-	5,5,5	0.78	0	5,5,5	0.45	0
2	GOL	D	502	-	5,5,5	0.94	0	5,5,5	1.57	2 (40%)
2	GOL	D	503	-	5,5,5	0.54	0	5,5,5	1.74	2 (40%)
2	GOL	D	504	-	5,5,5	0.71	0	5,5,5	1.27	1 (20%)
2	GOL	D	505	-	5,5,5	0.97	0	5,5,5	1.40	1 (20%)
3	SO4	D	506	-	4,4,4	0.73	0	6,6,6	0.51	0
3	SO4	D	507	-	4,4,4	0.75	0	6,6,6	0.34	0
3	SO4	D	508	-	4,4,4	1.64	2 (50%)	6,6,6	0.80	0
3	SO4	D	509	-	4,4,4	1.16	0	6,6,6	1.48	2 (33%)
3	SO4	D	510	-	4,4,4	0.86	0	6,6,6	0.47	0
3	SO4	D	511	-	4,4,4	1.10	0	6,6,6	1.67	2 (33%)
3	SO4	D	512	-	4,4,4	0.79	0	6,6,6	1.54	2 (33%)
3	SO4	D	513	-	4,4,4	0.90	0	6,6,6	0.47	0
3	SO4	D	514	-	4,4,4	0.81	0	6,6,6	0.35	0
3	SO4	D	515	-	4,4,4	0.73	0	6,6,6	0.54	0
3	SO4	D	516	-	4,4,4	0.79	0	6,6,6	0.49	0
3	SO4	D	517	-	4,4,4	1.15	1 (25%)	6,6,6	0.75	0
2	GOL	E	501	-	5,5,5	0.48	0	5,5,5	0.27	0
2	GOL	E	502	-	5,5,5	0.55	0	5,5,5	0.44	0
2	GOL	E	503	-	5,5,5	0.71	0	5,5,5	1.68	1 (20%)
2	GOL	E	504	-	5,5,5	0.75	0	5,5,5	0.81	0
2	GOL	E	505	-	5,5,5	1.45	0	5,5,5	2.50	4 (80%)
2	GOL	E	506	-	5,5,5	0.33	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	E	507	-	4,4,4	0.67	0	6,6,6	0.64	0
3	SO4	E	508	-	4,4,4	1.18	0	6,6,6	0.63	0
3	SO4	E	509	-	4,4,4	1.20	0	6,6,6	0.99	0
3	SO4	E	510	-	4,4,4	0.84	0	6,6,6	0.22	0
3	SO4	E	511	-	4,4,4	1.29	1 (25%)	6,6,6	1.41	1 (16%)
3	SO4	E	512	-	4,4,4	0.89	0	6,6,6	0.69	0
3	SO4	E	513	-	4,4,4	0.83	0	6,6,6	1.20	1 (16%)
3	SO4	E	514	-	4,4,4	2.03	1 (25%)	6,6,6	1.20	1 (16%)
3	SO4	E	515	-	4,4,4	1.13	0	6,6,6	0.94	0
3	SO4	E	516	-	4,4,4	0.78	0	6,6,6	0.26	0
4	CIT	E	517	-	3,12,12	0.81	0	3,17,17	2.88	2 (66%)
2	GOL	F	501	-	5,5,5	0.78	0	5,5,5	0.30	0
2	GOL	F	502	-	5,5,5	0.47	0	5,5,5	0.62	0
2	GOL	F	503	-	5,5,5	0.64	0	5,5,5	0.41	0
2	GOL	F	504	-	5,5,5	0.21	0	5,5,5	0.48	0
3	SO4	F	505	-	4,4,4	0.94	0	6,6,6	0.50	0
3	SO4	F	506	-	4,4,4	0.74	0	6,6,6	0.31	0
3	SO4	F	507	-	4,4,4	0.72	0	6,6,6	0.36	0
3	SO4	F	508	-	4,4,4	1.42	1 (25%)	6,6,6	1.03	1 (16%)
3	SO4	F	509	-	4,4,4	0.83	0	6,6,6	0.58	0
3	SO4	F	510	-	4,4,4	0.97	0	6,6,6	0.41	0
3	SO4	F	511	-	4,4,4	1.12	0	6,6,6	0.46	0
3	SO4	F	512	-	4,4,4	0.85	0	6,6,6	0.86	0
3	SO4	F	513	-	4,4,4	0.89	0	6,6,6	1.34	1 (16%)
3	SO4	F	514	-	4,4,4	1.20	0	6,6,6	0.42	0
3	SO4	F	515	-	4,4,4	0.68	0	6,6,6	0.34	0
2	GOL	G	501	-	5,5,5	0.59	0	5,5,5	0.88	0
2	GOL	G	502	-	5,5,5	0.36	0	5,5,5	0.51	0
2	GOL	G	503	-	5,5,5	0.53	0	5,5,5	1.12	1 (20%)
2	GOL	G	504	-	5,5,5	0.48	0	5,5,5	0.87	0
3	SO4	G	505	-	4,4,4	0.54	0	6,6,6	0.72	0
3	SO4	G	506	-	4,4,4	1.35	1 (25%)	6,6,6	1.00	1 (16%)
3	SO4	G	507	-	4,4,4	0.96	0	6,6,6	0.39	0
3	SO4	G	508	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	G	509	-	4,4,4	1.10	1 (25%)	6,6,6	0.59	0
3	SO4	G	510	-	4,4,4	0.63	0	6,6,6	0.28	0
3	SO4	G	511	-	4,4,4	0.48	0	6,6,6	0.74	0
3	SO4	G	512	-	4,4,4	0.64	0	6,6,6	0.47	0
4	CIT	G	513	-	3,12,12	2.29	2 (66%)	3,17,17	2.28	2 (66%)
2	GOL	H	501	-	5,5,5	0.59	0	5,5,5	0.58	0
2	GOL	H	502	-	5,5,5	0.37	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	H	503	-	5,5,5	0.81	0	5,5,5	0.88	0
3	SO4	H	504	-	4,4,4	0.66	0	6,6,6	0.45	0
3	SO4	H	505	-	4,4,4	0.59	0	6,6,6	0.58	0
3	SO4	H	506	-	4,4,4	1.03	0	6,6,6	0.81	0
3	SO4	H	507	-	4,4,4	0.13	0	6,6,6	0.43	0
3	SO4	H	508	-	4,4,4	0.64	0	6,6,6	0.31	0
3	SO4	H	509	-	4,4,4	1.49	1 (25%)	6,6,6	0.75	0
3	SO4	H	510	-	4,4,4	0.78	0	6,6,6	0.35	0
3	SO4	H	511	-	4,4,4	0.54	0	6,6,6	0.44	0
3	SO4	H	512	-	4,4,4	0.74	0	6,6,6	0.76	0
3	SO4	H	513	-	4,4,4	0.55	0	6,6,6	0.89	0
3	SO4	H	514	-	4,4,4	0.24	0	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	509	-	-	0/4/4/4	0/0/0/0
3	SO4	B	510	-	-	0/0/0/0	0/0/0/0
3	SO4	B	511	-	-	0/0/0/0	0/0/0/0
3	SO4	B	512	-	-	0/0/0/0	0/0/0/0
3	SO4	B	513	-	-	0/0/0/0	0/0/0/0
3	SO4	B	514	-	-	0/0/0/0	0/0/0/0
3	SO4	B	515	-	-	0/0/0/0	0/0/0/0
3	SO4	B	516	-	-	0/0/0/0	0/0/0/0
3	SO4	B	517	-	-	0/0/0/0	0/0/0/0
3	SO4	B	518	-	-	0/0/0/0	0/0/0/0
3	SO4	B	519	-	-	0/0/0/0	0/0/0/0
4	CIT	B	520	-	-	0/6/16/16	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	GOL	C	505	-	-	0/4/4/4	0/0/0/0
3	SO4	C	506	-	-	0/0/0/0	0/0/0/0
3	SO4	C	507	-	-	0/0/0/0	0/0/0/0
3	SO4	C	508	-	-	0/0/0/0	0/0/0/0
3	SO4	C	509	-	-	0/0/0/0	0/0/0/0
3	SO4	C	510	-	-	0/0/0/0	0/0/0/0
3	SO4	C	511	-	-	0/0/0/0	0/0/0/0
3	SO4	C	512	-	-	0/0/0/0	0/0/0/0
3	SO4	C	513	-	-	0/0/0/0	0/0/0/0
3	SO4	C	514	-	-	0/0/0/0	0/0/0/0
3	SO4	C	515	-	-	0/0/0/0	0/0/0/0
3	SO4	C	516	-	-	0/0/0/0	0/0/0/0
3	SO4	C	517	-	-	0/0/0/0	0/0/0/0
3	SO4	C	518	-	-	0/0/0/0	0/0/0/0
4	CIT	C	519	-	-	0/6/16/16	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	GOL	D	503	-	-	0/4/4/4	0/0/0/0
2	GOL	D	504	-	-	0/4/4/4	0/0/0/0
2	GOL	D	505	-	-	0/4/4/4	0/0/0/0
3	SO4	D	506	-	-	0/0/0/0	0/0/0/0
3	SO4	D	507	-	-	0/0/0/0	0/0/0/0
3	SO4	D	508	-	-	0/0/0/0	0/0/0/0
3	SO4	D	509	-	-	0/0/0/0	0/0/0/0
3	SO4	D	510	-	-	0/0/0/0	0/0/0/0
3	SO4	D	511	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	512	-	-	0/0/0/0	0/0/0/0
3	SO4	D	513	-	-	0/0/0/0	0/0/0/0
3	SO4	D	514	-	-	0/0/0/0	0/0/0/0
3	SO4	D	515	-	-	0/0/0/0	0/0/0/0
3	SO4	D	516	-	-	0/0/0/0	0/0/0/0
3	SO4	D	517	-	-	0/0/0/0	0/0/0/0
2	GOL	E	501	-	-	0/4/4/4	0/0/0/0
2	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	GOL	E	503	-	-	0/4/4/4	0/0/0/0
2	GOL	E	504	-	-	0/4/4/4	0/0/0/0
2	GOL	E	505	-	-	0/4/4/4	0/0/0/0
2	GOL	E	506	-	-	0/4/4/4	0/0/0/0
3	SO4	E	507	-	-	0/0/0/0	0/0/0/0
3	SO4	E	508	-	-	0/0/0/0	0/0/0/0
3	SO4	E	509	-	-	0/0/0/0	0/0/0/0
3	SO4	E	510	-	-	0/0/0/0	0/0/0/0
3	SO4	E	511	-	-	0/0/0/0	0/0/0/0
3	SO4	E	512	-	-	0/0/0/0	0/0/0/0
3	SO4	E	513	-	-	0/0/0/0	0/0/0/0
3	SO4	E	514	-	-	0/0/0/0	0/0/0/0
3	SO4	E	515	-	-	0/0/0/0	0/0/0/0
3	SO4	E	516	-	-	0/0/0/0	0/0/0/0
4	CIT	E	517	-	-	0/6/16/16	0/0/0/0
2	GOL	F	501	-	-	0/4/4/4	0/0/0/0
2	GOL	F	502	-	-	0/4/4/4	0/0/0/0
2	GOL	F	503	-	-	0/4/4/4	0/0/0/0
2	GOL	F	504	-	-	0/4/4/4	0/0/0/0
3	SO4	F	505	-	-	0/0/0/0	0/0/0/0
3	SO4	F	506	-	-	0/0/0/0	0/0/0/0
3	SO4	F	507	-	-	0/0/0/0	0/0/0/0
3	SO4	F	508	-	-	0/0/0/0	0/0/0/0
3	SO4	F	509	-	-	0/0/0/0	0/0/0/0
3	SO4	F	510	-	-	0/0/0/0	0/0/0/0
3	SO4	F	511	-	-	0/0/0/0	0/0/0/0
3	SO4	F	512	-	-	0/0/0/0	0/0/0/0
3	SO4	F	513	-	-	0/0/0/0	0/0/0/0
3	SO4	F	514	-	-	0/0/0/0	0/0/0/0
3	SO4	F	515	-	-	0/0/0/0	0/0/0/0
2	GOL	G	501	-	-	0/4/4/4	0/0/0/0
2	GOL	G	502	-	-	0/4/4/4	0/0/0/0
2	GOL	G	503	-	-	0/4/4/4	0/0/0/0
2	GOL	G	504	-	-	0/4/4/4	0/0/0/0

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	519	CIT	C2-C3	-2.32	1.51	1.54
3	G	509	SO4	O2-S	-2.11	1.39	1.47
4	A	515	CIT	O7-C3	2.09	1.46	1.43
3	E	511	SO4	O4-S	2.11	1.55	1.47
3	D	517	SO4	O4-S	2.15	1.55	1.47
4	G	513	CIT	C2-C3	2.16	1.58	1.54
3	D	508	SO4	O2-S	2.22	1.54	1.47
3	D	508	SO4	O1-S	2.22	1.54	1.47
4	A	515	CIT	C2-C3	2.27	1.58	1.54
2	C	503	GOL	O3-C3	2.28	1.52	1.42
4	B	520	CIT	C4-C3	2.29	1.58	1.54
3	G	506	SO4	O4-S	2.35	1.55	1.47
3	F	508	SO4	O2-S	2.36	1.55	1.47
4	C	519	CIT	C4-C3	2.41	1.58	1.54
3	B	517	SO4	O3-S	2.53	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	SO4	O4-S	2.59	1.56	1.47
2	C	503	GOL	O1-C1	2.65	1.53	1.42
3	A	512	SO4	O1-S	2.66	1.56	1.47
4	G	513	CIT	O7-C3	2.67	1.47	1.43
3	H	509	SO4	O4-S	2.73	1.57	1.47
3	A	505	SO4	O2-S	2.77	1.56	1.47
2	C	503	GOL	O2-C2	3.20	1.53	1.43
3	E	514	SO4	O3-S	3.32	1.59	1.47
4	C	519	CIT	O7-C3	5.86	1.52	1.43
2	C	505	GOL	O3-C3	5.87	1.67	1.42
4	B	520	CIT	O7-C3	6.48	1.53	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	519	CIT	C3-C2-C1	-6.46	104.63	114.96
4	C	519	CIT	C4-C3-C2	-4.38	99.32	109.81
2	A	503	GOL	C3-C2-C1	-3.19	98.60	111.12
4	A	515	CIT	C4-C3-C2	-3.11	102.38	109.81
3	F	513	SO4	O4-S-O3	-2.90	97.20	108.98
2	E	503	GOL	O2-C2-C1	-2.77	95.95	108.65
2	B	507	GOL	O1-C1-C2	-2.64	97.36	110.18
4	G	513	CIT	C4-C3-C2	-2.55	103.71	109.81
3	D	511	SO4	O4-S-O3	-2.53	98.70	108.98
4	E	517	CIT	C3-C2-C1	-2.51	110.94	114.96
3	B	517	SO4	O2-S-O1	-2.49	101.59	109.50
3	E	513	SO4	O2-S-O1	-2.47	101.68	109.50
2	B	503	GOL	O3-C3-C2	-2.40	98.56	110.18
2	D	504	GOL	O1-C1-C2	-2.35	98.80	110.18
3	D	511	SO4	O2-S-O1	-2.34	102.07	109.50
3	A	507	SO4	O2-S-O1	-2.29	102.25	109.50
2	D	502	GOL	O2-C2-C3	-2.27	98.22	108.65
2	D	503	GOL	O1-C1-C2	-2.25	99.28	110.18
3	E	514	SO4	O2-S-O1	-2.19	102.55	109.50
3	G	506	SO4	O2-S-O1	-2.16	102.64	109.50
2	G	503	GOL	O1-C1-C2	-2.08	100.08	110.18
2	E	505	GOL	O2-C2-C1	-2.08	99.11	108.65
3	D	509	SO4	O2-S-O1	2.09	116.13	109.50
3	D	512	SO4	O4-S-O3	2.16	117.76	108.98
3	D	509	SO4	O4-S-O3	2.22	118.00	108.98
2	D	502	GOL	C3-C2-C1	2.23	119.87	111.12
3	F	508	SO4	O2-S-O1	2.23	116.58	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	GOL	O3-C3-C2	2.25	121.09	110.18
2	E	505	GOL	O3-C3-C2	2.32	121.45	110.18
2	D	503	GOL	O2-C2-C3	2.40	119.65	108.65
2	D	505	GOL	O2-C2-C3	2.55	120.34	108.65
2	E	505	GOL	O1-C1-C2	2.79	123.73	110.18
2	C	505	GOL	C3-C2-C1	2.82	122.18	111.12
3	D	512	SO4	O2-S-O1	2.86	118.56	109.50
2	A	503	GOL	O3-C3-C2	2.90	124.25	110.18
4	G	513	CIT	C3-C2-C1	2.97	119.71	114.96
3	E	511	SO4	O4-S-O3	3.13	121.69	108.98
4	B	520	CIT	C3-C4-C5	3.33	120.28	114.96
2	E	505	GOL	C3-C2-C1	3.54	125.01	111.12
2	C	503	GOL	O1-C1-C2	3.73	128.28	110.18
4	E	517	CIT	C3-C4-C5	4.27	121.79	114.96
4	B	520	CIT	C3-C2-C1	6.54	125.42	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

37 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	3	0
2	A	502	GOL	2	0
2	A	503	GOL	1	0
3	A	510	SO4	1	0
4	A	515	CIT	6	0
2	B	502	GOL	1	0
2	B	503	GOL	3	0
2	B	504	GOL	3	0
2	B	505	GOL	2	0
3	B	511	SO4	1	0
3	B	513	SO4	1	0
3	B	514	SO4	1	0
4	B	520	CIT	8	0
2	C	503	GOL	3	0
2	C	504	GOL	2	0
2	C	505	GOL	4	0
3	C	508	SO4	1	0
4	C	519	CIT	4	0
2	D	502	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	GOL	2	0
2	D	505	GOL	4	0
3	D	512	SO4	1	0
2	E	504	GOL	1	0
2	E	505	GOL	5	0
4	E	517	CIT	2	0
2	F	502	GOL	5	0
2	F	504	GOL	2	0
3	F	506	SO4	1	0
2	G	502	GOL	1	0
3	G	510	SO4	1	0
4	G	513	CIT	7	0
2	H	501	GOL	1	0
2	H	502	GOL	2	0
2	H	503	GOL	1	0
3	H	505	SO4	1	0
3	H	508	SO4	1	0
3	H	509	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	430/448 (95%)	-0.65	4 (0%) 85 89	8, 13, 35, 96	0
1	B	430/448 (95%)	-0.66	2 (0%) 91 94	9, 17, 36, 91	0
1	C	431/448 (96%)	-0.47	10 (2%) 64 71	9, 18, 50, 107	0
1	D	435/448 (97%)	-0.46	4 (0%) 85 89	14, 22, 45, 88	0
1	E	430/448 (95%)	-0.34	12 (2%) 56 65	14, 23, 56, 114	0
1	F	430/448 (95%)	-0.34	6 (1%) 78 82	16, 27, 53, 116	0
1	G	430/448 (95%)	-0.09	14 (3%) 50 58	15, 32, 61, 111	1 (0%)
1	H	430/448 (95%)	0.14	18 (4%) 40 47	22, 37, 61, 115	0
All	All	3446/3584 (96%)	-0.36	70 (2%) 68 75	8, 23, 53, 116	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	9.5
1	E	444	VAL	8.8
1	F	405	MET	8.4
1	C	444	VAL	7.3
1	F	444	VAL	7.1
1	G	444	VAL	7.0
1	E	405	MET	6.3
1	G	405	MET	6.1
1	H	405	MET	5.9
1	C	405	MET	5.0
1	C	443	ALA	4.9
1	A	444	VAL	4.5
1	C	14	ALA	4.3
1	H	443	ALA	4.2
1	D	14	ALA	4.2
1	E	443	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	15	SER	4.0
1	F	443	ALA	4.0
1	A	405	MET	3.9
1	E	406	GLU	3.5
1	G	377	ALA	3.4
1	B	405	MET	3.3
1	C	424	HIS	3.3
1	H	288	LEU	3.1
1	G	15	SER	3.1
1	H	146	ASN	3.1
1	G	443	ALA	3.1
1	H	118	ASN	3.1
1	D	405	MET	3.0
1	C	407	PRO	3.0
1	A	15	SER	3.0
1	H	127	ILE	3.0
1	E	442	PRO	2.9
1	H	406	GLU	2.9
1	F	15	SER	2.8
1	G	406	GLU	2.8
1	H	377	ALA	2.7
1	G	404	CYS	2.7
1	G	391	LYS	2.7
1	E	421	LEU	2.6
1	E	407	PRO	2.6
1	H	104	LYS	2.6
1	H	116	ILE	2.5
1	G	424	HIS	2.5
1	D	15	SER	2.4
1	G	378	GLU	2.4
1	C	320	LEU	2.3
1	E	424	HIS	2.3
1	G	16	MET	2.3
1	G	328	LEU	2.3
1	F	406	GLU	2.3
1	H	15	SER	2.3
1	A	406	GLU	2.3
1	H	424	HIS	2.3
1	C	421	LEU	2.2
1	D	127	ILE	2.2
1	E	377	ALA	2.2
1	C	423	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	406	GLU	2.2
1	H	103	ALA	2.2
1	F	127	ILE	2.1
1	H	378	GLU	2.1
1	H	16	MET	2.1
1	H	64	VAL	2.1
1	E	404	CYS	2.1
1	G	442	PRO	2.1
1	H	105	GLY	2.0
1	E	423	LYS	2.0
1	G	64	VAL	2.0
1	B	15	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	E	509	5/5	0.71	0.30	23.90	46,60,77,91	5
2	GOL	C	503	6/6	0.84	0.29	16.06	18,24,28,33	6
3	SO4	G	507	5/5	0.94	0.22	14.63	40,46,60,61	5
2	GOL	E	505	6/6	0.81	0.30	14.46	32,45,48,49	0
2	GOL	B	505	6/6	0.83	0.23	13.17	43,54,65,67	0
3	SO4	F	513	5/5	0.89	0.27	10.45	56,60,79,90	0
3	SO4	E	515	5/5	0.85	0.27	10.23	52,70,82,84	0
3	SO4	C	507	5/5	0.71	0.32	9.83	72,81,101,102	0
3	SO4	C	515	5/5	0.90	0.24	9.56	49,58,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	F	512	5/5	0.92	0.22	8.73	64,69,90,96	0
3	SO4	G	505	5/5	0.87	0.28	8.47	71,98,113,117	0
3	SO4	H	506	5/5	0.90	0.31	7.60	59,63,68,77	0
3	SO4	H	513	5/5	0.99	0.19	6.95	53,53,57,60	0
2	GOL	D	505	6/6	0.92	0.15	6.89	32,36,39,50	0
2	GOL	C	505	6/6	0.84	0.27	6.52	21,27,34,43	0
3	SO4	C	516	5/5	0.96	0.21	6.19	40,58,64,72	0
3	SO4	D	509	5/5	0.95	0.16	5.59	45,56,68,71	0
3	SO4	G	506	5/5	0.81	0.20	5.49	45,80,86,98	0
3	SO4	F	511	5/5	0.84	0.20	5.47	54,74,86,91	0
3	SO4	A	505	5/5	0.96	0.20	5.36	32,35,47,64	0
2	GOL	H	502	6/6	0.85	0.18	5.27	52,62,74,81	0
3	SO4	D	517	5/5	0.93	0.21	5.25	34,35,49,51	5
4	CIT	C	519	13/13	0.88	0.21	5.21	26,45,62,62	0
3	SO4	D	508	5/5	0.92	0.24	4.63	48,59,67,81	0
4	CIT	A	515	13/13	0.92	0.17	4.56	15,29,39,49	13
3	SO4	E	514	5/5	0.92	0.30	4.52	41,52,66,79	0
3	SO4	F	514	5/5	0.91	0.27	4.48	59,70,77,89	0
3	SO4	H	510	5/5	0.92	0.30	4.30	78,82,95,96	0
4	CIT	B	520	13/13	0.89	0.24	4.26	31,46,59,64	0
3	SO4	A	511	5/5	0.95	0.17	4.04	39,53,58,69	0
2	GOL	F	504	6/6	0.81	0.20	4.00	50,57,62,66	0
2	GOL	A	501	6/6	0.91	0.15	3.97	28,38,48,60	0
3	SO4	C	517	5/5	0.94	0.24	3.74	56,64,78,90	0
2	GOL	B	508	6/6	0.80	0.18	3.44	63,65,68,70	0
2	GOL	E	504	6/6	0.88	0.25	3.40	37,56,61,63	0
4	CIT	G	513	13/13	0.91	0.18	3.31	35,44,66,66	0
3	SO4	F	508	5/5	0.91	0.32	3.30	54,67,89,95	0
4	CIT	E	517	13/13	0.88	0.21	3.29	35,64,73,87	0
3	SO4	H	509	5/5	0.80	0.34	2.97	43,46,66,74	5
2	GOL	B	503	6/6	0.92	0.21	2.94	29,31,43,48	0
2	GOL	A	504	6/6	0.89	0.14	2.91	38,45,53,54	0
2	GOL	B	504	6/6	0.96	0.14	2.71	30,35,38,40	0
2	GOL	D	502	6/6	0.96	0.20	2.62	31,35,39,41	0
3	SO4	B	515	5/5	0.99	0.12	2.11	23,35,38,39	0
2	GOL	C	504	6/6	0.91	0.14	1.98	36,38,44,56	0
2	GOL	C	502	6/6	0.94	0.10	1.95	31,38,49,63	0
2	GOL	E	501	6/6	0.92	0.13	1.92	35,49,58,64	0
2	GOL	B	502	6/6	0.93	0.13	1.84	32,37,45,57	0
2	GOL	D	504	6/6	0.92	0.15	1.53	31,37,44,54	0
2	GOL	F	501	6/6	0.94	0.19	1.35	25,32,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	G	501	6/6	0.94	0.14	1.34	40,49,64,65	0
2	GOL	F	502	6/6	0.93	0.13	1.31	40,47,49,56	0
3	SO4	A	514	5/5	0.92	0.23	1.25	48,62,67,83	0
2	GOL	H	501	6/6	0.89	0.21	1.21	32,43,45,48	0
2	GOL	G	503	6/6	0.94	0.23	1.21	29,36,38,44	0
2	GOL	E	502	6/6	0.97	0.17	1.06	22,26,27,32	0
2	GOL	D	501	6/6	0.97	0.16	0.42	18,22,23,24	0
2	GOL	B	501	6/6	0.97	0.14	0.29	18,25,27,34	0
2	GOL	C	501	6/6	0.97	0.13	0.13	18,20,21,22	0
2	GOL	A	503	6/6	0.95	0.14	0.10	14,18,19,24	0
2	GOL	H	503	6/6	0.89	0.12	0.06	38,42,49,53	0
3	SO4	A	510	5/5	0.99	0.08	-0.59	23,24,26,37	0
3	SO4	G	509	5/5	1.00	0.07	-0.71	24,25,28,29	0
3	SO4	G	510	5/5	0.90	0.41	-	90,99,107,116	0
3	SO4	H	505	5/5	0.79	0.41	-	75,97,102,103	0
3	SO4	B	513	5/5	0.89	0.32	-	79,94,112,117	0
3	SO4	C	506	5/5	0.93	0.43	-	76,77,94,94	0
3	SO4	D	513	5/5	0.80	0.32	-	71,82,108,108	0
3	SO4	G	508	5/5	0.68	0.49	-	96,103,128,136	0
3	SO4	D	514	5/5	0.89	0.29	-	62,91,99,102	0
3	SO4	D	516	5/5	0.83	0.33	-	75,76,93,95	0
3	SO4	A	506	5/5	0.92	0.30	-	66,66,86,88	0
3	SO4	C	508	5/5	0.94	0.30	-	74,75,79,82	0
3	SO4	C	509	5/5	0.93	0.33	-	104,108,116,118	0
3	SO4	H	514	5/5	0.72	0.43	-	101,112,123,125	0
3	SO4	D	515	5/5	0.87	0.38	-	76,91,101,105	0
3	SO4	F	510	5/5	0.91	0.27	-	62,74,79,88	0
3	SO4	F	506	5/5	0.93	0.40	-	86,87,108,111	0
3	SO4	D	511	5/5	0.86	0.24	-	49,62,78,78	0
3	SO4	C	511	5/5	0.95	0.19	-	67,67,82,88	0
3	SO4	E	512	5/5	0.92	0.23	-	50,66,84,88	0
3	SO4	C	512	5/5	0.98	0.20	-	40,46,54,54	0
3	SO4	D	512	5/5	0.93	0.25	-	60,73,82,87	0
2	GOL	B	507	6/6	0.89	0.18	-	54,64,72,76	0
3	SO4	H	508	5/5	0.91	0.37	-	69,71,88,94	0
3	SO4	F	515	5/5	0.93	0.34	-	90,102,112,113	0
2	GOL	G	504	6/6	0.74	0.31	-	52,58,67,71	0
3	SO4	C	514	5/5	0.91	0.30	-	65,79,88,91	0
3	SO4	B	514	5/5	0.80	0.31	-	61,66,79,82	5
3	SO4	D	507	5/5	0.92	0.40	-	78,96,97,105	0
3	SO4	H	512	5/5	0.89	0.32	-	81,83,96,96	0
3	SO4	A	512	5/5	0.93	0.26	-	41,41,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	E	503	6/6	0.94	0.21	-	50,57,62,65	0
2	GOL	G	502	6/6	0.72	0.49	-	56,68,77,82	0
3	SO4	B	518	5/5	0.86	0.36	-	102,103,116,122	0
2	GOL	B	509	6/6	0.78	0.40	-	50,58,65,66	0
3	SO4	C	510	5/5	0.93	0.33	-	51,60,76,78	0
3	SO4	E	511	5/5	0.98	0.15	-	39,41,44,55	0
3	SO4	F	507	5/5	0.83	0.37	-	71,88,91,99	5
3	SO4	A	509	5/5	0.96	0.19	-	55,62,69,75	0
3	SO4	B	511	5/5	0.91	0.34	-	45,58,66,67	5
3	SO4	H	511	5/5	0.94	0.33	-	70,92,95,103	0
3	SO4	H	507	5/5	0.87	0.42	-	104,110,115,123	0
2	GOL	E	506	6/6	0.83	0.18	-	58,72,74,75	0
3	SO4	A	508	5/5	0.94	0.36	-	62,73,75,86	0
3	SO4	E	508	5/5	0.91	0.27	-	39,43,56,60	5
3	SO4	D	510	5/5	0.94	0.25	-	66,78,95,97	0
3	SO4	F	505	5/5	0.86	0.32	-	72,75,85,96	0
3	SO4	F	509	5/5	0.91	0.33	-	56,75,85,85	0
3	SO4	G	512	5/5	0.87	0.33	-	80,91,99,104	0
3	SO4	A	507	5/5	0.92	0.35	-	39,52,60,70	5
3	SO4	B	510	5/5	0.97	0.25	-	68,70,76,86	0
3	SO4	E	507	5/5	0.78	0.31	-	78,97,117,120	0
2	GOL	B	506	6/6	0.88	0.44	-	56,67,71,71	0
3	SO4	B	516	5/5	0.91	0.25	-	51,67,68,72	0
3	SO4	G	511	5/5	0.90	0.41	-	82,101,104,113	0
3	SO4	B	512	5/5	0.93	0.32	-	44,48,51,65	5
3	SO4	E	513	5/5	0.91	0.31	-	75,76,88,92	0
3	SO4	B	517	5/5	0.91	0.23	-	39,41,60,63	0
3	SO4	H	504	5/5	0.90	0.35	-	73,79,92,107	0
3	SO4	B	519	5/5	0.92	0.34	-	56,73,88,106	0
3	SO4	C	513	5/5	0.97	0.20	-	43,45,49,62	0
2	GOL	D	503	6/6	0.84	0.14	-	43,49,54,62	0
3	SO4	E	510	5/5	0.89	0.43	-	84,91,94,107	0
2	GOL	F	503	6/6	0.77	0.32	-	59,67,71,72	0
2	GOL	A	502	6/6	0.90	0.15	-	54,66,71,72	0
3	SO4	D	506	5/5	0.94	0.31	-	72,74,85,96	0
3	SO4	A	513	5/5	0.92	0.33	-	74,76,86,93	0
3	SO4	C	518	5/5	0.85	0.34	-	83,92,120,127	0
3	SO4	E	516	5/5	0.68	0.47	-	91,102,118,122	0

6.5 Other polymers (i)

There are no such residues in this entry.