



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:29 am GMT

PDB ID : 2B5R  
Title : 1B Lactamase / B Lactamase Inhibitor  
Authors : Rahat, O.; Albeck, S.; Meged, R.; Dym, O.; Screiber, G.; Israel Structural Proteomics Center (ISPC)  
Deposited on : 2005-09-29  
Resolution : 1.65 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

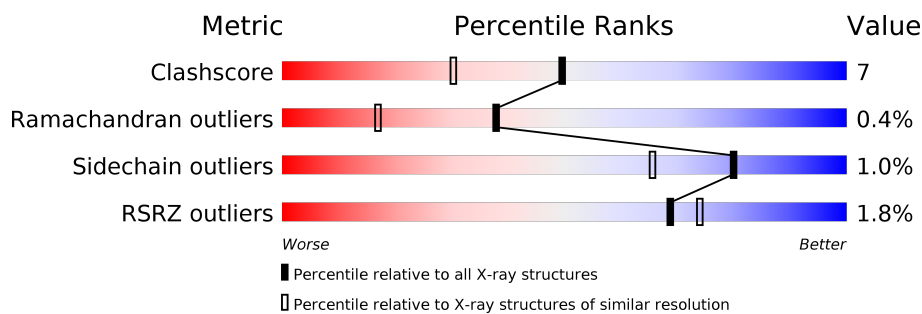
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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  $\geq 3$ , 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	263	 87% 12% .
1	B	263	 92% 7%
2	C	165	 6% 91% 8% .
2	D	165	 2% 88% 9% ..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7047 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 TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2026	1265	361	389	11			
1	B	263	Total	C	N	O	S	0	0	0
			2026	1265	361	389	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ILE	VAL	ENGINEERED	UNP P62593
A	104	TYR	GLU	ENGINEERED	UNP P62593
A	105	ASN	TYR	ENGINEERED	UNP P62593
B	84	ILE	VAL	ENGINEERED	UNP P62593
B	104	TYR	GLU	ENGINEERED	UNP P62593
B	105	ASN	TYR	ENGINEERED	UNP P62593

- Molecule 2 is a protein called Beta-lactamase inhibitory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	165	Total	C	N	O	S	0	0	0
			1235	778	207	243	7			
2	D	165	Total	C	N	O	S	0	0	0
			1235	778	207	243	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	136	Total	O	0	0
			136	136		
3	C	119	Total	O	0	0
			119	119		

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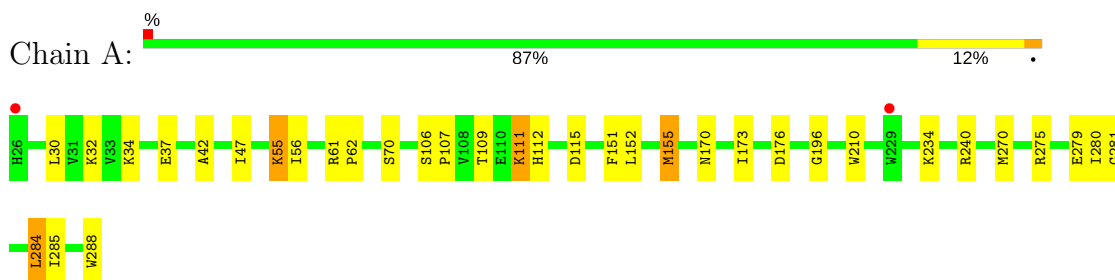
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	154	Total	O	0	0
			154	154		

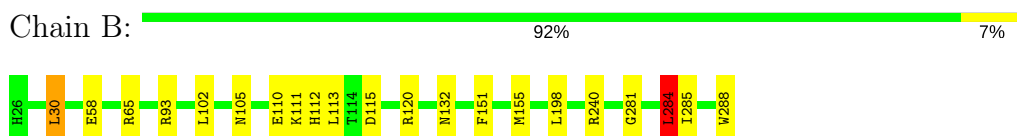
### 3 Residue-property plots [i](#)

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.

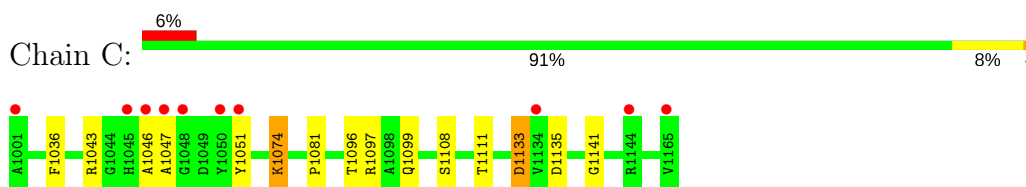
- Molecule 1: Beta-lactamase TEM



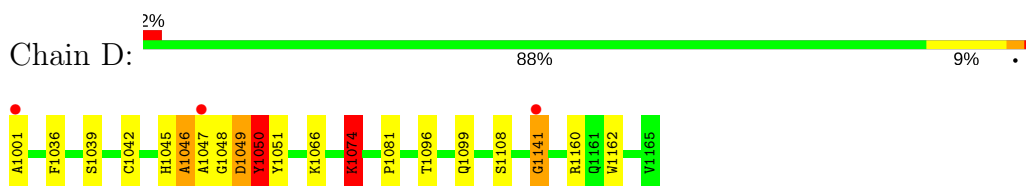
- Molecule 1: Beta-lactamase TEM



- Molecule 2: Beta-lactamase inhibitory protein



- Molecule 2: Beta-lactamase inhibitory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.80Å 124.47Å 157.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 1.65 48.31 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.30-1.65) 98.0 (48.31-1.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 1.65Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.190 , 0.222 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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	0.79	1/2060 (0.0%)	0.94	2/2790 (0.1%)
1	B	0.86	0/2060	0.98	7/2790 (0.3%)
2	C	0.84	0/1264	0.89	3/1715 (0.2%)
2	D	0.89	1/1264 (0.1%)	1.01	3/1715 (0.2%)
All	All	0.84	2/6648 (0.0%)	0.96	15/9010 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1042	CYS	CB-SG	5.57	1.91	1.82
1	A	210	TRP	CB-CG	5.06	1.59	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	TRP	CA-C-O	-14.65	89.34	120.10
1	B	288	TRP	N-CA-C	-11.88	78.91	111.00
2	D	1001	ALA	N-CA-C	-9.24	86.04	111.00
1	B	288	TRP	CA-CB-CG	7.26	127.50	113.70
1	B	288	TRP	CB-CA-C	-6.18	98.05	110.40
2	C	1133	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	D	1074	LYS	CD-CE-NZ	-5.80	98.36	111.70
1	B	65	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	C	1133	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	120	ARG	NE-CZ-NH1	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	284	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	155	MET	CB-CG-SD	-5.23	96.70	112.40
2	D	1050	TYR	N-CA-C	5.20	125.04	111.00
2	C	1074	LYS	CD-CE-NZ	-5.07	100.04	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1141	GLY	Peptide

## 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	2026	0	2036	35	0
1	B	2026	0	2036	17	0
2	C	1235	0	1170	16	0
2	D	1235	0	1168	23	0
3	A	116	0	0	2	0
3	B	136	0	0	3	0
3	C	119	0	0	6	0
3	D	154	0	0	5	0
All	All	7047	0	6410	86	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 (86) 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:196:GLY:HA3	3:A:2452:HOH:O	1.36	1.22
1:A:173:ILE:HD13	1:A:240:ARG:NH1	1.58	1.18
1:A:152:LEU:HD23	1:A:155:MET:CE	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD13	1:A:240:ARG:HH12	0.92	1.07
1:A:152:LEU:HD23	1:A:155:MET:HE3	1.31	1.06
1:A:152:LEU:HA	1:A:155:MET:HE3	1.38	1.06
2:D:1074:LYS:NZ	2:D:1141:GLY:HA2	1.69	1.06
1:A:55:LYS:HE3	1:A:56:ILE:H	1.20	1.03
1:A:173:ILE:CD1	1:A:240:ARG:HH12	1.77	0.97
2:D:1074:LYS:HZ1	2:D:1141:GLY:HA2	1.24	0.95
2:D:1048:GLY:O	2:D:1049:ASP:O	1.89	0.90
1:A:55:LYS:HE3	1:A:56:ILE:N	1.91	0.85
1:A:152:LEU:HA	1:A:155:MET:CE	2.07	0.84
2:C:1046:ALA:HA	2:C:1051:TYR:HB2	1.61	0.82
2:C:1096:THR:H	2:C:1099:GLN:HE21	1.26	0.79
1:A:55:LYS:CE	1:A:56:ILE:H	1.96	0.76
1:A:152:LEU:HD23	1:A:155:MET:HE1	1.68	0.75
2:D:1050:TYR:OH	3:D:2077:HOH:O	2.04	0.74
2:C:1135:ASP:OD1	3:C:2510:HOH:O	2.09	0.69
2:D:1074:LYS:NZ	2:D:1141:GLY:CA	2.51	0.69
2:D:1074:LYS:HZ2	2:D:1141:GLY:HA2	1.61	0.65
1:B:110:GLU:OE2	3:B:2142:HOH:O	2.15	0.64
1:A:270:MET:HG2	2:C:1047:ALA:HB1	1.79	0.64
2:D:1045:HIS:HD2	3:D:2009:HOH:O	1.81	0.63
2:D:1066:LYS:HE2	3:D:2552:HOH:O	1.97	0.63
2:D:1096:THR:H	2:D:1099:GLN:HE21	1.48	0.62
1:A:281:GLY:HA2	1:A:284:LEU:CD1	2.29	0.62
1:A:281:GLY:HA2	1:A:284:LEU:HD11	1.82	0.62
1:A:281:GLY:O	1:A:284:LEU:HD13	2.00	0.61
1:B:102:LEU:HD21	1:B:113:LEU:HD21	1.84	0.59
1:A:111:LYS:HE3	1:A:112:HIS:CE1	2.37	0.59
1:B:111:LYS:HE3	2:D:1036:PHE:O	2.02	0.59
2:C:1036:PHE:HZ	3:C:2518:HOH:O	1.88	0.57
2:C:1074:LYS:HE2	2:C:1141:GLY:HA2	1.86	0.57
2:D:1049:ASP:O	2:D:1051:TYR:N	2.37	0.57
1:B:132:ASN:ND2	3:D:2077:HOH:O	2.38	0.56
2:C:1043:ARG:HD2	3:C:2616:HOH:O	2.06	0.56
1:A:37:GLU:HG3	1:A:42:ALA:O	2.05	0.55
1:A:275:ARG:O	1:A:279:GLU:HG3	2.06	0.55
1:A:152:LEU:CD2	1:A:155:MET:HE3	2.22	0.55
1:A:107:PRO:HB2	3:C:2518:HOH:O	2.08	0.54
2:C:1097:ARG:HD3	3:C:2355:HOH:O	2.08	0.53
2:D:1160:ARG:HD3	2:D:1162:TRP:CZ2	2.44	0.53
1:B:102:LEU:CD2	1:B:113:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HB	1:A:176:ASP:HB2	1.92	0.52
1:A:281:GLY:O	1:A:284:LEU:CD1	2.58	0.52
2:D:1045:HIS:CE1	2:D:1047:ALA:HB2	2.46	0.51
1:A:280:ILE:O	1:A:284:LEU:HD12	2.11	0.50
1:B:112:HIS:ND1	1:B:115:ASP:OD2	2.44	0.49
2:C:1046:ALA:HA	2:C:1051:TYR:CB	2.38	0.49
2:D:1066:LYS:HD3	3:D:2399:HOH:O	2.13	0.49
1:A:47:ILE:HD11	1:A:62:PRO:HB3	1.95	0.48
2:C:1111:THR:HG22	3:C:2591:HOH:O	2.12	0.48
2:D:1074:LYS:HE3	2:D:1141:GLY:HA3	1.96	0.48
1:B:30:LEU:HD21	1:B:58:GLU:OE1	2.14	0.48
1:B:110:GLU:CG	3:B:2142:HOH:O	2.62	0.47
1:A:55:LYS:HA	1:A:55:LYS:HD2	1.71	0.47
1:A:170:ASN:ND2	3:A:2395:HOH:O	2.47	0.47
1:B:284:LEU:CD2	1:B:285:ILE:HG13	2.45	0.47
2:C:1046:ALA:O	2:C:1047:ALA:HB3	2.15	0.46
2:C:1043:ARG:HG2	2:C:1051:TYR:CE1	2.51	0.46
2:D:1081:PRO:HA	2:D:1108:SER:HA	1.98	0.46
1:B:281:GLY:O	1:B:284:LEU:HD22	2.16	0.45
2:C:1074:LYS:CE	2:C:1141:GLY:HA2	2.45	0.45
1:B:151:PHE:O	1:B:155:MET:HG2	2.17	0.45
1:B:105:ASN:OD1	2:D:1074:LYS:HE3	2.17	0.45
1:B:93:ARG:NH2	3:B:2533:HOH:O	2.51	0.44
2:D:1074:LYS:HZ2	2:D:1141:GLY:CA	2.26	0.44
2:D:1046:ALA:O	2:D:1047:ALA:HB3	2.18	0.43
1:A:151:PHE:CE2	1:A:155:MET:HE1	2.53	0.43
1:A:70:SER:O	1:A:234:LYS:HE3	2.18	0.43
1:B:111:LYS:HE2	2:D:1039:SER:OG	2.19	0.43
2:D:1074:LYS:HG3	2:D:1074:LYS:HZ3	1.34	0.43
1:B:112:HIS:HD1	1:B:115:ASP:CG	2.22	0.43
2:C:1081:PRO:HA	2:C:1108:SER:HA	2.00	0.42
1:B:111:LYS:CE	2:D:1036:PHE:O	2.67	0.42
1:A:115:ASP:N	1:A:115:ASP:OD1	2.53	0.42
2:C:1133:ASP:C	2:C:1133:ASP:OD1	2.58	0.42
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.77	0.42
2:D:1074:LYS:CE	2:D:1141:GLY:CA	2.98	0.41
1:A:285:ILE:HA	1:A:285:ILE:HD13	1.88	0.41
1:A:32:LYS:HE3	1:A:32:LYS:O	2.20	0.41
1:B:155:MET:SD	1:B:198:LEU:HD21	2.60	0.41
1:A:106:SER:HB3	1:A:109:THR:OG1	2.21	0.41
1:A:61:ARG:N	1:A:62:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1074:LYS:HZ3	2:C:1074:LYS:HG3	1.28	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	261/263 (99%)	257 (98%)	4 (2%)	0	100	100
1	B	261/263 (99%)	257 (98%)	4 (2%)	0	100	100
2	C	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
2	D	163/165 (99%)	157 (96%)	3 (2%)	3 (2%)	10	1
All	All	848/856 (99%)	827 (98%)	18 (2%)	3 (0%)	38	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1046	ALA
2	D	1049	ASP
2	D	1050	TYR

### 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	217/217 (100%)	213 (98%)	4 (2%)	64	40
1	B	217/217 (100%)	215 (99%)	2 (1%)	82	69
2	C	126/126 (100%)	126 (100%)	0	100	100
2	D	126/126 (100%)	125 (99%)	1 (1%)	85	73
All	All	686/686 (100%)	679 (99%)	7 (1%)	80	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	55	LYS
1	A	111	LYS
1	A	284	LEU
1	B	30	LEU
1	B	284	LEU
2	D	1074	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	132	ASN
2	C	1099	GLN
1	B	132	ASN
2	D	1045	HIS
2	D	1089	ASN
2	D	1099	GLN

### 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 [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	263/263 (100%)	-0.19	2 (0%) 86 88	8, 17, 32, 45	0
1	B	263/263 (100%)	-0.42	0 100 100	9, 14, 29, 36	0
2	C	165/165 (100%)	-0.03	10 (6%) 22 20	11, 18, 32, 50	0
2	D	165/165 (100%)	-0.29	3 (1%) 69 74	9, 14, 26, 41	0
All	All	856/856 (100%)	-0.25	15 (1%) 69 74	8, 16, 31, 50	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1046	ALA	6.3
2	C	1047	ALA	6.2
2	C	1001	ALA	5.3
2	C	1165	VAL	4.0
2	C	1050	TYR	3.8
2	C	1051	TYR	3.7
2	C	1144	ARG	3.5
2	D	1001	ALA	3.4
1	A	26	HIS	3.0
2	C	1045	HIS	2.6
2	C	1048	GLY	2.5
2	D	1047	ALA	2.4
1	A	229	TRP	2.2
2	D	1141	GLY	2.0
2	C	1134	VAL	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.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.