



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 1IZ5 / pdb_00001iz5
Title : Pyrococcus furiosus PCNA mutant (Met73Leu, Asp143Ala, Asp147Ala): orthorhombic form
Authors : Matsumiya, S.; Ishino, S.; Ishino, Y.; Morikawa, K.
Deposited on : 2002-09-23
Resolution : 1.80 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

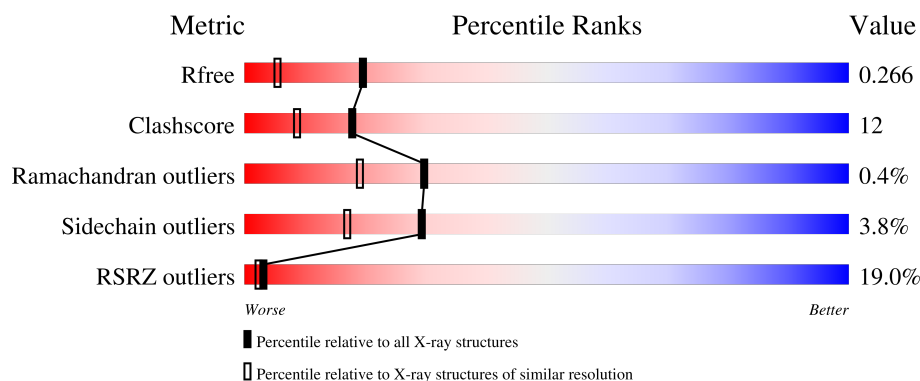
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	249	19% 72% 20% . .
1	B	249	18% 77% 16% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3919 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	240	Total	C	N	O	S	0	0	0
			1884	1208	300	369	7			
1	B	240	Total	C	N	O	S	0	0	0
			1884	1208	300	369	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	LEU	MET	engineered mutation	UNP O73947
A	143	ALA	ASP	engineered mutation	UNP O73947
A	147	ALA	ASP	engineered mutation	UNP O73947
B	73	LEU	MET	engineered mutation	UNP O73947
B	143	ALA	ASP	engineered mutation	UNP O73947
B	147	ALA	ASP	engineered mutation	UNP O73947

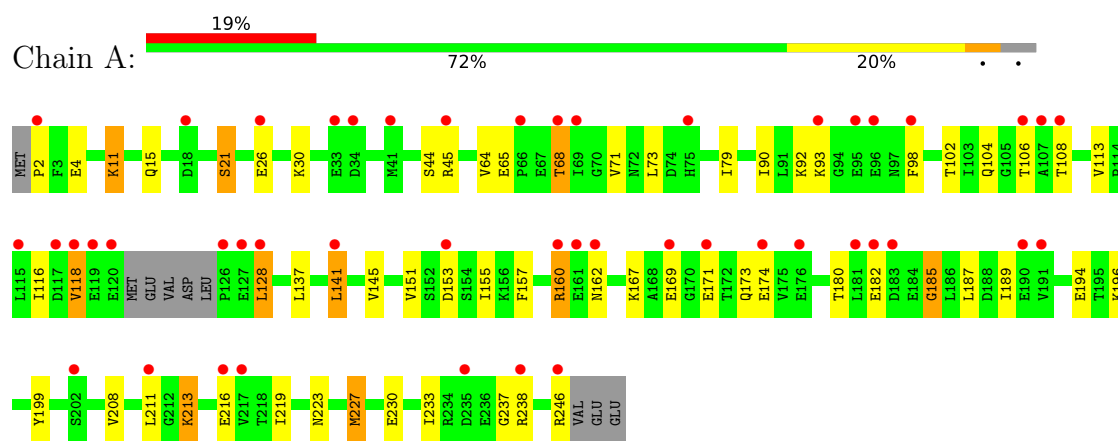
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		
2	B	75	Total	O	0	0
			75	75		

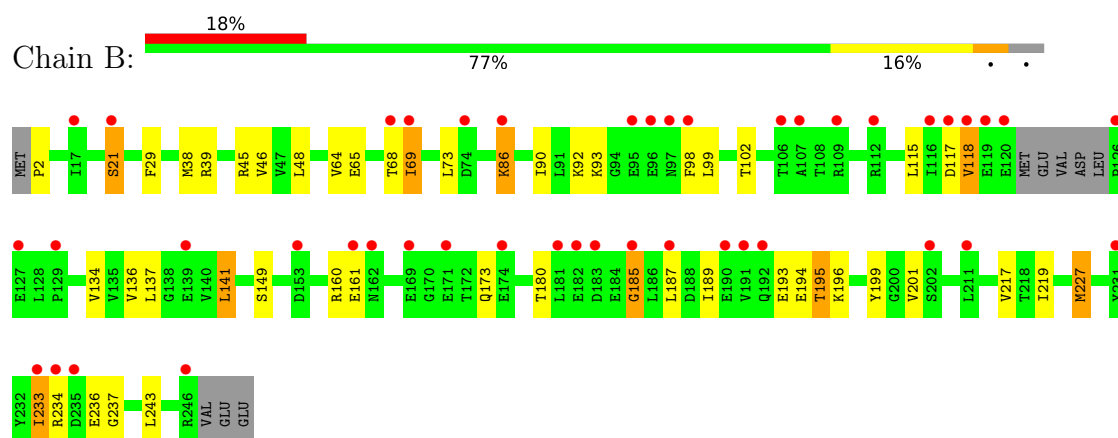
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.29Å 85.35Å 118.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 1.80 35.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.00-1.80) 99.3 (35.00-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.299 0.273 , 0.266	Depositor DCC
R_{free} test set	6093 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3919	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7629e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.35	0/1909	0.86	4/2569 (0.2%)
1	B	0.35	0/1909	0.85	2/2569 (0.1%)
All	All	0.35	0/3818	0.85	6/5138 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLY	N-CA-C	-6.32	106.82	114.66
1	B	185	GLY	N-CA-C	-6.25	106.91	114.66
1	A	21	SER	N-CA-C	5.96	120.16	112.41
1	A	106	THR	N-CA-C	-5.27	106.81	113.18
1	B	21	SER	N-CA-C	5.07	119.41	112.88
1	A	151	VAL	N-CA-C	5.03	118.55	113.47

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	1884	0	1936	48	0
1	B	1884	0	1936	54	0
2	A	76	0	0	4	0
2	B	75	0	0	8	0
All	All	3919	0	3872	94	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 12.

All (94) 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:173:GLN:HE21	1:B:180:THR:H	1.24	0.86
1:A:173:GLN:HE22	1:B:185:GLY:HA3	1.41	0.82
1:A:185:GLY:HA3	1:B:173:GLN:HE22	1.46	0.80
1:B:69:ILE:HD11	1:B:99:LEU:HD22	1.67	0.77
1:A:180:THR:H	1:B:173:GLN:HE21	1.30	0.76
1:A:2:PRO:HG2	1:A:64:VAL:HB	1.69	0.74
1:B:233:ILE:HG23	1:B:237:GLY:HA3	1.70	0.73
1:A:160:ARG:HD2	1:A:194:GLU:OE1	1.89	0.72
1:B:29:PHE:HB2	1:B:69:ILE:HG23	1.70	0.72
1:A:213:LYS:HB2	1:A:213:LYS:NZ	2.06	0.70
1:A:208:VAL:HA	1:A:211:LEU:HD13	1.76	0.67
1:A:157:PHE:HA	2:A:319:HOH:O	1.96	0.66
1:B:2:PRO:HG2	1:B:64:VAL:HB	1.77	0.65
1:B:194:GLU:OE2	1:B:196:LYS:HE3	1.96	0.65
1:B:69:ILE:HG13	1:B:115:LEU:HD22	1.80	0.64
1:A:30:LYS:HD3	1:A:68:THR:HB	1.81	0.63
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.65	0.62
1:B:29:PHE:N	2:B:313:HOH:O	2.32	0.62
1:A:26:GLU:HG2	1:A:71:VAL:O	2.00	0.60
1:B:193:GLU:O	1:B:195:THR:HG22	2.01	0.60
1:B:68:THR:HG22	2:B:313:HOH:O	2.02	0.59
1:A:26:GLU:HG3	1:A:116:ILE:HD11	1.83	0.59
1:B:38:MET:HG2	2:B:318:HOH:O	2.03	0.58
1:B:39:ARG:HD2	1:B:48:LEU:HD11	1.85	0.58
1:B:69:ILE:CD1	1:B:99:LEU:HD22	2.32	0.58
1:B:86:LYS:NZ	1:B:86:LYS:HB3	2.19	0.57
1:A:155:ILE:HD12	1:A:167:LYS:O	2.05	0.56
1:B:141:LEU:HD22	1:B:217:VAL:HG11	1.86	0.56
1:A:196:LYS:H	1:A:223:ASN:ND2	2.04	0.55
1:A:104:GLN:HG3	1:A:108:THR:HG22	1.87	0.55
1:B:68:THR:CG2	2:B:313:HOH:O	2.55	0.55
1:A:185:GLY:CA	1:B:173:GLN:HE22	2.17	0.54
1:A:137:LEU:HD13	2:A:262:HOH:O	2.08	0.54
1:A:213:LYS:HB2	1:A:213:LYS:HZ2	1.74	0.53
1:B:199:TYR:CZ	1:B:227:MET:HB3	2.43	0.53
1:A:26:GLU:OE2	1:A:118:VAL:HB	2.08	0.53
1:B:2:PRO:HD2	1:B:65:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:HE22	1:B:185:GLY:CA	2.15	0.53
1:A:45:ARG:NE	2:A:253:HOH:O	2.38	0.51
1:A:230:GLU:OE2	1:A:238:ARG:NH2	2.45	0.50
1:B:160:ARG:HD3	1:B:194:GLU:OE1	2.12	0.50
1:A:4:GLU:HG3	1:A:92:LYS:HG2	1.94	0.49
1:A:246:ARG:HD3	2:A:315:HOH:O	2.12	0.49
1:B:69:ILE:C	2:B:313:HOH:O	2.53	0.49
1:A:2:PRO:HD2	1:A:65:GLU:HB2	1.94	0.49
1:B:141:LEU:HD21	1:B:219:ILE:HD11	1.95	0.49
1:A:137:LEU:HD11	1:A:187:LEU:HD21	1.95	0.49
1:B:21:SER:OG	1:B:73:LEU:HD13	2.13	0.47
1:B:69:ILE:N	2:B:313:HOH:O	2.47	0.47
1:B:92:LYS:NZ	1:B:92:LYS:HB3	2.29	0.47
1:B:233:ILE:HG23	1:B:237:GLY:CA	2.42	0.47
1:A:137:LEU:HD12	1:A:187:LEU:HD11	1.97	0.47
1:B:45:ARG:NE	2:B:255:HOH:O	2.29	0.47
1:B:93:LYS:C	1:B:93:LYS:HD3	2.38	0.47
1:B:69:ILE:HG13	1:B:115:LEU:CD2	2.44	0.47
1:A:141:LEU:HD21	1:A:219:ILE:HD11	1.98	0.46
1:B:137:LEU:HG	1:B:187:LEU:HD21	1.96	0.46
1:A:173:GLN:NE2	1:B:185:GLY:HA3	2.21	0.46
1:A:182:GLU:OE2	1:A:182:GLU:N	2.47	0.46
1:A:21:SER:HB2	1:A:73:LEU:HD13	1.98	0.45
1:B:136:VAL:O	1:B:217:VAL:HG12	2.16	0.45
1:B:161:GLU:HA	1:B:161:GLU:OE1	2.16	0.45
1:A:199:TYR:CZ	1:A:227:MET:HB3	2.51	0.45
1:A:153:ASP:OD2	1:A:246:ARG:NH1	2.46	0.44
1:A:128:LEU:HD12	1:A:128:LEU:O	2.17	0.44
1:A:141:LEU:O	1:A:145:VAL:HG23	2.18	0.44
1:A:185:GLY:HA3	1:B:173:GLN:NE2	2.24	0.44
1:A:233:ILE:HG23	1:A:237:GLY:HA3	1.99	0.43
1:A:90:ILE:HB	1:A:102:THR:HB	1.99	0.43
1:A:45:ARG:HG2	1:A:45:ARG:NH1	2.33	0.43
1:B:234:ARG:C	1:B:236:GLU:H	2.26	0.43
1:A:169:GLU:HB3	1:A:174:GLU:HG2	2.01	0.43
1:B:98:PHE:C	1:B:98:PHE:CD1	2.96	0.43
1:A:11:LYS:O	1:A:15:GLN:HG3	2.18	0.43
1:B:86:LYS:HB3	1:B:86:LYS:HZ3	1.84	0.43
1:B:136:VAL:HG21	1:B:141:LEU:HD13	2.00	0.43
1:B:189:ILE:HG12	2:B:324:HOH:O	2.19	0.43
1:A:44:SER:O	1:A:45:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HD12	1:B:99:LEU:HD13	1.99	0.42
1:B:117:ASP:O	1:B:118:VAL:HB	2.18	0.42
1:B:134:VAL:HG12	1:B:136:VAL:HG13	2.02	0.42
1:A:98:PHE:CD1	1:A:98:PHE:C	2.98	0.41
1:B:160:ARG:O	1:B:161:GLU:C	2.63	0.41
1:A:213:LYS:HB2	1:A:213:LYS:HZ3	1.82	0.41
1:B:160:ARG:HG2	1:B:194:GLU:HG3	2.02	0.41
1:B:234:ARG:O	1:B:236:GLU:N	2.47	0.41
1:A:21:SER:CB	1:A:73:LEU:HD13	2.51	0.41
1:B:149:SER:HB3	1:B:201:VAL:HG11	2.02	0.41
1:B:29:PHE:HB2	1:B:69:ILE:CG2	2.46	0.41
1:B:90:ILE:HB	1:B:102:THR:HB	2.03	0.41
1:B:136:VAL:HA	1:B:187:LEU:HD23	2.01	0.41
1:A:79:ILE:HD12	1:A:113:VAL:HG22	2.03	0.40
1:A:162:ASN:HA	1:A:189:ILE:HG21	2.02	0.40
1:B:46:VAL:HG12	1:B:243:LEU:HD12	2.03	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	
1	A	236/249 (95%)	228 (97%)	7 (3%)	1 (0%)	30	19
1	B	236/249 (95%)	228 (97%)	7 (3%)	1 (0%)	30	19
All	All	472/498 (95%)	456 (97%)	14 (3%)	2 (0%)	30	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	B	118	VAL

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	208/217 (96%)	198 (95%)	10 (5%)	23	11
1	B	208/217 (96%)	202 (97%)	6 (3%)	37	25
All	All	416/434 (96%)	400 (96%)	16 (4%)	29	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	68	THR
1	A	93	LYS
1	A	128	LEU
1	A	141	LEU
1	A	160	ARG
1	A	171	GLU
1	A	213	LYS
1	A	216	GLU
1	A	227	MET
1	B	69	ILE
1	B	86	LYS
1	B	141	LEU
1	B	195	THR
1	B	227	MET
1	B	233	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	162	ASN
1	A	173	GLN
1	A	192	GLN
1	A	223	ASN
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	75	HIS
1	B	97	ASN
1	B	173	GLN
1	B	228	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 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	240/249 (96%)	1.16	47 (19%) 3 2	19, 31, 49, 71	0
1	B	240/249 (96%)	1.10	44 (18%) 3 2	19, 31, 49, 65	0
All	All	480/498 (96%)	1.13	91 (18%) 3 2	19, 31, 49, 71	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	VAL	10.8
1	B	162	ASN	5.9
1	A	128	LEU	5.5
1	A	26	GLU	4.9
1	A	126	PRO	4.9
1	A	41	MET	4.9
1	A	108	THR	4.8
1	B	118	VAL	4.6
1	B	69	ILE	4.4
1	B	117	ASP	4.2
1	A	117	ASP	4.2
1	B	126	PRO	4.0
1	A	183	ASP	4.0
1	B	153	ASP	4.0
1	A	174	GLU	3.8
1	B	190	GLU	3.7
1	A	107	ALA	3.6
1	A	153	ASP	3.6
1	A	162	ASN	3.5
1	B	181	LEU	3.5
1	A	68	THR	3.4
1	A	171	GLU	3.4
1	B	127	GLU	3.3
1	A	98	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLU	3.3
1	B	183	ASP	3.2
1	B	120	GLU	3.1
1	A	66	PRO	3.0
1	A	211	LEU	3.0
1	B	246	ARG	3.0
1	A	96	GLU	3.0
1	A	69	ILE	3.0
1	A	190	GLU	2.9
1	B	161	GLU	2.9
1	B	68	THR	2.9
1	A	95	GLU	2.9
1	A	182	GLU	2.9
1	B	139	GLU	2.9
1	A	34	ASP	2.8
1	B	235	ASP	2.8
1	A	246	ARG	2.8
1	B	202	SER	2.7
1	A	120	GLU	2.7
1	A	106	THR	2.7
1	A	235	ASP	2.6
1	A	176	GLU	2.6
1	B	95	GLU	2.6
1	B	171	GLU	2.5
1	B	106	THR	2.5
1	B	182	GLU	2.5
1	B	98	PHE	2.5
1	A	202	SER	2.5
1	A	127	GLU	2.5
1	B	96	GLU	2.5
1	B	119	GLU	2.5
1	A	45	ARG	2.4
1	B	174	GLU	2.4
1	B	185	GLY	2.4
1	A	33	GLU	2.3
1	A	169	GLU	2.3
1	B	116	ILE	2.3
1	B	97	ASN	2.3
1	B	109	ARG	2.3
1	B	234	ARG	2.3
1	A	216	GLU	2.3
1	B	169	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	231	TYR	2.3
1	A	75	HIS	2.3
1	A	160	ARG	2.3
1	A	238	ARG	2.2
1	A	191	VAL	2.2
1	A	115	LEU	2.2
1	A	141	LEU	2.2
1	B	74	ASP	2.2
1	B	192	GLN	2.2
1	B	211	LEU	2.2
1	A	18	ASP	2.2
1	B	191	VAL	2.2
1	A	181	LEU	2.2
1	B	187	LEU	2.2
1	A	93	LYS	2.2
1	A	161	GLU	2.1
1	A	2	PRO	2.1
1	B	112	ARG	2.1
1	B	233	ILE	2.1
1	B	86	LYS	2.1
1	B	129	PRO	2.1
1	B	21	SER	2.1
1	A	217	VAL	2.0
1	B	107	ALA	2.0
1	B	17	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.