Worldwide PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2017 – 01:30 AM EDT

PDB ID	:	1PZ3
Title	:	Crystal structure of a family 51 (GH51) alpha-L-arabinofuranosidase from Geobacillus stearothermophilus T6
Authors	:	Hoevel, K.; Shallom, D.; Niefind, K.; Belakhov, V.; Shoham, G.; Baasov, T.; Shoham, Y.; Schomburg, D.
Deposited on	:	unknown
Resolution	:	1.75 Å(reported)

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

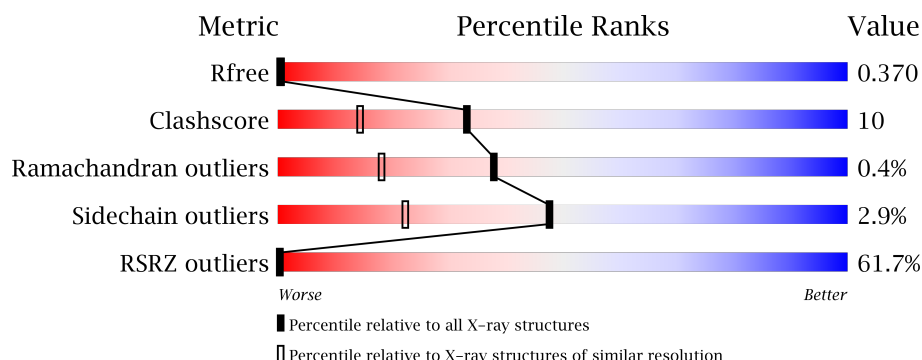|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	Percentile Ranks	Value
Rfree		0.370
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		2.9%
RSRZ outliers		61.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	502	66%　81%　16% ··
1	B	502	56%　83%　15% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9136 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 Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3990	2542	680	748	20			
1	B	497	Total	C	N	O	S	0	0	0
			3990	2542	680	748	20			

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	583	Total 583	O 583	0	0
3	B	561	Total 561	O 561	0	0

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 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: Alpha-L-arabinofuranosidase
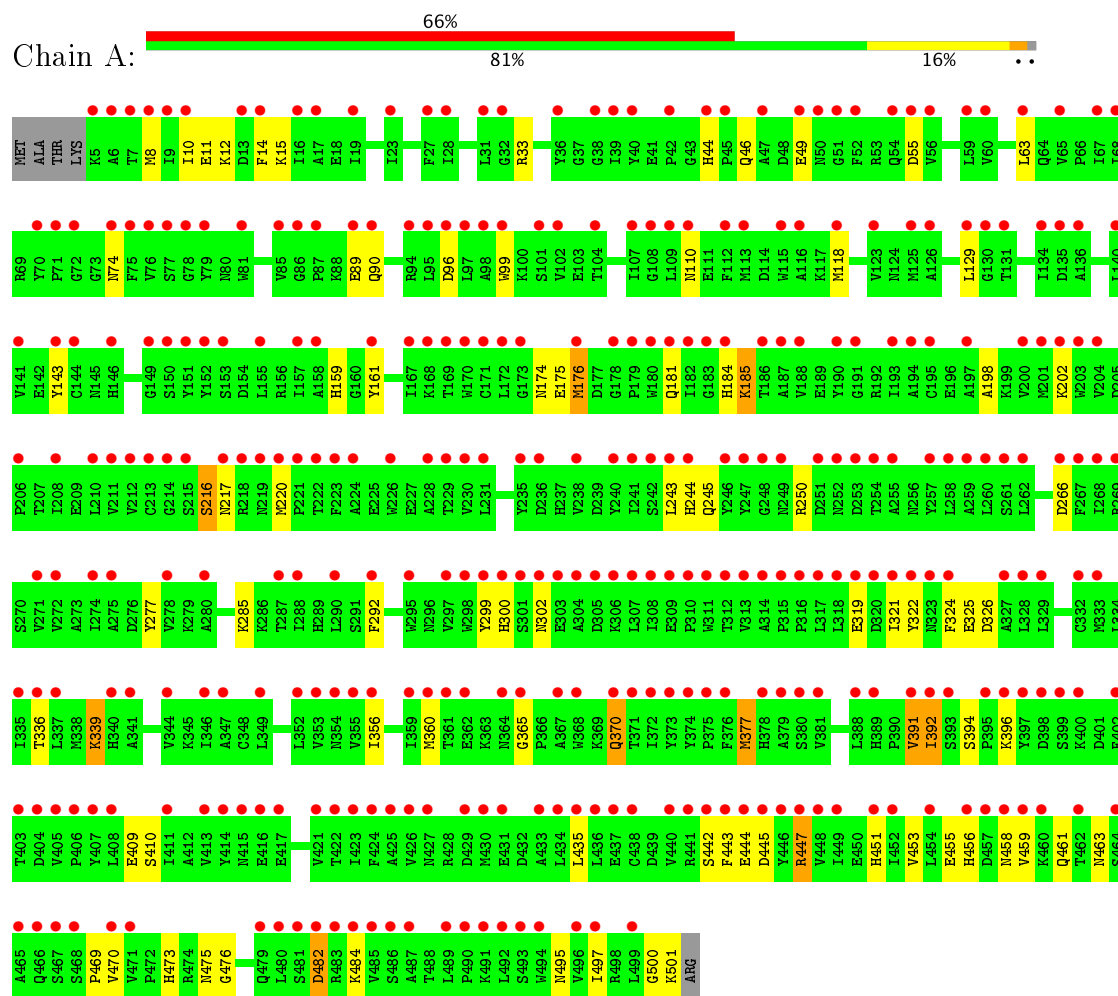
- Molecule 1: Alpha-L-arabinofuranosidase
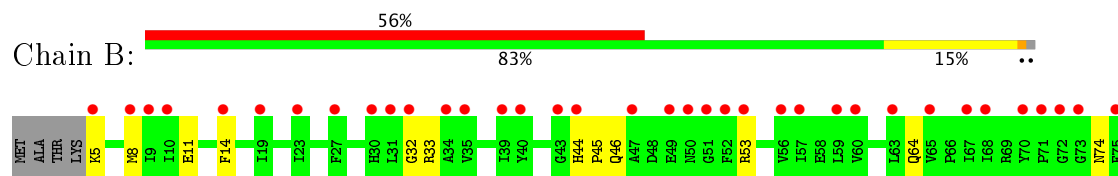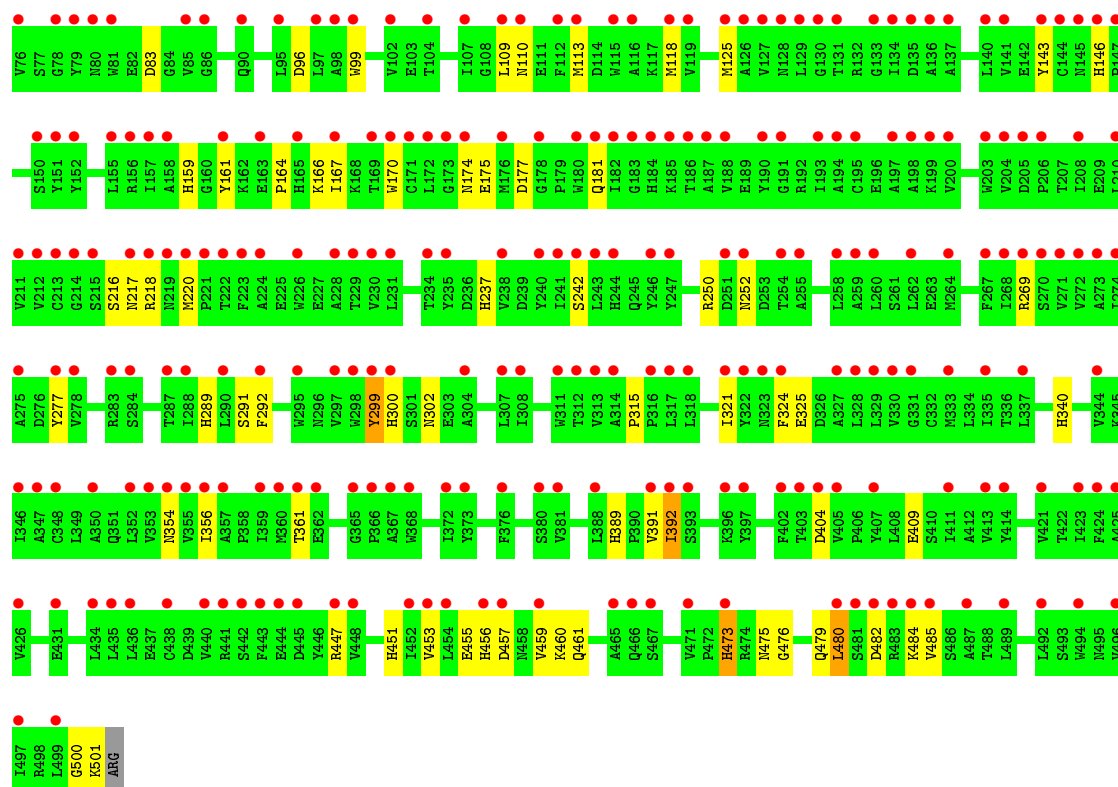
4   Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	179.43Å 179.43Å 100.23Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 120.00°	
Resolution (Å)	20.00 – 1.75	Depositor
	19.96 – 1.75	EDS
% Data completeness	(Not available) (20.00-1.75)	Depositor
(in resolution range)	98.3 (19.96-1.75)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 1.74Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.204	Depositor
	0.364 , 0.370	DCC
R_{free} test set	5990 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 66.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9136	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 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.66	0/4091	0.84	8/5558 (0.1%)
1	B	0.63	0/4091	0.83	7/5558 (0.1%)
All	All	0.64	0/8182	0.84	15/11116 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	33	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	33	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	457	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	177	ASP	CB-CG-OD2	6.98	124.58	118.30
1	A	33	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	96	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	83	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	266	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	404	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	377	MET	CG-SD-CE	-5.15	91.96	100.20
1	A	185	LYS	CD-CE-NZ	-5.14	99.87	111.70
1	A	55	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	96	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	482	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3891	86	0
1	B	3990	0	3891	71	0
2	A	6	0	8	3	0
2	B	6	0	8	2	0
3	A	583	0	0	28	4
3	B	561	0	0	26	3
All	All	9136	0	7798	155	4

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 10.

All (155) 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:319:GLU:CD	3:A:1038:HOH:O	1.67	1.24
1:B:392:ILE:HG21	3:B:1027:HOH:O	1.52	1.09
1:B:118:MET:CG	3:B:1026:HOH:O	2.06	1.03
1:B:118:MET:SD	3:B:1026:HOH:O	2.15	1.01
1:B:118:MET:HG3	3:B:1026:HOH:O	1.59	1.00
1:A:244:HIS:HE1	3:A:1069:HOH:O	1.45	1.00
1:B:175:GLU:OE1	3:B:959:HOH:O	1.83	0.96
1:A:451:HIS:CD2	1:A:497:ILE:HG12	2.01	0.94
1:A:319:GLU:OE1	3:A:1038:HOH:O	1.75	0.93
1:B:354:ASN:HD21	1:B:361:THR:H	1.22	0.88
1:A:244:HIS:CE1	3:A:1069:HOH:O	2.21	0.86
1:A:220:MET:SD	3:A:997:HOH:O	2.35	0.85
1:A:451:HIS:HD2	1:A:497:ILE:HG12	1.40	0.83
1:A:44:HIS:HD2	1:A:46:GLN:H	1.29	0.80
1:A:14:PHE:CZ	1:B:391:VAL:HG21	2.15	0.80
1:A:451:HIS:ND1	1:A:476:GLY:HA3	1.96	0.79
1:B:175:GLU:HG3	1:B:216:SER:HB3	1.63	0.78
1:A:451:HIS:CE1	1:A:495:ASN:HD22	2.03	0.77
1:A:463:ASN:HD21	1:A:470:VAL:H	1.34	0.75
1:A:220:MET:HE1	3:A:1079:HOH:O	1.85	0.74
1:A:175:GLU:CG	1:A:216:SER:HB3	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:SER:OG	3:B:1017:HOH:O	2.06	0.73
1:B:480:LEU:HD22	1:B:485:VAL:HG22	1.70	0.73
1:A:220:MET:SD	3:A:1079:HOH:O	2.46	0.73
1:B:166:LYS:HG2	3:B:789:HOH:O	1.89	0.71
1:B:11:GLU:HG2	1:B:14:PHE:HD1	1.54	0.70
1:A:220:MET:CE	3:A:1079:HOH:O	2.37	0.70
1:A:250:ARG:HH21	1:A:302:ASN:HD21	1.36	0.70
1:A:143:TYR:OH	1:A:159:HIS:HD2	1.75	0.70
1:B:175:GLU:CG	1:B:216:SER:HB3	2.22	0.69
1:B:456:HIS:CE1	1:B:461:GLN:HG2	2.29	0.68
1:B:220:MET:SD	3:B:1017:HOH:O	2.52	0.68
1:B:300:HIS:HD2	1:B:321:ILE:O	1.77	0.67
1:A:175:GLU:OE1	3:A:793:HOH:O	2.12	0.67
2:B:503:GOL:H2	3:B:505:HOH:O	1.94	0.66
1:A:451:HIS:HE1	1:A:495:ASN:HD22	1.41	0.66
1:A:14:PHE:CE2	1:B:391:VAL:HG21	2.30	0.65
1:B:456:HIS:HE1	1:B:461:GLN:HG2	1.63	0.64
1:A:184:HIS:HE1	3:A:676:HOH:O	1.81	0.64
1:B:250:ARG:HH21	1:B:302:ASN:HD21	1.45	0.63
1:A:360:MET:CE	3:A:669:HOH:O	2.47	0.63
1:A:44:HIS:CD2	1:A:46:GLN:H	2.16	0.63
1:B:11:GLU:CG	1:B:14:PHE:HD1	2.12	0.63
2:A:503:GOL:H2	3:A:546:HOH:O	1.98	0.62
1:A:300:HIS:HE1	1:A:326:ASP:OD2	1.82	0.62
1:B:299:TYR:CE1	1:B:300:HIS:CE1	2.88	0.61
1:B:217:ASN:CB	3:B:1017:HOH:O	2.48	0.61
1:A:360:MET:HE2	3:A:669:HOH:O	2.00	0.60
1:B:389:HIS:HD2	3:B:803:HOH:O	1.83	0.59
1:B:44:HIS:ND1	1:B:45:PRO:HD2	2.18	0.59
1:A:391:VAL:HB	1:B:14:PHE:CZ	2.37	0.59
1:A:473:HIS:HD2	1:A:475:ASN:H	1.50	0.58
1:B:174:ASN:HD22	1:B:181:GLN:HE22	1.51	0.58
1:B:143:TYR:OH	1:B:159:HIS:HD2	1.87	0.57
1:B:8:MET:HG3	1:B:392:ILE:HG22	1.87	0.57
1:B:500:GLY:O	1:B:501:LYS:HB2	2.04	0.57
1:B:300:HIS:CD2	1:B:321:ILE:O	2.57	0.57
1:B:64:GLN:NE2	3:B:600:HOH:O	2.38	0.57
1:B:11:GLU:HG2	1:B:14:PHE:CD1	2.39	0.56
1:B:146:HIS:HD2	3:B:611:HOH:O	1.88	0.56
1:B:299:TYR:CZ	1:B:300:HIS:CE1	2.94	0.56
1:A:10:ILE:O	1:A:442:SER:OG	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:CD	1:A:216:SER:HB3	2.26	0.55
1:A:300:HIS:HD2	3:A:656:HOH:O	1.89	0.55
1:A:49:GLU:HG2	3:A:768:HOH:O	2.05	0.55
1:A:175:GLU:HG2	1:A:216:SER:HB3	1.87	0.55
1:B:217:ASN:HB3	3:B:1017:HOH:O	2.06	0.54
1:A:12:LYS:O	1:A:15:LYS:NZ	2.30	0.54
1:B:174:ASN:HD22	1:B:181:GLN:NE2	2.05	0.54
1:B:167:ILE:HB	1:B:170:TRP:CZ2	2.43	0.54
1:A:325:GLU:HB3	1:A:459:VAL:HB	1.90	0.54
1:B:480:LEU:HD22	1:B:485:VAL:CG2	2.36	0.53
1:A:216:SER:HB2	3:A:997:HOH:O	2.07	0.53
1:B:164:PRO:HG2	1:B:166:LYS:HE2	1.88	0.53
1:A:74:ASN:HA	1:A:181:GLN:HE22	1.73	0.53
1:A:174:ASN:HD22	1:A:181:GLN:NE2	2.07	0.53
1:A:129:LEU:O	1:A:185:LYS:HE3	2.09	0.52
1:A:410:SER:HB3	3:A:1086:HOH:O	2.09	0.52
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.56	0.52
1:B:74:ASN:HA	1:B:181:GLN:HE22	1.75	0.52
1:B:456:HIS:HD2	3:B:921:HOH:O	1.92	0.52
1:A:14:PHE:CE2	1:B:391:VAL:CG2	2.93	0.52
1:A:198:ALA:O	1:A:202:LYS:HE3	2.10	0.51
1:B:354:ASN:ND2	1:B:361:THR:H	2.00	0.51
1:A:217:ASN:ND2	3:A:997:HOH:O	2.43	0.51
1:A:435:LEU:HD22	1:A:435:LEU:N	2.25	0.51
1:A:99:TRP:CH2	2:A:503:GOL:H31	2.45	0.51
1:A:89:GLU:HG2	1:A:90:GLN:NE2	2.25	0.51
1:A:456:HIS:CE1	1:A:461:GLN:HG2	2.46	0.51
1:B:409:GLU:OE1	3:B:1025:HOH:O	2.19	0.50
1:A:11:GLU:CG	1:A:14:PHE:HD1	2.24	0.50
1:A:216:SER:CB	3:A:997:HOH:O	2.59	0.50
1:A:391:VAL:O	1:A:391:VAL:HG12	2.12	0.50
1:B:453:VAL:HB	1:B:473:HIS:CD2	2.47	0.50
1:A:159:HIS:HE1	3:A:574:HOH:O	1.94	0.50
1:B:389:HIS:CD2	3:B:803:HOH:O	2.61	0.49
1:B:44:HIS:CD2	1:B:53:ARG:CZ	2.95	0.49
1:A:322:TYR:H	1:A:370:GLN:HE22	1.61	0.49
1:A:220:MET:CG	3:A:997:HOH:O	2.57	0.49
1:A:322:TYR:H	1:A:370:GLN:NE2	2.11	0.49
1:A:455:GLU:OE2	1:A:473:HIS:HE1	1.96	0.48
1:B:269:ARG:HG3	1:B:340:HIS:HE1	1.78	0.48
1:B:218:ARG:O	3:B:1018:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:CE1	1:A:453:VAL:HG22	2.49	0.48
1:A:44:HIS:HE1	1:A:365:GLY:O	1.95	0.48
1:B:109:LEU:O	1:B:113:MET:HG2	2.13	0.48
1:B:125:MET:HB3	1:B:170:TRP:CE3	2.49	0.48
1:B:325:GLU:HB3	1:B:459:VAL:HB	1.96	0.48
1:A:447:ARG:HD2	3:A:1042:HOH:O	2.14	0.48
1:B:217:ASN:HB2	3:B:1017:HOH:O	2.13	0.48
1:A:482:ASP:OD1	3:A:955:HOH:O	2.20	0.47
1:A:110:ASN:HB3	1:A:161:TYR:CZ	2.50	0.47
1:B:125:MET:HG2	1:B:170:TRP:CZ3	2.50	0.47
1:B:32:GLY:HA2	1:B:315:PRO:O	2.15	0.47
1:A:324:PHE:CZ	1:A:455:GLU:HA	2.50	0.46
1:A:339:LYS:HE3	1:A:409:GLU:OE2	2.15	0.46
1:A:245:GLN:NE2	3:A:685:HOH:O	2.48	0.46
1:A:11:GLU:HG2	1:A:14:PHE:HD1	1.81	0.46
1:B:299:TYR:CE1	1:B:300:HIS:HE1	2.33	0.46
1:B:242:SER:HA	1:B:291:SER:O	2.17	0.45
1:A:336:THR:HA	1:A:339:LYS:HG2	1.98	0.45
1:B:453:VAL:HB	1:B:473:HIS:NE2	2.31	0.45
1:A:339:LYS:HD2	3:A:993:HOH:O	2.17	0.45
1:B:159:HIS:HE1	3:B:612:HOH:O	2.00	0.45
1:B:99:TRP:CH2	2:B:503:GOL:H31	2.52	0.44
1:B:252:ASN:HD21	1:B:460:LYS:HE3	1.81	0.43
1:A:463:ASN:ND2	1:A:470:VAL:H	2.10	0.43
1:A:456:HIS:HE1	1:A:469:PRO:HB2	1.83	0.43
1:A:11:GLU:HG2	1:A:14:PHE:CD1	2.54	0.43
1:A:484:LYS:NZ	1:A:484:LYS:HB2	2.33	0.43
1:A:321:ILE:HA	1:A:370:GLN:HE22	1.84	0.43
1:B:220:MET:CG	3:B:1017:HOH:O	2.66	0.42
1:A:63:LEU:HD23	1:A:377:MET:HG3	2.02	0.42
1:B:146:HIS:HE1	3:B:687:HOH:O	2.02	0.42
1:B:473:HIS:CE1	3:B:988:HOH:O	2.72	0.42
1:A:392:ILE:CD1	1:A:394:SER:HB3	2.49	0.42
1:A:10:ILE:HG22	1:A:443:PHE:CE1	2.55	0.42
1:A:500:GLY:O	1:A:501:LYS:HB2	2.20	0.42
1:B:110:ASN:HB3	1:B:161:TYR:CZ	2.55	0.42
1:A:243:LEU:N	1:A:243:LEU:HD12	2.35	0.42
1:B:289:HIS:HE1	3:B:839:HOH:O	2.03	0.42
1:B:237:HIS:HD2	3:B:867:HOH:O	2.03	0.41
1:B:479:GLN:NE2	3:B:820:HOH:O	2.53	0.41
1:A:456:HIS:HD2	1:A:458:ASN:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:HIS:CE1	1:B:475:ASN:HB2	2.56	0.41
1:A:220:MET:HB3	1:A:220:MET:HE2	1.85	0.41
1:A:447:ARG:NE	3:A:1018:HOH:O	2.53	0.41
1:A:99:TRP:CZ2	2:A:503:GOL:H31	2.56	0.41
1:A:175:GLU:HB2	3:A:1069:HOH:O	2.20	0.41
1:A:10:ILE:HG22	1:A:443:PHE:HE1	1.86	0.41
1:A:176:MET:O	1:A:184:HIS:HD2	2.04	0.41
1:B:324:PHE:CZ	1:B:455:GLU:HA	2.55	0.40
1:B:451:HIS:CG	1:B:476:GLY:HA3	2.57	0.40
1:A:10:ILE:HA	3:A:834:HOH:O	2.22	0.40
1:A:11:GLU:HA	1:A:442:SER:HG	1.87	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:763:HOH:O	3:B:511:HOH:O[6_554]	2.07	0.13
3:A:1063:HOH:O	3:B:992:HOH:O[1_554]	2.13	0.07
3:A:1041:HOH:O	3:B:688:HOH:O[1_554]	2.16	0.04
3:A:507:HOH:O	3:A:564:HOH:O[2_655]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/502 (99%)	471 (95%)	22 (4%)	2 (0%)	38	18
1	B	495/502 (99%)	477 (96%)	16 (3%)	2 (0%)	38	18
All	All	990/1004 (99%)	948 (96%)	38 (4%)	4 (0%)	38	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	TYR
1	B	299	TYR
1	A	356	ILE
1	B	356	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/434 (99%)	415 (96%)	15 (4%)	41	16
1	B	430/434 (99%)	420 (98%)	10 (2%)	56	31
All	All	860/868 (99%)	835 (97%)	25 (3%)	48	22

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	118	MET
1	A	176	MET
1	A	216	SER
1	A	277	TYR
1	A	285	LYS
1	A	292	PHE
1	A	339	LYS
1	A	370	GLN
1	A	391	VAL
1	A	392	ILE
1	A	396	LYS
1	A	444	GLU
1	A	445	ASP
1	A	447	ARG
1	B	5	LYS
1	B	46	GLN
1	B	277	TYR
1	B	292	PHE
1	B	392	ILE

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Mol	Chain	Res	Type
1	B	447	ARG
1	B	473	HIS
1	B	480	LEU
1	B	482	ASP
1	B	484	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	64	GLN
1	A	159	HIS
1	A	181	GLN
1	A	184	HIS
1	A	219	ASN
1	A	237	HIS
1	A	245	GLN
1	A	300	HIS
1	A	302	ASN
1	A	370	GLN
1	A	451	HIS
1	A	456	HIS
1	A	463	ASN
1	A	473	HIS
1	A	495	ASN
1	B	64	GLN
1	B	146	HIS
1	B	159	HIS
1	B	181	GLN
1	B	252	ASN
1	B	289	HIS
1	B	300	HIS
1	B	302	ASN
1	B	354	ASN
1	B	461	GLN
1	B	475	ASN
1	B	479	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	GOL	A	503	-	5,5,5	0.67	0	5,5,5	0.96	1 (20%)
2	GOL	B	503	-	5,5,5	0.64	0	5,5,5	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	503	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	GOL	O2-C2-C1	2.06	118.55	108.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	3	0
2	B	503	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	497/502 (99%)	2.61	331 (66%)	0	0	13, 23, 40, 56	0
1	B	497/502 (99%)	2.32	282 (56%)	0	0	16, 23, 37, 47	0
All	All	994/1004 (99%)	2.47	613 (61%)	0	0	13, 23, 39, 56	0

All (613) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	10.6
1	A	252	ASN	7.8
1	A	457	ASP	7.5
1	A	251	ASP	7.3
1	A	441	ARG	7.2
1	A	435	LEU	7.1
1	B	170	TRP	6.9
1	A	402	PHE	6.5
1	A	180	TRP	6.3
1	A	241	ILE	6.1
1	B	312	THR	6.0
1	A	10	ILE	5.9
1	A	482	ASP	5.9
1	A	440	VAL	5.8
1	A	151	TYR	5.8
1	B	217	ASN	5.6
1	A	115	TRP	5.6
1	B	180	TRP	5.5
1	B	440	VAL	5.5
1	A	308	ILE	5.5
1	B	212	VAL	5.5
1	B	311	TRP	5.4
1	A	479	GLN	5.4
1	A	212	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	482	ASP	5.2
1	B	438	CYS	5.2
1	B	241	ILE	5.1
1	B	43	GLY	5.1
1	A	200	VAL	5.1
1	B	481	SER	5.0
1	A	444	GLU	5.0
1	A	313	VAL	5.0
1	A	314	ALA	4.9
1	A	423	ILE	4.9
1	A	393	SER	4.9
1	A	445	ASP	4.8
1	A	485	VAL	4.8
1	A	95	LEU	4.7
1	A	448	VAL	4.7
1	B	141	VAL	4.7
1	A	442	SER	4.7
1	B	308	ILE	4.7
1	A	443	PHE	4.7
1	B	172	LEU	4.7
1	B	203	TRP	4.6
1	A	327	ALA	4.6
1	A	112	PHE	4.6
1	B	307	LEU	4.5
1	A	421	VAL	4.5
1	B	213	CYS	4.5
1	A	173	GLY	4.4
1	A	99	TRP	4.4
1	B	220	MET	4.4
1	B	480	LEU	4.3
1	A	426	VAL	4.3
1	A	136	ALA	4.3
1	B	129	LEU	4.3
1	B	317	LEU	4.3
1	B	81	TRP	4.3
1	A	267	PHE	4.3
1	B	51	GLY	4.3
1	A	407	TYR	4.3
1	A	332	CYS	4.2
1	A	411	ILE	4.2
1	A	97	LEU	4.2
1	A	436	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	492	LEU	4.2
1	A	288	ILE	4.2
1	A	329	LEU	4.2
1	A	403	THR	4.2
1	A	157	ILE	4.2
1	B	443	PHE	4.2
1	A	70	TYR	4.2
1	A	413	VAL	4.2
1	B	31	LEU	4.1
1	B	444	GLU	4.1
1	A	346	ILE	4.1
1	A	438	CYS	4.1
1	A	311	TRP	4.1
1	A	28	ILE	4.1
1	A	75	PHE	4.1
1	A	242	SER	4.1
1	B	321	ILE	4.0
1	A	220	MET	4.0
1	B	214	GLY	4.0
1	A	39	ILE	4.0
1	A	480	LEU	4.0
1	B	95	LEU	4.0
1	A	257	TYR	4.0
1	A	188	VAL	4.0
1	A	204	VAL	4.0
1	B	76	VAL	4.0
1	B	292	PHE	4.0
1	A	247	TYR	3.9
1	A	213	CYS	3.9
1	A	454	LEU	3.9
1	B	267	PHE	3.9
1	A	36	TYR	3.9
1	A	42	PRO	3.9
1	A	459	VAL	3.9
1	B	413	VAL	3.9
1	B	403	THR	3.9
1	A	31	LEU	3.9
1	A	143	TYR	3.9
1	A	376	PHE	3.9
1	B	109	LEU	3.8
1	A	259	ALA	3.8
1	A	268	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	408	LEU	3.8
1	B	456	HIS	3.8
1	A	218	ARG	3.8
1	B	10	ILE	3.8
1	B	39	ILE	3.8
1	B	359	ILE	3.8
1	A	492	LEU	3.8
1	B	243	LEU	3.8
1	A	312	THR	3.8
1	A	471	VAL	3.8
1	A	255	ALA	3.8
1	A	352	LEU	3.8
1	A	72	GLY	3.7
1	B	157	ILE	3.7
1	A	172	LEU	3.7
1	B	258	LEU	3.7
1	A	27	PHE	3.7
1	B	9	ILE	3.7
1	A	483	ARG	3.7
1	B	144	CYS	3.7
1	A	486	SER	3.7
1	A	328	LEU	3.7
1	A	68	ILE	3.7
1	A	243	LEU	3.7
1	A	333	MET	3.7
1	A	367	ALA	3.6
1	B	314	ALA	3.6
1	A	52	PHE	3.6
1	A	150	SER	3.6
1	A	317	LEU	3.6
1	B	313	VAL	3.6
1	B	173	GLY	3.6
1	B	151	TYR	3.6
1	A	59	LEU	3.6
1	B	107	ILE	3.6
1	B	178	GLY	3.6
1	B	288	ILE	3.6
1	A	405	VAL	3.6
1	B	271	VAL	3.6
1	B	466	GLN	3.6
1	A	406	PRO	3.6
1	A	322	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	63	LEU	3.6
1	A	102	VAL	3.6
1	A	223	PHE	3.6
1	B	60	VAL	3.6
1	B	204	VAL	3.6
1	A	187	ALA	3.6
1	B	322	TYR	3.6
1	A	290	LEU	3.6
1	A	434	LEU	3.6
1	A	497	ILE	3.6
1	B	200	VAL	3.6
1	B	346	ILE	3.6
1	B	423	ILE	3.6
1	B	136	ALA	3.5
1	B	78	GLY	3.5
1	B	473	HIS	3.5
1	B	99	TRP	3.5
1	A	304	ALA	3.5
1	A	318	LEU	3.5
1	A	9	ILE	3.5
1	A	141	VAL	3.5
1	A	344	VAL	3.5
1	A	470	VAL	3.5
1	B	195	CYS	3.5
1	B	348	CYS	3.5
1	B	404	ASP	3.5
1	B	275	ALA	3.5
1	A	258	LEU	3.5
1	B	388	LEU	3.5
1	A	230	VAL	3.5
1	B	167	ILE	3.5
1	B	14	PHE	3.5
1	B	112	PHE	3.5
1	B	50	ASN	3.5
1	B	240	TYR	3.5
1	A	262	LEU	3.5
1	B	337	LEU	3.5
1	A	496	VAL	3.5
1	B	208	ILE	3.5
1	B	283	ARG	3.5
1	B	424	PHE	3.5
1	B	445	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	275	ALA	3.5
1	A	210	LEU	3.4
1	A	217	ASN	3.4
1	B	226	TRP	3.4
1	A	466	GLN	3.4
1	B	467	SER	3.4
1	B	52	PHE	3.4
1	B	397	TYR	3.4
1	A	489	LEU	3.4
1	B	459	VAL	3.4
1	A	193	ILE	3.4
1	A	295	TRP	3.4
1	A	494	TRP	3.4
1	B	75	PHE	3.4
1	A	315	PRO	3.4
1	B	431	GLU	3.4
1	A	140	LEU	3.4
1	B	246	TYR	3.4
1	B	435	LEU	3.4
1	B	116	ALA	3.4
1	B	234	THR	3.4
1	A	17	ALA	3.4
1	A	155	LEU	3.4
1	A	161	TYR	3.4
1	B	344	VAL	3.4
1	B	421	VAL	3.4
1	A	229	THR	3.4
1	A	81	TRP	3.4
1	A	272	VAL	3.3
1	A	355	VAL	3.3
1	B	210	LEU	3.3
1	A	417	GLU	3.3
1	A	336	THR	3.3
1	B	483	ARG	3.3
1	A	431	GLU	3.3
1	A	298	TRP	3.3
1	A	60	VAL	3.3
1	A	499	LEU	3.3
1	B	85	VAL	3.3
1	B	278	VAL	3.3
1	A	359	ILE	3.3
1	B	368	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	462	THR	3.3
1	B	182	ILE	3.3
1	A	365	GLY	3.3
1	B	436	LEU	3.3
1	A	208	ILE	3.3
1	A	356	ILE	3.3
1	B	19	ILE	3.3
1	B	23	ILE	3.3
1	B	72	GLY	3.3
1	A	399	SER	3.2
1	A	468	SER	3.2
1	A	56	VAL	3.2
1	B	158	ALA	3.2
1	A	184	HIS	3.2
1	B	146	HIS	3.2
1	A	182	ILE	3.2
1	A	429	ASP	3.2
1	A	146	HIS	3.2
1	B	489	LEU	3.2
1	B	494	TRP	3.2
1	B	367	ALA	3.2
1	B	231	LEU	3.2
1	A	14	PHE	3.2
1	B	376	PHE	3.2
1	A	78	GLY	3.2
1	A	481	SER	3.2
1	B	269	ARG	3.1
1	A	108	GLY	3.1
1	A	397	TYR	3.1
1	B	70	TYR	3.1
1	B	299	TYR	3.1
1	A	215	SER	3.1
1	B	188	VAL	3.1
1	A	158	ALA	3.1
1	A	379	ALA	3.1
1	B	40	TYR	3.1
1	B	143	TYR	3.1
1	B	49	GLU	3.1
1	B	224	ALA	3.1
1	B	223	PHE	3.1
1	B	130	GLY	3.1
1	B	255	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	251	ASP	3.0
1	B	57	ILE	3.0
1	A	425	ALA	3.0
1	A	404	ASP	3.0
1	B	230	VAL	3.0
1	A	449	ILE	3.0
1	B	335	ILE	3.0
1	B	218	ARG	3.0
1	A	278	VAL	3.0
1	B	65	VAL	3.0
1	B	155	LEU	3.0
1	B	328	LEU	3.0
1	B	471	VAL	3.0
1	B	152	TYR	3.0
1	B	235	TYR	3.0
1	B	392	ILE	3.0
1	B	402	PHE	3.0
1	A	430	MET	3.0
1	B	113	MET	3.0
1	A	269	ARG	3.0
1	B	252	ASN	3.0
1	A	372	ILE	3.0
1	B	71	PRO	3.0
1	B	206	PRO	3.0
1	A	76	VAL	3.0
1	A	349	LEU	3.0
1	B	119	VAL	3.0
1	A	360	MET	2.9
1	B	228	ALA	2.9
1	A	107	ILE	2.9
1	B	268	ILE	2.9
1	B	171	CYS	2.9
1	B	44	HIS	2.9
1	A	337	LEU	2.9
1	A	222	THR	2.9
1	B	300	HIS	2.9
1	A	19	ILE	2.9
1	B	161	TYR	2.9
1	A	130	GLY	2.9
1	A	123	VAL	2.9
1	A	271	VAL	2.9
1	B	290	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	381	VAL	2.9
1	A	395	PRO	2.9
1	A	274	ILE	2.9
1	A	335	ILE	2.9
1	B	356	ILE	2.9
1	A	190	TYR	2.9
1	A	7	THR	2.9
1	A	144	CYS	2.9
1	B	287	THR	2.9
1	A	226	TRP	2.9
1	B	353	VAL	2.9
1	B	150	SER	2.9
1	A	219	ASN	2.9
1	B	131	THR	2.9
1	B	357	ALA	2.9
1	B	487	ALA	2.9
1	B	27	PHE	2.8
1	A	5	LYS	2.8
1	A	63	LEU	2.8
1	A	353	VAL	2.8
1	A	8	MET	2.8
1	B	186	THR	2.8
1	A	452	ILE	2.8
1	A	299	TYR	2.8
1	B	215	SER	2.8
1	A	85	VAL	2.8
1	A	324	PHE	2.8
1	B	219	ASN	2.8
1	A	244	HIS	2.8
1	A	49	GLU	2.8
1	A	96	ASP	2.8
1	A	260	LEU	2.8
1	A	176	MET	2.8
1	B	284	SER	2.8
1	A	51	GLY	2.8
1	A	86	GLY	2.8
1	B	86	GLY	2.8
1	B	191	GLY	2.8
1	B	457	ASP	2.8
1	A	302	ASN	2.8
1	B	333	MET	2.8
1	A	388	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	396	LYS	2.8
1	B	352	LEU	2.8
1	A	261	SER	2.8
1	B	32	GLY	2.8
1	A	47	ALA	2.8
1	A	300	HIS	2.8
1	B	145	ASN	2.8
1	A	297	VAL	2.7
1	B	59	LEU	2.7
1	A	38	GLY	2.7
1	B	193	ILE	2.7
1	A	309	GLU	2.7
1	A	246	TYR	2.7
1	A	446	TYR	2.7
1	B	190	TYR	2.7
1	B	318	LEU	2.7
1	A	266	ASP	2.7
1	B	30	HIS	2.7
1	A	287	THR	2.7
1	A	67	ILE	2.7
1	A	135	ASP	2.7
1	A	197	ALA	2.7
1	B	221	PRO	2.7
1	A	374	TYR	2.7
1	B	407	TYR	2.7
1	B	97	LEU	2.7
1	B	441	ARG	2.7
1	B	80	ASN	2.7
1	A	167	ILE	2.7
1	A	248	GLY	2.7
1	B	448	VAL	2.7
1	A	153	SER	2.7
1	B	393	SER	2.7
1	A	447	ARG	2.6
1	A	183	GLY	2.6
1	A	13	ASP	2.6
1	B	360	MET	2.6
1	A	238	VAL	2.6
1	B	414	TYR	2.6
1	B	454	LEU	2.6
1	A	206	PRO	2.6
1	B	372	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	240	TYR	2.6
1	A	203	TRP	2.6
1	B	125	MET	2.6
1	A	71	PRO	2.6
1	A	321	ILE	2.6
1	B	163	GLU	2.6
1	A	211	VAL	2.6
1	B	238	VAL	2.6
1	B	391	VAL	2.6
1	B	79	TYR	2.6
1	B	184	HIS	2.6
1	A	464	SER	2.6
1	B	316	PRO	2.6
1	B	447	ARG	2.6
1	B	134	ILE	2.6
1	A	253	ASP	2.6
1	A	44	HIS	2.6
1	A	170	TRP	2.5
1	B	68	ILE	2.5
1	B	453	VAL	2.5
1	A	40	TYR	2.5
1	B	373	TYR	2.5
1	A	169	THR	2.5
1	A	292	PHE	2.5
1	B	298	TRP	2.5
1	A	149	GLY	2.5
1	B	411	ILE	2.5
1	A	65	VAL	2.5
1	A	235	TYR	2.5
1	A	362	GLU	2.5
1	A	101	SER	2.5
1	A	224	ALA	2.5
1	B	137	ALA	2.5
1	B	273	ALA	2.5
1	A	179	PRO	2.5
1	A	104	THR	2.5
1	A	371	THR	2.5
1	B	329	LEU	2.5
1	A	320	ASP	2.5
1	B	362	GLU	2.5
1	A	194	ALA	2.5
1	A	228	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	90	GLN	2.5
1	A	458	ASN	2.5
1	B	323	ASN	2.5
1	B	354	ASN	2.5
1	B	222	THR	2.5
1	A	380	SER	2.5
1	A	493	SER	2.5
1	A	424	PHE	2.5
1	A	89	GLU	2.5
1	B	355	VAL	2.5
1	B	115	TRP	2.5
1	A	98	ALA	2.4
1	A	487	ALA	2.4
1	A	378	HIS	2.4
1	A	456	HIS	2.4
1	B	361	THR	2.4
1	A	195	CYS	2.4
1	B	183	GLY	2.4
1	A	316	PRO	2.4
1	B	434	LEU	2.4
1	A	319	GLU	2.4
1	B	90	GLN	2.4
1	B	176	MET	2.4
1	B	485	VAL	2.4
1	A	134	ILE	2.4
1	A	465	ALA	2.4
1	B	497	ILE	2.4
1	A	254	THR	2.4
1	A	416	GLU	2.4
1	B	254	THR	2.4
1	A	50	ASN	2.4
1	A	310	PRO	2.4
1	A	340	HIS	2.4
1	A	113	MET	2.4
1	A	118	MET	2.4
1	B	242	SER	2.4
1	A	116	ALA	2.4
1	B	347	ALA	2.4
1	A	400	LYS	2.4
1	B	426	VAL	2.4
1	A	231	LEU	2.4
1	B	169	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	370	GLN	2.4
1	A	202	LYS	2.4
1	B	187	ALA	2.4
1	B	127	VAL	2.3
1	B	405	VAL	2.3
1	B	260	LEU	2.3
1	B	499	LEU	2.3
1	B	118	MET	2.3
1	B	350	ALA	2.3
1	B	104	THR	2.3
1	A	323	ASN	2.3
1	A	354	ASN	2.3
1	A	398	ASP	2.3
1	A	23	ILE	2.3
1	A	392	ILE	2.3
1	A	168	LYS	2.3
1	B	47	ALA	2.3
1	B	465	ALA	2.3
1	B	229	THR	2.3
1	B	174	ASN	2.3
1	A	201	MET	2.3
1	B	297	VAL	2.3
1	B	452	ILE	2.3
1	A	341	ALA	2.3
1	A	490	PRO	2.3
1	A	77	SER	2.3
1	B	5	LYS	2.3
1	A	32	GLY	2.3
1	B	165	HIS	2.3
1	B	244	HIS	2.3
1	B	140	LEU	2.3
1	B	262	LEU	2.3
1	B	274	ILE	2.3
1	A	306	LYS	2.3
1	A	460	LYS	2.3
1	B	185	LYS	2.3
1	B	425	ALA	2.3
1	A	303	GLU	2.3
1	B	324	PHE	2.3
1	A	191	GLY	2.3
1	A	131	THR	2.2
1	A	368	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	2.2
1	B	194	ALA	2.2
1	B	304	ALA	2.2
1	A	236	ASP	2.2
1	B	135	ASP	2.2
1	A	389	HIS	2.2
1	B	197	ALA	2.2
1	B	211	VAL	2.2
1	B	484	LYS	2.2
1	A	427	ASN	2.2
1	B	67	ILE	2.2
1	A	125	MET	2.2
1	B	264	MET	2.2
1	A	361	THR	2.2
1	A	214	GLY	2.2
1	A	249	ASN	2.2
1	A	280	ALA	2.2
1	B	34	ALA	2.2
1	B	110	ASN	2.2
1	B	330	VAL	2.2
1	B	496	VAL	2.2
1	A	491	LYS	2.2
1	A	181	GLN	2.2
1	A	373	TYR	2.2
1	B	198	ALA	2.2
1	B	102	VAL	2.2
1	A	45	PRO	2.2
1	A	87	PRO	2.2
1	A	129	LEU	2.2
1	A	221	PRO	2.2
1	A	437	GLU	2.2
1	A	6	ALA	2.2
1	A	152	TYR	2.1
1	B	147	PRO	2.1
1	B	366	PRO	2.1
1	B	56	VAL	2.1
1	B	73	GLY	2.1
1	A	94	ARG	2.1
1	B	380	SER	2.1
1	B	442	SER	2.1
1	A	364	ASN	2.1
1	A	375	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	55	ASP	2.1
1	B	331	GLY	2.1
1	B	181	GLN	2.1
1	B	272	VAL	2.1
1	A	301	SER	2.1
1	A	126	ALA	2.1
1	A	347	ALA	2.1
1	B	199	LYS	2.1
1	A	110	ASN	2.1
1	B	128	ASN	2.1
1	A	109	LEU	2.1
1	A	171	CYS	2.1
1	B	259	ALA	2.1
1	B	156	ARG	2.1
1	A	178	GLY	2.1
1	B	133	GLY	2.1
1	B	396	LYS	2.1
1	A	305	ASP	2.1
1	A	422	THR	2.1
1	A	414	TYR	2.1
1	B	277	TYR	2.1
1	A	381	VAL	2.1
1	A	433	ALA	2.1
1	B	35	VAL	2.1
1	B	327	ALA	2.1
1	A	16	ILE	2.1
1	B	270	SER	2.1
1	A	54	GLN	2.0
1	B	126	ALA	2.0
1	A	415	ASN	2.0
1	B	53	ARG	2.0
1	B	295	TRP	2.0
1	A	186	THR	2.0
1	B	205	ASP	2.0
1	B	365	GLY	2.0
1	B	8	MET	2.0
1	A	451	HIS	2.0
1	A	467	SER	2.0
1	A	484	LYS	2.0
1	A	79	TYR	2.0
1	B	247	TYR	2.0
1	A	391	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASN	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	GOL	B	503	6/6	0.81	0.20	0.17	25,28,32,35	0
2	GOL	A	503	6/6	0.78	0.20	-0.25	24,27,31,32	0

6.5　Other polymers (i)

There are no such residues in this entry.