



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:40 AM GMT

PDB ID : 2I4L  
Title : Rhodopseudomonas palustris prolyl-tRNA synthetase  
Authors : Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.  
Deposited on : 2006-08-22  
Resolution : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

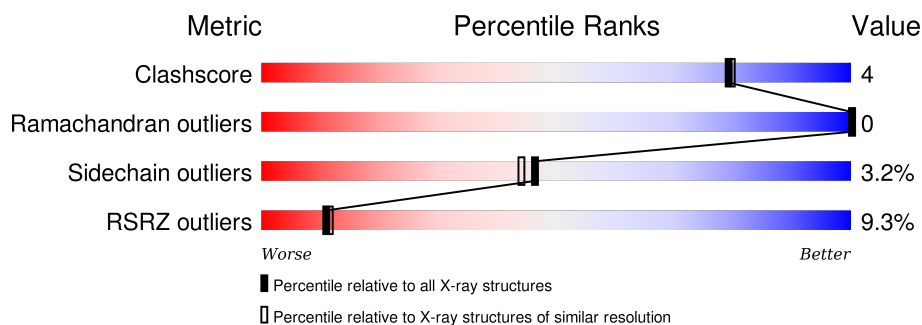
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	458	<div> <div>16%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	458	<div> <div>9%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	C	458	<div> <div>2%</div> <div>89%</div> <div>6%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11092 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3479	2201	618	646	14			
1	B	441	Total	C	N	O	S	0	0	0
			3495	2211	620	650	14			
1	C	441	Total	C	N	O	S	0	0	0
			3495	2211	620	650	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
A	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
A	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
A	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
A	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
A	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
A	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
A	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
A	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
B	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
B	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
B	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
B	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
B	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
B	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
B	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
B	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-19	MET	-	EXPRESSION TAG	UNP Q6N5P6
C	-18	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-17	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-16	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-15	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-14	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-13	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-12	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-11	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-10	HIS	-	EXPRESSION TAG	UNP Q6N5P6
C	-9	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-8	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	-7	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-6	LEU	-	EXPRESSION TAG	UNP Q6N5P6
C	-5	VAL	-	EXPRESSION TAG	UNP Q6N5P6
C	-4	PRO	-	EXPRESSION TAG	UNP Q6N5P6
C	-3	ARG	-	EXPRESSION TAG	UNP Q6N5P6
C	-2	GLY	-	EXPRESSION TAG	UNP Q6N5P6
C	-1	SER	-	EXPRESSION TAG	UNP Q6N5P6
C	0	HIS	-	EXPRESSION TAG	UNP Q6N5P6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	129	Total O 129 129	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	222	Total 222	O 222	0	0
2	C	272	Total 272	O 272	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.84Å 212.56Å 150.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 46.72 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.6 ((Not available)-2.00) 94.5 (46.72-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.221 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 119990 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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 [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	0.64	0/3554	0.69	1/4807 (0.0%)
1	B	0.70	0/3570	0.71	0/4828
1	C	0.80	0/3570	0.75	1/4828 (0.0%)
All	All	0.72	0/10694	0.72	2/14463 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	420	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	3479	0	3448	19	1
1	B	3495	0	3466	23	0
1	C	3495	0	3466	32	0
2	A	129	0	0	1	0
2	B	222	0	0	0	0
2	C	272	0	0	0	0
All	All	11092	0	10380	73	1

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 4.

All (73) 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:C:12:LYS:HD2	1:C:12:LYS:N	1.49	1.25
1:C:12:LYS:H	1:C:12:LYS:CD	1.52	1.13
1:C:92:GLU:OE1	1:C:140:ARG:CZ	2.16	0.93
1:A:347:ARG:HH12	1:A:436:ARG:HD3	1.34	0.92
1:C:12:LYS:H	1:C:12:LYS:HD2	0.73	0.88
1:B:12:LYS:H	1:B:12:LYS:HE3	1.41	0.82
1:C:408:ARG:CG	1:C:408:ARG:HH11	1.91	0.82
1:C:408:ARG:HH11	1:C:408:ARG:HG3	1.44	0.82
1:C:305:ASP:OD1	1:C:307:THR:HG22	1.85	0.77
1:C:131:ASN:HD21	1:C:160:ALA:HB1	1.56	0.70
1:C:347:ARG:NH1	1:C:437:LEU:O	2.23	0.68
1:C:408:ARG:H	1:C:408:ARG:HD2	1.61	0.64
1:C:195:MET:HG2	1:C:255:ALA:HB1	1.81	0.63
1:A:347:ARG:NH1	1:A:436:ARG:HD3	2.12	0.62
1:C:408:ARG:NH1	1:C:408:ARG:HG3	2.04	0.62
1:B:71:MET:H	1:B:134:HIS:HD2	1.45	0.62
1:A:354:LYS:HD3	1:A:407:PRO:HG2	1.82	0.62
1:B:92:GLU:OE1	1:B:140:ARG:NH2	2.33	0.61
1:B:354:LYS:HD2	1:B:407:PRO:HG2	1.82	0.61
1:C:92:GLU:OE1	1:C:140:ARG:NH1	2.34	0.61
1:A:195:MET:HG2	1:A:255:ALA:HB1	1.84	0.60
1:B:71:MET:H	1:B:134:HIS:CD2	2.20	0.60
1:B:354:LYS:HD2	1:B:407:PRO:CG	2.31	0.60
1:C:71:MET:H	1:C:134:HIS:HD2	1.48	0.60
1:A:131:ASN:C	1:A:131:ASN:HD22	2.04	0.60
1:B:300:ASN:HD22	1:B:310:PRO:HA	1.66	0.59
1:B:12:LYS:N	1:B:12:LYS:HE3	2.14	0.59
1:B:12:LYS:H	1:B:12:LYS:CE	2.14	0.58
1:C:131:ASN:HD22	1:C:131:ASN:C	2.07	0.58
1:C:365:ASP:O	1:C:369:ARG:HG3	2.04	0.57
1:A:92:GLU:OE1	1:A:140:ARG:NH1	2.38	0.56
1:C:71:MET:H	1:C:134:HIS:CD2	2.23	0.56
1:C:408:ARG:H	1:C:408:ARG:CD	2.18	0.56
1:A:131:ASN:HD21	1:A:160:ALA:HB1	1.72	0.54
1:C:408:ARG:NH1	1:C:408:ARG:CG	2.60	0.54
1:A:92:GLU:OE1	1:A:140:ARG:CZ	2.55	0.54
1:C:12:LYS:N	1:C:12:LYS:CD	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD21	1:B:8:LEU:HD23	1.91	0.52
1:C:114:ILE:HG21	1:C:161:TYR:CG	2.46	0.51
1:A:217:GLY:O	1:A:279:ARG:NH2	2.43	0.50
1:B:140:ARG:HG2	1:B:155:PHE:HE2	1.77	0.50
1:B:349:THR:HA	1:B:379:LEU:O	2.12	0.49
1:A:140:ARG:HD2	2:A:510:HOH:O	2.14	0.48
1:B:195:MET:HG2	1:B:255:ALA:HB1	1.95	0.48
1:B:202:ILE:O	1:B:202:ILE:HG22	2.14	0.47
1:C:428:LEU:HD11	1:C:433:VAL:HB	1.96	0.47
1:A:92:GLU:OE1	1:A:140:ARG:NH2	2.48	0.47
1:C:428:LEU:CD1	1:C:433:VAL:HB	2.45	0.47
1:B:353:LEU:HD11	1:B:404:HIS:HB3	1.97	0.47
1:A:233:PRO:HB3	1:A:237:VAL:HG21	1.97	0.47
1:B:347:ARG:NH1	1:B:437:LEU:O	2.49	0.46
1:C:408:ARG:HG2	1:C:408:ARG:HH11	1.80	0.45
1:A:278:THR:OG1	1:A:279:ARG:N	2.49	0.44
1:A:114:ILE:HG21	1:A:161:TYR:CG	2.52	0.44
1:C:428:LEU:HD11	1:C:433:VAL:CB	2.48	0.44
1:A:42:TRP:CH2	1:A:321:SER:HB2	2.53	0.43
1:C:92:GLU:OE1	1:C:140:ARG:NE	2.48	0.43
1:B:428:LEU:HD11	1:B:433:VAL:HA	2.01	0.43
1:A:193:ILE:HD11	1:A:228:LEU:HD23	2.00	0.42
1:B:354:LYS:HD2	1:B:407:PRO:HG3	1.99	0.42
1:B:125:TYR:HB3	1:B:303:GLY:HA2	2.00	0.42
1:C:215:GLU:HG2	1:C:216:THR:HG23	2.02	0.42
1:C:131:ASN:HD22	1:C:132:LEU:N	2.18	0.41
1:B:140:ARG:HG2	1:B:155:PHE:CE2	2.55	0.41
1:C:125:TYR:HB2	1:C:165:VAL:HG21	2.02	0.41
1:B:357:ASP:OD2	1:B:360:THR:HG23	2.20	0.41
1:C:215:GLU:HG2	1:C:216:THR:N	2.35	0.41
1:C:354:LYS:HG2	1:C:357:ASP:HB2	2.02	0.41
1:A:162:SER:O	1:A:313:GLY:HA2	2.21	0.41
1:C:162:SER:O	1:C:313:GLY:HA2	2.21	0.40
1:B:-2:GLY:HA3	1:B:375:GLY:HA2	2.03	0.40
1:A:14:ASN:OD1	1:A:28:ARG:HD2	2.20	0.40
1:A:117:ILE:HG12	1:B:33:ARG:HD3	2.03	0.40

All (1) 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:144:ARG:NH2	1:A:259:ASP:OD1[3_555]	2.14	0.06

### 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	437/458 (95%)	424 (97%)	13 (3%)	0	100	100
1	B	439/458 (96%)	426 (97%)	13 (3%)	0	100	100
1	C	439/458 (96%)	430 (98%)	9 (2%)	0	100	100
All	All	1315/1374 (96%)	1280 (97%)	35 (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	359/376 (96%)	342 (95%)	17 (5%)	32	27
1	B	361/376 (96%)	352 (98%)	9 (2%)	55	55
1	C	361/376 (96%)	352 (98%)	9 (2%)	55	55
All	All	1081/1128 (96%)	1046 (97%)	35 (3%)	46	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	LYS
1	A	13	GLU
1	A	69	LEU
1	A	105	LEU
1	A	131	ASN
1	A	134	HIS
1	A	144	ARG
1	A	158	LYS
1	A	198	GLU
1	A	218	GLU
1	A	253	VAL
1	A	282	GLU
1	A	322	ARG
1	A	386	ARG
1	A	410	LEU
1	A	436	ARG
1	B	3	LEU
1	B	12	LYS
1	B	105	LEU
1	B	134	HIS
1	B	158	LYS
1	B	307	THR
1	B	308	ASP
1	B	366	GLN
1	B	410	LEU
1	C	-1	SER
1	C	12	LYS
1	C	105	LEU
1	C	131	ASN
1	C	134	HIS
1	C	158	LYS
1	C	198	GLU
1	C	215	GLU
1	C	408	ARG

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	131	ASN
1	A	229	ASN
1	B	134	HIS
1	B	300	ASN

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Mol	Chain	Res	Type
1	C	131	ASN
1	C	134	HIS
1	C	300	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](#)

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 ⓘ

### 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	439/458 (95%)	0.91	74 (16%) 2 3	20, 31, 51, 62	0
1	B	441/458 (96%)	0.48	39 (8%) 12 13	19, 27, 47, 65	0
1	C	441/458 (96%)	0.01	10 (2%) 64 64	14, 24, 41, 55	0
All	All	1321/1374 (96%)	0.46	123 (9%) 11 11	14, 28, 47, 65	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	8.5
1	B	430	LEU	7.4
1	A	202	ILE	7.1
1	A	271	PRO	6.9
1	A	270	VAL	6.9
1	A	268	SER	6.3
1	B	202	ILE	6.2
1	A	266	TYR	6.0
1	A	276	LEU	5.8
1	A	253	VAL	5.8
1	A	272	GLU	5.2
1	A	269	GLU	5.0
1	A	274	ASN	4.8
1	C	202	ILE	4.7
1	B	408	ARG	4.5
1	A	252	SER	4.4
1	B	438	THR	4.4
1	A	408	ARG	4.3
1	A	411	ALA	4.3
1	A	223	ILE	4.2
1	A	224	ASP	4.2
1	B	360	THR	4.1
1	A	275	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	137	TRP	4.1
1	B	411	ALA	4.0
1	A	156	LEU	4.0
1	A	261	HIS	3.9
1	B	433	VAL	3.9
1	B	70	LEU	3.7
1	A	225	ARG	3.6
1	A	320	VAL	3.6
1	B	432	ASP	3.6
1	A	50	LEU	3.6
1	B	405	VAL	3.6
1	B	366	GLN	3.5
1	B	135	ILE	3.4
1	B	429	ALA	3.4
1	A	155	PHE	3.3
1	B	373	ALA	3.3
1	A	305	ASP	3.3
1	B	431	ALA	3.3
1	A	-2	GLY	3.2
1	A	42	TRP	3.1
1	A	205	ASP	3.1
1	B	363	ALA	3.0
1	B	367	LEU	3.0
1	B	308	ASP	3.0
1	A	139	PHE	2.9
1	A	39	ILE	2.9
1	A	135	ILE	2.9
1	A	226	ASP	2.9
1	B	156	LEU	2.9
1	B	428	LEU	2.9
1	A	309	ALA	2.9
1	C	438	THR	2.9
1	A	43	LEU	2.8
1	A	304	PRO	2.8
1	A	308	ASP	2.8
1	A	227	VAL	2.8
1	A	149	VAL	2.7
1	A	307	THR	2.7
1	B	69	LEU	2.7
1	A	251	THR	2.7
1	B	416	GLU	2.7
1	B	73	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	2.6
1	C	408	ARG	2.6
1	B	369	ARG	2.6
1	A	157	MET	2.6
1	A	47	HIS	2.5
1	B	414	LYS	2.5
1	B	435	ALA	2.5
1	B	50	LEU	2.4
1	B	374	LYS	2.4
1	A	236	ASN	2.4
1	A	41	ALA	2.4
1	B	406	GLY	2.4
1	A	73	THR	2.4
1	A	264	ALA	2.4
1	B	407	PRO	2.4
1	B	137	TRP	2.4
1	A	222	TYR	2.4
1	A	106	TYR	2.4
1	A	254	TYR	2.4
1	A	303	GLY	2.4
1	A	70	LEU	2.3
1	B	364	CYS	2.3
1	A	49	VAL	2.3
1	A	165	VAL	2.3
1	B	412	GLU	2.3
1	C	135	ILE	2.3
1	A	40	TYR	2.3
1	C	156	LEU	2.3
1	B	309	ALA	2.3
1	A	413	GLY	2.2
1	B	304	PRO	2.2
1	A	136	GLN	2.2
1	A	369	ARG	2.2
1	A	94	LEU	2.2
1	B	71	MET	2.2
1	C	201	PRO	2.2
1	A	16	LYS	2.2
1	A	265	ARG	2.2
1	A	386	ARG	2.2
1	A	216	THR	2.2
1	A	278	THR	2.2
1	B	305	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	SER	2.1
1	C	305	ASP	2.1
1	C	304	PRO	2.1
1	A	53	ILE	2.1
1	C	205	ASP	2.1
1	A	13	GLU	2.1
1	A	125	TYR	2.1
1	A	138	LYS	2.1
1	C	137	TRP	2.1
1	B	72	PRO	2.1
1	B	49	VAL	2.0
1	A	277	ASN	2.0
1	A	214	ALA	2.0
1	A	242	ASP	2.0
1	A	249	GLN	2.0
1	A	229	ASN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.