

wwPDB X-ray Structure Validation Summary Report (i)

Feb 6, 2024 – 04:44 PM EST

PDB ID : 2GJW

Title : RNA Recognition and Cleavage by an Splicing Endonuclease

Authors: Xue, S.; Calvin, K.; Li, H.

Deposited on : 2006-03-31

Resolution : 2.85 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

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

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

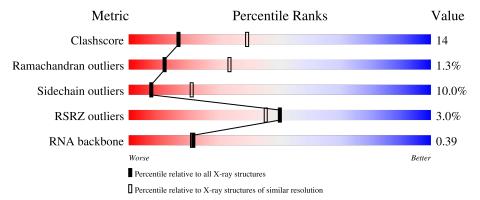
Validation Pipeline (wwPDB-VP) : 2.36

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 2.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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	y of chai	n		
			21%					
1	Е	19	47%		16%	11%	21%	5%
			32%					
1	I	19	42%		32%		16%	11%
			33%	•				
2	F	12	25%	33%		25%	1	L7%
			42%					
2	J	12	33%	17%		33%	1	L7%
			29%					
3	Н	7	29%		43%		29%	



Mol	Chain	Length	Quality of cha	ain	
			29%		
3	L	7	57%	29%	14%
			2%		
4	A	313	62%	30%	6% •
			.% •		
4	В	313	70%	24%	
			.% •		
4	С	313	66%	29%	• •
			.% •	_	
4	D	313	62%	29%	5% •



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11778 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 RNA chain called 5'-R(*GP*CP*GP*AP*CP*CP*GP*AP*CP*CP*AP*(D U)P*AP*GP*CP*UP*GP*CP*A)-3'.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	E	18	Total 379				P 17	0	0	0
1	I	19	Total 401			O 127	P 18	0	0	0

• Molecule 2 is a RNA chain called 5'-R(*UP*GP*CP*AP*GP*CP*GP*UP*CP*AP*(A 23))-3'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Г	19	Total	С	N	О	Р	0	0	0
2	I'	12	258	115	48	83	12	0	U	U
2	Т	12	Total	С	N	О	Р	0	0	0
2	J	12	258	115	48	83	12		U	U

• Molecule 3 is a RNA chain called 5'-R(*AP*GP*GP*UP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	Н	7	Total	С	N	О	Р	0	0	0
3	11	'	148	67	28	47	6	0	U	U
9	Т	7	Total	С	N	О	Р	0	0	0
3	L	1	148	67	28	47	6	U	U	U

• Molecule 4 is a protein called tRNA-splicing endonuclease.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
4	A	308	Total 2569	C 1642	N 445	O 476	S 6	0	0	0
4	В	304	Total 2529	C 1618	N 433	O 472	S 6	0	0	0
4	С	307	Total 2559	C 1636	N 442	O 475	S 6	0	0	0



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	D	304	Total 2529	C 1618	N 433	O 472	S 6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP O29362
A	-3	HIS	-	expression tag	UNP O29362
A	-2	HIS	-	expression tag	UNP O29362
A	-1	HIS	-	expression tag	UNP O29362
A	0	HIS	-	expression tag	UNP O29362
A	1	HIS	-	expression tag	UNP O29362
A	2	HIS	-	expression tag	UNP O29362
A	3	HIS	-	expression tag	UNP O29362
A	4	HIS	-	expression tag	UNP O29362
A	155	VAL	ILE	see remark 999	UNP O29362
В	-5	MET	-	expression tag	UNP O29362
В	-4	HIS	-	expression tag	UNP O29362
В	-3	HIS	-	expression tag	UNP O29362
В	-2	HIS	-	expression tag	UNP O29362
В	-1	HIS	_	expression tag	UNP O29362
В	0	HIS	-	expression tag	UNP O29362
В	1	HIS	-	expression tag	UNP O29362
В	2	HIS	-	expression tag	UNP O29362
В	3	HIS	-	expression tag	UNP O29362
В	71	VAL	ILE	see remark 999	UNP O29362
С	-5	MET	-	expression tag	UNP O29362
С	-4	HIS	-	expression tag	UNP O29362
С	-3	HIS	-	expression tag	UNP O29362
С	-2	HIS	-	expression tag	UNP O29362
С	-1	HIS	-	expression tag	UNP O29362
С	0	HIS	-	expression tag	UNP O29362
С	1	HIS	-	expression tag	UNP O29362
С	2	HIS	-	expression tag	UNP O29362
С	3	HIS	-	expression tag	UNP O29362
С	71	VAL	ILE	see remark 999	UNP O29362
D	-4	MET	-	expression tag	UNP O29362
D	-3	HIS	-	expression tag	UNP O29362
D	-2	HIS	_	expression tag	UNP O29362
D	-1	HIS	_	expression tag	UNP O29362
D	0	HIS	_	expression tag	UNP O29362
D	1	HIS	-	expression tag	UNP O29362



Chain	Residue	Modelled	Actual	Comment	Reference
D	2	HIS	-	expression tag	UNP O29362
D	3	HIS	-	expression tag	UNP O29362
D	4	HIS	-	expression tag	UNP O29362
D	155	VAL	ILE	see remark 999	UNP O29362



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.

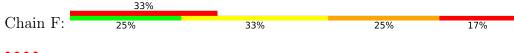
• Molecule 1: 5'-R(*GP*CP*GP*AP*CP*CP*GP*AP*CP*CP*AP*(DU)P*AP*GP*CP*UP*GP*CP*A)-3'



• Molecule 1: 5'-R(*GP*CP*GP*AP*CP*CP*GP*AP*CP*CP*AP*(DU)P*AP*GP*CP*UP*GP*CP*A)-3'

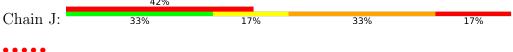


• Molecule 2: 5'-R(*UP*GP*CP*AP*GP*CP*GP*GP*UP*CP*AP*(A23))-3'





• Molecule 2: 5'-R(*UP*GP*CP*AP*GP*CP*GP*GP*UP*CP*AP*(A23))-3'





• Molecule 3: 5'-R(*AP*GP*GP*UP*CP*GP*C)-3'





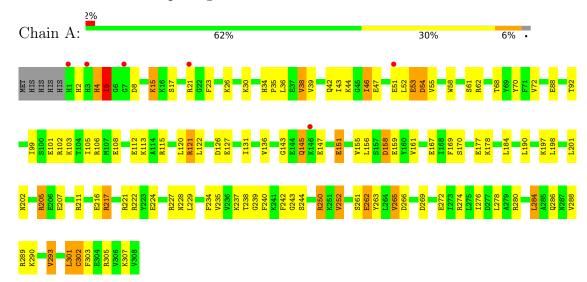




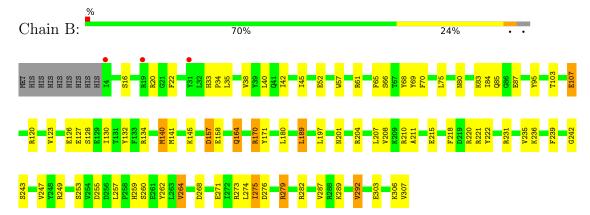


A15 G16 G17 U18 G20 G20

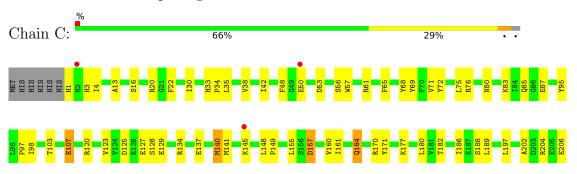
• Molecule 4: tRNA-splicing endonuclease



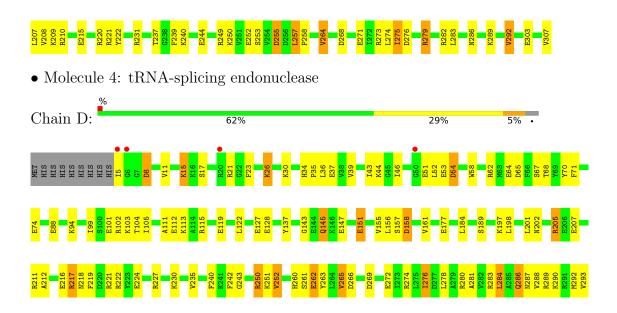
• Molecule 4: tRNA-splicing endonuclease



• Molecule 4: tRNA-splicing endonuclease











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	89.97Å 140.41Å 82.05Å	Depositor
a, b, c, α , β , γ	90.00° 111.68° 90.00°	Depositor
Resolution (Å)	35.09 - 2.85	Depositor
resolution (A)	35.10 - 2.73	EDS
% Data completeness	83.9 (35.09-2.85)	Depositor
(in resolution range)	77.0 (35.10-2.73)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) > 1$	2.03 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R R.	0.247 , 0.296	Depositor
R, R_{free}	0.250 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 55.3	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	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 53.62 % 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 4.1074e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities 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: A23

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	Bo	nd lengths	В	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	Е	0.93	0/423	1.67	6/657~(0.9%)
1	I	1.02	0/448	1.72	7/696 (1.0%)
2	F	1.12	0/260	2.10	16/404 (4.0%)
2	J	1.17	0/260	2.06	9/404 (2.2%)
3	Н	1.09	1/165~(0.6%)	2.38	6/256 (2.3%)
3	L	1.12	1/165~(0.6%)	2.34	8/256 (3.1%)
4	A	0.66	0/2617	0.74	1/3511 (0.0%)
4	В	0.64	0/2573	0.73	0/3451
4	С	0.63	0/2606	0.75	0/3496
4	D	0.64	0/2573	0.76	0/3451
All	All	0.72	$2/12090 \ (0.0\%)$	1.04	53/16582 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\textup{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	L	17	G	P-OP2	-5.37	1.39	1.49
3	Н	17	G	P-OP1	-5.21	1.40	1.49

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
3	L	20	G	OP1-P-OP2	-16.68	94.58	119.60
2	J	4	G	OP1-P-OP2	-15.20	96.80	119.60
3	L	17	G	OP1-P-OP2	-15.18	96.84	119.60
2	F	4	G	OP1-P-OP2	-15.14	96.89	119.60
3	Н	20	G	OP1-P-OP2	-15.04	97.04	119.60

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	Е	379	0	198	11	0
1	I	401	0	209	8	0
2	F	258	0	130	9	0
2	J	258	0	130	6	0
3	Н	148	0	78	4	0
3	L	148	0	78	4	0
4	A	2569	0	2576	108	0
4	В	2529	0	2545	70	0
4	С	2559	0	2569	75	0
4	D	2529	0	2545	92	0
All	All	11778	0	11058	325	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 14.

The worst 5 of 325 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:F:3:U:H5'	4:B:306:LYS:HD3	1.47	0.96
4:B:201:ASN:HB3	4:C:4:ILE:HG22	1.47	0.93
4:A:288:VAL:HG23	4:A:290:LYS:HG3	1.50	0.93
4:A:235:VAL:HG21	4:A:252:VAL:CG1	2.05	0.86
4:B:201:ASN:HB3	4:C:4:ILE:CG2	2.04	0.86

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	entiles
4	A	306/313 (98%)	276 (90%)	25 (8%)	5 (2%)	9	28
4	В	302/313~(96%)	282 (93%)	16 (5%)	4 (1%)	12	33
4	C	305/313 (97%)	282 (92%)	19 (6%)	4 (1%)	12	33
4	D	302/313~(96%)	274 (91%)	25 (8%)	3 (1%)	15	40
All	All	1215/1252 (97%)	1114 (92%)	85 (7%)	16 (1%)	12	33

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	5	ILE
4	A	252	VAL
4	В	157	ASP
4	С	140	MET
4	С	157	ASP

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
4	A	276/281 (98%)	240 (87%)	36 (13%)	4 11
4	В	272/281 (97%)	252 (93%)	20 (7%)	13 35
4	С	275/281 (98%)	254 (92%)	21 (8%)	13 33
4	D	272/281 (97%)	239 (88%)	33 (12%)	5 13
All	All	1095/1124~(97%)	985 (90%)	110 (10%)	7 21

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	С	83	LYS
4	С	257	LEU
4	D	307	LYS
4	D	250	ARG



Mol	Chain	Res	Type
4	С	107	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	199	ASN
4	D	202	ASN
4	D	287	ASN
4	D	286	GLN
4	В	286	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Ε	16/19 (84%)	6 (37%)	0
1	I	17/19 (89%)	7 (41%)	1 (5%)
2	F	11/12 (91%)	5 (45%)	1 (9%)
2	J	11/12 (91%)	5 (45%)	1 (9%)
3	Н	6/7 (85%)	3 (50%)	1 (16%)
3	L	6/7 (85%)	4 (66%)	0
All	All	67/76 (88%)	30 (44%)	4 (5%)

5 of 30 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Е	4	С
1	Е	5	G
1	Е	13	A
1	Е	15	A
1	Е	19	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	4	G
3	Н	19	С
1	I	20	С
2	J	4	G



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

2 non-standard protein/DNA/RNA residues are 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).

Mol Ty	Trme	Type Chain	Chain	Chain	Chain	Dag	Link	Bond lengths				Bond angles		
	туре		Res	S LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2				
2	A23	F	14	2	19,28,29	2.89	3 (15%)	19,43,46	5.26	9 (47%)				
2	A23	J	14	2	19,28,29	3.13	4 (21%)	19,43,46	5.86	9 (47%)				

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A23	F	14	2	-	2/3/35/36	0/4/4/4
2	A23	J	14	2	-	2/3/35/36	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\mathring{A})$	Ideal(A)
2	J	14	A23	C4-N3	-12.03	1.19	1.35
2	F	14	A23	C4-N3	-11.04	1.20	1.35
2	J	14	A23	C5-N7	-3.85	1.25	1.39
2	F	14	A23	C5-N7	-3.67	1.26	1.39
2	J	14	A23	C6-N1	-3.51	1.21	1.37

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	J	14	A23	C4-C5-N7	-15.97	92.75	109.40
2	F	14	A23	C4-C5-N7	-12.96	95.89	109.40
2	J	14	A23	C5-C6-N6	12.86	139.90	120.35
2	F	14	A23	C5-C6-N6	11.45	137.75	120.35
2	J	14	A23	C1'-N9-C4	10.07	144.33	126.64



There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	14	A23	C3'-C4'-C5'-O5'
2	F	14	A23	O4'-C4'-C5'-O5'
2	J	14	A23	C3'-C4'-C5'-O5'
2	J	14	A23	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	14	A23	3	0
2	J	14	A23	1	0

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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	E	17/19 (89%)	1.27	4 (23%) 0 0	58, 84, 175, 191	0
1	I	18/19 (94%)	1.33	6 (33%) 0 0	49, 90, 181, 186	0
2	F	11/12 (91%)	1.57	4 (36%) 0 0	46, 66, 182, 189	0
2	J	11/12 (91%)	1.62	5 (45%) 0 0	50, 68, 164, 165	0
3	Н	7/7 (100%)	1.49	2 (28%) 0 0	57, 86, 139, 148	0
3	L	7/7 (100%)	1.98	2 (28%) 0 0	57, 88, 163, 178	0
4	A	308/313 (98%)	-0.08	6 (1%) 66 64	28, 57, 91, 122	0
4	В	304/313 (97%)	-0.08	3 (0%) 82 81	26, 52, 92, 120	0
4	С	307/313 (98%)	-0.10	3 (0%) 82 81	31, 54, 93, 125	0
4	D	304/313 (97%)	-0.06	4 (1%) 77 76	29, 54, 89, 121	0
All	All	$1294/1328 \ (97\%)$	0.00	39 (3%) 50 45	26, 56, 99, 191	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	6	GLY	6.5
1	I	21	A	6.3
3	L	21	С	5.9
4	D	5	ILE	5.4
2	F	5	С	4.9

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	A23	F	14	25/26	0.92	0.18	51,54,68,70	0
2	A23	J	14	25/26	0.93	0.19	71,73,77,80	0

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.

