



# wwPDB X-ray Structure Validation Summary Report

Aug 29, 2014 – 06:57 AM EDT

PDB ID : 2JK5  
Title : Potassium Channel KcsA in complex with Tetrabutylammonium in high K  
Authors : Lenaeus, M.J.; Focia, P.J.; Wagner, T.; Gross, A.  
Deposited on : 2008-08-15  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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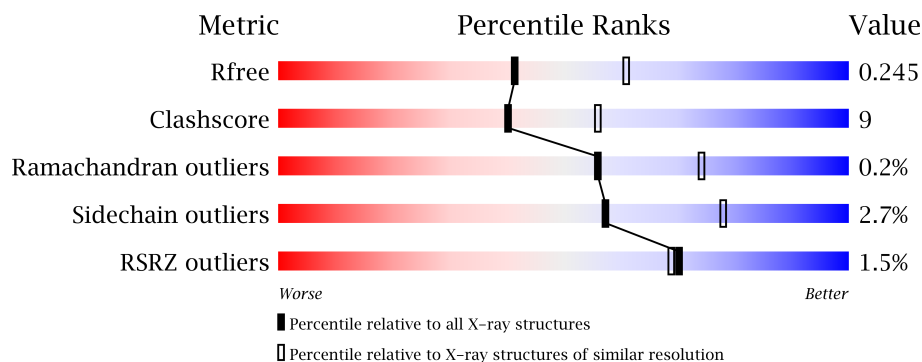
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	219	
2	B	212	
3	C	124	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	K	C	1127	-	X
5	K	C	1129	-	X
7	L2C	C	1132	-	X
8	TBA	C	1133[A]	-	X
8	TBA	C	1133[B]	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
9	HP6	C	1134	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4420 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	7	0
			1687	1061	283	337	6			

- Molecule 2 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	2	0
			1664	1033	286	340	5			

- Molecule 3 is a protein called VOLTAGE-GATED POTASSIUM CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	1	0
			778	510	133	133	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	CYS	LEU	CONFLICT	UNP P0A334

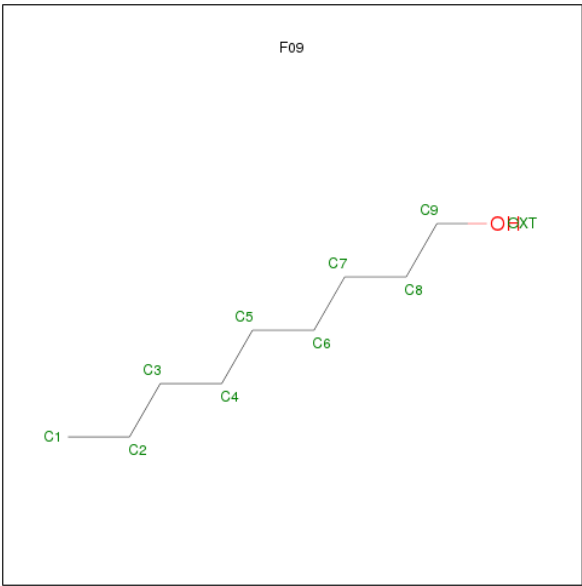
- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Co	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

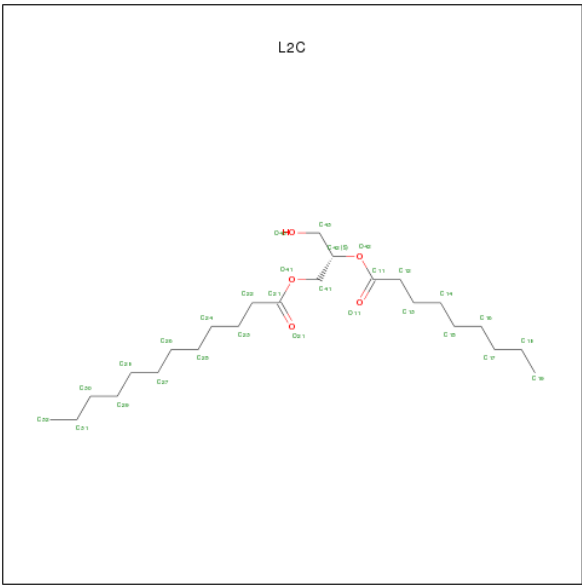
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total	K	0	0
			6	6		

- Molecule 6 is NONAN-1-OL (three-letter code: F09) (formula: C<sub>9</sub>H<sub>20</sub>O).



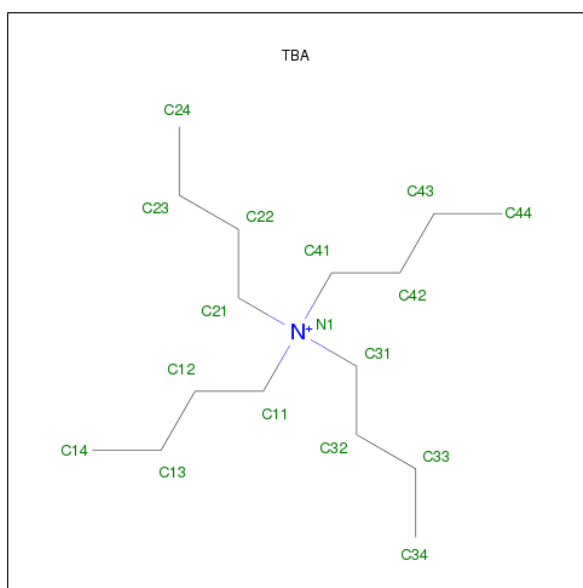
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			10	9	1		

- Molecule 7 is (2S)-3-HYDROXY-2-(NONANOYLOXY)PROPYLLAURATE (three-letter code: L2C) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>5</sub>).



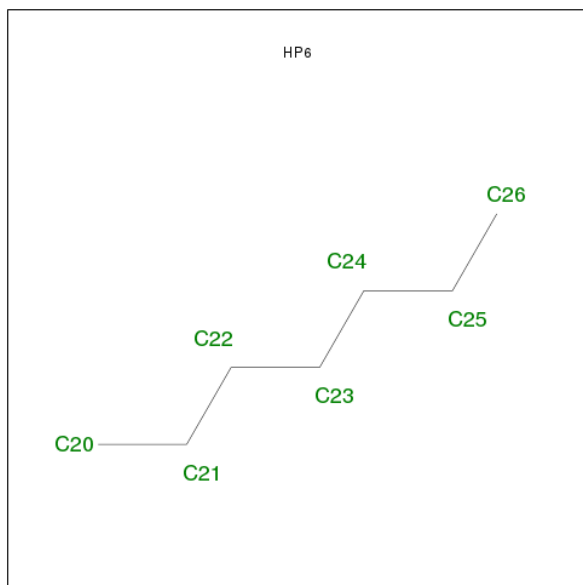
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			29	24	5		

- Molecule 8 is TETRABUTYLAMMONIUM ION (three-letter code: TBA) (formula:  $C_{16}H_{36}N$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	C	N	1
			34	32	2	
					0	

- Molecule 9 is HEPTANE (three-letter code: HP6) (formula:  $C_7H_{16}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	C		0
			7	7		
					0	

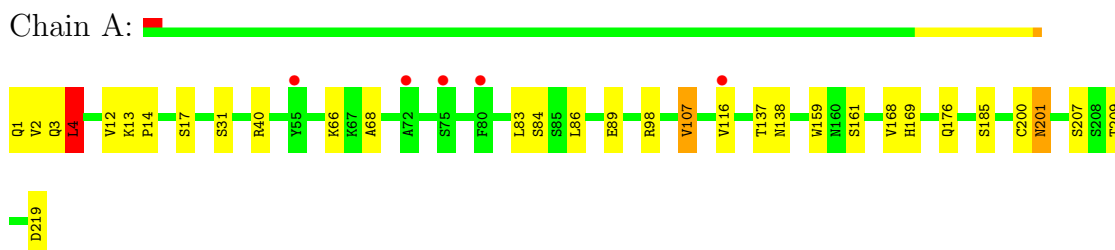
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	72	Total 72	O 72	0	0
10	B	81	Total 81	O 81	0	0
10	C	51	Total 51	O 51	0	0

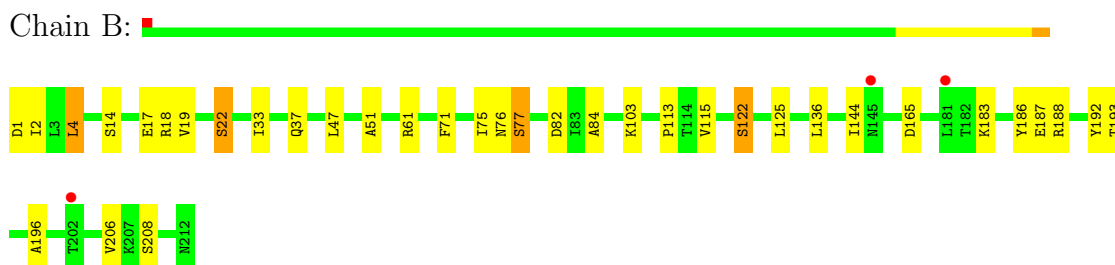
### 3 Residue-property plots

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.

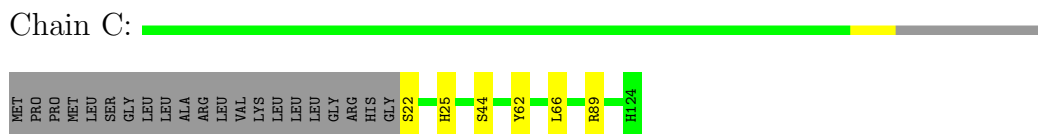
- Molecule 1: ANTIBODY FAB FRAGMENT LIGHT CHAIN



- Molecule 2: ANTIBODY FAB FRAGMENT HEAVY CHAIN



- Molecule 3: VOLTAGE-GATED POTASSIUM CHANNEL





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.15Å 156.15Å 76.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 49.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.40) 99.5 (49.38-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
R, $R_{free}$	0.202 , 0.249 0.202 , 0.245	Depositor DCC
$R_{free}$ test set	1790 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.8	EDS
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 35723 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L2C, CO, K, HP6, TBA, F09

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	0.51	0/1730	0.60	1/2368 (0.0%)
2	B	0.53	0/1701	0.62	0/2309
3	C	0.65	0/798	0.63	0/1097
All	All	0.55	0/4229	0.62	1/5774 (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	4	LEU	CA-CB-CG	5.46	127.86	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1616	25	0
2	B	1664	0	1591	35	0
3	C	778	0	789	5	0
4	C	1	0	0	0	0
5	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	10	0	19	1	0
7	C	29	0	46	6	0
8	C	34	0	72	9	0
9	C	7	0	16	1	0
10	A	72	0	0	3	0
10	B	81	0	0	5	0
10	C	51	0	0	2	0
All	All	4420	0	4149	79	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 79 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:C:1132:L2C:H121	7:C:1132:L2C:H412	1.32	1.10
2:B:193:THR:HG22	2:B:208:SER:HB3	1.44	0.95
2:B:193:THR:HG22	2:B:208:SER:CB	1.97	0.95
2:B:18:ARG:HH11	2:B:76[A]:ASN:HD21	1.04	0.93
2:B:1:ASP:OD1	10:B:2002:HOH:O	1.85	0.93

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	223/219 (102%)	213 (96%)	9 (4%)	1 (0%)	43	61
2	B	212/212 (100%)	203 (96%)	9 (4%)	0	100	100
3	C	102/124 (82%)	99 (97%)	3 (3%)	0	100	100
All	All	537/555 (97%)	515 (96%)	21 (4%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	VAL

### 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	187/185 (101%)	180 (96%)	7 (4%)	45	66
2	B	192/190 (101%)	186 (97%)	6 (3%)	52	74
3	C	75/92 (82%)	75 (100%)	0	100	100
All	All	454/467 (97%)	441 (97%)	13 (3%)	57	76

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219[A]	ASP
1	A	219[B]	ASP
2	B	122	SER
1	A	201	ASN
2	B	77	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	ASN
3	C	25	HIS
2	B	137	ASN
1	A	201	ASN
2	B	190	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z  > 2$
6	F09	C	1131	-	9,9,9	1.24	1 (11%)	8,8,8	0.52	0
7	L2C	C	1132	-	28,28,28	1.36	3 (10%)	30,30,30	1.56	3 (10%)
8	TBA	C	1133[A]	-	16,16,16	1.33	4 (25%)	18,18,18	0.94	0
8	TBA	C	1133[B]	-	16,16,16	0.76	0	18,18,18	0.64	0
9	HP6	C	1134	-	6,6,6	0.33	0	5,5,5	0.33	0

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
6	F09	C	1131	-	-	0/7/7/7	0/0/0/0
7	L2C	C	1132	-	-	2/30/30/30	0/0/0/0
8	TBA	C	1133[A]	-	-	0/20/20/20	0/0/0/0
8	TBA	C	1133[B]	-	-	0/20/20/20	0/0/0/0
9	HP6	C	1134	-	-	0/4/4/4	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1132	L2C	O41-C21	4.35	1.46	1.33
7	C	1132	L2C	O42-C11	4.17	1.46	1.34
6	C	1131	F09	OXT-C9	-3.64	1.22	1.42
7	C	1132	L2C	C25-C24	-2.89	1.34	1.51
8	C	1133[A]	TBA	C41-N1	-2.70	1.43	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1132	L2C	O42-C11-C12	5.87	124.05	111.54
7	C	1132	L2C	O41-C21-C22	3.24	121.83	111.90
7	C	1132	L2C	O42-C11-O11	-2.54	116.89	123.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1132	L2C	C42-O42-C11-C12
7	C	1132	L2C	C42-O42-C11-O11

There are no ring outliers.

## 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	219/219 (100%)	-0.13	5 (2%) 57 55	30, 51, 62, 70	3 (1%)
2	B	212/212 (100%)	-0.11	3 (1%) 72 71	22, 47, 69, 75	5 (2%)
3	C	103/124 (83%)	-0.16	0 100 100	19, 26, 50, 56	2 (1%)
All	All	534/555 (96%)	-0.13	8 (1%) 70 69	19, 46, 65, 75	10 (1%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	3.0
1	A	75	SER	2.7
1	A	116	VAL	2.5
2	B	145	ASN	2.3
1	A	55	TYR	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K	C	1129	1/1	0.18	24.00	26,26,26,26	1
9	HP6	C	1134	7/7	0.33	16.97	48,51,54,54	0
7	L2C	C	1132	29/29	0.25	6.50	47,59,69,72	0
8	TBA	C	1133[B]	17/17	0.17	4.38	20,21,21,21	17
8	TBA	C	1133[A]	17/17	0.17	4.38	23,23,24,24	17
5	K	C	1127	1/1	0.22	2.77	27,27,27,27	1
6	F09	C	1131	10/10	0.20	0.93	56,59,60,61	0
5	K	C	1126	1/1	0.18	0.81	22,22,22,22	1
5	K	C	1128	1/1	0.11	-1.14	18,18,18,18	1
4	CO	C	1124	1/1	0.06	-2.05	42,42,42,42	1
5	K	C	1125	1/1	0.13	-2.69	16,16,16,16	1
5	K	C	1130	1/1	0.80	-	63,63,63,63	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.