WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:22 PM GMT

PDB ID	:	1TAQ
Title	:	STRUCTURE OF TAQ DNA POLYMERASE
Authors	:	Kim, Y.; Eom, S.H.; Wang, J.; Lee, D.-S.; Suh, S.W.; Steitz, T.A.
Deposited on	:	1996-06-04
Resolution	:	2.40 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 2.40 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
Clashscore		22
Ramachandran outliers		4.5%
Sidechain outliers		11.3%
RSRZ outliers		7.4%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
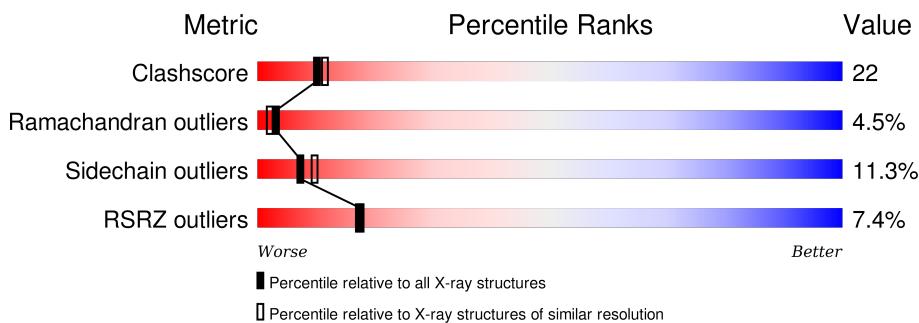
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	832	7% / 54% / 35% / 8% / ·
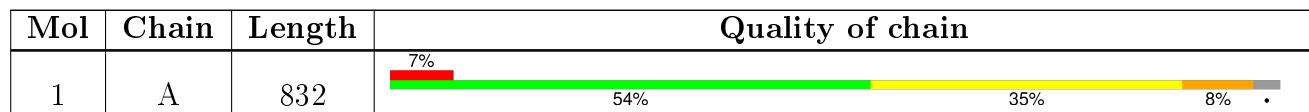
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	900	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6747 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 TAQ DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	807	Total 6432	C 4102	N 1145	O 1168	S 17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	CYS	SER	CONFLICT	UNP P19821
A	576	CYS	SER	CONFLICT	UNP P19821
A	577	CYS	SER	CONFLICT	UNP P19821
A	597	GLY	ALA	CONFLICT	UNP P19821

- Molecule 2 is SUGAR (B-2-OCTYLGLUCOSIDE) (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).
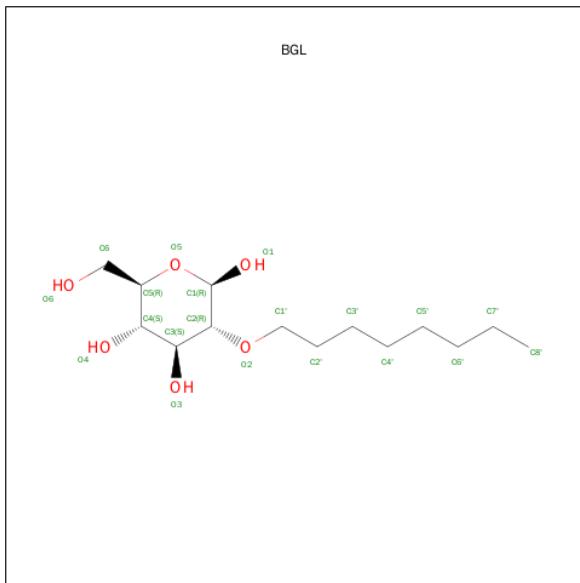
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 20	C 14	O 6	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	294	Total 294	O 294	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: TAQ DNA POLYMERASE
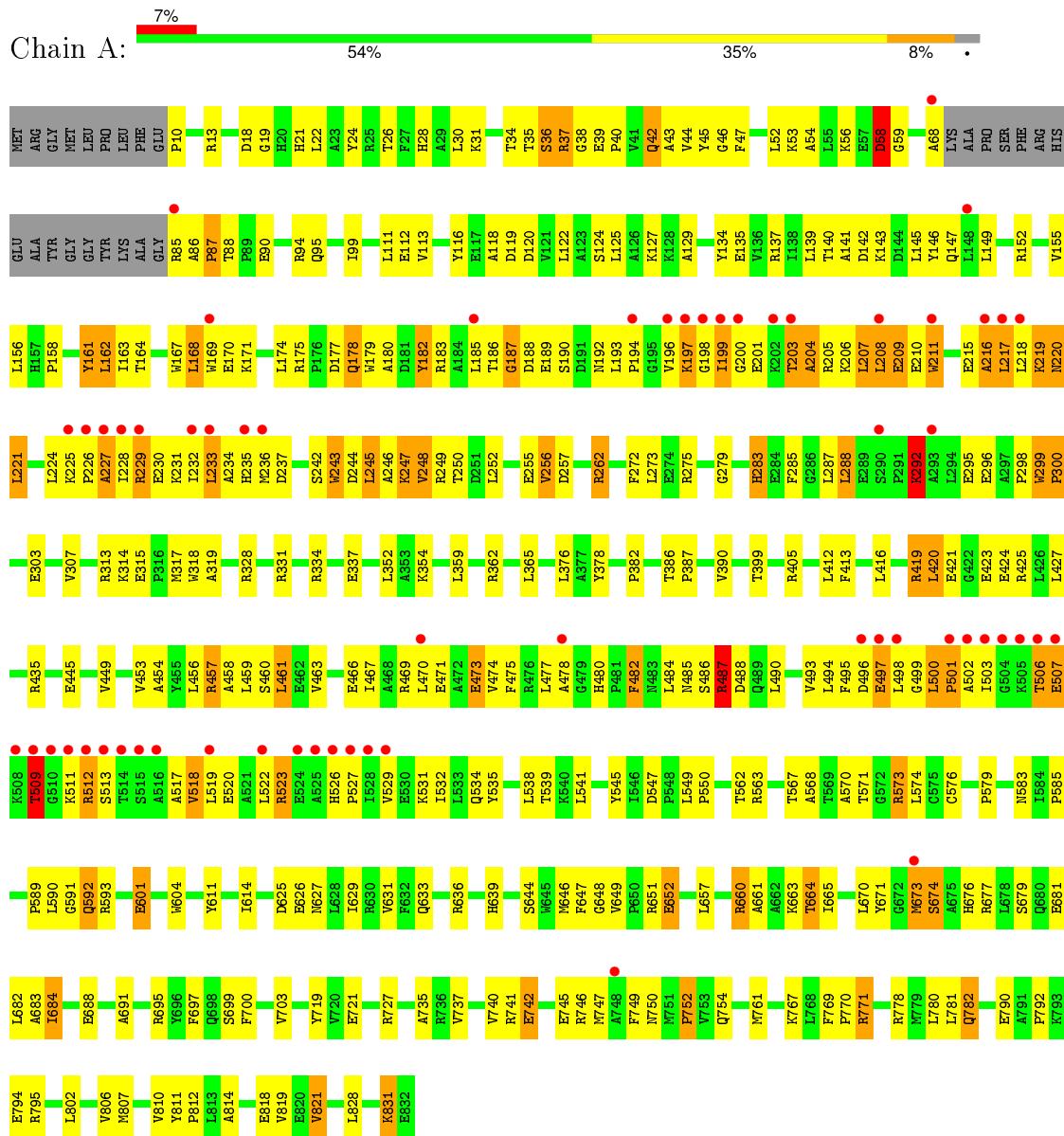
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.42Å 107.42Å 170.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.40 53.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.40) 72.8 (53.71-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.06 (at 2.39Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.323 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 105.0	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning [2]	$<|L|>=0.47$, $<L^2>=0.30$	Xtriage
Outliers	0 of 32776 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 (i)

5.1 Standard geometry (i)

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

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	0.47	0/6568	0.76	4/8891 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	A	509	THR	N-CA-C	6.39	128.26	111.00
1	A	359	LEU	CA-CB-CG	5.73	128.49	115.30
1	A	58	ASP	N-CA-C	5.34	125.41	111.00
1	A	135	GLU	N-CA-C	-5.09	97.25	111.00

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	6432	0	6525	283	0
2	A	20	0	27	2	0
3	A	1	0	0	0	0
4	A	294	0	0	9	0
All	All	6747	0	6552	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 22.

All (284) 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:34:THR:HG22	1:A:40:PRO:HA	1.49	0.95
1:A:295:GLU:HG2	1:A:331:ARG:HG2	1.50	0.92
1:A:207:LEU:HD23	1:A:210:GLU:HB2	1.52	0.90
1:A:127:LYS:HG3	1:A:250:THR:HB	1.52	0.88
1:A:34:THR:HB	1:A:38:GLY:O	1.74	0.88
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.55	0.88
1:A:292:LYS:HA	1:A:292:LYS:HE2	1.64	0.78
1:A:68:ALA:HB2	1:A:112:GLU:HB2	1.62	0.78
1:A:44:VAL:HA	1:A:99:ILE:HD11	1.64	0.78
1:A:146:TYR:O	1:A:149:LEU:HB2	1.84	0.77
1:A:111:LEU:HD23	1:A:125:LEU:HD11	1.66	0.77
1:A:592:GLN:HG3	1:A:828:LEU:HD11	1.67	0.76
1:A:140:THR:HG21	1:A:145:LEU:HD12	1.67	0.75
1:A:183:ARG:HE	1:A:245:LEU:HD21	1.52	0.75
1:A:224:LEU:HB3	1:A:229:ARG:HB2	1.68	0.74
1:A:470:LEU:O	1:A:474:VAL:HG23	1.88	0.72
1:A:18:ASP:O	1:A:22:LEU:HG	1.90	0.72
1:A:207:LEU:HB3	1:A:211:TRP:HE1	1.55	0.71
1:A:168:LEU:HD11	1:A:179:TRP:CD1	2.25	0.71
1:A:421:GLU:HA	1:A:427:LEU:HD21	1.72	0.71
1:A:660:ARG:O	1:A:664:THR:HG23	1.90	0.71
1:A:196:VAL:HB	1:A:204:ALA:HB2	1.73	0.71
1:A:466:GLU:HA	1:A:469:ARG:CZ	2.22	0.70
1:A:198:GLY:HA2	1:A:203:THR:HA	1.73	0.70
1:A:376:LEU:HD22	1:A:420:LEU:HD22	1.73	0.70
1:A:585:PRO:O	1:A:591:GLY:HA3	1.91	0.70
1:A:116:TYR:CZ	1:A:252:LEU:HD12	2.28	0.69
1:A:53:LYS:HA	1:A:56:LYS:HD3	1.75	0.68
1:A:186:THR:HG22	1:A:187:GLY:H	1.59	0.68
1:A:147:GLN:CD	1:A:248:VAL:HG21	2.14	0.67
1:A:684:ILE:HG23	1:A:688:GLU:HB3	1.78	0.65
1:A:207:LEU:HB3	1:A:211:TRP:NE1	2.11	0.64
1:A:592:GLN:HG3	1:A:828:LEU:CD1	2.26	0.64
1:A:129:ALA:O	1:A:134:TYR:HB2	1.98	0.64
1:A:205:ARG:HA	1:A:208:LEU:HG	1.78	0.64
1:A:244:ASP:O	1:A:247:LYS:HB2	1.98	0.64
1:A:197:LYS:HD3	1:A:227:ALA:HB2	1.80	0.63
1:A:574:LEU:HD12	1:A:782:GLN:HE21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:HB3	1:A:252:LEU:HD21	1.80	0.63
1:A:639:HIS:CD2	1:A:663:LYS:HA	2.34	0.62
1:A:458:ALA:HA	1:A:461:LEU:HD23	1.81	0.62
1:A:386:THR:O	1:A:390:VAL:HG23	1.99	0.62
1:A:771:ARG:HB3	1:A:802:LEU:HD21	1.81	0.62
1:A:231:LYS:HA	1:A:234:ALA:HB3	1.82	0.61
1:A:285:PHE:HA	1:A:288:LEU:HD21	1.82	0.61
1:A:146:TYR:HB2	1:A:179:TRP:CZ3	2.35	0.61
1:A:474:VAL:HG11	1:A:484:LEU:HD21	1.82	0.61
1:A:216:ALA:HA	1:A:221:LEU:HB3	1.83	0.61
1:A:571:THR:HG21	1:A:754:GLN:OE1	2.01	0.60
1:A:68:ALA:HB2	1:A:112:GLU:CB	2.30	0.60
1:A:526:HIS:HB2	1:A:529:VAL:HG22	1.84	0.60
1:A:399:THR:O	1:A:405:ARG:HD3	2.02	0.60
1:A:200:GLY:O	1:A:201:GLU:HG2	2.02	0.59
1:A:124:SER:OG	1:A:252:LEU:HD23	2.02	0.59
1:A:18:ASP:OD2	1:A:21:HIS:HB2	2.01	0.59
1:A:819:VAL:HG12	1:A:821:VAL:HG12	1.83	0.59
1:A:527:PRO:O	1:A:531:LYS:HG2	2.03	0.58
1:A:482:PHE:H	1:A:482:PHE:HD1	1.51	0.58
1:A:182:TYR:CE2	1:A:208:LEU:HD13	2.38	0.58
1:A:425:ARG:HB2	4:A:1075:HOH:O	2.03	0.58
1:A:273:LEU:HB3	1:A:279:GLY:HA2	1.86	0.58
1:A:471:GLU:HG2	1:A:475:PHE:CZ	2.38	0.58
1:A:216:ALA:CA	1:A:221:LEU:HB3	2.33	0.58
1:A:697:PHE:HE1	1:A:703:VAL:HG12	1.68	0.58
1:A:721:GLU:O	1:A:752:PRO:HB3	2.04	0.57
2:A:833:BGL:H1'2	2:A:833:BGL:O1	2.04	0.57
1:A:227:ALA:H	1:A:230:GLU:HB3	1.68	0.57
1:A:771:ARG:HH11	1:A:771:ARG:HG2	1.69	0.57
1:A:769:PHE:HB3	1:A:770:PRO:HD3	1.85	0.57
1:A:661:ALA:O	1:A:665:ILE:HG13	2.05	0.57
1:A:182:TYR:CZ	1:A:208:LEU:HD13	2.40	0.56
1:A:86:ALA:CB	1:A:87:PRO:HD3	2.31	0.56
1:A:458:ALA:O	1:A:461:LEU:HG	2.05	0.56
1:A:507:GLU:C	1:A:513:SER:HB2	2.25	0.56
1:A:30:LEU:HD13	1:A:45:TYR:HD2	1.69	0.56
1:A:13:ARG:NH1	1:A:13:ARG:HB2	2.21	0.56
1:A:534:GLN:O	1:A:538:LEU:HB2	2.05	0.56
1:A:199:ILE:HG13	1:A:226:PRO:O	2.04	0.56
1:A:127:LYS:HG3	1:A:250:THR:CB	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:HA	1:A:247:LYS:HG3	1.88	0.56
1:A:423:GLU:O	1:A:427:LEU:HG	2.06	0.56
1:A:671:TYR:CE1	1:A:673:MET:HA	2.40	0.56
1:A:218:LEU:O	1:A:219:LYS:HB2	2.06	0.56
1:A:249:ARG:HG3	1:A:252:LEU:HD21	1.88	0.55
1:A:454:ALA:O	1:A:457:ARG:HG3	2.06	0.55
1:A:473:GLU:HG2	1:A:531:LYS:HE2	1.87	0.55
1:A:673:MET:HG2	1:A:677:ARG:HB3	1.87	0.55
1:A:43:ALA:HB3	1:A:95:GLN:OE1	2.06	0.55
1:A:319:ALA:O	1:A:362:ARG:NH2	2.39	0.55
1:A:226:PRO:O	1:A:228:ILE:N	2.40	0.55
1:A:19:GLY:HA2	1:A:47:PHE:HE2	1.72	0.55
1:A:547:ASP:O	1:A:550:PRO:HD2	2.07	0.54
1:A:227:ALA:N	1:A:230:GLU:HB3	2.21	0.54
1:A:207:LEU:O	1:A:209:GLU:N	2.41	0.54
1:A:216:ALA:HB2	1:A:221:LEU:HD12	1.90	0.54
1:A:466:GLU:HA	1:A:469:ARG:NH2	2.23	0.54
1:A:147:GLN:NE2	1:A:248:VAL:HG21	2.23	0.53
1:A:767:LYS:O	1:A:770:PRO:HD2	2.09	0.53
1:A:445:GLU:HG3	1:A:562:THR:O	2.07	0.53
1:A:215:GLU:OE1	1:A:218:LEU:HB2	2.09	0.53
1:A:627:ASN:O	1:A:631:VAL:HG23	2.09	0.53
1:A:742:GLU:O	1:A:746:ARG:HD3	2.08	0.53
1:A:467:ILE:HD13	1:A:539:THR:HG22	1.91	0.53
1:A:299:TRP:CG	1:A:300:PRO:N	2.77	0.53
1:A:216:ALA:HB2	1:A:221:LEU:HB3	1.90	0.53
1:A:85:ARG:N	1:A:88:THR:HG1	2.07	0.53
1:A:227:ALA:HA	1:A:231:LYS:HG2	1.90	0.52
1:A:780:LEU:HD11	1:A:790:GLU:HB2	1.91	0.52
1:A:10:PRO:HG3	1:A:152:ARG:HH12	1.74	0.52
1:A:590:LEU:HG	1:A:593:ARG:NH2	2.24	0.52
1:A:520:GLU:O	1:A:523:ARG:HG2	2.09	0.52
1:A:229:ARG:HD2	1:A:229:ARG:C	2.31	0.52
1:A:162:LEU:O	1:A:164:THR:HG23	2.10	0.52
1:A:141:ALA:HB2	1:A:158:PRO:HG2	1.92	0.52
1:A:585:PRO:HG2	1:A:591:GLY:CA	2.40	0.51
1:A:116:TYR:CE2	1:A:252:LEU:HD12	2.46	0.51
1:A:53:LYS:O	1:A:56:LYS:HB2	2.10	0.51
1:A:149:LEU:HD11	1:A:163:ILE:O	2.10	0.51
1:A:741:ARG:O	1:A:745:GLU:HG3	2.11	0.51
1:A:180:ALA:HA	1:A:245:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:O	1:A:463:VAL:HG23	2.11	0.50
1:A:648:GLY:CA	2:A:833:BGL:H5'1	2.41	0.50
1:A:143:LYS:HB3	1:A:179:TRP:HH2	1.76	0.50
1:A:217:LEU:CD2	1:A:218:LEU:HG	2.42	0.50
1:A:216:ALA:CB	1:A:221:LEU:HB3	2.42	0.50
1:A:735:ALA:HB3	1:A:741:ARG:HB3	1.93	0.50
1:A:778:ARG:HG3	1:A:790:GLU:HB3	1.94	0.50
1:A:646:MET:O	1:A:695:ARG:HD3	2.12	0.50
1:A:737:VAL:HB	1:A:740:VAL:HB	1.93	0.50
1:A:174:LEU:HD12	1:A:178:GLN:OE1	2.12	0.50
1:A:674:SER:OG	1:A:677:ARG:HB2	2.11	0.50
1:A:792:PRO:O	1:A:795:ARG:HB2	2.11	0.50
1:A:636:ARG:HH11	1:A:636:ARG:HG2	1.77	0.50
1:A:229:ARG:NH1	1:A:233:LEU:HD11	2.26	0.49
1:A:626:GLU:CD	1:A:626:GLU:H	2.14	0.49
1:A:503:ILE:HG21	1:A:517:ALA:HB1	1.94	0.49
1:A:217:LEU:HB2	1:A:232:ILE:HG23	1.94	0.49
1:A:262:ARG:N	1:A:262:ARG:HD2	2.28	0.49
1:A:36:SER:O	1:A:37:ARG:HG3	2.12	0.49
1:A:673:MET:O	1:A:677:ARG:HD3	2.13	0.49
1:A:545:TYR:OH	1:A:583:ASN:HB2	2.12	0.49
1:A:541:LEU:HD23	1:A:590:LEU:HD13	1.94	0.49
1:A:207:LEU:CD2	1:A:210:GLU:HB2	2.35	0.49
1:A:314:LYS:HE3	1:A:315:GLU:OE2	2.13	0.49
1:A:54:ALA:CB	1:A:139:LEU:HD12	2.43	0.49
1:A:198:GLY:HA2	1:A:203:THR:CA	2.41	0.49
1:A:143:LYS:O	1:A:179:TRP:CZ3	2.66	0.49
1:A:629:ILE:HD13	1:A:814:ALA:HB1	1.95	0.49
1:A:295:GLU:O	1:A:331:ARG:HA	2.13	0.48
1:A:691:ALA:O	1:A:695:ARG:HG3	2.13	0.48
1:A:19:GLY:HA2	1:A:47:PHE:CE2	2.49	0.48
1:A:248:VAL:O	1:A:248:VAL:HG23	2.13	0.48
1:A:262:ARG:HD2	1:A:262:ARG:H	1.78	0.48
1:A:137:ARG:HB3	1:A:156:LEU:HD13	1.94	0.48
1:A:211:TRP:CZ3	1:A:228:ILE:HA	2.49	0.48
1:A:747:MET:HA	1:A:750:ASN:HB3	1.95	0.48
1:A:230:GLU:O	1:A:233:LEU:HD12	2.14	0.48
1:A:487:ARG:NH2	1:A:511:LYS:HE2	2.29	0.47
1:A:683:ALA:O	1:A:684:ILE:HD12	2.14	0.47
1:A:604:TRP:CE3	1:A:790:GLU:HG2	2.48	0.47
1:A:633:GLN:NE2	1:A:814:ALA:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:O	1:A:216:ALA:HB3	2.13	0.47
1:A:26:THR:HB	1:A:46:GLY:HA3	1.96	0.47
1:A:651:ARG:HG3	1:A:652:GLU:N	2.29	0.47
1:A:236:MET:O	1:A:237:ASP:HB2	2.14	0.47
1:A:719:TYR:CD1	1:A:727:ARG:HG3	2.49	0.47
1:A:42:GLN:NE2	1:A:42:GLN:H	2.12	0.47
1:A:34:THR:CG2	1:A:40:PRO:HA	2.34	0.47
1:A:208:LEU:N	1:A:211:TRP:HE1	2.13	0.47
1:A:625:ASP:OD2	1:A:700:PHE:HD1	1.98	0.47
1:A:272:PHE:HA	1:A:275:ARG:NH1	2.30	0.47
1:A:186:THR:OG1	1:A:208:LEU:HD21	2.15	0.46
1:A:119:ASP:HA	1:A:122:LEU:HD12	1.96	0.46
1:A:155:VAL:HB	1:A:163:ILE:HB	1.97	0.46
1:A:164:THR:O	1:A:167:TRP:HB3	2.15	0.46
1:A:629:ILE:O	1:A:633:GLN:HG2	2.16	0.46
1:A:545:TYR:O	1:A:549:LEU:HD22	2.15	0.46
1:A:563:ARG:O	1:A:576:CYS:HA	2.16	0.46
1:A:207:LEU:HD11	1:A:228:ILE:HG12	1.96	0.46
1:A:295:GLU:H	1:A:295:GLU:CD	2.19	0.46
1:A:246:ALA:C	1:A:248:VAL:H	2.19	0.46
1:A:424:GLU:HG2	4:A:953:HOH:O	2.16	0.46
1:A:673:MET:O	1:A:674:SER:CB	2.65	0.45
1:A:299:TRP:O	1:A:300:PRO:C	2.54	0.45
1:A:68:ALA:HB3	1:A:113:VAL:O	2.16	0.45
1:A:376:LEU:HD11	1:A:413:PHE:CE1	2.52	0.45
1:A:498:LEU:HD12	1:A:499:GLY:H	1.80	0.45
1:A:313:ARG:HD3	1:A:318:TRP:O	2.16	0.45
1:A:671:TYR:HA	1:A:749:PHE:HE1	1.81	0.45
1:A:507:GLU:OE1	1:A:517:ALA:HB2	2.17	0.45
1:A:477:LEU:O	1:A:478:ALA:HB3	2.16	0.45
1:A:44:VAL:HA	1:A:99:ILE:CD1	2.41	0.45
1:A:485:ASN:O	1:A:487:ARG:N	2.49	0.45
1:A:466:GLU:HG2	1:A:469:ARG:HH22	1.80	0.45
1:A:174:LEU:HD21	1:A:209:GLU:HB3	1.99	0.45
1:A:249:ARG:HG3	1:A:252:LEU:CD2	2.46	0.45
1:A:475:PHE:CZ	1:A:482:PHE:O	2.69	0.45
1:A:243:TRP:HD1	1:A:244:ASP:N	2.14	0.45
1:A:522:LEU:N	1:A:522:LEU:HD12	2.32	0.45
1:A:40:PRO:HD2	1:A:94:ARG:HH12	1.82	0.44
1:A:299:TRP:CD2	1:A:299:TRP:C	2.88	0.44
1:A:244:ASP:HA	1:A:247:LYS:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:HB2	1:A:59:GLY:H	1.61	0.44
1:A:518:VAL:O	1:A:519:LEU:HB3	2.17	0.44
1:A:111:LEU:HD22	1:A:256:VAL:HG11	1.99	0.44
1:A:140:THR:O	1:A:158:PRO:HD3	2.18	0.44
1:A:307:VAL:HG23	4:A:1126:HOH:O	2.17	0.44
1:A:40:PRO:HD2	1:A:94:ARG:NH1	2.32	0.44
1:A:482:PHE:CE2	1:A:493:VAL:HG21	2.52	0.44
1:A:604:TRP:HE3	1:A:790:GLU:HG2	1.83	0.44
1:A:601:GLU:HG3	4:A:1155:HOH:O	2.16	0.44
1:A:471:GLU:HG3	1:A:484:LEU:HD12	2.00	0.44
1:A:778:ARG:HD2	1:A:790:GLU:OE1	2.17	0.44
1:A:303:GLU:HA	4:A:1057:HOH:O	2.16	0.44
1:A:198:GLY:O	1:A:199:ILE:HB	2.18	0.44
1:A:761:MET:HB2	4:A:910:HOH:O	2.18	0.44
1:A:611:TYR:HB3	1:A:614:ILE:HB	2.00	0.44
1:A:697:PHE:CE1	1:A:703:VAL:HG12	2.52	0.43
1:A:506:THR:HG21	4:A:1145:HOH:O	2.16	0.43
1:A:296:GLU:OE2	1:A:334:ARG:NH1	2.51	0.43
1:A:674:SER:HG	1:A:677:ARG:HB2	1.83	0.43
1:A:317:MET:SD	1:A:362:ARG:HB2	2.58	0.43
1:A:456:LEU:HB3	4:A:984:HOH:O	2.18	0.43
1:A:207:LEU:HD22	1:A:211:TRP:CD1	2.54	0.43
1:A:807:MET:O	1:A:810:VAL:HG12	2.19	0.43
1:A:487:ARG:HH21	1:A:511:LYS:HE2	1.84	0.43
1:A:541:LEU:HD11	1:A:585:PRO:HD3	2.01	0.43
1:A:771:ARG:NH1	1:A:771:ARG:HG2	2.32	0.43
1:A:24:TYR:CZ	1:A:28:HIS:HE1	2.35	0.43
1:A:378:TYR:CD1	1:A:567:THR:HB	2.53	0.43
1:A:470:LEU:HD13	1:A:531:LYS:HE3	2.01	0.43
1:A:639:HIS:HD2	1:A:663:LYS:HA	1.79	0.43
1:A:529:VAL:O	1:A:532:ILE:HG22	2.19	0.43
1:A:570:ALA:HB1	1:A:747:MET:HE1	2.00	0.43
1:A:283:HIS:ND1	1:A:283:HIS:O	2.52	0.43
1:A:190:SER:O	1:A:192:ASN:N	2.52	0.43
1:A:255:GLU:O	1:A:256:VAL:C	2.57	0.42
1:A:246:ALA:C	1:A:248:VAL:N	2.72	0.42
1:A:490:LEU:O	1:A:494:LEU:HG	2.19	0.42
1:A:484:LEU:O	1:A:485:ASN:HB2	2.19	0.42
1:A:496:ASP:C	1:A:497:GLU:HG3	2.39	0.42
1:A:229:ARG:HH11	1:A:233:LEU:HD11	1.84	0.42
1:A:589:PRO:O	1:A:593:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:HB2	1:A:179:TRP:CE3	2.54	0.42
1:A:58:ASP:O	1:A:137:ARG:NH2	2.53	0.42
1:A:412:LEU:O	1:A:416:LEU:HB2	2.20	0.42
1:A:35:THR:O	1:A:37:ARG:N	2.52	0.42
1:A:352:LEU:HD11	1:A:387:PRO:HG2	2.01	0.42
1:A:137:ARG:NH1	1:A:156:LEU:HD21	2.35	0.42
1:A:283:HIS:C	1:A:283:HIS:ND1	2.73	0.42
1:A:199:ILE:CG1	1:A:227:ALA:HB3	2.49	0.41
1:A:47:PHE:HB3	1:A:99:ILE:CD1	2.50	0.41
1:A:147:GLN:CD	1:A:180:ALA:HB2	2.41	0.41
1:A:34:THR:HG22	1:A:40:PRO:CA	2.34	0.41
1:A:99:ILE:HA	1:A:99:ILE:HD13	1.72	0.41
1:A:802:LEU:O	1:A:806:VAL:HG23	2.19	0.41
1:A:224:LEU:HG	1:A:225:LYS:H	1.85	0.41
1:A:647:PHE:O	1:A:649:VAL:HG13	2.20	0.41
1:A:209:GLU:H	1:A:209:GLU:CD	2.24	0.41
1:A:567:THR:O	1:A:568:ALA:HB3	2.21	0.41
1:A:795:ARG:HG3	1:A:795:ARG:HH11	1.85	0.41
1:A:354:LYS:HE3	1:A:354:LYS:HB3	1.93	0.41
1:A:193:LEU:N	1:A:194:PRO:HD3	2.34	0.41
1:A:828:LEU:O	1:A:828:LEU:HG	2.21	0.41
1:A:230:GLU:O	1:A:234:ALA:HB2	2.20	0.41
1:A:466:GLU:HA	1:A:469:ARG:NH1	2.35	0.41
1:A:419:ARG:NE	1:A:419:ARG:HA	2.36	0.41
1:A:501:PRO:HB2	1:A:502:ALA:H	1.60	0.41
1:A:811:TYR:HA	1:A:812:PRO:HD2	1.86	0.41
1:A:256:VAL:O	1:A:256:VAL:HG13	2.21	0.41
1:A:220:ASN:O	1:A:221:LEU:HB2	2.21	0.41
1:A:500:LEU:HA	1:A:501:PRO:HD3	1.84	0.41
1:A:175:ARG:HB2	1:A:177:ASP:OD1	2.21	0.41
1:A:174:LEU:HD12	1:A:178:GLN:CD	2.41	0.40
1:A:47:PHE:HB3	1:A:99:ILE:HD11	2.03	0.40
1:A:676:HIS:O	1:A:679:SER:HB3	2.21	0.40
1:A:573:ARG:NH1	4:A:1034:HOH:O	2.54	0.40
1:A:204:ALA:HA	1:A:211:TRP:HZ2	1.86	0.40
1:A:535:TYR:O	1:A:539:THR:HG23	2.21	0.40
1:A:185:LEU:HD12	1:A:185:LEU:O	2.21	0.40
1:A:794:GLU:O	1:A:795:ARG:HG2	2.21	0.40
1:A:193:LEU:HD13	1:A:242:SER:OG	2.22	0.40
1:A:199:ILE:HD11	1:A:226:PRO:HB2	2.03	0.40
1:A:512:ARG:O	1:A:512:ARG:HD2	2.22	0.40

There are no symmetry-related clashes.

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	803/832 (96%)	675 (84%)	92 (12%)	36 (4%)	3 2

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	87	PRO
1	A	161	TYR
1	A	208	LEU
1	A	220	ASN
1	A	221	LEU
1	A	256	VAL
1	A	292	LYS
1	A	299	TRP
1	A	487	ARG
1	A	501	PRO
1	A	674	SER
1	A	31	LYS
1	A	36	SER
1	A	188	ASP
1	A	203	THR
1	A	219	LYS
1	A	509	THR
1	A	58	ASP
1	A	197	LYS
1	A	204	ALA
1	A	227	ALA
1	A	486	SER
1	A	39	GLU
1	A	216	ALA

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Mol	Chain	Res	Type
1	A	831	LYS
1	A	199	ILE
1	A	300	PRO
1	A	118	ALA
1	A	287	LEU
1	A	507	GLU
1	A	673	MET
1	A	187	GLY
1	A	382	PRO
1	A	248	VAL
1	A	298	PRO

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	665/683 (97%)	590 (89%)	75 (11%)	7	10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	52	LEU
1	A	90	GLU
1	A	142	ASP
1	A	161	TYR
1	A	162	LEU
1	A	168	LEU
1	A	169	TRP
1	A	170	GLU
1	A	171	LYS
1	A	178	GLN
1	A	182	TYR
1	A	189	GLU
1	A	206	LYS
1	A	207	LEU

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Mol	Chain	Res	Type
1	A	209	GLU
1	A	211	TRP
1	A	217	LEU
1	A	229	ARG
1	A	233	LEU
1	A	235	HIS
1	A	243	TRP
1	A	245	LEU
1	A	247	LYS
1	A	257	ASP
1	A	262	ARG
1	A	283	HIS
1	A	288	LEU
1	A	292	LYS
1	A	328	ARG
1	A	337	GLU
1	A	365	LEU
1	A	419	ARG
1	A	420	LEU
1	A	435	ARG
1	A	449	VAL
1	A	453	VAL
1	A	457	ARG
1	A	460	SER
1	A	461	LEU
1	A	473	GLU
1	A	480	HIS
1	A	482	PHE
1	A	487	ARG
1	A	488	ASP
1	A	495	PHE
1	A	497	GLU
1	A	500	LEU
1	A	506	THR
1	A	509	THR
1	A	512	ARG
1	A	518	VAL
1	A	523	ARG
1	A	573	ARG
1	A	579	PRO
1	A	592	GLN
1	A	601	GLU

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Mol	Chain	Res	Type
1	A	644	SER
1	A	652	GLU
1	A	657	LEU
1	A	660	ARG
1	A	664	THR
1	A	670	LEU
1	A	681	GLU
1	A	682	LEU
1	A	684	ILE
1	A	699	SER
1	A	742	GLU
1	A	752	PRO
1	A	771	ARG
1	A	781	LEU
1	A	782	GLN
1	A	818	GLU
1	A	821	VAL
1	A	831	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	28	HIS
1	A	154	HIS
1	A	485	ASN
1	A	534	GLN
1	A	566	GLN
1	A	639	HIS
1	A	782	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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	BGL	A	833	-	19,20,20	1.15	1 (5%)	23,25,25	2.39	8 (34%)

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	BGL	A	833	-	-	0/11/31/31	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	833	BGL	C4-C5	3.46	1.60	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	833	BGL	O5-C5-C4	-3.90	102.36	109.68
2	A	833	BGL	C1-O5-C5	-3.70	106.62	113.47
2	A	833	BGL	C1-C2-C3	-3.01	105.14	110.45
2	A	833	BGL	C3-C4-C5	-2.74	105.43	110.20
2	A	833	BGL	O6-C6-C5	3.14	121.69	111.33
2	A	833	BGL	O4-C4-C3	3.26	117.68	110.34
2	A	833	BGL	O3-C3-C2	3.55	118.28	109.87
2	A	833	BGL	C6-C5-C4	5.69	127.05	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	833	BGL	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	807/832 (96%)	0.12	60 (7%)	17	17	10, 43, 98, 100	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	9.1
1	A	217	LEU	8.6
1	A	510	GLY	8.5
1	A	525	ALA	8.0
1	A	208	LEU	7.3
1	A	232	ILE	6.0
1	A	512	ARG	5.9
1	A	529	VAL	5.9
1	A	514	THR	5.9
1	A	506	THR	5.7
1	A	233	LEU	5.5
1	A	198	GLY	5.4
1	A	501	PRO	5.4
1	A	236	MET	5.1
1	A	203	THR	5.1
1	A	515	SER	5.1
1	A	227	ALA	5.0
1	A	226	PRO	5.0
1	A	511	LYS	4.7
1	A	199	ILE	4.6
1	A	194	PRO	4.6
1	A	509	THR	4.4
1	A	504	GLY	4.2
1	A	513	SER	4.1
1	A	519	LEU	4.0
1	A	229	ARG	4.0
1	A	516	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	211	TRP	3.9
1	A	202	LYS	3.3
1	A	508	LYS	3.3
1	A	528	ILE	3.3
1	A	507	GLU	3.3
1	A	68	ALA	3.2
1	A	478	ALA	3.2
1	A	524	GLU	3.2
1	A	502	ALA	3.2
1	A	522	LEU	3.2
1	A	470	LEU	3.1
1	A	526	HIS	3.0
1	A	197	LYS	3.0
1	A	225	LYS	3.0
1	A	235	HIS	2.9
1	A	196	VAL	2.9
1	A	169	TRP	2.8
1	A	503	ILE	2.7
1	A	185	LEU	2.7
1	A	527	PRO	2.6
1	A	505	LYS	2.6
1	A	218	LEU	2.4
1	A	673	MET	2.4
1	A	498	LEU	2.3
1	A	496	ASP	2.3
1	A	748	ALA	2.2
1	A	290	SER	2.2
1	A	85	ARG	2.2
1	A	497	GLU	2.2
1	A	148	LEU	2.1
1	A	293	ALA	2.1
1	A	216	ALA	2.1
1	A	200	GLY	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.

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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
3	ZN	A	900	1/1	0.75	0.39	4.98	58,58,58,58	0
2	BGL	A	833	20/20	0.97	0.12	0.49	2,24,46,57	0

6.5 Other polymers (i)

There are no such residues in this entry.