



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:55 PM GMT

PDB ID : 5EW3  
Title : Human Vascular Endothelial Growth Factor Receptor 2 (KDR) Kinase Domain  
in complex with AAL993  
Authors : Stark, W.; Goepfert, A.  
Deposited on : 2015-11-20  
Resolution : 2.50 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

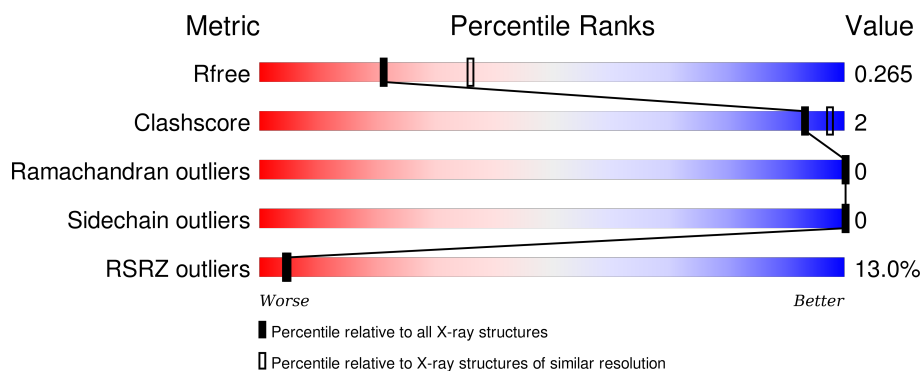
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	316	<div> <div>8%</div> <div>83%</div> <div>13%</div> </div>
1	B	316	<div> <div>15%</div> <div>80%</div> <div>16%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4453 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 Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2190	1410	378	386	16			
1	B	266	Total	C	N	O	S	0	0	0
			2133	1375	365	377	16			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P35968
A	?	-	GLY	deletion	UNP P35968
A	?	-	ALA	deletion	UNP P35968
A	?	-	ARG	deletion	UNP P35968
A	?	-	PHE	deletion	UNP P35968
A	?	-	ARG	deletion	UNP P35968
A	?	-	GLN	deletion	UNP P35968
A	?	-	GLY	deletion	UNP P35968
A	?	-	LYS	deletion	UNP P35968
A	?	-	ASP	deletion	UNP P35968
A	?	-	TYR	deletion	UNP P35968
A	?	-	VAL	deletion	UNP P35968
A	?	-	GLY	deletion	UNP P35968
A	?	-	ALA	deletion	UNP P35968
A	?	-	ILE	deletion	UNP P35968
A	?	-	PRO	deletion	UNP P35968
A	?	-	VAL	deletion	UNP P35968
A	?	-	ASP	deletion	UNP P35968
A	?	-	LEU	deletion	UNP P35968
A	?	-	LYS	deletion	UNP P35968
A	?	-	ARG	deletion	UNP P35968
A	?	-	ARG	deletion	UNP P35968
A	?	-	LEU	deletion	UNP P35968
A	?	-	ASP	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968

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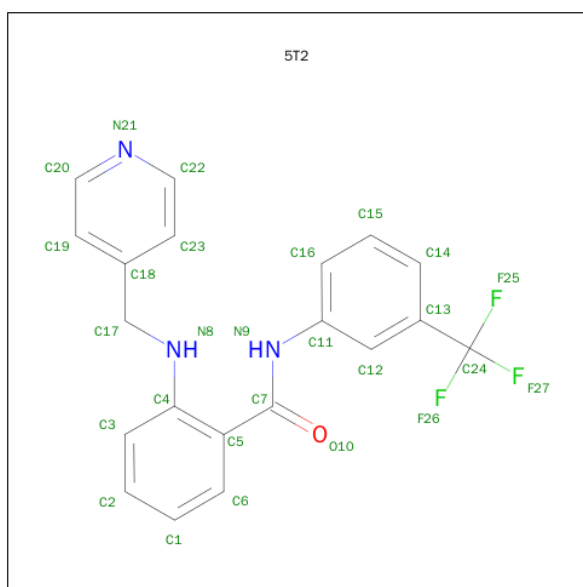
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P35968
A	?	-	THR	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	GLN	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	ALA	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	GLY	deletion	UNP P35968
A	?	-	PHE	deletion	UNP P35968
A	?	-	VAL	deletion	UNP P35968
A	?	-	GLU	deletion	UNP P35968
A	?	-	GLU	deletion	UNP P35968
A	?	-	LYS	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	LEU	deletion	UNP P35968
A	?	-	SER	deletion	UNP P35968
A	?	-	ASP	deletion	UNP P35968
A	?	-	VAL	deletion	UNP P35968
A	?	-	GLU	deletion	UNP P35968
A	?	-	GLU	deletion	UNP P35968
A	?	-	GLU	deletion	UNP P35968
B	?	-	LYS	deletion	UNP P35968
B	?	-	GLY	deletion	UNP P35968
B	?	-	ALA	deletion	UNP P35968
B	?	-	ARG	deletion	UNP P35968
B	?	-	PHE	deletion	UNP P35968
B	?	-	ARG	deletion	UNP P35968
B	?	-	GLN	deletion	UNP P35968
B	?	-	GLY	deletion	UNP P35968
B	?	-	LYS	deletion	UNP P35968
B	?	-	ASP	deletion	UNP P35968
B	?	-	TYR	deletion	UNP P35968
B	?	-	VAL	deletion	UNP P35968
B	?	-	GLY	deletion	UNP P35968
B	?	-	ALA	deletion	UNP P35968
B	?	-	ILE	deletion	UNP P35968
B	?	-	PRO	deletion	UNP P35968
B	?	-	VAL	deletion	UNP P35968
B	?	-	ASP	deletion	UNP P35968

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P35968
B	?	-	LYS	deletion	UNP P35968
B	?	-	ARG	deletion	UNP P35968
B	?	-	ARG	deletion	UNP P35968
B	?	-	LEU	deletion	UNP P35968
B	?	-	ASP	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	ILE	deletion	UNP P35968
B	?	-	THR	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	GLN	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	ALA	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	GLY	deletion	UNP P35968
B	?	-	PHE	deletion	UNP P35968
B	?	-	VAL	deletion	UNP P35968
B	?	-	GLU	deletion	UNP P35968
B	?	-	GLU	deletion	UNP P35968
B	?	-	LYS	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	LEU	deletion	UNP P35968
B	?	-	SER	deletion	UNP P35968
B	?	-	ASP	deletion	UNP P35968
B	?	-	VAL	deletion	UNP P35968
B	?	-	GLU	deletion	UNP P35968
B	?	-	GLU	deletion	UNP P35968
B	?	-	GLU	deletion	UNP P35968

- Molecule 2 is 2-(pyridin-4-ylmethylamino)- {N}-[3-(trifluoromethyl)phenyl]benzamide (three-letter code: 5T2) (formula: C<sub>20</sub>H<sub>16</sub>F<sub>3</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	20	3	3	1		
2	B	1	Total	C	F	N	O	0	0
			27	20	3	3	1		

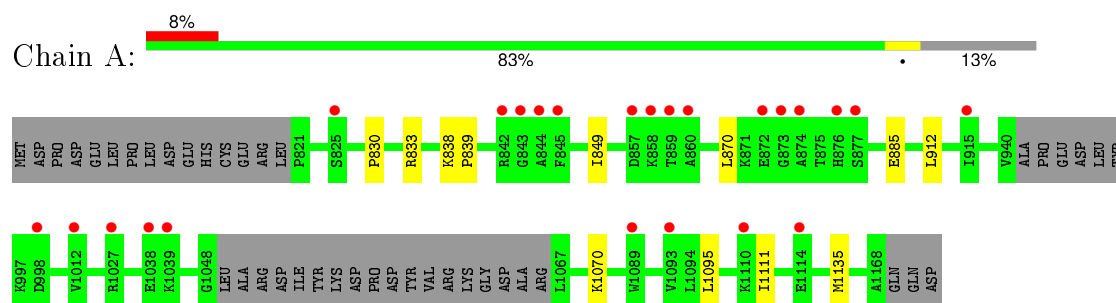
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	26	Total	O	0	0
			26	26		

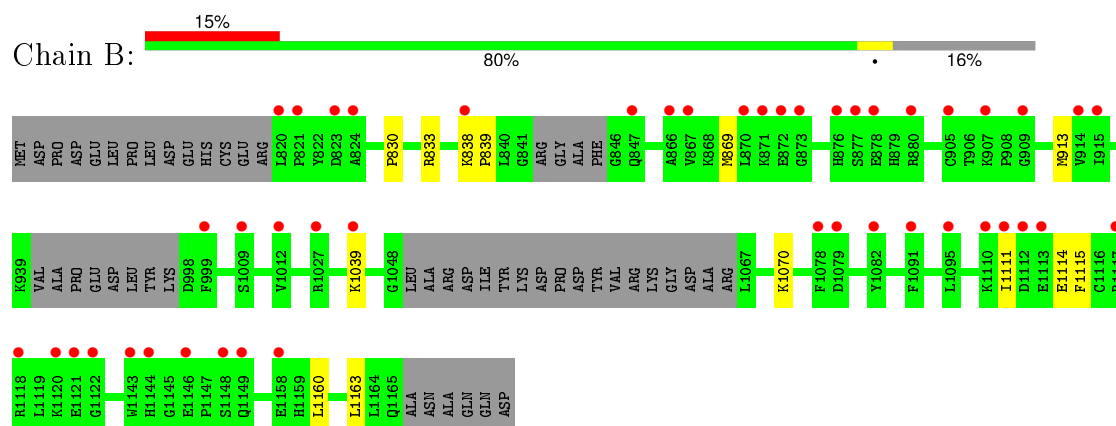
### 3 Residue-property plots [i](#)

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: Vascular endothelial growth factor receptor 2



- Molecule 1: Vascular endothelial growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.50Å 55.76Å 89.76Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	19.68 – 2.50 19.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.68-2.50) 98.9 (19.68-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.50Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.218 , 0.254 0.233 , 0.265	Depositor DCC
$R_{free}$ test set	665 reflections (2.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.8	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23051 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5T2

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	0.41	0/2243	0.61	0/3027
1	B	0.41	0/2184	0.61	0/2948
All	All	0.41	0/4427	0.61	0/5975

There are no bond length outliers.

There are no bond angle outliers.

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	2190	0	2204	9	0
1	B	2133	0	2145	8	0
2	A	27	0	16	1	0
2	B	27	0	16	0	0
3	A	50	0	0	0	0
3	B	26	0	0	0	0
All	All	4453	0	4381	17	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 2.

All (17) 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:1039:LYS:HG2	1:B:1039:LYS:O	2.05	0.56
1:B:1160:LEU:HA	1:B:1163:LEU:HD12	1.88	0.55
1:A:1070:LYS:CE	1:A:1111:ILE:HD11	2.39	0.52
1:B:869:MET:HG3	1:B:913:MET:HG2	1.93	0.51
1:A:1070:LYS:HE3	1:A:1111:ILE:HD11	1.93	0.49
1:B:1070:LYS:CE	1:B:1111:ILE:HD11	2.42	0.49
1:A:885:GLU:CD	2:A:1201:5T2:H7	2.40	0.42
1:A:839:PRO:HA	1:A:849:ILE:HG22	2.01	0.42
1:A:1095:LEU:HD22	1:A:1135:MET:HE2	2.00	0.42
1:B:1114:GLU:O	1:B:1115:PHE:HB3	2.20	0.42
1:B:838:LYS:HA	1:B:839:PRO:HD3	1.98	0.42
1:A:838:LYS:HA	1:A:839:PRO:HD3	1.98	0.41
1:B:1070:LYS:HE3	1:B:1111:ILE:HD11	2.03	0.41
1:A:1095:LEU:HD13	1:A:1135:MET:HE1	2.01	0.41
1:A:870:LEU:HD12	1:A:912:LEU:HB3	2.04	0.40
1:B:830:PRO:HG2	1:B:833:ARG:HD3	2.02	0.40
1:A:830:PRO:HG2	1:A:833:ARG:HD3	2.03	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	268/316 (85%)	259 (97%)	9 (3%)	0	100	100
1	B	258/316 (82%)	252 (98%)	6 (2%)	0	100	100
All	All	526/632 (83%)	511 (97%)	15 (3%)	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	237/275 (86%)	237 (100%)	0	100	100
1	B	233/275 (85%)	233 (100%)	0	100	100
All	All	470/550 (86%)	470 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

2 ligands are 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	5T2	A	1201	-	29,29,29	1.08	0	40,40,40	1.17	4 (10%)
2	5T2	B	1201	-	29,29,29	1.16	0	40,40,40	1.18	4 (10%)

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	5T2	A	1201	-	-	0/19/19/19	0/3/3/3
2	5T2	B	1201	-	-	0/19/19/19	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	5T2	F26-C24-C13	-2.50	107.65	112.92
2	A	1201	5T2	C19-C20-N21	-2.41	119.46	123.64
2	A	1201	5T2	F26-C24-C13	-2.30	108.08	112.92
2	A	1201	5T2	C23-C22-N21	-2.21	119.81	123.64
2	B	1201	5T2	C19-C20-N21	-2.11	119.98	123.64
2	B	1201	5T2	C22-N21-C20	2.14	121.99	116.84
2	B	1201	5T2	C17-N8-C4	2.37	127.47	121.84
2	A	1201	5T2	C22-N21-C20	2.38	122.57	116.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	5T2	1	0

## 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

### 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	274/316 (86%)	0.52	24 (8%) 12 13	31, 53, 87, 108	0
1	B	266/316 (84%)	0.94	46 (17%) 2 2	38, 66, 102, 129	0
All	All	540/632 (85%)	0.73	70 (12%) 5 4	31, 60, 96, 129	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1039	LYS	7.3
1	A	860	ALA	6.0
1	A	859	THR	5.7
1	B	1117	ARG	5.4
1	B	1112	ASP	5.1
1	B	872	GLU	4.3
1	A	858	LYS	4.2
1	A	842	ARG	4.1
1	B	915	ILE	4.0
1	A	876	HIS	4.0
1	A	857	ASP	3.9
1	B	1148	SER	3.8
1	B	838	LYS	3.7
1	B	1113	GLU	3.6
1	B	867	VAL	3.3
1	B	1149	GLN	3.3
1	B	1121	GLU	3.2
1	B	820	LEU	3.2
1	B	1158	GLU	3.2
1	B	876	HIS	3.2
1	B	1027	ARG	3.2
1	B	877	SER	3.1
1	A	1114	GLU	3.1
1	B	1082	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1110	LYS	3.0
1	A	1110	LYS	2.9
1	A	1039	LYS	2.9
1	A	872	GLU	2.8
1	B	847	GLN	2.8
1	B	873	GLY	2.7
1	B	999	PHE	2.7
1	A	843	GLY	2.7
1	B	866	ALA	2.7
1	A	998	ASP	2.7
1	A	1027	ARG	2.6
1	B	1120	LYS	2.6
1	B	870	LEU	2.6
1	B	1144	HIS	2.6
1	A	874	ALA	2.5
1	A	1012	VAL	2.5
1	B	871	LYS	2.5
1	B	824	ALA	2.5
1	B	1079	ASP	2.5
1	B	880	ARG	2.5
1	A	1089	TRP	2.5
1	B	909	GLY	2.5
1	B	1146	GLU	2.5
1	B	907	LYS	2.4
1	B	1118	ARG	2.4
1	B	914	VAL	2.4
1	B	1111	ILE	2.4
1	A	915	ILE	2.3
1	A	844	ALA	2.3
1	B	823	ASP	2.3
1	B	878	GLU	2.3
1	B	1078	PHE	2.2
1	B	1091	PHE	2.2
1	B	1143	TRP	2.2
1	A	1093	VAL	2.2
1	A	873	GLY	2.2
1	A	1038	GLU	2.2
1	B	821	PRO	2.1
1	B	1095	LEU	2.1
1	B	1012	VAL	2.1
1	A	845	PHE	2.1
1	B	905	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	825	SER	2.1
1	B	1122	GLY	2.1
1	B	1009	SER	2.0
1	A	877	SER	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	5T2	A	1201	27/27	0.96	0.17	-0.32	27,39,42,46	0
2	5T2	B	1201	27/27	0.95	0.18	-0.55	45,53,58,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.