



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 10:26 AM EST

PDB ID : 6WXY  
Title : crystal structure of cA6-bound Card1  
Authors : Rostol, J.; Xie, W.; Patel, D.J.; Marraffini, L.  
Deposited on : 2020-05-12  
Resolution : 2.10 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 : 2.16  
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) : 2.16

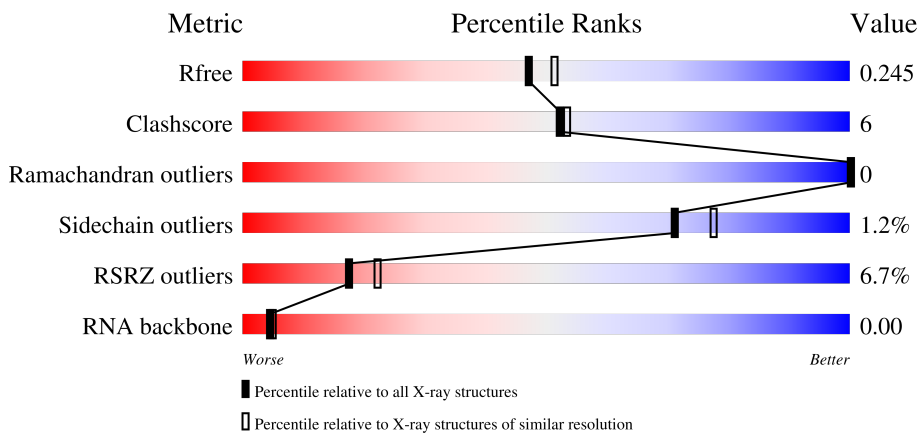
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

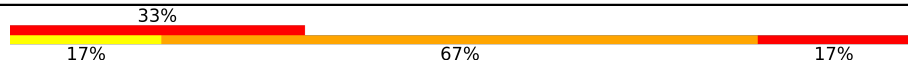
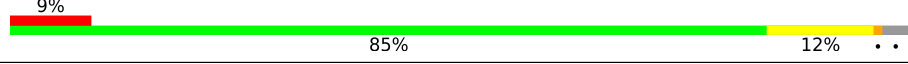
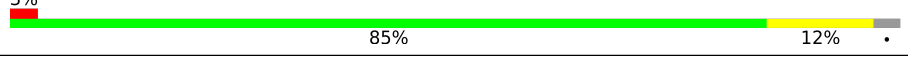
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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  $\geq 3$ , 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	6	
2	B	382	
2	C	382	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6534 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 RNA chain called cA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	6	132	60	30	36	6	0	0	0

- Molecule 2 is a protein called Card1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	372	3092	1991	506	585	10	0	0	0
2	C	372	3092	1991	506	585	10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	GLY	-	expression tag	UNP F2NWD3
B	375	SER	-	expression tag	UNP F2NWD3
B	376	GLY	-	expression tag	UNP F2NWD3
B	377	HIS	-	expression tag	UNP F2NWD3
B	378	HIS	-	expression tag	UNP F2NWD3
B	379	HIS	-	expression tag	UNP F2NWD3
B	380	HIS	-	expression tag	UNP F2NWD3
B	381	HIS	-	expression tag	UNP F2NWD3
B	382	HIS	-	expression tag	UNP F2NWD3
C	374	GLY	-	expression tag	UNP F2NWD3
C	375	SER	-	expression tag	UNP F2NWD3
C	376	GLY	-	expression tag	UNP F2NWD3
C	377	HIS	-	expression tag	UNP F2NWD3
C	378	HIS	-	expression tag	UNP F2NWD3
C	379	HIS	-	expression tag	UNP F2NWD3
C	380	HIS	-	expression tag	UNP F2NWD3
C	381	HIS	-	expression tag	UNP F2NWD3
C	382	HIS	-	expression tag	UNP F2NWD3

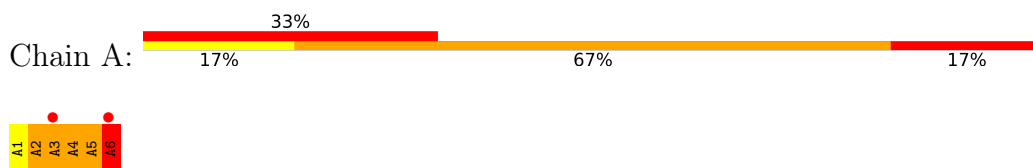
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	92	Total O 92 92	0	0
3	C	125	Total O 125 125	0	0

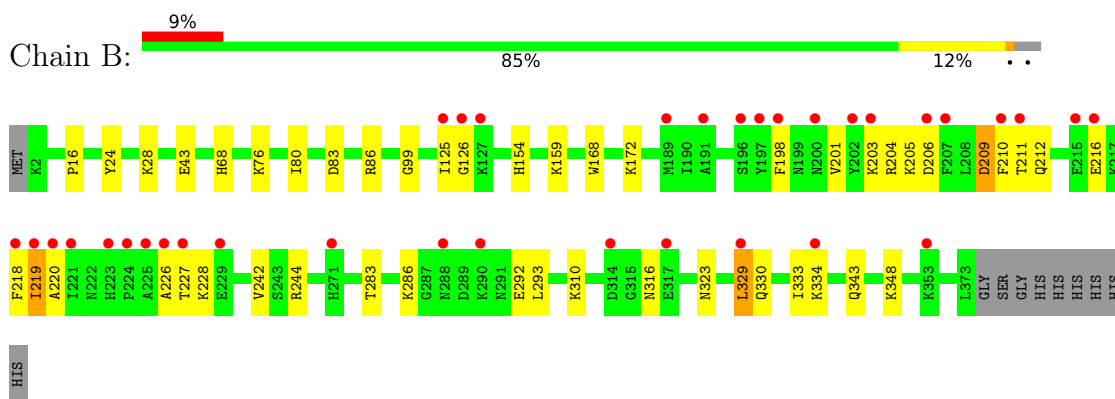
### 3 Residue-property plots [i](#)

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.

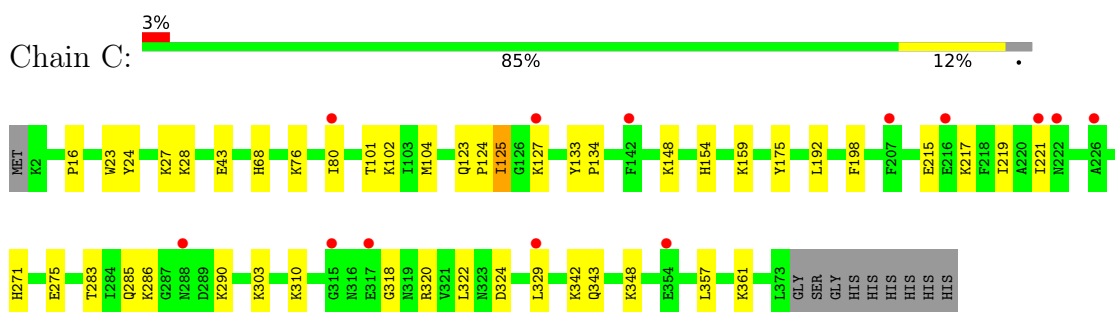
- Molecule 1: cA6



- Molecule 2: Card1



- Molecule 2: Card1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.91Å 124.76Å 42.26Å 90.00° 96.79° 90.00°	Depositor
Resolution (Å)	85.85 – 2.10 85.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (85.85-2.10) 98.4 (85.85-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.18_3855	Depositor
R, $R_{free}$	0.206 , 0.245 0.206 , 0.245	Depositor DCC
$R_{free}$ test set	2519 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.43% 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	0.98	1/149 (0.7%)	1.37	2/230 (0.9%)
2	B	0.40	0/3157	0.58	1/4257 (0.0%)
2	C	0.39	0/3157	0.53	0/4257
All	All	0.42	1/6463 (0.0%)	0.59	3/8744 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	A	O3'-P	-6.18	1.53	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	329	LEU	CA-CB-CG	-8.04	96.80	115.30
1	A	6	A	C3'-C2'-C1'	-5.43	97.16	101.50
1	A	6	A	C2'-C3'-O3'	5.03	121.75	113.70

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	132	0	66	10	0
2	B	3092	0	3063	36	0
2	C	3092	0	3063	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	92	0	0	3	0
3	C	125	0	0	6	0
All	All	6534	0	6192	69	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 6.

All (69) 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:C:101:THR:H	2:C:104:MET:HE3	1.37	0.90
2:C:285:GLN:HB2	2:C:290:LYS:HE3	1.67	0.77
1:A:6:A:H1'	2:B:125:ILE:HD13	1.67	0.76
1:A:5:A:O2'	2:B:125:ILE:HG23	1.89	0.72
2:B:203:LYS:HB2	2:B:206:ASP:O	1.95	0.66
2:C:101:THR:N	2:C:104:MET:HE3	2.11	0.64
2:B:219:ILE:HG22	2:B:226:ALA:O	1.98	0.63
2:B:293:LEU:HD11	2:B:333:ILE:HD11	1.80	0.62
2:B:43:GLU:HG3	2:B:68:HIS:NE2	2.18	0.59
1:A:5:A:C5	2:B:16:PRO:HG3	2.38	0.58
2:C:271:HIS:HA	3:C:438:HOH:O	2.03	0.58
2:B:283:THR:HG22	2:B:292:GLU:HG2	1.86	0.56
2:B:323:ASN:HD21	2:C:322:LEU:HD23	1.70	0.56
2:C:123:GLN:HG2	3:C:508:HOH:O	2.05	0.56
2:C:124:PRO:HB2	2:C:127:LYS:HB2	1.87	0.55
1:A:5:A:C4	2:B:125:ILE:HG22	2.42	0.55
2:C:192:LEU:HA	2:C:221:ILE:HD13	1.89	0.55
2:C:329:LEU:HD13	2:C:343:GLN:HB2	1.88	0.55
2:C:43:GLU:HG3	2:C:68:HIS:NE2	2.23	0.54
1:A:3:A:C8	1:A:3:A:H3'	2.43	0.54
2:C:148:LYS:NZ	3:C:406:HOH:O	2.38	0.54
2:B:125:ILE:HG13	2:B:126:GLY:H	1.73	0.54
2:B:329:LEU:HD22	2:B:343:GLN:CD	2.28	0.54
2:B:329:LEU:HD22	2:B:343:GLN:OE1	2.08	0.53
2:C:342:LYS:HD2	3:C:424:HOH:O	2.08	0.52
2:C:215:GLU:O	2:C:219:ILE:HG13	2.10	0.52
2:C:275:GLU:OE1	3:C:401:HOH:O	2.19	0.52
1:A:3:A:O4'	2:C:125:ILE:HG12	2.09	0.52
2:B:212:GLN:HB2	2:B:242:VAL:HG13	1.91	0.52
2:B:99:GLY:O	2:C:102:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:A:C4	2:B:16:PRO:HG3	2.45	0.51
2:B:209:ASP:HB3	2:B:244:ARG:HG3	1.93	0.51
2:B:316:ASN:OD1	2:B:316:ASN:N	2.41	0.51
2:B:24:TYR:CZ	2:B:28:LYS:HG3	2.45	0.50
2:B:218:PHE:C	2:B:220:ALA:H	2.15	0.49
1:A:2:A:C4	2:C:16:PRO:HG3	2.47	0.49
1:A:1:A:H5'	1:A:6:A:H5'	1.95	0.48
2:B:348:LYS:NZ	3:B:406:HOH:O	2.36	0.47
2:C:101:THR:H	2:C:104:MET:CE	2.17	0.47
2:C:24:TYR:CZ	2:C:28:LYS:HG3	2.49	0.47
2:C:23:TRP:CZ2	2:C:27:LYS:HE3	2.49	0.47
2:C:303:LYS:HG3	3:C:418:HOH:O	2.14	0.47
2:B:198:PHE:HA	2:B:201:VAL:HG12	1.97	0.46
2:C:320:ARG:NH1	2:C:324:ASP:OD2	2.47	0.46
2:B:168:TRP:O	2:B:172:LYS:HG3	2.16	0.46
2:C:101:THR:HG23	2:C:104:MET:CE	2.47	0.45
2:C:133:TYR:CD1	2:C:134:PRO:HA	2.51	0.45
2:B:204:ARG:NH2	3:B:408:HOH:O	2.48	0.45
2:B:154:HIS:O	2:B:286:LYS:HE3	2.16	0.45
2:B:218:PHE:C	2:B:220:ALA:N	2.70	0.45
2:B:83:ASP:OD1	2:B:86:ARG:NH2	2.48	0.45
2:C:124:PRO:HB2	2:C:127:LYS:HD3	1.99	0.44
2:C:76:LYS:O	2:C:80:ILE:HG23	2.18	0.44
2:B:159:LYS:HE3	2:B:159:LYS:HB2	1.66	0.44
2:B:219:ILE:HG13	2:B:228:LYS:HB2	1.99	0.44
2:C:217:LYS:HE2	2:C:217:LYS:HA	2.00	0.43
2:C:154:HIS:O	2:C:286:LYS:HE3	2.18	0.42
2:B:205:LYS:HA	2:B:205:LYS:HD3	1.90	0.41
2:B:201:VAL:HG13	2:B:210:PHE:CZ	2.55	0.41
1:A:5:A:C8	2:B:125:ILE:HA	2.55	0.41
2:B:330:GLN:O	2:B:334:LYS:HB3	2.20	0.41
2:B:329:LEU:HA	2:B:329:LEU:HD12	1.81	0.41
2:C:318:GLY:HA2	2:C:357:LEU:HD23	2.02	0.41
2:C:159:LYS:HG2	2:C:283:THR:HB	2.03	0.41
2:C:175:TYR:CD2	2:C:348:LYS:HE2	2.56	0.41
2:B:76:LYS:O	2:B:80:ILE:HG23	2.21	0.40
2:B:219:ILE:HG21	2:B:227:THR:C	2.41	0.40
3:B:452:HOH:O	2:C:101:THR:HB	2.22	0.40
2:C:198:PHE:CE2	2:C:221:ILE:HD11	2.57	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	
2	B	370/382 (97%)	354 (96%)	16 (4%)	0	100	100
2	C	370/382 (97%)	361 (98%)	9 (2%)	0	100	100
All	All	740/764 (97%)	715 (97%)	25 (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	
2	B	344/352 (98%)	339 (98%)	5 (2%)	65	71
2	C	344/352 (98%)	341 (99%)	3 (1%)	78	84
All	All	688/704 (98%)	680 (99%)	8 (1%)	71	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	209	ASP
2	B	211	THR
2	B	216	GLU
2	B	219	ILE
2	B	310	LYS
2	C	125	ILE
2	C	310	LYS
2	C	361	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	13	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	5/6 (83%)	5 (100%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	A
1	A	5	A
1	A	6	A

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

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	6/6 (100%)	1.23	2 (33%) <b>0</b> <b>0</b>	52, 71, 91, 113	0
2	B	372/382 (97%)	0.75	35 (9%) <b>8</b> <b>11</b>	31, 50, 93, 110	0
2	C	372/382 (97%)	0.55	13 (3%) 44 50	27, 47, 70, 92	0
All	All	750/770 (97%)	0.66	50 (6%) <b>17</b> <b>22</b>	27, 48, 87, 113	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	210	PHE	11.9
2	B	207	PHE	7.8
2	B	219	ILE	6.6
2	C	207	PHE	5.2
2	B	225	ALA	4.6
2	C	315	GLY	4.5
2	C	142	PHE	4.1
1	A	6	A	4.0
2	B	202	TYR	4.0
2	C	221	ILE	3.7
2	B	206	ASP	3.4
2	B	226	ALA	3.4
2	B	314	ASP	3.3
2	B	191	ALA	3.2
2	C	216	GLU	3.2
2	B	125	ILE	3.2
2	C	222	ASN	3.1
2	B	353	LYS	3.0
2	B	220	ALA	2.9
2	B	196	SER	2.9
2	B	215	GLU	2.9
2	B	198	PHE	2.8
2	B	203	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	200	ASN	2.8
2	B	224	PRO	2.8
2	B	211	THR	2.7
2	B	218	PHE	2.6
2	B	223	HIS	2.6
2	B	127	LYS	2.5
1	A	3	A	2.5
2	B	329	LEU	2.5
2	B	271	HIS	2.4
2	C	288	ASN	2.4
2	B	216	GLU	2.4
2	B	126	GLY	2.4
2	B	317	GLU	2.3
2	C	354	GLU	2.3
2	B	290	LYS	2.3
2	B	288	ASN	2.3
2	C	127	LYS	2.3
2	B	229	GLU	2.2
2	B	334	LYS	2.2
2	B	221	ILE	2.2
2	B	197	TYR	2.1
2	B	189	MET	2.1
2	C	317	GLU	2.1
2	B	227	THR	2.1
2	C	226	ALA	2.1
2	C	80	ILE	2.0
2	C	329	LEU	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 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.