



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:11 PM GMT

PDB ID : 4ILL  
Title : Recognition and Cleavage of a non-structured CRISPR RNA by its Processing  
Endoribonuclease Cas6  
Authors : Shao, Y.; Li, H.  
Deposited on : 2012-12-31  
Resolution : 2.48 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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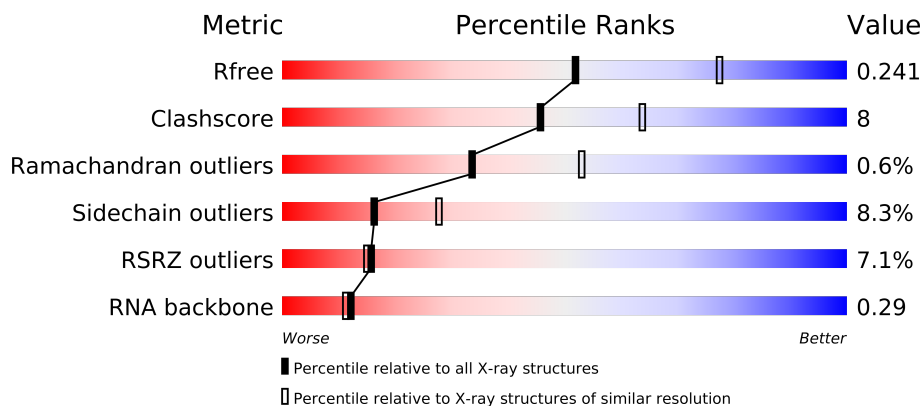
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.48 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))
$R_{free}$	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)
RNA backbone	1838	1007 (3.06-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
2	C	24	
2	R	24	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5206 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CRISPR-associated endoribonuclease Cas6 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2217	1440	381	392	4			
1	B	278	Total	C	N	O	S	0	0	0
			2215	1438	380	393	4			

- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*CP\*UP\*AP\*AP\*UP\*CP\*UP\*AP\*CP\*UP\*AP\*UP\*AP\*GP\*AP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	19	Total	C	N	O	P	0	0	0
			406	183	76	128	19			
2	C	17	Total	C	N	O	P	0	0	0
			356	162	64	114	16			

- Molecule 3 is water.

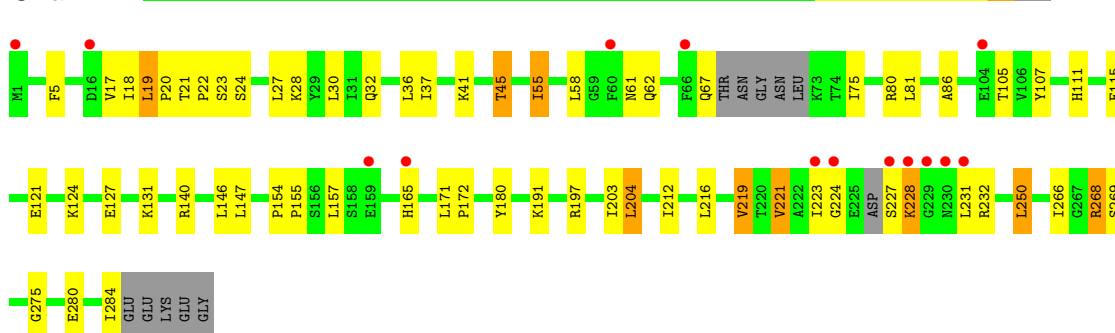
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	R	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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

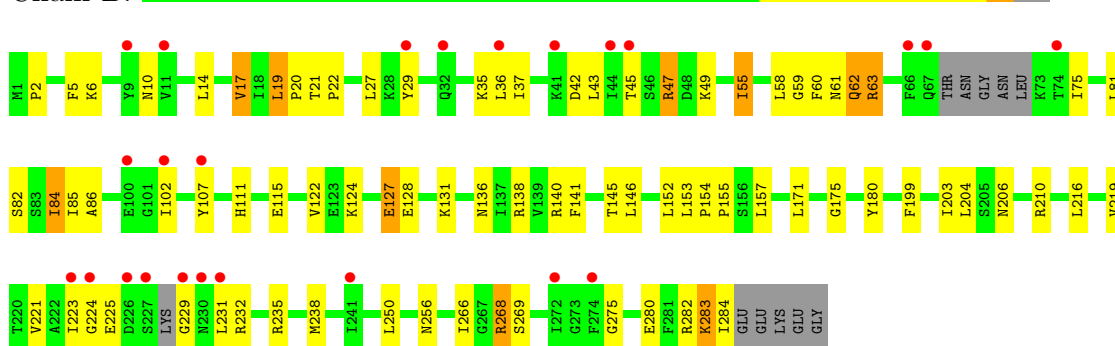
- Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain A:



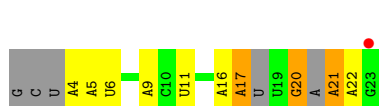
- Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain B:



- Molecule 2: RNA (5'-R(\*GP\*CP\*UP\*AP\*AP\*UP\*CP\*UP\*AP\*CP\*UP\*AP\*UP\*AP\*GP\*AP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*G)-3')

Chain R:



- Molecule 2: RNA (5'-R(\*GP\*CP\*UP\*AP\*AP\*UP\*CP\*UP\*AP\*CP\*UP\*AP\*UP\*AP\*GP\*AP\*AP\*UP\*UP\*GP\*AP\*AP\*AP\*G)-3')

Chain C:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.74Å 68.54Å 79.83Å 90.00° 119.12° 90.00°	Depositor
Resolution (Å)	32.00 – 2.48 41.89 – 2.48	Depositor EDS
% Data completeness (in resolution range)	91.2 (32.00-2.48) 90.9 (41.89-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, $R_{free}$	0.204 , 0.239 0.205 , 0.241	Depositor DCC
$R_{free}$ test set	1959 reflections (8.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.3	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.2	EDS
Estimated twinning fraction	0.034 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24962 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.30	0/2258	0.54	0/3040
1	B	0.31	0/2256	0.56	0/3038
2	C	0.29	0/398	0.81	0/618
2	R	0.33	0/454	0.93	0/702
All	All	0.31	0/5366	0.62	0/7398

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2217	0	2333	32	0
1	B	2215	0	2324	50	0
2	C	356	0	181	5	0
2	R	406	0	206	6	0
3	A	10	0	0	0	0
3	B	1	0	0	0	0
3	R	1	0	0	0	0
All	All	5206	0	5044	85	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 8.

All (85) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:ASN:O	1:B:63:ARG:N	2.16	0.79
1:A:121:GLU:HB3	1:A:124:LYS:HG2	1.74	0.70
1:A:23:SER:OG	1:A:67:GLN:NE2	2.28	0.67
1:B:6:LYS:HG3	1:B:84:ILE:HD11	1.76	0.66
1:B:225:GLU:OE1	1:B:229:GLY:N	2.30	0.64
1:A:223:ILE:HB	1:A:232:ARG:HB2	1.79	0.63
1:B:14:LEU:HD11	1:B:102:ILE:HD12	1.81	0.63
1:A:140:ARG:NH1	1:A:280:GLU:OE1	2.31	0.62
1:A:171:LEU:HD11	1:B:171:LEU:HD11	1.81	0.62
1:B:29:TYR:OH	1:B:35:LYS:NZ	2.34	0.61
1:A:165:HIS:O	1:B:210:ARG:NH2	2.35	0.60
1:A:212:ILE:O	1:B:235:ARG:NH1	2.35	0.58
1:B:140:ARG:NH1	1:B:280:GLU:OE1	2.37	0.57
1:A:36:LEU:HD12	1:A:37:ILE:HG13	1.87	0.56
1:A:19:LEU:HD22	1:A:75:ILE:HG13	1.87	0.56
1:B:128:GLU:HA	1:B:131:LYS:HD3	1.87	0.56
1:B:27:LEU:HD22	1:B:85:ILE:HD11	1.85	0.56
1:A:203:ILE:HD12	1:B:203:ILE:HD12	1.88	0.56
1:B:235:ARG:HB2	2:C:5:A:C5	2.42	0.55
1:B:36:LEU:HD12	1:B:37:ILE:HG13	1.89	0.55
1:B:42:ASP:N	1:B:42:ASP:OD2	2.38	0.54
1:B:55:ILE:HG13	1:B:55:ILE:O	2.08	0.53
1:B:175:GLY:H	1:B:206:ASN:HB3	1.73	0.53
1:A:191:LYS:HE2	1:A:197:ARG:HH12	1.74	0.52
1:B:2:PRO:HG2	1:B:122:VAL:HG21	1.90	0.52
1:A:219:VAL:HG12	1:A:221:VAL:HG12	1.92	0.52
1:B:266:ILE:O	1:B:275:GLY:HA3	2.10	0.52
2:R:20:G:H5'	2:R:21:A:H3'	1.91	0.52
2:R:20:G:C5'	2:R:21:A:H3'	2.40	0.51
1:A:227:SER:OG	1:A:228:LYS:N	2.45	0.50
2:R:4:A:H62	1:B:136:ASN:HD21	1.60	0.50
1:B:5:PHE:O	1:B:86:ALA:HA	2.11	0.49
1:A:41:LYS:O	1:A:45:THR:OG1	2.30	0.49
1:B:10:ASN:OD1	1:B:115:GLU:HB2	2.12	0.49
1:B:49:LYS:NZ	2:C:12:A:OP1	2.45	0.49
1:B:20:PRO:HB3	1:B:107:TYR:CE1	2.48	0.48
1:B:59:GLY:HA3	1:B:82:SER:O	2.13	0.47
1:A:28:LYS:HE3	1:A:32:GLN:NE2	2.29	0.47
1:B:283:LYS:HA	1:B:283:LYS:HD2	1.73	0.47
1:B:219:VAL:HG21	1:B:238:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268:ARG:HG3	1:A:269:SER:N	2.31	0.46
1:A:24:SER:O	1:A:55:ILE:HD11	2.15	0.46
1:A:228:LYS:HD3	1:A:228:LYS:HA	1.76	0.46
1:A:55:ILE:O	1:A:55:ILE:HG13	2.14	0.46
1:B:283:LYS:HE2	1:B:284:ILE:H	1.82	0.45
1:A:204:LEU:HD13	1:A:250:LEU:HD21	1.99	0.45
1:B:19:LEU:HD12	1:B:19:LEU:HA	1.85	0.45
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.81	0.45
1:B:58:LEU:HD13	1:B:81:LEU:HD23	1.97	0.44
1:B:223:ILE:HB	1:B:232:ARG:HB2	1.99	0.44
1:A:266:ILE:O	1:A:275:GLY:HA3	2.17	0.44
1:A:61:ASN:HB3	1:A:62:GLN:H	1.57	0.44
1:A:5:PHE:O	1:A:86:ALA:HA	2.18	0.44
1:B:60:PHE:CG	1:B:61:ASN:N	2.85	0.44
1:B:17:VAL:HG23	1:B:75:ILE:HG13	2.00	0.44
1:B:153:LEU:HD12	1:B:154:PRO:HD2	2.00	0.44
1:A:21:THR:HA	1:A:22:PRO:HA	1.87	0.43
1:B:27:LEU:HB3	1:B:55:ILE:HD13	2.00	0.43
2:R:20:G:H1'	2:R:22:A:C5	2.54	0.43
1:A:24:SER:HB2	1:A:55:ILE:HG13	2.01	0.43
1:B:47:ARG:HG3	1:B:47:ARG:H	1.48	0.43
2:C:14:A:H2'	2:C:15:G:C8	2.54	0.43
1:B:199:PHE:O	1:B:203:ILE:HG12	2.19	0.42
2:C:10:C:O2'	2:C:11:U:H5'	2.19	0.42
2:C:16:A:O2'	2:C:17:A:O5'	2.34	0.42
1:B:124:LYS:O	1:B:127:GLU:HB2	2.20	0.42
1:B:141:PHE:HD1	1:B:145:THR:HG1	1.63	0.42
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.84	0.42
1:A:20:PRO:HB3	1:A:107:TYR:CE1	2.55	0.42
1:A:17:VAL:O	1:A:75:ILE:N	2.38	0.41
1:B:21:THR:HA	1:B:22:PRO:HA	1.90	0.41
1:B:283:LYS:HG3	1:B:283:LYS:HZ2	1.62	0.41
2:R:4:A:H62	1:B:136:ASN:ND2	2.18	0.41
1:A:147:LEU:CD1	1:A:172:PRO:HB3	2.51	0.41
1:B:61:ASN:HB2	1:B:62:GLN:NE2	2.36	0.41
1:B:268:ARG:HG3	1:B:269:SER:N	2.36	0.41
1:B:138:ARG:HH22	1:B:282:ARG:NH2	2.18	0.41
1:A:27:LEU:HB3	1:A:55:ILE:HD13	2.03	0.41
1:B:154:PRO:HA	1:B:155:PRO:HD3	1.87	0.41
1:B:43:LEU:HA	1:B:43:LEU:HD12	1.87	0.41
1:B:61:ASN:C	1:B:63:ARG:H	2.24	0.41
2:R:16:A:H2''	2:R:17:A:H5'	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:58:LEU:HD13	1:A:81:LEU:HD23	2.02	0.40
1:A:30:LEU:HD21	1:A:105:THR:HG22	2.03	0.40
1:B:58:LEU:HA	1:B:59:GLY:HA3	1.77	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	272/289 (94%)	266 (98%)	5 (2%)	1 (0%)	43	64
1	B	272/289 (94%)	265 (97%)	5 (2%)	2 (1%)	30	48
All	All	544/578 (94%)	531 (98%)	10 (2%)	3 (1%)	33	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	A	224	GLY
1	B	224	GLY

### 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	246/256 (96%)	225 (92%)	21 (8%)	15	26
1	B	246/256 (96%)	226 (92%)	20 (8%)	17	29
All	All	492/512 (96%)	451 (92%)	41 (8%)	16	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	19	LEU
1	A	45	THR
1	A	55	ILE
1	A	80	ARG
1	A	111	HIS
1	A	115	GLU
1	A	127	GLU
1	A	131	LYS
1	A	146	LEU
1	A	157	LEU
1	A	180	TYR
1	A	204	LEU
1	A	216	LEU
1	A	219	VAL
1	A	221	VAL
1	A	228	LYS
1	A	231	LEU
1	A	250	LEU
1	A	268	ARG
1	A	284	ILE
1	B	17	VAL
1	B	19	LEU
1	B	45	THR
1	B	47	ARG
1	B	55	ILE
1	B	63	ARG
1	B	84	ILE
1	B	111	HIS
1	B	127	GLU
1	B	146	LEU
1	B	157	LEU
1	B	180	TYR
1	B	204	LEU
1	B	216	LEU
1	B	221	VAL
1	B	231	LEU
1	B	250	LEU
1	B	256	ASN
1	B	268	ARG
1	B	283	LYS

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

Mol	Chain	Res	Type
1	A	67	GLN
1	B	62	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	16/24 (66%)	7 (43%)	2 (12%)
2	R	16/24 (66%)	7 (43%)	0
All	All	32/48 (66%)	14 (43%)	2 (6%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	5	A
2	R	6	U
2	R	9	A
2	R	11	U
2	R	17	A
2	R	20	G
2	R	21	A
2	C	3	U
2	C	5	A
2	C	6	U
2	C	9	A
2	C	10	C
2	C	11	U
2	C	17	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	2	C
2	C	16	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	278/289 (96%)	0.47	14 (5%) 28 28	50, 70, 97, 125	0
1	B	278/289 (96%)	0.67	24 (8%) 11 10	56, 85, 112, 129	0
2	C	17/24 (70%)	0.87	3 (17%) 2 2	70, 87, 134, 139	0
2	R	19/24 (79%)	0.35	1 (5%) 25 26	57, 83, 123, 131	0
All	All	592/626 (94%)	0.57	42 (7%) 16 15	50, 76, 111, 139	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	SER	7.8
1	B	231	LEU	6.5
2	C	17	A	5.8
1	A	228	LYS	4.8
1	A	229	GLY	4.8
1	A	1	MET	4.6
1	B	230	ASN	4.5
1	B	32	GLN	4.4
1	A	230	ASN	4.2
2	R	23	G	4.1
1	A	66	PHE	4.0
1	B	226	ASP	3.7
1	B	272	ILE	3.4
1	B	107	TYR	3.4
1	A	165	HIS	3.3
1	B	102	ILE	3.3
2	C	9	A	3.2
1	A	159	GLU	3.1
1	A	16	ASP	3.1
1	B	44	ILE	3.1
1	B	29	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLY	3.0
1	B	100	GLU	2.9
1	B	223	ILE	2.8
1	B	66	PHE	2.8
1	A	227	SER	2.7
1	B	36	LEU	2.6
1	B	11	VAL	2.6
1	A	231	LEU	2.5
1	A	224	GLY	2.4
1	B	224	GLY	2.4
1	B	67	GLN	2.2
1	B	274	PHE	2.2
1	A	60	PHE	2.2
1	A	104	GLU	2.1
1	B	41	LYS	2.1
1	B	9	TYR	2.1
1	B	74	THR	2.1
1	A	223	ILE	2.1
1	B	45	THR	2.1
1	B	241	ILE	2.1
2	C	16	A	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.