



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 04:23 PM EST

PDB ID : 5MOM  
Title : Crystal Structure of PCNA encoding the hypomorphic mutation S228I  
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Deposited on : 2016-12-14  
Resolution : 2.27 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-20028442
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-20028442

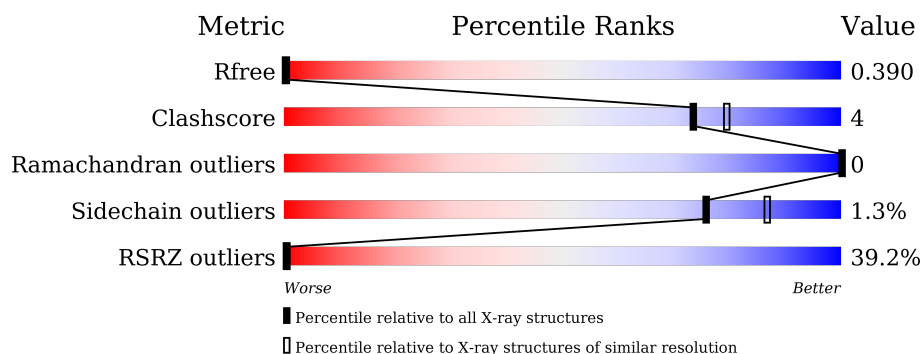
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	258	<div> <div>48%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	B	258	<div> <div>29%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	C	258	<div> <div>37%</div> <div>85%</div> <div>10%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5731 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	251	Total	C	N	O	S	0	0	0
			1869	1189	303	361	16			
1	B	249	Total	C	N	O	S	0	0	0
			1879	1193	305	365	16			
1	C	248	Total	C	N	O	S	0	0	0
			1831	1168	292	355	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

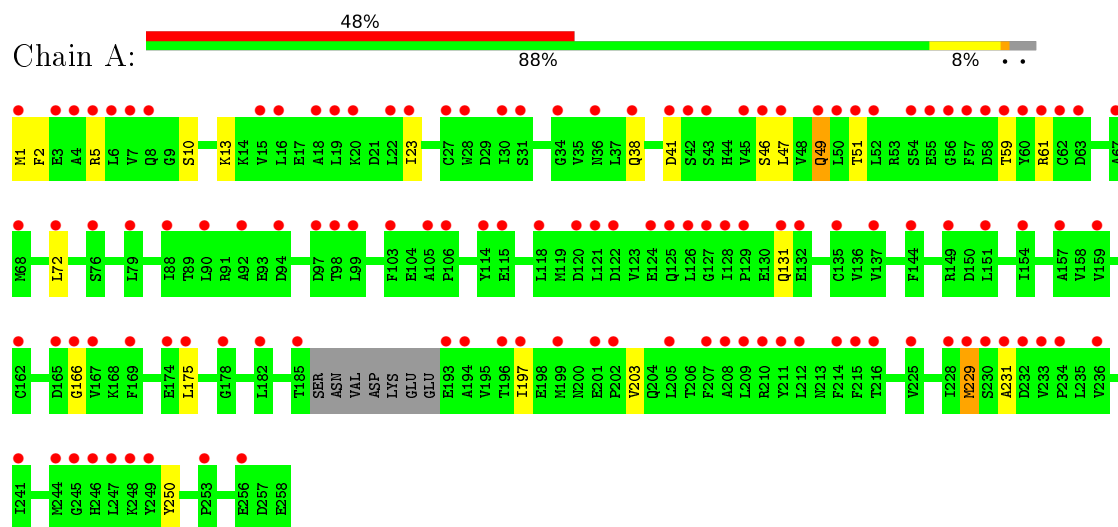
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	75	Total	O	0	0
			75	75		
2	C	41	Total	O	0	0
			41	41		

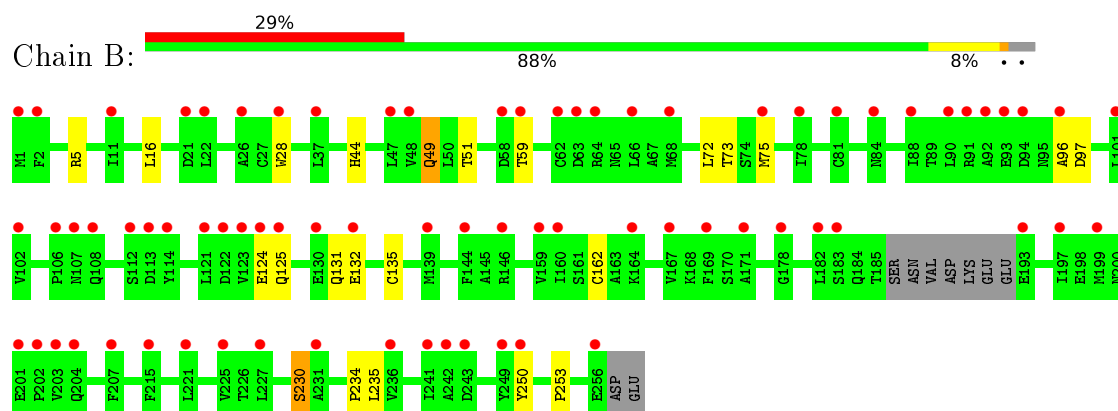
### 3 Residue-property plots [i](#)

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.

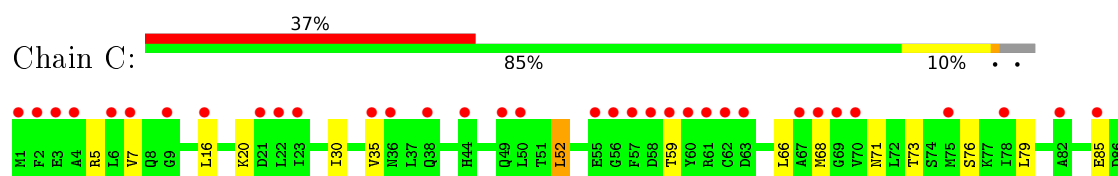
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.95Å 162.95Å 140.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.07 – 2.27 89.07 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.07-2.27) 100.0 (89.07-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.199 , 0.216 0.387 , 0.390	Depositor DCC
$R_{free}$ test set	4473 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	5731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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	0.37	0/1894	0.66	1/2564 (0.0%)
1	B	0.48	0/1904	0.70	0/2575
1	C	0.38	0/1856	0.66	3/2517 (0.1%)
All	All	0.42	0/5654	0.67	4/7656 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	175	LEU	CA-CB-CG	8.97	135.93	115.30
1	C	121	LEU	CA-CB-CG	6.05	129.21	115.30
1	C	52	LEU	CA-CB-CG	5.76	128.55	115.30
1	C	175	LEU	CA-CB-CG	5.45	127.83	115.30

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	1869	0	1851	14	0
1	B	1879	0	1884	17	0
1	C	1831	0	1798	15	0
2	A	36	0	0	3	1
2	B	75	0	0	2	0
2	C	41	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5731	0	5533	46	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 4.

All (46) 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:C:230:SER:OG	2:C:301:HOH:O	1.80	0.91
1:A:131:GLN:OE1	2:A:301:HOH:O	1.99	0.80
1:B:16:LEU:HD21	1:B:75:MET:CE	2.19	0.72
1:B:16:LEU:HD21	1:B:75:MET:HE3	1.71	0.71
1:A:203:VAL:HG11	1:A:229:MET:HG2	1.72	0.71
1:B:73:THR:OG1	2:B:301:HOH:O	2.13	0.66
1:B:5:ARG:HB3	1:B:59:THR:HB	1.78	0.64
1:A:49:GLN:OE1	1:A:51:THR:HG23	2.00	0.62
1:C:66:LEU:HD13	1:C:68:MET:HG3	1.82	0.62
1:B:49:GLN:OE1	1:B:51:THR:HG23	2.06	0.56
1:C:96:ALA:HB1	1:C:118:LEU:HD23	1.88	0.56
1:A:41:ASP:OD1	1:A:46:SER:N	2.18	0.55
1:C:5:ARG:HB3	1:C:59:THR:HB	1.89	0.55
1:A:131:GLN:HE22	1:A:250:TYR:HE2	1.57	0.53
1:B:44:HIS:HE1	1:B:124:GLU:OE2	1.93	0.52
1:A:5:ARG:HB3	1:A:59:THR:HB	1.93	0.51
1:C:119:MET:HE2	1:C:121:LEU:HD11	1.93	0.51
1:A:1:MET:SD	1:A:2:PHE:N	2.83	0.51
1:B:132:GLU:HG3	1:B:230:SER:CB	2.41	0.50
1:C:71:ASN:HB2	1:C:119:MET:SD	2.52	0.49
1:B:124:GLU:O	1:B:125:GLN:HB2	2.11	0.49
1:A:166:GLY:HA2	1:A:197:ILE:HD13	1.94	0.49
1:B:16:LEU:CD2	1:B:75:MET:HE3	2.43	0.49
1:B:135:CYS:SG	1:B:162:CYS:SG	3.08	0.48
1:B:131:GLN:NE2	2:B:306:HOH:O	2.47	0.48
1:B:234:PRO:HA	1:B:253:PRO:HD3	1.96	0.48
1:B:132:GLU:HG3	1:B:230:SER:HB3	1.97	0.47
1:A:38:GLN:HG2	1:A:47:LEU:HD11	1.96	0.47
1:B:28:TRP:HE1	1:B:72:LEU:HD21	1.80	0.47
1:C:184:GLN:HG3	1:C:195:VAL:O	2.16	0.46
1:C:254:LYS:O	1:C:255:ILE:HG13	2.15	0.46
1:C:30:ILE:HD12	1:C:35:VAL:HG22	1.97	0.46
1:A:1:MET:HE1	1:A:61:ARG:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLN:OE1	2:C:302:HOH:O	2.21	0.45
1:A:231:ALA:CB	2:A:305:HOH:O	2.64	0.45
1:C:85:GLU:N	1:C:85:GLU:OE1	2.50	0.44
1:C:7:VAL:HA	1:C:87:ILE:HD13	1.98	0.44
1:A:10:SER:HA	1:A:13:LYS:HD3	2.00	0.43
1:A:231:ALA:HB3	2:A:305:HOH:O	2.19	0.42
1:B:235:LEU:O	1:B:250:TYR:HA	2.20	0.42
1:A:23:ILE:HG13	1:A:72:LEU:HD12	2.01	0.42
1:C:16:LEU:HG	1:C:79:LEU:HD12	2.02	0.42
1:B:96:ALA:O	1:B:97:ASP:HB2	2.20	0.41
1:C:20:LYS:HD3	1:C:76:SER:OG	2.20	0.41
1:B:28:TRP:CZ2	1:B:75:MET:CE	3.03	0.41
1:C:169:PHE:O	1:C:179:ASN:HA	2.21	0.41

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)
2:A:328:HOH:O	2:C:329:HOH:O[8_554]	2.17	0.03

## 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	247/258 (96%)	238 (96%)	9 (4%)	0	100	100
1	B	245/258 (95%)	239 (98%)	6 (2%)	0	100	100
1	C	244/258 (95%)	240 (98%)	4 (2%)	0	100	100
All	All	736/774 (95%)	717 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	199/226 (88%)	197 (99%)	2 (1%)	82	91
1	B	206/226 (91%)	204 (99%)	2 (1%)	82	91
1	C	193/226 (85%)	189 (98%)	4 (2%)	61	76
All	All	598/678 (88%)	590 (99%)	8 (1%)	76	87

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	229	MET
1	B	49	GLN
1	B	230	SER
1	C	52	LEU
1	C	73	THR
1	C	118	LEU
1	C	121	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	44	HIS
1	B	200	ASN
1	C	184	GLN
1	C	200	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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, 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	251/258 (97%)	2.39	123 (49%) 0 0	45, 64, 97, 114	0
1	B	249/258 (96%)	1.73	75 (30%) 1 1	35, 53, 90, 106	0
1	C	248/258 (96%)	2.09	95 (38%) 0 0	43, 61, 102, 118	0
All	All	748/774 (96%)	2.07	293 (39%) 0 0	35, 60, 97, 118	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	9.2
1	C	1	MET	9.1
1	B	1	MET	8.8
1	A	175	LEU	8.5
1	A	165	ASP	8.3
1	C	4	ALA	7.9
1	C	59	THR	7.6
1	A	232	ASP	7.5
1	A	129	PRO	7.5
1	C	117	LYS	7.4
1	A	62	CYS	7.4
1	A	54	SER	7.2
1	A	233	VAL	7.0
1	B	123	VAL	7.0
1	C	6	LEU	6.9
1	B	93	GLU	6.9
1	A	127	GLY	6.8
1	A	185	THR	6.6
1	A	57	PHE	6.6
1	C	97	ASP	6.4
1	C	90	LEU	6.4
1	C	105	ALA	6.3
1	C	88	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	193	GLU	6.2
1	C	22	LEU	6.1
1	C	91	ARG	5.9
1	C	167	VAL	5.9
1	C	89	THR	5.9
1	A	4	ALA	5.8
1	A	105	ALA	5.8
1	C	106	PRO	5.7
1	A	60	TYR	5.6
1	C	92	ALA	5.6
1	A	42	SER	5.6
1	C	211	TYR	5.6
1	A	121	LEU	5.5
1	A	43	SER	5.4
1	A	174	GLU	5.4
1	A	256	GLU	5.3
1	C	100	ALA	5.2
1	C	118	LEU	5.2
1	A	169	PHE	5.1
1	B	107	ASN	5.0
1	A	23	ILE	5.0
1	B	125	GLN	5.0
1	C	67	ALA	5.0
1	B	183	SER	4.9
1	A	1	MET	4.8
1	C	3	GLU	4.6
1	A	90	LEU	4.5
1	A	63	ASP	4.5
1	A	229	MET	4.4
1	C	99	LEU	4.4
1	C	122	ASP	4.2
1	B	113	ASP	4.2
1	B	231	ALA	4.1
1	A	6	LEU	4.1
1	A	126	LEU	4.1
1	C	75	MET	4.1
1	C	164	LYS	4.1
1	A	7	VAL	4.1
1	C	162	CYS	4.1
1	A	162	CYS	4.0
1	A	166	GLY	4.0
1	C	96	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	3.9
1	C	108	GLN	3.9
1	A	178	GLY	3.8
1	C	196	THR	3.8
1	A	228	ILE	3.8
1	C	87	ILE	3.8
1	A	128	ILE	3.7
1	A	209	LEU	3.7
1	A	59	THR	3.7
1	A	31	SER	3.7
1	A	114	TYR	3.6
1	A	135	CYS	3.6
1	A	122	ASP	3.6
1	A	167	VAL	3.6
1	C	93	GLU	3.6
1	C	7	VAL	3.6
1	C	55	GLU	3.6
1	B	202	PRO	3.6
1	B	106	PRO	3.5
1	A	137	VAL	3.5
1	A	56	GLY	3.5
1	B	101	LEU	3.5
1	B	62	CYS	3.5
1	A	27	CYS	3.4
1	C	63	ASP	3.4
1	B	28	TRP	3.4
1	C	23	ILE	3.4
1	B	96	ALA	3.4
1	C	38	GLN	3.4
1	A	97	ASP	3.4
1	C	61	ARG	3.4
1	B	81	CYS	3.4
1	A	230	SER	3.4
1	A	28	TRP	3.4
1	B	199	MET	3.4
1	B	90	LEU	3.4
1	C	57	PHE	3.4
1	A	212	LEU	3.4
1	B	144	PHE	3.4
1	C	234	PRO	3.3
1	A	154	ILE	3.3
1	B	102	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	164	LYS	3.3
1	B	84	ASN	3.3
1	A	182	LEU	3.3
1	B	2	PHE	3.3
1	A	38	GLN	3.3
1	C	129	PRO	3.3
1	C	121	LEU	3.3
1	A	236	VAL	3.3
1	C	62	CYS	3.2
1	A	124	GLU	3.2
1	A	103	PHE	3.2
1	C	111	VAL	3.2
1	C	60	TYR	3.2
1	C	44	HIS	3.2
1	C	69	GLY	3.2
1	A	45	VAL	3.1
1	B	122	ASP	3.1
1	A	8	GLN	3.1
1	B	256	GLU	3.1
1	C	68	MET	3.1
1	B	182	LEU	3.1
1	B	92	ALA	3.1
1	C	9	GLY	3.1
1	A	50	LEU	3.1
1	C	116	MET	3.1
1	C	58	ASP	3.0
1	A	34	GLY	3.0
1	B	88	ILE	3.0
1	C	171	ALA	3.0
1	C	179	ASN	3.0
1	B	215	PHE	3.0
1	A	99	LEU	3.0
1	A	41	ASP	3.0
1	A	247	LEU	2.9
1	B	91	ARG	2.9
1	C	107	ASN	2.9
1	C	78	ILE	2.9
1	A	76	SER	2.9
1	B	242	ALA	2.9
1	B	160	ILE	2.9
1	A	5	ARG	2.9
1	B	112	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	194	ALA	2.8
1	B	146	ARG	2.8
1	C	94	ASP	2.8
1	B	114	TYR	2.8
1	A	19	LEU	2.8
1	A	196	THR	2.8
1	C	112	SER	2.8
1	C	184	GLN	2.8
1	B	241	ILE	2.8
1	A	144	PHE	2.7
1	B	94	ASP	2.7
1	A	22	LEU	2.7
1	C	35	VAL	2.7
1	A	18	ALA	2.7
1	C	115	GLU	2.7
1	B	108	GLN	2.7
1	B	193	GLU	2.7
1	B	249	TYR	2.7
1	C	102	VAL	2.7
1	A	20	LYS	2.6
1	A	98	THR	2.6
1	B	68	MET	2.6
1	B	178	GLY	2.6
1	A	197	ILE	2.6
1	C	98	THR	2.6
1	A	94	ASP	2.6
1	B	26	ALA	2.6
1	C	126	LEU	2.6
1	A	234	PRO	2.6
1	B	167	VAL	2.6
1	C	2	PHE	2.6
1	A	211	TYR	2.6
1	A	205	LEU	2.6
1	B	159	VAL	2.6
1	A	15	VAL	2.5
1	A	30	ILE	2.5
1	A	72	LEU	2.5
1	B	124	GLU	2.5
1	C	70	VAL	2.5
1	A	61	ARG	2.5
1	C	208	ALA	2.5
1	C	128	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	2.5
1	A	125	GLN	2.5
1	A	207	PHE	2.5
1	A	92	ALA	2.5
1	B	22	LEU	2.5
1	B	75	MET	2.5
1	C	169	PHE	2.5
1	A	3	GLU	2.5
1	B	204	GLN	2.5
1	A	52	LEU	2.5
1	C	50	LEU	2.5
1	A	132	GLU	2.4
1	C	183	SER	2.4
1	A	67	ALA	2.4
1	A	106	PRO	2.4
1	C	220	PRO	2.4
1	A	120	ASP	2.4
1	B	21	ASP	2.4
1	A	202	PRO	2.4
1	A	214	PHE	2.4
1	A	225	VAL	2.4
1	C	123	VAL	2.4
1	C	233	VAL	2.4
1	A	49	GLN	2.4
1	B	227	LEU	2.4
1	B	132	GLU	2.4
1	B	139	MET	2.4
1	B	171	ALA	2.4
1	C	197	ILE	2.4
1	A	16	LEU	2.4
1	A	151	LEU	2.4
1	A	231	ALA	2.4
1	C	194	ALA	2.4
1	B	225	VAL	2.4
1	A	248	LYS	2.4
1	A	131	GLN	2.4
1	A	159	VAL	2.4
1	C	163	ALA	2.3
1	A	244	MET	2.3
1	A	215	PHE	2.3
1	C	156	ASP	2.3
1	B	47	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	221	LEU	2.3
1	A	199	MET	2.3
1	B	11	ILE	2.3
1	B	197	ILE	2.3
1	A	149	ARG	2.3
1	B	63	ASP	2.3
1	A	201	GLU	2.3
1	B	64	ARG	2.3
1	A	241	ILE	2.3
1	C	244	MET	2.3
1	C	82	ALA	2.3
1	C	223	SER	2.3
1	B	130	GLU	2.3
1	B	201	GLU	2.3
1	C	85	GLU	2.3
1	A	118	LEU	2.2
1	A	246	HIS	2.2
1	A	58	ASP	2.2
1	B	243	ASP	2.2
1	A	115	GLU	2.2
1	B	250	TYR	2.2
1	C	250	TYR	2.2
1	A	36	ASN	2.2
1	C	153	HIS	2.2
1	C	139	MET	2.2
1	A	249	TYR	2.2
1	B	203	VAL	2.2
1	A	51	THR	2.2
1	A	208	ALA	2.2
1	B	59	THR	2.2
1	C	228	ILE	2.2
1	A	47	LEU	2.2
1	A	245	GLY	2.2
1	B	236	VAL	2.2
1	C	147	ILE	2.2
1	B	37	LEU	2.2
1	C	16	LEU	2.2
1	B	58	ASP	2.2
1	B	48	VAL	2.1
1	A	216	THR	2.1
1	C	144	PHE	2.1
1	B	78	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	MET	2.1
1	A	55	GLU	2.1
1	C	113	ASP	2.1
1	A	210	ARG	2.1
1	A	253	PRO	2.1
1	B	169	PHE	2.1
1	B	207	PHE	2.1
1	C	103	PHE	2.1
1	C	49	GLN	2.0
1	C	181	LYS	2.0
1	A	157	ALA	2.0
1	C	21	ASP	2.0
1	C	214	PHE	2.0
1	A	88	ILE	2.0
1	B	66	LEU	2.0
1	B	121	LEU	2.0
1	C	36	ASN	2.0
1	A	46	SER	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.