



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:56 AM GMT

PDB ID : 3GM1  
Title : Crystal Structure of the Focal Adhesion Targeting (FAT) Domain of Pyk2 in Complex with Paxillin LD4 Motif-Derived Peptides  
Authors : Lulo, J.E.; Yuzawa, S.; Schlessinger, J.  
Deposited on : 2009-03-12  
Resolution : 2.95 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

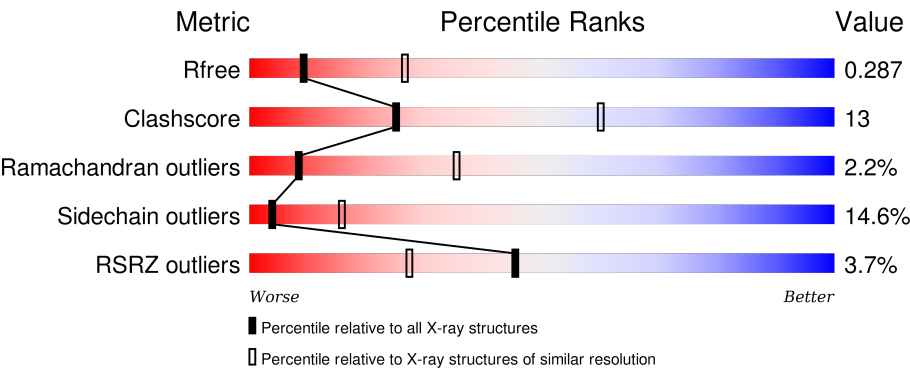
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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 <sub>free</sub>	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	153	<div><div></div><div>61%24%7%8%</div></div>
1	B	153	<div><div></div><div>62%25%5%8%</div></div>
2	C	13	<div><div>8%</div><div>46%31%8%15%</div></div>
2	D	13	<div><div>23%</div><div>62%31%8%</div></div>
2	E	13	<div><div>8%</div><div>31%38%15%15%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (46%), green (69%), yellow (23%), and orange (8%). The segments are stacked horizontally, with the red segment starting from the left and the orange segment at the far right. The percentages are labeled above each segment.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2528 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 Protein tyrosine kinase 2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1069	670	186	209	4			
1	B	141	Total	C	N	O	S	0	0	0
			1078	675	188	211	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	857	GLY	-	EXPRESSION TAG	UNP Q14289
A	858	SER	-	EXPRESSION TAG	UNP Q14289
A	859	HIS	-	EXPRESSION TAG	UNP Q14289
A	860	MET	-	EXPRESSION TAG	UNP Q14289
A	899	ALA	CYS	ENGINEERED	UNP Q14289
B	857	GLY	-	EXPRESSION TAG	UNP Q14289
B	858	SER	-	EXPRESSION TAG	UNP Q14289
B	859	HIS	-	EXPRESSION TAG	UNP Q14289
B	860	MET	-	EXPRESSION TAG	UNP Q14289
B	899	ALA	CYS	ENGINEERED	UNP Q14289

- Molecule 2 is a protein called Paxillin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	S	0	0	0
			87	52	14	20	1			
2	F	13	Total	C	N	O	S	0	0	0
			98	59	16	22	1			
2	C	11	Total	C	N	O	S	0	0	0
			86	52	14	19	1			
2	D	12	Total	C	N	O	S	0	0	0
			93	56	15	21	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total 7	O 7	0	0
3	B	7	Total 7	O 7	0	0
3	C	2	Total 2	O 2	0	0
3	D	1	Total 1	O 1	0	0

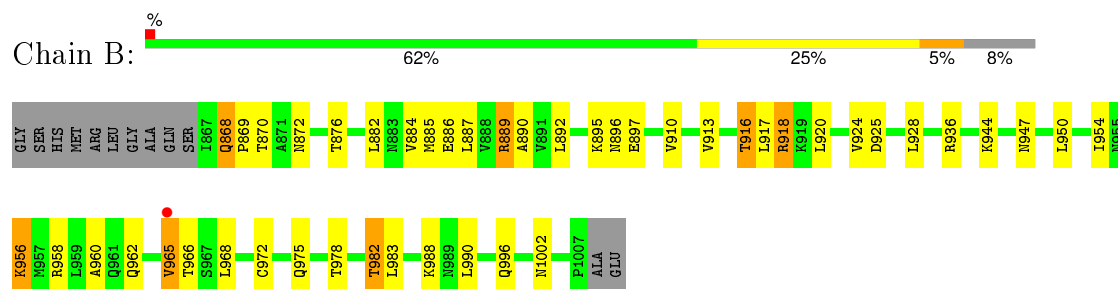
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

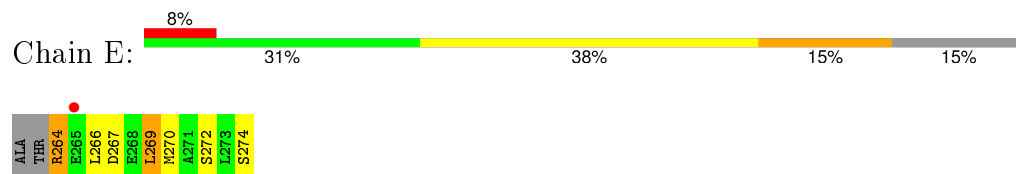
- Molecule 1: Protein tyrosine kinase 2 beta



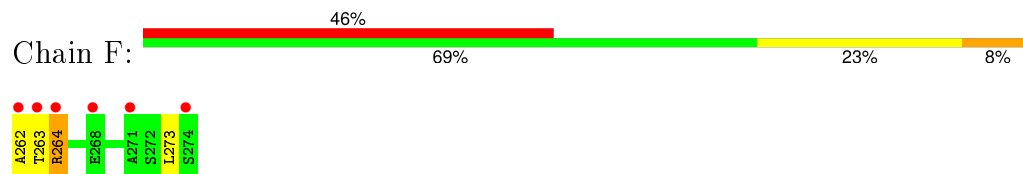
- Molecule 1: Protein tyrosine kinase 2 beta



- Molecule 2: Paxillin

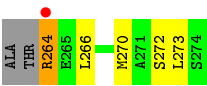


- Molecule 2: Paxillin

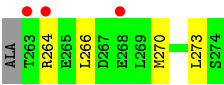


- Molecule 2: Paxillin





● Molecule 2: Paxillin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.77Å 73.77Å 156.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.67 – 2.95 42.67 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.67-2.95) 97.8 (42.67-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.233 , 0.290 0.227 , 0.287	Depositor DCC
$R_{free}$ test set	459 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 9465 reflections (0.021%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9940e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/1079	0.69	1/1466 (0.1%)
1	B	0.52	0/1088	0.66	0/1479
2	C	0.55	0/85	0.67	0/112
2	D	0.46	0/92	0.71	0/122
2	E	0.54	0/86	0.77	0/112
2	F	0.58	0/97	0.73	0/129
All	All	0.53	0/2527	0.68	1/3420 (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	983	LEU	CA-CB-CG	5.31	127.51	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	1069	0	1123	23	0
1	B	1078	0	1127	32	0
2	C	86	0	85	7	0
2	D	93	0	92	2	0
2	E	87	0	85	6	0
2	F	98	0	97	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	7	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
All	All	2528	0	2609	65	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 13.

All (65) 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:B:889:ARG:HG2	1:B:890:ALA:N	1.76	0.98
1:B:918:ARG:HG2	1:B:918:ARG:HH11	1.30	0.92
1:B:885:MET:HE3	2:C:266:LEU:HB2	1.63	0.80
1:B:870:THR:HG21	2:C:266:LEU:HD23	1.65	0.77
1:A:996:GLN:HE21	1:A:1000:LEU:HD11	1.54	0.73
1:B:956:LYS:HG2	1:B:975:GLN:HB3	1.72	0.71
1:B:887:LEU:HA	1:B:916:THR:HG21	1.76	0.67
1:A:911:LYS:HG3	2:F:273:LEU:HD11	1.76	0.66
2:C:264:ARG:HB2	2:C:264:ARG:NH1	2.11	0.66
1:A:956:LYS:HG2	1:A:975:GLN:HB3	1.78	0.66
1:B:884:VAL:HG22	1:B:920:LEU:HD11	1.80	0.64
1:A:964:ALA:O	1:A:965:VAL:HG22	2.01	0.61
1:B:886:GLU:HG2	1:B:889:ARG:HH11	1.66	0.61
1:B:918:ARG:CG	1:B:918:ARG:HH11	2.08	0.59
1:B:870:THR:HG22	1:B:988:LYS:HE2	1.84	0.58
1:A:910:VAL:HG21	1:A:957:MET:HG3	1.86	0.58
1:B:913:VAL:O	1:B:916:THR:HG22	2.04	0.57
1:B:887:LEU:HA	1:B:916:THR:CG2	2.34	0.57
1:B:885:MET:CE	2:C:266:LEU:HB2	2.34	0.57
1:B:918:ARG:HA	2:D:266:LEU:HD21	1.86	0.56
1:B:924:VAL:HG21	1:B:990:LEU:HD21	1.86	0.56
1:B:928:LEU:O	1:B:936:ARG:HD2	2.06	0.56
1:A:948:LYS:O	1:A:952:GLU:HG3	2.06	0.56
1:A:963:ASN:O	1:A:969:SER:HA	2.06	0.55
1:A:885:MET:HG2	2:E:266:LEU:HD13	1.88	0.55
1:A:931:LEU:HB2	1:A:932:PRO:HD2	1.89	0.55
1:B:889:ARG:HG2	1:B:890:ALA:H	1.70	0.53
1:B:925:ASP:HA	1:B:928:LEU:HD12	1.91	0.52
2:C:264:ARG:HB2	2:C:264:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:270:MET:O	2:C:273:LEU:HB2	2.10	0.52
1:A:996:GLN:HE21	1:A:1000:LEU:CD1	2.23	0.50
1:A:932:PRO:HD3	1:A:1001:ALA:HB2	1.92	0.50
1:A:870:THR:HG23	2:E:267:ASP:OD1	2.11	0.50
1:B:956:LYS:HG2	1:B:975:GLN:CB	2.40	0.50
1:B:978:THR:O	1:B:982:THR:HG22	2.11	0.49
1:A:872:ASN:ND2	2:E:264:ARG:HB2	2.27	0.49
1:A:947:ASN:N	1:A:947:ASN:HD22	2.11	0.48
1:B:910:VAL:HG11	1:B:954:ILE:HD13	1.94	0.48
1:A:978:THR:O	1:A:982:THR:HG23	2.14	0.48
1:B:965:VAL:O	1:B:965:VAL:HG12	2.14	0.48
1:B:918:ARG:HG2	1:B:918:ARG:NH1	2.10	0.47
1:A:883:ASN:ND2	1:A:919:LYS:HD2	2.31	0.46
1:B:882:LEU:O	1:B:885:MET:HB2	2.16	0.46
1:B:920:LEU:HD21	1:B:990:LEU:HD23	1.98	0.45
1:B:956:LYS:HE3	1:B:975:GLN:OE1	2.16	0.45
2:E:266:LEU:O	2:E:270:MET:N	2.50	0.44
1:A:940:GLU:HA	1:A:943:GLN:HE21	1.81	0.44
2:F:262:ALA:HA	2:F:264:ARG:HH22	1.82	0.44
1:B:868:GLN:HB2	1:B:869:PRO:HD2	1.99	0.44
1:B:960:ALA:HB2	1:B:972:CYS:HB3	2.00	0.44
1:B:872:ASN:HD21	2:C:264:ARG:NH2	2.15	0.44
1:B:897:GLU:OE2	1:B:897:GLU:HA	2.18	0.43
2:F:263:THR:O	2:F:263:THR:HG22	2.17	0.43
1:A:892:LEU:HA	1:A:892:LEU:HD23	1.88	0.43
1:A:924:VAL:HG12	1:A:928:LEU:HD22	2.00	0.42
2:E:264:ARG:NH1	2:E:267:ASP:OD2	2.53	0.42
1:B:917:LEU:HD23	1:B:950:LEU:HD22	2.02	0.42
2:E:269:LEU:O	2:E:272:SER:HB3	2.20	0.41
2:F:262:ALA:HA	2:F:264:ARG:HH12	1.85	0.41
1:B:918:ARG:CG	1:B:918:ARG:NH1	2.75	0.41
1:A:917:LEU:HD23	1:A:950:LEU:HD22	2.02	0.41
2:D:266:LEU:O	2:D:270:MET:HG2	2.21	0.41
1:A:898:LEU:HA	1:A:898:LEU:HD23	1.68	0.41
1:A:935:SER:C	1:A:937:THR:N	2.72	0.41
1:A:928:LEU:N	1:A:929:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	138/153 (90%)	123 (89%)	13 (9%)	2 (1%)	14	49
1	B	139/153 (91%)	124 (89%)	11 (8%)	4 (3%)	6	27
2	C	9/13 (69%)	8 (89%)	0	1 (11%)	0	2
2	D	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
2	E	9/13 (69%)	9 (100%)	0	0	100	100
2	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	316/358 (88%)	284 (90%)	25 (8%)	7 (2%)	8	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	965	VAL
1	B	965	VAL
1	B	896	ASN
1	B	1002	ASN
2	C	272	SER
1	A	929	PRO
1	B	895	LYS

### 5.3.2 Protein sidechains

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	122/132 (92%)	103 (84%)	19 (16%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	123/132 (93%)	107 (87%)	16 (13%)	5	20
2	C	10/11 (91%)	9 (90%)	1 (10%)	9	32
2	D	11/11 (100%)	9 (82%)	2 (18%)	2	9
2	E	10/11 (91%)	7 (70%)	3 (30%)	0	1
2	F	11/11 (100%)	10 (91%)	1 (9%)	12	38
All	All	287/308 (93%)	245 (85%)	42 (15%)	4	16

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	894	LEU
1	A	896	ASN
1	A	898	LEU
1	A	900	GLN
1	A	918	ARG
1	A	919	LYS
1	A	920	LEU
1	A	928	LEU
1	A	943	GLN
1	A	945	LEU
1	A	947	ASN
1	A	956	LYS
1	A	958	ARG
1	A	962	GLN
1	A	968	LEU
1	A	982	THR
1	A	983	LEU
1	A	988	LYS
1	A	1003	LEU
2	E	264	ARG
2	E	269	LEU
2	E	274	SER
2	F	264	ARG
1	B	868	GLN
1	B	876	THR
1	B	889	ARG
1	B	892	LEU
1	B	916	THR
1	B	918	ARG
1	B	944	LYS

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Mol	Chain	Res	Type
1	B	947	ASN
1	B	956	LYS
1	B	958	ARG
1	B	962	GLN
1	B	966	THR
1	B	968	LEU
1	B	982	THR
1	B	983	LEU
1	B	996	GLN
2	C	264	ARG
2	D	264	ARG
2	D	273	LEU

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

Mol	Chain	Res	Type
1	A	872	ASN
1	A	883	ASN
1	A	943	GLN
1	A	947	ASN
1	A	989	ASN
1	A	996	GLN
1	B	872	ASN
1	B	883	ASN
1	B	943	GLN
1	B	947	ASN
1	B	989	ASN

### 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 [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	140/153 (91%)	0.12	0 <span>100</span> <span>100</span>	32, 47, 64, 71	0
1	B	141/153 (92%)	0.24	1 (0%) <span>89</span> <span>76</span>	36, 52, 72, 78	0
2	C	11/13 (84%)	0.53	1 (9%) <span>11</span> <span>6</span>	64, 65, 78, 81	0
2	D	12/13 (92%)	1.94	3 (25%) <span>1</span> <span>1</span>	95, 97, 105, 107	0
2	E	11/13 (84%)	0.75	1 (9%) <span>11</span> <span>6</span>	79, 81, 94, 94	0
2	F	13/13 (100%)	2.06	6 (46%) <span>0</span> <span>0</span>	76, 79, 94, 94	0
All	All	328/358 (91%)	0.35	12 (3%) <span>45</span> <span>27</span>	32, 52, 91, 107	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	264	ARG	4.4
2	F	263	THR	4.3
2	D	263	THR	4.0
2	F	262	ALA	3.8
2	D	268	GLU	3.8
2	F	264	ARG	3.2
2	F	268	GLU	2.9
1	B	965	VAL	2.7
2	F	274	SER	2.6
2	F	271	ALA	2.5
2	C	264	ARG	2.3
2	E	265	GLU	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.