

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

Dec 16, 2023 – 05:59 PM EST

PDB ID : 4PJE

Title : Structure of human MR1-Ac-6-FP in complex with human MAIT B-B10 TCR

Authors : Birkinshaw, R.W.; Rossjohn, J.

2014-05-12 Deposited on

1.95 Å(reported) Resolution

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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

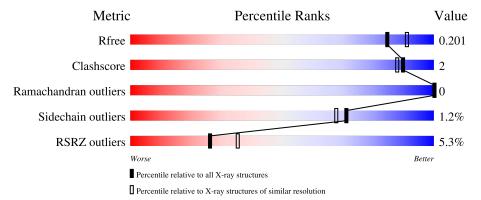
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	٨	071	4%	
1	A	271	92%	5% •
1		071	6%	
1	С	271	89%	• 7%
		400		
2	В	100	96%	• •
			9%	
2	D	100	94%	
			11%	
3	E	205	87%	5% 8%



Mol	Chain	Length	Quality of chain	
3	G	205	91%	5% •
4	F	245	92%	6% •
4	Н	245	92%	6% •



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14211 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 Major histocompatibility complex class I-related gene protein.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	261	Total 2153	C 1381	N 370	O 392	S 10	0	0	0
1	С	252	Total 2065	C 1323	N 358	O 374	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	engineered mutation UNP (	
С	0	MET	-	initiating methionine	UNP Q95460
С	261	SER	CYS	engineered mutation	UNP Q95460

• Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	R	99	Total C N O		О	S	0	0	0	
	Ъ	99	808	514	136	155	3			
9	D	97	Total	С	N	О	S	0	0	0
2	D	91	781	499	129	150	3	0	U	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called TCR-alpha.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
3	Е	189	Total 1471	C 934	N 235	O 292	S 10	0	1	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	G	197	Total 1535	C 967	N 247	O 311	S 10	0	1	0

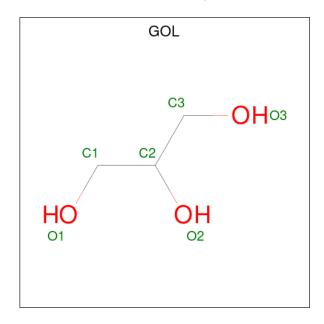
• Molecule 4 is a protein called TCR-beta.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	F	240	Total 1950	C 1223	N 344	O 373	S 10	0	9	0
4	Н	240	Total 1888	C 1183	1 1	O 361	S 9	0	1	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	С	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



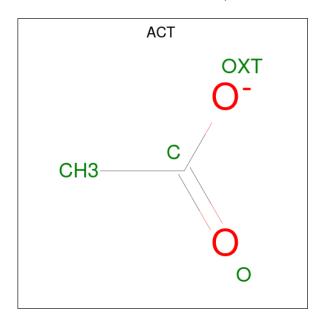
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0
6	Н	1	Total C O 6 3 3	0	0

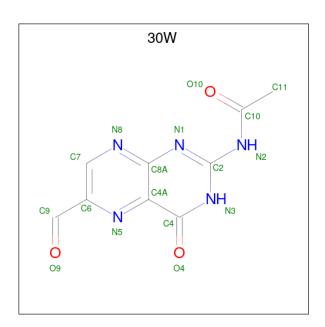
• Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	Е	1	Total C O 4 2 2	0	0

 $\bullet$  Molecule 8 is N-(6-formyl-4-oxo-3,4-dihydropteridin-2-yl)acetamide (three-letter code: 30W) (formula:  $C_9H_7N_5O_3).$ 





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 16			0	0
8	С	1	Total 16		N 5	0	0

• Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Na 1 1	0	0
9	Н	1	Total Na 1 1	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	265	Total O 265 265	0	0
10	В	106	Total O 106 106	0	0
10	С	216	Total O 216 216	0	0
10	D	70	Total O 70 70	0	0
10	Е	146	Total O 146 146	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	222	Total O 222 222	0	0
10	G	214	Total O 214 214	0	0
10	Н	224	Total O 224 224	0	0



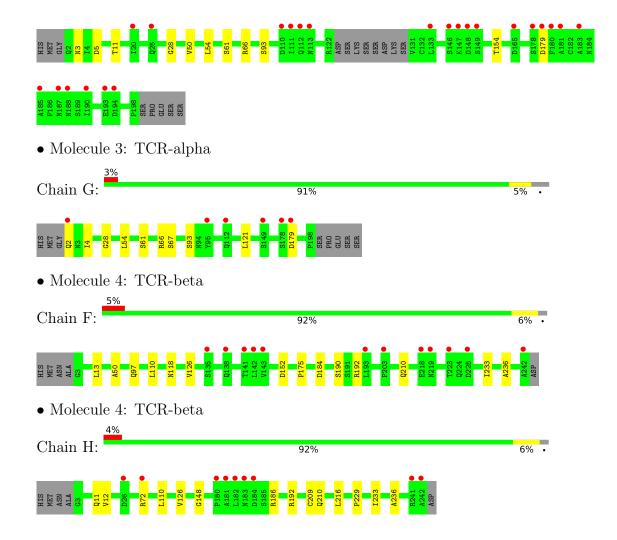
## 3 Residue-property plots (i)

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: Major histocompatibility complex class I-related gene protein









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	219.04Å 72.46Å 143.36Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.50^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	28.55 - 1.95	Depositor
resolution (A)	28.44 - 1.95	EDS
% Data completeness	97.8 (28.55-1.95)	Depositor
(in resolution range)	97.7 (28.44-1.95)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.97 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
D D.	0.171 , 0.197	Depositor
$R, R_{free}$	0.173 , $0.201$	DCC
$R_{free}$ test set	7803 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 51.8	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14211	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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: GOL, ACT, NA, CL, 30W

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
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.55	0/2217	0.61	0/3012
1	С	0.52	0/2126	0.61	0/2888
2	В	0.49	0/831	0.62	0/1131
2	D	0.42	0/804	0.62	0/1097
3	Е	0.50	0/1504	0.64	0/2042
3	G	0.53	0/1569	0.67	0/2129
4	F	0.50	0/2000	0.65	0/2723
4	Н	0.51	0/1938	0.67	0/2640
All	All	0.51	0/12989	0.64	0/17662

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	A	2153	0	2046	9	0
1	С	2065	0	1942	7	0
2	В	808	0	746	1	0
2	D	781	0	712	1	0
3	Е	1471	0	1366	7	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1535	0	1426	5	0
4	F	1950	0	1829	11	0
4	Н	1888	0	1769	10	0
5	A	1	0	0	0	0
5	С	1	0	0	0	0
5	F	1	0	0	0	0
6	A	12	0	16	0	0
6	В	12	0	16	0	0
6	D	6	0	8	1	0
6	F	12	0	16	2	0
6	Н	6	0	8	0	0
7	A	8	0	6	0	0
7	Ε	4	0	3	0	0
8	A	16	0	6	0	0
8	С	16	0	6	0	0
9	F	1	0	0	0	0
9	Н	1	0	0	0	0
10	A	265	0	0	1	0
10	В	106	0	0	0	0
10	С	216	0	0	0	0
10	D	70	0	0	1	0
10	Е	146	0	0	0	0
10	F	222	0	0	0	0
10	G	214	0	0	0	0
10	Н	224	0	0	2	0
All	All	14211	0	11921	44	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 2.

The worst 5 of 44 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)
3:G:66[B]:ARG:HH11	3:G:66[B]:ARG:HG2	1.39	0.85
1:A:65:LEU:HA	4:F:97:GLN:HE22	1.50	0.76
4:H:148:GLY:O	4:H:186[A]:ARG:HD2	1.96	0.67
4:H:72:ARG:HG2	4:H:72:ARG:HH11	1.62	0.64
4:F:118:ASN:HB3	6:F:303:GOL:H2	1.80	0.64

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
1	A	255/271 (94%)	251 (98%)	4 (2%)	0	100	100
1	С	244/271 (90%)	240 (98%)	4 (2%)	0	100	100
2	В	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
2	D	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
3	E	186/205 (91%)	182 (98%)	4 (2%)	0	100	100
3	G	196/205 (96%)	194 (99%)	2 (1%)	0	100	100
4	F	247/245 (101%)	244 (99%)	3 (1%)	0	100	100
4	Н	239/245 (98%)	236 (99%)	3 (1%)	0	100	100
All	All	1559/1642~(95%)	1537 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	A	$229/241\ (95\%)$	227 (99%)	2 (1%)	78 77
1	С	$216/241\ (90\%)$	214 (99%)	2 (1%)	78 77
2	В	89/95~(94%)	87 (98%)	2 (2%)	52 44
2	D	85/95~(90%)	83 (98%)	2 (2%)	49 40
3	E	159/181 (88%)	158 (99%)	1 (1%)	86 85
3	G	169/181 (93%)	164 (97%)	5 (3%)	41 30



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
4	F	209/212 (99%)	208 (100%)	1 (0%)	88	88	
4	Н	$202/212\ (95\%)$	201 (100%)	1 (0%)	88	88	
All	All	1358/1458 (93%)	1342 (99%)	16 (1%)	71	68	

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	179	ASP
3	G	121	LEU
3	Е	179	ASP
3	G	67	SER
2	D	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
4	F	97	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 for Mogul analysis.

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	Trino	Chain	Dag	Link	Bo	nd leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	В	101	-	5,5,5	0.13	0	5,5,5	0.20	0
7	ACT	A	305	-	3,3,3	1.10	0	3,3,3	0.91	0
6	GOL	Н	302	-	5,5,5	0.09	0	5,5,5	0.25	0
6	GOL	В	102	-	5,5,5	0.28	0	5,5,5	0.55	0
6	GOL	A	303	-	5,5,5	0.20	0	5,5,5	0.58	0
6	GOL	F	303	-	5,5,5	0.27	0	5,5,5	0.66	0
8	30W	A	306	1	16,17,18	0.60	0	18,24,25	2.84	3 (16%)
7	ACT	Е	301	-	3,3,3	1.04	0	3,3,3	1.06	0
8	30W	С	302	1	16,17,18	0.60	1 (6%)	18,24,25	2.80	3 (16%)
6	GOL	F	304	-	5,5,5	0.15	0	5,5,5	0.50	0
7	ACT	A	304	-	3,3,3	1.10	0	3,3,3	0.95	0
6	GOL	A	302	-	5,5,5	0.22	0	5,5,5	0.52	0
6	GOL	D	101	-	5,5,5	0.09	0	5,5,5	0.39	0

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
6	GOL	В	101	_	-	0/4/4/4	-
6	GOL	Н	302	-	-	1/4/4/4	-
6	GOL	В	102	-	-	0/4/4/4	-
6	GOL	A	303	-	-	2/4/4/4	-
6	GOL	F	303	-	-	2/4/4/4	-
8	30W	A	306	1	-	0/4/4/6	0/2/2/2
8	30W	С	302	1	-	0/4/4/6	0/2/2/2
6	GOL	F	304	-	-	4/4/4/4	-
6	GOL	A	302	-	-	0/4/4/4	-
6	GOL	D	101	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
8	С	302	30W	C2-N2	-2.01	1.33	1.37



The worst	5	of	6	bond	angle	outliers	are	listed	below:
TITO WOLDS	$\mathbf{O}$	$O_{\mathbf{I}}$	$\circ$	Oliu	WII SIC	Outiloid	COL C	IIDUCA	DOIOW.

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
8	С	302	30W	N2-C2-N3	9.48	132.45	117.98
8	A	306	30W	N2-C2-N3	9.32	132.21	117.98
8	A	306	30W	N2-C2-N1	-6.38	109.05	117.72
8	С	302	30W	N2-C2-N1	-5.96	109.62	117.72
8	С	302	30W	C4A-C8A-N1	-2.86	119.09	123.18

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	101	GOL	O1-C1-C2-C3
6	F	304	GOL	O1-C1-C2-C3
6	F	304	GOL	C1-C2-C3-O3
6	F	304	GOL	O1-C1-C2-O2
6	A	303	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	303	GOL	2	0
6	D	101	GOL	1	0

### 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	261/271 (96%)	-0.11	10 (3%) 40 50	18, 27, 51, 73	1 (0%)
1	С	252/271 (92%)	0.03	15 (5%) 21 30	20, 32, 58, 94	0
2	В	99/100 (99%)	-0.14	0 100 100	21, 33, 56, 65	0
2	D	97/100 (97%)	0.43	9 (9%) 8 14	26, 52, 82, 96	0
3	E	189/205 (92%)	0.43	23 (12%) 4 6	20, 39, 84, 109	0
3	G	197/205 (96%)	-0.07	6 (3%) 50 59	20, 30, 54, 71	6 (3%)
4	F	240/245 (97%)	-0.04	12 (5%) 28 39	19, 33, 65, 193	2 (0%)
4	Н	240/245 (97%)	-0.14	9 (3%) 40 50	22, 31, 55, 78	4 (1%)
All	All	1575/1642 (95%)	0.02	84 (5%) 26 35	18, 32, 66, 193	13 (0%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	VAL	7.6
3	Е	179	ASP	6.1
3	Е	149	SER	5.9
4	Н	182	LEU	5.4
3	Е	178	SER	5.1

#### 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)

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	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
7	ACT	A	305	4/4	0.26	0.23	97,97,97,99	0
6	GOL	F	304	6/6	0.60	0.29	58,60,62,64	0
7	ACT	Е	301	4/4	0.61	0.23	49,49,52,58	0
6	GOL	D	101	6/6	0.80	0.25	47,52,54,57	0
6	GOL	A	302	6/6	0.84	0.28	32,36,37,39	6
6	GOL	F	303	6/6	0.87	0.29	31,42,46,47	0
6	GOL	A	303	6/6	0.89	0.17	32,42,46,49	0
5	CL	A	301	1/1	0.92	0.06	59,59,59,59	0
6	GOL	Н	302	6/6	0.92	0.10	35,36,38,39	6
7	ACT	A	304	4/4	0.95	0.14	40,62,64,64	0
9	NA	Н	301	1/1	0.95	0.05	32,32,32,32	0
6	GOL	В	101	6/6	0.96	0.09	23,25,28,29	0
8	30W	С	302	16/17	0.97	0.18	23,26,28,29	0
6	GOL	В	102	6/6	0.97	0.13	23,24,28,32	6
5	CL	С	301	1/1	0.98	0.05	34,34,34,34	0
8	30W	A	306	16/17	0.98	0.13	23,24,25,27	0
9	NA	F	302	1/1	0.99	0.15	27,27,27,27	0
5	CL	F	301	1/1	0.99	0.05	41,41,41,41	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

