



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:21 PM UTC

PDB ID : 5MOM / pdb_00005mom
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

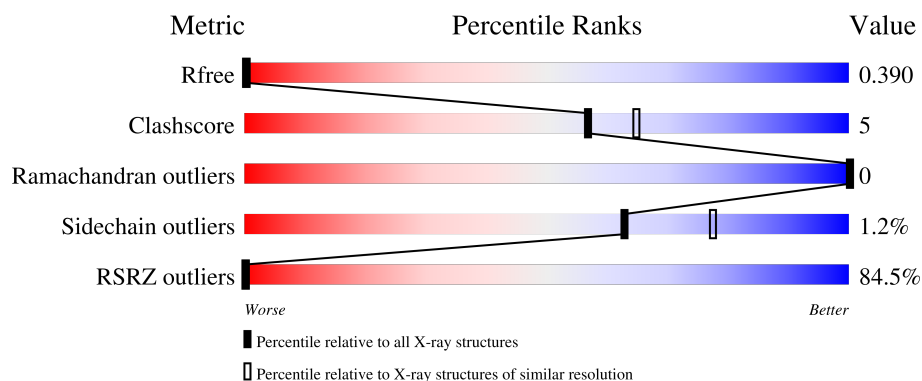
1 Overall quality at a glance

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	258	90% 88% 9% .
1	B	258	71% 87% 9% .
1	C	258	84% 84% 12% .

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

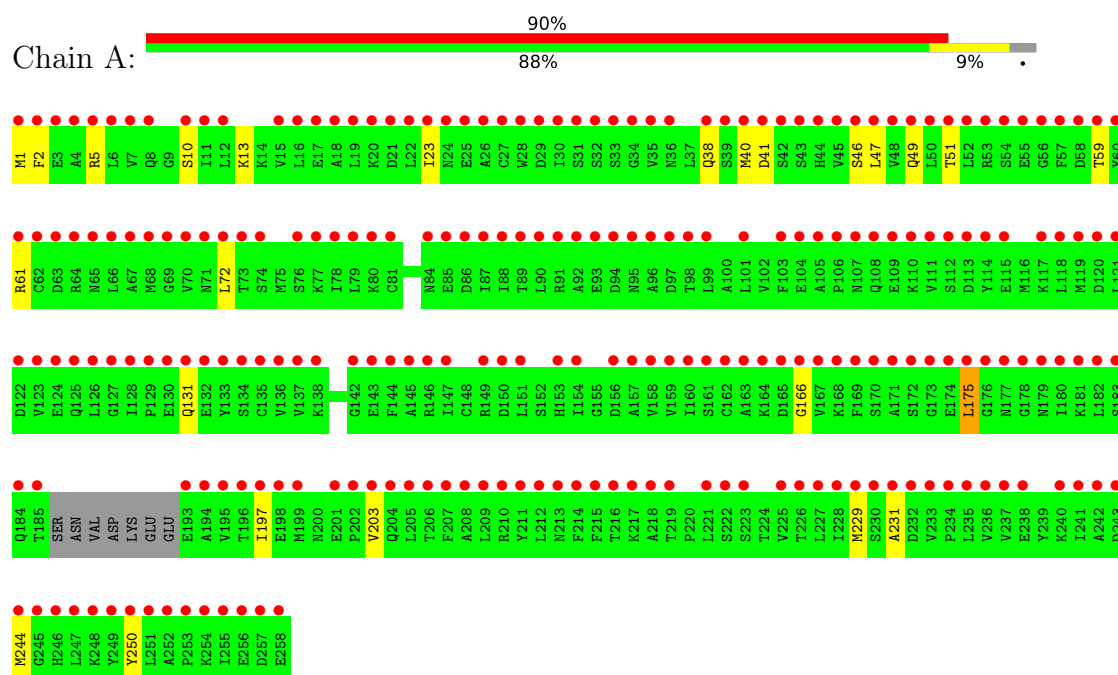
- Molecule 2 is water.

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		

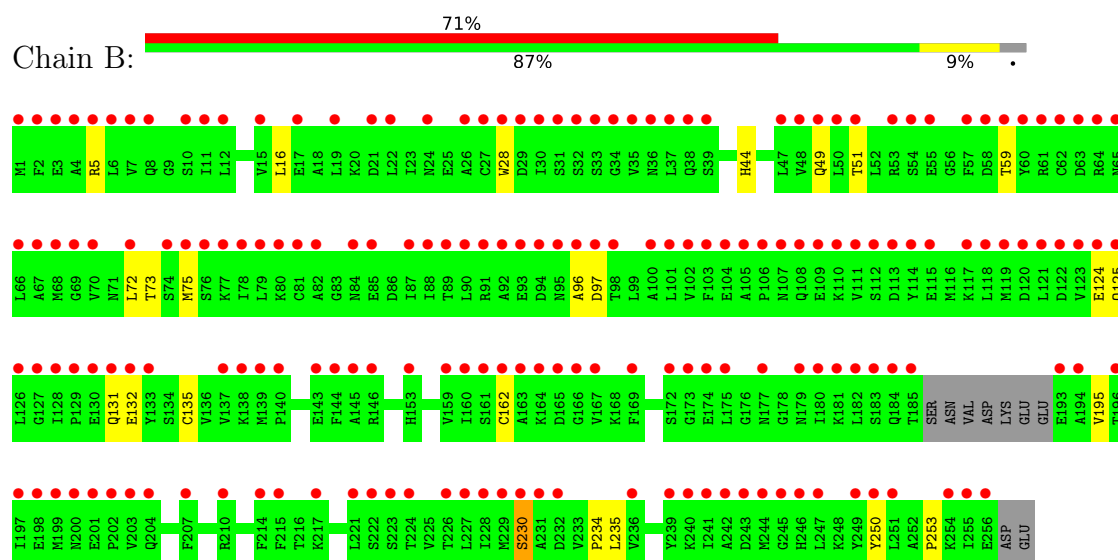
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

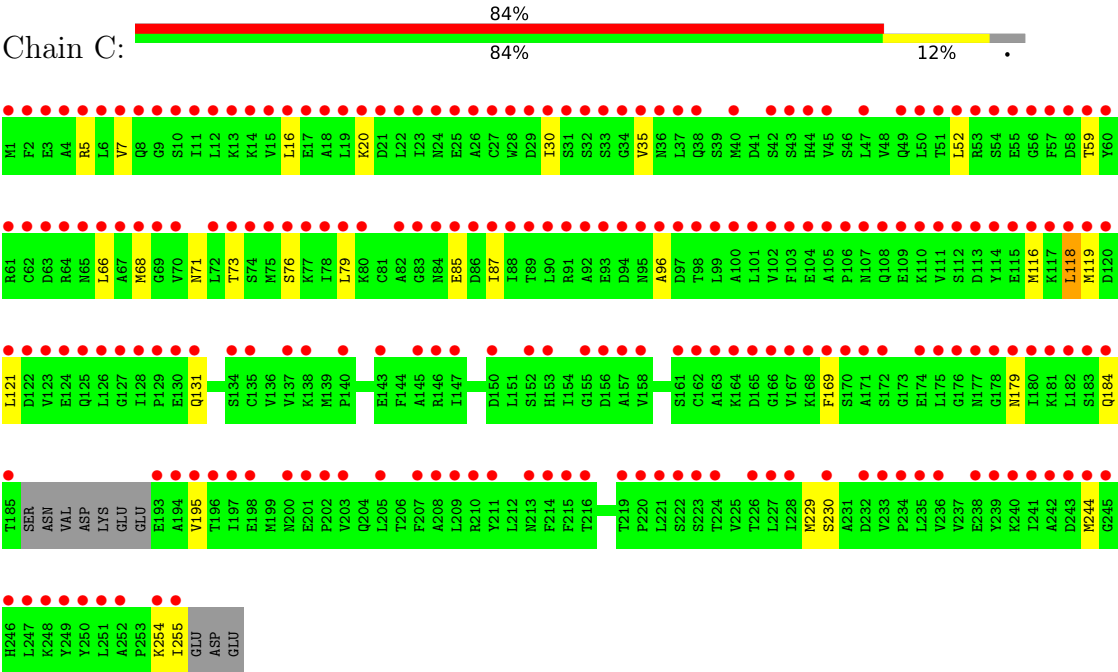
- Molecule 1: Proliferating cell nuclear antigen



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.216 0.389 , 0.390	Depositor DCC
R_{free} test set	4471 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.31	0/1894	0.61	1/2564 (0.0%)
1	B	0.43	0/1904	0.70	0/2575
1	C	0.32	0/1856	0.62	0/2517
All	All	0.36	0/5654	0.64	1/7656 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	175	LEU	CA-CB-CG	5.61	135.93	116.30

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	17	0
1	B	1879	0	1884	17	0
1	C	1831	0	1798	17	0
2	A	36	0	0	3	1
2	B	75	0	0	2	0
2	C	41	0	0	2	1
All	All	5731	0	5533	51	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 5.

All (51) 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	1.00
1:A:131:GLN:OE1	2:A:301:HOH:O	1.99	0.80
1:B:28:TRP:CZ2	1:B:75:MET:HE1	2.19	0.78
1:B:16:LEU:HD21	1:B:75:MET:CE	2.19	0.72
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:16:LEU:HD11	1:B:75:MET:HE2	1.79	0.64
1:B:5:ARG:HB3	1:B:59:THR:HB	1.78	0.64
1:B:16:LEU:HD21	1:B:75:MET:HE3	1.81	0.63
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:A:1:MET:HE1	1:A:61:ARG:HG2	1.92	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: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:30:ILE:HD12	1:C:35:VAL:HG22	1.97	0.46
1:C:254:LYS:O	1:C:255:ILE:HG13	2.15	0.46
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:A:244:MET:HE3	1:A:244:MET:HB2	1.71	0.44
1:C:85:GLU:OE1	1:C:85:GLU:N	2.50	0.44
1:C:229:MET:HE2	1:C:229:MET:HB3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:229:MET:HE2	1:A:229:MET:HB2	1.73	0.42
1:C:244:MET:HE3	1:C:244:MET:HB2	1.65	0.42
1:A:40:MET:HE3	1:A:40:MET:HB3	1.98	0.41
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:C:116:MET:HE2	1:C:116:MET:HB3	1.90	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%)	198 (100%)	1 (0%)	81	89
1	B	206/226 (91%)	204 (99%)	2 (1%)	68	81
1	C	193/226 (85%)	189 (98%)	4 (2%)	47	63
All	All	598/678 (88%)	591 (99%)	7 (1%)	63	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	B	195	VAL
1	B	230	SER
1	C	52	LEU
1	C	73	THR
1	C	118	LEU
1	C	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	179	ASN
1	B	38	GLN
1	B	44	HIS
1	B	49	GLN
1	B	84	ASN
1	B	179	ASN
1	C	177	ASN
1	C	179	ASN
1	C	184	GLN
1	C	246	HIS

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	251/258 (97%)	4.35	231 (92%) 0 0	45, 64, 97, 114	0
1	B	249/258 (96%)	3.06	184 (73%) 0 0	35, 53, 90, 106	0
1	C	248/258 (96%)	4.13	217 (87%) 0 0	43, 61, 102, 118	0
All	All	748/774 (96%)	3.85	632 (84%) 0 0	35, 60, 97, 118	0

All (632) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ASP	13.3
1	C	4	ALA	11.5
1	C	117	LYS	11.0
1	A	193	GLU	10.5
1	C	255	ILE	10.4
1	A	127	GLY	10.3
1	A	129	PRO	10.0
1	C	59	THR	9.7
1	C	193	GLU	9.7
1	A	174	GLU	9.6
1	A	185	THR	9.6
1	A	233	VAL	9.6
1	C	3	GLU	9.3
1	C	108	GLN	9.2
1	C	6	LEU	9.2
1	A	165	ASP	9.1
1	B	125	GLN	8.9
1	C	106	PRO	8.9
1	C	123	VAL	8.8
1	C	122	ASP	8.8
1	C	1	MET	8.7
1	B	123	VAL	8.7
1	A	63	ASP	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	2	PHE	8.4
1	C	165	ASP	8.3
1	B	1	MET	8.3
1	A	175	LEU	8.1
1	A	256	GLU	8.1
1	C	121	LEU	8.0
1	A	54	SER	8.0
1	A	1	MET	8.0
1	C	100	ALA	8.0
1	C	91	ARG	8.0
1	A	6	LEU	7.9
1	A	257	ASP	7.9
1	C	58	ASP	7.9
1	C	92	ALA	7.9
1	C	107	ASN	7.9
1	C	105	ALA	7.8
1	A	60	TYR	7.8
1	A	62	CYS	7.8
1	B	95	ASN	7.7
1	A	121	LEU	7.7
1	C	97	ASP	7.6
1	A	169	PHE	7.6
1	B	93	GLU	7.5
1	C	243	ASP	7.4
1	B	96	ALA	7.4
1	C	129	PRO	7.2
1	A	107	ASN	7.2
1	C	9	GLY	7.1
1	C	95	ASN	7.1
1	A	4	ALA	7.1
1	C	69	GLY	7.0
1	C	67	ALA	7.0
1	C	90	LEU	7.0
1	C	96	ALA	6.9
1	C	118	LEU	6.9
1	C	85	GLU	6.9
1	A	106	PRO	6.9
1	C	124	GLU	6.9
1	C	125	GLN	6.8
1	A	258	GLU	6.8
1	B	256	GLU	6.8
1	C	99	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	88	ILE	6.8
1	A	105	ALA	6.7
1	A	154	ILE	6.7
1	A	122	ASP	6.6
1	C	35	VAL	6.6
1	C	94	ASP	6.6
1	C	113	ASP	6.6
1	B	130	GLU	6.6
1	A	57	PHE	6.6
1	A	128	ILE	6.6
1	A	44	HIS	6.5
1	A	126	LEU	6.5
1	C	22	LEU	6.5
1	B	243	ASP	6.5
1	A	255	ILE	6.5
1	B	94	ASP	6.5
1	A	56	GLY	6.4
1	C	7	VAL	6.4
1	A	96	ALA	6.4
1	B	108	GLN	6.4
1	C	89	THR	6.4
1	A	43	SER	6.3
1	B	183	SER	6.3
1	A	8	GLN	6.3
1	A	20	LYS	6.3
1	C	56	GLY	6.3
1	C	93	GLU	6.3
1	B	146	ARG	6.2
1	A	30	ILE	6.2
1	B	164	LYS	6.2
1	A	135	CYS	6.2
1	C	126	LEU	6.1
1	A	7	VAL	6.1
1	A	3	GLU	6.1
1	B	59	THR	6.1
1	B	107	ASN	6.1
1	C	127	GLY	6.1
1	A	58	ASP	6.0
1	C	87	ILE	6.0
1	C	8	GLN	6.0
1	C	119	MET	6.0
1	B	58	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	232	ASP	5.9
1	A	198	GLU	5.9
1	C	115	GLU	5.9
1	C	128	ILE	5.9
1	A	97	ASP	5.8
1	A	42	SER	5.8
1	A	66	LEU	5.8
1	A	132	GLU	5.8
1	C	70	VAL	5.8
1	B	193	GLU	5.8
1	A	90	LEU	5.7
1	A	64	ARG	5.7
1	A	45	VAL	5.7
1	A	95	ASN	5.7
1	A	162	CYS	5.7
1	C	185	THR	5.7
1	C	63	ASP	5.6
1	B	185	THR	5.6
1	C	114	TYR	5.6
1	A	254	LYS	5.6
1	A	38	GLN	5.5
1	A	229	MET	5.5
1	C	64	ARG	5.5
1	C	57	PHE	5.5
1	C	66	LEU	5.5
1	A	34	GLY	5.4
1	A	166	GLY	5.4
1	C	102	VAL	5.4
1	A	201	GLU	5.4
1	A	49	GLN	5.4
1	C	23	ILE	5.4
1	A	115	GLU	5.4
1	B	62	CYS	5.4
1	A	28	TRP	5.4
1	C	55	GLU	5.4
1	A	131	GLN	5.3
1	B	124	GLU	5.3
1	C	29	ASP	5.3
1	A	23	ILE	5.3
1	A	55	GLU	5.3
1	A	36	ASN	5.3
1	C	116	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	61	ARG	5.3
1	A	2	PHE	5.2
1	A	103	PHE	5.2
1	A	149	ARG	5.2
1	A	214	PHE	5.2
1	A	244	MET	5.2
1	B	84	ASN	5.2
1	C	21	ASP	5.2
1	A	93	GLU	5.2
1	B	64	ARG	5.2
1	C	130	GLU	5.2
1	B	122	ASP	5.2
1	A	53	ARG	5.2
1	C	44	HIS	5.2
1	A	212	LEU	5.2
1	C	16	LEU	5.2
1	A	182	LEU	5.1
1	C	80	LYS	5.1
1	C	164	LYS	5.1
1	C	25	GLU	5.1
1	A	183	SER	5.1
1	A	59	THR	5.1
1	B	242	ALA	5.1
1	A	130	GLU	5.1
1	B	28	TRP	5.1
1	C	38	GLN	5.1
1	A	137	VAL	5.1
1	B	63	ASP	5.0
1	A	230	SER	5.0
1	B	231	ALA	5.0
1	A	80	LYS	5.0
1	A	52	LEU	5.0
1	A	108	GLN	5.0
1	A	5	ARG	4.9
1	C	211	TYR	4.9
1	C	30	ILE	4.9
1	C	12	LEU	4.9
1	C	5	ARG	4.9
1	A	161	SER	4.9
1	C	110	LYS	4.9
1	A	113	ASP	4.9
1	A	164	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	4.8
1	A	202	PRO	4.8
1	A	210	ARG	4.8
1	C	52	LEU	4.8
1	A	194	ALA	4.8
1	A	27	CYS	4.8
1	B	109	GLU	4.8
1	C	109	GLU	4.8
1	C	101	LEU	4.8
1	C	246	HIS	4.8
1	A	124	GLU	4.8
1	C	68	MET	4.8
1	A	91	ARG	4.7
1	C	78	ILE	4.7
1	B	167	VAL	4.7
1	B	120	ASP	4.7
1	C	65	ASN	4.7
1	B	128	ILE	4.7
1	C	175	LEU	4.7
1	C	244	MET	4.7
1	C	61	ARG	4.7
1	A	41	ASP	4.7
1	A	22	LEU	4.7
1	C	220	PRO	4.7
1	A	211	TYR	4.7
1	A	231	ALA	4.7
1	B	91	ARG	4.6
1	A	247	LEU	4.6
1	C	86	ASP	4.6
1	A	35	VAL	4.6
1	C	98	THR	4.6
1	B	106	PRO	4.6
1	B	92	ALA	4.6
1	B	26	ALA	4.5
1	B	105	ALA	4.5
1	A	119	MET	4.5
1	A	32	SER	4.5
1	C	103	PHE	4.5
1	A	24	ASN	4.5
1	A	120	ASP	4.5
1	A	159	VAL	4.4
1	C	112	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	4.4
1	C	72	LEU	4.4
1	A	167	VAL	4.4
1	A	179	ASN	4.4
1	C	196	THR	4.4
1	B	115	GLU	4.4
1	B	8	GLN	4.4
1	A	94	ASP	4.4
1	B	36	ASN	4.4
1	C	171	ALA	4.4
1	A	205	LEU	4.4
1	B	80	LYS	4.4
1	C	111	VAL	4.4
1	A	177	ASN	4.4
1	C	242	ALA	4.3
1	B	81	CYS	4.3
1	A	101	LEU	4.3
1	A	181	LYS	4.3
1	B	97	ASP	4.3
1	A	206	THR	4.3
1	A	153	HIS	4.3
1	B	118	LEU	4.3
1	A	76	SER	4.3
1	C	208	ALA	4.3
1	A	118	LEU	4.3
1	C	27	CYS	4.3
1	C	233	VAL	4.2
1	A	40	MET	4.2
1	B	121	LEU	4.2
1	B	175	LEU	4.2
1	A	199	MET	4.2
1	A	196	THR	4.2
1	A	236	VAL	4.2
1	A	249	TYR	4.2
1	C	75	MET	4.2
1	C	28	TRP	4.2
1	B	61	ARG	4.2
1	A	109	GLU	4.2
1	B	21	ASP	4.2
1	B	144	PHE	4.2
1	B	3	GLU	4.2
1	A	243	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	CYS	4.1
1	B	85	GLU	4.1
1	B	66	LEU	4.1
1	C	60	TYR	4.1
1	C	250	TYR	4.1
1	A	98	THR	4.1
1	A	87	ILE	4.1
1	C	184	GLN	4.1
1	B	101	LEU	4.1
1	A	246	HIS	4.1
1	A	133	TYR	4.1
1	C	51	THR	4.1
1	B	160	ILE	4.1
1	B	70	VAL	4.1
1	A	242	ALA	4.0
1	A	252	ALA	4.0
1	A	72	LEU	4.0
1	A	178	GLY	4.0
1	B	117	LYS	4.0
1	B	102	VAL	4.0
1	A	253	PRO	4.0
1	C	49	GLN	4.0
1	C	84	ASN	4.0
1	C	162	CYS	4.0
1	A	163	ALA	4.0
1	C	120	ASP	4.0
1	A	19	LEU	4.0
1	C	135	CYS	4.0
1	A	197	ILE	4.0
1	A	176	GLY	3.9
1	B	240	LYS	3.9
1	A	88	ILE	3.9
1	C	53	ARG	3.9
1	C	167	VAL	3.9
1	A	184	GLN	3.9
1	C	163	ALA	3.9
1	C	214	PHE	3.9
1	B	249	TYR	3.9
1	A	209	LEU	3.9
1	A	18	ALA	3.9
1	A	228	ILE	3.9
1	A	114	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	98	THR	3.9
1	B	113	ASP	3.8
1	B	2	PHE	3.8
1	B	131	GLN	3.8
1	B	244	MET	3.8
1	C	240	LYS	3.8
1	B	246	HIS	3.8
1	C	82	ALA	3.8
1	C	104	GLU	3.8
1	B	197	ILE	3.8
1	A	111	VAL	3.8
1	B	110	LYS	3.8
1	A	160	ILE	3.8
1	C	34	GLY	3.8
1	C	153	HIS	3.8
1	A	51	THR	3.8
1	A	29	ASP	3.8
1	B	194	ALA	3.8
1	C	194	ALA	3.8
1	A	240	LYS	3.8
1	B	221	LEU	3.8
1	C	83	GLY	3.7
1	A	84	ASN	3.7
1	B	87	ILE	3.7
1	B	88	ILE	3.7
1	A	12	LEU	3.7
1	A	17	GLU	3.7
1	A	69	GLY	3.7
1	C	54	SER	3.7
1	A	248	LYS	3.7
1	C	182	LEU	3.6
1	A	21	ASP	3.6
1	B	232	ASP	3.6
1	A	157	ALA	3.6
1	B	165	ASP	3.6
1	C	179	ASN	3.6
1	A	123	VAL	3.6
1	C	74	SER	3.6
1	C	134	SER	3.6
1	A	151	LEU	3.6
1	B	126	LEU	3.6
1	A	70	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	31	SER	3.5
1	B	77	LYS	3.5
1	A	216	THR	3.5
1	B	127	GLY	3.5
1	C	197	ILE	3.5
1	A	125	GLN	3.5
1	C	221	LEU	3.5
1	B	55	GLU	3.5
1	B	132	GLU	3.5
1	B	203	VAL	3.5
1	B	19	LEU	3.5
1	A	136	VAL	3.4
1	A	195	VAL	3.4
1	C	77	LYS	3.4
1	A	104	GLU	3.4
1	B	11	ILE	3.4
1	B	72	LEU	3.4
1	A	144	PHE	3.4
1	A	146	ARG	3.4
1	C	178	GLY	3.4
1	A	77	LYS	3.4
1	B	103	PHE	3.4
1	A	234	PRO	3.4
1	B	226	THR	3.4
1	B	69	GLY	3.4
1	A	11	ILE	3.4
1	A	110	LYS	3.4
1	A	221	LEU	3.4
1	A	227	LEU	3.4
1	B	89	THR	3.4
1	B	104	GLU	3.4
1	B	138	LYS	3.4
1	A	150	ASP	3.4
1	A	156	ASP	3.4
1	B	196	THR	3.3
1	B	250	TYR	3.3
1	B	159	VAL	3.3
1	C	36	ASN	3.3
1	B	119	MET	3.3
1	B	201	GLU	3.3
1	C	137	VAL	3.3
1	C	177	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	57	PHE	3.3
1	C	73	THR	3.3
1	A	203	VAL	3.3
1	B	65	ASN	3.3
1	B	153	HIS	3.3
1	A	172	SER	3.3
1	C	43	SER	3.3
1	C	152	SER	3.3
1	A	245	GLY	3.2
1	A	65	ASN	3.2
1	B	12	LEU	3.2
1	C	241	ILE	3.2
1	B	31	SER	3.2
1	A	250	TYR	3.2
1	B	67	ALA	3.2
1	A	73	THR	3.2
1	B	32	SER	3.2
1	B	7	VAL	3.2
1	C	138	LYS	3.2
1	B	6	LEU	3.2
1	C	205	LEU	3.2
1	C	230	SER	3.1
1	A	85	GLU	3.1
1	A	204	GLN	3.1
1	A	147	ILE	3.1
1	C	210	ARG	3.1
1	A	207	PHE	3.1
1	B	74	SER	3.1
1	A	225	VAL	3.1
1	A	47	LEU	3.1
1	A	79	LEU	3.1
1	A	235	LEU	3.1
1	A	241	ILE	3.1
1	C	17	GLU	3.1
1	C	76	SER	3.1
1	A	48	VAL	3.1
1	A	251	LEU	3.1
1	A	143	GLU	3.1
1	A	89	THR	3.1
1	A	215	PHE	3.1
1	B	184	GLN	3.1
1	C	213	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	3.1
1	B	22	LEU	3.1
1	A	180	ILE	3.0
1	A	222	SER	3.0
1	B	29	ASP	3.0
1	C	156	ASP	3.0
1	A	158	VAL	3.0
1	B	17	GLU	3.0
1	C	238	GLU	3.0
1	B	39	SER	3.0
1	A	168	LYS	3.0
1	C	24	ASN	3.0
1	B	111	VAL	3.0
1	A	78	ILE	3.0
1	B	60	TYR	3.0
1	B	204	GLN	3.0
1	B	112	SER	3.0
1	C	166	GLY	3.0
1	B	214	PHE	3.0
1	B	163	ALA	3.0
1	A	15	VAL	3.0
1	B	30	ILE	3.0
1	C	31	SER	3.0
1	C	223	SER	2.9
1	A	138	LYS	2.9
1	C	181	LYS	2.9
1	C	42	SER	2.9
1	B	254	LYS	2.9
1	C	234	PRO	2.9
1	C	146	ARG	2.9
1	A	218	ALA	2.9
1	C	79	LEU	2.9
1	B	199	MET	2.9
1	A	86	ASP	2.9
1	A	237	VAL	2.8
1	A	226	THR	2.8
1	C	155	GLY	2.8
1	B	227	LEU	2.8
1	C	252	ALA	2.8
1	A	10	SER	2.8
1	B	54	SER	2.8
1	C	200	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	162	CYS	2.8
1	A	67	ALA	2.8
1	B	68	MET	2.8
1	C	20	LYS	2.8
1	C	158	VAL	2.8
1	C	216	THR	2.7
1	B	33	SER	2.7
1	C	183	SER	2.7
1	B	181	LYS	2.7
1	A	16	LEU	2.7
1	B	79	LEU	2.7
1	B	137	VAL	2.7
1	B	174	GLU	2.7
1	A	217	LYS	2.7
1	B	37	LEU	2.7
1	B	182	LEU	2.7
1	B	4	ALA	2.7
1	C	195	VAL	2.7
1	C	203	VAL	2.7
1	B	166	GLY	2.7
1	C	11	ILE	2.7
1	A	25	GLU	2.7
1	A	68	MET	2.7
1	B	229	MET	2.7
1	B	47	LEU	2.7
1	C	235	LEU	2.7
1	C	251	LEU	2.7
1	B	49	GLN	2.7
1	C	13	LYS	2.7
1	C	37	LEU	2.7
1	B	215	PHE	2.6
1	B	35	VAL	2.6
1	B	222	SER	2.6
1	B	223	SER	2.6
1	A	171	ALA	2.6
1	A	238	GLU	2.6
1	A	173	GLY	2.6
1	C	176	GLY	2.6
1	B	5	ARG	2.6
1	C	224	THR	2.6
1	A	112	SER	2.6
1	B	161	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	161	SER	2.6
1	C	172	SER	2.6
1	C	201	GLU	2.6
1	C	145	ALA	2.6
1	B	255	ILE	2.6
1	C	143	GLU	2.5
1	B	230	SER	2.5
1	C	170	SER	2.5
1	B	133	TYR	2.5
1	A	208	ALA	2.5
1	B	27	CYS	2.5
1	B	200	ASN	2.5
1	C	150	ASP	2.5
1	B	245	GLY	2.5
1	C	169	PHE	2.5
1	C	207	PHE	2.5
1	B	15	VAL	2.5
1	B	48	VAL	2.5
1	C	228	ILE	2.5
1	B	75	MET	2.5
1	A	71	ASN	2.5
1	A	219	THR	2.5
1	B	224	THR	2.5
1	B	180	ILE	2.5
1	C	26	ALA	2.5
1	B	78	ILE	2.4
1	C	19	LEU	2.4
1	C	14	LYS	2.4
1	C	131	GLN	2.4
1	A	142	GLY	2.4
1	A	39	SER	2.4
1	A	134	SER	2.4
1	A	26	ALA	2.4
1	B	202	PRO	2.4
1	A	46	SER	2.4
1	C	180	ILE	2.4
1	C	254	LYS	2.4
1	C	18	ALA	2.4
1	B	207	PHE	2.4
1	C	15	VAL	2.4
1	B	50	LEU	2.4
1	C	247	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	173	GLY	2.3
1	C	222	SER	2.3
1	B	53	ARG	2.3
1	B	179	ASN	2.3
1	B	239	TYR	2.3
1	C	239	TYR	2.3
1	B	140	PRO	2.3
1	C	45	VAL	2.3
1	A	99	LEU	2.3
1	C	227	LEU	2.3
1	B	210	ARG	2.3
1	A	74	SER	2.3
1	C	32	SER	2.3
1	C	147	ILE	2.3
1	B	169	PHE	2.2
1	C	202	PRO	2.2
1	A	145	ALA	2.2
1	B	145	ALA	2.2
1	C	219	THR	2.2
1	C	226	THR	2.2
1	A	33	SER	2.2
1	C	47	LEU	2.2
1	C	157	ALA	2.2
1	B	251	LEU	2.2
1	A	213	ASN	2.2
1	B	24	ASN	2.2
1	B	177	ASN	2.2
1	C	40	MET	2.2
1	A	81	CYS	2.2
1	B	217	LYS	2.2
1	B	82	ALA	2.2
1	B	100	ALA	2.2
1	C	33	SER	2.2
1	B	114	TYR	2.2
1	B	247	LEU	2.2
1	B	236	VAL	2.2
1	B	139	MET	2.2
1	B	129	PRO	2.2
1	A	223	SER	2.2
1	C	50	LEU	2.1
1	C	236	VAL	2.1
1	C	198	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	38	GLN	2.1
1	B	51	THR	2.1
1	B	76	SER	2.1
1	A	117	LYS	2.1
1	B	241	ILE	2.1
1	C	168	LYS	2.1
1	C	174	GLU	2.1
1	C	140	PRO	2.1
1	B	34	GLY	2.1
1	C	245	GLY	2.1
1	B	198	GLU	2.1
1	C	215	PHE	2.1
1	A	170	SER	2.0
1	B	10	SER	2.0
1	C	249	TYR	2.0
1	C	248	LYS	2.0
1	B	143	GLU	2.0
1	B	172	SER	2.0
1	C	10	SER	2.0
1	C	209	LEU	2.0
1	B	228	ILE	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 oligosaccharides 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.