



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:32 PM UTC

PDB ID : 3GR2 / pdb\_00003gr2  
Title : AmpC beta-lactamase in complex with Fragment-based Inhibitor  
Authors : Teotico, D.T.; Shoichet, B.K.  
Deposited on : 2009-03-24  
Resolution : 1.80 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 Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

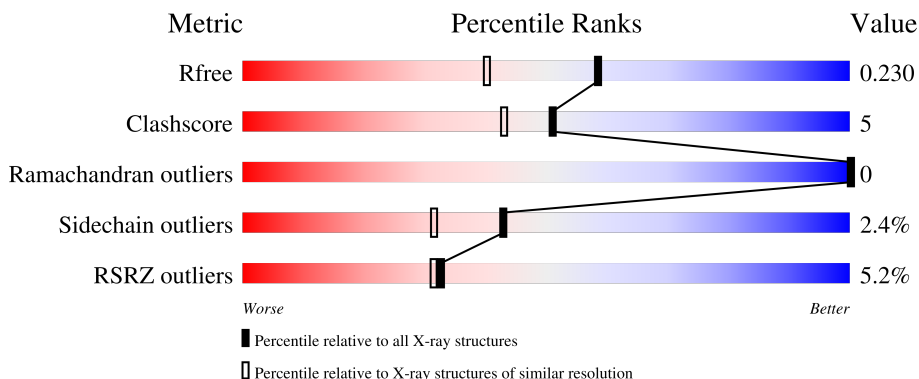
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


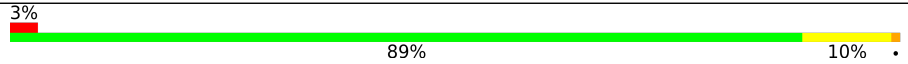
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	358	
1	B	358	

## 2 Entry composition [i](#)

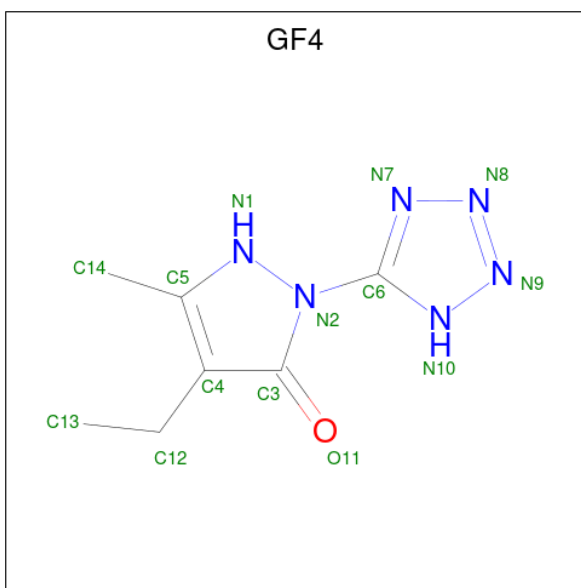
There are 3 unique types of molecules in this entry. The entry contains 6344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	358	Total 2907	C 1864	N 497	O 538	S 8	22	33	0
1	B	358	Total 2903	C 1865	N 498	O 532	S 8	29	31	0

- Molecule 2 is 4-ethyl-5-methyl-2-(1H-tetrazol-5-yl)-1,2-dihydro-3H-pyrazol-3-one (CCD ID: GF4) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 7	N 6	O 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	252	Total 252	O 252	0	0

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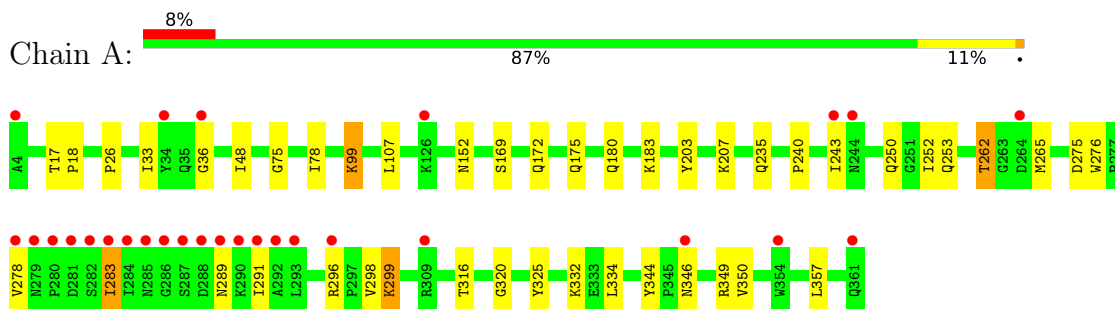
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	268	Total 268	O 268	0	0

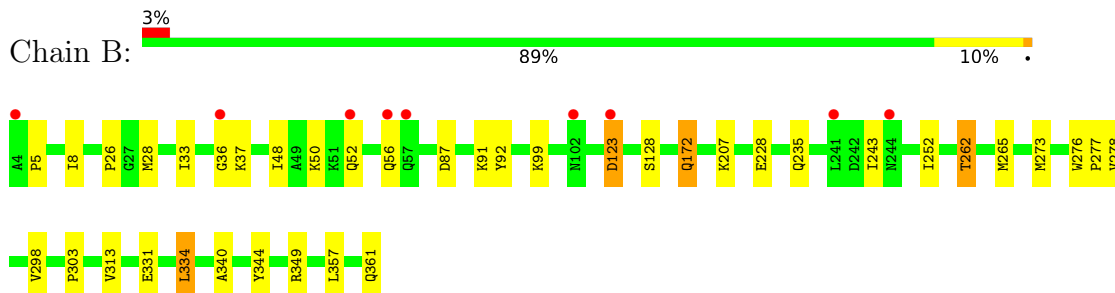
### 3 Residue-property plots [i](#)

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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.53Å 76.55Å 98.01Å 90.00° 116.36° 90.00°	Depositor
Resolution (Å)	32.44 – 1.80 32.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.44-1.80) 98.7 (32.44-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.79Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.205 , 0.229 0.203 , 0.230	Depositor DCC
$R_{free}$ test set	3612 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GF4

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	0.45	0/3157	0.78	4/4307 (0.1%)
1	B	0.50	3/3149 (0.1%)	0.76	1/4296 (0.0%)
All	All	0.48	3/6306 (0.0%)	0.77	5/8603 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	LYS	CE-NZ	9.34	1.77	1.49
1	B	37	LYS	CG-CD	-6.57	1.32	1.52
1	B	207	LYS	CG-CD	-6.15	1.33	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	LYS	CD-CE-NZ	6.07	131.32	111.90
1	A	299	LYS	CD-CE-NZ	5.70	130.14	111.90
1	B	207	LYS	CB-CG-CD	5.66	124.31	111.30
1	A	332	LYS	CG-CD-CE	5.45	123.83	111.30
1	A	183	LYS	CD-CE-NZ	-5.35	94.79	111.90

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	2907	0	2882	37	0
1	B	2903	0	2893	24	0
2	A	14	0	10	4	0
3	A	252	0	0	1	0
3	B	268	0	0	1	0
All	All	6344	0	5785	60	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 5.

All (60) 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:152[B]:ASN:HD21	2:A:1:GF4:H13	1.19	1.03
1:B:172:GLN:HE21	1:B:172:GLN:HA	1.27	0.99
1:A:262[A]:THR:HG23	1:A:265[A]:MET:HG3	1.60	0.84
1:A:320:GLY:H	2:A:1:GF4:HN10	1.24	0.84
1:B:172:GLN:HA	1:B:172:GLN:NE2	1.94	0.79
1:A:152[B]:ASN:ND2	2:A:1:GF4:H13	1.97	0.78
1:A:262[A]:THR:CG2	1:A:265[A]:MET:SD	2.76	0.73
1:A:262[A]:THR:HG23	1:A:265[A]:MET:CG	2.19	0.73
1:B:56:GLN:HG3	3:B:538:HOH:O	1.89	0.70
1:B:172:GLN:HE21	1:B:172:GLN:CA	2.01	0.70
1:B:123:ASP:OD1	1:B:123:ASP:N	2.27	0.66
1:A:262[A]:THR:HG23	1:A:265[A]:MET:SD	2.41	0.60
1:B:243[A]:ILE:CD1	1:B:252:ILE:HD12	2.32	0.59
1:B:262[A]:THR:HG23	1:B:265[A]:MET:HG2	1.83	0.59
1:A:262[B]:THR:HG21	1:A:296:ARG:HB3	1.84	0.57
1:B:262[B]:THR:CG2	1:B:298:VAL:HG12	2.35	0.56
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.88	0.55
1:B:5:PRO:HD2	1:B:8:ILE:HD12	1.90	0.54
1:A:240:PRO:HA	1:A:243:ILE:HD12	1.90	0.54
1:A:169:SER:OG	1:A:172[A]:GLN:HG3	2.08	0.53
1:B:262[A]:THR:HG23	1:B:265[A]:MET:CG	2.38	0.53
1:A:276:TRP:CZ3	1:A:278[B]:VAL:HG22	2.46	0.51
1:A:262[A]:THR:HG22	1:A:265[A]:MET:SD	2.50	0.51
1:A:243:ILE:HD13	1:A:252[A]:ILE:CD1	2.42	0.50
1:A:175[B]:GLN:HG3	1:A:180:GLN:NE2	2.27	0.49
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.27	0.49
1:B:344:TYR:CE1	1:B:349:ARG:HG2	2.47	0.49
1:A:275:ASP:O	1:A:278[A]:VAL:HG22	2.13	0.48
1:A:289:ASN:OD1	1:A:291:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HB	1:A:350:VAL:HG11	1.97	0.47
1:B:50:LYS:O	1:B:52:GLN:NE2	2.48	0.46
1:A:36:GLY:HA2	1:A:235[B]:GLN:HE22	1.79	0.46
1:A:175[B]:GLN:HG3	1:A:180:GLN:HE21	1.81	0.46
1:A:325:TYR:HB2	1:A:349[B]:ARG:HG2	1.98	0.46
1:A:344:TYR:OH	1:A:349[B]:ARG:HG3	2.16	0.46
1:A:262[B]:THR:HG21	1:A:296:ARG:CB	2.46	0.45
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.98	0.45
1:A:17:THR:HB	1:A:18:PRO:HD3	1.98	0.45
1:B:334[B]:LEU:HG	1:B:357:LEU:HD22	1.99	0.44
1:B:334[A]:LEU:HD22	1:B:357:LEU:HD22	1.99	0.44
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.53	0.43
1:B:56:GLN:HB3	1:B:228:GLU:HG3	2.01	0.43
1:A:316:THR:OG1	1:A:349[B]:ARG:NH2	2.51	0.43
1:A:175[B]:GLN:HE21	1:A:180:GLN:HG3	1.83	0.43
1:A:334:LEU:HG	1:A:357:LEU:HD22	2.01	0.43
1:A:152[A]:ASN:HD21	2:A:1:GF4:H13	1.84	0.43
1:B:36:GLY:HA2	1:B:235[B]:GLN:HE22	1.83	0.43
1:A:262[B]:THR:OG1	1:A:298:VAL:HG12	2.18	0.42
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.54	0.42
1:A:26:PRO:HB3	1:A:48:ILE:HD11	2.01	0.42
1:A:203:TYR:HA	1:A:207:LYS:O	2.19	0.42
1:A:262[B]:THR:CG2	1:A:296:ARG:HB3	2.50	0.41
1:A:346:ASN:HB2	3:A:522:HOH:O	2.21	0.41
1:B:28[B]:MET:SD	1:B:340:ALA:HB2	2.60	0.40
1:B:273:MET:HG3	1:B:313:VAL:HG13	2.03	0.40
1:A:107:LEU:HD22	1:B:303:PRO:HD3	2.02	0.40
1:A:99:LYS:H	1:A:99:LYS:HG2	1.58	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	389/358 (109%)	379 (97%)	10 (3%)	0	100	100
1	B	388/358 (108%)	381 (98%)	7 (2%)	0	100	100
All	All	777/716 (108%)	760 (98%)	17 (2%)	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	324/292 (111%)	317 (98%)	7 (2%)	45	34
1	B	324/292 (111%)	311 (96%)	13 (4%)	28	15
All	All	648/584 (111%)	628 (97%)	20 (3%)	43	23

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	250[A]	GLN
1	A	250[B]	GLN
1	A	262[A]	THR
1	A	262[B]	THR
1	A	283	ILE
1	A	299	LYS
1	B	99	LYS
1	B	123	ASP
1	B	128[A]	SER
1	B	128[B]	SER
1	B	172	GLN
1	B	262[A]	THR
1	B	262[B]	THR
1	B	278[A]	VAL
1	B	278[B]	VAL
1	B	331	GLU
1	B	334[A]	LEU

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Mol	Chain	Res	Type
1	B	334[B]	LEU
1	B	361	GLN

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	GLN
1	A	137	ASN
1	A	180	GLN
1	A	253	GLN
1	A	279	ASN
1	A	346	ASN
1	B	6	GLN
1	B	23	GLN
1	B	56	GLN
1	B	137	ASN
1	B	172	GLN
1	B	249	GLN
1	B	256	GLN
1	B	285	ASN
1	B	361	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GF4	A	1	-	15,15,15	2.94	6 (40%)	17,21,21	3.07	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GF4	A	1	-	-	0/3/6/6	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	GF4	C5-C4	6.09	1.50	1.38
2	A	1	GF4	N9-N8	5.80	1.41	1.30
2	A	1	GF4	N10-N9	4.83	1.41	1.35
2	A	1	GF4	N7-N8	3.09	1.40	1.36
2	A	1	GF4	O11-C3	3.04	1.29	1.23
2	A	1	GF4	C3-N2	-3.01	1.32	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GF4	C3-C4-C5	-6.17	102.61	107.55
2	A	1	GF4	N10-C6-N7	5.75	115.56	108.58
2	A	1	GF4	C14-C5-N1	4.45	124.94	119.40
2	A	1	GF4	C12-C4-C3	4.35	128.45	122.13
2	A	1	GF4	C6-N10-N9	-3.79	104.12	109.63
2	A	1	GF4	C12-C4-C5	2.89	128.93	125.46
2	A	1	GF4	C14-C5-C4	-2.85	126.38	131.20
2	A	1	GF4	C13-C12-C4	-2.30	106.19	112.42
2	A	1	GF4	N7-N8-N9	-2.29	107.76	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GF4	4	0

## 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

### 6.1 Protein, DNA and RNA chains

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	358/358 (100%)	0.43	28 (7%) 19 17	13, 24, 39, 67	49 (13%)
1	B	358/358 (100%)	0.23	9 (2%) 58 58	12, 25, 33, 38	48 (13%)
All	All	716/716 (100%)	0.33	37 (5%) 33 31	12, 25, 35, 67	97 (13%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASN	7.1
1	A	283	ILE	6.9
1	A	284	ILE	6.8
1	A	291	ILE	6.6
1	A	282	SER	6.2
1	A	281	ASP	5.5
1	A	287	SER	5.2
1	A	286	GLY	5.0
1	A	280	PRO	4.9
1	A	290	LYS	4.7
1	A	278[A]	VAL	4.7
1	A	293	LEU	4.5
1	A	288	ASP	4.2
1	B	123	ASP	4.1
1	B	56	GLN	4.1
1	A	292	ALA	3.9
1	A	4	ALA	3.7
1	A	285	ASN	3.5
1	B	102	ASN	3.2
1	B	52	GLN	3.2
1	A	354[A]	TRP	3.2
1	A	36	GLY	3.1
1	A	346	ASN	3.1
1	A	361	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	2.9
1	B	57	GLN	2.9
1	B	36	GLY	2.9
1	B	241	LEU	2.8
1	A	279	ASN	2.7
1	A	296	ARG	2.6
1	B	4	ALA	2.6
1	A	244	ASN	2.3
1	A	34	TYR	2.3
1	A	126	LYS	2.3
1	A	243	ILE	2.1
1	A	264	ASP	2.1
1	A	309	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GF4	A	1	14/14	0.86	0.11	38,40,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.