Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BLP
Title	:	STRUCTURAL BASIS FOR THE INACTIVATION OF THE P54 MUTANT OF BETA-LACTAMASE FROM STAPHYLOCOCCUS AUREUS PC1
Authors	:	Herzberg, O.
Deposited on	:	1993-09-23
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

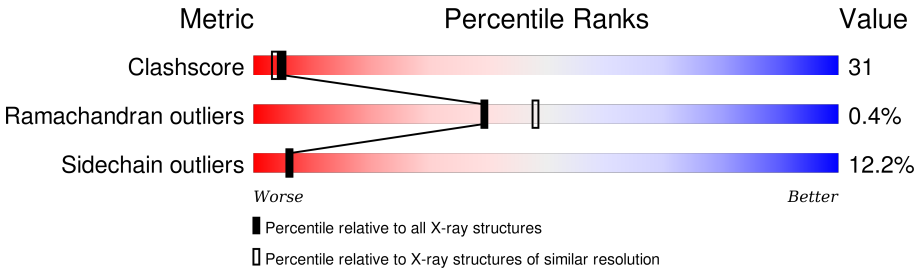
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	257	47% 38% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2108 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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1982	1264	334	381	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ASN	ASP	ENGINEERED MUTATION	UNP P00807

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		

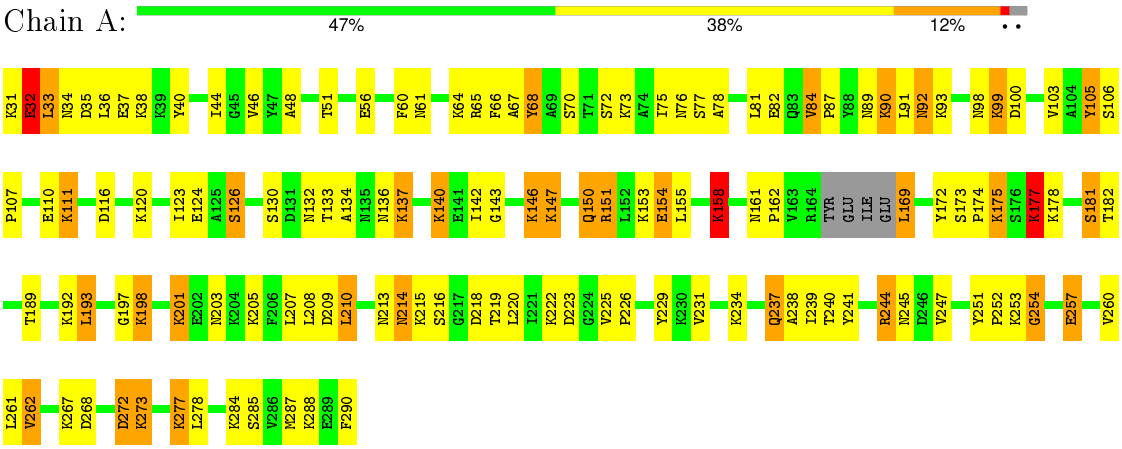
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

- Molecule 1: BETA-LACTAMASE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	54.90Å 96.00Å 137.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2108	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.24	3/2010 (0.1%)	1.82	38/2697 (1.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	SER	CA-CB	7.29	1.63	1.52
1	A	181	SER	CB-OG	5.83	1.49	1.42
1	A	70	SER	CB-OG	5.59	1.49	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	LYS	N-CA-CB	10.01	128.61	110.60
1	A	151	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	A	68	TYR	CB-CG-CD1	-7.86	116.29	121.00
1	A	261	LEU	CB-CA-C	7.45	124.36	110.20
1	A	40	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	A	65	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	234	LYS	N-CA-CB	7.21	123.58	110.60
1	A	37	GLU	CG-CD-OE2	7.15	132.59	118.30
1	A	244	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	154	GLU	OE1-CD-OE2	6.96	131.65	123.30
1	A	158	LYS	CA-CB-CG	6.86	128.49	113.40
1	A	238	ALA	CB-CA-C	6.54	119.90	110.10
1	A	105	TYR	N-CA-CB	6.47	122.24	110.60
1	A	100	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	268	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	177	LYS	CA-CB-CG	6.10	126.83	113.40
1	A	98	ASN	N-CA-CB	6.10	121.58	110.60
1	A	134	ALA	N-CA-CB	6.09	118.63	110.10
1	A	290	PHE	CB-CA-C	6.09	122.58	110.40
1	A	137	LYS	N-CA-CB	6.08	121.54	110.60
1	A	257	GLU	CG-CD-OE1	6.00	130.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	273	LYS	N-CA-CB	5.85	121.13	110.60
1	A	214	ASN	CB-CA-C	5.64	121.69	110.40
1	A	210	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	116	ASP	N-CA-CB	5.51	120.53	110.60
1	A	237	GLN	OE1-CD-NE2	5.46	134.46	121.90
1	A	245	ASN	CB-CG-ND2	5.45	129.79	116.70
1	A	262	VAL	O-C-N	5.42	131.38	122.70
1	A	35	ASP	O-C-N	5.38	131.31	122.70
1	A	35	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	272	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	32	GLU	CG-CD-OE1	5.26	128.82	118.30
1	A	220	LEU	CB-CA-C	5.25	120.18	110.20
1	A	237	GLN	CB-CA-C	-5.25	99.90	110.40
1	A	181	SER	N-CA-CB	5.21	118.32	110.50
1	A	150	GLN	CA-CB-CG	5.10	124.63	113.40
1	A	51	THR	OG1-CB-CG2	5.07	121.67	110.00
1	A	37	GLU	CG-CD-OE1	-5.03	108.25	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	1982	0	2069	126	0
2	A	126	0	0	13	0
All	All	2108	0	2069	126	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 31.

All (126) 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:146:LYS:HD2	1:A:147:LYS:HG2	1.26	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HB2	1:A:177:LYS:NZ	1.74	1.01
1:A:64:LYS:HB2	2:A:307:HOH:O	1.60	1.00
1:A:198:LYS:N	1:A:198:LYS:HE3	1.79	0.97
1:A:146:LYS:HD2	1:A:147:LYS:CG	1.95	0.96
1:A:68:TYR:OH	1:A:162:PRO:HA	1.65	0.95
1:A:110:GLU:HG3	1:A:111:LYS:HD2	1.57	0.87
1:A:169:LEU:N	2:A:416:HOH:O	2.10	0.84
1:A:198:LYS:HE3	1:A:198:LYS:H	1.40	0.84
1:A:146:LYS:CD	1:A:147:LYS:HG2	2.10	0.81
1:A:89:ASN:ND2	1:A:90:LYS:HD2	1.96	0.80
1:A:222:LYS:HE3	1:A:231:VAL:O	1.82	0.79
1:A:105:TYR:CZ	1:A:107:PRO:HG3	2.19	0.77
1:A:201:LYS:CE	1:A:205:LYS:HD2	2.16	0.75
1:A:44:ILE:HD11	1:A:278:LEU:HD11	1.70	0.74
1:A:177:LYS:HB2	1:A:177:LYS:HZ3	1.49	0.73
1:A:201:LYS:HA	1:A:201:LYS:HE3	1.72	0.72
1:A:146:LYS:HG3	1:A:147:LYS:H	1.57	0.69
1:A:33:LEU:HD12	1:A:36:LEU:HD12	1.73	0.69
1:A:215:LYS:HE2	1:A:215:LYS:HA	1.73	0.69
1:A:64:LYS:HD3	1:A:66:PHE:CZ	2.30	0.67
1:A:257:GLU:OE1	2:A:292:HOH:O	2.13	0.66
1:A:92:ASN:ND2	2:A:345:HOH:O	2.27	0.66
1:A:87:PRO:HB2	1:A:89:ASN:OD1	1.96	0.65
1:A:177:LYS:HB2	1:A:177:LYS:HZ2	1.62	0.65
1:A:189:THR:O	1:A:193:LEU:HB2	1.96	0.65
1:A:150:GLN:O	1:A:154:GLU:HG3	1.97	0.65
1:A:175:LYS:HA	1:A:175:LYS:NZ	2.12	0.64
1:A:198:LYS:N	1:A:198:LYS:CE	2.56	0.64
1:A:175:LYS:N	1:A:175:LYS:HD2	2.13	0.63
1:A:222:LYS:CE	1:A:231:VAL:O	2.46	0.63
1:A:207:LEU:HA	1:A:210:LEU:HD12	1.79	0.63
1:A:151:ARG:HH21	1:A:198:LYS:HD2	1.64	0.62
1:A:229:TYR:HE2	1:A:287:MET:CE	2.12	0.62
1:A:87:PRO:HG2	1:A:90:LYS:NZ	2.16	0.60
1:A:155:LEU:O	1:A:192:LYS:HE3	2.02	0.59
1:A:82:GLU:OE2	2:A:293:HOH:O	2.16	0.59
1:A:229:TYR:HE2	1:A:287:MET:HE2	1.67	0.58
1:A:103:VAL:O	1:A:106:SER:OG	2.20	0.58
1:A:126:SER:O	1:A:130:SER:HA	2.04	0.57
1:A:105:TYR:HB3	1:A:132:ASN:HD22	1.68	0.57
1:A:198:LYS:HE3	2:A:293:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HE2	2:A:315:HOH:O	2.06	0.56
1:A:146:LYS:HG2	2:A:402:HOH:O	2.05	0.56
1:A:64:LYS:HD3	1:A:66:PHE:HZ	1.70	0.56
1:A:89:ASN:CG	1:A:90:LYS:HD2	2.25	0.56
1:A:201:LYS:HE3	1:A:205:LYS:HD2	1.86	0.56
1:A:136:ASN:O	1:A:140:LYS:HG2	2.05	0.56
1:A:48:ALA:HA	1:A:260:VAL:O	2.06	0.56
1:A:99:LYS:HE2	1:A:99:LYS:O	2.05	0.56
1:A:192:LYS:NZ	2:A:387:HOH:O	2.39	0.55
1:A:151:ARG:NH2	1:A:198:LYS:HD2	2.22	0.54
1:A:89:ASN:HD21	1:A:90:LYS:HD2	1.70	0.54
1:A:229:TYR:CE2	1:A:287:MET:HE2	2.41	0.54
1:A:87:PRO:HG2	1:A:90:LYS:HZ1	1.73	0.53
1:A:201:LYS:O	1:A:205:LYS:HD3	2.09	0.53
1:A:201:LYS:HG3	1:A:205:LYS:HE2	1.90	0.53
1:A:209:ASP:OD2	2:A:412:HOH:O	2.18	0.52
1:A:120:LYS:O	1:A:124:GLU:HG3	2.09	0.52
1:A:219:THR:OG1	2:A:397:HOH:O	2.19	0.51
1:A:75:ILE:O	1:A:78:ALA:HB3	2.10	0.51
1:A:105:TYR:CE1	1:A:107:PRO:HG3	2.45	0.51
1:A:175:LYS:HZ3	1:A:175:LYS:HA	1.75	0.51
1:A:201:LYS:HG3	1:A:205:LYS:CD	2.40	0.50
1:A:285:SER:O	1:A:288:LYS:HB2	2.11	0.50
1:A:197:GLY:C	1:A:198:LYS:HE3	2.30	0.50
1:A:161:ASN:ND2	1:A:178:LYS:HA	2.27	0.50
1:A:81:LEU:HD21	1:A:123:ILE:HD13	1.93	0.50
1:A:237:GLN:HG3	1:A:244:ARG:HD2	1.93	0.49
1:A:201:LYS:HE2	1:A:205:LYS:HD2	1.91	0.48
1:A:169:LEU:CA	2:A:416:HOH:O	2.58	0.48
1:A:68:TYR:HH	1:A:162:PRO:HA	1.73	0.48
1:A:192:LYS:CE	2:A:387:HOH:O	2.61	0.47
1:A:174:PRO:HD3	1:A:241:TYR:CE2	2.49	0.47
1:A:247:VAL:HG12	1:A:262:VAL:HG13	1.95	0.47
1:A:143:GLY:O	1:A:147:LYS:HG3	2.14	0.47
1:A:237:GLN:HG3	1:A:244:ARG:HH11	1.79	0.47
1:A:172:TYR:O	1:A:240:THR:OG1	2.27	0.46
1:A:267:LYS:HD2	1:A:272:ASP:HB3	1.97	0.46
1:A:197:GLY:CA	1:A:198:LYS:HE3	2.45	0.46
1:A:201:LYS:CG	1:A:205:LYS:HE2	2.46	0.46
1:A:209:ASP:OD1	1:A:213:ASN:ND2	2.50	0.45
1:A:215:LYS:HA	1:A:218:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:O	1:A:158:LYS:NZ	2.43	0.45
1:A:91:LEU:HB3	1:A:120:LYS:HB2	1.97	0.45
1:A:201:LYS:HA	1:A:201:LYS:CE	2.43	0.45
1:A:222:LYS:HG3	1:A:231:VAL:HG11	1.99	0.45
1:A:201:LYS:O	1:A:205:LYS:CD	2.65	0.45
1:A:229:TYR:CE2	1:A:287:MET:CE	2.98	0.45
1:A:64:LYS:HG2	1:A:66:PHE:CE1	2.52	0.45
1:A:215:LYS:HE2	1:A:215:LYS:CA	2.46	0.45
1:A:146:LYS:HD2	1:A:147:LYS:CD	2.47	0.44
1:A:222:LYS:HG3	1:A:231:VAL:CG1	2.48	0.44
1:A:84:VAL:O	1:A:203:ASN:ND2	2.49	0.44
1:A:68:TYR:HE1	1:A:72:SER:HB3	1.82	0.44
1:A:146:LYS:HG3	1:A:147:LYS:N	2.29	0.43
1:A:103:VAL:HG22	1:A:133:THR:CA	2.49	0.43
1:A:77:SER:O	1:A:81:LEU:HG	2.19	0.43
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.73	0.43
1:A:60:PHE:CE1	1:A:61:ASN:ND2	2.87	0.43
1:A:251:TYR:HA	1:A:252:PRO:HD3	1.88	0.43
1:A:76:ASN:O	1:A:142:ILE:HD11	2.19	0.42
1:A:146:LYS:CG	1:A:147:LYS:H	2.30	0.42
1:A:229:TYR:CD1	1:A:229:TYR:N	2.87	0.42
1:A:99:LYS:HE2	1:A:99:LYS:CA	2.49	0.42
1:A:253:LYS:O	1:A:254:GLY:C	2.58	0.42
1:A:192:LYS:O	1:A:197:GLY:HA2	2.20	0.42
1:A:103:VAL:HG22	1:A:133:THR:HA	2.01	0.42
1:A:143:GLY:O	1:A:146:LYS:HE3	2.20	0.41
1:A:173:SER:C	1:A:175:LYS:H	2.22	0.41
1:A:201:LYS:CA	1:A:201:LYS:HE3	2.47	0.41
1:A:48:ALA:O	1:A:56:GLU:HA	2.21	0.41
1:A:201:LYS:HG3	1:A:205:LYS:CE	2.50	0.41
1:A:223:ASP:OD2	1:A:277:LYS:NZ	2.52	0.41
1:A:61:ASN:O	1:A:64:LYS:HB3	2.20	0.41
1:A:44:ILE:HG22	1:A:46:VAL:HG23	2.02	0.41
1:A:105:TYR:C	1:A:107:PRO:HD3	2.41	0.41
1:A:201:LYS:HD3	1:A:205:LYS:HE2	2.03	0.41
1:A:237:GLN:HG3	1:A:244:ARG:CD	2.51	0.41
1:A:67:ALA:HB2	1:A:172:TYR:CD1	2.56	0.41
1:A:181:SER:OG	1:A:182:THR:N	2.54	0.41
1:A:92:ASN:HD22	1:A:92:ASN:N	2.19	0.40
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.88	0.40
1:A:105:TYR:HB3	1:A:132:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TYR:HD1	1:A:229:TYR:N	2.19	0.40
1:A:32:GLU:HG2	1:A:34:ASN:HD22	1.87	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	249/257 (97%)	241 (97%)	7 (3%)	1 (0%)	39 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	GLY

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	221/227 (97%)	194 (88%)	27 (12%)	6 6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS

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Mol	Chain	Res	Type
1	A	32	GLU
1	A	33	LEU
1	A	38	LYS
1	A	73	LYS
1	A	84	VAL
1	A	90	LYS
1	A	92	ASN
1	A	93	LYS
1	A	99	LYS
1	A	111	LYS
1	A	137	LYS
1	A	140	LYS
1	A	146	LYS
1	A	147	LYS
1	A	158	LYS
1	A	169	LEU
1	A	175	LYS
1	A	177	LYS
1	A	193	LEU
1	A	198	LYS
1	A	201	LYS
1	A	214	ASN
1	A	216	SER
1	A	239	ILE
1	A	277	LYS
1	A	284	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	92	ASN
1	A	136	ASN
1	A	161	ASN
1	A	213	ASN
1	A	245	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.