

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

## May 25, 2020 - 07:55 am BST

PDB ID	:	4H3H
$\operatorname{Title}$	:	Crystal structure of a ternary complex of human symplekin NTD, human Ssu72
		and a RNA poymerase II CTD peptide phosphorylated at SER-7
Authors	:	Xiang, K.; Tong, L.
Deposited on	:	2012-09-13
$\operatorname{Resolution}$	:	2.20  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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594(2.20-2.20)
Ramachandran outliers	138981	$5503 \ (2.20-2.20)$
Sidechain outliers	138945	5504(2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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	351	<sup>2%</sup> 78%	10%	• 10%						
1	D	351	<sup>2%</sup> <b>78</b> %	9%	• 11%						
2	В	214	70%	16%	• 12%						
2	Е	214	% 69%	18%	• 10%						
3	F	10	<u>30%</u> 50% <u>30%</u>		20%						



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8208 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		At	oms		ZeroOcc	AltConf	Trace	
1	А	317	Total 2506	C 1596	N 433	O 464	S 13	0	0	0
1	D	311	Total 2461	C 1569	N 422	O 457	S 13	0	0	0

• Molecule 1 is a protein called Symplekin.

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	EXPRESSION TAG	UNP Q92797
A	11	GLY	-	EXPRESSION TAG	UNP Q92797
A	12	SER	-	EXPRESSION TAG	UNP Q92797
A	13	SER	-	EXPRESSION TAG	UNP Q92797
A	14	HIS	-	EXPRESSION TAG	UNP Q92797
A	15	HIS	-	EXPRESSION TAG	UNP Q92797
A	16	HIS	-	EXPRESSION TAG	UNP Q92797
А	17	HIS	-	EXPRESSION TAG	UNP Q92797
A	18	HIS	-	EXPRESSION TAG	UNP Q92797
А	19	HIS	-	EXPRESSION TAG	UNP Q92797
A	20	SER	-	EXPRESSION TAG	UNP Q92797
А	21	SER	-	EXPRESSION TAG	UNP Q92797
А	22	GLY	-	EXPRESSION TAG	UNP Q92797
A	23	LEU	-	EXPRESSION TAG	UNP Q92797
A	24	VAL	-	EXPRESSION TAG	UNP Q92797
A	25	PRO	-	EXPRESSION TAG	UNP Q92797
A	26	ARG	-	EXPRESSION TAG	UNP Q92797
А	27	GLY	-	EXPRESSION TAG	UNP Q92797
A	28	SER	-	EXPRESSION TAG	UNP Q92797
A	29	HIS	-	EXPRESSION TAG	UNP Q92797
D	10	MET	-	EXPRESSION TAG	UNP Q92797
D	11	GLY	-	EXPRESSION TAG	UNP Q92797
D	12	SER	-	EXPRESSION TAG	UNP Q92797
D	13	SER	-	EXPRESSION TAG	UNP Q92797
D	14	HIS	-	EXPRESSION TAG	UNP Q92797

There are 40 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
D	15	HIS	-	EXPRESSION TAG	UNP Q92797
D	16	HIS	-	EXPRESSION TAG	UNP Q92797
D	17	HIS	-	EXPRESSION TAG	UNP Q92797
D	18	HIS	-	EXPRESSION TAG	UNP Q92797
D	19	HIS	-	EXPRESSION TAG	UNP Q92797
D	20	SER	-	EXPRESSION TAG	UNP Q92797
D	21	SER	-	EXPRESSION TAG	UNP Q92797
D	22	GLY	-	EXPRESSION TAG	UNP Q92797
D	23	LEU	-	EXPRESSION TAG	UNP Q92797
D	24	VAL	-	EXPRESSION TAG	UNP Q92797
D	25	PRO	-	EXPRESSION TAG	UNP Q92797
D	26	ARG	-	EXPRESSION TAG	UNP Q92797
D	27	GLY	-	EXPRESSION TAG	UNP Q92797
D	28	SER	-	EXPRESSION TAG	UNP Q92797
D	29	HIS	-	EXPRESSION TAG	UNP Q92797

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• Molecule 2 is a protein called RNA polymerase II subunit A C-terminal domain phosphatase SSU72.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			ZeroOcc	AltConf	Trace
9	9 D 190	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0	
	D	109	1546	960	272	303	11	0	0	U
0	9 F	192	Total	С	Ν	Ο	S	0	0	0
			1565	971	275	308	11		0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-19	MET	-	EXPRESSION TAG	UNP Q9NP77
В	-18	GLY	-	EXPRESSION TAG	UNP Q9NP77
В	-17	SER	-	EXPRESSION TAG	UNP Q9NP77
В	-16	SER	-	EXPRESSION TAG	UNP Q9NP77
В	-15	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-14	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-13	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-12	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-11	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-10	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	-9	SER	-	EXPRESSION TAG	UNP Q9NP77
В	-8	SER	-	EXPRESSION TAG	UNP Q9NP77
В	-7	GLY	-	EXPRESSION TAG	UNP Q9NP77
В	-6	LEU	-	EXPRESSION TAG	UNP Q9NP77

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-5	VAL	-	EXPRESSION TAG	UNP Q9NP77
В	-4	PRO	-	EXPRESSION TAG	UNP Q9NP77
В	-3	ARG	_	EXPRESSION TAG	UNP Q9NP77
В	-2	GLY	-	EXPRESSION TAG	UNP Q9NP77
В	-1	SER	-	EXPRESSION TAG	UNP Q9NP77
В	0	HIS	-	EXPRESSION TAG	UNP Q9NP77
В	12	SER	CYS	ENGINEERED MUTATION	UNP Q9NP77
Е	-19	MET	-	EXPRESSION TAG	UNP Q9NP77
Е	-18	GLY	-	EXPRESSION TAG	UNP Q9NP77
Е	-17	SER	-	EXPRESSION TAG	UNP Q9NP77
Е	-16	SER	-	EXPRESSION TAG	UNP Q9NP77
Е	-15	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-14	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-13	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-12	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-11	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-10	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	-9	SER	-	EXPRESSION TAG	UNP Q9NP77
Е	-8	SER	-	EXPRESSION TAG	UNP Q9NP77
Е	-7	GLY	-	EXPRESSION TAG	UNP Q9NP77
Е	-6	LEU	-	EXPRESSION TAG	UNP Q9NP77
Е	-5	VAL	-	EXPRESSION TAG	UNP Q9NP77
Е	-4	PRO	-	EXPRESSION TAG	UNP Q9NP77
Е	-3	ARG	-	EXPRESSION TAG	UNP Q9NP77
Е	-2	GLY	-	EXPRESSION TAG	UNP Q9NP77
Е	-1	SER	-	EXPRESSION TAG	UNP Q9NP77
Е	0	HIS	-	EXPRESSION TAG	UNP Q9NP77
Е	12	SER	CYS	ENGINEERED MUTATION	UNP Q9NP77

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• Molecule 3 is a protein called Pol II CTD peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total 62	C 37	N 8	O 16	Р 1	0	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	В	1	Total 5	0 4	Р 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	20	Total         O           20         20	0	0
5	В	16	Total         O           16         16	0	0
5	D	14	Total         O           14         14	0	0
5	Ε	13	Total O 13 13	0	0



# 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 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: Symplekin



30%

20%

# 

# 103 <th 103</th

• Molecule 3: Pol II CTD peptide

30%

50%

Chain F:





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.82Å 97.74Å 104.60Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $98.63^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	50.00 - 2.20	Depositor
Resolution (A)	48.87 - 2.20	EDS
% Data completeness	99.7 (50.00-2.20)	Depositor
(in resolution range)	99.7 (48.87-2.20)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.57 (at 2.20 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D.	0.198 , $0.227$	Depositor
$\Pi, \Pi_{free}$	0.196 , $0.223$	DCC
$R_{free}$ test set	3400 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , $37.1$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$\boxed{ F_o, F_c \text{ correlation} }$	0.95	EDS
Total number of atoms	8208	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.63% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SEP

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	Chain	Bond lengths		Bond angles	
	Chain	RMSZ   # Z  > 5		RMSZ	# Z  > 5
1	А	0.84	1/2544~(0.0%)	0.81	2/3449~(0.1%)
1	D	0.76	0/2497	0.77	4/3385~(0.1%)
2	В	0.84	2/1574~(0.1%)	0.82	3/2124~(0.1%)
2	Е	0.81	0/1594	0.82	3/2152~(0.1%)
3	F	0.80	0/54	0.77	0/73
All	All	0.81	3/8263~(0.0%)	0.80	12/11183~(0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	340	PRO	N-CD	10.51	1.62	1.47
2	В	161	CYS	CB-SG	-7.93	1.68	1.82
2	В	147	GLU	CD-OE1	5.23	1.31	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	218	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	D	218	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	В	139	VAL	CB-CA-C	-6.22	99.58	111.40
1	D	218	ARG	CG-CD-NE	-5.99	99.22	111.80
2	Е	34	ARG	NE-CZ-NH1	5.76	123.18	120.30

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	А	2506	0	2610	44	0
1	D	2461	0	2566	22	0
2	В	1546	0	1493	36	0
2	Е	1565	0	1510	38	0
3	F	62	0	50	2	0
4	В	5	0	0	0	0
5	А	20	0	0	2	0
5	В	16	0	0	0	0
5	D	14	0	0	0	0
5	Ē	13	0	0	0	0
All	All	8208	0	8229	135	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 8.

The worst 5 of 135 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)
2:B:135:HIS:HD2	2:B:189:HIS:CE1	1.72	1.06
2:B:135:HIS:HD2	2:B:189:HIS:HE1	1.00	0.98
2:B:135:HIS:CD2	2:B:189:HIS:HE1	1.84	0.95
2:E:99:GLN:HE21	2:E:99:GLN:H	1.13	0.94
1:A:339:MET:HB3	1:A:340:PRO:HD3	1.48	0.94

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentil	$\mathbf{les}$
1	А	315/351~(90%)	310 (98%)	5(2%)	0	100 10	0
1	D	309/351~(88%)	306 (99%)	3 (1%)	0	100 10	0
2	В	187/214~(87%)	184 (98%)	3~(2%)	0	100 10	0
2	Е	190/214~(89%)	185 (97%)	4 (2%)	1 (0%)	29 31	
3	F	5/10~(50%)	5(100%)	0	0	100 10	0
All	All	1006/1140~(88%)	990 (98%)	15(2%)	1 (0%)	51 60	)

analysed, and the total number of residues.

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Е	5	PRO

#### 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
1	А	283/315~(90%)	268~(95%)	15~(5%)	22 27
1	D	278/315~(88%)	266~(96%)	12 (4%)	29 36
2	В	177/199~(89%)	166 (94%)	11~(6%)	18 21
2	Е	180/199~(90%)	166 (92%)	14 (8%)	12 13
3	F	7/9~(78%)	6 (86%)	1 (14%)	3 2
All	All	925/1037~(89%)	872 (94%)	53 (6%)	20 24

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	130	THR
1	D	109	LYS
2	Е	171	GLU
2	В	168	MET
1	D	33	SER



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	D	81	GLN
1	D	220	HIS
2	Е	163	GLN
1	D	154	GLN
1	D	282	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Cl	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Pos	Tink	B	Bond lengths			Bond angles		
			I nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2							
3	SEP	F	7	3	8,9,10	1.38	1 (12%)	8,12,14	1.44	2 (25%)							

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	F	7	3	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	$\mathbf{F}$	7	SEP	P-O1P	2.99	1.60	1.50

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	F	7	SEP	OG-CB-CA	2.33	110.41	108.14
3	F	7	SEP	P-OG-CB	-2.04	112.69	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	7	SEP	CB-OG-P-O2P
3	F	7	SEP	N-CA-CB-OG
3	F	7	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Iol Type Chain Res Li	Tink	Bond lengths			Bond angles				
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	В	201	-	4,4,4	0.85	0	$^{6,6,6}$	0.67	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

# 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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	317/351~(90%)	-0.07	6 (1%) 66 65	17, 31, 49, 66	0
1	D	311/351~(88%)	0.02	7 (2%) 60 58	20, 34, 67, 83	0
2	В	189/214~(88%)	0.03	1 (0%) 91 90	18, 35, 61, 74	0
2	Е	192/214~(89%)	-0.05	3 (1%) 72 70	20, 34, 57, 72	0
3	F	7/10~(70%)	1.78	3~(42%) 0 0	44, 49, 55, 56	0
All	All	1016/1140 (89%)	-0.01	20 (1%) 65 63	17, 33, 61, 83	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	148	ARG	6.5
3	F	4	THR	4.1
1	D	45	LEU	3.4
1	D	205	ARG	3.4
1	А	149	VAL	3.3

# 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
3	SEP	F	7	10/11	0.99	0.13	$26,\!37,\!43,\!43$	0

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



# 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	PO4	В	201	5/5	0.99	0.18	$35,\!37,\!38,\!39$	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

