



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:12 PM GMT

PDB ID : 2E8Y
Title : Crystal structure of pullulanase type I from Bacillus subtilis str. 168
Authors : Mikami, B.; Malle, D.; Utsumi, S.; Iwamoto, H.; Katsuya, Y.
Deposited on : 2007-01-24
Resolution : 2.11 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

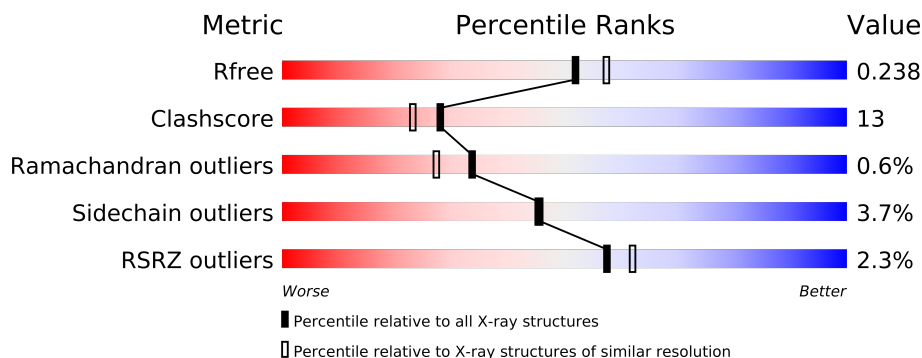
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.11 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}	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	718	
1	B	718	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	A	751	-	X
3	ACT	B	752	-	X
4	GOL	A	761	X	X
4	GOL	B	762	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12049 atoms, of which 0 are hydrogen and 0 are deuterium.

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 AmyX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5672	3615	975	1060	22			
1	B	712	Total	C	N	O	S	0	0	0
			5672	3615	975	1060	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LYS	MET	CONFLICT	UNP O34587
B	365	LYS	MET	CONFLICT	UNP O34587

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

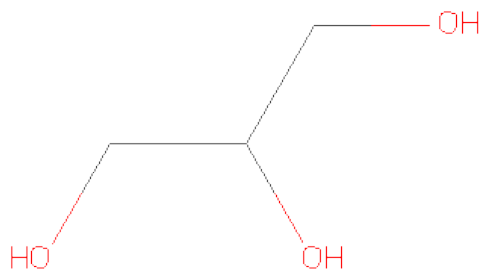
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

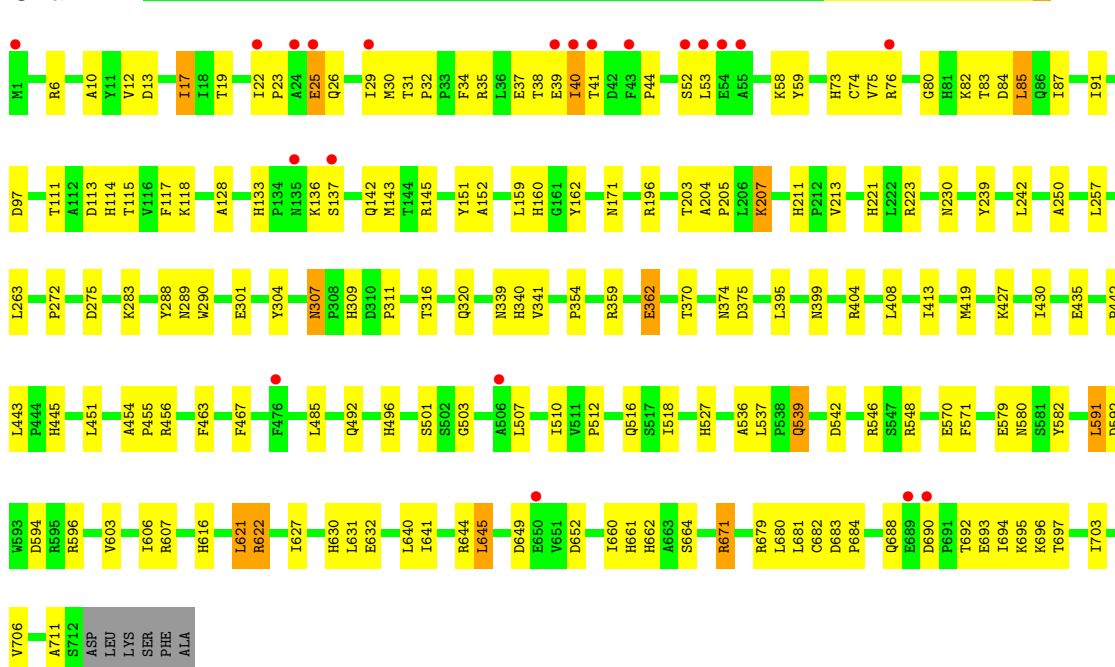
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	333	Total 333	O 333	0	0
5	B	350	Total 350	O 350	0	0

3 Residue-property plots

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

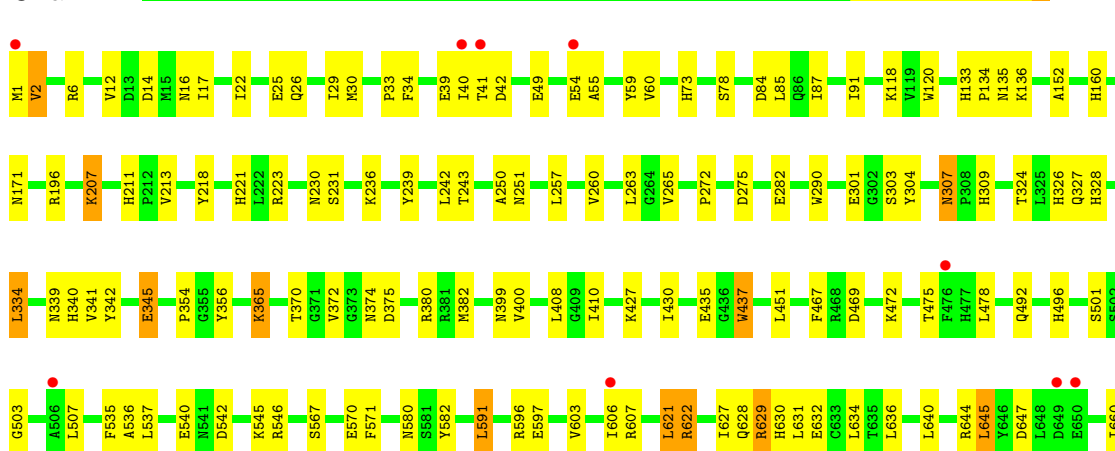
• Molecule 1: AmyX protein

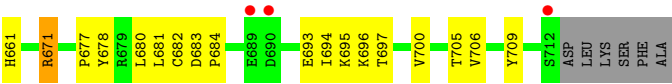
Chain A:



• Molecule 1: AmyX protein

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.56Å 127.68Å 189.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.11 47.34 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.11) 99.3 (47.34-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.238 0.202 , 0.238	Depositor DCC
R_{free} test set	9861 reflections (10.03%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 98917 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12049	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.32	0/5820	0.58	0/7902
1	B	0.33	0/5820	0.59	0/7902
All	All	0.32	0/11640	0.59	0/15804

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5672	0	5521	153	0
1	B	5672	0	5521	133	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	3	3	0
3	B	4	0	3	0	0
4	A	6	0	4	1	0
4	B	6	0	4	0	0
5	A	333	0	0	11	0
5	B	350	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12049	0	11056	284	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (284) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:LYS:H	1:A:207:LYS:HE2	1.00	1.07
1:B:230:ASN:HD21	1:B:250:ALA:H	1.03	1.00
1:A:230:ASN:HD21	1:A:250:ALA:H	1.10	1.00
1:A:207:LYS:HE2	1:A:207:LYS:N	1.75	0.99
1:A:87:ILE:H	1:A:171:ASN:HD21	1.12	0.92
1:A:111:THR:HG22	1:A:113:ASP:H	1.35	0.91
1:B:640:LEU:HD21	1:B:660:ILE:HD11	1.50	0.91
1:A:207:LYS:CE	1:A:207:LYS:H	1.86	0.89
1:A:660:ILE:HB	1:A:706:VAL:CG1	2.05	0.87
1:A:660:ILE:HB	1:A:706:VAL:HG13	1.57	0.86
1:A:263:LEU:HD22	1:A:606:ILE:HD11	1.57	0.86
1:A:160:HIS:HD2	1:A:196:ARG:H	1.21	0.84
1:B:160:HIS:HD2	1:B:196:ARG:H	1.22	0.83
1:A:339:ASN:HD21	1:A:340:HIS:HD2	1.26	0.82
1:A:496:HIS:HE1	1:A:503:GLY:H	1.27	0.82
1:B:263:LEU:HD22	1:B:606:ILE:HD11	1.63	0.80
1:B:230:ASN:HD21	1:B:250:ALA:N	1.80	0.80
1:A:339:ASN:ND2	1:A:340:HIS:HD2	1.81	0.78
1:B:22:ILE:HD12	1:B:59:TYR:HE1	1.48	0.78
1:B:22:ILE:HD13	1:B:30:MET:O	1.83	0.78
1:B:251:ASN:HB2	1:B:597:GLU:OE1	1.83	0.78
1:B:339:ASN:ND2	1:B:340:HIS:HD2	1.81	0.77
1:B:660:ILE:CG2	1:B:706:VAL:HB	2.15	0.77
1:A:87:ILE:N	1:A:171:ASN:HD21	1.82	0.77
1:A:87:ILE:H	1:A:171:ASN:ND2	1.83	0.76
1:B:87:ILE:H	1:B:171:ASN:ND2	1.85	0.74
1:B:39:GLU:HG3	1:B:40:ILE:HG13	1.68	0.74
1:B:341:VAL:H	1:B:374:ASN:HD21	1.33	0.74
1:B:677:PRO:HG3	1:B:695:LYS:HE2	1.68	0.74
1:B:603:VAL:O	1:B:606:ILE:HG13	1.87	0.73
1:A:22:ILE:HD13	1:A:30:MET:O	1.88	0.72
1:B:87:ILE:H	1:B:171:ASN:HD21	1.35	0.72
1:B:496:HIS:HE1	1:B:503:GLY:H	1.36	0.71
1:B:339:ASN:HD21	1:B:340:HIS:HD2	1.36	0.71
1:B:660:ILE:HG23	1:B:706:VAL:HB	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:GLN:HG3	5:A:957:HOH:O	1.90	0.71
1:B:622:ARG:HD3	5:B:913:HOH:O	1.90	0.70
1:B:22:ILE:HD12	1:B:59:TYR:CE1	2.25	0.70
1:A:542:ASP:HB3	3:A:751:ACT:H2	1.73	0.70
1:A:621:LEU:HD23	1:A:627:ILE:HA	1.72	0.70
1:B:207:LYS:CD	1:B:207:LYS:H	2.03	0.69
1:A:456:ARG:HD3	5:A:1051:HOH:O	1.91	0.69
1:B:22:ILE:HD11	1:B:34:PHE:HZ	1.56	0.69
1:B:207:LYS:H	1:B:207:LYS:HD2	1.57	0.68
1:A:603:VAL:O	1:A:606:ILE:HG13	1.93	0.68
1:A:692:THR:HG22	5:A:1088:HOH:O	1.92	0.68
1:B:54:GLU:HG3	1:B:55:ALA:H	1.58	0.68
1:B:14:ASP:HB3	1:B:17:ILE:HD13	1.76	0.68
1:A:87:ILE:HG13	1:A:171:ASN:HD21	1.59	0.68
1:A:435:GLU:HG2	5:A:989:HOH:O	1.95	0.67
1:A:571:PHE:HZ	1:A:591:LEU:HD22	1.59	0.66
1:A:671:ARG:HG2	1:A:697:THR:HG22	1.78	0.66
1:B:621:LEU:HD23	1:B:627:ILE:HA	1.79	0.65
1:B:133:HIS:HB3	1:B:136:LYS:HB2	1.77	0.65
1:B:307:ASN:HD21	1:B:309:HIS:HB2	1.62	0.63
1:A:341:VAL:H	1:A:374:ASN:HD21	1.46	0.63
1:A:307:ASN:HD21	1:A:309:HIS:HB2	1.63	0.63
1:A:492:GLN:HG2	1:A:507:LEU:HD11	1.80	0.63
1:A:242:LEU:HD23	5:A:820:HOH:O	1.99	0.63
1:B:211:HIS:HD2	1:B:213:VAL:H	1.48	0.62
1:A:230:ASN:HD21	1:A:250:ALA:N	1.89	0.62
1:A:307:ASN:ND2	1:A:309:HIS:H	1.97	0.62
1:A:316:THR:O	1:A:320:GLN:HG3	1.98	0.62
1:A:413:ILE:HB	5:A:896:HOH:O	1.99	0.62
1:B:540:GLU:O	1:B:545:LYS:HE3	1.99	0.62
1:B:339:ASN:ND2	1:B:340:HIS:CD2	2.67	0.61
1:B:207:LYS:HD2	1:B:207:LYS:N	2.15	0.61
1:A:211:HIS:CD2	1:A:213:VAL:HG22	2.36	0.61
1:A:6:ARG:HD3	1:A:84:ASP:OD2	2.00	0.61
1:A:73:HIS:HB2	1:A:85:LEU:HB2	1.82	0.61
1:A:546:ARG:HH11	3:A:751:ACT:CH3	2.13	0.60
1:B:606:ILE:HD12	1:B:607:ARG:N	2.16	0.60
1:A:38:THR:HB	1:A:41:THR:OG1	2.01	0.60
1:B:22:ILE:HD11	1:B:34:PHE:CZ	2.37	0.60
1:A:339:ASN:ND2	1:A:340:HIS:CD2	2.68	0.59
1:B:211:HIS:CD2	1:B:213:VAL:HG22	2.37	0.59
1:B:469:ASP:OD2	1:B:475:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:LYS:HE2	1:B:365:LYS:N	2.17	0.59
1:A:52:SER:C	1:A:53:LEU:HD12	2.24	0.59
1:A:133:HIS:HB3	1:A:136:LYS:HB3	1.83	0.58
1:A:87:ILE:HG13	1:A:171:ASN:ND2	2.17	0.58
1:B:307:ASN:ND2	1:B:309:HIS:H	2.01	0.58
1:B:91:ILE:HD12	1:B:354:PRO:O	2.04	0.58
1:A:22:ILE:HD12	1:A:59:TYR:CE1	2.39	0.58
1:A:622:ARG:HD3	5:A:939:HOH:O	2.01	0.58
1:A:13:ASP:HB2	1:A:17:ILE:HD11	1.84	0.58
1:A:118:LYS:HG2	1:A:152:ALA:HB2	1.86	0.57
1:A:680:LEU:HD12	1:A:688:GLN:HG3	1.85	0.57
1:B:54:GLU:HG3	1:B:55:ALA:N	2.19	0.57
1:B:472:LYS:NZ	1:B:475:THR:HG22	2.20	0.57
1:B:631:LEU:C	1:B:631:LEU:HD23	2.25	0.57
1:A:340:HIS:HE1	5:A:830:HOH:O	1.88	0.56
1:A:40:ILE:HG22	1:A:40:ILE:O	2.05	0.56
1:B:660:ILE:HD13	1:B:700:VAL:HG21	1.88	0.56
1:A:128:ALA:HA	1:A:143:MET:HG3	1.87	0.55
1:B:571:PHE:HZ	1:B:591:LEU:HD22	1.70	0.55
1:B:339:ASN:HD21	1:B:340:HIS:CD2	2.22	0.55
1:A:211:HIS:HD2	1:A:213:VAL:H	1.54	0.55
1:B:356:TYR:O	1:B:380:ARG:HD3	2.06	0.54
1:B:1:MET:HG2	1:B:2:VAL:N	2.23	0.54
1:A:694:ILE:C	1:A:694:ILE:HD12	2.28	0.54
1:B:606:ILE:C	1:B:606:ILE:HD12	2.28	0.54
1:B:16:ASN:C	1:B:17:ILE:HD12	2.28	0.54
1:B:1:MET:HG2	1:B:2:VAL:HG23	1.90	0.54
1:A:111:THR:HB	1:A:114:HIS:O	2.08	0.54
1:B:221:HIS:CD2	1:B:223:ARG:H	2.26	0.54
1:A:546:ARG:HD3	3:A:751:ACT:H1	1.90	0.53
1:A:571:PHE:CZ	1:A:591:LEU:HD22	2.42	0.53
1:B:91:ILE:CD1	1:B:354:PRO:O	2.56	0.53
1:A:22:ILE:HD11	1:A:34:PHE:CZ	2.44	0.53
1:B:17:ILE:N	1:B:17:ILE:HD12	2.23	0.53
1:A:26:GLN:NE2	1:A:29:ILE:HD12	2.23	0.53
1:A:211:HIS:HD2	1:A:213:VAL:HG22	1.72	0.53
1:A:661:HIS:HE1	5:A:813:HOH:O	1.92	0.53
1:B:345:GLU:CD	1:B:345:GLU:H	2.11	0.53
1:A:463:PHE:HA	1:A:518:ILE:HB	1.89	0.53
1:A:370:THR:HG23	1:A:375:ASP:OD2	2.09	0.53
1:A:91:ILE:HD12	1:A:354:PRO:O	2.09	0.53
1:B:260:VAL:HG13	1:B:265:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:ILE:HD11	1:A:34:PHE:HZ	1.75	0.52
1:A:606:ILE:HD12	1:A:606:ILE:C	2.30	0.52
1:B:694:ILE:O	1:B:694:ILE:HD12	2.08	0.52
1:B:6:ARG:HD3	1:B:84:ASP:OD2	2.10	0.52
1:A:23:PRO:HG2	1:A:26:GLN:HB2	1.92	0.51
1:A:221:HIS:CD2	1:A:223:ARG:HB3	2.45	0.51
1:B:160:HIS:CD2	1:B:196:ARG:H	2.13	0.51
1:B:49:GLU:CG	1:B:60:VAL:HB	2.40	0.51
1:B:570:GLU:HB2	1:B:606:ILE:HG12	1.92	0.51
1:A:22:ILE:HD12	1:A:59:TYR:HE1	1.76	0.51
1:B:118:LYS:HG2	1:B:152:ALA:HB2	1.92	0.51
1:B:435:GLU:HB2	1:B:437:TRP:CE2	2.45	0.51
1:A:309:HIS:O	1:A:311:PRO:HD3	2.11	0.50
1:B:630:HIS:O	1:B:645:LEU:HA	2.11	0.50
1:B:263:LEU:CD2	1:B:606:ILE:HD11	2.39	0.50
1:B:536:ALA:C	1:B:537:LEU:HD12	2.32	0.50
1:B:303:SER:HA	5:B:877:HOH:O	2.12	0.50
1:A:630:HIS:O	1:A:645:LEU:HA	2.12	0.50
1:A:496:HIS:CE1	1:A:503:GLY:H	2.18	0.49
1:B:324:THR:HA	1:B:327:GLN:HE21	1.78	0.49
1:A:204:ALA:N	1:A:205:PRO:HD3	2.27	0.49
1:B:260:VAL:CG1	1:B:265:VAL:HG21	2.42	0.49
1:B:41:THR:HG22	1:B:42:ASP:N	2.27	0.49
1:B:695:LYS:O	1:B:697:THR:N	2.45	0.49
1:B:694:ILE:HD12	1:B:694:ILE:C	2.33	0.49
1:A:76:ARG:HD2	1:A:82:LYS:HE2	1.94	0.49
1:A:413:ILE:HD13	1:A:456:ARG:CZ	2.43	0.49
1:B:492:GLN:HG2	1:B:507:LEU:HD11	1.95	0.49
1:A:536:ALA:C	1:A:537:LEU:HD12	2.33	0.48
1:A:631:LEU:C	1:A:631:LEU:HD23	2.33	0.48
1:A:263:LEU:CD2	1:A:606:ILE:HD11	2.35	0.48
1:A:496:HIS:HE1	1:A:503:GLY:N	2.03	0.48
1:A:12:VAL:HG23	1:A:85:LEU:HD22	1.94	0.48
1:A:682:CYS:O	1:A:706:VAL:HA	2.12	0.48
1:B:49:GLU:HG2	1:B:60:VAL:HB	1.95	0.48
1:B:41:THR:CG2	1:B:42:ASP:N	2.77	0.48
1:A:679:ARG:CZ	1:A:693:GLU:HG3	2.43	0.48
1:A:31:THR:HB	1:A:32:PRO:HD2	1.96	0.48
1:A:91:ILE:CD1	1:A:354:PRO:O	2.62	0.48
1:B:73:HIS:HE1	5:B:845:HOH:O	1.96	0.48
1:A:570:GLU:HB2	1:A:606:ILE:HG12	1.95	0.47
1:B:677:PRO:CG	1:B:695:LYS:HE2	2.42	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:485:LEU:HA	1:A:548:ARG:HD3	1.96	0.47
1:A:359:ARG:HB3	1:A:442:PRO:HG2	1.95	0.47
1:A:111:THR:HG22	1:A:113:ASP:N	2.16	0.47
1:B:282:GLU:OE2	1:B:309:HIS:HE1	1.96	0.47
1:A:136:LYS:HD3	1:A:162:TYR:OH	2.13	0.47
1:B:631:LEU:HD23	1:B:632:GLU:N	2.30	0.47
1:A:290:TRP:CD2	1:A:582:TYR:HA	2.49	0.47
1:B:334:LEU:HD22	1:B:400:VAL:HG11	1.96	0.47
1:A:221:HIS:CD2	1:A:223:ARG:H	2.33	0.47
1:A:145:ARG:HB2	1:A:151:TYR:CE1	2.50	0.47
1:B:427:LYS:O	1:B:430:ILE:HG23	2.15	0.47
1:A:339:ASN:HD21	1:A:340:HIS:CD2	2.17	0.47
1:A:75:VAL:HG23	1:A:83:THR:HG22	1.97	0.46
1:B:12:VAL:HG13	1:B:12:VAL:O	2.16	0.46
1:A:694:ILE:HD12	1:A:694:ILE:O	2.16	0.46
1:A:454:ALA:N	1:A:455:PRO:CD	2.78	0.46
1:B:370:THR:HG23	1:B:375:ASP:OD2	2.16	0.46
1:A:683:ASP:HB2	1:A:684:PRO:CD	2.45	0.46
1:B:671:ARG:HG2	1:B:697:THR:HG22	1.96	0.46
1:A:10:ALA:CB	1:A:75:VAL:HG21	2.46	0.46
1:A:26:GLN:HE22	1:A:29:ILE:HD12	1.80	0.46
1:A:203:THR:C	1:A:205:PRO:HD3	2.35	0.46
1:A:73:HIS:HD2	5:A:993:HOH:O	1.99	0.46
1:A:695:LYS:O	1:A:697:THR:N	2.42	0.46
1:B:571:PHE:CZ	1:B:591:LEU:HD22	2.50	0.46
1:B:133:HIS:CG	1:B:134:PRO:HD2	2.51	0.46
1:B:660:ILE:CD1	1:B:700:VAL:HG21	2.44	0.45
1:A:445:HIS:HD2	1:B:632:GLU:OE2	1.99	0.45
1:A:536:ALA:O	1:A:537:LEU:HD12	2.16	0.45
1:B:496:HIS:HE1	1:B:503:GLY:N	2.09	0.45
1:A:223:ARG:HD2	4:A:761:GOL:O3	2.16	0.45
1:A:76:ARG:CZ	1:A:80:GLY:HA2	2.46	0.45
1:A:548:ARG:NH1	1:A:703:ILE:CD1	2.78	0.45
1:A:548:ARG:NH1	1:A:703:ILE:HD11	2.32	0.45
1:B:25:GLU:CD	1:B:25:GLU:H	2.20	0.45
1:A:19:THR:HG23	1:A:58:LYS:HE3	1.99	0.45
1:B:681:LEU:HD13	1:B:681:LEU:C	2.37	0.45
1:A:512:PRO:HD2	1:A:516:GLN:NE2	2.32	0.45
1:B:478:LEU:HD11	1:B:535:PHE:CD2	2.52	0.45
1:B:370:THR:OG1	1:B:372:VAL:HG22	2.18	0.44
1:B:207:LYS:HZ2	1:B:207:LYS:H	1.64	0.44
1:B:33:PRO:HD2	1:B:78:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:THR:HA	1:B:324:THR:HG21	1.99	0.44
1:A:616:HIS:HB3	1:A:652:ASP:OD2	2.18	0.44
1:A:679:ARG:NH2	1:A:693:GLU:HG3	2.32	0.44
1:A:362:GLU:HB3	1:B:636:LEU:HB3	1.99	0.44
1:B:496:HIS:CE1	1:B:501:SER:HA	2.53	0.44
1:B:661:HIS:HE1	5:B:891:HOH:O	2.00	0.44
1:A:288:TYR:CD1	1:A:289:ASN:N	2.86	0.44
1:A:160:HIS:CD2	1:A:196:ARG:H	2.14	0.44
1:B:496:HIS:CE1	1:B:503:GLY:H	2.25	0.44
1:A:413:ILE:HD13	1:A:456:ARG:NH2	2.32	0.44
1:A:640:LEU:HD21	1:A:660:ILE:CG2	2.48	0.44
1:A:39:GLU:O	1:A:40:ILE:HB	2.17	0.43
1:A:359:ARG:NH2	1:A:443:LEU:HD11	2.33	0.43
1:B:472:LYS:HZ1	1:B:475:THR:HG22	1.81	0.43
1:A:73:HIS:HB2	1:A:85:LEU:CB	2.46	0.43
1:A:136:LYS:HG2	1:A:137:SER:H	1.83	0.43
1:A:221:HIS:HD2	1:A:223:ARG:HB3	1.83	0.43
1:B:12:VAL:HB	1:B:85:LEU:HD21	2.01	0.43
1:A:136:LYS:HG2	1:A:137:SER:N	2.33	0.43
1:B:682:CYS:O	1:B:706:VAL:HA	2.19	0.43
1:B:26:GLN:NE2	1:B:29:ILE:HD12	2.34	0.43
1:A:117:PHE:O	1:A:152:ALA:HA	2.18	0.43
1:B:221:HIS:HD2	1:B:223:ARG:H	1.67	0.43
1:A:37:GLU:N	1:A:74:CYS:O	2.49	0.43
1:B:542:ASP:O	1:B:546:ARG:HG3	2.19	0.42
1:B:683:ASP:HB2	1:B:684:PRO:CD	2.49	0.42
1:A:606:ILE:HD12	1:A:607:ARG:N	2.35	0.42
1:B:661:HIS:HD2	1:B:705:THR:OG1	2.02	0.42
1:A:592:ASP:OD1	1:A:594:ASP:HB2	2.18	0.42
1:A:39:GLU:O	1:A:40:ILE:CB	2.68	0.42
1:B:591:LEU:HA	1:B:591:LEU:HD23	1.95	0.42
1:A:395:LEU:O	1:A:399:ASN:HA	2.20	0.42
1:B:628:GLN:HA	1:B:628:GLN:HE21	1.84	0.42
1:B:290:TRP:CD2	1:B:582:TYR:HA	2.54	0.42
1:B:365:LYS:CA	1:B:365:LYS:HE2	2.49	0.42
1:B:275:ASP:HA	1:B:301:GLU:HA	2.00	0.42
1:A:501:SER:HB3	1:A:510:ILE:HB	2.00	0.42
1:A:527:HIS:CE1	1:A:579:GLU:HB2	2.55	0.42
1:A:230:ASN:ND2	1:A:250:ALA:H	1.94	0.42
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.87	0.42
1:B:221:HIS:CD2	1:B:223:ARG:HB3	2.55	0.42
1:B:370:THR:HG22	1:B:410:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:LYS:HB2	1:A:283:LYS:HE3	1.75	0.42
1:A:275:ASP:HA	1:A:301:GLU:HA	2.02	0.42
1:A:640:LEU:HD13	1:A:641:ILE:N	2.35	0.41
1:B:472:LYS:HZ1	1:B:475:THR:CG2	2.32	0.41
1:B:231:SER:OG	1:B:236:LYS:HE3	2.20	0.41
1:A:35:ARG:HH12	1:A:44:PRO:HB3	1.85	0.41
1:A:640:LEU:C	1:A:640:LEU:HD13	2.40	0.41
1:A:662:HIS:NE2	1:A:664:SER:OG	2.52	0.41
1:B:680:LEU:HD13	1:B:680:LEU:C	2.40	0.41
1:A:38:THR:OG1	1:A:73:HIS:ND1	2.49	0.41
1:A:26:GLN:HG3	1:A:30:MET:HE1	2.03	0.41
1:B:342:TYR:HA	5:B:940:HOH:O	2.20	0.41
1:A:38:THR:HG22	1:A:39:GLU:N	2.35	0.41
1:B:324:THR:HA	1:B:327:GLN:NE2	2.35	0.41
1:B:239:TYR:CZ	1:B:304:TYR:HB2	2.56	0.41
1:A:307:ASN:HD22	1:A:307:ASN:C	2.22	0.41
1:A:35:ARG:NH1	1:A:44:PRO:HB3	2.35	0.41
1:A:17:ILE:HG13	1:A:17:ILE:O	2.20	0.41
1:A:680:LEU:HD13	1:A:680:LEU:C	2.41	0.41
1:A:539:GLN:HG2	5:A:1058:HOH:O	2.20	0.41
1:A:39:GLU:C	1:A:40:ILE:HG13	2.41	0.41
1:A:681:LEU:C	1:A:681:LEU:HD13	2.41	0.41
1:A:239:TYR:CZ	1:A:304:TYR:HB2	2.56	0.41
1:A:427:LYS:HB3	1:A:430:ILE:HG23	2.02	0.41
1:B:211:HIS:HE1	5:B:1049:HOH:O	2.04	0.40
1:A:73:HIS:CB	1:A:85:LEU:HB2	2.48	0.40
1:B:695:LYS:HE3	5:B:1107:HOH:O	2.21	0.40
1:B:1:MET:CG	1:B:2:VAL:N	2.84	0.40
1:A:631:LEU:HD23	1:A:632:GLU:N	2.37	0.40
1:B:324:THR:O	1:B:328:HIS:HD2	2.03	0.40
1:B:681:LEU:HB2	1:B:709:TYR:CE2	2.57	0.40
1:B:218:TYR:CZ	1:B:567:SER:HA	2.56	0.40
1:A:115:THR:HB	1:A:159:LEU:HD12	2.03	0.40
1:B:678:TYR:O	1:B:693:GLU:HA	2.22	0.40
1:B:307:ASN:C	1:B:307:ASN:HD22	2.24	0.40
1:B:133:HIS:CB	1:B:136:LYS:HB2	2.49	0.40
1:B:629:ARG:NH2	1:B:647:ASP:OD1	2.45	0.40
1:B:120:TRP:CE2	1:B:382:MET:HG3	2.57	0.40
1:B:326:HIS:HE1	1:B:399:ASN:O	2.04	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	710/718 (99%)	683 (96%)	21 (3%)	6 (1%)	27	19
1	B	710/718 (99%)	685 (96%)	22 (3%)	3 (0%)	43	39
All	All	1420/1436 (99%)	1368 (96%)	43 (3%)	9 (1%)	33	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	696	LYS
1	B	696	LYS
1	A	25	GLU
1	A	649	ASP
1	B	2	VAL
1	A	272	PRO
1	A	711	ALA
1	B	272	PRO

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	608/615 (99%)	585 (96%)	23 (4%)	44	44
1	B	608/615 (99%)	586 (96%)	22 (4%)	47	47
All	All	1216/1230 (99%)	1171 (96%)	45 (4%)	45	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	25	GLU
1	A	85	LEU
1	A	97	ASP
1	A	207	LYS
1	A	257	LEU
1	A	307	ASN
1	A	362	GLU
1	A	404	ARG
1	A	408	LEU
1	A	419	MET
1	A	451	LEU
1	A	467	PHE
1	A	539	GLN
1	A	580	ASN
1	A	591	LEU
1	A	596	ARG
1	A	621	LEU
1	A	622	ARG
1	A	644	ARG
1	A	645	LEU
1	A	671	ARG
1	A	690	ASP
1	B	135	ASN
1	B	207	LYS
1	B	242	LEU
1	B	257	LEU
1	B	307	ASN
1	B	334	LEU
1	B	345	GLU
1	B	365	LYS
1	B	408	LEU
1	B	437	TRP
1	B	451	LEU
1	B	467	PHE
1	B	580	ASN
1	B	591	LEU
1	B	596	ARG
1	B	621	LEU
1	B	622	ARG
1	B	629	ARG
1	B	634	LEU
1	B	644	ARG

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Mol	Chain	Res	Type
1	B	645	LEU
1	B	671	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	133	HIS
1	A	135	ASN
1	A	160	HIS
1	A	171	ASN
1	A	180	GLN
1	A	199	GLN
1	A	211	HIS
1	A	221	HIS
1	A	230	ASN
1	A	248	GLN
1	A	307	ASN
1	A	309	HIS
1	A	312	GLN
1	A	327	GLN
1	A	339	ASN
1	A	340	HIS
1	A	374	ASN
1	A	445	HIS
1	A	496	HIS
1	A	516	GLN
1	A	527	HIS
1	A	549	GLN
1	A	580	ASN
1	A	583	GLN
1	A	628	GLN
1	A	661	HIS
1	B	26	GLN
1	B	73	HIS
1	B	133	HIS
1	B	142	GLN
1	B	160	HIS
1	B	171	ASN
1	B	180	GLN
1	B	211	HIS
1	B	221	HIS

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Mol	Chain	Res	Type
1	B	230	ASN
1	B	248	GLN
1	B	251	ASN
1	B	307	ASN
1	B	309	HIS
1	B	312	GLN
1	B	327	GLN
1	B	339	ASN
1	B	340	HIS
1	B	374	ASN
1	B	496	HIS
1	B	516	GLN
1	B	527	HIS
1	B	549	GLN
1	B	580	ASN
1	B	604	HIS
1	B	628	GLN
1	B	661	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	ACT	A	751	-	1,3,3	0.26	0	0,3,3	0.00	-
4	GOL	A	761	-	5,5,5	4.57	5 (100%)	5,5,5	5.77	3 (60%)
3	ACT	B	752	-	1,3,3	0.63	0	0,3,3	0.00	-
4	GOL	B	762	-	5,5,5	4.60	5 (100%)	5,5,5	5.76	3 (60%)

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
3	ACT	A	751	-	-	0/0/0/0	0/0/0/0
4	GOL	A	761	-	-	0/4/4/4	0/0/0/0
3	ACT	B	752	-	-	0/0/0/0	0/0/0/0
4	GOL	B	762	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	762	GOL	C3-C2	-7.76	1.20	1.52
4	A	761	GOL	C3-C2	-7.72	1.20	1.52
4	B	762	GOL	O1-C1	4.42	1.61	1.42
4	A	761	GOL	O1-C1	4.35	1.61	1.42
4	B	762	GOL	O3-C3	3.04	1.55	1.42
4	B	762	GOL	O2-C2	-3.01	1.34	1.43
4	A	761	GOL	C1-C2	-3.00	1.40	1.52
4	A	761	GOL	O3-C3	2.98	1.55	1.42
4	B	762	GOL	C1-C2	-2.82	1.40	1.52
4	A	761	GOL	O2-C2	-2.82	1.34	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	761	GOL	O3-C3-C2	10.54	161.16	109.71
4	B	762	GOL	O3-C3-C2	10.54	161.16	109.71
4	A	761	GOL	O2-C2-C3	6.64	138.45	108.22
4	B	762	GOL	O2-C2-C3	6.57	138.15	108.22
4	B	762	GOL	O1-C1-C2	3.31	125.87	109.71
4	A	761	GOL	O1-C1-C2	3.24	125.53	109.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	712/718 (99%)	-0.09	21 (2%)	49 53	15, 24, 47, 70	0
1	B	712/718 (99%)	-0.20	12 (1%)	67 71	13, 23, 42, 59	0
All	All	1424/1436 (99%)	-0.14	33 (2%)	57 62	13, 24, 44, 70	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.0
1	A	40	ILE	6.8
1	B	1	MET	5.0
1	A	39	GLU	4.6
1	A	650	GLU	4.4
1	A	135	ASN	4.2
1	A	25	GLU	3.9
1	B	40	ILE	3.8
1	A	54	GLU	3.8
1	B	506	ALA	3.7
1	A	506	ALA	3.5
1	B	54	GLU	3.3
1	B	689	GLU	3.2
1	A	43	PHE	3.0
1	A	53	LEU	3.0
1	B	649	ASP	2.9
1	B	650	GLU	2.9
1	B	476	PHE	2.7
1	A	24	ALA	2.7
1	A	476	PHE	2.6
1	A	689	GLU	2.6
1	A	29	ILE	2.5
1	A	55	ALA	2.4
1	A	41	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	690	ASP	2.4
1	B	606	ILE	2.3
1	B	690	ASP	2.3
1	B	41	THR	2.2
1	A	52	SER	2.2
1	A	137	SER	2.1
1	A	22	ILE	2.1
1	A	76	ARG	2.1
1	B	712	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	761	6/6	0.29	9.66	37,41,42,43	0
3	ACT	B	752	4/4	0.23	4.16	33,33,33,35	0
3	ACT	A	751	4/4	0.12	2.70	26,28,29,31	0
4	GOL	B	762	6/6	0.17	1.86	34,37,39,43	0
2	CA	A	741	1/1	0.12	0.51	19,19,19,19	0
2	CA	B	742	1/1	0.09	-1.05	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.