



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 04:08 PM JST

PDB ID : 7FCL  
Title : Zebrafish SIGIRR TIR domain  
Authors : Wang, X.; Zhou, J.  
Deposited on : 2021-07-15  
Resolution : 3.04 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.

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	:	2.29
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)	:	2.29

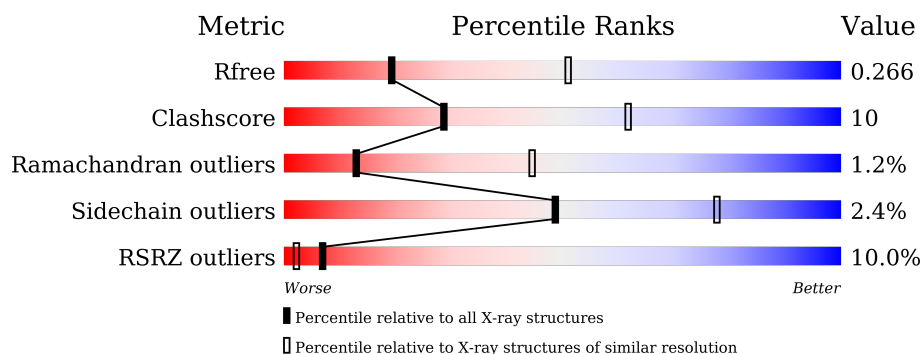
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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	155	<div> <div>9%</div> <div>65%</div> <div>27%</div> <div>6%</div> </div>
1	B	155	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
1	C	155	<div> <div>11%</div> <div>72%</div> <div>21%</div> <div>6%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3621 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 SIGIRR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1207	773	211	215	8			
1	B	146	Total	C	N	O	S	0	0	0
			1207	773	211	215	8			
1	C	146	Total	C	N	O	S	0	0	0
			1207	773	211	215	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	MET	-	initiating methionine	UNP K9K3G6
A	218	ASN	ASP	engineered mutation	UNP K9K3G6
A	328	HIS	-	expression tag	UNP K9K3G6
A	329	HIS	-	expression tag	UNP K9K3G6
A	330	HIS	-	expression tag	UNP K9K3G6
A	331	HIS	-	expression tag	UNP K9K3G6
A	332	HIS	-	expression tag	UNP K9K3G6
A	333	HIS	-	expression tag	UNP K9K3G6
B	179	MET	-	initiating methionine	UNP K9K3G6
B	218	ASN	ASP	engineered mutation	UNP K9K3G6
B	328	HIS	-	expression tag	UNP K9K3G6
B	329	HIS	-	expression tag	UNP K9K3G6
B	330	HIS	-	expression tag	UNP K9K3G6
B	331	HIS	-	expression tag	UNP K9K3G6
B	332	HIS	-	expression tag	UNP K9K3G6
B	333	HIS	-	expression tag	UNP K9K3G6
C	179	MET	-	initiating methionine	UNP K9K3G6
C	218	ASN	ASP	engineered mutation	UNP K9K3G6
C	328	HIS	-	expression tag	UNP K9K3G6
C	329	HIS	-	expression tag	UNP K9K3G6
C	330	HIS	-	expression tag	UNP K9K3G6
C	331	HIS	-	expression tag	UNP K9K3G6
C	332	HIS	-	expression tag	UNP K9K3G6

*Continued on next page...*

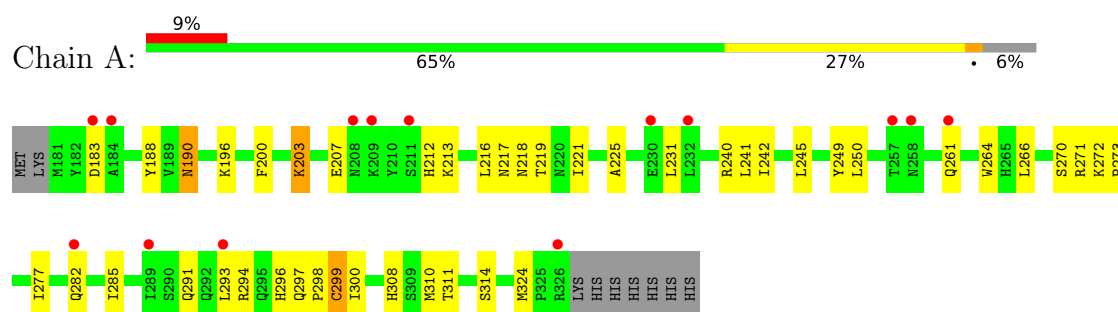
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	333	HIS	-	expression tag	UNP K9K3G6

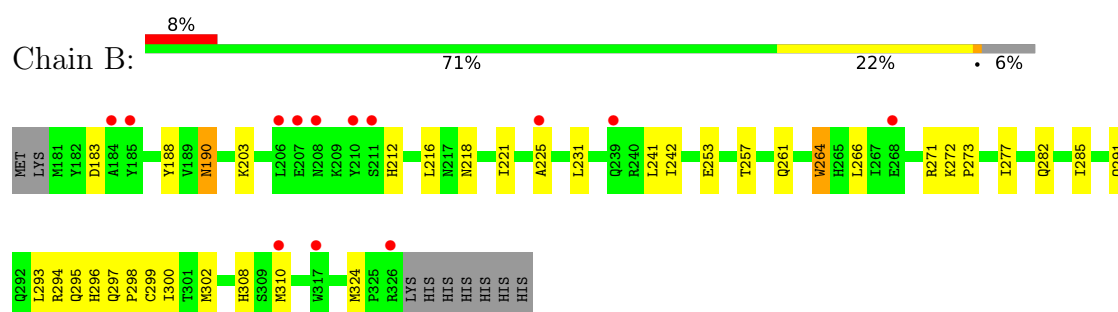
### 3 Residue-property plots [i](#)

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.

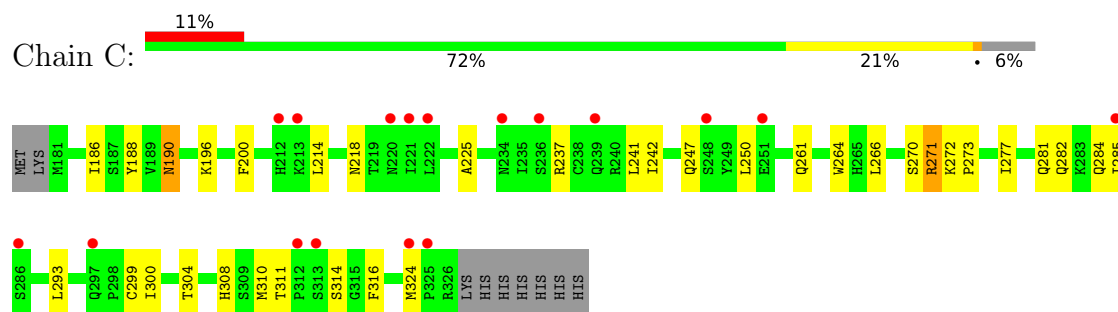
#### • Molecule 1: SIGIRR protein



#### • Molecule 1: SIGIRR protein



#### • Molecule 1: SIGIRR protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.00Å 145.36Å 75.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.56 – 3.04 42.00 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.56-3.04) 99.2 (42.00-3.04)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.239 , 0.273 0.245 , 0.266	Depositor DCC
$R_{free}$ test set	478 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.438 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.416 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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	0.59	1/1237 (0.1%)	0.77	1/1675 (0.1%)
1	B	0.57	0/1237	0.74	0/1675
1	C	0.57	0/1237	0.78	0/1675
All	All	0.58	1/3711 (0.0%)	0.76	1/5025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	CYS	CB-SG	-5.61	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	LYS	CD-CE-NZ	5.80	125.05	111.70

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	1207	0	1202	29	0
1	B	1207	0	1202	23	0
1	C	1207	0	1203	21	1
All	All	3621	0	3607	70	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 10.

All (70) 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:B:291:GLN:O	1:B:295:GLN:OE1	1.61	1.17
1:B:291:GLN:C	1:B:295:GLN:OE1	2.29	0.69
1:B:190:ASN:O	1:B:190:ASN:ND2	2.24	0.68
1:A:225:ALA:O	1:A:261:GLN:NE2	2.27	0.67
1:B:225:ALA:O	1:B:261:GLN:NE2	2.30	0.64
1:A:217:ASN:ND2	1:A:219:THR:OG1	2.31	0.63
1:C:190:ASN:ND2	1:C:190:ASN:O	2.29	0.63
1:C:225:ALA:O	1:C:261:GLN:NE2	2.32	0.62
1:B:282:GLN:HA	1:B:285:ILE:HG12	1.83	0.61
1:C:282:GLN:HA	1:C:285:ILE:HG12	1.82	0.61
1:A:203:LYS:HE2	1:A:216:LEU:HD21	1.86	0.58
1:B:277:ILE:HD12	1:B:282:GLN:HE21	1.69	0.57
1:A:242:ILE:HD11	1:A:324:MET:CE	2.34	0.57
1:C:242:ILE:HD11	1:C:324:MET:CE	2.35	0.56
1:B:221:ILE:HB	1:B:231:LEU:HD22	1.86	0.56
1:B:294:ARG:O	1:B:297:GLN:HB2	2.05	0.56
1:C:293:LEU:O	1:C:300:ILE:HD11	2.05	0.56
1:B:272:LYS:HA	1:B:299:CYS:O	2.06	0.56
1:C:242:ILE:HD11	1:C:324:MET:HE2	1.88	0.56
1:A:293:LEU:O	1:A:300:ILE:HD11	2.07	0.55
1:C:186:ILE:HD11	1:C:214:LEU:HD22	1.89	0.53
1:B:242:ILE:HD11	1:B:324:MET:CE	2.39	0.53
1:B:293:LEU:O	1:B:300:ILE:HD11	2.10	0.51
1:A:298:PRO:HG3	1:B:264:TRP:CD2	2.46	0.51
1:A:183:ASP:OD2	1:A:212:HIS:HA	2.11	0.50
1:A:190:ASN:O	1:A:190:ASN:ND2	2.43	0.49
1:A:272:LYS:HA	1:A:299:CYS:O	2.12	0.49
1:B:203:LYS:HE2	1:B:216:LEU:HD21	1.93	0.49
1:B:241:LEU:HD21	1:B:266:LEU:HD22	1.95	0.49
1:A:277:ILE:HD12	1:A:282:GLN:HE21	1.78	0.49
1:C:272:LYS:HA	1:C:299:CYS:O	2.12	0.49
1:C:188:TYR:O	1:C:218:ASN:HA	2.13	0.49
1:C:277:ILE:HD12	1:C:282:GLN:HE21	1.77	0.48
1:B:242:ILE:HD11	1:B:324:MET:HE2	1.97	0.47
1:A:213:LYS:HE3	1:A:213:LYS:HB3	1.77	0.46
1:B:188:TYR:O	1:B:218:ASN:HA	2.15	0.46
1:C:241:LEU:HD21	1:C:266:LEU:HD22	1.96	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:O	1:A:218:ASN:HA	2.16	0.46
1:C:250:LEU:CD1	1:C:285:ILE:HD12	2.46	0.46
1:C:247:GLN:OE1	1:C:284:GLN:HB3	2.16	0.46
1:A:241:LEU:HD23	1:A:273:PRO:HB3	1.97	0.45
1:B:190:ASN:OD1	1:B:218:ASN:ND2	2.45	0.45
1:C:196:LYS:HG2	1:C:200:PHE:CE2	2.52	0.45
1:A:207:GLU:HG2	1:A:212:HIS:O	2.18	0.44
1:A:294:ARG:O	1:A:297:GLN:HB2	2.17	0.44
1:C:304:THR:O	1:C:316:PHE:HD2	2.00	0.43
1:A:242:ILE:HD11	1:A:324:MET:HE1	1.98	0.43
1:C:241:LEU:HD23	1:C:273:PRO:HB3	2.00	0.43
1:A:298:PRO:HD2	1:B:296:HIS:CD2	2.53	0.43
1:A:242:ILE:HD11	1:A:324:MET:HE2	2.00	0.43
1:A:291:GLN:HG2	1:A:294:ARG:HH21	1.84	0.43
1:C:270:SER:O	1:C:271:ARG:HB2	2.19	0.43
1:A:241:LEU:HD21	1:A:266:LEU:HD22	1.99	0.42
1:A:272:LYS:HE2	1:A:272:LYS:HB2	1.76	0.42
1:C:311:THR:O	1:C:314:SER:HB2	2.19	0.42
1:C:218:ASN:OD1	1:C:218:ASN:N	2.51	0.42
1:A:245:LEU:HD12	1:A:249:TYR:CD1	2.54	0.41
1:A:270:SER:O	1:A:271:ARG:HB2	2.20	0.41
1:B:253:GLU:O	1:B:257:THR:HG22	2.19	0.41
1:A:221:ILE:HB	1:A:231:LEU:HD22	2.01	0.41
1:A:250:LEU:CD1	1:A:285:ILE:HD12	2.51	0.41
1:A:196:LYS:HG2	1:A:200:PHE:CE2	2.55	0.41
1:B:183:ASP:OD2	1:B:212:HIS:HA	2.20	0.41
1:B:293:LEU:HB3	1:B:302:MET:SD	2.61	0.41
1:A:240:ARG:HD3	1:A:240:ARG:HA	1.95	0.41
1:A:311:THR:O	1:A:314:SER:HB2	2.21	0.41
1:B:241:LEU:HD23	1:B:273:PRO:HB3	2.04	0.40
1:A:296:HIS:CD2	1:B:298:PRO:HD2	2.55	0.40
1:C:247:GLN:HG2	1:C:284:GLN:OE1	2.21	0.40
1:C:281:GLN:O	1:C:284:GLN:N	2.48	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:C:299:CYS:CB	1:C:299:CYS:SG[3_556]	1.81	0.39

## 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	144/155 (93%)	138 (96%)	5 (4%)	1 (1%)	22	57
1	B	144/155 (93%)	138 (96%)	4 (3%)	2 (1%)	11	40
1	C	144/155 (93%)	138 (96%)	4 (3%)	2 (1%)	11	40
All	All	432/465 (93%)	414 (96%)	13 (3%)	5 (1%)	13	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	310	MET
1	B	310	MET
1	A	310	MET
1	B	271	ARG
1	C	271	ARG

### 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	137/146 (94%)	134 (98%)	3 (2%)	52	79
1	B	137/146 (94%)	134 (98%)	3 (2%)	52	79
1	C	137/146 (94%)	133 (97%)	4 (3%)	42	74
All	All	411/438 (94%)	401 (98%)	10 (2%)	49	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	264	TRP
1	A	308	HIS
1	B	190	ASN
1	B	264	TRP
1	B	308	HIS
1	C	190	ASN
1	C	237	ARG
1	C	264	TRP
1	C	308	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	282	GLN
1	B	295	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 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	146/155 (94%)	0.51	14 (9%) <b>8</b> <b>2</b>	44, 76, 94, 101	0
1	B	146/155 (94%)	0.57	13 (8%) <b>9</b> <b>3</b>	44, 75, 96, 102	0
1	C	146/155 (94%)	0.65	17 (11%) <b>4</b> <b>1</b>	43, 75, 94, 102	0
All	All	438/465 (94%)	0.58	44 (10%) <b>7</b> <b>2</b>	43, 75, 96, 102	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	312	PRO	7.0
1	A	258	ASN	5.8
1	C	313	SER	5.4
1	A	184	ALA	5.0
1	C	236	SER	4.5
1	C	324	MET	4.3
1	A	208	ASN	4.1
1	C	234	ASN	4.1
1	A	230	GLU	3.8
1	C	212	HIS	3.8
1	C	286	SER	3.7
1	B	207	GLU	3.4
1	C	285	ILE	3.4
1	A	326	ARG	3.4
1	B	185	TYR	3.1
1	B	326	ARG	3.1
1	B	268	GLU	3.1
1	B	210	TYR	3.1
1	C	220	ASN	3.0
1	B	206	LEU	2.9
1	B	239	GLN	2.9
1	C	325	PRO	2.8
1	B	225	ALA	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	261	GLN	2.6
1	A	183	ASP	2.6
1	A	293	LEU	2.6
1	C	251	GLU	2.6
1	A	257	THR	2.6
1	B	310	MET	2.6
1	A	211	SER	2.6
1	A	209	LYS	2.6
1	C	297	GLN	2.5
1	A	289	ILE	2.5
1	C	221	ILE	2.5
1	A	282	GLN	2.4
1	C	213	LYS	2.4
1	B	184	ALA	2.4
1	B	317	TRP	2.3
1	B	208	ASN	2.3
1	B	211	SER	2.3
1	A	232	LEU	2.2
1	C	239	GLN	2.2
1	C	222	LEU	2.2
1	C	248	SER	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 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.