



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:41 pm GMT

PDB ID : 3TG9
Title : The crystal structure of penicillin binding protein from *Bacillus halodurans*
Authors : Zhang, Z.; Satyanarayana, L.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-08-17
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

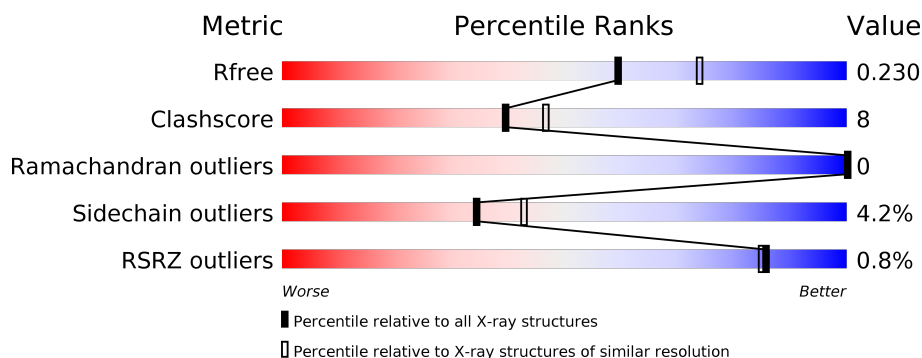
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	356	
1	B	356	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5404 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 Penicillin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2551	1650	420	465	16			
1	B	326	Total	C	N	O	S	0	0	0
			2586	1672	422	477	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q9KAM0
A	0	VAL	-	EXPRESSION TAG	UNP Q9KAM0
A	333	ALA	-	EXPRESSION TAG	UNP Q9KAM0
A	334	GLU	-	EXPRESSION TAG	UNP Q9KAM0
A	335	ASN	-	EXPRESSION TAG	UNP Q9KAM0
A	336	LEU	-	EXPRESSION TAG	UNP Q9KAM0
A	337	TYR	-	EXPRESSION TAG	UNP Q9KAM0
A	338	PHE	-	EXPRESSION TAG	UNP Q9KAM0
A	339	GLN	-	EXPRESSION TAG	UNP Q9KAM0
A	340	SER	-	EXPRESSION TAG	UNP Q9KAM0
A	341	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	342	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	343	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	344	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	345	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	346	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	347	TRP	-	EXPRESSION TAG	UNP Q9KAM0
A	348	SER	-	EXPRESSION TAG	UNP Q9KAM0
A	349	HIS	-	EXPRESSION TAG	UNP Q9KAM0
A	350	PRO	-	EXPRESSION TAG	UNP Q9KAM0
A	351	GLN	-	EXPRESSION TAG	UNP Q9KAM0
A	352	PHE	-	EXPRESSION TAG	UNP Q9KAM0
A	353	GLU	-	EXPRESSION TAG	UNP Q9KAM0
A	354	LYS	-	EXPRESSION TAG	UNP Q9KAM0
B	-1	MET	-	EXPRESSION TAG	UNP Q9KAM0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP Q9KAM0
B	333	ALA	-	EXPRESSION TAG	UNP Q9KAM0
B	334	GLU	-	EXPRESSION TAG	UNP Q9KAM0
B	335	ASN	-	EXPRESSION TAG	UNP Q9KAM0
B	336	LEU	-	EXPRESSION TAG	UNP Q9KAM0
B	337	TYR	-	EXPRESSION TAG	UNP Q9KAM0
B	338	PHE	-	EXPRESSION TAG	UNP Q9KAM0
B	339	GLN	-	EXPRESSION TAG	UNP Q9KAM0
B	340	SER	-	EXPRESSION TAG	UNP Q9KAM0
B	341	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	342	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	343	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	344	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	345	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	346	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	347	TRP	-	EXPRESSION TAG	UNP Q9KAM0
B	348	SER	-	EXPRESSION TAG	UNP Q9KAM0
B	349	HIS	-	EXPRESSION TAG	UNP Q9KAM0
B	350	PRO	-	EXPRESSION TAG	UNP Q9KAM0
B	351	GLN	-	EXPRESSION TAG	UNP Q9KAM0
B	352	PHE	-	EXPRESSION TAG	UNP Q9KAM0
B	353	GLU	-	EXPRESSION TAG	UNP Q9KAM0
B	354	LYS	-	EXPRESSION TAG	UNP Q9KAM0

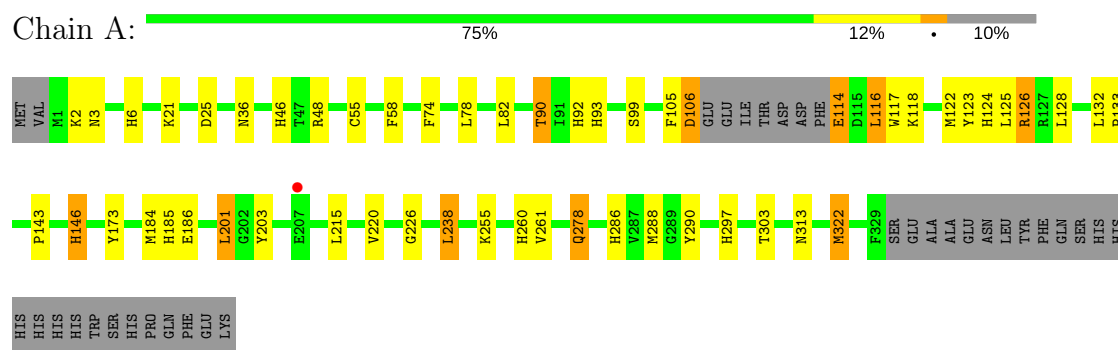
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	161	Total O 161 161	0	0
2	B	106	Total O 106 106	0	0

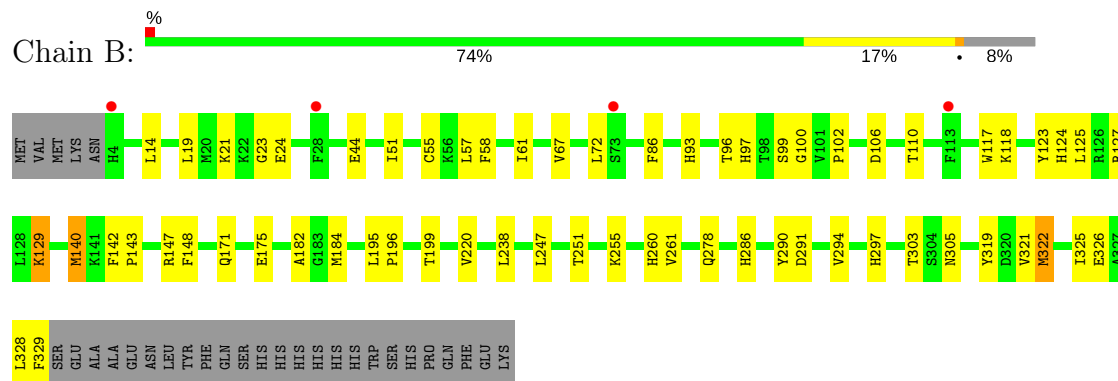
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Penicillin-binding protein



• Molecule 1: Penicillin-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.24Å 79.80Å 74.44Å 90.00° 100.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.20) 99.8 (50.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.230	Depositor DCC
R_{free} test set	1915 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5404	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/2629	0.56	1/3573 (0.0%)
1	B	0.33	0/2666	0.51	0/3627
All	All	0.36	0/5295	0.53	1/7200 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LEU	CA-CB-CG	-5.40	102.88	115.30

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	2551	0	2449	46	0
1	B	2586	0	2466	42	0
2	A	161	0	0	6	0
2	B	106	0	0	5	0
All	All	5404	0	4915	84	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 (84) 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:105:PHE:HA	1:A:106:ASP:HB2	1.15	1.12
1:A:105:PHE:HA	1:A:106:ASP:CB	1.93	0.99
1:A:3:ASN:H	1:A:6:HIS:HD2	1.15	0.89
1:A:3:ASN:H	1:A:6:HIS:CD2	1.89	0.88
1:A:105:PHE:CA	1:A:106:ASP:HB2	2.01	0.87
1:A:118:LYS:HA	1:B:124:HIS:HE1	1.39	0.87
1:A:114:GLU:HB2	1:A:117:TRP:H	1.38	0.87
1:B:102:PRO:HD3	1:B:140:MET:HE2	1.60	0.83
1:A:118:LYS:HA	1:B:124:HIS:CE1	2.19	0.77
1:B:129:LYS:HG3	2:B:434:HOH:O	1.84	0.76
1:B:297:HIS:HD2	2:B:437:HOH:O	1.68	0.76
1:A:124:HIS:HE1	1:B:118:LYS:HA	1.55	0.71
1:A:290:TYR:OH	1:A:297:HIS:HE1	1.76	0.68
1:A:143:PRO:O	1:A:146:HIS:HB2	1.96	0.66
1:A:322:MET:HG2	2:A:428:HOH:O	1.97	0.64
1:B:251:THR:O	1:B:255:LYS:HG3	1.98	0.63
1:A:185:HIS:HE1	2:A:462:HOH:O	1.83	0.62
1:A:297:HIS:HD2	2:A:390:HOH:O	1.82	0.62
1:B:67:VAL:HA	1:B:72:LEU:O	2.00	0.61
1:A:124:HIS:CE1	1:B:118:LYS:HA	2.35	0.60
1:B:290:TYR:OH	1:B:297:HIS:HE1	1.86	0.59
1:A:286:HIS:HD2	2:A:390:HOH:O	1.85	0.58
1:B:286:HIS:HE1	2:B:369:HOH:O	1.87	0.58
1:B:93:HIS:HB3	1:B:99:SER:HA	1.85	0.58
1:A:255:LYS:O	1:A:260:HIS:HE1	1.86	0.58
1:A:114:GLU:C	1:A:116:LEU:N	2.58	0.56
1:B:142:PHE:CD2	1:B:147:ARG:NH1	2.74	0.56
1:B:57:LEU:O	1:B:61:ILE:HG13	2.06	0.56
1:B:322:MET:HE1	2:B:437:HOH:O	2.05	0.55
1:A:74:PHE:O	1:A:90:THR:HG23	2.07	0.54
1:A:123:TYR:HA	1:A:220:VAL:HB	1.89	0.53
1:A:21:LYS:HE3	1:A:25:ASP:O	2.08	0.52
1:A:58:PHE:HE1	1:A:238:LEU:HD22	1.74	0.51
1:B:106:ASP:O	1:B:110:THR:HG22	2.11	0.51
1:B:123:TYR:HA	1:B:220:VAL:HB	1.92	0.51
1:A:3:ASN:N	1:A:6:HIS:HD2	1.96	0.51
1:A:55:CYS:SG	1:A:226:GLY:HA2	2.50	0.51
1:A:322:MET:HE1	2:A:390:HOH:O	2.10	0.51
1:B:142:PHE:HB2	1:B:143:PRO:HD2	1.94	0.49
1:B:297:HIS:CE1	1:B:319:TYR:HB2	2.46	0.49
1:B:148:PHE:CD1	1:B:261:VAL:HG11	2.47	0.49
1:A:36:ASN:HA	1:A:203:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:HG2	1:A:117:TRP:HD1	1.78	0.48
1:A:123:TYR:O	1:A:126:ARG:HD2	2.14	0.47
1:A:3:ASN:N	1:A:6:HIS:CD2	2.72	0.47
1:A:2:LYS:HZ2	1:A:2:LYS:HG2	1.51	0.47
1:A:93:HIS:HB3	1:A:99:SER:HA	1.97	0.47
1:B:184:MET:SD	1:B:238:LEU:HB2	2.54	0.47
1:B:51:ILE:HD11	1:B:55:CYS:HB3	1.97	0.47
1:B:86:PHE:HD1	1:B:140:MET:HE1	1.80	0.47
1:A:58:PHE:CE1	1:A:238:LEU:HD22	2.49	0.46
1:A:173:TYR:C	1:A:173:TYR:CD2	2.88	0.46
1:A:46:HIS:HD2	1:A:186:GLU:OE2	1.98	0.46
1:B:117:TRP:CZ3	1:B:125:LEU:HD11	2.51	0.46
1:A:55:CYS:HB2	1:A:58:PHE:CD2	2.51	0.46
1:B:58:PHE:CE1	1:B:238:LEU:HD13	2.51	0.45
1:A:114:GLU:C	1:A:116:LEU:H	2.20	0.45
1:B:100:GLY:O	1:B:140:MET:HG3	2.17	0.45
1:B:171:GLN:O	1:B:175:GLU:HG3	2.17	0.45
1:B:325:ILE:O	1:B:328:LEU:HB2	2.16	0.45
1:A:105:PHE:CA	1:A:106:ASP:CB	2.78	0.45
1:A:90:THR:HG22	1:A:92:HIS:N	2.31	0.45
1:A:184:MET:SD	1:A:238:LEU:HB2	2.57	0.44
1:B:182:ALA:HB2	1:B:247:LEU:HD21	2.00	0.44
1:B:195:LEU:HD22	1:B:199:THR:HG21	1.99	0.44
1:B:127:ARG:HB2	1:B:129:LYS:HD3	1.99	0.44
1:B:14:LEU:HD22	1:B:321:VAL:HG21	2.00	0.43
1:B:19:LEU:HD23	1:B:19:LEU:C	2.38	0.43
1:A:255:LYS:O	1:A:260:HIS:CE1	2.69	0.43
1:B:195:LEU:HA	1:B:196:PRO:HD3	1.89	0.43
1:A:78:LEU:HD11	1:A:82:LEU:HD12	2.01	0.43
1:B:326:GLU:O	1:B:329:PHE:HB2	2.18	0.43
1:B:86:PHE:CD1	1:B:140:MET:HE1	2.55	0.42
1:B:58:PHE:CD1	1:B:58:PHE:N	2.86	0.42
1:B:21:LYS:HE3	1:B:23:GLY:O	2.19	0.42
1:A:132:LEU:HB2	1:A:133:PRO:HD3	2.02	0.42
1:A:278:GLN:HE21	1:A:278:GLN:HB3	1.49	0.41
1:A:117:TRP:CZ3	1:A:125:LEU:HD11	2.55	0.41
1:A:146:HIS:HD2	2:A:475:HOH:O	2.03	0.41
1:A:201:LEU:O	1:A:313:ASN:HB2	2.20	0.41
1:B:255:LYS:O	1:B:260:HIS:HE1	2.04	0.41
1:B:291:ASP:HB2	1:B:294:VAL:HB	2.02	0.41
1:B:303:THR:HB	2:B:450:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:O	1:B:97:HIS:HB2	2.20	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	318/356 (89%)	304 (96%)	14 (4%)	0	100	100
1	B	324/356 (91%)	309 (95%)	15 (5%)	0	100	100
All	All	642/712 (90%)	613 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	270/302 (89%)	254 (94%)	16 (6%)	23	26
1	B	274/302 (91%)	267 (97%)	7 (3%)	51	64
All	All	544/604 (90%)	521 (96%)	23 (4%)	34	43

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	90	THR
1	A	106	ASP
1	A	114	GLU
1	A	116	LEU
1	A	122	MET
1	A	126	ARG
1	A	128	LEU
1	A	146	HIS
1	A	201	LEU
1	A	215	LEU
1	A	261	VAL
1	A	278	GLN
1	A	288	MET
1	A	303	THR
1	A	322	MET
1	B	24	GLU
1	B	44	GLU
1	B	129	LYS
1	B	140	MET
1	B	278	GLN
1	B	305	ASN
1	B	322	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	45	HIS
1	A	124	HIS
1	A	260	HIS
1	A	278	GLN
1	A	286	HIS
1	A	297	HIS
1	B	45	HIS
1	B	124	HIS
1	B	149	HIS
1	B	245	HIS
1	B	260	HIS
1	B	278	GLN
1	B	286	HIS
1	B	297	HIS
1	B	305	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 carbohydrates 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	322/356 (90%)	-0.21	1 (0%) 93 93	21, 28, 46, 71	0
1	B	326/356 (91%)	0.08	4 (1%) 79 77	23, 38, 55, 73	0
All	All	648/712 (91%)	-0.06	5 (0%) 86 85	21, 32, 53, 73	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	HIS	3.1
1	B	113	PHE	2.8
1	A	207	GLU	2.5
1	B	73	SER	2.3
1	B	28	PHE	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.