



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 1XX2 / pdb_00001xx2
Title : Refinement of P99 beta-lactamase from *Enterobacter cloacae*
Authors : Knox, J.R.; Sun, T.
Deposited on : 2004-11-03
Resolution : 1.88 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

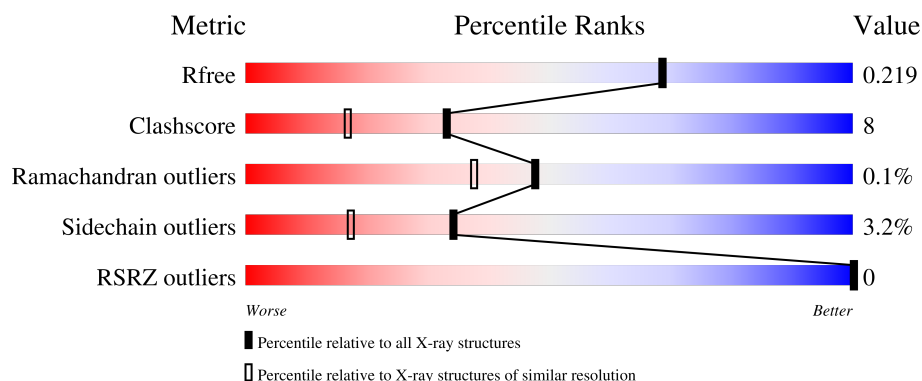
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	361	 78% 19% ..
1	B	361	 79% 18% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6085 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	359	Total	C	N	O	S	0	9	0
			2828	1816	480	520	12			
1	B	359	Total	C	N	O	S	0	8	0
			2817	1806	478	521	12			

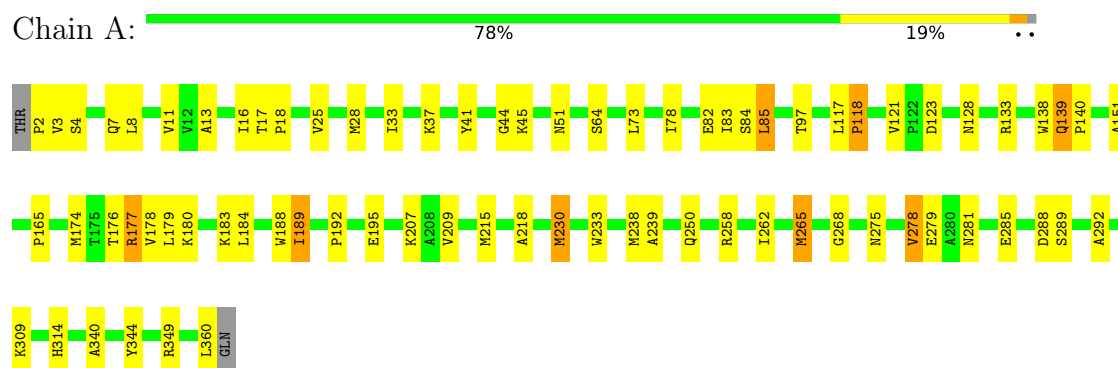
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	242	Total	O	0	0
			242	242		
2	B	198	Total	O	0	0
			198	198		

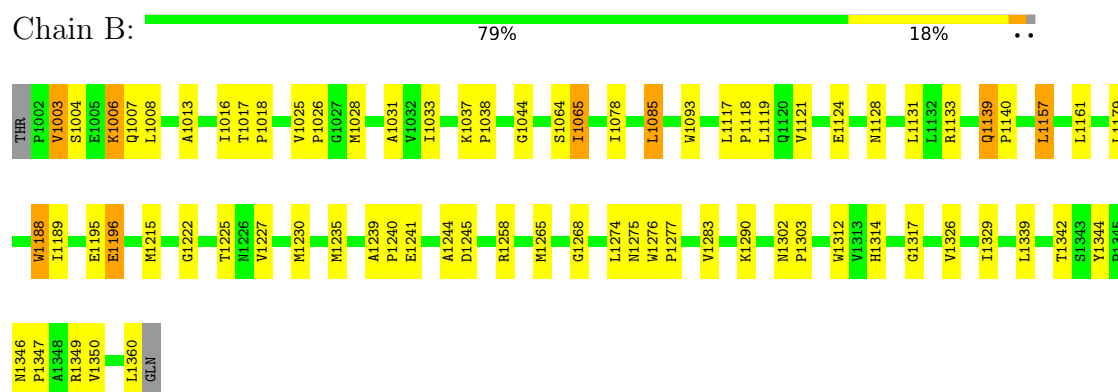
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.50Å 83.47Å 95.46Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	10.00 – 1.88 10.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	77.4 (10.00-1.88) 77.4 (10.00-1.88)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.53 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.214 0.180 , 0.219	Depositor DCC
R_{free} test set	2293 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6085	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.47	0/2904	1.03	19/3965 (0.5%)
1	B	0.47	0/2893	1.04	26/3951 (0.7%)
All	All	0.47	0/5797	1.03	45/7916 (0.6%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ILE	N-CA-C	-10.93	102.41	111.81
1	B	1189	ILE	N-CA-C	-10.88	102.45	111.81
1	A	121	VAL	N-CA-C	-10.17	99.89	108.63
1	B	1121	VAL	N-CA-C	-9.06	100.84	108.63
1	A	25	VAL	CA-C-N	8.03	127.32	118.97
1	A	25	VAL	C-N-CA	8.03	127.32	118.97
1	B	1239	ALA	CA-C-N	7.21	127.22	119.28
1	B	1239	ALA	C-N-CA	7.21	127.22	119.28
1	B	1016	ILE	N-CA-C	7.20	117.99	110.72
1	A	16	ILE	N-CA-C	7.14	117.94	110.72
1	B	1044	GLY	N-CA-C	7.05	125.14	112.02
1	B	1314	HIS	N-CA-C	6.69	117.42	108.38
1	A	97	THR	N-CA-C	6.32	120.99	113.28
1	B	1268	GLY	N-CA-C	-6.29	105.24	112.79
1	A	268	GLY	N-CA-C	-6.01	105.57	112.79
1	A	37	LYS	CA-C-N	5.85	127.15	119.84
1	A	37	LYS	C-N-CA	5.85	127.15	119.84
1	A	64	SER	N-CA-C	5.82	119.85	112.87
1	B	1064	SER	N-CA-C	5.79	119.44	112.38
1	A	292	ALA	N-CA-C	5.71	117.50	111.28
1	A	314	HIS	N-CA-C	5.67	117.41	108.96
1	A	178	VAL	N-CA-C	5.65	116.09	111.62
1	B	1244	ALA	N-CA-C	5.64	117.51	111.36
1	B	1117	LEU	CA-C-N	5.60	125.54	119.78
1	B	1117	LEU	C-N-CA	5.60	125.54	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1329	ILE	CA-C-N	5.54	125.64	119.32
1	B	1329	ILE	C-N-CA	5.54	125.64	119.32
1	A	118	PRO	N-CA-C	5.46	119.90	111.21
1	B	1139	GLN	CA-C-N	5.46	125.38	119.76
1	B	1139	GLN	C-N-CA	5.46	125.38	119.76
1	A	44	GLY	N-CA-C	5.42	123.89	112.17
1	B	1196	GLU	N-CA-C	5.37	117.83	111.33
1	B	1312	TRP	N-CA-C	-5.33	99.09	108.20
1	A	239	ALA	CA-C-N	5.32	124.98	119.56
1	A	239	ALA	C-N-CA	5.32	124.98	119.56
1	B	1222	GLY	N-CA-C	5.20	123.93	115.46
1	B	1006	LYS	N-CA-C	-5.18	105.70	112.23
1	B	1117	LEU	N-CA-C	-5.17	103.26	109.83
1	A	188	TRP	N-CA-C	5.11	116.95	109.24
1	A	117	LEU	N-CA-C	-5.09	103.17	109.64
1	B	1179	LEU	N-CA-C	5.09	116.52	111.07
1	B	1118	PRO	N-CA-C	5.08	119.30	111.21
1	B	1093	TRP	CA-C-N	5.06	124.72	119.56
1	B	1093	TRP	C-N-CA	5.06	124.72	119.56
1	B	1065	ILE	N-CA-C	-5.05	106.44	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2828	0	2815	51	0
1	B	2817	0	2795	37	0
2	A	242	0	0	5	0
2	B	198	0	0	3	0
All	All	6085	0	5610	88	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 8.

All (88) 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:258:ARG:HH12	1:A:275:ASN:HD21	1.06	0.91
1:B:1258:ARG:HH12	1:B:1275:ASN:HD21	1.22	0.87
1:A:275:ASN:O	1:A:278[A]:VAL:HG13	1.76	0.85
1:B:1283:VAL:HG12	1:B:1350:VAL:HG11	1.60	0.81
1:A:258:ARG:HH12	1:A:275:ASN:ND2	1.83	0.75
1:A:33:ILE:HG21	1:A:238:MET:HE1	1.69	0.74
1:A:258:ARG:NH1	1:A:275:ASN:HD21	1.86	0.73
1:A:230:MET:HE3	1:A:230:MET:HA	1.69	0.73
1:B:1128:ASN:HB2	2:B:295:HOH:O	1.89	0.71
1:A:230:MET:HA	1:A:230:MET:CE	2.23	0.68
1:A:45[B]:LYS:HZ3	1:A:51:ASN:HD21	1.46	0.63
1:B:1196:GLU:HG3	2:B:396:HOH:O	2.00	0.62
1:A:45[B]:LYS:NZ	1:A:51:ASN:HD21	1.97	0.60
1:A:82:GLU:O	1:A:83[B]:ILE:HD12	2.02	0.59
1:A:128:ASN:HB2	2:A:441:HOH:O	2.02	0.58
1:B:1157:LEU:HD22	1:B:1161:LEU:HG	1.86	0.58
1:A:7:GLN:O	1:A:11:VAL:HG23	2.04	0.58
1:A:13:ALA:O	1:A:17:THR:HG23	2.04	0.57
1:A:189:ILE:HD13	1:A:218:ALA:HB1	1.86	0.56
1:A:139:GLN:HG2	2:A:488:HOH:O	2.05	0.56
1:A:258:ARG:HH22	1:A:275:ASN:HD22	1.53	0.56
1:A:83[B]:ILE:CD1	1:A:165:PRO:HG2	2.38	0.54
1:A:258:ARG:HH22	1:A:275:ASN:ND2	2.05	0.54
1:B:1230:MET:CE	1:B:1326[B]:VAL:HG11	2.37	0.54
1:B:1004:SER:HB3	1:B:1007:GLN:HB2	1.89	0.54
1:B:1017:THR:OG1	1:B:1018:PRO:HD3	2.08	0.53
1:B:1033:ILE:HD13	1:B:1235:MET:HG3	1.89	0.53
1:B:1028:MET:HG3	1:B:1339:LEU:O	2.10	0.52
1:A:344:TYR:CE2	1:A:349:ARG:HG2	2.44	0.52
1:A:309[A]:LYS:N	1:A:309[A]:LYS:HD2	2.25	0.52
1:A:78:ILE:HG12	1:A:83[B]:ILE:HG22	1.92	0.52
1:B:1133[B]:ARG:NH1	2:B:242:HOH:O	2.43	0.51
1:A:207:LYS:HG2	1:A:209:VAL:HG13	1.92	0.51
1:A:281:ASN:O	1:A:285:GLU:HG2	2.10	0.51
1:B:1225:THR:HG21	1:B:1230:MET:HG2	1.93	0.50
1:A:192:PRO:HG2	1:A:195[B]:GLU:HB2	1.93	0.50
1:B:1258:ARG:HH12	1:B:1275:ASN:ND2	2.02	0.50
1:B:1230:MET:CE	1:B:1326[A]:VAL:HG21	2.42	0.49
1:A:183:LYS:N	1:A:183:LYS:HD2	2.27	0.49
1:B:1346:ASN:HB2	1:B:1347:PRO:HD3	1.94	0.49
1:A:45[B]:LYS:NZ	1:A:51:ASN:ND2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1188:TRP:CZ2	1:B:1195[A]:GLU:HG3	2.49	0.48
1:A:2:PRO:O	1:A:3:VAL:C	2.56	0.48
1:B:1037:LYS:HG2	1:B:1038:PRO:HD2	1.94	0.48
1:A:133[A]:ARG:HH11	1:A:133[A]:ARG:HG3	1.79	0.47
1:A:8:LEU:HD23	1:A:41:TYR:OH	2.15	0.47
1:A:138:TRP:CH2	1:A:140:PRO:HB3	2.50	0.47
1:B:1302:ASN:HA	1:B:1303:PRO:C	2.39	0.47
1:B:1302:ASN:OD1	1:B:1303:PRO:HA	2.15	0.46
1:A:73:LEU:HD22	1:A:174:MET:HE2	1.98	0.45
1:B:1065:ILE:HG13	1:B:1317:GLY:HA3	1.98	0.45
1:A:4:SER:HB3	1:A:7:GLN:HB2	1.99	0.45
1:A:78:ILE:HD11	1:A:85:LEU:HD13	1.99	0.45
1:A:17:THR:OG1	1:A:18:PRO:HD3	2.16	0.45
1:B:1131:LEU:HD13	1:B:1215:MET:HG2	1.99	0.45
1:B:1031:ALA:HB2	1:B:1227:VAL:HG22	1.99	0.44
1:A:177:ARG:HD3	2:A:583:HOH:O	2.17	0.44
1:A:133[B]:ARG:NH1	2:A:574:HOH:O	2.50	0.44
1:A:83[B]:ILE:HG23	1:A:84:SER:N	2.32	0.44
1:A:118:PRO:O	1:A:151:ALA:HB1	2.17	0.44
1:B:1225:THR:CG2	1:B:1230:MET:HG2	2.48	0.44
1:A:28:MET:HE2	1:A:340:ALA:HB2	2.00	0.44
1:A:192:PRO:HG2	1:A:195[A]:GLU:HB2	2.00	0.43
1:A:4:SER:HB3	1:A:7:GLN:OE1	2.18	0.43
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.34	0.43
1:B:1290:LYS:HE2	1:B:1290:LYS:HB3	1.63	0.43
1:B:1025:VAL:HA	1:B:1026:PRO:HD3	1.89	0.43
1:B:1276:TRP:CD2	1:B:1277:PRO:HA	2.54	0.42
1:B:1344:TYR:CZ	1:B:1349:ARG:HG2	2.54	0.42
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.54	0.42
1:B:1004:SER:HB3	1:B:1007:GLN:HE21	1.85	0.42
1:B:1003:VAL:HG12	1:B:1004:SER:O	2.19	0.42
1:B:1346:ASN:N	1:B:1347:PRO:CD	2.82	0.42
1:A:8:LEU:CD1	1:A:360:LEU:HD21	2.50	0.42
1:A:262:ILE:HD12	1:A:262:ILE:N	2.35	0.41
1:A:176:THR:HA	1:A:180:LYS:HE3	2.02	0.41
1:A:265:MET:HE3	2:A:527:HOH:O	2.20	0.41
1:A:230:MET:HE2	1:A:233:TRP:HB3	2.03	0.41
1:B:1008:LEU:HD13	1:B:1360:LEU:HD21	2.02	0.41
1:B:1139:GLN:HA	1:B:1140:PRO:HD3	1.87	0.41
1:B:1078:ILE:HD13	1:B:1085:LEU:HD22	2.02	0.41
1:B:1240:PRO:HD2	1:B:1241:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1258:ARG:HH22	1:B:1275:ASN:HD22	1.69	0.41
1:A:288:ASP:OD2	1:A:289:SER:N	2.54	0.41
1:B:1025:VAL:HG13	1:B:1342:THR:HG22	2.03	0.40
1:A:33:ILE:CG2	1:A:238:MET:HE1	2.46	0.40
1:A:179:LEU:HD23	1:A:184:LEU:HD12	2.03	0.40
1:B:1013:ALA:O	1:B:1017:THR:HG23	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	366/361 (101%)	358 (98%)	8 (2%)	0	100	100
1	B	365/361 (101%)	357 (98%)	7 (2%)	1 (0%)	36	26
All	All	731/722 (101%)	715 (98%)	15 (2%)	1 (0%)	48	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1003	VAL

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	294/287 (102%)	284 (97%)	10 (3%)	32	16
1	B	293/287 (102%)	284 (97%)	9 (3%)	35	18
All	All	587/574 (102%)	568 (97%)	19 (3%)	34	17

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	123	ASP
1	A	139	GLN
1	A	177	ARG
1	A	215	MET
1	A	230	MET
1	A	265	MET
1	A	278[A]	VAL
1	A	278[B]	VAL
1	A	279	GLU
1	B	1006	LYS
1	B	1085	LEU
1	B	1119	LEU
1	B	1124	GLU
1	B	1157	LEU
1	B	1188	TRP
1	B	1245	ASP
1	B	1265	MET
1	B	1274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	GLN
1	A	51	ASN
1	A	57	GLN
1	A	137	ASN
1	A	186	HIS
1	A	190	ASN
1	A	242	ASN
1	A	250	GLN
1	A	275	ASN
1	B	1007	GLN

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Mol	Chain	Res	Type
1	B	1035	GLN
1	B	1051	ASN
1	B	1057	GLN
1	B	1095	GLN
1	B	1128	ASN
1	B	1137	ASN
1	B	1190	ASN
1	B	1228	GLN
1	B	1256	GLN
1	B	1275	ASN
1	B	1281	ASN
1	B	1346	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	359/361 (99%)	-1.94	0 100 100	8, 21, 40, 80	9 (2%)
1	B	359/361 (99%)	-1.94	0 100 100	8, 20, 38, 69	9 (2%)
All	All	718/722 (99%)	-1.94	0 100 100	8, 21, 39, 80	18 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.