

wwPDB X-ray Structure Validation Summary Report (i)

Dec 6, 2023 – 07:10 pm GMT

PDB ID	:	1W4C
Title	:	P4 protein from Bacteriophage PHI12 apo state
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Deposited on	:	2004-07-22
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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 <=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	А	331	67%	18% · 13%			
1	В	331	66%	23% • 8%			
1	С	331	67%	22% • 8%			
1	D	331	5% 66%	19% · 13%			
1	Е	331	66%	23% • 8%			



Mol	Chain	Length	Quality of chai	n	
		224	6%		
1	F	331	66%	23%	• 8%
1	C	991	1%		
	G	391	67%	21%	• 8%
1	Н	331	66%	19%	13%
-		001	9%	1370	1370
1	Ι	331	66%	19%	13%
	-		8%		
1	J	331	68%	21%	• 8%
1	K	221	10%	210/	201/
	Λ	001	<u>68%</u>	21%	• 8%
1	L	331	68%	17%	13%
			11%		
1	М	331	66%	22%	• 8%
-	NT	001	10%	_	
	N	331	66%	23%	• 8%
1	0	331	650/	249/	80/
		001	12%	2470	• 076
1	Р	331	66%	23%	• 8%
			11%		
1	Q	331	66%	23%	• 8%
1	D	991	9%		
	n	391	66%	23%	• 8%
1	S	331	66%	23%	. 8%
			9%	20,0	0,0
1	Т	331	66%	23%	• 8%
		224	11%		
	U	331	66%	19% •	13%
1	V	321		220/	00/
	v	001	<u> </u>	22%	• ŏ%
1	W	331	66%	23%	• 8%
			8%		
1	Х	331	68%	18%	• 13%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 57270 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	289	Total	C	N 270	0	S 7	0	0	1	
			21/1 Tetal	1301 C	079 N	424	1 C				
1	В	304		1424	N 200	449	57	0	0	0	
			2288 TExteri	1434	399 N	448	(C				
1	С	304		1422	N 200	440	57	0	0	0	
			2288 TExteri	1433	399 N	449	(C				
1	D	289		1961	N 270	49.4	57	0	0	1	
			2171 Tutul	1301	379 N	424	(
1	Е	304	Total	U 1 4 9 4	N 200	140	5	0	0	0	
			2289	1434	399	449	(
1	F	304	Total	C	N	0	S	0	0	0	
			2289	1434	399	449	7 				
1	G	304	Total	C	N	0	S	0	0	0	
			2289	1434	399	449	<u>'/</u>				
1	Н	Н	289	Total	С	Ν	0	S	0	0	1
			2171	1361	379	424	7	_	_		
1	T	Ι	I 289	Total	С	Ν	0	S	0	0	1
	-	200	2171	1361	379	424	7			-	
1	J	304	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
			2289	1434	399	449	7	Ŭ			
1	K	304	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
		501	2289	1434	399	449	7	Ŭ	Ŭ		
1	L	289	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	1	
	Ľ	205	2171	1361	379	424	7	0	0	1	
1	М	304	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0	
1	111	504	2289	1434	399	449	7	0	0	0	
1	Ν	304	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	11	504	2289	1434	399	449	7	U	0	0	
1	0	204	Total	С	Ν	0	S	0	0	0	
	U	304	2289	1434	399	449	7		U	U	
1	D	204	Total	С	Ν	Ο	S	0	0	0	
	Г	304	2289	1434	399	449	7	U	U	0	

• Molecule 1 is a protein called NTPASE P4.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	204	Total	С	Ν	0	S	0	0	0
	Q	504	2289	1434	399	449	7	0	0	0
1	D	204	Total	С	Ν	0	S	0	0	0
	n	504	2289	1434	399	449	7	0	0	0
1	q	304	Total	С	Ν	0	S	0	0	0
	G	304	2289	1434	399	449	7	0	0	0
1	т	304	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	T	504	2289	1434	399	449	7	0	0	0
1	II	U 289	Total	С	Ν	Ο	\mathbf{S}	0	0	1
1	U		2171	1361	379	424	7	0	0	L
1	V	304	Total	С	Ν	Ο	S	0	0	0
1	v	504	2289	1434	399	449	7	0	0	0
1	W	304	Total	С	Ν	0	S	0	0	0
1	vv	504	2289	1434	399	449	7	0	0	0
1	v	280	Total	С	Ν	0	S	0	0	1
		289	2171	1361	379	424	$\overline{7}$		0	

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	110	Total O 110 110	0	0
2	В	119	Total O 119 119	0	0
2	С	129	Total O 129 129	0	0
2	D	145	Total O 145 145	0	0
2	Ε	143	Total O 143 143	0	0
2	F	151	Total O 151 151	0	0
2	G	101	Total O 101 101	0	0
2	Н	178	Total O 178 178	0	0
2	Ι	193	Total O 193 193	0	0
2	J	159	Total O 159 159	0	0
2	К	122	Total O 122 122	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	93	Total O 93 93	0	0
2	М	169	Total O 169 169	0	0
2	Ν	202	Total O 202 202	0	0
2	О	144	Total O 144 144	0	0
2	Р	103	Total O 103 103	0	0
2	Q	93	Total O 93 93	0	0
2	R	110	Total O 110 110	0	0
2	S	146	Total O 146 146	0	0
2	Т	88	Total O 88 88	0	0
2	U	73	Total O 73 73	0	0
2	V	118	Total O 118 118	0	0
2	W	120	Total O 120 120	0	0
2	Х	153	Total O 153 153	0	0



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: NTPASE P4































4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	115.40Å 126.30Å 155.60Å	Deneriten
a, b, c, α , β , γ	90.00° 91.60° 90.50°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	20.00 - 2.50	Depositor
Resolution (A)	20.01 - 2.50	EDS
% Data completeness	96.0 (20.00-2.50)	Depositor
(in resolution range)	95.9 (20.01-2.50)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.35 (at 2.50 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.251 , 0.224	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.221 , 0.248	DCC
R_{free} test set	14484 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 59.2	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
	0.004 for h,-k,-l	
Estimated twinning fraction	0.006 for -h,k,-l	Xtriage
	0.001 for -h,-k,l	
F_o, F_c correlation	0.93	EDS
Total number of atoms	57270	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	0/2208	0.66	0/2991	
1	В	0.34	0/2324	0.65	0/3145	
1	С	0.35	0/2323	0.64	0/3142	
1	D	0.37	0/2208	0.65	0/2991	
1	Ε	0.36	0/2325	0.65	0/3146	
1	F	0.36	0/2325	0.65	0/3146	
1	G	0.36	0/2325	0.64	0/3146	
1	Н	0.39	0/2208	0.66	0/2991	
1	Ι	0.40	0/2208	0.67	0/2991	
1	J	0.37	0/2325	0.65	0/3146	
1	Κ	0.35	0/2325	0.65	0/3146	
1	L	0.36	0/2208	0.66	0/2991	
1	М	0.37	0/2325	0.65	0/3146	
1	Ν	0.36	0/2325	0.65	0/3146	
1	0	0.36	0/2325	0.64	0/3146	
1	Р	0.34	0/2325	0.65	0/3146	
1	Q	0.35	0/2325	0.64	0/3146	
1	R	0.35	0/2325	0.64	0/3146	
1	S	0.36	0/2325	0.64	0/3146	
1	Т	0.35	0/2325	0.64	0/3146	
1	U	0.36	0/2208	0.65	0/2991	
1	V	0.35	0/2325	0.64	0/3146	
1	W	0.35	0/2325	0.65	0/3146	
1	X	0.38	0/2208	0.66	0/2991	
All	All	0.36	0/54978	0.65	0/74414	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2171	0	2147	70	0
1	В	2288	0	2271	75	0
1	С	2288	0	2266	81	0
1	D	2171	0	2147	72	1
1	Е	2289	0	2271	80	1
1	F	2289	0	2271	83	0
1	G	2289	0	2271	66	0
1	Н	2171	0	2147	74	1
1	Ι	2171	0	2147	82	0
1	J	2289	0	2271	66	0
1	Κ	2289	0	2271	78	0
1	L	2171	0	2147	69	0
1	М	2289	0	2271	98	0
1	Ν	2289	0	2271	90	1
1	0	2289	0	2271	91	0
1	Р	2289	0	2271	90	0
1	Q	2289	0	2271	88	0
1	R	2289	0	2271	86	0
1	S	2289	0	2271	78	0
1	Т	2289	0	2271	82	0
1	U	2171	0	2147	80	0
1	V	2289	0	2271	76	0
1	W	2289	0	2271	89	1
1	Х	2171	0	2147	76	1
2	А	110	0	0	6	0
2	В	119	0	0	5	0
2	С	129	0	0	3	0
2	D	145	0	0	4	0
2	Ε	143	0	0	11	0
2	F	151	0	0	9	0
2	G	101	0	0	1	0
2	Н	178	0	0	9	0
2	Ι	193	0	0	11	0
2	J	159	0	0	2	0
2	Κ	122	0	0	2	0
2	L	93	0	0	4	0
2	М	169	0	0	12	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ν	202	0	0	5	0
2	0	144	0	0	6	0
2	Р	103	0	0	8	0
2	Q	93	0	0	6	0
2	R	110	0	0	3	0
2	S	146	0	0	8	0
2	Т	88	0	0	4	0
2	U	73	0	0	7	0
2	V	118	0	0	5	0
2	W	120	0	0	7	0
2	Х	153	0	0	6	0
All	All	57270	0	53631	1731	3

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 16.

The worst 5 of 1731 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:I:39:SER:HA	1:M:115:GLU:OE2	1.15	1.28
1:I:39:SER:HA	1:M:115:GLU:CD	1.56	1.26
1:S:251:ARG:HD2	1:T:236:THR:HG23	1.27	1.15
1:K:251:ARG:HD2	1:L:236:THR:HG23	1.14	1.13
1:T:251:ARG:HD2	1:U:236:THR:HG23	1.15	1.13

All (3) 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:H:115:GLU:OE2	1:N:39:SER:OG[1_655]	1.92	0.28
1:E:39:SER:CB	1:W:115:GLU:OE1[1_645]	2.04	0.16
1:D:115:GLU:OE2	1:X:38:GLU:O[1_545]	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	Perce	entiles
1	А	285/331~(86%)	265~(93%)	16 (6%)	4 (1%)	11	20
1	В	298/331~(90%)	286 (96%)	7 (2%)	5(2%)	9	16
1	С	298/331~(90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	D	285/331~(86%)	266 (93%)	15~(5%)	4 (1%)	11	20
1	Е	298/331~(90%)	288 (97%)	5 (2%)	5 (2%)	9	16
1	F	298/331~(90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	G	298/331~(90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	Н	285/331~(86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	Ι	285/331~(86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	J	298/331~(90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	К	298/331~(90%)	284 (95%)	9 (3%)	5 (2%)	9	16
1	L	285/331~(86%)	265 (93%)	16 (6%)	4 (1%)	11	20
1	М	298/331~(90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	N	298/331~(90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	Ο	298/331~(90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	Р	298/331~(90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	Q	298/331~(90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	R	298/331~(90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	S	298/331~(90%)	288 (97%)	5 (2%)	5 (2%)	9	16
1	Т	298/331~(90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	U	285/331~(86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	V	298/331~(90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	W	298/331~(90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	X	285/331~(86%)	265 (93%)	16 (6%)	4 (1%)	11	20
All	All	7061/7944 (89%)	6723 (95%)	225 (3%)	113 (2%)	9	17

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	236	THR
1	С	236	THR



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	Е	236	THR
1	F	236	THR
1	G	236	THR

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	234/265~(88%)	225~(96%)	9~(4%)	33	58
1	В	247/265~(93%)	238~(96%)	9~(4%)	35	61
1	С	246/265~(93%)	237~(96%)	9 (4%)	34	60
1	D	234/265~(88%)	225~(96%)	9~(4%)	33	58
1	Ε	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	F	247/265~(93%)	238~(96%)	9~(4%)	35	61
1	G	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	Н	234/265~(88%)	225~(96%)	9 (4%)	33	58
1	Ι	234/265~(88%)	225~(96%)	9 (4%)	33	58
1	J	247/265~(93%)	238 (96%)	9 (4%)	35	61
1	K	247/265~(93%)	238 (96%)	9 (4%)	35	61
1	L	234/265~(88%)	225~(96%)	9~(4%)	33	58
1	М	247/265~(93%)	238~(96%)	9 (4%)	35	61
1	Ν	247/265~(93%)	238~(96%)	9 (4%)	35	61
1	Ο	247/265~(93%)	238 (96%)	9 (4%)	35	61
1	Р	247/265~(93%)	238 (96%)	9 (4%)	35	61
1	Q	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	R	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	S	247/265~(93%)	237 (96%)	10 (4%)	31	56
1	Т	247/265~(93%)	237 (96%)	10 (4%)	31	56
1	U	234/265~(88%)	225 (96%)	9 (4%)	33	58



Mol	Chain	Analysed	Rotameric	Outliers	Percentile	
1	V	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	W	247/265~(93%)	237~(96%)	10 (4%)	31	56
1	Х	234/265~(88%)	225~(96%)	9~(4%)	33	58
All	All	5836/6360~(92%)	5612 (96%)	224 (4%)	33	58

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5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	М	257	LEU
1	Х	262	ASP
1	Р	271	THR
1	Х	192	LYS
1	V	194	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such side chains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	V	3	HIS
1	V	268	GLN
1	Х	253	ASN
1	J	62	ASN
1	Ι	291	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 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 (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	289/331~(87%)	0.22	25 (8%) 10 10	0	25, 38, 90, 114	0
1	В	304/331~(91%)	0.44	40 (13%) 3 3	;	26, 39, 89, 118	0
1	С	304/331~(91%)	0.20	22 (7%) 15 16	6	24, 37, 89, 119	0
1	D	289/331~(87%)	0.12	18 (6%) 20 21	1	22, 36, 90, 113	0
1	Ε	304/331~(91%)	0.32	35 (11%) 4 4		23, 37, 90, 119	0
1	F	304/331~(91%)	0.15	20 (6%) 18 19	9	23, 37, 89, 118	0
1	G	304/331~(91%)	0.29	24 (7%) 12 12	2	25, 38, 88, 119	0
1	Н	289/331~(87%)	0.18	20 (6%) 16 17	7	20, 34, 90, 113	0
1	Ι	289/331~(87%)	0.40	29 (10%) 7 6	5	19,33,90,113	0
1	J	304/331~(91%)	0.22	27 (8%) 9 9		20, 34, 88, 118	0
1	Κ	304/331~(91%)	0.30	32 (10%) 6 6	5	24, 38, 89, 119	0
1	L	289/331~(87%)	0.39	28 (9%) 7 7		25, 39, 90, 114	0
1	М	304/331~(91%)	0.42	35 (11%) 4 4		18, 34, 89, 119	0
1	Ν	304/331~(91%)	0.44	34 (11%) 5 4		19, 34, 90, 119	0
1	Ο	304/331~(91%)	0.20	24 (7%) 12 12	2	23, 36, 89, 119	0
1	Р	304/331~(91%)	0.38	39 (12%) 3 3	;	26, 39, 90, 119	0
1	Q	304/331~(91%)	0.54	36 (11%) 4 4		27, 40, 90, 119	0
1	R	304/331~(91%)	0.35	29 (9%) 8 8		23, 37, 89, 119	0
1	S	304/331~(91%)	0.20	23 (7%) 13 14	4	22, 37, 89, 118	0
1	Т	304/331~(91%)	0.33	29 (9%) 8 8		24, 40, 89, 118	0
1	U	289/331 (87%)	0.43	37 (12%) 3 3	3	27, 40, 91, 114	0
1	V	304/331 (91%)	0.30	34 (11%) 5 4	2	$26, 39, \overline{89, 119}$	0
1	W	304/331~(91%)	0.27	37 (12%) 4 3	3	25, 38, 90, 118	0
1	Х	289/331~(87%)	0.24	25 (8%) 10 10	0	21, 36, 91, 114	0



Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
All	All	7191/7944~(90%)	0.31	702 (9%) 7 7	18, 37, 91, 119	0

The worst 5 of 702 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	133	ASN	8.9
1	Ι	79	GLY	8.3
1	Ν	309	GLY	7.9
1	Κ	240	ASP	7.9
1	Т	240	ASP	7.8

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.

