



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2026 – 07:18 pm BST

PDB ID : 9SJH / pdb_00009sjh
Title : Crystal structure of apo GHdex dextranase (BT3087), E360A catalytic mutant
Authors : Feasey, M.; Basle, A.; van den Berg, B.
Deposited on : 2025-08-31
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

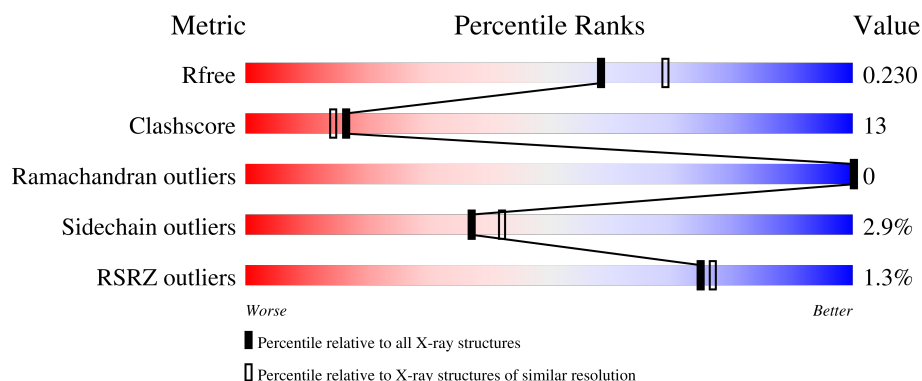
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	577	2% 75% 21% ...
1	B	577	% 79% 17% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9950 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 Cycloisomaltooligosaccharide glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	568	Total	C	N	O	S	0	0	0
			4500	2859	754	865	22			
1	A	570	Total	C	N	O	S	0	0	0
			4520	2871	760	867	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	initiating methionine	UNP Q8A368
B	25	GLY	-	expression tag	UNP Q8A368
B	360	ALA	GLU	engineered mutation	UNP Q8A368
B	593	LEU	-	expression tag	UNP Q8A368
B	594	GLU	-	expression tag	UNP Q8A368
B	595	HIS	-	expression tag	UNP Q8A368
B	596	HIS	-	expression tag	UNP Q8A368
B	597	HIS	-	expression tag	UNP Q8A368
B	598	HIS	-	expression tag	UNP Q8A368
B	599	HIS	-	expression tag	UNP Q8A368
B	600	HIS	-	expression tag	UNP Q8A368
A	24	MET	-	initiating methionine	UNP Q8A368
A	25	GLY	-	expression tag	UNP Q8A368
A	360	ALA	GLU	engineered mutation	UNP Q8A368
A	593	LEU	-	expression tag	UNP Q8A368
A	594	GLU	-	expression tag	UNP Q8A368
A	595	HIS	-	expression tag	UNP Q8A368
A	596	HIS	-	expression tag	UNP Q8A368
A	597	HIS	-	expression tag	UNP Q8A368
A	598	HIS	-	expression tag	UNP Q8A368
A	599	HIS	-	expression tag	UNP Q8A368
A	600	HIS	-	expression tag	UNP Q8A368

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0

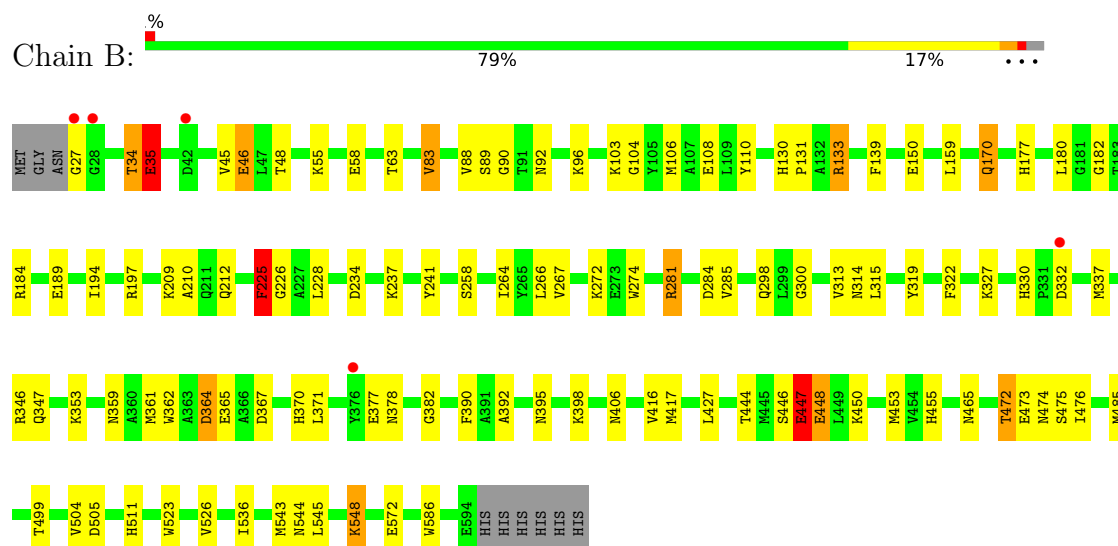
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	380	Total 380	O 380	0	0
4	A	384	Total 384	O 384	0	0

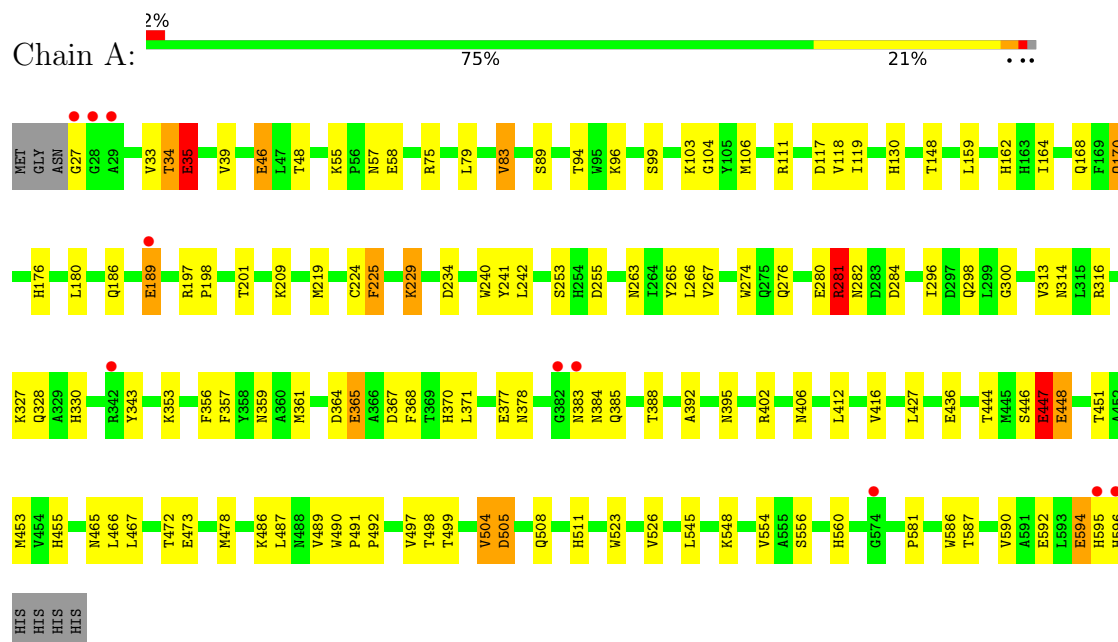
3 Residue-property plots

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

• Molecule 1: Cycloisomaltooligosaccharide glucanotransferase



• Molecule 1: Cycloisomaltooligosaccharide glucanotransferase



4 Data and refinement statistics

Property	Value
Space group	P 41 21 2
Cell constants a, b, c, α , β , γ	92.86Å 92.86Å 330.68Å 90.00° 90.00° 90.00°
Resolution (Å)	89.40 – 2.10 89.40 – 2.10
% Data completeness (in resolution range)	99.9 (89.40-2.10) 99.9 (89.40-2.10)
R_{merge}	0.89
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.10Å)
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88), REFMAC 5.8.0430 (refmacat 0.4.88)
R, R_{free}	0.190 , 0.230 0.190 , 0.230
R_{free} test set	4264 reflections (4.98%)
Wilson B-factor (Å ²)	35.4
Anisotropy	0.408
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.2
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$
Estimated twinning fraction	No twinning to report.
F_o, F_c correlation	0.96
Total number of atoms	9950
Average B, all atoms (Å ²)	40.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.58	0/4640	1.23	29/6306 (0.5%)
1	B	0.57	0/4618	1.21	27/6276 (0.4%)
All	All	0.58	0/9258	1.22	56/12582 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	GLU	CB-CG-CD	16.20	140.13	112.60
1	A	35	GLU	CB-CG-CD	14.15	136.65	112.60
1	B	447	GLU	CB-CG-CD	13.15	134.95	112.60
1	B	35	GLU	N-CA-CB	-12.28	89.74	110.49
1	A	35	GLU	N-CA-CB	-12.25	89.79	110.49
1	A	447	GLU	CB-CG-CD	11.44	132.05	112.60
1	A	448	GLU	CB-CG-CD	10.57	130.57	112.60
1	B	448	GLU	CB-CG-CD	9.84	129.32	112.60
1	A	46	GLU	N-CA-CB	-9.48	94.25	110.17
1	A	83	VAL	N-CA-CB	-9.20	100.40	112.36
1	B	447	GLU	CB-CA-C	8.42	124.76	110.79
1	B	83	VAL	N-CA-CB	-7.58	103.88	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	46	GLU	CB-CA-C	7.18	122.21	110.22
1	A	451	THR	CA-CB-OG1	-6.89	99.26	109.60
1	A	48	THR	CA-CB-OG1	-6.81	99.38	109.60
1	A	595	HIS	CB-CA-C	6.80	120.43	109.27
1	B	364	ASP	CB-CA-C	6.52	122.25	109.72
1	B	46	GLU	CB-CG-CD	6.50	123.65	112.60
1	B	377	GLU	CB-CA-C	-6.47	100.99	110.96
1	A	447	GLU	CB-CA-C	6.46	121.51	110.79
1	A	444	THR	CA-CB-OG1	-6.43	99.96	109.60
1	B	444	THR	CA-CB-OG1	-6.39	100.01	109.60
1	B	332	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	48	THR	CA-CB-OG1	-6.20	100.30	109.60
1	A	526	VAL	N-CA-CB	6.19	118.96	110.54
1	A	377	GLU	CB-CA-C	-6.14	101.16	110.92
1	A	83	VAL	N-CA-C	-6.13	107.16	113.10
1	B	505	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	201	THR	CA-CB-OG1	-5.91	100.74	109.60
1	B	83	VAL	N-CA-C	-5.81	107.10	113.43
1	A	548	LYS	N-CA-CB	-5.77	100.87	109.69
1	B	34	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	189	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	94	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	34	THR	CA-C-N	5.59	132.23	121.54
1	A	34	THR	C-N-CA	5.59	132.23	121.54
1	B	150	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	473	GLU	CB-CG-CD	-5.48	103.28	112.60
1	B	63	THR	CA-CB-OG1	-5.44	101.43	109.60
1	B	170	GLN	CB-CA-C	5.34	119.85	109.33
1	B	526	VAL	N-CA-CB	5.33	117.78	110.54
1	A	170	GLN	CB-CA-C	5.31	119.52	109.37
1	B	364	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	225	PHE	CA-C-N	-5.22	117.74	122.80
1	B	225	PHE	C-N-CA	-5.22	117.74	122.80
1	A	594	GLU	CB-CG-CD	5.19	121.43	112.60
1	B	133	ARG	CG-CD-NE	-5.18	100.60	112.00
1	A	504	VAL	CA-C-N	-5.16	115.31	122.74
1	A	504	VAL	C-N-CA	-5.16	115.31	122.74
1	B	548	LYS	N-CA-CB	-5.15	101.80	109.69
1	B	189	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	34	THR	CA-C-N	5.09	131.27	121.54
1	B	34	THR	C-N-CA	5.09	131.27	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	436	GLU	N-CA-CB	5.02	117.95	110.22

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	ARG	Sidechain
1	B	184	ARG	Sidechain
1	B	281	ARG	Sidechain

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	4520	0	4303	123	0
1	B	4500	0	4288	106	0
2	A	80	0	0	4	0
2	B	85	0	0	4	0
3	B	1	0	0	0	0
4	A	384	0	0	80	0
4	B	380	0	0	70	0
All	All	9950	0	8591	230	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 13.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:VAL:HG12	4:A:897:HOH:O	1.21	1.31
1:A:448:GLU:HB2	4:A:900:HOH:O	1.30	1.29
1:B:92:ASN:HB3	4:B:1097:HOH:O	1.12	1.28
1:B:106:MET:HG2	4:B:1066:HOH:O	1.11	1.24
1:B:536:ILE:HG21	4:B:996:HOH:O	1.07	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:HB2	4:B:898:HOH:O	1.06	1.21
1:A:581:PRO:HD2	4:A:1102:HOH:O	1.43	1.15
1:A:314:ASN:HB2	4:A:1064:HOH:O	1.48	1.10
1:B:210:ALA:HB2	4:B:832:HOH:O	1.48	1.08
1:A:118:VAL:HA	4:A:804:HOH:O	1.53	1.07
1:A:427:LEU:HB2	4:A:1015:HOH:O	1.54	1.04
1:A:263:ASN:HB3	4:A:817:HOH:O	1.56	1.04
1:A:383:ASN:HB3	4:A:1088:HOH:O	1.57	1.02
1:B:90:GLY:HA2	4:B:843:HOH:O	1.58	1.01
1:B:225:PHE:HE2	4:B:835:HOH:O	1.43	1.01
1:A:255:ASP:HB3	4:A:1087:HOH:O	1.59	1.00
1:B:314:ASN:HB2	4:B:1048:HOH:O	1.61	1.00
1:A:487:LEU:HG	4:A:807:HOH:O	1.61	0.98
1:B:225:PHE:CE2	4:B:835:HOH:O	2.18	0.93
1:B:367:ASP:H	1:B:370:HIS:HD2	1.19	0.91
1:B:209:LYS:HE3	4:B:1117:HOH:O	1.71	0.90
1:A:367:ASP:H	1:A:370:HIS:HD2	1.20	0.89
1:A:111:ARG:HD3	4:A:1021:HOH:O	1.75	0.87
1:B:27:GLY:HA3	4:B:915:HOH:O	1.73	0.87
1:B:194:ILE:HG23	4:B:1088:HOH:O	1.75	0.85
1:B:346:ARG:HD3	4:B:1051:HOH:O	1.76	0.85
1:B:453:MET:SD	4:B:1065:HOH:O	2.33	0.84
1:A:466:LEU:HD13	4:A:1168:HOH:O	1.77	0.84
1:A:365:GLU:OE2	4:A:801:HOH:O	1.95	0.84
1:A:356:PHE:CD1	4:A:813:HOH:O	2.30	0.83
1:B:382:GLY:HA3	4:B:850:HOH:O	1.78	0.83
1:A:497:VAL:HB	4:A:807:HOH:O	1.77	0.82
1:A:554:VAL:HG21	4:A:1102:HOH:O	1.79	0.82
1:B:347:GLN:OE1	2:B:716:SO4:O1	1.97	0.82
1:B:511:HIS:HD2	1:B:586:TRP:HE1	1.29	0.81
1:B:322:PHE:HD2	4:B:818:HOH:O	1.65	0.80
1:B:194:ILE:HG12	4:B:1004:HOH:O	1.80	0.80
1:B:395:ASN:HD21	1:B:406:ASN:H	1.29	0.79
1:A:511:HIS:HD2	1:A:586:TRP:HE1	1.31	0.78
1:A:162:HIS:HB2	4:A:912:HOH:O	1.82	0.78
1:A:592:GLU:HG2	4:A:897:HOH:O	1.83	0.76
1:A:159:LEU:HA	4:A:912:HOH:O	1.86	0.75
1:A:427:LEU:HD13	4:A:1031:HOH:O	1.85	0.75
2:A:708:SO4:O1	4:A:803:HOH:O	2.05	0.75
1:B:108:GLU:HB3	4:B:1085:HOH:O	1.85	0.75
1:A:276:GLN:OE1	4:A:802:HOH:O	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NE	4:A:806:HOH:O	2.21	0.74
1:A:556:SER:HA	4:A:835:HOH:O	1.88	0.73
1:A:298:GLN:HE21	1:A:300:GLY:H	1.37	0.73
1:B:511:HIS:CD2	1:B:586:TRP:HE1	2.07	0.72
1:A:455:HIS:HD2	4:A:927:HOH:O	1.71	0.72
1:A:253:SER:HB2	4:A:817:HOH:O	1.89	0.71
1:A:590:VAL:HG22	4:A:1168:HOH:O	1.88	0.71
1:A:117:ASP:O	4:A:804:HOH:O	2.08	0.71
1:A:359:ASN:HB2	4:A:849:HOH:O	1.90	0.70
1:A:511:HIS:CD2	1:A:586:TRP:HE1	2.08	0.70
1:A:395:ASN:HD21	1:A:406:ASN:H	1.36	0.70
1:A:498:THR:OG1	4:A:805:HOH:O	2.09	0.69
1:B:45:VAL:HG13	4:B:971:HOH:O	1.92	0.69
1:B:298:GLN:HE21	1:B:300:GLY:H	1.39	0.69
1:A:130:HIS:ND1	2:A:706:SO4:O2	2.25	0.69
1:A:587:THR:HA	4:A:835:HOH:O	1.92	0.69
1:B:272:LYS:HE3	4:B:1084:HOH:O	1.94	0.68
1:A:170:GLN:HG3	4:A:994:HOH:O	1.93	0.68
1:B:371:LEU:HD21	4:B:1101:HOH:O	1.94	0.67
1:A:267:VAL:HG13	4:A:1069:HOH:O	1.95	0.66
1:A:39:VAL:HG12	4:A:808:HOH:O	1.95	0.66
1:B:395:ASN:ND2	1:B:406:ASN:H	1.93	0.66
1:A:119:ILE:HD12	4:A:839:HOH:O	1.94	0.66
1:B:274:TRP:HD1	4:B:818:HOH:O	1.79	0.66
1:B:455:HIS:HD2	4:B:890:HOH:O	1.79	0.65
1:A:412:LEU:HG	4:A:811:HOH:O	1.96	0.65
1:A:282:ASN:HB3	4:A:891:HOH:O	1.97	0.65
1:A:395:ASN:ND2	1:A:406:ASN:H	1.96	0.64
1:A:361:MET:HE2	1:A:371:LEU:HD23	1.78	0.64
1:A:176:HIS:CD2	4:A:936:HOH:O	2.50	0.64
1:B:177:HIS:HE1	1:B:234:ASP:OD2	1.81	0.64
1:A:328:GLN:CG	4:A:1125:HOH:O	2.45	0.63
1:B:212:GLN:HB3	4:B:1098:HOH:O	1.99	0.62
1:A:416:VAL:CG2	4:A:811:HOH:O	2.47	0.62
1:B:475:SER:HB2	4:B:1053:HOH:O	1.98	0.61
1:A:359:ASN:HD21	1:A:378:ASN:HD21	1.47	0.61
1:B:226:GLY:HA2	4:B:837:HOH:O	2.00	0.61
1:A:383:ASN:HB2	1:A:385:GLN:HE21	1.65	0.60
1:A:119:ILE:HG23	4:A:839:HOH:O	2.01	0.60
1:B:298:GLN:NE2	1:B:300:GLY:H	2.00	0.60
1:A:298:GLN:NE2	1:A:300:GLY:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:HG23	4:A:811:HOH:O	2.02	0.59
1:B:285:VAL:HG23	4:B:983:HOH:O	2.02	0.58
1:B:177:HIS:HD2	1:B:228:LEU:H	1.51	0.58
1:B:427:LEU:HD21	1:B:453:MET:HE2	1.85	0.58
1:B:472:THR:HG23	4:B:1068:HOH:O	2.03	0.58
1:B:274:TRP:CD1	4:B:818:HOH:O	2.53	0.58
1:A:229:LYS:HD3	1:A:265:TYR:OH	2.03	0.58
1:B:485:MET:HB3	4:B:996:HOH:O	2.03	0.57
1:B:180:LEU:HB2	4:B:983:HOH:O	2.03	0.57
1:B:362:TRP:HA	4:B:884:HOH:O	2.04	0.57
1:B:361:MET:HE2	1:B:371:LEU:HD23	1.85	0.57
1:A:453:MET:SD	4:A:1006:HOH:O	2.57	0.56
1:A:427:LEU:HD21	1:A:453:MET:HE2	1.87	0.56
1:B:315:LEU:HD21	4:B:835:HOH:O	2.05	0.56
1:A:357:PHE:C	4:A:813:HOH:O	2.47	0.56
1:B:182:GLY:HA2	4:B:1102:HOH:O	2.05	0.56
1:B:359:ASN:HD21	1:B:378:ASN:HD21	1.54	0.55
1:B:416:VAL:HB	4:B:813:HOH:O	2.07	0.55
1:B:274:TRP:CD1	4:B:859:HOH:O	2.59	0.55
1:A:330:HIS:HD2	4:A:1111:HOH:O	1.90	0.55
1:B:473:GLU:OE2	4:B:801:HOH:O	2.18	0.55
1:B:34:THR:H	1:B:35:GLU:HG2	1.72	0.55
1:B:417:MET:HB3	4:B:814:HOH:O	2.06	0.55
1:A:478:MET:HE3	4:A:1066:HOH:O	2.07	0.55
1:A:34:THR:H	1:A:35:GLU:HG2	1.72	0.54
1:A:209:LYS:HD2	4:A:978:HOH:O	2.06	0.54
1:B:392:ALA:HB1	1:B:523:TRP:CZ3	2.42	0.54
1:A:280:GLU:HG3	4:A:856:HOH:O	2.07	0.54
1:B:446:SER:OG	1:B:448:GLU:HG3	2.07	0.54
1:A:367:ASP:H	1:A:370:HIS:CD2	2.12	0.54
1:B:177:HIS:CD2	1:B:228:LEU:H	2.26	0.54
1:A:359:ASN:ND2	1:A:378:ASN:HD21	2.06	0.54
1:B:103:LYS:HE3	4:B:1104:HOH:O	2.06	0.54
1:B:264:ILE:HG22	4:B:837:HOH:O	2.08	0.53
1:B:367:ASP:H	1:B:370:HIS:CD2	2.11	0.53
1:B:390:PHE:HD2	4:B:814:HOH:O	1.90	0.53
1:A:242:LEU:HD12	4:A:841:HOH:O	2.09	0.53
1:A:328:GLN:HG2	4:A:1125:HOH:O	2.07	0.53
1:A:328:GLN:HG3	4:A:1125:HOH:O	2.07	0.53
1:A:266:LEU:HB3	4:A:841:HOH:O	2.10	0.53
1:A:446:SER:OG	1:A:448:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HD2	4:B:1064:HOH:O	2.09	0.52
1:A:75:ARG:NH2	4:A:820:HOH:O	2.42	0.52
1:B:130:HIS:HB2	4:B:1107:HOH:O	2.09	0.52
1:B:319:TYR:HE1	4:B:835:HOH:O	1.92	0.52
1:A:219:MET:HE2	4:A:1113:HOH:O	2.08	0.52
1:B:106:MET:HE3	4:B:1066:HOH:O	2.08	0.51
1:B:104:GLY:H	1:B:465:ASN:HD21	1.58	0.51
1:A:327:LYS:HG2	1:A:353:LYS:HD2	1.93	0.51
1:A:35:GLU:HG3	4:A:1040:HOH:O	2.10	0.51
1:B:398:LYS:NZ	2:B:710:SO4:O3	2.43	0.51
1:A:119:ILE:HG12	4:A:808:HOH:O	2.11	0.51
1:A:448:GLU:HG2	4:A:1114:HOH:O	2.10	0.51
1:B:474:ASN:HB2	4:B:968:HOH:O	2.11	0.51
1:A:103:LYS:HA	1:A:465:ASN:HD21	1.75	0.51
1:B:212:GLN:CB	4:B:1098:HOH:O	2.58	0.50
1:A:356:PHE:HD1	4:A:813:HOH:O	1.81	0.50
1:B:139:PHE:HB2	4:B:811:HOH:O	2.11	0.50
1:A:392:ALA:HB1	1:A:523:TRP:CZ3	2.46	0.50
1:A:560:HIS:CG	4:A:808:HOH:O	2.64	0.50
1:B:267:VAL:HG11	1:B:274:TRP:CD2	2.47	0.50
1:B:103:LYS:HA	1:B:465:ASN:HD21	1.76	0.49
1:B:447:GLU:H	1:B:447:GLU:CD	2.17	0.49
1:B:180:LEU:HD22	1:B:284:ASP:HB3	1.95	0.49
1:B:359:ASN:ND2	1:B:378:ASN:HD21	2.11	0.49
1:A:104:GLY:H	1:A:465:ASN:HD21	1.59	0.48
1:A:511:HIS:HE1	4:A:973:HOH:O	1.96	0.48
1:B:46:GLU:HB2	4:B:1118:HOH:O	2.13	0.48
1:A:504:VAL:O	1:A:505:ASP:HB3	2.13	0.48
1:A:504:VAL:HG12	1:A:505:ASP:HB2	1.95	0.48
1:A:189:GLU:HG2	4:A:1089:HOH:O	2.13	0.48
1:A:240:TRP:HB2	4:A:1069:HOH:O	2.13	0.48
1:B:104:GLY:H	1:B:465:ASN:ND2	2.11	0.48
1:A:499:THR:HA	1:A:511:HIS:O	2.14	0.48
1:B:106:MET:CE	4:B:1066:HOH:O	2.61	0.47
1:B:264:ILE:HG23	4:B:1022:HOH:O	2.13	0.47
1:B:572:GLU:HG2	4:B:817:HOH:O	2.15	0.47
1:A:104:GLY:H	1:A:465:ASN:ND2	2.12	0.47
1:B:106:MET:CG	4:B:1066:HOH:O	1.97	0.47
1:B:476:ILE:HG21	1:B:543:MET:HG3	1.96	0.47
1:B:212:GLN:HG2	4:B:1098:HOH:O	2.14	0.47
1:A:267:VAL:HG11	1:A:274:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD3	4:A:814:HOH:O	2.15	0.47
1:A:106:MET:HG2	4:A:834:HOH:O	2.14	0.47
1:B:212:GLN:CG	4:B:1098:HOH:O	2.63	0.47
1:A:545:LEU:HD13	4:A:1146:HOH:O	2.15	0.47
1:B:55:LYS:HB2	1:B:58:GLU:CD	2.41	0.46
1:B:511:HIS:HE1	4:B:963:HOH:O	1.98	0.46
1:B:237:LYS:HG3	4:B:1040:HOH:O	2.15	0.46
1:A:384:ASN:HB2	4:A:854:HOH:O	2.14	0.46
1:A:388:THR:CG2	4:A:849:HOH:O	2.63	0.46
1:B:96:LYS:HE3	4:B:870:HOH:O	2.15	0.46
1:B:327:LYS:HG2	1:B:353:LYS:HD2	1.97	0.46
1:B:170:GLN:HG3	4:B:926:HOH:O	2.16	0.46
1:A:33:VAL:HG11	4:A:809:HOH:O	2.16	0.45
1:B:337:MET:HE1	4:B:1115:HOH:O	2.16	0.45
1:B:499:THR:HA	1:B:511:HIS:O	2.16	0.45
1:B:110:TYR:HB3	4:B:1085:HOH:O	2.16	0.45
1:B:241:TYR:HA	1:B:267:VAL:HA	1.99	0.44
1:A:402:ARG:N	2:A:707:SO4:O4	2.46	0.44
1:B:322:PHE:CD2	4:B:818:HOH:O	2.50	0.44
1:B:159:LEU:HD23	4:B:863:HOH:O	2.18	0.44
1:A:282:ASN:CB	4:A:891:HOH:O	2.59	0.44
1:A:416:VAL:HG21	4:A:811:HOH:O	2.16	0.44
1:B:450:LYS:HE2	4:B:1127:HOH:O	2.17	0.43
1:B:536:ILE:CG2	4:B:996:HOH:O	1.96	0.43
1:A:57:ASN:HD21	1:A:99:SER:HB3	1.83	0.43
1:A:164:ILE:HG12	4:A:912:HOH:O	2.18	0.43
1:B:266:LEU:HA	4:B:837:HOH:O	2.18	0.43
1:B:476:ILE:CG2	1:B:543:MET:HG3	2.48	0.43
1:A:225:PHE:C	1:A:225:PHE:CD1	2.97	0.43
1:A:316:ARG:HD3	1:A:343:TYR:CE1	2.54	0.43
1:A:368:PHE:HD2	4:A:1055:HOH:O	2.00	0.43
1:A:416:VAL:HB	4:A:829:HOH:O	2.19	0.43
1:A:383:ASN:HB2	1:A:385:GLN:NE2	2.33	0.43
1:A:79:LEU:HD22	1:A:466:LEU:HG	2.00	0.43
1:B:330:HIS:HD2	4:B:960:HOH:O	2.02	0.42
1:A:490:TRP:CG	1:A:491:PRO:HA	2.54	0.42
1:B:545:LEU:HD12	4:B:1090:HOH:O	2.18	0.42
1:B:131:PRO:HD2	2:B:706:SO4:O2	2.19	0.42
1:A:281:ARG:HA	1:A:281:ARG:HD3	1.65	0.42
1:A:148:THR:HB	2:A:705:SO4:O4	2.20	0.42
1:A:508:GLN:HG2	4:A:1146:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:N	4:A:845:HOH:O	2.53	0.42
1:B:225:PHE:CD1	1:B:225:PHE:C	2.97	0.41
1:A:57:ASN:HB3	1:A:96:LYS:NZ	2.35	0.41
1:A:168:GLN:NE2	1:A:170:GLN:OE1	2.53	0.41
1:B:548:LYS:HB3	2:B:718:SO4:O1	2.20	0.41
1:B:504:VAL:HG21	4:B:823:HOH:O	2.20	0.41
1:A:33:VAL:CG1	4:A:809:HOH:O	2.69	0.41
1:A:180:LEU:HD22	1:A:284:ASP:HB3	2.01	0.41
1:A:241:TYR:HA	1:A:267:VAL:HA	2.03	0.41
1:A:492:PRO:HB2	4:A:1055:HOH:O	2.20	0.41
1:B:35:GLU:HG2	1:B:35:GLU:H	0.81	0.41
1:B:88:VAL:HA	4:B:1072:HOH:O	2.21	0.41
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.95	0.41
1:A:224:CYS:HB3	1:A:296:ILE:CG2	2.51	0.41
1:A:35:GLU:HG2	1:A:35:GLU:H	0.85	0.41
1:A:55:LYS:HB2	1:A:58:GLU:HG3	2.03	0.40
1:A:467:LEU:HD23	4:A:1071:HOH:O	2.21	0.40
1:A:364:ASP:CG	4:A:801:HOH:O	2.64	0.40
1:A:46:GLU:HG2	4:A:1103:HOH:O	2.21	0.40
1:A:447:GLU:CD	1:A:447:GLU:H	2.28	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	568/577 (98%)	545 (96%)	23 (4%)	0	100	100
1	B	566/577 (98%)	549 (97%)	17 (3%)	0	100	100
All	All	1134/1154 (98%)	1094 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	479/485 (99%)	464 (97%)	15 (3%)	35	39
1	B	477/485 (98%)	464 (97%)	13 (3%)	39	45
All	All	956/970 (99%)	928 (97%)	28 (3%)	37	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	GLU
1	B	83	VAL
1	B	89	SER
1	B	133	ARG
1	B	225	PHE
1	B	258	SER
1	B	281	ARG
1	B	313	VAL
1	B	364	ASP
1	B	365	GLU
1	B	447	GLU
1	B	472	THR
1	B	544	ASN
1	A	35	GLU
1	A	83	VAL
1	A	89	SER
1	A	186	GLN
1	A	225	PHE
1	A	229	LYS
1	A	281	ARG
1	A	313	VAL
1	A	365	GLU
1	A	447	GLU
1	A	472	THR
1	A	486	LYS
1	A	489	VAL
1	A	594	GLU

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Mol	Chain	Res	Type
1	A	596	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
1	B	92	ASN
1	B	114	ASN
1	B	168	GLN
1	B	177	HIS
1	B	288	ASN
1	B	295	GLN
1	B	298	GLN
1	B	309	ASN
1	B	330	HIS
1	B	359	ASN
1	B	370	HIS
1	B	395	ASN
1	B	455	HIS
1	B	465	ASN
1	B	479	ASN
1	B	511	HIS
1	B	565	GLN
1	A	57	ASN
1	A	92	ASN
1	A	114	ASN
1	A	168	GLN
1	A	186	GLN
1	A	288	ASN
1	A	295	GLN
1	A	298	GLN
1	A	309	ASN
1	A	330	HIS
1	A	359	ASN
1	A	370	HIS
1	A	385	GLN
1	A	395	ASN
1	A	455	HIS
1	A	465	ASN
1	A	479	ASN
1	A	511	HIS
1	A	565	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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	710	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	711	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	A	707	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	B	707	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	A	708	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	A	704	-	4,4,4	0.33	0	6,6,6	0.14	0
2	SO4	A	713	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	B	702	-	4,4,4	0.42	0	6,6,6	0.16	0
2	SO4	B	716	-	4,4,4	0.28	0	6,6,6	0.17	0
2	SO4	B	713	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	B	705	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	B	708	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	B	704	-	4,4,4	0.34	0	6,6,6	0.19	0
2	SO4	A	703	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	B	703	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	A	711	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	A	714	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	A	712	-	4,4,4	0.34	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	706	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	B	712	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	A	701	-	4,4,4	0.44	0	6,6,6	0.18	0
2	SO4	B	710	-	4,4,4	0.30	0	6,6,6	0.06	0
2	SO4	A	715	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	A	705	-	4,4,4	0.35	0	6,6,6	0.23	0
2	SO4	A	709	-	4,4,4	0.40	0	6,6,6	0.23	0
2	SO4	B	717	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	B	715	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	A	716	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	B	709	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	B	718	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	A	702	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	B	701	-	4,4,4	0.39	0	6,6,6	0.15	0
2	SO4	A	706	-	4,4,4	0.34	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	707	SO4	1	0
2	A	708	SO4	1	0
2	B	716	SO4	1	0
2	B	706	SO4	1	0
2	B	710	SO4	1	0
2	A	705	SO4	1	0
2	B	718	SO4	1	0
2	A	706	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	570/577 (98%)	-0.08	10 (1%) 67 70	24, 36, 56, 119	0
1	B	568/577 (98%)	-0.09	5 (0%) 81 83	26, 36, 57, 104	0
All	All	1138/1154 (98%)	-0.09	15 (1%) 75 77	24, 36, 57, 119	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	GLY	4.6
1	A	29	ALA	4.4
1	B	27	GLY	3.7
1	A	383	ASN	3.5
1	A	595	HIS	3.5
1	A	28	GLY	3.0
1	A	27	GLY	3.0
1	A	596	HIS	2.7
1	B	376	TYR	2.3
1	A	342	ARG	2.2
1	A	574	GLY	2.2
1	A	189	GLU	2.2
1	A	382	GLY	2.1
1	B	332	ASP	2.1
1	B	42	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	715	5/5	0.58	0.13	80,92,105,119	0
2	SO4	B	716	5/5	0.72	0.14	75,76,92,95	0
2	SO4	B	712	5/5	0.76	0.11	86,89,95,107	0
2	SO4	A	705	5/5	0.77	0.13	61,84,90,100	0
2	SO4	B	705	5/5	0.79	0.10	77,95,97,113	0
2	SO4	A	715	5/5	0.81	0.09	70,80,96,98	0
2	SO4	B	713	5/5	0.82	0.09	87,95,105,106	0
2	SO4	B	718	5/5	0.84	0.09	89,91,95,100	0
2	SO4	B	706	5/5	0.84	0.09	72,80,90,91	0
2	SO4	B	710	5/5	0.84	0.08	69,72,74,76	0
2	SO4	A	708	5/5	0.86	0.09	50,55,61,71	0
2	SO4	B	711	5/5	0.86	0.08	77,83,89,99	0
2	SO4	B	717	5/5	0.87	0.08	83,84,87,93	0
2	SO4	B	708	5/5	0.87	0.09	58,58,66,82	0
2	SO4	A	714	5/5	0.87	0.08	70,71,76,86	0
2	SO4	A	704	5/5	0.87	0.08	71,77,84,88	0
2	SO4	B	707	5/5	0.89	0.08	72,74,80,89	0
2	SO4	A	710	5/5	0.89	0.08	66,70,78,84	0
2	SO4	A	713	5/5	0.89	0.07	69,77,81,84	0
2	SO4	A	702	5/5	0.89	0.10	67,77,87,104	0
2	SO4	A	706	5/5	0.89	0.08	69,72,76,83	0
2	SO4	A	711	5/5	0.90	0.07	65,68,76,80	0
2	SO4	A	707	5/5	0.90	0.07	72,78,81,87	0
2	SO4	B	704	5/5	0.91	0.08	62,76,86,97	0
2	SO4	A	701	5/5	0.92	0.08	56,56,61,61	0
2	SO4	B	703	5/5	0.93	0.08	64,74,83,84	0
2	SO4	A	712	5/5	0.93	0.07	48,57,67,89	0
2	SO4	B	709	5/5	0.93	0.07	63,65,68,75	0
2	SO4	A	709	5/5	0.93	0.06	55,60,64,66	0
2	SO4	A	703	5/5	0.93	0.09	61,69,71,73	0
2	SO4	A	716	5/5	0.93	0.07	57,61,70,78	0
3	NA	B	714	1/1	0.94	0.20	55,55,55,55	0
2	SO4	B	701	5/5	0.95	0.09	45,54,55,55	0
2	SO4	B	702	5/5	0.95	0.07	65,67,77,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.