

# wwPDB X-ray Structure Validation Summary Report (i)

### Sep 17, 2023 – 12:16 AM EDT

PDB ID	:	4X23
Title	:	CRYSTAL STRUCTURE OF CENP-C IN COMPLEX WITH THE NUCLE-
		OSOME CORE PARTICLE
Authors	:	Jiang, J.S.
Deposited on	:	2014-11-25
Resolution	:	3.50  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
$\mathrm{EDS}$	:	2.35.1
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)	:	2.35.1

# 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 3.50 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.



Motric	Whole archive	Similar resolution
Wiethic	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	I	147	74%	25%						
-	-		1470							
1	S	147	78%	22%	·					
2	J	147	75%	24%	·					
2	Т	147	77%	22%	•					
3	А	98	80%	17%	•					



Chain Length Quality of chain Mol Е 3 98 85% 14% . 3 Κ 9883% 14% • .% 3 Ο 98 81% 19% В 794 81% 19% .% F 47977% 23% L 794 76% 24% Р 4 7976% 23% С 510277% 23%  $\mathbf{G}$ 102588% 12% М 102582% 18% .% Q 510281% 19% D 90 6 82% 18% 6 Η 90 84% 16% 6Ν 90 82% 18% .% R 6 90 83% 14% U 72516% 80% 7 $\mathbf{V}$ 2544% 36% 8% 12% 7W 258% 88% • 7Х 2552% 32% 16%





# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23974 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 DNA chain called DNA (147-MER).

Mol	Chain	Residues		Atoms					AltConf	Trace
1	Ι	146	Total 2975	C 1413	N 540	O 876	Р 146	0	0	0
1	S	146	Total 2975	C 1413	N 540	O 876	Р 146	0	0	0

• Molecule 2 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues		Atoms					AltConf	Trace
2	J	146	Total 3011	C 1425	N 564	0 876	Р 146	0	0	0
2	Т	146	Total 3011	C 1425	N 564	O 876	Р 146	0	0	0

- Mol Chain Residues Atoms ZeroOcc AltConf Trace S Total С Ν Ο 3 0 0 А 950 7754911451363 Total С Ν Ο  $\mathbf{S}$ 3 Ε 980 0 0 797 5041511393 С S Ν Total 0 3 Κ 0 0 0 957594821421323 S С Ν Total Ο 3 Ο 98 0 0 0 3 791 501148139
- Molecule 3 is a protein called Histone H3.

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	133	ILE	-	expression tag	UNP P02299
А	134	GLU	-	expression tag	UNP P02299
А	135	GLY	-	expression tag	UNP P02299
А	136	GLY	-	expression tag	UNP P02299



Chain	Residue	Modelled	Actual	Comment	Reference
А	137	LEU	-	expression tag	UNP P02299
Е	133	ILE	-	expression tag	UNP P02299
E	134	GLU	-	expression tag	UNP P02299
E	135	GLY	-	expression tag	UNP P02299
E	136	GLY	-	expression tag	UNP P02299
E	137	LEU	-	expression tag	UNP P02299
K	133	ILE	-	expression tag	UNP P02299
K	134	GLU	-	expression tag	UNP P02299
K	135	GLY	-	expression tag	UNP P02299
K	136	GLY	-	expression tag	UNP P02299
K	137	LEU	-	expression tag	UNP P02299
0	133	ILE	-	expression tag	UNP P02299
0	134	GLU	-	expression tag	UNP P02299
0	135	GLY	-	expression tag	UNP P02299
0	136	GLY	-	expression tag	UNP P02299
0	137	LEU	-	expression tag	UNP P02299

• Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	В	70	Total	С	Ν	Ο	S	0	0	0
4	T D	19	622	392	120	109	1		0	0
4	F	70	Total	С	Ν	Ο	S	0	0	0
4	4 F	19	626	395	121	109	1			
4	т	70	Total	С	Ν	0	S	0	0	0
4	L	19	626	395	121	109	1	0		0
4	4 P	79	Total	С	Ν	0	S	0	0	0
4			626	395	121	109	1			0

• Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
5	5 C	102	Total	С	Ν	0	S	0	0	0	
0		102	780	491	151	137	1	0	0	0	
5	С	102	Total	С	Ν	0	S	12	19	0	0
0	5 G		776	489	151	135	1		U	0	
Б	м	109	Total	С	Ν	0	S	12	0	0	
0		102	780	491	151	137	1			0	
Б	5 Q	Q 102	Total	С	Ν	0	S	11	0	0	
0			780	491	151	137	1			U	

• Molecule 6 is a protein called Histone H2B.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6 D	00	Total	С	Ν	0	S	0	0	0
0		90	703	444	123	134	2	0	0	0
6	Ц	90	Total	С	Ν	0	S	2	0	0
0	11		703	444	123	134	2	5		0
6	N	00	Total	С	Ν	0	S	2	0	0
0	1 N	90	703	444	123	134	2	5	0	0
6	6 R	88	Total	С	Ν	0	S	0	0	0
0			691	438	121	130	2			0

• Molecule 7 is a protein called CENP-C.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	7 V	22	Total C N O	0	0	0
•	•		203  128  43  32	0	Ŭ	0
7	I	5	Total C N O	0	0	0
1	U	5	40 $24$ $11$ $5$	0	0	0
7	v	01	Total C N O	0	0	0
(	Λ	21	$196 \ 123 \ 42 \ 31$	0		0
7	7 W	0	Total C N O	0	0	0
	vv	0	25 13 7 5	0	U	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: DNA (147-MER)

• Molecule 3: Histone H3





#### 

 $\bullet$  Molecule 5: Histone H2A

Chain G:	88%	12%
<b>S15</b> V26 V42 V42 V48 E60 G66 G66 T76 R76	D89 192 1100 1101	
• Molecule 5: Histon	ne H2A	
Chain M:	82%	18%
815 N18 N18 R19 R26 R26 R28 R31 R31 R31 R34 R31 R34 R34 R34	R41 E60 666 666 184 1101 1101 1114 1115 1115 1115 1115	
• Molecule 5: Histon	ne H2A	
Chain Q:	81%	19%
S15 F24 P25 V26 V34 X34 X34 R34 R41 R41 V42 V42	E55 E60 E60 E63 E63 E63 C65 M7 M7 M7 M81 H81 H81 H81 H81 H81 H81 H81 H81 H81 H	
• Molecule 6: Histon	ne H2B	
Chain D:	82%	18%
E32 146 146 188 188 188 188 188 188 188 188 188 18	185 186 186 190 190 190 190 111 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17 <b>1</b> 17	
• Molecule 6: Histon	ne H2B	
Chain H:	84%	16%
833 833 146 146 149 149 149 168 168 168 168	1385 1387 1387 1387 1387 1387 1388 1388 1388	
• Molecule 6: Histon	ne H2B	
Chain N:	82%	18%
532 137 137 146 146 146 168 168 168 168 168 168 168 168 168 173 174	875 876 186 186 187 187 187 186 198 103 1103 1103 1103 1118 1118 1118 1118	
• Molecule 6: Histon	ne H2B	
Chain B:	930/	14%



E32 V45 146 149 158 158	E73 474 876 876 876 186 186 186 186 186 186 186 190 101 101 811 811 811	SER	
• Molecule 7	7: CENP-C		
Chain V:	44%	36%	8% 12%
PRO ASN V712 S715 N716 N716 T717 T718 R719 R719	7725 7726 7726 7728 7728 7729 7739 7733 7731 7731 7731 7731 7733 7733		
• Molecule 7	7: CENP-C		
Chain U:	16% ·	80%	
PRO ASN VAL ARG ARG SER SER SER R719 R719	L720 PRO PRO LEU TYP TYP GLY GLY GLY ARG GLU ARG GLU ASP TYR TYR TYR		
• Molecule 7	7: CENP-C		
Chain X:	52%	32%	16%
PRO ASN VAL R713 R714 S715 N716 R716 R717 R717 1718	K719 E729 P732 Y733 GLN GLN		
• Molecule 7	7: CENP-C		
Chain W:	8% •	88%	
PRO ASN VAL ARG ARG S715 N716 N716 ILE	ARG LEU LEU PPRO CLU CLU CLU ARG ARG CLY ARG ARG CLY ARG CLU ARG ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP		



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	102.99Å 176.10Å 208.85Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Pecolution(Å)	49.54 - 3.50	Depositor
Resolution (A)	49.54 - 3.40	EDS
% Data completeness	99.9 (49.54-3.50)	Depositor
(in resolution range)	$92.1 \ (49.54 - 3.40)$	EDS
R <sub>merge</sub>	0.12	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.01 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690), CNS 1.3	Depositor
D D.	0.236 , $0.286$	Depositor
$\Pi, \Pi_{free}$	0.239 , $0.287$	DCC
$R_{free}$ test set	2000 reflections $(3.78%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	111.6	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.25,75.1	EDS
L-test for twinning <sup>2</sup>	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23974	wwPDB-VP
Average B, all atoms $(Å^2)$	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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).

Mal	Mol Chain		Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	Ι	0.49	0/3333	0.88	0/5137		
1	S	0.49	0/3333	0.88	0/5137		
2	J	0.50	0/3381	0.87	0/5221		
2	Т	0.50	0/3381	0.87	0/5221		
3	А	0.20	0/785	0.39	0/1054		
3	Е	0.20	0/807	0.36	0/1082		
3	Κ	0.20	0/769	0.36	0/1034		
3	0	0.20	0/801	0.36	0/1075		
4	В	0.20	0/629	0.37	0/844		
4	F	0.20	0/633	0.37	0/848		
4	L	0.20	0/633	0.38	0/848		
4	Р	0.20	0/633	0.37	0/848		
5	С	0.20	0/790	0.42	0/1068		
5	G	0.19	0/786	0.36	0/1063		
5	М	0.20	0/790	0.35	0/1068		
5	Q	0.20	0/790	0.36	0/1068		
6	D	0.20	0/714	0.37	0/963		
6	Н	0.21	0/714	0.37	0/963		
6	Ν	0.21	0/714	0.38	0/963		
6	R	0.21	0/702	0.40	0/947		
7	U	0.17	0/39	0.32	0/50		
7	V	0.23	0/207	0.53	0/276		
7	W	0.18	0/24	0.30	0/30		
7	Х	0.25	0/200	0.56	0/266		
All	All	0.38	0/25588	0.70	0/37074		

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	Ι	2975	0	1639	27	0
1	S	2975	0	1639	24	0
2	J	3011	0	1639	28	0
2	Т	3011	0	1639	27	0
3	А	775	0	811	14	0
3	Е	797	0	839	14	0
3	Κ	759	0	785	12	0
3	0	791	0	828	17	0
4	В	622	0	652	12	0
4	F	626	0	663	13	0
4	L	626	0	663	13	0
4	Р	626	0	663	18	0
5	С	780	0	822	16	0
5	G	776	0	818	11	0
5	М	780	0	822	18	0
5	Q	780	0	822	17	0
6	D	703	0	720	11	0
6	Н	703	0	720	11	0
6	Ν	703	0	720	15	0
6	R	691	0	710	10	0
7	U	40	0	40	1	0
7	V	203	0	208	9	0
7	W	25	0	23	2	0
7	Х	196	0	199	7	0
All	All	23974	0	19084	246	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 6.

The worst 5 of 246 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)
5:M:60:GLU:OE2	7:W:717:ARG:HD2	1.63	0.99
5:M:60:GLU:OE2	7:W:717:ARG:CD	2.24	0.86
4:P:29:ILE:HD11	4:P:55:ARG:HG2	1.68	0.73



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Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å		
7:V:729:GLU:HG3	7:X:733:TYR:HB2	1.71	0.72		
4:F:29:ILE:HD11	4:F:55:ARG:HG2	1.72	0.71		

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	Perce	ntiles
3	А	93/98~(95%)	89 (96%)	4 (4%)	0	100	100
3	Е	96/98~(98%)	91 (95%)	4 (4%)	1 (1%)	15	54
3	K	93/98~(95%)	89 (96%)	4 (4%)	0	100	100
3	Ο	96/98~(98%)	94 (98%)	2 (2%)	0	100	100
4	В	77/79~(98%)	74 (96%)	3 (4%)	0	100	100
4	F	77/79~(98%)	74 (96%)	3 (4%)	0	100	100
4	L	77/79~(98%)	74 (96%)	3 (4%)	0	100	100
4	Р	77/79~(98%)	74 (96%)	3 (4%)	0	100	100
5	С	100/102~(98%)	95 (95%)	5 (5%)	0	100	100
5	G	100/102~(98%)	95 (95%)	5 (5%)	0	100	100
5	М	100/102~(98%)	95 (95%)	5 (5%)	0	100	100
5	Q	100/102~(98%)	95 (95%)	5 (5%)	0	100	100
6	D	88/90~(98%)	84 (96%)	2 (2%)	2 (2%)	6	36
6	Н	88/90~(98%)	85 (97%)	3 (3%)	0	100	100
6	Ν	88/90~(98%)	84 (96%)	4 (4%)	0	100	100
6	R	86/90~(96%)	84 (98%)	1 (1%)	1 (1%)	13	50
7	U	3/25~(12%)	2 (67%)	1 (33%)	0	100	100
7	V	20/25~(80%)	11 (55%)	7 (35%)	2 (10%)	0	7



001000	Contributed from provide page							
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles	
7	W	1/25~(4%)	1 (100%)	0	0	100	100	
7	Х	19/25~(76%)	12~(63%)	7 (37%)	0	100	100	
All	All	1479/1576~(94%)	1402 (95%)	71 (5%)	6 (0%)	34	72	

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	V	726	TRP
6	R	101	GLY
6	D	100	PRO
6	D	101	GLY
7	V	725	TYR

#### 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	А	82/84~(98%)	82 (100%)	0	100 100
3	Ε	84/84~(100%)	84 (100%)	0	100 100
3	Κ	78/84~(93%)	78 (100%)	0	100 100
3	Ο	83/84~(99%)	82~(99%)	1 (1%)	71 87
4	В	63/64~(98%)	63 (100%)	0	100 100
4	F	64/64~(100%)	64 (100%)	0	100 100
4	L	64/64~(100%)	62~(97%)	2(3%)	40 70
4	Р	64/64~(100%)	63~(98%)	1 (2%)	62 83
5	С	79/79~(100%)	79~(100%)	0	100 100
5	G	78/79~(99%)	78 (100%)	0	100 100
5	М	79/79~(100%)	79~(100%)	0	100 100
5	Q	79/79~(100%)	$78 \ (99\%)$	1 (1%)	69 86
6	D	77/77~(100%)	77 (100%)	0	100 100
6	Н	77/77~(100%)	77~(100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
6	Ν	77/77~(100%)	77~(100%)	0	100	100
6	R	75/77~(97%)	75 (100%)	0	100	100
7	U	3/24~(12%)	3~(100%)	0	100	100
7	V	21/24~(88%)	19 (90%)	2(10%)	8	34
7	W	3/24~(12%)	3~(100%)	0	100	100
7	Х	20/24~(83%)	19 (95%)	1 (5%)	24	58
All	All	1250/1312~(95%)	1242 (99%)	8 (1%)	86	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Х	732	ASP
5	Q	34	ARG
3	0	41	TYR
4	L	84	MET
4	Р	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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			$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	Ι	146/147~(99%)	-0.52	0	100	100		126, 188, 227, 250	0
1	S	146/147~(99%)	-0.29	0	100	100		146,211,254,271	0
2	J	146/147~(99%)	-0.39	0	100	100		125, 188, 228, 241	0
2	Т	146/147~(99%)	-0.28	0	100	100		161, 212, 253, 266	0
3	А	95/98~(96%)	-0.18	0	100	100		70,109,157,168	0
3	Е	98/98~(100%)	-0.20	0	100	100		74,102,143,161	0
3	K	95/98~(96%)	-0.09	0	100	100		86, 119, 160, 175	0
3	Ο	98/98~(100%)	-0.04	1 (1	%) 8	2 77	7	78, 127, 186, 220	0
4	В	79/79~(100%)	-0.07	0	100	100		71, 106, 146, 158	0
4	F	79/79~(100%)	-0.07	1 (1	%) [7	7 71		75, 97, 136, 149	0
4	L	79/79~(100%)	-0.07	0	100	100		73,112,147,159	0
4	Р	79/79~(100%)	-0.10	0	100	100		82, 119, 150, 163	0
5	С	102/102~(100%)	-0.25	0	100	100		72,109,143,167	0
5	G	102/102~(100%)	-0.18	0	100	100		73,100,136,162	4(3%)
5	М	102/102~(100%)	-0.19	0	100	100		79,116,154,168	4(3%)
5	Q	102/102~(100%)	-0.20	1 (0	%) 8	2 77	7	83,115,158,179	4(3%)
6	D	90/90~(100%)	-0.23	0	100	100		79,109,138,156	0
6	Н	90/90~(100%)	-0.20	0	100	100		73,102,141,155	1 (1%)
6	Ν	90/90~(100%)	-0.21	0	100	100		82, 114, 149, 159	1 (1%)
6	R	88/90~(97%)	-0.14	1 (1	%) 8	0 75	5	83, 116, 149, 171	0
7	U	5/25~(20%)	-0.19	0	100	100		137, 155, 164, 178	0
7	V	$22/25\ (88\%)$	-0.14	0	100	100		86, 126, 159, 176	0
7	W	3/25~(12%)	0.06	0	100	100		159, 159, 168, 179	0
7	Х	21/25~(84%)	-0.22	0	100	100		$93, 135, 160, \overline{194}$	0



Mol	Chain	Analysed	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
All	All	2103/2164~(97%)	-0.22	4 (0%) 95 93	70, 124, 226, 271	14 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	0	81	ASP	3.2
4	F	102	GLY	2.3
5	Q	24	PHE	2.3
6	R	49	THR	2.1

## 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.

