



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2017 – 01:27 PM EDT

PDB ID : 5XJB  
Title : The Crystal Structure of the Minimal Core Domain of the Microtubule Depolymerizer KIF2C Complexed with ADP-Mg-BeFx  
Authors : Ogawa, T.; Jiang, X.; Hirokawa, N.  
Deposited on : unknown  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure 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/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

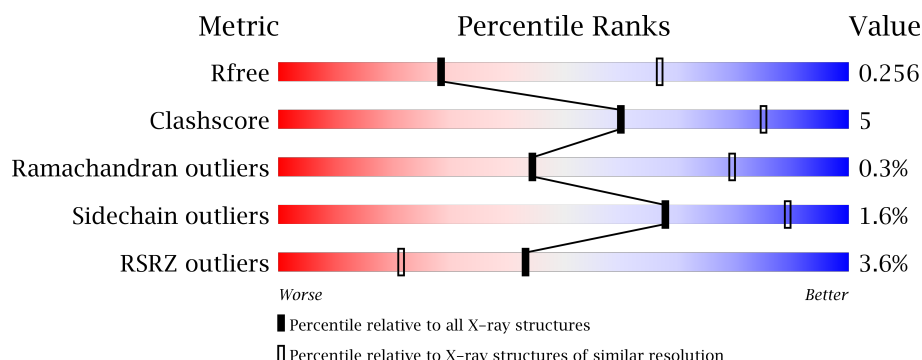
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	426	 4% 70% 8% 20%
1	B	426	 2% 71% 7% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEF	A	602	-	-	X	X
3	BEF	B	602	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5344 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 Kinesin-like protein KIF2C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2663	1678	472	492	21			
1	B	333	Total	C	N	O	S	0	0	0
			2612	1650	460	481	21			

There are 48 discrepancies between the modelled and reference sequences:

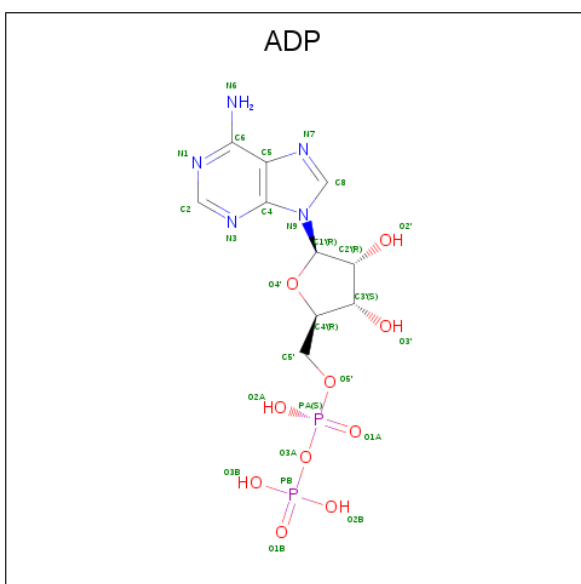
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	initiating methionine	UNP Q922S8
A	168	ALA	-	expression tag	UNP Q922S8
A	169	SER	-	expression tag	UNP Q922S8
A	170	MET	-	expression tag	UNP Q922S8
A	171	THR	-	expression tag	UNP Q922S8
A	172	GLY	-	expression tag	UNP Q922S8
A	173	GLY	-	expression tag	UNP Q922S8
A	174	GLN	-	expression tag	UNP Q922S8
A	175	GLN	-	expression tag	UNP Q922S8
A	176	MET	-	expression tag	UNP Q922S8
A	177	GLY	-	expression tag	UNP Q922S8
A	178	ARG	-	expression tag	UNP Q922S8
A	179	ASP	-	expression tag	UNP Q922S8
A	180	PRO	-	expression tag	UNP Q922S8
A	181	ASN	-	expression tag	UNP Q922S8
A	182	SER	-	expression tag	UNP Q922S8
A	183	SER	-	expression tag	UNP Q922S8
A	586	HIS	-	expression tag	UNP Q922S8
A	587	HIS	-	expression tag	UNP Q922S8
A	588	HIS	-	expression tag	UNP Q922S8
A	589	HIS	-	expression tag	UNP Q922S8
A	590	HIS	-	expression tag	UNP Q922S8
A	591	HIS	-	expression tag	UNP Q922S8
A	592	HIS	-	expression tag	UNP Q922S8
B	167	MET	-	initiating methionine	UNP Q922S8

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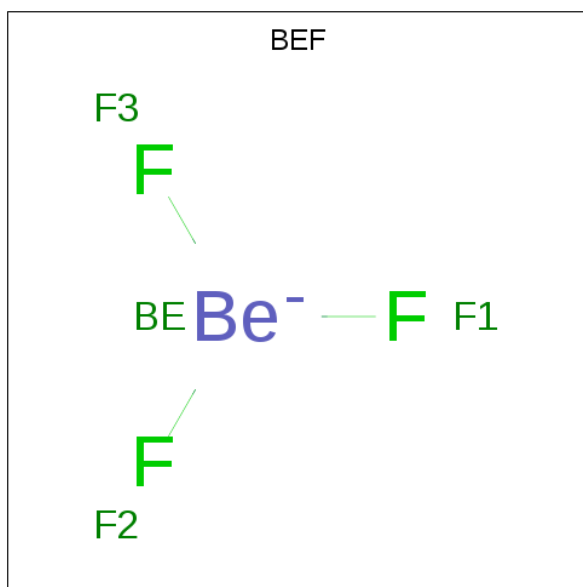
Chain	Residue	Modelled	Actual	Comment	Reference
B	168	ALA	-	expression tag	UNP Q922S8
B	169	SER	-	expression tag	UNP Q922S8
B	170	MET	-	expression tag	UNP Q922S8
B	171	THR	-	expression tag	UNP Q922S8
B	172	GLY	-	expression tag	UNP Q922S8
B	173	GLY	-	expression tag	UNP Q922S8
B	174	GLN	-	expression tag	UNP Q922S8
B	175	GLN	-	expression tag	UNP Q922S8
B	176	MET	-	expression tag	UNP Q922S8
B	177	GLY	-	expression tag	UNP Q922S8
B	178	ARG	-	expression tag	UNP Q922S8
B	179	ASP	-	expression tag	UNP Q922S8
B	180	PRO	-	expression tag	UNP Q922S8
B	181	ASN	-	expression tag	UNP Q922S8
B	182	SER	-	expression tag	UNP Q922S8
B	183	SER	-	expression tag	UNP Q922S8
B	586	HIS	-	expression tag	UNP Q922S8
B	587	HIS	-	expression tag	UNP Q922S8
B	588	HIS	-	expression tag	UNP Q922S8
B	589	HIS	-	expression tag	UNP Q922S8
B	590	HIS	-	expression tag	UNP Q922S8
B	591	HIS	-	expression tag	UNP Q922S8
B	592	HIS	-	expression tag	UNP Q922S8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Be	F	0	0
			4	1	3		
3	B	1	Total	Be	F	0	0
			4	1	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	O	0	0
			2	2		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- 4% 70% 8% 20%
- MET ALA SER MET THR GLY GLN MET GLY ARG ASP PRO ASN SER VAL ARG ARG LYS SER CYS ILE VAL LYS GLU MET GLY LYS MET ASN LYS ARG GLU GLU LYS ARG ALA GLN ASN SER GLU LEU ARG ILE LYS ARG ALA GLN THR TYR ASP SER PHE MET

- Chain B:
-



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.45 Å   166.59 Å   75.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-3.10) 99.9 (29.48-3.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 3.11 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.201   ,   0.261 0.209   ,   0.256	Depositor DCC
$R_{free}$ test set	1061 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: MG, BEF, ADP

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	0.64	3/2700 (0.1%)	1.05	12/3627 (0.3%)
1	B	0.61	0/2649	0.88	5/3558 (0.1%)
All	All	0.63	3/5349 (0.1%)	0.97	17/7185 (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
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	SER	CA-CB	-5.82	1.44	1.52
1	A	455	GLY	CA-C	5.66	1.60	1.51
1	A	529	ASN	C-N	5.02	1.45	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	ASN	CB-CA-C	-19.35	71.70	110.40
1	A	529	ASN	O-C-N	13.54	144.37	122.70
1	A	529	ASN	N-CA-C	-13.42	74.76	111.00
1	A	529	ASN	CA-C-N	-11.37	92.20	117.20
1	A	535	PHE	CB-CA-C	-10.12	90.16	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	535	PHE	Peptide
1	A	584	LEU	Peptide
1	B	534	PRO	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	2663	0	2676	36	1
1	B	2612	0	2637	23	1
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	4	0	0	3	0
3	B	4	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	1	0
5	B	2	0	0	0	0
All	All	5344	0	5337	57	2

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.

The worst 5 of 57 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:464:SER:N	3:B:602:BEF:F3	1.80	1.04
1:A:528:GLN:O	1:A:530:LYS:CB	2.13	0.97
1:A:528:GLN:O	1:A:529:ASN:C	2.03	0.96
1:A:463:SER:N	1:A:465:ARG:HG2	1.85	0.91
1:B:463:SER:OG	3:B:602:BEF:F3	1.75	0.91

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:OE2	1:A:301:GLU:OE2[2_655]	1.78	0.42
1:B:301:GLU:OE2	1:B:301:GLU:OE2[2_655]	1.88	0.32

## 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	331/426 (78%)	300 (91%)	30 (9%)	1 (0%)	44	79
1	B	323/426 (76%)	304 (94%)	18 (6%)	1 (0%)	44	79
All	All	654/852 (77%)	604 (92%)	48 (7%)	2 (0%)	44	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ILE
1	B	250	ILE

### 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	288/374 (77%)	283 (98%)	5 (2%)	66	88
1	B	284/374 (76%)	280 (99%)	4 (1%)	71	90
All	All	572/748 (76%)	563 (98%)	9 (2%)	68	89

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	PHE
1	B	484	PHE
1	B	339	THR
1	A	419	GLU
1	B	286	LEU

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

Mol	Chain	Res	Type
1	A	467	HIS
1	B	467	HIS
1	B	303	GLN
1	A	390	ASN
1	B	390	ASN

### 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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	ADP	A	601	4	25,29,29	1.22	3 (12%)	24,45,45	1.81	5 (20%)
3	BEF	A	602	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ADP	B	601	4	25,29,29	1.14	3 (12%)	24,45,45	1.91	5 (20%)
3	BEF	B	602	-	0,3,3	0.00	-	0,3,3	0.00	-

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	ADP	A	601	4	-	0/12/32/32	0/3/3/3
3	BEF	A	602	-	-	0/0/0/0	0/0/0/0
2	ADP	B	601	4	-	0/12/32/32	0/3/3/3
3	BEF	B	602	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C2-N3	2.19	1.35	1.32
2	A	601	ADP	C2-N3	2.34	1.36	1.32
2	B	601	ADP	O4'-C1'	2.63	1.44	1.41
2	B	601	ADP	C5-C4	3.13	1.47	1.40
2	A	601	ADP	O4'-C1'	3.19	1.45	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	N3-C2-N1	-6.16	123.49	128.86
2	A	601	ADP	N3-C2-N1	-5.89	123.73	128.86
2	B	601	ADP	C5'-C4'-C3'	-3.58	101.64	115.29
2	A	601	ADP	O5'-PA-O1A	-2.59	98.80	109.25
2	B	601	ADP	C4-C5-N7	-2.32	107.17	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	BEF	3	0
3	B	602	BEF	3	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 [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	341/426 (80%)	0.02	17 (4%) 30 13	30, 73, 127, 165	0
1	B	333/426 (78%)	-0.12	7 (2%) 64 43	46, 74, 122, 144	0
All	All	674/852 (79%)	-0.05	24 (3%) 43 21	30, 74, 126, 165	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	SER	4.7
1	A	528	GLN	4.2
1	A	455	GLY	4.2
1	A	456	GLN	3.7
1	A	388	ASN	3.5

### 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
3	BEF	B	602	4/4	0.54	0.53	5.98	104,122,124,127	0
3	BEF	A	602	4/4	0.58	0.38	3.59	102,110,114,115	0
2	ADP	A	601	27/27	0.95	0.15	-0.44	67,78,99,107	0
2	ADP	B	601	27/27	0.96	0.14	-0.71	67,84,99,119	0
4	MG	A	603	1/1	0.82	0.10	-	66,66,66,66	0
4	MG	B	603	1/1	0.73	0.13	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.