



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:54 am BST

PDB ID : 5XU1  
Title : Structure of a non-canonical ABC transporter from *Streptococcus pneumoniae* R6  
Authors : Yang, H.B.; Jiang, Y.L.; Hou, W.T.; Chen, M.T.; Chen, Y.; Zhou, C.Z.  
Deposited on : 2017-06-22  
Resolution : 3.30 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

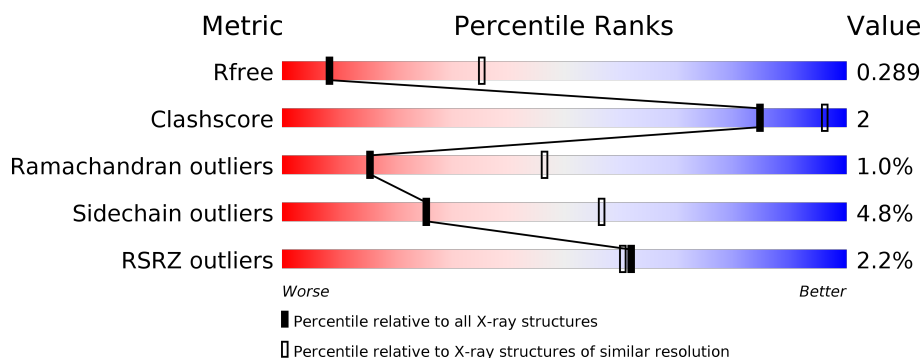
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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	245	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	245	<div> <div>82%</div> <div>10%</div> <div>•</div> <div>8%</div> </div>
2	M	419	<div> <div>%</div> <div>82%</div> <div>11%</div> <div>•</div> <div>7%</div> </div>
2	S	419	<div> <div>4%</div> <div>79%</div> <div>10%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9287 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 ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1712	1080	296	331	5			
1	B	226	Total	C	N	O	S	0	0	0
			1752	1101	306	340	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q8DQF8
A	-10	GLY	-	expression tag	UNP Q8DQF8
A	-9	GLY	-	expression tag	UNP Q8DQF8
A	-8	SER	-	expression tag	UNP Q8DQF8
A	-7	HIS	-	expression tag	UNP Q8DQF8
A	-6	HIS	-	expression tag	UNP Q8DQF8
A	-5	HIS	-	expression tag	UNP Q8DQF8
A	-4	HIS	-	expression tag	UNP Q8DQF8
A	-3	HIS	-	expression tag	UNP Q8DQF8
A	-2	HIS	-	expression tag	UNP Q8DQF8
A	-1	GLY	-	expression tag	UNP Q8DQF8
A	0	THR	-	expression tag	UNP Q8DQF8
B	-11	MET	-	expression tag	UNP Q8DQF8
B	-10	GLY	-	expression tag	UNP Q8DQF8
B	-9	GLY	-	expression tag	UNP Q8DQF8
B	-8	SER	-	expression tag	UNP Q8DQF8
B	-7	HIS	-	expression tag	UNP Q8DQF8
B	-6	HIS	-	expression tag	UNP Q8DQF8
B	-5	HIS	-	expression tag	UNP Q8DQF8
B	-4	HIS	-	expression tag	UNP Q8DQF8
B	-3	HIS	-	expression tag	UNP Q8DQF8
B	-2	HIS	-	expression tag	UNP Q8DQF8
B	-1	GLY	-	expression tag	UNP Q8DQF8
B	0	THR	-	expression tag	UNP Q8DQF8

- Molecule 2 is a protein called ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	390	Total	C	N	O	S	0	0	0
			2950	1890	486	562	12			
2	S	378	Total	C	N	O	S	0	0	0
			2855	1830	469	543	13			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

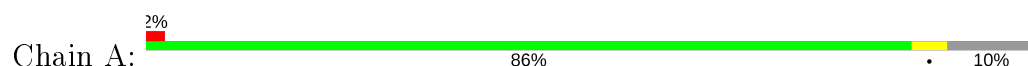
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	5	Total	O	0	0
			5	5		
4	M	2	Total	O	0	0
			2	2		
4	S	7	Total	O	0	0
			7	7		

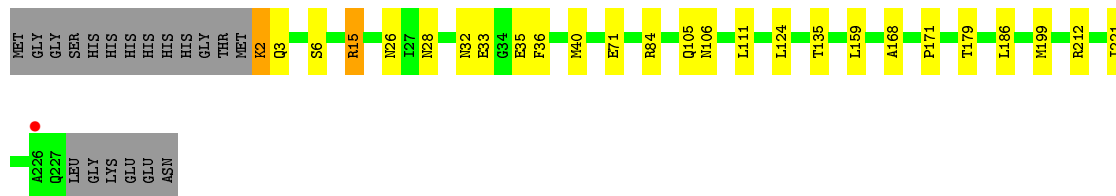
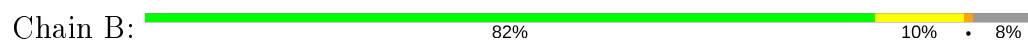
### 3 Residue-property plots [i](#)

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

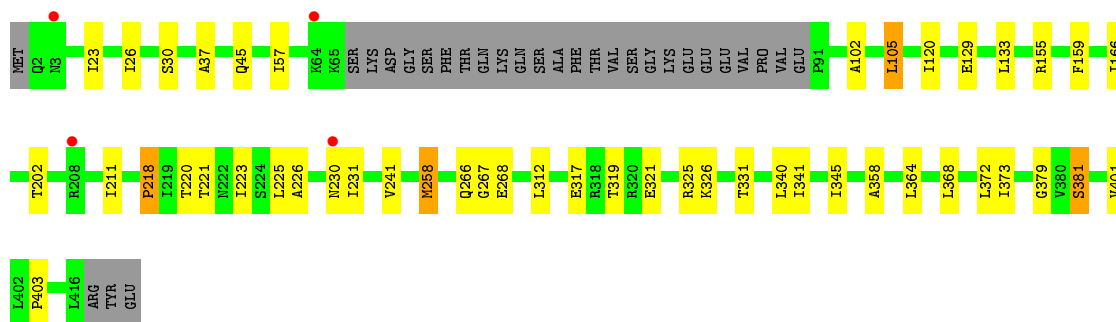
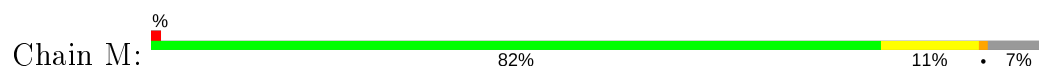
- Molecule 1: ABC transporter ATP-binding protein



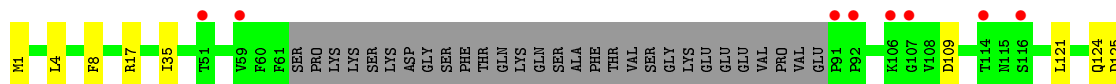
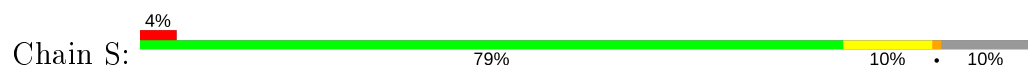
- Molecule 1: ABC transporter ATP-binding protein

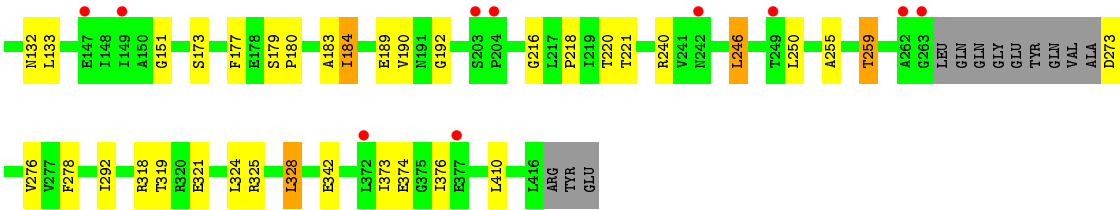


- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.05Å 154.99Å 205.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.19 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.30) 99.3 (49.19-3.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.234 , 0.289 0.234 , 0.289	Depositor DCC
$R_{free}$ test set	1727 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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

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	0.40	0/1732	0.66	0/2333
1	B	0.41	0/1773	0.67	0/2389
2	M	0.42	0/2989	0.63	0/4040
2	S	0.43	0/2891	0.64	0/3906
All	All	0.42	0/9385	0.65	0/12668

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 [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	1712	0	1761	2	0
1	B	1752	0	1796	7	0
2	M	2950	0	3072	20	0
2	S	2855	0	2978	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
4	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	7	0	0	1	0
All	All	9287	0	9607	43	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 (43) 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)
2:M:45:GLN:HE22	2:M:373:ILE:HG23	1.58	0.68
1:B:26:ASN:OD1	1:B:28:ASN:ND2	2.27	0.68
2:S:151:GLY:HA3	2:S:184:ILE:HD11	1.78	0.65
2:M:340:LEU:HD11	2:M:401:VAL:HG12	1.87	0.57
2:S:324:LEU:O	2:S:328:LEU:HD22	2.06	0.56
2:S:373:ILE:HG22	2:S:376:ILE:HD11	1.86	0.56
2:M:166:ILE:HD11	2:M:218:PRO:HB2	1.88	0.55
2:M:159:PHE:HA	2:M:223:ILE:HD11	1.91	0.53
1:B:84:ARG:NH1	2:M:326:LYS:O	2.45	0.50
2:S:319:THR:HG22	2:S:410:LEU:HD11	1.93	0.50
2:M:133:LEU:CD2	2:M:225:LEU:HD11	2.43	0.48
2:S:35:ILE:HD13	2:S:292:ILE:HG22	1.94	0.48
2:M:321:GLU:OE2	2:M:325:ARG:NH2	2.49	0.46
1:A:168:ALA:HB1	1:A:171:PRO:HG3	1.98	0.45
1:B:35:GLU:OE2	1:B:212:ARG:NH1	2.47	0.45
2:M:120:ILE:HA	2:M:129:GLU:HA	1.99	0.45
1:B:168:ALA:HB1	1:B:171:PRO:HG3	1.99	0.45
2:M:341:ILE:O	2:M:345:ILE:HG12	2.17	0.45
2:S:133:LEU:HD22	2:S:190:VAL:HG11	1.98	0.45
2:M:211:ILE:HG23	2:M:373:ILE:HD11	1.98	0.45
2:M:37:ALA:HB1	2:M:379:GLY:HA3	1.99	0.44
2:S:121:LEU:HG	2:S:190:VAL:HG22	1.99	0.44
2:M:220:THR:HG23	2:M:225:LEU:HD13	2.00	0.44
1:B:2:LYS:O	1:B:33:GLU:N	2.46	0.43
2:S:318:ARG:NH2	2:S:342:GLU:OE1	2.51	0.43
2:S:177:PHE:HB2	2:S:183:ALA:HB2	2.00	0.43
2:M:226:ALA:HA	2:M:231:ILE:O	2.18	0.43
2:M:312:LEU:HG	2:M:403:PRO:HG3	2.01	0.43
2:S:255:ALA:O	2:S:259:THR:OG1	2.35	0.43
1:B:168:ALA:O	1:B:199:MET:HA	2.18	0.42
2:M:23:ILE:HA	2:M:26:ILE:HG12	2.01	0.42
2:M:102:ALA:HB2	2:M:258:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:321:GLU:OE2	2:S:325:ARG:NH2	2.53	0.42
2:S:132:ASN:N	2:S:216:GLY:O	2.46	0.42
2:S:220:THR:OG1	2:S:221:THR:N	2.53	0.42
2:M:220:THR:OG1	2:M:221:THR:N	2.53	0.41
2:M:57:ILE:HD12	2:M:241:VAL:HG21	2.02	0.41
2:M:230:ASN:CG	2:S:192:GLY:HA3	2.40	0.41
2:S:246:LEU:HD22	2:S:250:LEU:HD12	2.01	0.41
1:A:56:MET:HB3	1:A:80:LEU:HG	2.01	0.41
2:S:240:ARG:HD2	4:S:503:HOH:O	2.21	0.41
2:M:30:SER:HA	2:M:358:ALA:HB2	2.03	0.40
1:B:32:ASN:O	1:B:35:GLU:HB2	2.22	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	217/245 (89%)	209 (96%)	7 (3%)	1 (0%)	29	61
1	B	224/245 (91%)	206 (92%)	16 (7%)	2 (1%)	17	48
2	M	386/419 (92%)	354 (92%)	26 (7%)	6 (2%)	9	36
2	S	372/419 (89%)	343 (92%)	26 (7%)	3 (1%)	19	51
All	All	1199/1328 (90%)	1112 (93%)	75 (6%)	12 (1%)	15	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	372	LEU
2	M	368	LEU
2	S	276	VAL
1	B	15	ARG

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Mol	Chain	Res	Type
2	M	267	GLY
2	M	381	SER
1	A	95	PHE
2	M	105	LEU
2	M	268	GLU
2	S	374	GLU
2	S	180	PRO
1	B	221	ILE

### 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	189/208 (91%)	183 (97%)	6 (3%)	39	67
1	B	193/208 (93%)	178 (92%)	15 (8%)	12	38
2	M	327/353 (93%)	316 (97%)	11 (3%)	37	65
2	S	317/353 (90%)	300 (95%)	17 (5%)	22	53
All	All	1026/1122 (91%)	977 (95%)	49 (5%)	25	56

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	116	VAL
1	A	134	LEU
1	A	137	ARG
1	A	138	SER
1	A	196	THR
1	B	2	LYS
1	B	3	GLN
1	B	6	SER
1	B	15	ARG
1	B	36	PHE
1	B	40	MET
1	B	71	GLU

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Mol	Chain	Res	Type
1	B	105	GLN
1	B	106	ASN
1	B	111	LEU
1	B	124	LEU
1	B	135	THR
1	B	159	LEU
1	B	179	THR
1	B	186	LEU
2	M	105	LEU
2	M	155	ARG
2	M	202	THR
2	M	218	PRO
2	M	258	MET
2	M	266	GLN
2	M	317	GLU
2	M	319	THR
2	M	331	THR
2	M	364	LEU
2	M	381	SER
2	S	1	MET
2	S	4	LEU
2	S	8	PHE
2	S	17	ARG
2	S	109	ASP
2	S	124	GLN
2	S	125	ASP
2	S	173	SER
2	S	179	SER
2	S	184	ILE
2	S	189	GLU
2	S	218	PRO
2	S	246	LEU
2	S	259	THR
2	S	273	ASP
2	S	278	PHE
2	S	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	45	GLN
2	M	118	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	221/245 (90%)	-0.08	4 (1%) 68 67	53, 76, 102, 125	0
1	B	226/245 (92%)	-0.17	1 (0%) 92 93	58, 78, 114, 141	0
2	M	390/419 (93%)	-0.16	4 (1%) 82 82	54, 78, 120, 148	0
2	S	378/419 (90%)	0.12	18 (4%) 30 28	50, 88, 132, 149	0
All	All	1215/1328 (91%)	-0.06	27 (2%) 62 60	50, 80, 125, 149	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	ALA	4.0
2	S	106	LYS	3.3
2	S	377	GLU	3.0
2	M	208	ARG	2.9
2	S	51	THR	2.8
2	S	262	ALA	2.7
2	S	147	GLU	2.7
2	M	3	ASN	2.7
2	S	116	SER	2.6
1	A	14	TYR	2.5
2	S	263	GLY	2.4
2	S	242	ASN	2.4
2	S	203	SER	2.4
2	S	249	THR	2.4
2	S	91	PRO	2.3
2	S	149	ILE	2.3
2	S	204	PRO	2.2
2	M	64	LYS	2.2
2	S	59	VAL	2.2
1	A	20	GLU	2.2
2	M	230	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	S	114	THR	2.1
1	A	22	GLN	2.1
2	S	372	LEU	2.1
1	A	115	GLY	2.0
2	S	107	GLY	2.0
2	S	92	PRO	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. 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( $\text{\AA}^2$ )	Q<0.9
3	MG	B	301	1/1	0.93	0.25	49,49,49,49	0
3	MG	A	301	1/1	0.97	0.43	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.