



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2016 – 11:18 AM EDT

PDB ID : 5E0T  
Title : Human PCNA mutant - S228I  
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Deposited on : 2015-09-29  
Resolution : 2.67 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

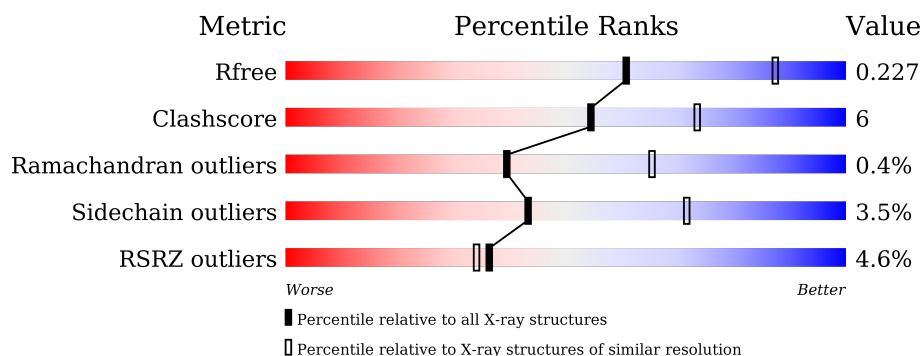
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	261	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	261	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	261	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6040 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1909	1204	313	376	16			
1	B	253	Total	C	N	O	S	0	0	0
			1953	1228	318	391	16			
1	C	252	Total	C	N	O	S	0	0	0
			1942	1222	317	387	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ILE	SER	engineered mutation	UNP P12004
B	228	ILE	SER	engineered mutation	UNP P12004
C	228	ILE	SER	engineered mutation	UNP P12004

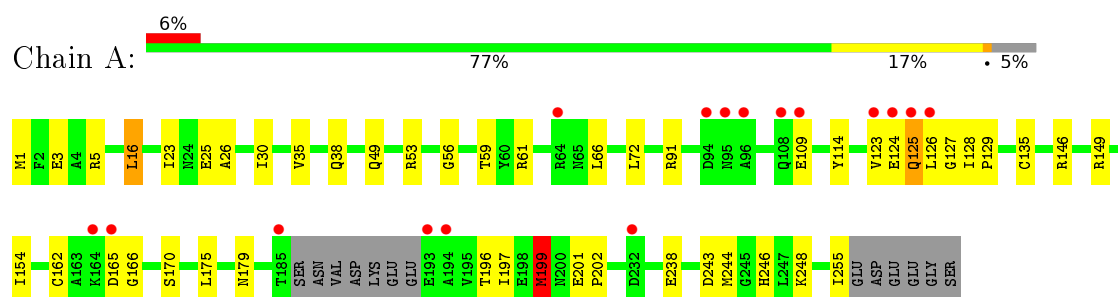
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	74	Total	O	0	0
			74	74		
2	C	92	Total	O	0	0
			92	92		

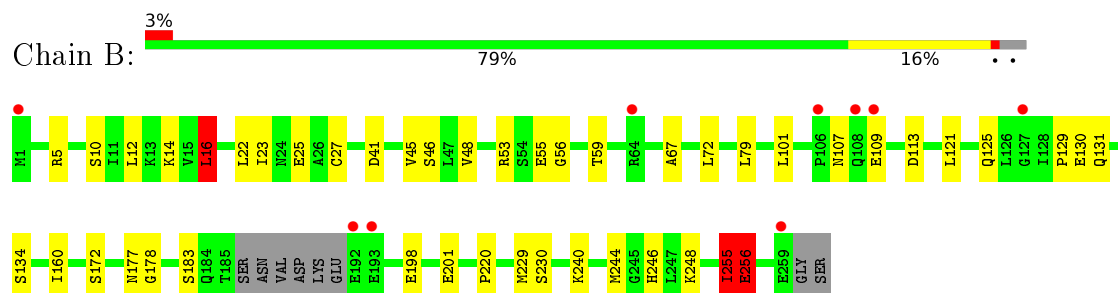
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

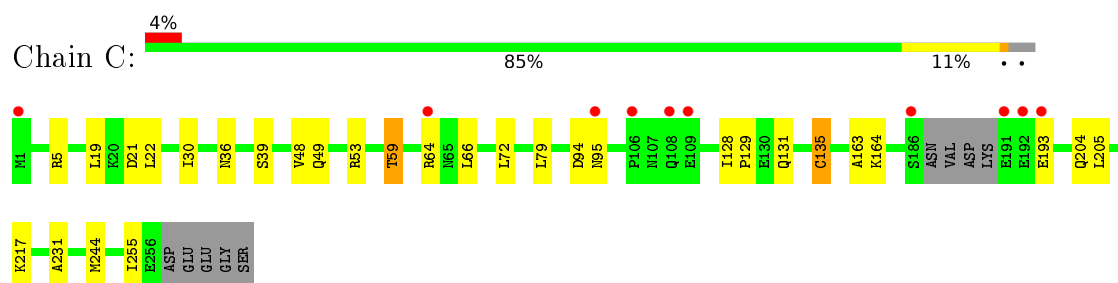
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.32Å 162.32Å 139.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.85 – 2.67 42.85 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.85-2.67) 99.8 (42.85-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.189 , 0.226 0.189 , 0.227	Depositor DCC
$R_{free}$ test set	2140 reflections (3.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 53660 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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

### 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	0.65	0/1934	0.75	2/2612 (0.1%)
1	B	0.68	0/1978	0.79	1/2671 (0.0%)
1	C	0.74	2/1967 (0.1%)	0.80	1/2656 (0.0%)
All	All	0.69	2/5879 (0.0%)	0.78	4/7939 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	135	CYS	CB-SG	-5.16	1.73	1.81
1	C	131	GLN	CG-CD	5.01	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LEU	CA-CB-CG	-8.86	94.93	115.30
1	B	16	LEU	CA-CB-CG	-8.33	96.15	115.30
1	C	53	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	199	MET	CA-CB-CG	-5.13	104.59	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	B	107	ASN	Peptide

## 5.2 Too-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 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	1909	0	1929	26	0
1	B	1953	0	1957	36	1
1	C	1942	0	1952	15	0
2	A	70	0	0	1	0
2	B	74	0	0	5	0
2	C	92	0	0	2	0
All	All	6040	0	5838	75	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 6.

All (75) 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:A:3:GLU:OE2	1:A:91:ARG:NH1	2.08	0.86
1:B:53:ARG:HD2	2:B:304:HOH:O	1.91	0.69
1:B:255:ILE:H	1:B:255:ILE:HD12	1.56	0.68
1:C:164:LYS:O	2:C:301:HOH:O	2.13	0.67
1:B:41:ASP:OD1	1:B:46:SER:HB3	1.97	0.65
1:A:49:GLN:HG3	1:A:128:ILE:HD11	1.79	0.65
1:C:36:ASN:HD21	1:C:49:GLN:HE21	1.46	0.62
1:B:45:VAL:HG22	2:B:301:HOH:O	2.00	0.61
1:C:64:ARG:NH2	1:C:94:ASP:O	2.33	0.61
1:B:130:GLU:H	1:B:130:GLU:CD	2.07	0.57
1:C:5:ARG:HB3	1:C:59:THR:HB	1.87	0.56
1:A:5:ARG:HB3	1:A:59:THR:HB	1.85	0.56
1:A:199:MET:HE3	1:A:202:PRO:N	2.21	0.56
1:A:125:GLN:NE2	1:A:126:LEU:H	2.03	0.55
1:A:238:GLU:OE2	1:A:248:LYS:HE2	2.07	0.55
1:B:256:GLU:N	1:B:256:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HG2	1:A:49:GLN:HG2	1.89	0.54
1:B:255:ILE:HG22	1:B:256:GLU:OE1	2.08	0.54
1:B:5:ARG:HB3	1:B:59:THR:HB	1.90	0.53
1:B:255:ILE:N	1:B:255:ILE:HD12	2.23	0.53
1:B:130:GLU:OE1	1:B:130:GLU:N	2.30	0.53
1:A:246:HIS:CD2	1:A:248:LYS:HG3	2.44	0.52
1:A:166:GLY:HA2	1:A:197:ILE:HD13	1.92	0.51
1:B:14:LYS:HD3	1:B:220:PRO:HB2	1.93	0.51
1:A:199:MET:HE3	1:A:201:GLU:C	2.31	0.51
1:B:240:LYS:NZ	2:B:302:HOH:O	2.45	0.50
1:B:25:GLU:HB3	1:B:121:LEU:HD11	1.93	0.50
1:B:27:CYS:SG	1:B:67:ALA:HB1	2.52	0.49
1:A:30:ILE:HB	1:A:66:LEU:HB2	1.95	0.49
1:A:53:ARG:NH2	1:A:243:ASP:O	2.45	0.49
1:B:10:SER:O	1:B:14:LYS:HG3	2.13	0.48
1:B:255:ILE:O	1:B:256:GLU:HB3	2.14	0.47
1:A:125:GLN:NE2	1:A:127:GLY:H	2.13	0.47
1:A:53:ARG:NH1	2:A:303:HOH:O	2.48	0.47
1:C:30:ILE:HB	1:C:66:LEU:HB2	1.96	0.47
1:B:172:SER:CB	1:B:177:ASN:HB3	2.46	0.46
1:A:109:GLU:OE1	1:B:183:SER:HB2	2.16	0.45
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.46	0.45
1:B:240:LYS:NZ	2:B:303:HOH:O	2.27	0.45
1:B:56:GLY:HA3	1:B:244:MET:HE3	1.98	0.45
1:B:240:LYS:HD2	1:B:240:LYS:HA	1.71	0.45
1:C:163:ALA:HB1	2:C:347:HOH:O	2.17	0.45
1:B:53:ARG:NH2	2:B:302:HOH:O	2.24	0.44
1:A:114:TYR:CD1	1:B:178:GLY:HA3	2.53	0.44
1:C:193:GLU:H	1:C:193:GLU:HG2	1.51	0.43
1:B:16:LEU:HD13	1:B:79:LEU:CD1	2.49	0.43
1:B:23:ILE:HG13	1:B:72:LEU:CD1	2.49	0.43
1:C:205:LEU:HD21	1:C:231:ALA:HA	2.02	0.42
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.78	0.42
1:C:19:LEU:HD21	1:C:48:VAL:HG11	2.02	0.42
1:B:130:GLU:N	1:B:130:GLU:CD	2.71	0.42
1:B:23:ILE:HG22	1:B:41:ASP:HA	2.02	0.42
1:A:146:ARG:HE	1:A:149:ARG:HH22	1.66	0.42
1:B:109:GLU:H	1:B:109:GLU:CD	2.24	0.42
1:A:135:CYS:SG	1:A:162:CYS:HB3	2.60	0.41
1:B:101:LEU:HD12	1:B:101:LEU:N	2.35	0.41
1:B:22:LEU:HD23	1:B:48:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:HB2	1:B:230:SER:HA	2.03	0.41
1:C:64:ARG:NE	1:C:94:ASP:HB3	2.36	0.41
1:A:1:MET:HE1	1:A:61:ARG:NH1	2.35	0.41
1:B:229:MET:HB2	1:B:229:MET:HE2	1.72	0.41
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.92	0.41
1:A:30:ILE:HD12	1:A:35:VAL:HG22	2.03	0.41
1:B:160:ILE:HG21	1:B:229:MET:HE1	2.03	0.41
1:A:56:GLY:HA3	1:A:244:MET:HG2	2.02	0.41
1:A:23:ILE:HG21	1:A:26:ALA:HB2	2.02	0.41
1:B:129:PRO:HA	1:B:130:GLU:OE1	2.21	0.41
1:C:255:ILE:HG21	1:C:255:ILE:HD13	1.85	0.41
1:A:154:ILE:HD13	1:A:175:LEU:HD11	2.02	0.40
1:C:21:ASP:OD2	1:C:217:LYS:NZ	2.47	0.40
1:A:128:ILE:HA	1:A:129:PRO:HD3	1.88	0.40
1:A:23:ILE:HB	1:A:72:LEU:HD12	2.03	0.40
1:B:246:HIS:CD2	1:B:248:LYS:HG3	2.56	0.40
1:A:170:SER:OG	1:A:179:ASN:HB3	2.21	0.40
1:C:22:LEU:HA	1:C:22:LEU:HD12	1.90	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:B:198:GLU:OE2	1:B:198:GLU:OE2[8_555]	1.89	0.31

## 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	244/261 (94%)	241 (99%)	2 (1%)	1 (0%)	39	65
1	B	249/261 (95%)	245 (98%)	2 (1%)	2 (1%)	24	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	248/261 (95%)	245 (99%)	3 (1%)	0	100	100
All	All	741/783 (95%)	731 (99%)	7 (1%)	3 (0%)	39	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	GLU
1	B	255	ILE
1	A	165	ASP

### 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	216/228 (95%)	209 (97%)	7 (3%)	46	74
1	B	221/228 (97%)	213 (96%)	8 (4%)	42	70
1	C	220/228 (96%)	212 (96%)	8 (4%)	42	70
All	All	657/684 (96%)	634 (96%)	23 (4%)	43	71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	25	GLU
1	A	123	VAL
1	A	125	GLN
1	A	196	THR
1	A	199	MET
1	A	255	ILE
1	B	16	LEU
1	B	55	GLU
1	B	113	ASP
1	B	125	GLN
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	201	GLU
1	B	255	ILE
1	B	256	GLU
1	C	39	SER
1	C	59	THR
1	C	72	LEU
1	C	79	LEU
1	C	95	ASN
1	C	135	CYS
1	C	204	GLN
1	C	244	MET

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

Mol	Chain	Res	Type
1	A	125	GLN
1	C	36	ASN
1	C	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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	248/261 (95%)	-0.02	16 (6%) 22 20	32, 49, 82, 104	0
1	B	253/261 (96%)	-0.01	9 (3%) 46 45	33, 49, 86, 117	0
1	C	252/261 (96%)	-0.07	10 (3%) 42 40	25, 42, 80, 104	0
All	All	753/783 (96%)	-0.03	35 (4%) 36 34	25, 47, 83, 117	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	ASN	4.5
1	A	232	ASP	4.4
1	A	108	GLN	4.0
1	C	64	ARG	4.0
1	B	192	GLU	4.0
1	B	1	MET	4.0
1	B	193	GLU	3.8
1	C	192	GLU	3.8
1	A	126	LEU	3.7
1	B	127	GLY	3.7
1	C	191	GLU	3.2
1	A	124	GLU	3.1
1	A	193	GLU	3.1
1	A	109	GLU	3.1
1	A	95	ASN	3.0
1	B	109	GLU	2.9
1	C	1	MET	2.9
1	A	125	GLN	2.8
1	C	108	GLN	2.8
1	C	186	SER	2.8
1	B	259	GLU	2.7
1	A	194	ALA	2.7
1	C	106	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	64	ARG	2.6
1	A	185	THR	2.5
1	B	106	PRO	2.4
1	A	165	ASP	2.4
1	A	96	ALA	2.4
1	A	164	LYS	2.4
1	B	64	ARG	2.3
1	B	108	GLN	2.2
1	C	193	GLU	2.2
1	A	123	VAL	2.2
1	A	94	ASP	2.2
1	C	109	GLU	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.