WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:38 PM GMT

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	:	2003-07-09
Resolution	:	1.75 Å(reported)

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

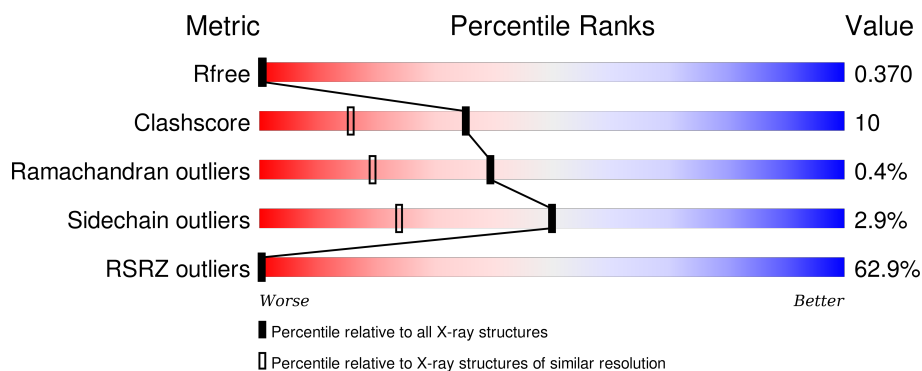|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (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		62.9%

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$_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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.

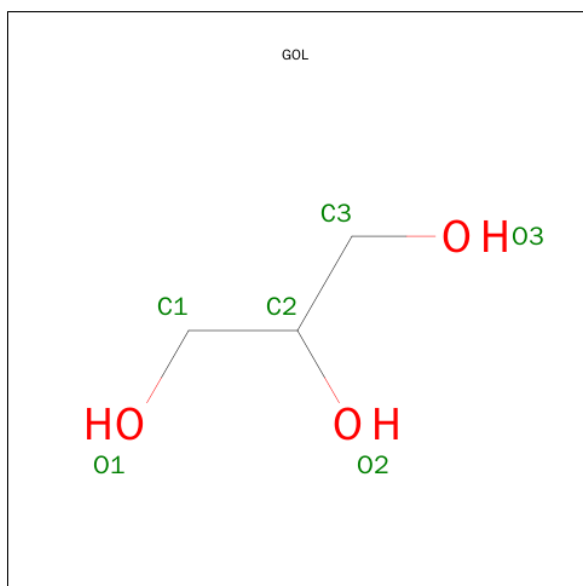| Mol	Chain	Length	Quality of chain
1	A	502	67% / 81% 16% ••
1	B	502	57% / 83% 15% ••

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 3990	C 2542	N 680	O 748	S 20	0	0	0
1	B	497	Total 3990	C 2542	N 680	O 748	S 20	0	0	0

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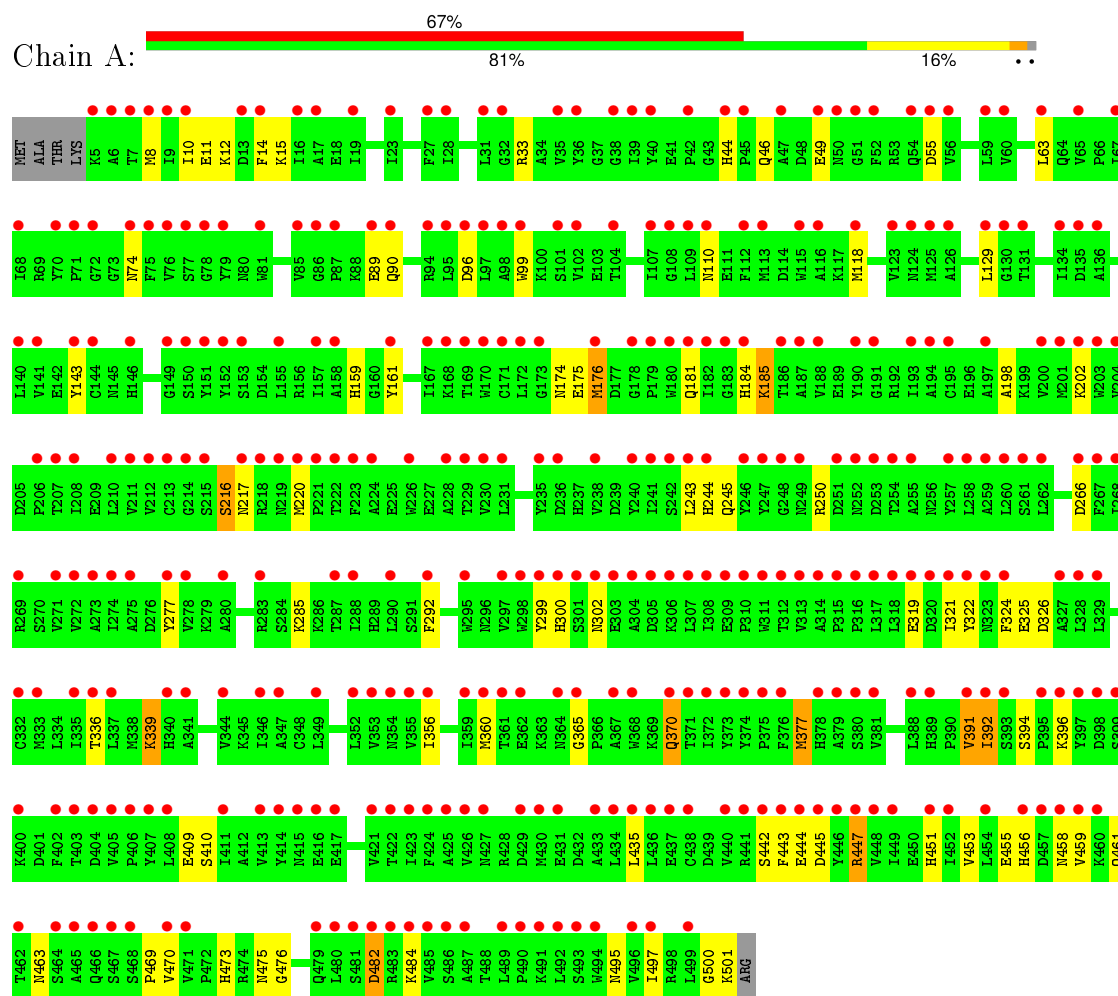

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is water.

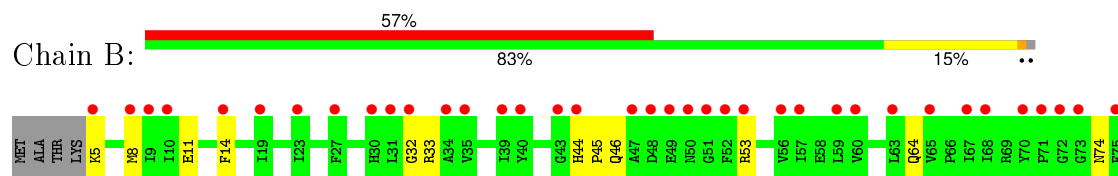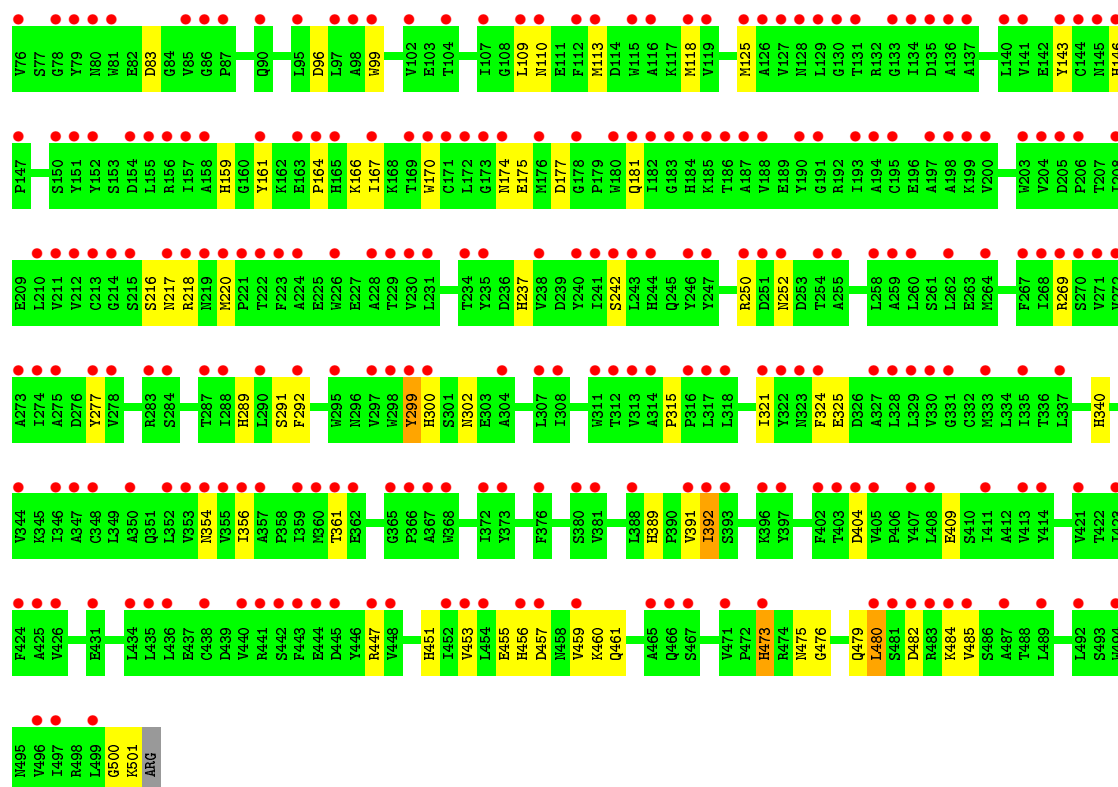| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	583	Total O 583 583	0	0
3	B	561	Total O 561 561	0	0

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: Alpha-L-arabinofuranosidase

- Molecule 1: Alpha-L-arabinofuranosidase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	179.43Å 179.43Å 100.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.75 19.96 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.75) 98.3 (19.96-1.75)	Depositor 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 0.364 , 0.370	Depositor 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
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 119689 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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:14:PHE:CZ	1:B:391:VAL:HG21	2.15	0.80
1:A:44:HIS:HD2	1:A:46:GLN:H	1.29	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:410:SER:HB3	3:A:1086:HOH:O	2.09	0.52
1:A:129:LEU:O	1:A:185:LYS:HE3	2.09	0.52
1:B:74:ASN:HA	1:B:181:GLN:HE22	1.75	0.52
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.56	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:99:TRP:CH2	2:A:503:GOL:H31	2.45	0.51
1:A:435:LEU:N	1:A:435:LEU:HD22	2.25	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:216:SER:CB	3:A:997:HOH:O	2.59	0.50
1:A:11:GLU:CG	1:A:14:PHE:HD1	2.24	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:B:217:ASN:HB2	3:B:1017:HOH:O	2.13	0.48
1:A:447:ARG:HD2	3:A:1042:HOH:O	2.14	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:B:453:VAL:HB	1:B:473:HIS:NE2	2.31	0.45
1:A:336:THR:HA	1:A:339:LYS:HG2	1.98	0.45
1:B:159:HIS:HE1	3:B:612:HOH:O	2.00	0.45
1:A:339:LYS:HD2	3:A:993:HOH:O	2.17	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:B:146:HIS:HE1	3:B:687:HOH:O	2.02	0.42
1:A:63:LEU:HD23	1:A:377:MET:HG3	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:B:289:HIS:HE1	3:B:839:HOH:O	2.03	0.42
1:A:243:LEU:N	1:A:243:LEU:HD12	2.35	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:99:TRP:CZ2	2:A:503:GOL:H31	2.56	0.41
1:A:447:ARG:NE	3:A:1018:HOH:O	2.53	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%)	39	19
1	B	495/502 (99%)	477 (96%)	16 (3%)	2 (0%)	39	19
All	All	990/1004 (99%)	948 (96%)	38 (4%)	4 (0%)	39	19

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%)	43	17
1	B	430/434 (99%)	420 (98%)	10 (2%)	58	33
All	All	860/868 (99%)	835 (97%)	25 (3%)	50	24

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	1.00	1 (20%)
2	GOL	B	503	-	5,5,5	0.63	0	5,5,5	0.87	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	2.16	118.55	108.65

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%)	2.64	337 (67%)	0	0	13, 23, 40, 56	0
1	B	497/502 (99%)	2.35	288 (57%)	0	0	16, 23, 37, 47	0
All	All	994/1004 (99%)	2.50	625 (62%)	0	0	13, 23, 39, 56	0

All (625) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	10.7
1	A	252	ASN	7.9
1	A	457	ASP	7.5
1	A	251	ASP	7.4
1	A	435	LEU	7.2
1	A	441	ARG	7.2
1	B	170	TRP	7.0
1	A	402	PHE	6.5
1	A	180	TRP	6.4
1	A	241	ILE	6.2
1	B	312	THR	6.0
1	A	10	ILE	6.0
1	A	482	ASP	5.9
1	A	440	VAL	5.8
1	A	151	TYR	5.8
1	A	115	TRP	5.7
1	B	217	ASN	5.7
1	B	180	TRP	5.6
1	B	311	TRP	5.5
1	A	308	ILE	5.5
1	B	440	VAL	5.5
1	B	212	VAL	5.5
1	A	479	GLN	5.4
1	A	212	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	438	CYS	5.2
1	B	241	ILE	5.2
1	B	482	ASP	5.2
1	B	43	GLY	5.1
1	A	200	VAL	5.1
1	B	481	SER	5.1
1	A	314	ALA	5.0
1	A	313	VAL	5.0
1	A	423	ILE	5.0
1	A	444	GLU	5.0
1	A	393	SER	5.0
1	A	445	ASP	4.8
1	A	485	VAL	4.8
1	A	95	LEU	4.8
1	A	442	SER	4.7
1	B	308	ILE	4.7
1	A	448	VAL	4.7
1	B	141	VAL	4.7
1	B	203	TRP	4.7
1	B	172	LEU	4.7
1	A	327	ALA	4.7
1	A	443	PHE	4.7
1	B	307	LEU	4.6
1	A	112	PHE	4.6
1	A	421	VAL	4.6
1	B	213	CYS	4.6
1	A	99	TRP	4.5
1	A	173	GLY	4.5
1	B	480	LEU	4.4
1	B	81	TRP	4.4
1	A	136	ALA	4.4
1	B	220	MET	4.4
1	B	129	LEU	4.3
1	B	317	LEU	4.3
1	A	426	VAL	4.3
1	B	51	GLY	4.3
1	A	332	CYS	4.3
1	A	411	ILE	4.3
1	A	97	LEU	4.3
1	A	436	LEU	4.3
1	B	492	LEU	4.3
1	A	407	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	267	PHE	4.3
1	A	288	ILE	4.3
1	A	329	LEU	4.3
1	A	157	ILE	4.2
1	A	403	THR	4.2
1	A	70	TYR	4.2
1	A	413	VAL	4.2
1	B	443	PHE	4.2
1	B	31	LEU	4.2
1	A	311	TRP	4.1
1	A	346	ILE	4.1
1	A	438	CYS	4.1
1	A	28	ILE	4.1
1	B	444	GLU	4.1
1	A	242	SER	4.1
1	B	321	ILE	4.1
1	A	75	PHE	4.1
1	B	214	GLY	4.1
1	A	39	ILE	4.1
1	A	480	LEU	4.1
1	B	95	LEU	4.1
1	A	257	TYR	4.0
1	A	220	MET	4.0
1	A	188	VAL	4.0
1	A	204	VAL	4.0
1	B	76	VAL	4.0
1	A	213	CYS	4.0
1	B	292	PHE	4.0
1	A	454	LEU	4.0
1	A	247	TYR	4.0
1	A	36	TYR	3.9
1	B	267	PHE	3.9
1	A	31	LEU	3.9
1	A	459	VAL	3.9
1	B	413	VAL	3.9
1	A	42	PRO	3.9
1	B	109	LEU	3.9
1	B	403	THR	3.9
1	A	143	TYR	3.9
1	A	259	ALA	3.9
1	A	268	ILE	3.9
1	A	408	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	376	PHE	3.9
1	A	492	LEU	3.8
1	B	10	ILE	3.8
1	B	39	ILE	3.8
1	B	243	LEU	3.8
1	B	359	ILE	3.8
1	A	255	ALA	3.8
1	B	456	HIS	3.8
1	A	352	LEU	3.8
1	A	471	VAL	3.8
1	A	312	THR	3.8
1	A	218	ARG	3.8
1	A	172	LEU	3.8
1	B	258	LEU	3.8
1	B	157	ILE	3.8
1	A	72	GLY	3.8
1	B	9	ILE	3.8
1	B	144	CYS	3.8
1	A	328	LEU	3.7
1	A	27	PHE	3.7
1	A	486	SER	3.7
1	A	243	LEU	3.7
1	A	68	ILE	3.7
1	A	367	ALA	3.7
1	A	483	ARG	3.7
1	B	314	ALA	3.7
1	A	317	LEU	3.7
1	B	173	GLY	3.7
1	A	150	SER	3.7
1	A	59	LEU	3.7
1	B	313	VAL	3.7
1	B	107	ILE	3.7
1	B	288	ILE	3.7
1	B	178	GLY	3.7
1	A	52	PHE	3.6
1	A	333	MET	3.6
1	B	151	TYR	3.6
1	B	63	LEU	3.6
1	A	405	VAL	3.6
1	B	271	VAL	3.6
1	A	187	ALA	3.6
1	A	322	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	PRO	3.6
1	A	290	LEU	3.6
1	A	434	LEU	3.6
1	A	102	VAL	3.6
1	B	60	VAL	3.6
1	B	136	ALA	3.6
1	B	204	VAL	3.6
1	A	497	ILE	3.6
1	B	346	ILE	3.6
1	B	423	ILE	3.6
1	B	99	TRP	3.6
1	B	78	GLY	3.6
1	A	223	PHE	3.6
1	B	322	TYR	3.6
1	A	304	ALA	3.6
1	A	318	LEU	3.6
1	B	200	VAL	3.6
1	B	466	GLN	3.6
1	B	195	CYS	3.6
1	B	348	CYS	3.6
1	A	9	ILE	3.6
1	B	473	HIS	3.6
1	B	275	ALA	3.6
1	A	141	VAL	3.6
1	A	258	LEU	3.6
1	A	344	VAL	3.6
1	A	470	VAL	3.6
1	B	388	LEU	3.6
1	B	167	ILE	3.6
1	A	230	VAL	3.5
1	A	262	LEU	3.5
1	B	337	LEU	3.5
1	B	404	ASP	3.5
1	B	208	ILE	3.5
1	A	275	ALA	3.5
1	B	50	ASN	3.5
1	B	226	TRP	3.5
1	B	14	PHE	3.5
1	B	112	PHE	3.5
1	B	240	TYR	3.5
1	A	210	LEU	3.5
1	A	496	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASN	3.5
1	A	295	TRP	3.5
1	A	494	TRP	3.5
1	B	424	PHE	3.5
1	A	489	LEU	3.5
1	B	445	ASP	3.5
1	B	467	SER	3.5
1	A	193	ILE	3.5
1	B	283	ARG	3.5
1	B	52	PHE	3.5
1	A	140	LEU	3.5
1	B	397	TYR	3.5
1	B	435	LEU	3.5
1	B	459	VAL	3.5
1	B	116	ALA	3.5
1	A	466	GLN	3.4
1	A	315	PRO	3.4
1	A	17	ALA	3.4
1	A	155	LEU	3.4
1	B	75	PHE	3.4
1	B	246	TYR	3.4
1	A	81	TRP	3.4
1	B	431	GLU	3.4
1	B	344	VAL	3.4
1	B	421	VAL	3.4
1	B	210	LEU	3.4
1	A	161	TYR	3.4
1	B	234	THR	3.4
1	A	298	TRP	3.4
1	A	272	VAL	3.4
1	A	355	VAL	3.4
1	A	229	THR	3.4
1	A	499	LEU	3.4
1	A	359	ILE	3.4
1	B	368	TRP	3.4
1	A	336	THR	3.4
1	A	417	GLU	3.4
1	A	60	VAL	3.3
1	B	85	VAL	3.3
1	B	278	VAL	3.3
1	B	182	ILE	3.3
1	A	431	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	483	ARG	3.3
1	B	436	LEU	3.3
1	A	365	GLY	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	A	462	THR	3.3
1	B	72	GLY	3.3
1	B	158	ALA	3.3
1	A	399	SER	3.3
1	A	468	SER	3.3
1	A	182	ILE	3.3
1	A	56	VAL	3.2
1	B	489	LEU	3.2
1	B	494	TRP	3.2
1	A	184	HIS	3.2
1	B	146	HIS	3.2
1	B	367	ALA	3.2
1	A	146	HIS	3.2
1	B	231	LEU	3.2
1	A	429	ASP	3.2
1	A	78	GLY	3.2
1	A	481	SER	3.2
1	A	108	GLY	3.2
1	A	14	PHE	3.2
1	B	376	PHE	3.2
1	A	158	ALA	3.2
1	A	379	ALA	3.2
1	A	397	TYR	3.2
1	B	70	TYR	3.2
1	B	299	TYR	3.2
1	B	269	ARG	3.2
1	A	215	SER	3.1
1	B	188	VAL	3.1
1	B	224	ALA	3.1
1	B	40	TYR	3.1
1	B	143	TYR	3.1
1	B	255	ALA	3.1
1	B	130	GLY	3.1
1	B	49	GLU	3.1
1	B	57	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	223	PHE	3.1
1	A	425	ALA	3.1
1	A	449	ILE	3.1
1	B	335	ILE	3.1
1	B	230	VAL	3.1
1	B	251	ASP	3.1
1	B	155	LEU	3.1
1	B	328	LEU	3.1
1	A	404	ASP	3.0
1	B	392	ILE	3.0
1	A	278	VAL	3.0
1	B	65	VAL	3.0
1	B	471	VAL	3.0
1	B	152	TYR	3.0
1	B	218	ARG	3.0
1	B	235	TYR	3.0
1	A	372	ILE	3.0
1	B	402	PHE	3.0
1	A	349	LEU	3.0
1	B	228	ALA	3.0
1	B	252	ASN	3.0
1	B	171	CYS	3.0
1	A	107	ILE	3.0
1	B	268	ILE	3.0
1	A	269	ARG	3.0
1	A	430	MET	3.0
1	B	113	MET	3.0
1	A	76	VAL	3.0
1	B	71	PRO	3.0
1	B	119	VAL	3.0
1	B	206	PRO	3.0
1	A	337	LEU	3.0
1	A	19	ILE	3.0
1	B	44	HIS	3.0
1	B	290	LEU	3.0
1	A	130	GLY	2.9
1	A	360	MET	2.9
1	A	222	THR	2.9
1	B	161	TYR	2.9
1	A	226	TRP	2.9
1	A	274	ILE	2.9
1	A	335	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	300	HIS	2.9
1	B	356	ILE	2.9
1	A	123	VAL	2.9
1	A	144	CYS	2.9
1	A	271	VAL	2.9
1	B	381	VAL	2.9
1	A	395	PRO	2.9
1	A	190	TYR	2.9
1	B	353	VAL	2.9
1	B	357	ALA	2.9
1	B	487	ALA	2.9
1	A	63	LEU	2.9
1	A	7	THR	2.9
1	B	150	SER	2.9
1	B	287	THR	2.9
1	A	219	ASN	2.9
1	A	452	ILE	2.9
1	A	353	VAL	2.9
1	B	131	THR	2.9
1	B	27	PHE	2.9
1	A	299	TYR	2.9
1	B	215	SER	2.9
1	A	85	VAL	2.9
1	B	186	THR	2.9
1	A	260	LEU	2.8
1	A	5	LYS	2.8
1	A	324	PHE	2.8
1	A	8	MET	2.8
1	B	219	ASN	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	A	244	HIS	2.8
1	A	388	LEU	2.8
1	B	352	LEU	2.8
1	B	284	SER	2.8
1	A	47	ALA	2.8
1	A	96	ASP	2.8
1	B	32	GLY	2.8
1	A	49	GLU	2.8
1	A	261	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	302	ASN	2.8
1	A	176	MET	2.8
1	B	59	LEU	2.8
1	B	457	ASP	2.8
1	A	300	HIS	2.8
1	B	145	ASN	2.8
1	A	297	VAL	2.8
1	B	193	ILE	2.8
1	B	333	MET	2.8
1	A	38	GLY	2.8
1	B	318	LEU	2.8
1	A	396	LYS	2.8
1	A	67	ILE	2.7
1	A	246	TYR	2.7
1	A	446	TYR	2.7
1	B	190	TYR	2.7
1	A	197	ALA	2.7
1	B	97	LEU	2.7
1	A	309	GLU	2.7
1	B	30	HIS	2.7
1	A	266	ASP	2.7
1	A	167	ILE	2.7
1	A	287	THR	2.7
1	A	374	TYR	2.7
1	B	407	TYR	2.7
1	B	221	PRO	2.7
1	A	135	ASP	2.7
1	A	248	GLY	2.7
1	B	80	ASN	2.7
1	B	448	VAL	2.7
1	A	183	GLY	2.7
1	B	454	LEU	2.7
1	B	441	ARG	2.7
1	A	153	SER	2.7
1	B	393	SER	2.7
1	A	238	VAL	2.7
1	B	372	ILE	2.7
1	B	414	TYR	2.7
1	A	203	TRP	2.7
1	A	13	ASP	2.7
1	A	206	PRO	2.7
1	A	447	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	360	MET	2.6
1	A	321	ILE	2.6
1	A	240	TYR	2.6
1	A	211	VAL	2.6
1	B	238	VAL	2.6
1	B	391	VAL	2.6
1	A	71	PRO	2.6
1	B	134	ILE	2.6
1	B	79	TYR	2.6
1	A	464	SER	2.6
1	A	170	TRP	2.6
1	B	125	MET	2.6
1	B	163	GLU	2.6
1	B	184	HIS	2.6
1	B	316	PRO	2.6
1	B	68	ILE	2.6
1	A	44	HIS	2.6
1	A	253	ASP	2.6
1	B	298	TRP	2.6
1	B	447	ARG	2.6
1	B	453	VAL	2.6
1	B	411	ILE	2.6
1	A	40	TYR	2.6
1	B	373	TYR	2.6
1	A	149	GLY	2.6
1	A	169	THR	2.5
1	A	65	VAL	2.5
1	A	224	ALA	2.5
1	B	137	ALA	2.5
1	B	273	ALA	2.5
1	A	292	PHE	2.5
1	A	235	TYR	2.5
1	B	329	LEU	2.5
1	A	101	SER	2.5
1	A	194	ALA	2.5
1	A	228	ALA	2.5
1	A	179	PRO	2.5
1	B	115	TRP	2.5
1	A	362	GLU	2.5
1	A	104	THR	2.5
1	A	371	THR	2.5
1	A	98	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	487	ALA	2.5
1	A	458	ASN	2.5
1	B	323	ASN	2.5
1	B	354	ASN	2.5
1	A	195	CYS	2.5
1	A	320	ASP	2.5
1	A	380	SER	2.5
1	A	493	SER	2.5
1	B	355	VAL	2.5
1	B	222	THR	2.5
1	B	362	GLU	2.5
1	A	424	PHE	2.5
1	B	434	LEU	2.5
1	B	183	GLY	2.5
1	A	378	HIS	2.5
1	A	456	HIS	2.5
1	A	89	GLU	2.5
1	A	90	GLN	2.5
1	B	361	THR	2.5
1	A	316	PRO	2.5
1	A	134	ILE	2.5
1	B	497	ILE	2.5
1	A	465	ALA	2.5
1	A	319	GLU	2.4
1	B	485	VAL	2.4
1	A	116	ALA	2.4
1	A	231	LEU	2.4
1	B	347	ALA	2.4
1	A	50	ASN	2.4
1	A	254	THR	2.4
1	B	90	GLN	2.4
1	B	254	THR	2.4
1	A	310	PRO	2.4
1	A	340	HIS	2.4
1	B	242	SER	2.4
1	B	426	VAL	2.4
1	B	176	MET	2.4
1	A	416	GLU	2.4
1	B	187	ALA	2.4
1	B	260	LEU	2.4
1	B	499	LEU	2.4
1	B	169	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	113	MET	2.4
1	A	118	MET	2.4
1	B	127	VAL	2.4
1	B	405	VAL	2.4
1	B	350	ALA	2.4
1	A	400	LYS	2.4
1	A	23	ILE	2.4
1	A	392	ILE	2.4
1	A	370	GLN	2.4
1	A	202	LYS	2.4
1	B	47	ALA	2.4
1	B	465	ALA	2.4
1	B	104	THR	2.4
1	A	323	ASN	2.4
1	A	354	ASN	2.4
1	B	118	MET	2.3
1	B	452	ILE	2.3
1	A	398	ASP	2.3
1	A	341	ALA	2.3
1	B	297	VAL	2.3
1	B	174	ASN	2.3
1	B	229	THR	2.3
1	B	140	LEU	2.3
1	B	262	LEU	2.3
1	B	274	ILE	2.3
1	A	32	GLY	2.3
1	A	77	SER	2.3
1	B	425	ALA	2.3
1	A	168	LYS	2.3
1	A	490	PRO	2.3
1	A	201	MET	2.3
1	A	368	TRP	2.3
1	B	165	HIS	2.3
1	B	244	HIS	2.3
1	A	191	GLY	2.3
1	B	98	ALA	2.3
1	B	194	ALA	2.3
1	B	304	ALA	2.3
1	B	324	PHE	2.3
1	B	5	LYS	2.3
1	A	303	GLU	2.3
1	B	197	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	131	THR	2.3
1	A	306	LYS	2.3
1	A	460	LYS	2.3
1	B	67	ILE	2.3
1	B	185	LYS	2.3
1	A	236	ASP	2.3
1	B	135	ASP	2.3
1	B	211	VAL	2.3
1	A	280	ALA	2.2
1	A	389	HIS	2.2
1	B	34	ALA	2.2
1	A	427	ASN	2.2
1	A	214	GLY	2.2
1	B	330	VAL	2.2
1	B	496	VAL	2.2
1	A	249	ASN	2.2
1	B	110	ASN	2.2
1	A	361	THR	2.2
1	B	198	ALA	2.2
1	A	125	MET	2.2
1	B	264	MET	2.2
1	B	484	LYS	2.2
1	A	129	LEU	2.2
1	A	373	TYR	2.2
1	B	102	VAL	2.2
1	A	6	ALA	2.2
1	A	45	PRO	2.2
1	A	87	PRO	2.2
1	A	221	PRO	2.2
1	A	491	LYS	2.2
1	A	181	GLN	2.2
1	A	152	TYR	2.2
1	B	56	VAL	2.2
1	B	73	GLY	2.2
1	A	437	GLU	2.2
1	B	147	PRO	2.2
1	B	366	PRO	2.2
1	B	380	SER	2.2
1	B	442	SER	2.2
1	B	331	GLY	2.2
1	A	126	ALA	2.2
1	A	347	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	364	ASN	2.2
1	B	272	VAL	2.2
1	A	375	PRO	2.1
1	A	94	ARG	2.1
1	A	301	SER	2.1
1	A	55	ASP	2.1
1	A	109	LEU	2.1
1	A	171	CYS	2.1
1	B	259	ALA	2.1
1	A	178	GLY	2.1
1	B	133	GLY	2.1
1	A	110	ASN	2.1
1	B	128	ASN	2.1
1	B	181	GLN	2.1
1	A	433	ALA	2.1
1	B	327	ALA	2.1
1	A	16	ILE	2.1
1	A	381	VAL	2.1
1	B	35	VAL	2.1
1	A	414	TYR	2.1
1	B	277	TYR	2.1
1	B	199	LYS	2.1
1	A	422	THR	2.1
1	B	156	ARG	2.1
1	A	305	ASP	2.1
1	B	295	TRP	2.1
1	B	126	ALA	2.1
1	B	270	SER	2.1
1	B	396	LYS	2.1
1	A	415	ASN	2.1
1	B	365	GLY	2.1
1	A	54	GLN	2.0
1	A	186	THR	2.0
1	A	391	VAL	2.0
1	A	467	SER	2.0
1	A	79	TYR	2.0
1	B	247	TYR	2.0
1	A	273	ALA	2.0
1	B	53	ARG	2.0
1	A	451	HIS	2.0
1	B	205	ASP	2.0
1	B	408	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASN	2.0
1	B	8	MET	2.0
1	A	35	VAL	2.0
1	A	277	TYR	2.0
1	A	484	LYS	2.0
1	A	124	ASN	2.0
1	A	283	ARG	2.0
1	B	250	ARG	2.0
1	B	87	PRO	2.0
1	B	164	PRO	2.0
1	A	207	THR	2.0
1	B	48	ASP	2.0
1	B	154	ASP	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.