



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2025 – 10:11 AM EDT

PDB ID : 9MTN / pdb\_00009mtn  
Title : Crystal structure of KwaB  
Authors : Zhiying, Z.; Dinshaw, J.P.  
Deposited on : 2025-01-11  
Resolution : 3.92 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

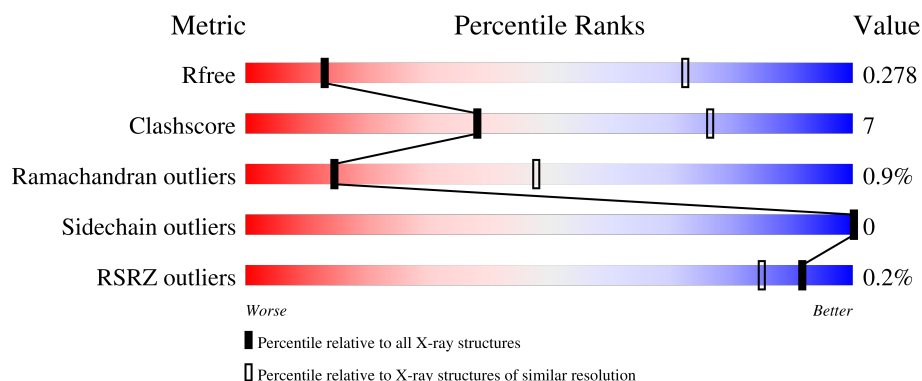
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.92 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))
$R_{free}$	164625	1175 (4.14-3.70)
Clashscore	180529	1045 (4.12-3.72)
Ramachandran outliers	177936	1006 (4.12-3.72)
Sidechain outliers	177891	1185 (4.14-3.70)
RSRZ outliers	164620	1175 (4.14-3.70)

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  $\geq 3$ , 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	315	 74% 23% . .
1	B	315	 80% 15% 5%
1	C	315	 80% 15% 5%
1	K	315	 77% 18% 5%

## 2 Entry composition

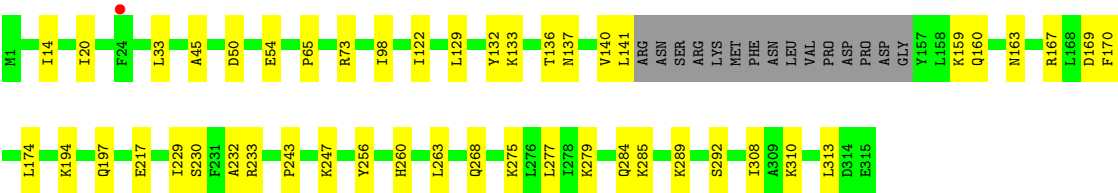
There is only 1 type of molecule in this entry. The entry contains 9722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kiwa protein KwaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2477	1583	412	477	5			
1	K	300	Total	C	N	O	S	0	0	0
			2421	1550	401	465	5			
1	B	298	Total	C	N	O	S	0	0	0
			2402	1538	396	463	5			
1	C	300	Total	C	N	O	S	0	0	0
			2422	1553	398	466	5			





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	283.11Å 283.11Å 76.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.28 – 3.92 33.28 – 3.92	Depositor EDS
% Data completeness (in resolution range)	86.1 (33.28-3.92) 86.1 (33.28-3.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.238 , 0.275 0.243 , 0.278	Depositor DCC
$R_{free}$ test set	1754 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.9	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 113.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.106 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.31	0/2514	0.65	4/3383 (0.1%)
1	B	0.22	0/2437	0.52	0/3280
1	C	0.24	0/2458	0.54	0/3309
1	K	0.27	0/2456	0.62	0/3305
All	All	0.26	0/9865	0.59	4/13277 (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	49	ILE	CA-C-N	6.30	129.01	120.38
1	A	49	ILE	C-N-CA	6.30	129.01	120.38
1	A	47	GLY	CA-C-N	5.23	131.52	121.54
1	A	47	GLY	C-N-CA	5.23	131.52	121.54

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	2477	0	2542	48	0
1	B	2402	0	2470	32	0
1	C	2422	0	2490	30	0
1	K	2421	0	2494	35	0
All	All	9722	0	9996	133	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 7.

All (133) 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:130:ALA:HB3	1:A:176:SER:HB3	1.72	0.69
1:A:11:SER:HA	1:A:14:ILE:HB	1.78	0.66
1:A:268:GLN:HB2	1:A:277:LEU:HD12	1.79	0.64
1:A:49:ILE:HG22	1:A:53:LYS:HB2	1.79	0.64
1:K:133:LYS:HE3	1:K:169:ASP:H	1.63	0.64
1:A:142:ARG:HD2	1:A:158:LEU:HB3	1.80	0.62
1:A:206:ALA:HB2	1:A:239:SER:HB2	1.81	0.61
1:A:254:ILE:HG23	1:A:269:ILE:HG12	1.82	0.61
1:C:167:ARG:HE	1:C:169:ASP:H	1.50	0.60
1:A:145:ARG:NH2	1:A:155:ASP:OD1	2.36	0.58
1:B:211:ARG:NH2	1:B:223:GLU:OE2	2.37	0.58
1:B:136:THR:H	1:B:167:ARG:HH12	1.52	0.57
1:K:66:LEU:HD22	1:K:81:ASP:HB3	1.86	0.57
1:K:238:ILE:HD13	1:K:291:MET:HB2	1.85	0.57
1:K:136:THR:HB	1:K:138:LEU:HD23	1.87	0.57
1:B:292:SER:O	1:B:310:LYS:NZ	2.38	0.57
1:C:132:TYR:HB3	1:C:174:LEU:HG	1.87	0.56
1:C:141:LEU:HB2	1:C:160:GLN:HA	1.87	0.56
1:C:194:LYS:HB3	1:C:197:GLN:HE22	1.71	0.55
1:A:71:ASP:N	1:A:71:ASP:OD1	2.38	0.55
1:B:279:LYS:O	1:B:284:GLN:NE2	2.39	0.55
1:B:127:LYS:HE2	1:B:177:ILE:HD11	1.89	0.54
1:K:78:PHE:HB2	1:K:183:ILE:HB	1.89	0.54
1:A:49:ILE:O	1:A:53:LYS:N	2.38	0.54
1:A:53:LYS:HG3	1:A:57:ILE:HB	1.90	0.54
1:C:159:LYS:NZ	1:C:160:GLN:O	2.40	0.54
1:K:206:ALA:HB2	1:K:239:SER:HB2	1.89	0.54
1:A:299:ASP:HB2	1:K:256:TYR:HE2	1.73	0.53
1:A:139:ALA:HB1	1:K:169:ASP:HA	1.91	0.53
1:B:71:ASP:N	1:B:71:ASP:OD1	2.38	0.53
1:B:268:GLN:HB2	1:B:277:LEU:HB2	1.91	0.53
1:A:120:ILE:HB	1:A:131:LEU:HB2	1.91	0.52
1:A:141:LEU:HD11	1:K:140:VAL:HG11	1.92	0.52
1:B:299:ASP:HB2	1:C:256:TYR:HE2	1.76	0.51
1:B:33:LEU:HD21	1:B:98:ILE:HG21	1.92	0.51
1:A:279:LYS:O	1:A:284:GLN:NE2	2.44	0.51
1:B:44:ILE:HD11	1:C:140:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PRO:HG3	1:C:73:ARG:HD2	1.93	0.51
1:A:270:ASN:HB3	1:A:277:LEU:HD21	1.93	0.51
1:K:162:PRO:HB3	1:K:165:ILE:HB	1.92	0.51
1:K:110:ASN:ND2	1:K:114:ASP:OD2	2.44	0.50
1:A:87:GLU:OE1	1:A:91:LYS:NZ	2.43	0.50
1:B:194:LYS:HB3	1:B:197:GLN:HE22	1.75	0.50
1:A:211:ARG:NH2	1:A:223:GLU:OE2	2.44	0.50
1:K:174:LEU:HD21	1:K:189:LEU:HG	1.94	0.50
1:B:71:ASP:OD2	1:B:73:ARG:NH1	2.45	0.50
1:C:292:SER:O	1:C:310:LYS:NZ	2.38	0.50
1:A:32:LYS:HB3	1:A:106:TYR:HB2	1.92	0.49
1:A:194:LYS:HB3	1:A:197:GLN:HE22	1.77	0.49
1:K:211:ARG:NH2	1:K:223:GLU:OE2	2.44	0.49
1:K:285:LYS:HE2	1:K:289:LYS:HE3	1.94	0.49
1:A:190:GLU:HA	1:A:195:PHE:HB3	1.94	0.49
1:K:20:ILE:HG21	1:K:45:ALA:HB2	1.94	0.49
1:K:40:ALA:HA	1:K:43:SER:HB3	1.95	0.49
1:B:74:LYS:NZ	1:C:73:ARG:O	2.39	0.49
1:B:141:LEU:HD23	1:B:162:PRO:HG2	1.95	0.48
1:C:229:ILE:HD12	1:C:232:ALA:HB3	1.95	0.48
1:B:270:ASN:HB3	1:B:277:LEU:HD21	1.96	0.48
1:A:51:LYS:HG2	1:A:170:PHE:HB2	1.96	0.48
1:B:73:ARG:HE	1:C:308:ILE:HD12	1.77	0.48
1:K:67:LEU:HD13	1:K:183:ILE:HG13	1.95	0.48
1:C:230:SER:HA	1:C:233:ARG:HE	1.78	0.48
1:A:229:ILE:HA	1:A:232:ALA:HB3	1.95	0.47
1:C:50:ASP:O	1:C:54:GLU:N	2.44	0.47
1:C:136:THR:OG1	1:C:167:ARG:NH1	2.44	0.47
1:A:49:ILE:HA	1:A:52:ILE:HB	1.97	0.47
1:A:56:ILE:HD11	1:A:175:PHE:CZ	2.50	0.47
1:C:20:ILE:HG21	1:C:45:ALA:HB2	1.96	0.47
1:B:190:GLU:OE2	1:B:233:ARG:NH1	2.45	0.47
1:C:285:LYS:HE2	1:C:289:LYS:HE3	1.96	0.46
1:C:260:HIS:HB3	1:C:263:LEU:HB2	1.98	0.46
1:C:132:TYR:HD2	1:C:174:LEU:HD21	1.79	0.46
1:C:268:GLN:HB2	1:C:277:LEU:HB2	1.98	0.46
1:A:217:GLU:HA	1:A:275:LYS:HD3	1.96	0.46
1:B:229:ILE:HD12	1:B:232:ALA:HB3	1.97	0.46
1:C:279:LYS:O	1:C:284:GLN:NE2	2.48	0.46
1:K:183:ILE:HD12	1:K:189:LEU:HD11	1.98	0.46
1:B:167:ARG:O	1:C:140:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:HB3	1:A:188:THR:HG21	1.98	0.45
1:K:229:ILE:HD12	1:K:232:ALA:HB3	1.98	0.45
1:K:138:LEU:HB3	1:K:139:ALA:H	1.67	0.45
1:K:260:HIS:HB3	1:K:263:LEU:HB2	1.97	0.45
1:B:88:GLU:OE2	1:B:116:LYS:NZ	2.44	0.45
1:B:132:TYR:HD2	1:B:174:LEU:HD21	1.80	0.45
1:B:216:ILE:HG23	1:B:278:ILE:HD12	1.98	0.45
1:K:162:PRO:HG3	1:K:165:ILE:HD12	1.98	0.45
1:K:168:LEU:HD12	1:K:168:LEU:HA	1.84	0.45
1:A:136:THR:HG1	1:A:167:ARG:HH12	1.60	0.44
1:B:304:ILE:HG13	1:C:313:LEU:HD12	1.99	0.44
1:B:173:ASP:HB2	1:B:174:LEU:HD23	1.99	0.44
1:B:229:ILE:HG23	1:B:233:ARG:HH21	1.82	0.44
1:A:10:ILE:HD12	1:A:129:LEU:HD12	1.99	0.44
1:A:73:ARG:NH2	1:A:311:ASP:OD2	2.47	0.44
1:K:190:GLU:OE2	1:K:233:ARG:NH2	2.51	0.44
1:A:280:THR:HG23	1:A:283:SER:H	1.82	0.44
1:C:217:GLU:HA	1:C:275:LYS:HD3	2.00	0.44
1:A:56:ILE:HA	1:A:62:LEU:HD22	1.98	0.44
1:A:37:GLU:O	1:A:41:LEU:N	2.44	0.44
1:K:44:ILE:HD12	1:K:168:LEU:HD23	2.00	0.44
1:B:222:LEU:HD12	1:B:284:GLN:HG2	2.00	0.44
1:A:49:ILE:H	1:A:49:ILE:HG13	1.52	0.43
1:A:304:ILE:HG23	1:K:313:LEU:HB2	2.01	0.43
1:B:136:THR:H	1:B:167:ARG:NH1	2.16	0.43
1:C:33:LEU:HD21	1:C:98:ILE:HG21	2.01	0.43
1:K:56:ILE:HA	1:K:62:LEU:HD22	1.99	0.43
1:B:88:GLU:HA	1:B:91:LYS:HB2	2.01	0.42
1:C:14:ILE:HD13	1:C:14:ILE:HA	1.90	0.42
1:A:48:PHE:O	1:A:52:ILE:N	2.47	0.42
1:C:122:ILE:N	1:C:129:LEU:O	2.51	0.42
1:A:135:LYS:HZ1	1:A:138:LEU:HD12	1.84	0.42
1:B:20:ILE:HG21	1:B:45:ALA:HB2	2.01	0.42
1:B:217:GLU:HA	1:B:275:LYS:HD3	2.01	0.42
1:A:74:LYS:HB2	1:A:74:LYS:HE2	1.85	0.42
1:A:158:LEU:HD21	1:K:112:PHE:CZ	2.55	0.42
1:C:243:PRO:HA	1:C:247:LYS:HD2	2.01	0.42
1:A:47:GLY:C	1:A:49:ILE:H	2.28	0.41
1:K:79:LYS:HG2	1:K:182:TYR:HE1	1.85	0.41
1:K:37:GLU:O	1:K:41:LEU:N	2.53	0.41
1:B:24:PHE:HZ	1:B:166:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:107:ASN:HA	1:K:108:PRO:HD3	1.96	0.41
1:B:41:LEU:HA	1:B:44:ILE:HB	2.02	0.41
1:A:14:ILE:HD13	1:A:14:ILE:HA	1.96	0.41
1:A:115:VAL:HG11	1:A:166:LEU:HD21	2.02	0.41
1:K:186:HIS:CD2	1:K:233:ARG:HH12	2.39	0.41
1:C:133:LYS:HD3	1:C:167:ARG:HH21	1.85	0.41
1:A:18:SER:OG	1:A:19:GLY:N	2.54	0.41
1:A:79:LYS:HB3	1:A:79:LYS:HE2	1.87	0.41
1:A:46:GLU:HG3	1:A:48:PHE:H	1.86	0.41
1:K:11:SER:HB3	1:K:57:ILE:HD12	2.03	0.41
1:A:44:ILE:HD13	1:A:44:ILE:HA	1.96	0.40
1:A:306:MET:HB2	1:K:313:LEU:HD21	2.04	0.40
1:K:270:ASN:HB3	1:K:277:LEU:HD21	2.02	0.40
1:C:160:GLN:HE22	1:C:163:ASN:HB2	1.85	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	303/315 (96%)	276 (91%)	26 (9%)	1 (0%)	37 70
1	B	294/315 (93%)	278 (95%)	14 (5%)	2 (1%)	19 54
1	C	296/315 (94%)	276 (93%)	18 (6%)	2 (1%)	19 54
1	K	296/315 (94%)	274 (93%)	16 (5%)	6 (2%)	6 33
All	All	1189/1260 (94%)	1104 (93%)	74 (6%)	11 (1%)	14 48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	VAL

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Mol	Chain	Res	Type
1	C	170	PHE
1	A	169	ASP
1	K	162	PRO
1	K	196	HIS
1	B	139	ALA
1	K	76	ALA
1	K	164	GLU
1	C	137	ASN
1	K	65	PRO
1	K	161	LEU

### 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	281/289 (97%)	281 (100%)	0	100	100
1	B	273/289 (94%)	273 (100%)	0	100	100
1	C	275/289 (95%)	275 (100%)	0	100	100
1	K	275/289 (95%)	275 (100%)	0	100	100
All	All	1104/1156 (96%)	1104 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	K	103	GLN
1	K	110	ASN
1	K	186	HIS
1	K	297	GLN
1	B	103	GLN
1	B	192	GLN
1	C	103	GLN

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Mol	Chain	Res	Type
1	C	185	ASN
1	C	186	HIS
1	C	192	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/315 (97%)	-0.45	1 (0%) 90 81	98, 137, 186, 218	0
1	B	298/315 (94%)	-0.47	0 100 100	159, 219, 251, 266	0
1	C	300/315 (95%)	-0.41	1 (0%) 90 81	120, 172, 225, 252	0
1	K	300/315 (95%)	-0.50	0 100 100	90, 133, 180, 205	0
All	All	1205/1260 (95%)	-0.46	2 (0%) 92 85	90, 161, 238, 266	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ARG	2.2
1	C	24	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 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.