



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:41 pm GMT

PDB ID : 1RYN  
Title : Structure of the Chloroplast Group II Intron Splicing Factor CRS2  
Authors : Ostheimer, G.J.; Barkan, A.; Matthews, B.W.  
Deposited on : 2003-12-22  
Resolution : 1.75 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

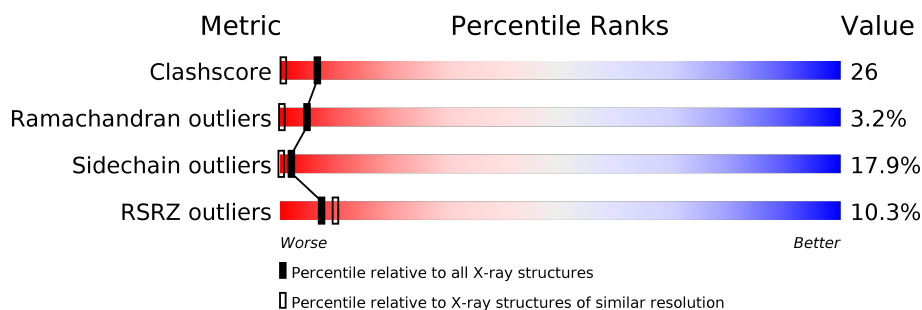
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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	202	<div> <div>10%</div> <div>49%</div> <div>34%</div> <div>11%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1557 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 CRS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1515	963	269	279	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	CLONING ARTIFACT	UNP Q9M5P4
A	43	ASN	ILE	ENGINEERED	UNP Q9M5P4
A	45	PHE	SER	ENGINEERED	UNP Q9M5P4
A	51	THR	ILE	ENGINEERED	UNP Q9M5P4
A	194	LEU	-	EXPRESSION TAG	UNP Q9M5P4
A	195	GLU	-	EXPRESSION TAG	UNP Q9M5P4
A	196	HIS	-	EXPRESSION TAG	UNP Q9M5P4
A	197	HIS	-	EXPRESSION TAG	UNP Q9M5P4
A	198	HIS	-	EXPRESSION TAG	UNP Q9M5P4
A	199	HIS	-	EXPRESSION TAG	UNP Q9M5P4
A	200	HIS	-	EXPRESSION TAG	UNP Q9M5P4
A	201	HIS	-	EXPRESSION TAG	UNP Q9M5P4

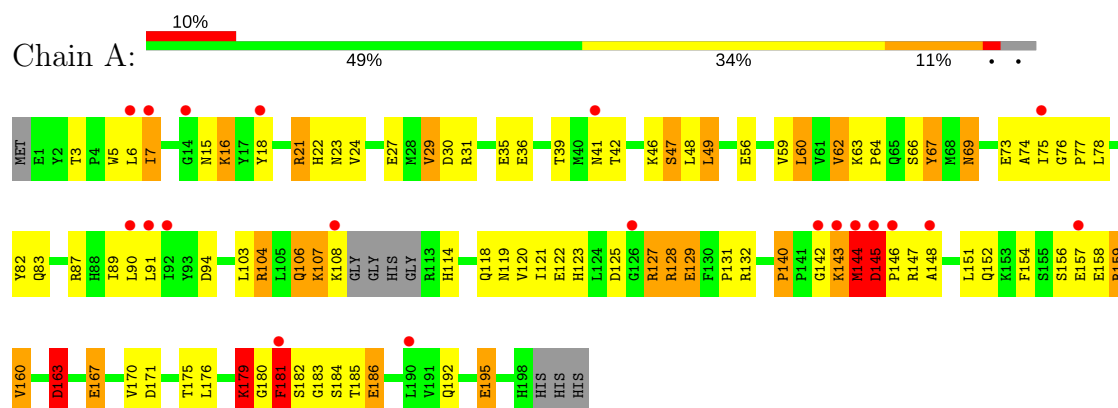
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		

### 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: protein CRS2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.70Å 56.49Å 69.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.75 19.85 – 1.75	Depositor EDS
% Data completeness (in resolution range)	91.0 (15.00-1.75) 91.4 (19.85-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.76Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.195 , 0.278 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 113.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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](#)

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	1.05	13/1548 (0.8%)	1.47	30/2096 (1.4%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	MET	CA-CB	-8.25	1.35	1.53
1	A	181	PHE	N-CA	7.85	1.62	1.46
1	A	27	GLU	CD-OE2	7.31	1.33	1.25
1	A	186	GLU	CD-OE2	6.39	1.32	1.25
1	A	167	GLU	CD-OE2	6.37	1.32	1.25
1	A	129	GLU	CD-OE2	6.30	1.32	1.25
1	A	122	GLU	CD-OE2	6.15	1.32	1.25
1	A	158	GLU	CD-OE2	6.09	1.32	1.25
1	A	56	GLU	CD-OE2	5.88	1.32	1.25
1	A	36	GLU	CD-OE2	5.85	1.32	1.25
1	A	157	GLU	CD-OE2	5.79	1.32	1.25
1	A	35	GLU	CD-OE2	5.69	1.31	1.25
1	A	73	GLU	CD-OE2	5.29	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	PHE	CA-C-N	13.78	147.52	117.20
1	A	143	LYS	C-N-CA	11.37	150.12	121.70
1	A	181	PHE	CA-C-O	-9.78	99.56	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	MET	CB-CG-SD	8.34	137.42	112.40
1	A	30	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	181	PHE	O-C-N	-7.70	110.38	122.70
1	A	181	PHE	CA-CB-CG	-7.68	95.46	113.90
1	A	144	MET	CB-CA-C	7.20	124.81	110.40
1	A	143	LYS	O-C-N	-6.65	112.06	122.70
1	A	163	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	181	PHE	C-N-CA	6.54	138.05	121.70
1	A	163	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	182	SER	C-N-CA	6.34	135.61	122.30
1	A	140	PRO	C-N-CD	-6.15	107.08	120.60
1	A	62	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	125	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	144	MET	CG-SD-CE	-6.00	90.60	100.20
1	A	30	ASP	CB-CG-OD1	5.91	123.61	118.30
1	A	144	MET	CA-CB-CG	-5.87	103.32	113.30
1	A	181	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	145	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	104	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	62	VAL	N-CA-CB	-5.60	99.17	111.50
1	A	145	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	21	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	29	VAL	CB-CA-C	5.49	121.82	111.40
1	A	125	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	171	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	A	143	LYS	CA-C-N	5.17	128.58	117.20
1	A	125	ASP	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLY	Peptide
1	A	181	PHE	Mainchain

## 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	1515	0	1504	79	0
2	A	42	0	0	4	0
All	All	1557	0	1504	79	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 26.

All (79) 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:A:21:ARG:HH12	1:A:152:GLN:NE2	1.49	1.08
1:A:6:LEU:HD23	1:A:60:LEU:HD12	1.37	1.03
1:A:46:LYS:HD3	1:A:66:SER:HB3	1.38	1.03
1:A:103:LEU:H	1:A:192:GLN:HE21	1.12	0.94
1:A:6:LEU:HD23	1:A:60:LEU:CD1	2.06	0.86
1:A:6:LEU:HD21	1:A:62:VAL:HG21	1.62	0.82
1:A:175:THR:HA	1:A:179:LYS:HB2	1.60	0.81
1:A:75:ILE:CD1	1:A:91:LEU:HD11	2.11	0.80
1:A:46:LYS:HD3	1:A:66:SER:CB	2.14	0.78
1:A:75:ILE:HD13	1:A:91:LEU:HD11	1.65	0.77
1:A:103:LEU:H	1:A:192:GLN:NE2	1.82	0.77
1:A:42:THR:HB	1:A:49:LEU:HD13	1.66	0.77
1:A:146:PRO:C	1:A:147:ARG:HD3	2.13	0.69
1:A:31:ARG:HH12	1:A:167:GLU:CG	2.05	0.68
1:A:21:ARG:HH12	1:A:152:GLN:HE21	1.41	0.68
1:A:154:PHE:HB2	1:A:159:ARG:HD2	1.77	0.67
1:A:140:PRO:HG2	1:A:146:PRO:HB3	1.77	0.66
1:A:21:ARG:NH1	1:A:152:GLN:NE2	2.34	0.65
1:A:6:LEU:CD2	1:A:60:LEU:HD12	2.22	0.65
1:A:31:ARG:HH12	1:A:167:GLU:HG2	1.60	0.65
1:A:128:ARG:HD3	1:A:128:ARG:N	2.11	0.65
1:A:7:ILE:HD13	1:A:7:ILE:N	2.12	0.65
1:A:23:ASN:HB3	2:A:228:HOH:O	1.96	0.64
1:A:107:LYS:NZ	1:A:185:THR:HG21	2.17	0.59
1:A:31:ARG:NH1	1:A:167:GLU:HG2	2.18	0.59
1:A:29:VAL:HG11	1:A:63:LYS:HG3	1.85	0.58
1:A:29:VAL:CG1	1:A:63:LYS:HG3	2.35	0.57
1:A:6:LEU:C	1:A:7:ILE:HD13	2.25	0.57
1:A:148:ALA:O	1:A:152:GLN:HB2	2.04	0.57
1:A:69:ASN:OD1	1:A:69:ASN:N	2.29	0.55
1:A:107:LYS:O	1:A:108:LYS:HB3	2.06	0.54
1:A:6:LEU:CD2	1:A:62:VAL:HG21	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD21	1:A:62:VAL:CG2	2.34	0.54
1:A:31:ARG:CG	1:A:170:VAL:HG21	2.38	0.54
1:A:5:TRP:NE1	2:A:240:HOH:O	2.33	0.54
1:A:128:ARG:H	1:A:128:ARG:HD3	1.73	0.53
1:A:140:PRO:CG	1:A:146:PRO:HB3	2.38	0.53
1:A:107:LYS:HZ3	1:A:176:LEU:HD11	1.73	0.53
1:A:31:ARG:HG2	1:A:170:VAL:HG21	1.89	0.53
1:A:163:ASP:OD2	1:A:163:ASP:N	2.42	0.52
1:A:146:PRO:O	1:A:147:ARG:HD3	2.11	0.51
1:A:107:LYS:HZ1	1:A:185:THR:HG21	1.75	0.50
1:A:15:ASN:HB2	1:A:16:LYS:HE3	1.93	0.50
1:A:120:VAL:O	1:A:121:ILE:C	2.48	0.49
1:A:89:ILE:HG22	1:A:91:LEU:CD2	2.43	0.49
1:A:60:LEU:N	1:A:60:LEU:HD23	2.27	0.48
1:A:31:ARG:HG2	1:A:170:VAL:CG2	2.43	0.47
1:A:24:VAL:HG12	1:A:94:ASP:HB3	1.97	0.47
1:A:5:TRP:HB2	1:A:59:VAL:HG12	1.95	0.47
1:A:107:LYS:NZ	1:A:176:LEU:HD11	2.28	0.47
1:A:66:SER:O	1:A:67:TYR:HB2	2.15	0.46
1:A:107:LYS:NZ	1:A:176:LEU:CD1	2.78	0.46
1:A:143:LYS:C	1:A:145:ASP:H	2.09	0.46
1:A:47:SER:HB3	1:A:64:PRO:HA	1.98	0.46
1:A:42:THR:HB	1:A:49:LEU:CD1	2.41	0.45
1:A:49:LEU:CD1	1:A:49:LEU:N	2.79	0.45
1:A:7:ILE:CD1	1:A:7:ILE:N	2.79	0.45
1:A:119:ASN:ND2	1:A:123:HIS:HE1	2.15	0.44
1:A:31:ARG:HH12	1:A:167:GLU:HG3	1.78	0.43
1:A:127:ARG:HD3	1:A:128:ARG:HE	1.82	0.43
1:A:103:LEU:N	1:A:192:GLN:HE21	1.96	0.43
1:A:144:MET:HG2	1:A:144:MET:O	2.18	0.43
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.86	0.42
1:A:128:ARG:H	1:A:128:ARG:CD	2.32	0.42
1:A:106:GLN:O	1:A:131:PRO:HA	2.19	0.42
1:A:82:TYR:O	1:A:83:GLN:HB2	2.20	0.42
1:A:89:ILE:O	1:A:131:PRO:HD2	2.20	0.41
1:A:195:GLU:HG3	1:A:195:GLU:O	2.19	0.41
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.71	0.41
1:A:107:LYS:HZ3	1:A:176:LEU:CD1	2.32	0.41
1:A:159:ARG:O	1:A:160:VAL:C	2.58	0.41
1:A:7:ILE:HD12	1:A:90:LEU:HB3	2.03	0.41
1:A:41:ASN:HB2	2:A:229:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:N	1:A:77:PRO:HD2	2.36	0.41
1:A:147:ARG:N	1:A:147:ARG:HD3	2.35	0.40
1:A:145:ASP:C	1:A:147:ARG:H	2.24	0.40
1:A:181:PHE:HB3	1:A:183:GLY:O	2.20	0.40
1:A:47:SER:OG	1:A:74:ALA:HB1	2.22	0.40
1:A:114:HIS:HD2	2:A:221:HOH:O	2.04	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	190/202 (94%)	174 (92%)	10 (5%)	6 (3%)	<b>5</b> <b>0</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLY
1	A	129	GLU
1	A	67	TYR
1	A	179	LYS
1	A	145	ASP
1	A	160	VAL

### 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	162/170 (95%)	133 (82%)	29 (18%)	<b>2</b> <b>0</b>

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	7	ILE
1	A	16	LYS
1	A	18	TYR
1	A	22	HIS
1	A	39	THR
1	A	47	SER
1	A	49	LEU
1	A	60	LEU
1	A	69	ASN
1	A	78	LEU
1	A	87	ARG
1	A	104	ARG
1	A	106	GLN
1	A	107	LYS
1	A	118	GLN
1	A	127	ARG
1	A	128	ARG
1	A	132	ARG
1	A	144	MET
1	A	145	ASP
1	A	156	SER
1	A	159	ARG
1	A	163	ASP
1	A	179	LYS
1	A	181	PHE
1	A	184	SER
1	A	186	GLU
1	A	195	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	65	GLN
1	A	88	HIS
1	A	152	GLN

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	168	GLN
1	A	192	GLN

### 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](#)

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	194/202 (96%)	0.69	20 (10%) <b>7</b> <b>10</b>	24, 38, 73, 97	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	MET	6.6
1	A	143	LYS	5.2
1	A	146	PRO	4.9
1	A	142	GLY	4.7
1	A	148	ALA	3.7
1	A	91	LEU	3.0
1	A	18	TYR	2.9
1	A	41	ASN	2.7
1	A	157	GLU	2.5
1	A	181	PHE	2.5
1	A	14	GLY	2.5
1	A	145	ASP	2.4
1	A	75	ILE	2.3
1	A	6	LEU	2.3
1	A	7	ILE	2.3
1	A	126	GLY	2.2
1	A	92	ILE	2.2
1	A	190	LEU	2.1
1	A	90	LEU	2.1
1	A	108	LYS	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.