



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 PM GMT

PDB ID : 4NXK
Title : Crystal structure of Abp-D197A, a catalytic mutant of a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on : 2013-12-09
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

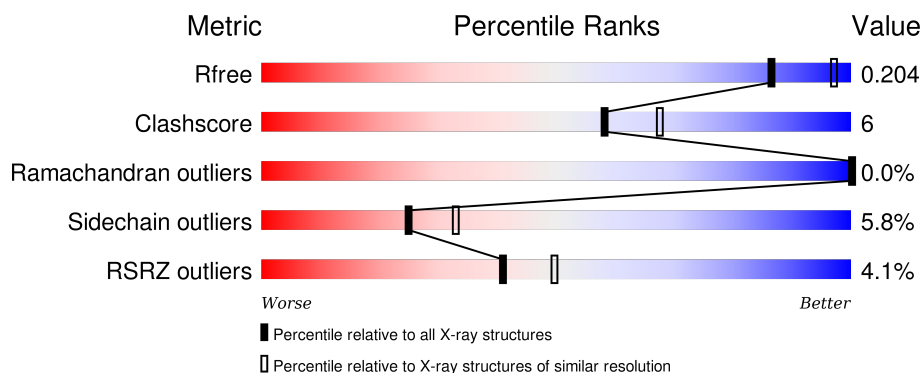
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	B	448	<div> <div>85%</div> <div>9%</div> <div>• •</div> </div>
1	C	448	<div> <div>2%</div> <div>83%</div> <div>10%</div> <div>• •</div> </div>
1	D	448	<div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
1	E	448	<div> <div>3%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	504	-	-	-	X
2	SO4	A	507	-	-	-	X
2	SO4	A	508	-	-	-	X
2	SO4	B	501	-	-	-	X
2	SO4	B	502	-	-	-	X
2	SO4	B	506	-	-	-	X
2	SO4	C	502	-	-	-	X
2	SO4	C	503	-	-	-	X
2	SO4	C	507	-	-	-	X
2	SO4	C	509	-	-	-	X
2	SO4	D	503	-	-	-	X
2	SO4	D	504	-	-	-	X
2	SO4	D	507	-	-	-	X
2	SO4	D	508	-	-	-	X
2	SO4	E	501	-	-	-	X
2	SO4	E	502	-	-	-	X
2	SO4	E	503	-	-	-	X
2	SO4	E	506	-	-	-	X
2	SO4	E	508	-	-	-	X
2	SO4	F	502	-	-	-	X
2	SO4	F	504	-	-	-	X
2	SO4	F	505	-	-	-	X
2	SO4	F	506	-	-	-	X
2	SO4	G	503	-	-	-	X
2	SO4	G	505	-	-	-	X
2	SO4	G	506	-	-	-	X
2	SO4	H	502	-	-	X	-
2	SO4	H	504	-	-	-	X
2	SO4	H	505	-	-	-	X
3	GOL	A	511	-	-	-	X
3	GOL	B	511	-	-	-	X
3	GOL	B	513	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	514	-	-	X	X
3	GOL	D	513	-	-	-	X
3	GOL	E	510	-	-	-	X
3	GOL	E	511	-	-	-	X
3	GOL	E	513	-	-	-	X
3	GOL	H	509	-	-	X	-
4	CIT	A	513	-	-	X	X
4	CIT	B	514	-	-	X	X
4	CIT	C	515	-	-	X	X
4	CIT	D	516	-	-	X	X
4	CIT	E	514	-	-	X	X
4	CIT	G	509	-	-	-	X

2 Entry composition

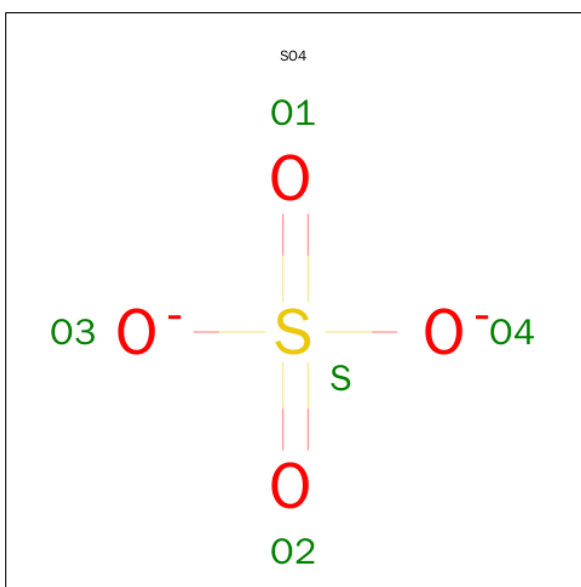
There are 5 unique types of molecules in this entry. The entry contains 31524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	4	0
			3494	2235	599	635	25			
1	B	430	Total	C	N	O	S	0	2	0
			3482	2227	598	632	25			
1	C	430	Total	C	N	O	S	0	2	0
			3479	2226	597	631	25			
1	D	435	Total	C	N	O	S	0	2	0
			3509	2247	604	633	25			
1	E	431	Total	C	N	O	S	0	2	0
			3481	2227	598	631	25			
1	F	430	Total	C	N	O	S	0	0	0
			3467	2218	596	628	25			
1	G	430	Total	C	N	O	S	0	2	0
			3479	2226	597	631	25			
1	H	430	Total	C	N	O	S	0	3	0
			3483	2230	597	629	27			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

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

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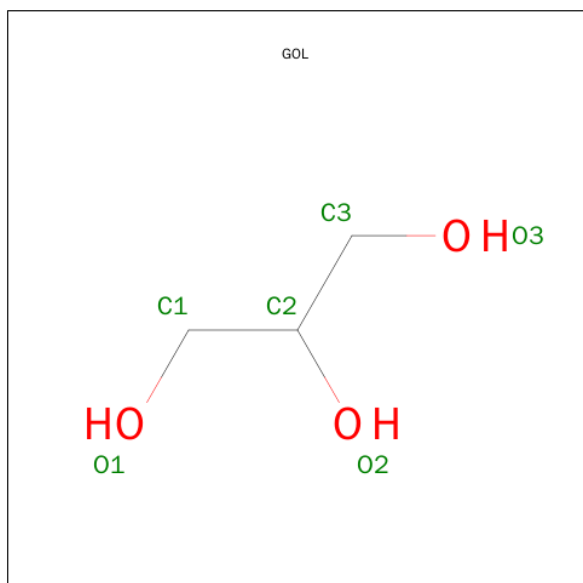
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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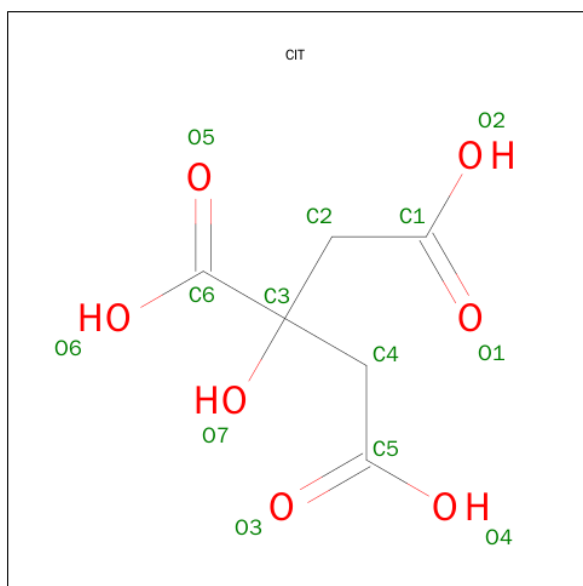
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0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

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

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



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

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

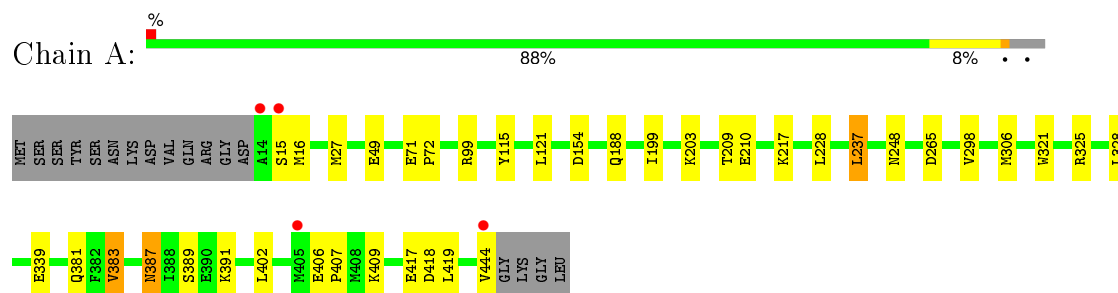
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	574	Total	O	0	0
			574	574		
5	B	491	Total	O	0	0
			491	491		
5	C	433	Total	O	0	0
			433	433		
5	D	402	Total	O	0	0
			402	402		
5	E	377	Total	O	0	0
			377	377		
5	F	299	Total	O	0	0
			299	299		
5	G	295	Total	O	0	0
			295	295		
5	H	191	Total	O	0	0
			191	191		

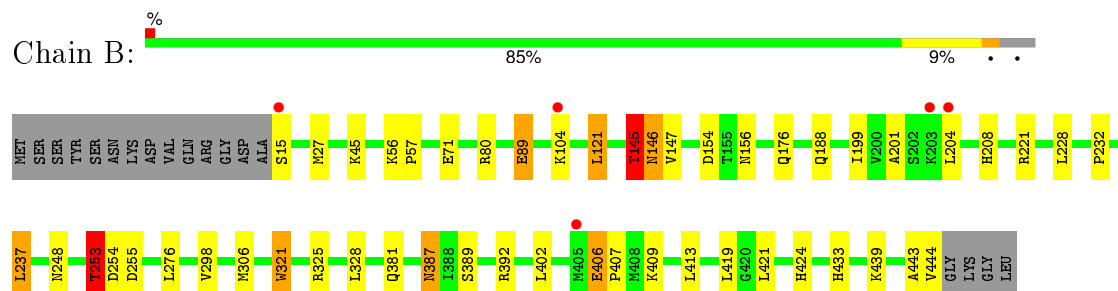
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

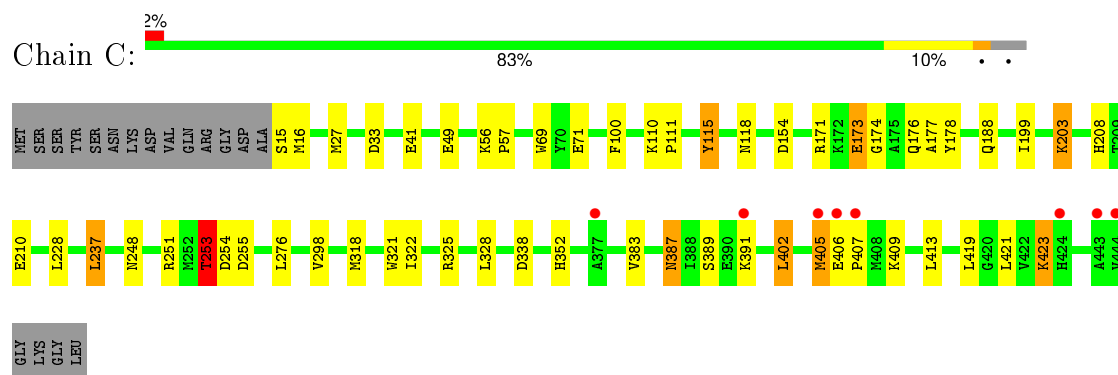
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



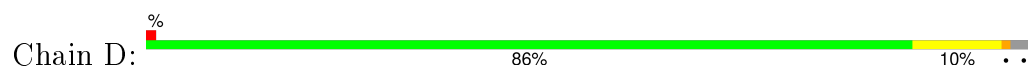
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

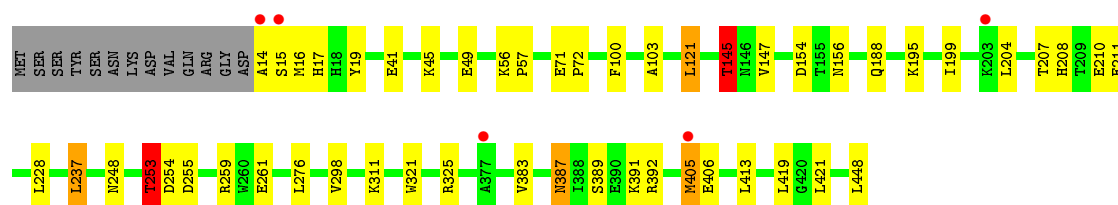


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

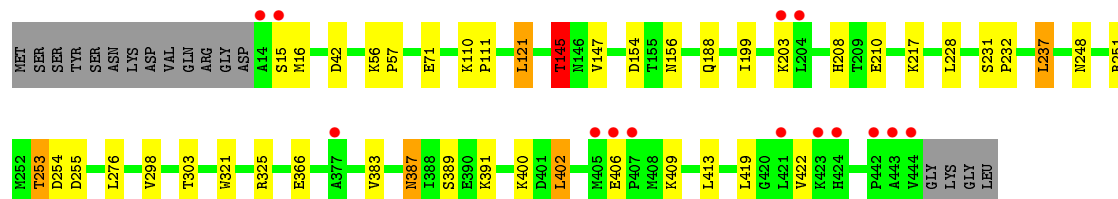
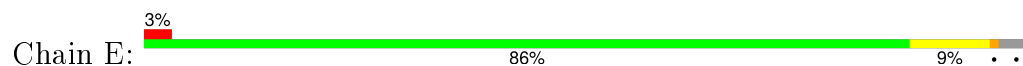


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

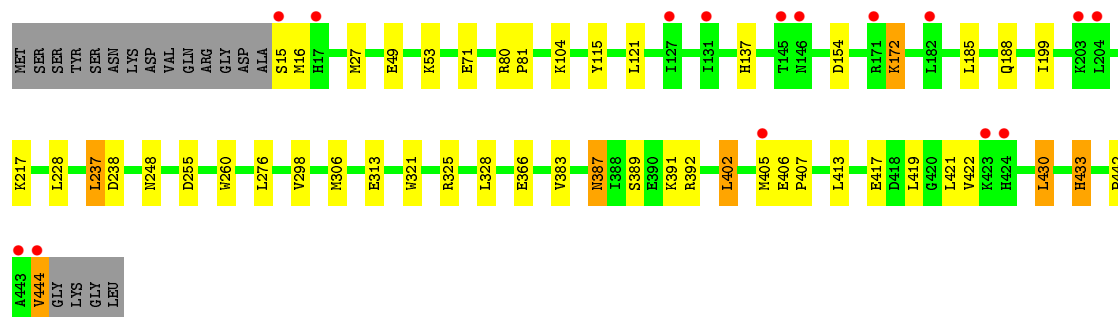
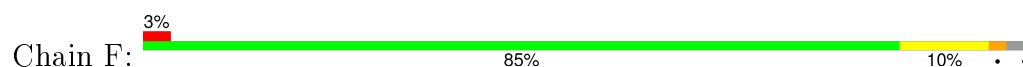




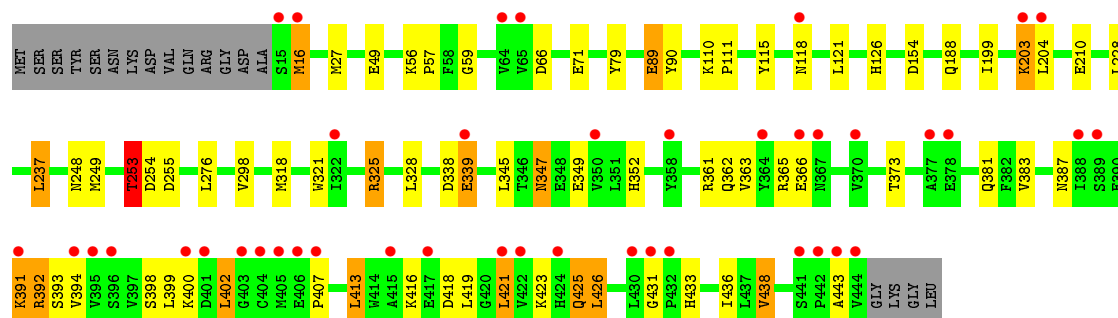
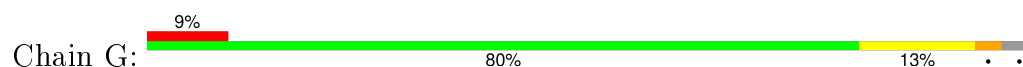
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



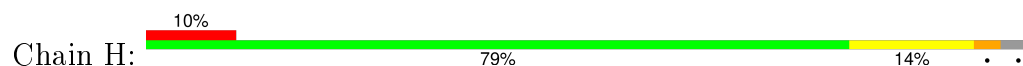
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

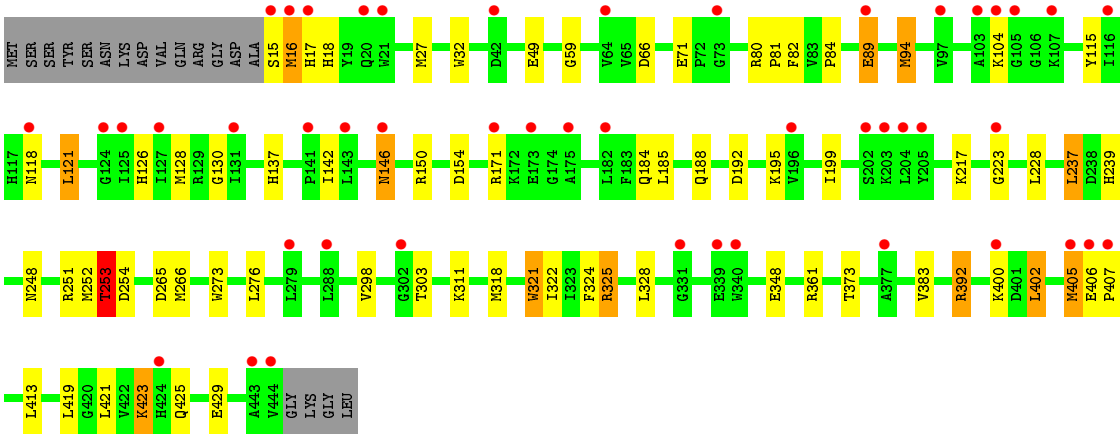


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.70Å 203.53Å 286.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 2.30 24.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (24.86-2.30) 96.4 (24.84-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.170 , 0.201 0.175 , 0.204	Depositor DCC
R_{free} test set	13610 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.972	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 269366 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31524	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	1.07	0/3608	0.92	7/4898 (0.1%)
1	B	1.03	1/3587 (0.0%)	0.91	9/4869 (0.2%)
1	C	0.99	4/3587 (0.1%)	0.89	8/4869 (0.2%)
1	D	0.95	1/3617 (0.0%)	0.90	9/4906 (0.2%)
1	E	0.88	0/3589	0.86	6/4873 (0.1%)
1	F	0.87	1/3569 (0.0%)	0.88	8/4845 (0.2%)
1	G	0.86	0/3587	0.90	6/4869 (0.1%)
1	H	0.81	0/3594	0.87	10/4877 (0.2%)
All	All	0.94	7/28738 (0.0%)	0.89	63/39006 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	TYR	CG-CD1	-5.57	1.31	1.39
1	D	325	ARG	CZ-NH1	5.39	1.40	1.33
1	C	173	GLU	CD-OE1	5.30	1.31	1.25
1	C	115	TYR	CG-CD2	-5.23	1.32	1.39
1	B	321	TRP	CG-CD1	-5.20	1.29	1.36
1	F	325	ARG	CZ-NH2	5.08	1.39	1.33
1	C	69	TRP	CZ3-CH2	-5.07	1.31	1.40

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	C	154	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	C	171	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	E	154	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	D	405	MET	CG-SD-CE	8.29	113.46	100.20
1	H	325	ARG	NE-CZ-NH2	-7.84	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	154	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	C	171	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	H	154	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	E	325	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	H	392	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	325	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	392	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	B	154	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	154	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	325	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	F	154	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	D	154	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	F	325	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	253	THR	N-CA-CB	-5.88	99.12	110.30
1	F	430	LEU	CB-CG-CD2	5.83	120.92	111.00
1	G	253	THR	N-CA-CB	-5.83	99.22	110.30
1	D	121	LEU	CB-CG-CD2	5.80	120.85	111.00
1	G	325	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	253	THR	N-CA-CB	-5.73	99.42	110.30
1	G	402	LEU	CB-CG-CD2	5.71	120.70	111.00
1	G	237	LEU	CA-CB-CG	-5.70	102.19	115.30
1	F	238	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	237	LEU	CA-CB-CG	-5.65	102.30	115.30
1	H	402	LEU	CB-CG-CD2	5.59	120.50	111.00
1	C	237	LEU	CA-CB-CG	-5.58	102.47	115.30
1	D	145	THR	CB-CA-C	-5.57	96.55	111.60
1	A	383	VAL	CA-CB-CG2	5.56	119.24	110.90
1	B	237	LEU	CA-CB-CG	-5.56	102.52	115.30
1	A	121	LEU	CB-CG-CD1	5.53	120.40	111.00
1	G	249	MET	CG-SD-CE	5.53	109.05	100.20
1	H	237	LEU	CA-CB-CG	-5.52	102.60	115.30
1	F	53	LYS	CB-CA-C	-5.46	99.47	110.40
1	A	237	LEU	CA-CB-CG	-5.45	102.78	115.30
1	C	402	LEU	CB-CG-CD2	5.39	120.16	111.00
1	F	402	LEU	CB-CG-CD2	5.39	120.16	111.00
1	D	237	LEU	CA-CB-CG	-5.38	102.92	115.30
1	C	33	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	392	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	145	THR	CB-CA-C	-5.32	97.23	111.60
1	B	325	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	F	172	LYS	CD-CE-NZ	5.29	123.86	111.70
1	H	80	ARG	NE-CZ-NH2	-5.28	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	392	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	H	94	MET	CG-SD-CE	5.21	108.54	100.20
1	A	99	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	F	237	LEU	CA-CB-CG	-5.14	103.47	115.30
1	H	253	THR	N-CA-CB	-5.14	100.54	110.30
1	B	253	THR	N-CA-CB	-5.13	100.55	110.30
1	A	402	LEU	CB-CG-CD1	5.13	119.72	111.00
1	H	405	MET	CB-CG-SD	5.12	127.77	112.40
1	E	402	LEU	CB-CG-CD2	5.11	119.68	111.00
1	B	80	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	H	121	LEU	CB-CG-CD2	5.08	119.64	111.00
1	B	255	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	121	LEU	CB-CG-CD2	5.07	119.61	111.00
1	E	121	LEU	CB-CG-CD2	5.06	119.61	111.00
1	B	145	THR	CB-CA-C	-5.01	98.08	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3376	35	0
1	B	3482	0	3360	28	0
1	C	3479	0	3361	46	0
1	D	3509	0	3408	36	0
1	E	3481	0	3365	21	0
1	F	3467	0	3347	18	0
1	G	3479	0	3361	56	0
1	H	3483	0	3373	73	0
2	A	45	0	0	0	0
2	B	40	0	0	0	0
2	C	45	0	0	1	0
2	D	55	0	0	3	0
2	E	45	0	0	0	0
2	F	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	30	0	0	0	0
2	H	35	0	0	3	0
3	A	18	0	24	3	0
3	B	30	0	40	3	0
3	C	30	0	37	9	0
3	D	24	0	31	6	0
3	E	24	0	31	5	0
3	F	24	0	32	3	0
3	G	12	0	16	3	0
3	H	18	0	24	11	0
4	A	13	0	5	15	0
4	B	13	0	5	6	0
4	C	13	0	5	8	0
4	D	13	0	5	9	0
4	E	13	0	5	7	0
4	G	13	0	5	3	0
5	A	574	0	0	14	0
5	B	491	0	0	8	0
5	C	433	0	0	13	0
5	D	402	0	0	6	0
5	E	377	0	0	5	0
5	F	299	0	0	5	0
5	G	295	0	0	22	0
5	H	191	0	0	25	0
All	All	31524	0	27216	331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:510:GOL:O3	3:E:510:GOL:C3	1.65	1.45
1:G:352:HIS:HB2	5:G:864:HOH:O	1.32	1.26
1:H:16:MET:CE	1:H:16:MET:HA	1.67	1.24
4:D:516:CIT:C6	4:D:516:CIT:O2	1.85	1.15
1:H:16:MET:HE3	1:H:16:MET:HA	1.12	1.09
1:G:203:LYS:HD3	1:G:203:LYS:H	1.17	1.08
4:D:516:CIT:O6	4:D:516:CIT:O2	1.78	1.02
1:C:210:GLU:HB2	4:C:515:CIT:H21	1.43	1.00
1:B:89:GLU:HG2	5:B:916:HOH:O	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:LYS:HA	5:H:670:HOH:O	1.68	0.94
1:C:118:ASN:HB3	5:C:1001:HOH:O	1.68	0.93
1:G:188[B]:GLN:HG3	5:G:683:HOH:O	1.68	0.92
1:E:188[A]:GLN:HG2	5:E:787:HOH:O	1.72	0.90
1:D:16:MET:HE3	5:D:782:HOH:O	1.70	0.89
1:H:252[B]:MET:CE	1:H:273:TRP:HB2	2.03	0.89
1:G:203:LYS:H	1:G:203:LYS:CD	1.82	0.89
1:G:203:LYS:HD3	1:G:203:LYS:N	1.90	0.86
1:H:146:ASN:HB3	5:H:720:HOH:O	1.76	0.85
1:H:16:MET:HE3	1:H:16:MET:CA	2.03	0.84
1:H:16:MET:CE	1:H:16:MET:CA	2.51	0.83
1:G:443:ALA:CB	5:G:754:HOH:O	2.23	0.83
1:A:210:GLU:H	4:A:513:CIT:H42	1.44	0.82
1:F:228:LEU:H	1:F:248:ASN:HD22	1.28	0.81
1:F:306:MET:HE3	5:F:646:HOH:O	1.81	0.80
1:H:128:MET:HE3	1:H:128:MET:HA	1.62	0.80
4:B:514:CIT:C1	4:B:514:CIT:O4	2.29	0.80
4:D:516:CIT:O6	4:D:516:CIT:C1	2.30	0.79
1:C:405:MET:HA	1:C:405:MET:CE	2.13	0.78
1:G:443:ALA:HB2	5:G:754:HOH:O	1.82	0.78
1:A:228:LEU:H	1:A:248:ASN:HD22	1.31	0.78
1:E:208:HIS:HA	4:E:514:CIT:O1	1.84	0.78
1:C:405:MET:HA	1:C:405:MET:HE2	1.66	0.77
1:H:252[B]:MET:HE2	1:H:273:TRP:HB2	1.64	0.77
1:A:210:GLU:H	4:A:513:CIT:C4	1.97	0.77
1:C:210:GLU:HB2	4:C:515:CIT:C2	2.15	0.77
1:B:443:ALA:O	1:B:444:VAL:HB	1.85	0.77
3:C:511:GOL:H11	5:C:681:HOH:O	1.85	0.76
1:B:228:LEU:H	1:B:248:ASN:HD22	1.32	0.76
1:H:228:LEU:H	1:H:248:ASN:HD22	1.34	0.75
4:C:515:CIT:O1	4:C:515:CIT:C6	2.29	0.75
1:A:210:GLU:HB2	4:A:513:CIT:H22	1.69	0.74
1:C:228:LEU:H	1:C:248:ASN:HD22	1.36	0.71
1:E:228:LEU:H	1:E:248:ASN:HD22	1.35	0.71
4:B:514:CIT:C6	4:B:514:CIT:O4	2.30	0.71
1:B:253:THR:HG23	1:B:254:ASP:O	1.89	0.71
1:G:210:GLU:HB2	4:G:509:CIT:H22	1.73	0.70
1:C:352:HIS:HB2	5:C:923:HOH:O	1.92	0.70
1:C:253:THR:HG23	1:C:254:ASP:O	1.91	0.70
1:G:228:LEU:H	1:G:248:ASN:HD22	1.40	0.69
1:A:210:GLU:HG2	4:A:513:CIT:H42	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:LYS:HD2	5:C:816:HOH:O	1.91	0.69
1:D:228:LEU:H	1:D:248:ASN:HD22	1.39	0.69
1:G:253:THR:HG23	1:G:254:ASP:O	1.93	0.68
1:H:32:TRP:CD2	3:H:509:GOL:H31	2.28	0.68
1:H:188:GLN:HG3	5:H:672:HOH:O	1.93	0.68
4:E:514:CIT:O7	4:E:514:CIT:O1	2.09	0.68
1:H:32:TRP:CG	3:H:509:GOL:H31	2.29	0.68
1:B:176:GLN:HB3	3:B:513:GOL:H31	1.75	0.67
4:B:514:CIT:C2	4:B:514:CIT:O4	2.38	0.67
1:G:349:GLU:HB3	1:G:413:LEU:CD1	2.25	0.67
1:H:82:PHE:HA	5:H:682:HOH:O	1.93	0.67
1:E:253:THR:HG23	1:E:254:ASP:O	1.94	0.66
1:H:142:ILE:HG12	5:H:777:HOH:O	1.93	0.66
1:D:208:HIS:HA	4:D:516:CIT:O2	1.95	0.66
1:A:210:GLU:CG	4:A:513:CIT:H22	2.26	0.66
1:C:177:ALA:H	3:C:514:GOL:H31	1.59	0.66
1:G:398:SER:HA	1:G:425:GLN:HB3	1.77	0.66
1:D:195:LYS:NZ	3:D:512:GOL:H32	2.11	0.65
1:A:210:GLU:HB2	4:A:513:CIT:C2	2.26	0.65
1:F:137:HIS:CE1	1:H:137:HIS:CE1	2.84	0.65
1:H:253:THR:HG23	1:H:254:ASP:O	1.97	0.65
1:G:433:HIS:HB2	5:G:698:HOH:O	1.96	0.65
1:A:417:GLU:HG3	5:A:1115:HOH:O	1.95	0.65
1:D:45:LYS:O	1:D:49:GLU:HG3	1.97	0.65
1:H:252[B]:MET:HE1	1:H:324:PHE:CZ	2.32	0.64
1:B:221:ARG:HH21	3:B:512:GOL:H2	1.62	0.64
4:E:514:CIT:C2	4:E:514:CIT:O3	2.46	0.64
1:C:118:ASN:HB3	5:C:1012:HOH:O	1.97	0.64
1:D:17:HIS:NE2	2:D:501:SO4:O3	2.30	0.64
1:C:423:LYS:HD2	1:C:423:LYS:H	1.63	0.64
1:H:192:ASP:OD1	5:H:617:HOH:O	2.15	0.64
4:A:513:CIT:H21	5:A:1173:HOH:O	1.99	0.63
1:H:252[B]:MET:CE	1:H:273:TRP:CB	2.74	0.63
1:H:195:LYS:NZ	3:H:509:GOL:H2	2.13	0.63
1:D:253:THR:HG23	1:D:254:ASP:O	1.98	0.62
1:G:421:LEU:HD21	5:G:754:HOH:O	1.99	0.62
1:A:210:GLU:CB	4:A:513:CIT:H22	2.29	0.61
1:C:176:GLN:HB3	3:C:514:GOL:H2	1.82	0.61
3:E:510:GOL:C3	3:E:510:GOL:HO3	2.08	0.60
1:C:208:HIS:HA	4:C:515:CIT:O1	2.01	0.60
1:C:208:HIS:CA	4:C:515:CIT:O1	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:VAL:HG13	5:A:1092:HOH:O	2.02	0.60
1:G:407:PRO:HB2	5:G:754:HOH:O	2.02	0.60
1:H:251:ARG:HH12	3:H:509:GOL:H11	1.66	0.59
1:D:207:THR:N	2:D:504:SO4:O1	2.36	0.59
1:H:248:ASN:ND2	5:H:748:HOH:O	2.34	0.59
1:G:16:MET:HE2	1:G:16:MET:N	2.18	0.59
1:G:391:LYS:HD2	5:G:765:HOH:O	2.02	0.59
1:C:188[B]:GLN:HG2	5:C:946:HOH:O	2.01	0.59
1:C:253:THR:CG2	1:C:254:ASP:O	2.51	0.58
1:C:423:LYS:CD	1:C:423:LYS:H	2.15	0.58
1:B:406:GLU:HB2	1:B:407:PRO:HD2	1.85	0.58
1:D:195:LYS:HZ1	3:D:512:GOL:H32	1.68	0.58
1:B:208:HIS:ND1	4:B:514:CIT:H41	2.18	0.58
1:E:210:GLU:HB2	4:E:514:CIT:H21	1.84	0.58
1:A:265:ASP:HB3	5:A:822:HOH:O	2.03	0.58
1:D:259:ARG:NH2	1:D:261:GLU:OE1	2.37	0.57
1:G:349:GLU:HB3	1:G:413:LEU:HD12	1.86	0.57
1:H:81:PRO:O	5:H:743:HOH:O	2.17	0.57
1:A:188[B]:GLN:HG2	5:A:857:HOH:O	2.03	0.57
1:G:79:TYR:O	5:G:764:HOH:O	2.17	0.57
1:B:146:ASN:HB3	5:B:924:HOH:O	2.03	0.57
1:E:253:THR:CG2	1:E:254:ASP:O	2.52	0.57
1:H:130:GLY:O	5:H:621:HOH:O	2.18	0.57
1:D:211:GLU:N	4:D:516:CIT:O1	2.32	0.57
1:H:130:GLY:C	5:H:621:HOH:O	2.44	0.57
1:B:188[B]:GLN:HG3	5:B:961:HOH:O	2.03	0.57
1:B:253:THR:CG2	1:B:254:ASP:O	2.53	0.57
1:G:347:ASN:HD22	1:G:347:ASN:C	2.08	0.56
1:E:56:LYS:HD2	5:E:890:HOH:O	2.05	0.56
1:G:254:ASP:OD1	3:G:508:GOL:C1	2.53	0.56
1:H:253:THR:CG2	1:H:254:ASP:O	2.54	0.56
1:G:387:ASN:ND2	1:G:431:GLY:O	2.37	0.56
1:H:16:MET:HE2	1:H:17:HIS:H	1.71	0.55
1:A:210:GLU:HG3	4:A:513:CIT:H22	1.89	0.55
1:C:405:MET:CA	1:C:405:MET:CE	2.84	0.55
4:E:514:CIT:H21	4:E:514:CIT:O3	2.06	0.55
1:F:49:GLU:OE2	1:F:115:TYR:OH	2.22	0.55
1:A:49[A]:GLU:OE2	1:A:115:TYR:OH	2.24	0.55
1:H:425[B]:GLN:NE2	5:H:622:HOH:O	2.38	0.55
1:H:84:PRO:HG2	2:H:502:SO4:O3	2.07	0.55
1:H:146:ASN:OD1	1:H:146:ASN:N	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASP:OD1	5:E:963:HOH:O	2.18	0.54
1:H:59:GLY:O	5:H:765:HOH:O	2.19	0.54
1:G:399:LEU:HD23	5:G:692:HOH:O	2.07	0.54
1:H:49:GLU:OE2	1:H:115:TYR:OH	2.25	0.54
1:G:253:THR:CG2	1:G:254:ASP:O	2.54	0.54
1:G:210:GLU:HG2	4:G:509:CIT:H42	1.90	0.54
1:C:49:GLU:OE2	1:C:115:TYR:OH	2.25	0.54
1:C:255:ASP:OD1	3:C:510:GOL:H12	2.07	0.54
1:G:210:GLU:H	4:G:509:CIT:H42	1.73	0.54
1:D:208:HIS:CA	4:D:516:CIT:O2	2.55	0.54
1:G:254:ASP:OD1	3:G:508:GOL:H11	2.07	0.54
1:G:59:GLY:C	5:G:814:HOH:O	2.46	0.54
1:F:366:GLU:HG3	5:F:802:HOH:O	2.06	0.53
1:H:84:PRO:CG	2:H:502:SO4:O3	2.57	0.53
1:G:362:GLN:NE2	5:G:861:HOH:O	2.27	0.53
1:H:223:GLY:N	5:H:759:HOH:O	2.41	0.53
1:G:349:GLU:HB3	1:G:413:LEU:HD11	1.90	0.53
1:H:94:MET:HE1	1:H:185:LEU:HD21	1.91	0.53
1:D:253:THR:CG2	1:D:254:ASP:O	2.56	0.53
1:G:443:ALA:HB3	5:G:754:HOH:O	1.98	0.53
1:H:324:PHE:O	5:H:776:HOH:O	2.19	0.52
1:B:146:ASN:OD1	1:B:146:ASN:N	2.34	0.52
1:C:251:ARG:HH12	3:C:510:GOL:H11	1.73	0.52
1:A:210:GLU:CG	4:A:513:CIT:H42	2.38	0.52
1:D:311:LYS:N	2:D:510:SO4:O4	2.30	0.52
1:A:406:GLU:HB2	1:A:407:PRO:HD2	1.91	0.52
1:G:426:LEU:HD21	1:G:438:VAL:HG21	1.91	0.52
4:B:514:CIT:O1	4:B:514:CIT:O4	2.28	0.51
1:H:195:LYS:HZ3	3:H:509:GOL:H2	1.75	0.51
1:A:188[A]:GLN:OE1	5:A:774:HOH:O	2.19	0.51
1:B:443:ALA:O	1:B:444:VAL:CB	2.58	0.51
1:H:223:GLY:HA2	5:H:759:HOH:O	2.11	0.51
1:A:306:MET:CE	5:A:788:HOH:O	2.59	0.51
1:H:252[B]:MET:HE3	1:H:273:TRP:CB	2.40	0.51
1:H:142:ILE:CG1	5:H:777:HOH:O	2.55	0.51
1:B:232:PRO:HD2	5:B:1073:HOH:O	2.11	0.51
1:H:94:MET:CE	1:H:185:LEU:HD21	2.41	0.51
1:D:145:THR:CG2	5:D:999:HOH:O	2.59	0.51
1:B:439:LYS:NZ	5:B:895:HOH:O	2.40	0.50
1:F:260:TRP:CD2	1:F:433:HIS:CD2	3.00	0.50
1:C:208:HIS:C	4:C:515:CIT:O1	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:PRO:HB2	1:F:444:VAL:HG12	1.94	0.50
1:D:210:GLU:HB2	4:D:516:CIT:H41	1.93	0.50
2:C:505:SO4:O3	5:C:705:HOH:O	2.18	0.50
1:H:184:GLN:HA	5:H:779:HOH:O	2.11	0.50
1:C:210:GLU:CB	4:C:515:CIT:H21	2.27	0.50
1:H:311:LYS:N	2:H:506:SO4:O3	2.30	0.50
4:C:515:CIT:H22	5:C:630:HOH:O	2.11	0.49
1:C:405:MET:HA	1:C:405:MET:HE3	1.95	0.49
1:D:255:ASP:OD2	3:D:513:GOL:H31	2.11	0.49
1:C:188[B]:GLN:OE1	5:C:811:HOH:O	2.19	0.49
1:D:14:ALA:HA	1:D:19:TYR:CD2	2.47	0.49
1:A:210:GLU:N	4:A:513:CIT:H42	2.21	0.49
4:B:514:CIT:O5	4:B:514:CIT:O2	2.31	0.49
1:D:14:ALA:HA	1:D:19:TYR:HD2	1.77	0.49
1:A:209:THR:N	4:A:513:CIT:H41	2.28	0.49
1:G:338:ASP:C	5:G:699:HOH:O	2.50	0.49
1:A:16:MET:HE1	5:A:1055:HOH:O	2.13	0.48
1:A:387:ASN:HD22	1:A:389:SER:H	1.61	0.48
1:F:406:GLU:HB2	1:F:407:PRO:HD2	1.95	0.48
1:G:325:ARG:HD3	5:G:731:HOH:O	2.13	0.48
1:H:251:ARG:HH12	3:H:509:GOL:C1	2.26	0.48
1:G:361:ARG:NH1	1:G:373:THR:CG2	2.77	0.48
1:G:392:ARG:HB2	1:G:392:ARG:HH21	1.78	0.48
1:C:254:ASP:OD1	3:C:511:GOL:H31	2.13	0.48
1:H:128:MET:CE	1:H:128:MET:HA	2.40	0.48
4:E:514:CIT:O6	4:E:514:CIT:O1	2.30	0.48
1:G:255:ASP:OD1	3:G:507:GOL:H32	2.14	0.48
1:H:32:TRP:CD1	3:H:509:GOL:H31	2.49	0.47
1:H:32:TRP:CE2	3:H:509:GOL:C3	2.98	0.47
1:C:406:GLU:HB2	1:C:407:PRO:HD2	1.95	0.47
1:G:416:LYS:HE2	1:G:416:LYS:HB2	1.41	0.47
1:H:406:GLU:HB2	1:H:407:PRO:HD2	1.96	0.47
1:G:339:GLU:N	5:G:699:HOH:O	2.48	0.47
1:G:49[A]:GLU:OE2	1:G:115:TYR:OH	2.25	0.47
4:A:513:CIT:O7	4:A:513:CIT:O3	2.30	0.47
1:A:210:GLU:H	4:A:513:CIT:H41	1.75	0.47
1:H:171:ARG:NH1	1:H:171:ARG:HB2	2.30	0.47
1:C:338:ASP:HA	1:H:392:ARG:HE	1.80	0.47
1:H:361:ARG:NH1	1:H:373:THR:CG2	2.78	0.47
1:G:203:LYS:CD	1:G:203:LYS:N	2.55	0.46
1:D:254:ASP:OD1	3:D:513:GOL:C1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:GLU:HG3	5:C:667:HOH:O	2.15	0.46
1:H:195:LYS:HZ1	3:H:509:GOL:H2	1.81	0.46
1:H:266[B]:MET:HG2	1:H:321:TRP:CH2	2.50	0.46
1:H:94:MET:HE1	1:H:185:LEU:CD2	2.46	0.46
1:H:89:GLU:HB2	5:H:629:HOH:O	2.14	0.46
1:E:145:THR:HB	1:E:147:VAL:H	1.81	0.46
1:D:208:HIS:C	4:D:516:CIT:O2	2.54	0.46
1:E:254:ASP:OD1	3:E:511:GOL:O2	2.34	0.46
1:F:255:ASP:OD2	3:F:509:GOL:H12	2.16	0.45
1:H:239:HIS:HA	5:H:605:HOH:O	2.16	0.45
1:E:231[A]:SER:OG	1:E:251:ARG:NH1	2.50	0.45
1:B:145:THR:HB	1:B:147:VAL:H	1.81	0.45
1:A:217:LYS:HE3	3:A:512:GOL:C3	2.47	0.45
1:B:204:LEU:HD11	1:D:156:ASN:HD21	1.81	0.45
1:B:387:ASN:HD22	1:B:389:SER:H	1.63	0.45
1:H:406:GLU:N	1:H:406:GLU:OE1	2.50	0.45
1:D:195:LYS:HZ1	3:D:512:GOL:C3	2.29	0.45
1:A:49[B]:GLU:OE2	1:A:115:TYR:OH	2.28	0.45
1:H:223:GLY:CA	5:H:759:HOH:O	2.64	0.45
1:H:265:ASP:HB3	5:H:769:HOH:O	2.17	0.45
1:G:393:SER:HB3	5:G:732:HOH:O	2.16	0.45
1:H:146:ASN:CB	5:H:720:HOH:O	2.51	0.44
1:F:387:ASN:C	1:F:387:ASN:HD22	2.21	0.44
1:E:16:MET:HA	5:E:696:HOH:O	2.16	0.44
1:D:103:ALA:O	5:D:833:HOH:O	2.21	0.44
1:H:392:ARG:NH1	1:H:429:GLU:HB3	2.31	0.44
3:A:512:GOL:H32	5:A:1157:HOH:O	2.17	0.44
1:A:418[A]:ASP:OD1	5:A:1147:HOH:O	2.21	0.44
1:A:210:GLU:CB	4:A:513:CIT:H42	2.48	0.44
1:F:80:ARG:HA	1:F:81:PRO:HD3	1.85	0.44
1:E:255:ASP:OD1	3:E:511:GOL:H11	2.18	0.43
1:D:145:THR:HB	1:D:147:VAL:H	1.83	0.43
1:E:156:ASN:HD21	1:G:204:LEU:HD11	1.83	0.43
1:H:318:MET:O	1:H:322:ILE:HG12	2.19	0.43
1:C:406:GLU:N	1:C:406:GLU:OE1	2.50	0.43
1:A:306:MET:HE3	5:A:788:HOH:O	2.17	0.43
3:F:509:GOL:H11	5:F:770:HOH:O	2.18	0.43
1:D:211:GLU:HB2	4:D:516:CIT:O1	2.17	0.43
1:E:56:LYS:N	1:E:57:PRO:CD	2.81	0.43
1:F:185:LEU:O	1:F:188:GLN:HG2	2.18	0.43
1:B:176:GLN:CB	3:B:513:GOL:H31	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HG2	5:A:882:HOH:O	2.18	0.43
1:G:425:GLN:HA	5:G:692:HOH:O	2.18	0.43
1:F:217:LYS:CE	3:F:510:GOL:O2	2.67	0.43
1:D:448:LEU:C	5:D:780:HOH:O	2.56	0.43
1:H:16:MET:HB3	1:H:18:HIS:CD2	2.54	0.42
1:A:406:GLU:N	1:A:406:GLU:OE1	2.52	0.42
1:B:387:ASN:ND2	1:B:389:SER:H	2.17	0.42
1:D:254:ASP:OD1	3:D:513:GOL:H11	2.18	0.42
1:F:81:PRO:HD2	5:F:803:HOH:O	2.18	0.42
1:B:433:HIS:CD2	1:B:433:HIS:N	2.87	0.42
1:H:66:ASP:HA	1:H:126:HIS:HB2	2.01	0.42
1:E:303:THR:HB	5:E:811:HOH:O	2.20	0.42
1:H:104:LYS:O	1:H:104:LYS:HG3	2.19	0.42
1:E:231[A]:SER:OG	1:E:232:PRO:HA	2.19	0.42
1:A:339:GLU:HG3	5:A:922:HOH:O	2.19	0.42
1:H:32:TRP:CE2	3:H:509:GOL:H31	2.53	0.42
1:A:387:ASN:ND2	1:A:389:SER:H	2.18	0.42
1:C:318:MET:O	1:C:322:ILE:HG12	2.20	0.42
1:B:424:HIS:HB2	5:B:831:HOH:O	2.19	0.42
1:G:16:MET:HB2	1:G:16:MET:HE3	1.99	0.42
1:D:188:GLN:HB3	5:D:854:HOH:O	2.20	0.42
1:C:41:GLU:HB2	1:C:100:PHE:HA	2.01	0.42
1:F:313:GLU:OE2	1:F:433:HIS:HD2	2.02	0.42
1:G:436:ILE:HA	5:G:680:HOH:O	2.18	0.42
1:E:387:ASN:HD22	1:E:389:SER:H	1.67	0.42
1:E:387:ASN:ND2	1:E:389:SER:H	2.17	0.42
1:A:27:MET:HA	1:A:328:LEU:O	2.19	0.42
1:C:255:ASP:OD1	3:C:510:GOL:C1	2.67	0.42
1:B:201:ALA:N	5:B:1073:HOH:O	2.31	0.42
1:C:16:MET:CE	5:C:922:HOH:O	2.68	0.42
1:D:56:LYS:N	1:D:57:PRO:CD	2.82	0.42
1:G:89:GLU:HG2	1:G:90:TYR:CD2	2.55	0.42
1:H:150:ARG:HD2	5:H:638:HOH:O	2.20	0.42
1:A:217:LYS:HE3	3:A:512:GOL:O3	2.20	0.41
1:B:406:GLU:HB2	1:B:407:PRO:CD	2.50	0.41
1:F:387:ASN:ND2	1:F:389:SER:H	2.19	0.41
1:B:27:MET:HA	1:B:328:LEU:O	2.20	0.41
1:H:27:MET:HA	1:H:328:LEU:O	2.20	0.41
1:C:56:LYS:N	1:C:57:PRO:CD	2.83	0.41
1:B:156:ASN:HD21	1:D:204:LEU:HD11	1.85	0.41
1:C:41:GLU:CD	5:C:933:HOH:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:MET:HA	1:F:328:LEU:O	2.20	0.41
1:G:66:ASP:HA	1:G:126:HIS:HB2	2.03	0.41
1:H:128:MET:HE3	1:H:128:MET:CA	2.43	0.41
4:E:514:CIT:C6	4:E:514:CIT:O1	2.65	0.41
1:C:27:MET:HA	1:C:328:LEU:O	2.20	0.41
1:G:110:LYS:HB3	1:G:111:PRO:HD3	2.01	0.41
1:D:387:ASN:HD22	1:D:389:SER:H	1.69	0.41
1:G:318:MET:CE	1:G:345:LEU:HD23	2.50	0.41
1:B:306:MET:HE1	5:B:764:HOH:O	2.20	0.41
1:C:110:LYS:HB3	1:C:111:PRO:HD3	2.02	0.41
1:G:347:ASN:HD22	1:G:349:GLU:H	1.69	0.41
1:C:387:ASN:ND2	1:C:389:SER:H	2.18	0.41
1:C:174:GLY:H	3:C:514:GOL:H32	1.85	0.41
1:C:16:MET:HE2	5:C:922:HOH:O	2.20	0.41
1:C:423:LYS:N	1:C:423:LYS:CD	2.84	0.41
1:G:253:THR:HB	5:G:603:HOH:O	2.20	0.41
1:H:251:ARG:NH1	3:H:509:GOL:H11	2.34	0.41
1:D:387:ASN:ND2	1:D:389:SER:H	2.19	0.41
1:E:217:LYS:HE2	3:E:512:GOL:H2	2.02	0.41
1:G:56:LYS:N	1:G:57:PRO:CD	2.83	0.41
1:D:41:GLU:HB2	1:D:100:PHE:HA	2.03	0.41
1:G:423:LYS:N	5:G:852:HOH:O	2.52	0.41
1:H:423:LYS:HG2	5:H:643:HOH:O	2.20	0.41
5:A:997:HOH:O	1:C:203:LYS:HG2	2.21	0.41
1:E:110:LYS:HB3	1:E:111:PRO:HD3	2.03	0.40
1:B:56:LYS:N	1:B:57:PRO:CD	2.84	0.40
1:D:406:GLU:HG3	5:D:634:HOH:O	2.21	0.40
1:F:417:GLU:HG3	5:F:846:HOH:O	2.21	0.40
1:H:130:GLY:CA	5:H:621:HOH:O	2.69	0.40
1:A:387:ASN:HD22	1:A:387:ASN:C	2.23	0.40
1:G:27:MET:HA	1:G:328:LEU:O	2.21	0.40
1:C:177:ALA:H	3:C:514:GOL:C3	2.28	0.40
1:G:16:MET:HB3	5:G:811:HOH:O	2.21	0.40
1:D:387:ASN:C	1:D:387:ASN:HD22	2.24	0.40
1:C:387:ASN:HD22	1:C:389:SER:H	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/448 (97%)	419 (97%)	14 (3%)	0	100	100
1	B	430/448 (96%)	414 (96%)	16 (4%)	0	100	100
1	C	430/448 (96%)	419 (97%)	11 (3%)	0	100	100
1	D	435/448 (97%)	422 (97%)	13 (3%)	0	100	100
1	E	431/448 (96%)	419 (97%)	12 (3%)	0	100	100
1	F	428/448 (96%)	416 (97%)	12 (3%)	0	100	100
1	G	430/448 (96%)	416 (97%)	14 (3%)	0	100	100
1	H	431/448 (96%)	418 (97%)	12 (3%)	1 (0%)	52	64
All	All	3448/3584 (96%)	3343 (97%)	104 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	325	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/382 (97%)	359 (96%)	13 (4%)	43	58
1	B	370/382 (97%)	348 (94%)	22 (6%)	24	32
1	C	370/382 (97%)	351 (95%)	19 (5%)	29	39
1	D	372/382 (97%)	354 (95%)	18 (5%)	31	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	370/382 (97%)	348 (94%)	22 (6%)	24	32
1	F	368/382 (96%)	344 (94%)	24 (6%)	21	27
1	G	370/382 (97%)	339 (92%)	31 (8%)	14	16
1	H	371/382 (97%)	348 (94%)	23 (6%)	23	30
All	All	2963/3056 (97%)	2791 (94%)	172 (6%)	25	33

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	71	GLU
1	A	199	ILE
1	A	203	LYS
1	A	237	LEU
1	A	298	VAL
1	A	321	TRP
1	A	381	GLN
1	A	383	VAL
1	A	387	ASN
1	A	391	LYS
1	A	409	LYS
1	A	419	LEU
1	B	15	SER
1	B	45	LYS
1	B	71	GLU
1	B	89	GLU
1	B	104	LYS
1	B	121	LEU
1	B	145	THR
1	B	146	ASN
1	B	199	ILE
1	B	237	LEU
1	B	253	THR
1	B	276	LEU
1	B	298	VAL
1	B	321	TRP
1	B	381	GLN
1	B	387	ASN
1	B	402	LEU
1	B	406	GLU
1	B	409	LYS

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Mol	Chain	Res	Type
1	B	413	LEU
1	B	419	LEU
1	B	421	LEU
1	C	15	SER
1	C	71	GLU
1	C	199	ILE
1	C	203	LYS
1	C	237	LEU
1	C	253	THR
1	C	276	LEU
1	C	298	VAL
1	C	321	TRP
1	C	383	VAL
1	C	387	ASN
1	C	391	LYS
1	C	402	LEU
1	C	405	MET
1	C	409	LYS
1	C	413	LEU
1	C	419	LEU
1	C	421	LEU
1	C	423	LYS
1	D	15	SER
1	D	71	GLU
1	D	72	PRO
1	D	121	LEU
1	D	145	THR
1	D	199	ILE
1	D	237	LEU
1	D	253	THR
1	D	276	LEU
1	D	298	VAL
1	D	321	TRP
1	D	383	VAL
1	D	387	ASN
1	D	391	LYS
1	D	405	MET
1	D	413	LEU
1	D	419	LEU
1	D	421	LEU
1	E	15	SER
1	E	71	GLU

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Mol	Chain	Res	Type
1	E	121	LEU
1	E	145	THR
1	E	199	ILE
1	E	203	LYS
1	E	237	LEU
1	E	253	THR
1	E	276	LEU
1	E	298	VAL
1	E	321	TRP
1	E	366	GLU
1	E	383	VAL
1	E	387	ASN
1	E	391	LYS
1	E	400	LYS
1	E	402	LEU
1	E	406	GLU
1	E	409	LYS
1	E	413	LEU
1	E	419	LEU
1	E	422	VAL
1	F	15	SER
1	F	16	MET
1	F	71	GLU
1	F	104	LYS
1	F	121	LEU
1	F	172	LYS
1	F	199	ILE
1	F	237	LEU
1	F	276	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	405	MET
1	F	413	LEU
1	F	419	LEU
1	F	421	LEU
1	F	422	VAL
1	F	430	LEU

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Mol	Chain	Res	Type
1	F	433	HIS
1	F	444	VAL
1	G	16	MET
1	G	71	GLU
1	G	89	GLU
1	G	118	ASN
1	G	121	LEU
1	G	199	ILE
1	G	203	LYS
1	G	237	LEU
1	G	253	THR
1	G	276	LEU
1	G	298	VAL
1	G	321	TRP
1	G	339	GLU
1	G	347	ASN
1	G	363	VAL
1	G	365	ARG
1	G	366	GLU
1	G	381	GLN
1	G	383	VAL
1	G	391	LYS
1	G	392	ARG
1	G	394	VAL
1	G	400	LYS
1	G	402	LEU
1	G	413	LEU
1	G	418	ASP
1	G	419	LEU
1	G	421	LEU
1	G	425	GLN
1	G	426	LEU
1	G	438	VAL
1	H	15	SER
1	H	16	MET
1	H	71	GLU
1	H	89	GLU
1	H	118	ASN
1	H	121	LEU
1	H	146	ASN
1	H	199	ILE
1	H	237	LEU

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Mol	Chain	Res	Type
1	H	253	THR
1	H	276	LEU
1	H	298	VAL
1	H	303	THR
1	H	321	TRP
1	H	348	GLU
1	H	383	VAL
1	H	400	LYS
1	H	402	LEU
1	H	405	MET
1	H	413	LEU
1	H	419	LEU
1	H	421	LEU
1	H	423	LYS

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	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	18	HIS
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	248	ASN
1	D	356	ASN
1	D	387	ASN
1	E	18	HIS

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Mol	Chain	Res	Type
1	E	20	GLN
1	E	146	ASN
1	E	156	ASN
1	E	248	ASN
1	E	356	ASN
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	381	GLN
1	H	18	HIS
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 ⓘ

102 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	A	501	-	4,4,4	1.01	0	6,6,6	0.87	1 (16%)
2	SO4	A	502	-	4,4,4	1.18	1 (25%)	6,6,6	0.60	0
2	SO4	A	503	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	A	504	-	4,4,4	1.32	1 (25%)	6,6,6	1.68	1 (16%)
2	SO4	A	505	-	4,4,4	0.98	0	6,6,6	0.67	0
2	SO4	A	506	-	4,4,4	0.89	0	6,6,6	0.99	1 (16%)
2	SO4	A	507	-	4,4,4	2.07	2 (50%)	6,6,6	1.59	1 (16%)
2	SO4	A	508	-	4,4,4	1.32	0	6,6,6	1.13	0
2	SO4	A	509	-	4,4,4	0.66	0	6,6,6	0.46	0
3	GOL	A	510	-	5,5,5	0.74	0	5,5,5	0.98	0
3	GOL	A	511	-	5,5,5	0.36	0	5,5,5	0.43	0
3	GOL	A	512	-	5,5,5	0.56	0	5,5,5	0.58	0
4	CIT	A	513	-	3,12,12	3.57	1 (33%)	3,17,17	3.28	1 (33%)
2	SO4	B	501	-	4,4,4	1.47	0	6,6,6	1.18	1 (16%)
2	SO4	B	502	-	4,4,4	0.91	0	6,6,6	0.91	0
2	SO4	B	503	-	4,4,4	0.95	0	6,6,6	0.29	0
2	SO4	B	504	-	4,4,4	0.65	0	6,6,6	0.59	0
2	SO4	B	505	-	4,4,4	1.22	0	6,6,6	1.05	0
2	SO4	B	506	-	4,4,4	1.53	2 (50%)	6,6,6	0.91	0
2	SO4	B	507	-	4,4,4	0.80	0	6,6,6	0.47	0
2	SO4	B	508	-	4,4,4	1.02	0	6,6,6	0.59	0
3	GOL	B	509	-	5,5,5	0.74	0	5,5,5	0.66	0
3	GOL	B	510	-	5,5,5	0.69	0	5,5,5	0.63	0
3	GOL	B	511	-	5,5,5	0.43	0	5,5,5	1.66	1 (20%)
3	GOL	B	512	-	5,5,5	0.21	0	5,5,5	1.29	1 (20%)
3	GOL	B	513	-	5,5,5	0.68	0	5,5,5	1.07	1 (20%)
4	CIT	B	514	-	3,12,12	2.52	2 (66%)	3,17,17	4.68	1 (33%)
2	SO4	C	501	-	4,4,4	1.03	0	6,6,6	0.39	0
2	SO4	C	502	-	4,4,4	1.08	0	6,6,6	1.05	1 (16%)
2	SO4	C	503	-	4,4,4	0.93	0	6,6,6	1.04	1 (16%)
2	SO4	C	504	-	4,4,4	0.66	0	6,6,6	0.71	0
2	SO4	C	505	-	4,4,4	1.02	0	6,6,6	0.95	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	506	-	4,4,4	1.35	0	6,6,6	0.65	0
2	SO4	C	507	-	4,4,4	1.40	0	6,6,6	2.28	1 (16%)
2	SO4	C	508	-	4,4,4	0.74	0	6,6,6	0.35	0
2	SO4	C	509	-	4,4,4	1.40	1 (25%)	6,6,6	0.64	0
3	GOL	C	510	-	5,5,5	1.33	0	5,5,5	2.42	2 (40%)
3	GOL	C	511	-	5,5,5	0.65	0	5,5,5	1.20	0
3	GOL	C	512	-	5,5,5	0.35	0	5,5,5	1.91	2 (40%)
3	GOL	C	513	-	5,5,5	1.29	1 (20%)	5,5,5	1.81	2 (40%)
3	GOL	C	514	-	5,5,5	1.14	1 (20%)	5,5,5	0.95	0
4	CIT	C	515	-	3,12,12	2.85	2 (66%)	3,17,17	6.98	2 (66%)
2	SO4	D	501	-	4,4,4	0.67	0	6,6,6	0.72	0
2	SO4	D	502	-	4,4,4	1.01	0	6,6,6	0.69	0
2	SO4	D	503	-	4,4,4	0.83	0	6,6,6	0.45	0
2	SO4	D	504	-	4,4,4	0.66	0	6,6,6	0.88	1 (16%)
2	SO4	D	505	-	4,4,4	0.90	0	6,6,6	0.58	0
2	SO4	D	506	-	4,4,4	0.85	0	6,6,6	0.45	0
2	SO4	D	507	-	4,4,4	1.22	0	6,6,6	2.22	1 (16%)
2	SO4	D	508	-	4,4,4	1.22	0	6,6,6	0.35	0
2	SO4	D	509	-	4,4,4	0.85	0	6,6,6	0.40	0
2	SO4	D	510	-	4,4,4	0.92	0	6,6,6	0.50	0
2	SO4	D	511	-	4,4,4	0.72	0	6,6,6	0.25	0
3	GOL	D	512	-	5,5,5	1.06	1 (20%)	5,5,5	1.01	0
3	GOL	D	513	-	5,5,5	0.77	0	5,5,5	1.39	1 (20%)
3	GOL	D	514	-	5,5,5	0.24	0	5,5,5	0.27	0
3	GOL	D	515	-	5,5,5	0.48	0	5,5,5	0.91	0
4	CIT	D	516	-	3,12,12	2.38	1 (33%)	3,17,17	4.14	3 (100%)
2	SO4	E	501	-	4,4,4	1.34	1 (25%)	6,6,6	0.63	0
2	SO4	E	502	-	4,4,4	0.65	0	6,6,6	0.54	0
2	SO4	E	503	-	4,4,4	1.06	0	6,6,6	0.86	0
2	SO4	E	504	-	4,4,4	0.99	0	6,6,6	0.45	0
2	SO4	E	505	-	4,4,4	0.90	0	6,6,6	0.54	0
2	SO4	E	506	-	4,4,4	1.24	0	6,6,6	0.36	0
2	SO4	E	507	-	4,4,4	0.97	0	6,6,6	0.75	0
2	SO4	E	508	-	4,4,4	1.08	0	6,6,6	1.20	1 (16%)
2	SO4	E	509	-	4,4,4	0.88	0	6,6,6	0.81	0
3	GOL	E	510	-	5,5,5	2.73	2 (40%)	5,5,5	2.91	3 (60%)
3	GOL	E	511	-	5,5,5	0.37	0	5,5,5	0.51	0
3	GOL	E	512	-	5,5,5	0.58	0	5,5,5	0.88	0
3	GOL	E	513	-	5,5,5	0.77	0	5,5,5	1.40	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	E	514	-	3,12,12	1.40	0	3,17,17	3.27	1 (33%)
2	SO4	F	501	-	4,4,4	0.73	0	6,6,6	0.45	0
2	SO4	F	502	-	4,4,4	1.07	0	6,6,6	0.41	0
2	SO4	F	503	-	4,4,4	0.79	0	6,6,6	0.79	0
2	SO4	F	504	-	4,4,4	0.86	0	6,6,6	0.23	0
2	SO4	F	505	-	4,4,4	0.73	0	6,6,6	0.31	0
2	SO4	F	506	-	4,4,4	0.89	0	6,6,6	0.63	0
2	SO4	F	507	-	4,4,4	0.98	0	6,6,6	0.32	0
3	GOL	F	508	-	5,5,5	0.32	0	5,5,5	1.33	1 (20%)
3	GOL	F	509	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	F	510	-	5,5,5	0.39	0	5,5,5	0.50	0
3	GOL	F	511	-	5,5,5	0.62	0	5,5,5	0.54	0
2	SO4	G	501	-	4,4,4	1.21	1 (25%)	6,6,6	0.56	0
2	SO4	G	502	-	4,4,4	0.90	0	6,6,6	0.76	0
2	SO4	G	503	-	4,4,4	1.11	0	6,6,6	0.90	0
2	SO4	G	504	-	4,4,4	0.79	0	6,6,6	0.48	0
2	SO4	G	505	-	4,4,4	1.07	0	6,6,6	0.69	0
2	SO4	G	506	-	4,4,4	0.80	0	6,6,6	0.34	0
3	GOL	G	507	-	5,5,5	1.14	0	5,5,5	0.99	0
3	GOL	G	508	-	5,5,5	0.64	0	5,5,5	1.20	1 (20%)
4	CIT	G	509	-	3,12,12	2.16	1 (33%)	3,17,17	6.02	3 (100%)
2	SO4	H	501	-	4,4,4	1.34	1 (25%)	6,6,6	0.56	0
2	SO4	H	502	-	4,4,4	0.79	0	6,6,6	0.63	0
2	SO4	H	503	-	4,4,4	0.63	0	6,6,6	0.34	0
2	SO4	H	504	-	4,4,4	1.16	0	6,6,6	0.38	0
2	SO4	H	505	-	4,4,4	0.79	0	6,6,6	0.48	0
2	SO4	H	506	-	4,4,4	0.73	0	6,6,6	0.61	0
2	SO4	H	507	-	4,4,4	0.81	0	6,6,6	0.47	0
3	GOL	H	508	-	5,5,5	0.45	0	5,5,5	0.66	0
3	GOL	H	509	-	5,5,5	0.58	0	5,5,5	0.92	0
3	GOL	H	510	-	5,5,5	0.19	0	5,5,5	0.36	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	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0

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

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

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	CIT	C4-C3	-5.78	1.45	1.54
4	C	515	CIT	C2-C3	-4.15	1.48	1.54
4	D	516	CIT	C2-C3	-3.98	1.48	1.54
4	B	514	CIT	C4-C3	-3.63	1.49	1.54
4	C	515	CIT	C4-C3	-2.63	1.50	1.54
3	C	513	GOL	O2-C2	-2.42	1.36	1.43
2	G	501	SO4	O2-S	-2.33	1.39	1.47
2	A	502	SO4	O4-S	-2.20	1.39	1.47
4	B	514	CIT	C2-C3	-2.18	1.51	1.54
3	D	512	GOL	O3-C3	-2.00	1.33	1.42
2	E	501	SO4	O4-S	2.01	1.54	1.47
2	A	507	SO4	O3-S	2.05	1.54	1.47
2	H	501	SO4	O4-S	2.05	1.54	1.47
2	B	506	SO4	O1-S	2.13	1.54	1.47
2	B	506	SO4	O2-S	2.16	1.54	1.47
2	C	509	SO4	O1-S	2.16	1.54	1.47
2	A	504	SO4	O1-S	2.24	1.54	1.47
3	C	514	GOL	O3-C3	2.29	1.52	1.42
3	E	510	GOL	O2-C2	2.68	1.51	1.43
4	G	509	CIT	C2-C3	3.09	1.59	1.54
2	A	507	SO4	O4-S	3.18	1.58	1.47
3	E	510	GOL	O3-C3	5.25	1.65	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	515	CIT	C3-C2-C1	-11.55	96.50	114.96
4	B	514	CIT	C3-C4-C5	-7.88	102.37	114.96
4	E	514	CIT	C3-C2-C1	-5.61	105.98	114.96
4	A	513	CIT	C3-C4-C5	-5.33	106.43	114.96
2	D	507	SO4	O2-S-O1	-5.27	92.80	109.50
2	C	507	SO4	O2-S-O1	-5.21	92.99	109.50
4	D	516	CIT	C3-C2-C1	-4.51	107.75	114.96
3	C	510	GOL	O2-C2-C1	-4.24	89.20	108.65
4	D	516	CIT	C4-C3-C2	-3.62	101.15	109.81
2	A	507	SO4	O2-S-O1	-3.61	98.06	109.50
2	A	504	SO4	O4-S-O3	-3.42	95.09	108.98
4	C	515	CIT	C3-C4-C5	-3.34	109.62	114.96
3	C	513	GOL	O2-C2-C1	-3.17	94.09	108.65
3	C	512	GOL	O3-C3-C2	-3.11	95.09	110.18
3	B	512	GOL	O3-C3-C2	-2.61	97.53	110.18
3	C	513	GOL	O1-C1-C2	-2.43	98.39	110.18
2	B	501	SO4	O4-S-O3	-2.24	99.88	108.98
3	E	513	GOL	O1-C1-C2	-2.22	99.43	110.18
2	A	506	SO4	O4-S-O3	-2.18	100.13	108.98
3	B	513	GOL	C3-C2-C1	-2.17	102.60	111.12
2	D	504	SO4	O2-S-O1	-2.07	102.93	109.50
3	F	508	GOL	O1-C1-C2	-2.07	100.13	110.18
3	D	513	GOL	C3-C2-C1	-2.01	103.22	111.12
3	C	512	GOL	C3-C2-C1	2.03	119.07	111.12
2	A	501	SO4	O2-S-O1	2.05	116.01	109.50
2	C	505	SO4	O2-S-O1	2.19	116.44	109.50
2	C	503	SO4	O2-S-O1	2.23	116.57	109.50
4	G	509	CIT	C3-C4-C5	2.33	118.68	114.96
3	G	508	GOL	O2-C2-C3	2.45	119.89	108.65
2	C	502	SO4	O2-S-O1	2.46	117.28	109.50
3	E	510	GOL	O3-C3-C2	2.59	122.75	110.18
3	B	511	GOL	O1-C1-C2	2.63	122.92	110.18
3	C	510	GOL	O2-C2-C3	2.73	121.18	108.65
2	E	508	SO4	O2-S-O1	2.83	118.47	109.50
4	G	509	CIT	C4-C3-C2	3.54	118.28	109.81
3	E	510	GOL	O1-C1-C2	3.87	128.96	110.18
3	E	510	GOL	C3-C2-C1	4.02	126.89	111.12
4	D	516	CIT	C3-C4-C5	4.23	121.72	114.96
4	G	509	CIT	C3-C2-C1	9.53	130.20	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	512	GOL	3	0
4	A	513	CIT	15	0
3	B	512	GOL	1	0
3	B	513	GOL	2	0
4	B	514	CIT	6	0
2	C	505	SO4	1	0
3	C	510	GOL	3	0
3	C	511	GOL	2	0
3	C	514	GOL	4	0
4	C	515	CIT	8	0
2	D	501	SO4	1	0
2	D	504	SO4	1	0
2	D	510	SO4	1	0
3	D	512	GOL	3	0
3	D	513	GOL	3	0
4	D	516	CIT	9	0
3	E	510	GOL	2	0
3	E	511	GOL	2	0
3	E	512	GOL	1	0
4	E	514	CIT	7	0
3	F	509	GOL	2	0
3	F	510	GOL	1	0
3	G	507	GOL	1	0
3	G	508	GOL	2	0
4	G	509	CIT	3	0
2	H	502	SO4	2	0
2	H	506	SO4	1	0
3	H	509	GOL	11	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	431/448 (96%)	-0.61	4 (0%)	85 89	11, 17, 38, 100	0
1	B	430/448 (95%)	-0.57	5 (1%)	81 85	13, 23, 44, 96	0
1	C	430/448 (95%)	-0.44	8 (1%)	70 76	12, 24, 58, 108	0
1	D	435/448 (97%)	-0.42	5 (1%)	82 86	20, 28, 52, 109	0
1	E	431/448 (96%)	-0.26	14 (3%)	51 60	18, 29, 68, 123	0
1	F	430/448 (95%)	-0.05	15 (3%)	48 56	22, 37, 68, 113	0
1	G	430/448 (95%)	0.43	42 (9%)	10 14	20, 45, 79, 130	1 (0%)
1	H	430/448 (95%)	0.75	47 (10%)	7 11	29, 54, 82, 124	0
All	All	3447/3584 (96%)	-0.15	140 (4%)	41 50	11, 31, 70, 130	1 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	11.0
1	C	444	VAL	8.9
1	G	405	MET	8.4
1	F	444	VAL	8.3
1	E	444	VAL	7.8
1	E	14	ALA	7.7
1	F	405	MET	7.3
1	G	444	VAL	7.1
1	E	405	MET	6.3
1	C	405	MET	5.9
1	H	405	MET	5.9
1	H	204	LEU	5.8
1	G	377	ALA	5.6
1	E	15	SER	5.5
1	H	16	MET	5.4
1	H	203	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	443	ALA	5.2
1	B	15	SER	5.1
1	A	14	ALA	5.0
1	G	404	CYS	4.6
1	H	443	ALA	4.5
1	G	442	PRO	4.4
1	F	15	SER	4.3
1	H	127	ILE	4.3
1	F	203	LYS	4.2
1	F	204	LEU	4.2
1	G	424	HIS	4.2
1	D	14	ALA	4.0
1	G	391	LYS	4.0
1	H	205	TYR	4.0
1	H	104	LYS	4.0
1	A	444	VAL	3.9
1	G	401	ASP	3.9
1	G	15	SER	3.8
1	H	146	ASN	3.8
1	E	203	LYS	3.8
1	E	204	LEU	3.8
1	G	406	GLU	3.7
1	G	367	ASN	3.6
1	H	406	GLU	3.5
1	C	424	HIS	3.4
1	G	204	LEU	3.4
1	H	15	SER	3.4
1	E	377	ALA	3.3
1	G	430	LEU	3.3
1	H	131	ILE	3.3
1	F	443	ALA	3.3
1	A	405	MET	3.2
1	C	406	GLU	3.2
1	B	405	MET	3.2
1	E	443	ALA	3.2
1	G	403	GLY	3.1
1	G	400	LYS	3.1
1	H	424	HIS	3.1
1	C	443	ALA	3.0
1	H	182	LEU	3.0
1	H	143	LEU	3.0
1	H	17	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	407	PRO	2.9
1	G	388	ILE	2.8
1	B	204	LEU	2.8
1	G	421	LEU	2.8
1	H	279	LEU	2.8
1	E	406	GLU	2.8
1	E	421	LEU	2.8
1	G	378	GLU	2.7
1	D	15	SER	2.7
1	G	415	ALA	2.7
1	H	171	ARG	2.7
1	H	118	ASN	2.7
1	F	171	ARG	2.7
1	H	105	GLY	2.7
1	A	15	SER	2.6
1	H	97	VAL	2.6
1	H	288	LEU	2.6
1	G	407	PRO	2.6
1	H	377	ALA	2.6
1	G	366	GLU	2.5
1	G	203	LYS	2.5
1	E	442	PRO	2.5
1	G	64	VAL	2.5
1	H	103	ALA	2.5
1	H	125	ILE	2.5
1	H	42	ASP	2.5
1	F	17	HIS	2.5
1	H	339	GLU	2.4
1	H	196	VAL	2.4
1	H	202	SER	2.4
1	E	424	HIS	2.4
1	H	107	LYS	2.4
1	H	89	GLU	2.4
1	G	422	VAL	2.4
1	H	116	ILE	2.4
1	E	423	LYS	2.4
1	H	64	VAL	2.4
1	H	340	TRP	2.4
1	H	407	PRO	2.3
1	G	441	SER	2.3
1	G	358	TYR	2.3
1	G	389	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	118	ASN	2.3
1	H	73	GLY	2.2
1	B	203	LYS	2.2
1	F	127	ILE	2.2
1	G	370	VAL	2.2
1	H	223	GLY	2.2
1	G	396	SER	2.2
1	H	175	ALA	2.2
1	F	182	LEU	2.2
1	H	20	GLN	2.2
1	C	377	ALA	2.2
1	G	322	ILE	2.2
1	G	394	VAL	2.2
1	H	21	TRP	2.2
1	F	423	LYS	2.1
1	H	331	GLY	2.1
1	G	339	GLU	2.1
1	H	173	GLU	2.1
1	C	391	LYS	2.1
1	F	131	ILE	2.1
1	G	417	GLU	2.1
1	C	407	PRO	2.1
1	G	432	PRO	2.1
1	G	431	GLY	2.1
1	F	146	ASN	2.1
1	D	405	MET	2.1
1	F	145	THR	2.1
1	D	377	ALA	2.1
1	D	203	LYS	2.1
1	H	400	LYS	2.1
1	G	16	MET	2.1
1	H	141	PRO	2.1
1	B	104	LYS	2.0
1	G	350	VAL	2.0
1	G	395	VAL	2.0
1	H	124	GLY	2.0
1	H	302	GLY	2.0
1	G	364	TYR	2.0
1	G	65	VAL	2.0
1	F	424	HIS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	504	5/5	0.89	0.23	13.78	57,72,75,83	0
2	SO4	F	505	5/5	0.86	0.35	11.57	105,112,128,128	0
2	SO4	C	507	5/5	0.85	0.23	9.12	39,40,70,80	5
2	SO4	B	506	5/5	0.93	0.21	8.47	34,44,50,60	5
4	CIT	C	515	13/13	0.87	0.31	8.31	42,60,81,81	0
2	SO4	A	507	5/5	0.96	0.21	7.96	36,40,45,59	0
2	SO4	D	508	5/5	0.93	0.28	7.73	47,60,76,84	0
2	SO4	B	502	5/5	0.92	0.29	7.30	52,84,94,99	0
2	SO4	D	504	5/5	0.91	0.28	6.94	72,91,106,117	0
3	GOL	C	514	6/6	0.88	0.27	6.79	27,35,47,54	0
2	SO4	E	502	5/5	0.79	0.33	6.77	87,116,121,127	0
4	CIT	D	516	13/13	0.87	0.29	6.61	54,71,79,84	0
4	CIT	A	513	13/13	0.85	0.23	6.47	34,51,69,69	0
2	SO4	E	506	5/5	0.92	0.29	6.46	46,73,80,81	0
2	SO4	E	508	5/5	0.90	0.20	6.35	74,79,114,125	0
3	GOL	D	513	6/6	0.89	0.20	6.11	35,44,47,48	0
2	SO4	C	503	5/5	0.86	0.29	6.06	76,89,97,100	0
3	GOL	E	511	6/6	0.94	0.15	5.90	36,42,48,58	0
2	SO4	C	502	5/5	0.91	0.24	5.70	64,90,94,99	0
3	GOL	A	511	6/6	0.94	0.13	5.52	26,31,41,48	0
2	SO4	B	501	5/5	0.89	0.25	5.52	54,65,82,90	0
3	GOL	E	513	6/6	0.87	0.26	5.47	47,51,57,59	0
2	SO4	E	501	5/5	0.77	0.22	5.25	67,77,81,109	0
2	SO4	D	503	5/5	0.89	0.22	5.16	60,83,94,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	509	5/5	0.85	0.28	5.07	66,67,83,102	0
3	GOL	E	510	6/6	0.86	0.24	4.87	28,29,34,35	0
2	SO4	G	505	5/5	0.90	0.36	4.53	69,70,91,107	0
2	SO4	F	506	5/5	0.93	0.28	4.39	63,72,80,93	0
2	SO4	G	506	5/5	0.82	0.27	4.29	76,103,107,111	0
4	CIT	E	514	13/13	0.86	0.25	4.12	51,79,91,96	0
2	SO4	G	503	5/5	0.92	0.21	3.78	67,75,77,82	0
4	CIT	B	514	13/13	0.79	0.28	3.74	41,70,87,88	0
2	SO4	E	503	5/5	0.95	0.25	3.64	66,66,80,81	0
4	CIT	G	509	13/13	0.84	0.23	3.63	49,64,81,91	0
2	SO4	D	507	5/5	0.84	0.24	3.59	61,65,78,83	0
2	SO4	F	504	5/5	0.81	0.32	3.11	73,79,109,111	0
2	SO4	H	504	5/5	0.79	0.37	2.77	61,88,101,103	0
2	SO4	H	505	5/5	0.92	0.34	2.72	80,95,101,106	0
3	GOL	B	513	6/6	0.95	0.20	2.32	35,40,51,59	0
2	SO4	F	502	5/5	0.78	0.21	2.22	77,81,98,115	0
2	SO4	A	508	5/5	0.95	0.20	2.19	50,57,67,68	0
3	GOL	B	511	6/6	0.96	0.17	2.15	24,28,34,35	0
2	SO4	A	503	5/5	0.97	0.13	1.27	39,54,55,58	0
3	GOL	F	511	6/6	0.76	0.20	1.19	60,71,75,82	0
3	GOL	H	510	6/6	0.83	0.27	1.16	73,83,87,104	0
3	GOL	C	510	6/6	0.96	0.14	1.05	22,25,27,27	0
3	GOL	B	510	6/6	0.96	0.08	0.92	28,36,38,43	0
3	GOL	F	508	6/6	0.95	0.16	0.76	34,37,41,44	0
3	GOL	C	513	6/6	0.95	0.14	0.69	33,43,47,47	0
2	SO4	A	502	5/5	0.99	0.09	0.67	27,28,30,38	0
3	GOL	F	509	6/6	0.87	0.24	0.51	45,58,75,79	0
3	GOL	D	512	6/6	0.96	0.13	0.40	25,28,32,35	0
3	GOL	H	509	6/6	0.89	0.19	0.29	48,55,68,71	0
3	GOL	A	510	6/6	0.97	0.10	0.15	16,17,22,23	0
2	SO4	G	501	5/5	0.99	0.09	-0.01	29,29,34,36	0
2	SO4	H	501	5/5	0.89	0.16	-0.02	63,66,76,97	0
3	GOL	G	508	6/6	0.91	0.10	-0.60	34,41,46,52	0
3	GOL	G	507	6/6	0.95	0.12	-0.86	29,34,37,45	0
2	SO4	G	502	5/5	0.83	0.35	-	66,88,106,106	0
2	SO4	D	505	5/5	0.91	0.27	-	69,94,98,107	0
2	SO4	B	505	5/5	0.92	0.27	-	50,75,78,80	0
2	SO4	C	508	5/5	0.93	0.33	-	82,83,86,94	0
2	SO4	F	501	5/5	0.92	0.30	-	81,92,101,104	0
3	GOL	C	511	6/6	0.92	0.16	-	31,44,47,47	0
2	SO4	B	503	5/5	0.90	0.37	-	80,90,94,100	0
2	SO4	B	504	5/5	0.97	0.28	-	68,78,86,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	H	508	6/6	0.87	0.22	-	54,60,76,80	0
2	SO4	C	505	5/5	0.93	0.27	-	65,81,89,90	0
2	SO4	H	503	5/5	0.87	0.34	-	96,103,112,116	0
3	GOL	B	512	6/6	0.84	0.17	-	55,64,67,72	0
2	SO4	B	507	5/5	0.91	0.33	-	66,91,99,113	0
2	SO4	D	506	5/5	0.93	0.28	-	66,80,90,95	0
2	SO4	D	502	5/5	0.88	0.28	-	61,64,83,85	0
2	SO4	B	508	5/5	0.93	0.33	-	57,68,75,92	0
2	SO4	E	507	5/5	0.98	0.13	-	51,52,54,61	0
3	GOL	F	510	6/6	0.79	0.32	-	69,76,87,91	0
3	GOL	E	512	6/6	0.84	0.31	-	60,66,69,73	0
2	SO4	E	504	5/5	0.90	0.30	-	65,82,90,91	0
2	SO4	E	509	5/5	0.90	0.33	-	73,74,89,98	0
2	SO4	H	502	5/5	0.88	0.37	-	81,87,105,106	0
2	SO4	A	509	5/5	0.94	0.34	-	74,74,92,98	0
3	GOL	D	514	6/6	0.91	0.25	-	60,74,80,81	0
2	SO4	D	509	5/5	0.88	0.33	-	71,93,95,105	0
2	SO4	F	507	5/5	0.87	0.34	-	68,80,81,99	0
2	SO4	G	504	5/5	0.86	0.35	-	73,84,103,105	0
2	SO4	H	507	5/5	0.87	0.44	-	84,88,103,114	0
2	SO4	A	506	5/5	0.95	0.21	-	60,66,69,78	0
2	SO4	A	501	5/5	0.90	0.38	-	59,75,87,105	0
2	SO4	D	511	5/5	0.89	0.27	-	71,96,107,107	0
3	GOL	D	515	6/6	0.85	0.13	-	48,58,67,71	0
2	SO4	A	505	5/5	0.86	0.25	-	71,72,98,101	0
2	SO4	C	501	5/5	0.90	0.29	-	65,83,86,90	0
3	GOL	B	509	6/6	0.72	0.55	-	58,68,77,80	0
2	SO4	E	505	5/5	0.87	0.32	-	80,89,103,103	0
2	SO4	D	510	5/5	0.93	0.25	-	79,82,92,95	0
3	GOL	C	512	6/6	0.89	0.17	-	45,52,69,72	0
2	SO4	C	506	5/5	0.92	0.28	-	60,66,76,86	0
2	SO4	C	504	5/5	0.98	0.15	-	50,51,61,65	0
3	GOL	A	512	6/6	0.86	0.21	-	61,65,69,72	0
2	SO4	H	506	5/5	0.83	0.44	-	98,99,112,117	0
2	SO4	D	501	5/5	0.85	0.34	-	96,99,111,124	0
2	SO4	F	503	5/5	0.81	0.34	-	72,77,104,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.