



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2022 – 03:06 PM EDT

PDB ID : 7RGU
Title : The crystal structure of RocC bound to a transcriptional terminator
Authors : Kim, H.J.; Edwards, R.A.; Glover, J.N.M.
Deposited on : 2021-07-15
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.31.2
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) : 2.31.2

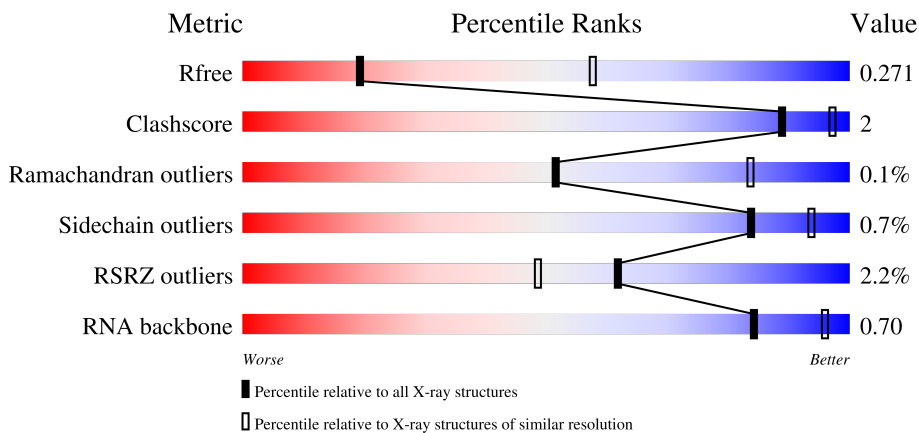
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	118	 2% 89% 5% 6%
1	C	118	 2% 89% 7% 4%
1	E	118	 86% 6% 8%
1	G	118	 2% 90% 8% 2%

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Mol	Chain	Length	Quality of chain
1	I	118	<p>3% 86% 11%</p>
1	K	118	<p>3% 84% 7% 9%</p>
1	M	118	<p>86% 10%</p>
1	O	118	<p>3% 77% 19%</p>
1	Q	118	<p>80% 7% 14%</p>
1	S	118	<p>3% 84% 14%</p>
2	B	28	<p>25% 75% 25%</p>
2	D	28	<p>11% 82% 18%</p>
2	F	28	<p>82% 14% 14%</p>
2	H	28	<p>86% 14%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20397 atoms, of which 9562 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 Repressor of competence, RNA Chaperone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	111	1777	556	889	167	161	4	0	1	0
1	C	110	1770	551	889	166	160	4	0	1	0
1	E	109	1762	547	889	164	158	4	0	1	0
1	G	115	1804	572	889	171	168	4	0	1	0
1	I	105	1712	528	872	156	152	4	0	1	0
1	K	107	1735	537	878	159	157	4	0	1	0
1	M	106	1726	532	878	158	154	4	0	1	0
1	O	95	1529	476	776	133	140	4	0	1	0
1	Q	102	1649	514	833	151	147	4	0	1	0
1	S	102	1649	514	833	151	147	4	0	1	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP A0A128QHZ1
A	10	PRO	-	expression tag	UNP A0A128QHZ1
A	11	LEU	-	expression tag	UNP A0A128QHZ1
A	12	GLY	-	expression tag	UNP A0A128QHZ1
A	13	SER	-	expression tag	UNP A0A128QHZ1
C	9	GLY	-	expression tag	UNP A0A128QHZ1
C	10	PRO	-	expression tag	UNP A0A128QHZ1
C	11	LEU	-	expression tag	UNP A0A128QHZ1
C	12	GLY	-	expression tag	UNP A0A128QHZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	SER	-	expression tag	UNP A0A128QHZ1
E	9	GLY	-	expression tag	UNP A0A128QHZ1
E	10	PRO	-	expression tag	UNP A0A128QHZ1
E	11	LEU	-	expression tag	UNP A0A128QHZ1
E	12	GLY	-	expression tag	UNP A0A128QHZ1
E	13	SER	-	expression tag	UNP A0A128QHZ1
G	9	GLY	-	expression tag	UNP A0A128QHZ1
G	10	PRO	-	expression tag	UNP A0A128QHZ1
G	11	LEU	-	expression tag	UNP A0A128QHZ1
G	12	GLY	-	expression tag	UNP A0A128QHZ1
G	13	SER	-	expression tag	UNP A0A128QHZ1
I	9	GLY	-	expression tag	UNP A0A128QHZ1
I	10	PRO	-	expression tag	UNP A0A128QHZ1
I	11	LEU	-	expression tag	UNP A0A128QHZ1
I	12	GLY	-	expression tag	UNP A0A128QHZ1
I	13	SER	-	expression tag	UNP A0A128QHZ1
K	9	GLY	-	expression tag	UNP A0A128QHZ1
K	10	PRO	-	expression tag	UNP A0A128QHZ1
K	11	LEU	-	expression tag	UNP A0A128QHZ1
K	12	GLY	-	expression tag	UNP A0A128QHZ1
K	13	SER	-	expression tag	UNP A0A128QHZ1
M	9	GLY	-	expression tag	UNP A0A128QHZ1
M	10	PRO	-	expression tag	UNP A0A128QHZ1
M	11	LEU	-	expression tag	UNP A0A128QHZ1
M	12	GLY	-	expression tag	UNP A0A128QHZ1
M	13	SER	-	expression tag	UNP A0A128QHZ1
O	9	GLY	-	expression tag	UNP A0A128QHZ1
O	10	PRO	-	expression tag	UNP A0A128QHZ1
O	11	LEU	-	expression tag	UNP A0A128QHZ1
O	12	GLY	-	expression tag	UNP A0A128QHZ1
O	13	SER	-	expression tag	UNP A0A128QHZ1
Q	9	GLY	-	expression tag	UNP A0A128QHZ1
Q	10	PRO	-	expression tag	UNP A0A128QHZ1
Q	11	LEU	-	expression tag	UNP A0A128QHZ1
Q	12	GLY	-	expression tag	UNP A0A128QHZ1
Q	13	SER	-	expression tag	UNP A0A128QHZ1
S	9	GLY	-	expression tag	UNP A0A128QHZ1
S	10	PRO	-	expression tag	UNP A0A128QHZ1
S	11	LEU	-	expression tag	UNP A0A128QHZ1
S	12	GLY	-	expression tag	UNP A0A128QHZ1
S	13	SER	-	expression tag	UNP A0A128QHZ1

- Molecule 2 is a RNA chain called Modified SL3 of RocR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	28	Total 821	262	234	93	204	28	0	0	0
2	D	28	Total 821	262	234	93	204	28	0	0	0
2	F	28	Total 821	262	234	93	204	28	0	0	0
2	H	28	Total 821	262	234	93	204	28	0	0	0

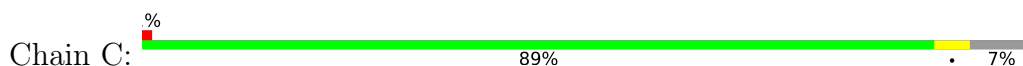
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Repressor of competence, RNA Chaperone



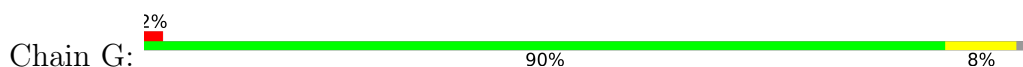
- Molecule 1: Repressor of competence, RNA Chaperone



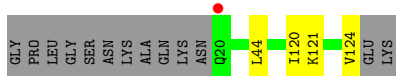
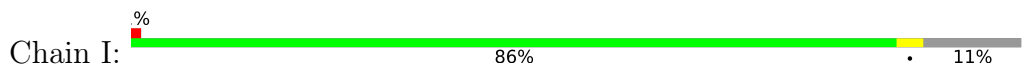
- Molecule 1: Repressor of competence, RNA Chaperone



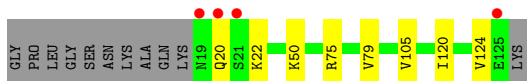
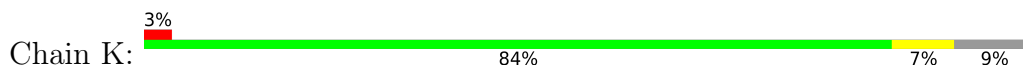
- Molecule 1: Repressor of competence, RNA Chaperone



- Molecule 1: Repressor of competence, RNA Chaperone



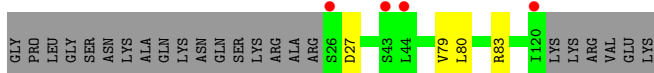
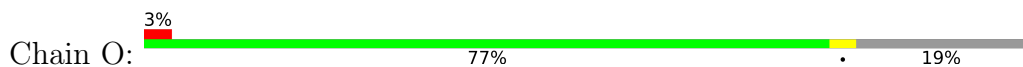
- Molecule 1: Repressor of competence, RNA Chaperone



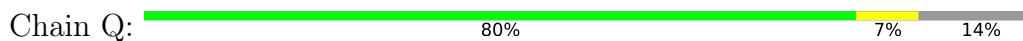
- Molecule 1: Repressor of competence, RNA Chaperone



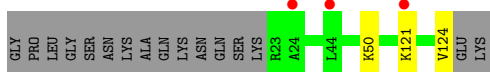
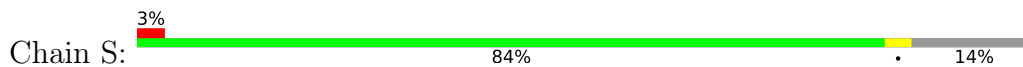
- Molecule 1: Repressor of competence, RNA Chaperone



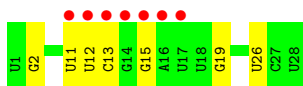
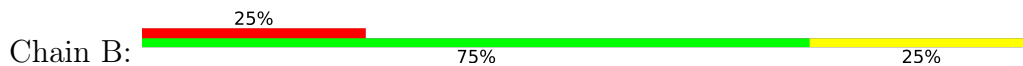
- Molecule 1: Repressor of competence, RNA Chaperone



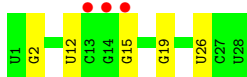
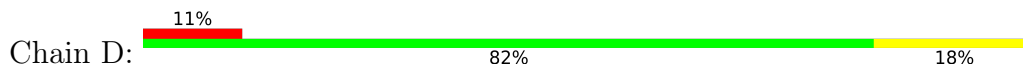
- Molecule 1: Repressor of competence, RNA Chaperone




- Molecule 2: Modified SL3 of RocR



- Molecule 2: Modified SL3 of RocR




- Molecule 2: Modified SL3 of RocR

Chain F:  82% 14%



● Molecule 2: Modified SL3 of RocR

Chain H:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.81Å 135.94Å 156.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 3.20 48.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.77-3.20) 91.5 (48.77-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.219 , 0.271 0.219 , 0.271	Depositor DCC
R_{free} test set	1463 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20397	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.26	0/901	0.42	0/1207
1	C	0.27	0/894	0.42	0/1197
1	E	0.27	0/886	0.42	0/1186
1	G	0.27	0/928	0.42	0/1243
1	I	0.26	0/853	0.41	0/1144
1	K	0.26	0/870	0.42	0/1167
1	M	0.26	0/861	0.42	0/1155
1	O	0.26	0/766	0.44	0/1032
1	Q	0.25	0/829	0.43	0/1113
1	S	0.25	0/829	0.42	0/1113
2	B	0.18	0/652	0.68	0/1012
2	D	0.20	0/652	0.70	0/1012
2	F	0.20	0/652	0.70	0/1012
2	H	0.19	0/652	0.69	0/1012
All	All	0.25	0/11225	0.51	0/15605

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	888	889	931	7	0
1	C	881	889	922	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	873	889	916	5	0
1	G	915	889	956	6	0
1	I	840	872	880	5	0
1	K	857	878	892	5	0
1	M	848	878	886	4	0
1	O	753	776	775	2	0
1	Q	816	833	854	8	0
1	S	816	833	854	2	0
2	B	587	234	298	2	0
2	D	587	234	298	1	0
2	F	587	234	298	2	0
2	H	587	234	298	0	0
All	All	10835	9562	10058	39	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.

The worst 5 of 39 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:Q:120:ILE:O	1:Q:124:VAL:HG13	1.97	0.63
1:C:29:LEU:HD11	1:C:80:LEU:HD22	1.80	0.63
1:K:50:LYS:HB2	1:K:105:VAL:HG21	1.81	0.62
1:Q:121:LYS:HA	1:Q:124:VAL:HG22	1.83	0.61
1:E:15:LYS:O	1:E:17:GLN:N	2.35	0.59

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	110/118 (93%)	108 (98%)	2 (2%)	0	100	100
1	C	109/118 (92%)	106 (97%)	3 (3%)	0	100	100
1	E	108/118 (92%)	106 (98%)	1 (1%)	1 (1%)	17	56
1	G	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
1	I	104/118 (88%)	102 (98%)	2 (2%)	0	100	100
1	K	106/118 (90%)	104 (98%)	2 (2%)	0	100	100
1	M	105/118 (89%)	101 (96%)	4 (4%)	0	100	100
1	O	94/118 (80%)	91 (97%)	3 (3%)	0	100	100
1	Q	101/118 (86%)	99 (98%)	2 (2%)	0	100	100
1	S	101/118 (86%)	99 (98%)	2 (2%)	0	100	100
All	All	1052/1180 (89%)	1024 (97%)	27 (3%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	ALA

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	95/99 (96%)	95 (100%)	0	100	100
1	C	94/99 (95%)	93 (99%)	1 (1%)	73	88
1	E	93/99 (94%)	93 (100%)	0	100	100
1	G	98/99 (99%)	97 (99%)	1 (1%)	76	90
1	I	90/99 (91%)	90 (100%)	0	100	100
1	K	92/99 (93%)	90 (98%)	2 (2%)	52	79
1	M	91/99 (92%)	91 (100%)	0	100	100
1	O	81/99 (82%)	80 (99%)	1 (1%)	71	88
1	Q	87/99 (88%)	86 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	87/99 (88%)	87 (100%)	0	100	100
All	All	908/990 (92%)	902 (99%)	6 (1%)	84	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	22	LYS
1	O	27	ASP
1	Q	118	MET
1	G	22	LYS
1	C	15	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	27/28 (96%)	4 (14%)	0
2	D	27/28 (96%)	4 (14%)	0
2	F	27/28 (96%)	4 (14%)	0
2	H	27/28 (96%)	4 (14%)	0
All	All	108/112 (96%)	16 (14%)	0

5 of 16 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	12	U
2	B	15	G
2	B	26	U
2	D	2	G

There are no RNA pucker outliers to report.

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 monosaccharides 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, 95th 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 ²)	Q<0.9
1	A	111/118 (94%)	0.03	1 (0%) 84 75	16, 28, 58, 81	0
1	C	110/118 (93%)	0.02	1 (0%) 84 75	12, 25, 54, 74	0
1	E	109/118 (92%)	-0.13	0 100 100	13, 25, 57, 64	0
1	G	115/118 (97%)	0.01	2 (1%) 70 57	17, 39, 64, 90	0
1	I	105/118 (88%)	0.19	1 (0%) 82 72	23, 39, 70, 91	0
1	K	107/118 (90%)	0.03	4 (3%) 41 26	25, 44, 79, 94	0
1	M	106/118 (89%)	-0.05	0 100 100	19, 32, 68, 91	0
1	O	95/118 (80%)	0.34	4 (4%) 36 23	29, 44, 81, 95	0
1	Q	102/118 (86%)	-0.10	0 100 100	24, 48, 70, 88	0
1	S	102/118 (86%)	0.31	3 (2%) 51 36	23, 46, 76, 93	0
2	B	28/28 (100%)	1.16	7 (25%) 0 0	37, 63, 181, 184	0
2	D	28/28 (100%)	0.59	3 (10%) 6 3	22, 54, 190, 191	0
2	F	28/28 (100%)	-0.08	0 100 100	28, 54, 85, 91	0
2	H	28/28 (100%)	0.04	0 100 100	31, 68, 93, 96	0
All	All	1174/1292 (90%)	0.09	26 (2%) 62 48	12, 39, 80, 191	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	14	G	5.4
1	O	26	SER	4.0
1	C	14	ASN	3.9
2	B	15	G	3.8
2	D	14	G	3.7

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 monosaccharides 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.