



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:45 am BST

PDB ID : 3QDJ  
Title : The complex between TCR DMF5 and human Class I MHC HLA-A2 with the bound MART-1(27-35) nonameric peptide  
Authors : Borbulevych, O.Y.; Baker, B.M.  
Deposited on : 2011-01-18  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

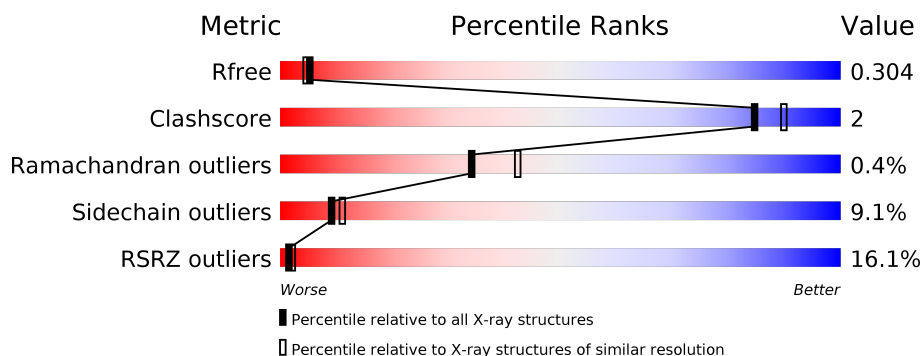
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	275	<div> <div>7%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	B	100	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
3	C	9	<div> <div>11%</div> <div>67%</div> <div>22%</div> <div>11%</div> </div>
4	D	199	<div> <div>30%</div> <div>85%</div> <div>15%</div> <div>.</div> </div>
5	E	242	<div> <div>21%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6646 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2255	1408	412	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			843	537	141	160	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called MART-1(27-35) peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			57	37	9	11			

- Molecule 4 is a protein called DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1546	965	255	318	8			

- Molecule 5 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1897	1191	333	365	8			

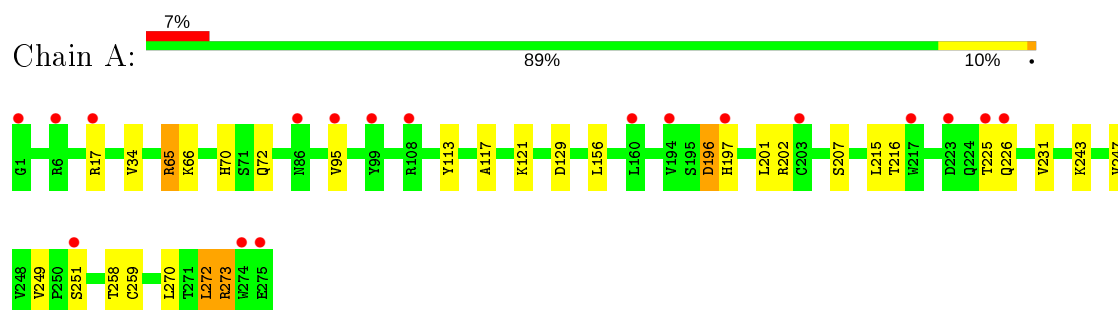
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total 24	O 24	0	0
6	B	13	Total 13	O 13	0	0
6	C	2	Total 2	O 2	0	0
6	D	6	Total 6	O 6	0	0
6	E	3	Total 3	O 3	0	0

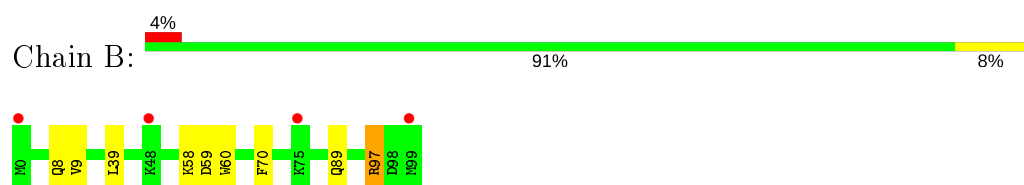
### 3 Residue-property plots [i](#)

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.

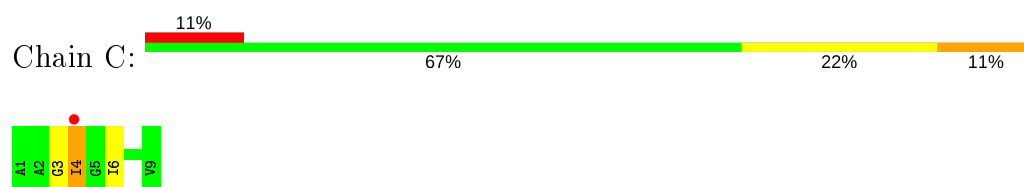
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



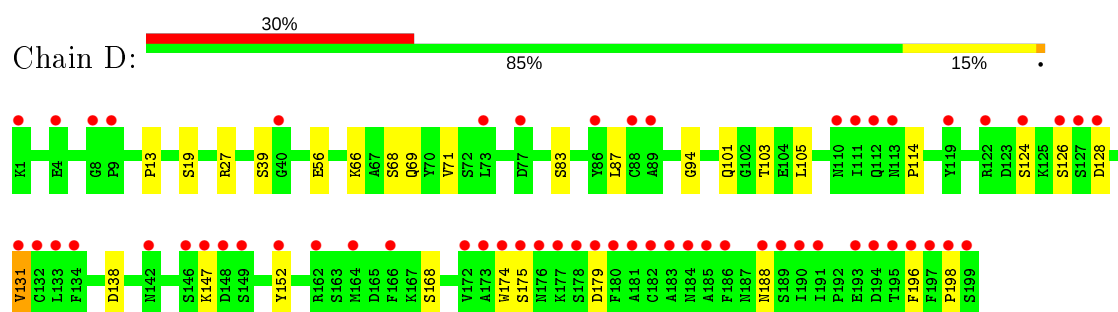
- Molecule 2: Beta-2-microglobulin



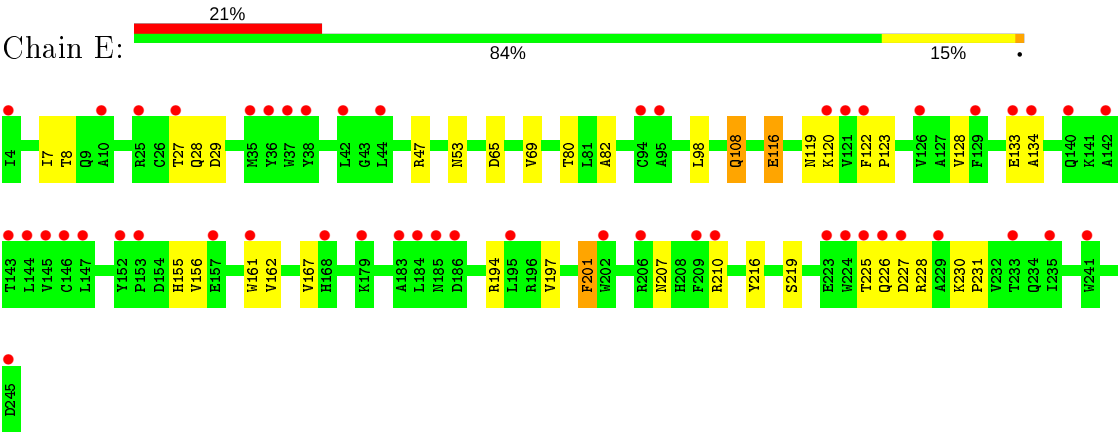
- Molecule 3: MART-1(27-35) peptide



- Molecule 4: DMF5 alpha chain



- Molecule 5: DMF5 beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.77Å 46.30Å 85.86Å 90.00° 106.55° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.30) 96.6 (19.85-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.240 , 0.299 0.246 , 0.304	Depositor DCC
$R_{free}$ test set	1887 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality

### 5.1 Standard geometry

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	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.68	0/2323	0.83	3/3152 (0.1%)
2	B	0.69	0/868	0.81	1/1169 (0.1%)
3	C	1.11	0/56	1.14	0/74
4	D	0.57	0/1579	0.71	0/2135
5	E	0.52	0/1946	0.70	0/2651
All	All	0.62	0/6772	0.77	4/9181 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	129	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	65	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	272	LEU	CA-CB-CG	5.45	127.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	3	GLY	Peptide



## 5.2 Too-close contacts ⓘ

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	2255	0	2109	11	0
2	B	843	0	812	3	0
3	C	57	0	67	2	0
4	D	1546	0	1460	6	0
5	E	1897	0	1808	13	0
6	A	24	0	0	0	0
6	B	13	0	0	0	0
6	C	2	0	0	0	0
6	D	6	0	0	0	0
6	E	3	0	0	0	0
All	All	6646	0	6256	30	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.

All (30) 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:A:72:GLN:NE2	5:E:53:ASN:OD1	2.32	0.62
3:C:4:ILE:O	3:C:4:ILE:CG1	2.48	0.61
3:C:4:ILE:HG12	3:C:4:ILE:O	2.03	0.59
4:D:114:PRO:HB3	4:D:138:ASP:HB3	1.91	0.53
5:E:225:THR:HG23	5:E:226:GLN:HG2	1.93	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.47
1:A:66:LYS:O	1:A:70:HIS:ND1	2.40	0.46
4:D:131:VAL:HG23	4:D:174:TRP:HB3	1.96	0.46
1:A:196:ASP:N	1:A:196:ASP:OD1	2.46	0.46
5:E:108:GLN:HG2	5:E:108:GLN:H	1.53	0.46
5:E:119:ASN:HB3	5:E:120:LYS:HD2	1.98	0.45
5:E:161:TRP:HB2	5:E:210:ARG:HB3	1.98	0.45
4:D:124:SER:OG	5:E:128:VAL:O	2.30	0.45
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.99	0.44
2:B:97:ARG:HG2	2:B:97:ARG:H	1.42	0.44
1:A:215:LEU:HD22	1:A:243:LYS:HD3	2.00	0.44
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:LYS:HB2	4:D:188:ASN:HD21	1.82	0.43
5:E:116:GLU:H	5:E:116:GLU:HG2	1.62	0.43
5:E:201:PHE:O	5:E:207:ASN:ND2	2.43	0.43
1:A:65:ARG:HB3	4:D:94:GLY:H	1.84	0.43
1:A:259:CYS:HB3	1:A:272:LEU:HB2	2.00	0.43
5:E:226:GLN:HB3	5:E:227:ASP:H	1.68	0.42
4:D:198:PRO:HG2	5:E:134:ALA:HB1	2.01	0.42
2:B:39:LEU:HA	2:B:39:LEU:HD23	1.85	0.42
5:E:230:LYS:HA	5:E:231:PRO:HD3	1.82	0.41
5:E:122:PHE:HA	5:E:123:PRO:HD3	1.93	0.41
1:A:258:THR:HG22	1:A:273:ARG:HG3	2.02	0.41
5:E:155:HIS:HB3	5:E:216:TYR:HB2	2.03	0.40

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	Percentiles	
1	A	274/275 (100%)	264 (96%)	9 (3%)	1 (0%)	34	42
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	197/199 (99%)	179 (91%)	17 (9%)	1 (0%)	29	35
5	E	240/242 (99%)	224 (93%)	15 (6%)	1 (0%)	34	42
All	All	816/825 (99%)	768 (94%)	45 (6%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
4	D	83	SER

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Mol	Chain	Res	Type
5	E	82	ALA

### 5.3.2 Protein sidechains ⓘ

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	232/231 (100%)	217 (94%)	15 (6%)	17	23
2	B	96/95 (101%)	90 (94%)	6 (6%)	18	24
3	C	5/5 (100%)	3 (60%)	2 (40%)	0	0
4	D	176/176 (100%)	155 (88%)	21 (12%)	5	5
5	E	204/204 (100%)	183 (90%)	21 (10%)	7	8
All	All	713/711 (100%)	648 (91%)	65 (9%)	9	11

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	34	VAL
1	A	95	VAL
1	A	113	TYR
1	A	121	LYS
1	A	156	LEU
1	A	196	ASP
1	A	197	HIS
1	A	207	SER
1	A	216	THR
1	A	225	THR
1	A	231	VAL
1	A	247	VAL
1	A	251	SER
1	A	273	ARG
2	B	8	GLN
2	B	9	VAL
2	B	58	LYS

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Mol	Chain	Res	Type
2	B	70	PHE
2	B	89	GLN
2	B	97	ARG
3	C	4	ILE
3	C	6	ILE
4	D	13	PRO
4	D	19	SER
4	D	27	ARG
4	D	39	SER
4	D	56	GLU
4	D	66	LYS
4	D	68	SER
4	D	69	GLN
4	D	71	VAL
4	D	87	LEU
4	D	101	GLN
4	D	103	THR
4	D	105	LEU
4	D	126	SER
4	D	128	ASP
4	D	131	VAL
4	D	152	TYR
4	D	168	SER
4	D	175	SER
4	D	179	ASP
4	D	196	PHE
5	E	7	ILE
5	E	8	THR
5	E	27	THR
5	E	28	GLN
5	E	29	ASP
5	E	47	ARG
5	E	65	ASP
5	E	69	VAL
5	E	80	THR
5	E	98	LEU
5	E	108	GLN
5	E	116	GLU
5	E	133	GLU
5	E	156	VAL
5	E	162	VAL
5	E	167	VAL

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Mol	Chain	Res	Type
5	E	194	ARG
5	E	197	VAL
5	E	201	PHE
5	E	219	SER
5	E	228	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	115	GLN
1	A	218	GLN
4	D	169	ASN
4	D	188	ASN
5	E	53	ASN
5	E	208	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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	275/275 (100%)	0.46	18 (6%)	18 24	48, 66, 102, 137	0
2	B	100/100 (100%)	0.36	4 (4%)	38 45	48, 61, 81, 87	0
3	C	9/9 (100%)	0.49	1 (11%)	5 7	53, 57, 60, 64	0
4	D	199/199 (100%)	1.62	59 (29%)	0 0	58, 93, 161, 176	0
5	E	242/242 (100%)	1.17	51 (21%)	1 1	52, 100, 130, 145	0
All	All	825/825 (100%)	0.94	133 (16%)	1 2	48, 77, 137, 176	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	146	SER	12.4
4	D	126	SER	12.0
5	E	184	LEU	8.6
4	D	190	ILE	7.3
4	D	132	CYS	6.6
4	D	113	ASN	6.4
4	D	196	PHE	5.9
4	D	199	SER	5.8
5	E	42	LEU	5.7
5	E	44	LEU	5.6
4	D	176	ASN	5.5
1	A	17	ARG	5.4
5	E	185	ASN	5.1
4	D	189	SER	5.0
1	A	1	GLY	4.8
5	E	229	ALA	4.8
4	D	179	ASP	4.6
4	D	112	GLN	4.5
4	D	184	ASN	4.3
4	D	180	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
5	E	183	ALA	4.3
5	E	168	HIS	4.3
4	D	173	ALA	4.2
5	E	206	ARG	4.0
4	D	147	LYS	4.0
4	D	188	ASN	4.0
4	D	177	LYS	3.9
4	D	198	PRO	3.9
4	D	162	ARG	3.9
4	D	164	MET	3.9
4	D	182	CYS	3.8
4	D	1	LYS	3.8
2	B	48	LYS	3.8
5	E	186	ASP	3.7
5	E	241	TRP	3.7
4	D	186	PHE	3.7
1	A	194	VAL	3.6
4	D	134	PHE	3.6
4	D	152	TYR	3.5
5	E	134	ALA	3.5
1	A	223	ASP	3.5
5	E	245	ASP	3.5
5	E	94	CYS	3.5
1	A	251	SER	3.5
5	E	120	LYS	3.4
4	D	194	ASP	3.4
5	E	209	PHE	3.4
4	D	124	SER	3.4
2	B	99[A]	MET	3.4
5	E	195	LEU	3.3
4	D	89	ALA	3.3
5	E	210	ARG	3.3
4	D	178	SER	3.3
5	E	37	TRP	3.3
4	D	172	VAL	3.2
4	D	195	THR	3.2
4	D	122	ARG	3.1
1	A	275	GLU	3.1
4	D	4	GLU	3.1
4	D	174	TRP	3.1
4	D	149	SER	3.1
4	D	111	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	142	ASN	3.1
5	E	140	GLN	3.1
4	D	185	ALA	3.1
4	D	77	ASP	3.1
4	D	133	LEU	3.1
5	E	161	TRP	3.1
4	D	193	GLU	3.1
5	E	133	GLU	3.0
4	D	197	PHE	3.0
5	E	129	PHE	3.0
4	D	110	ASN	3.0
5	E	35	MET	3.0
1	A	108	ARG	3.0
5	E	223	GLU	3.0
1	A	225	THR	2.9
5	E	145	VAL	2.9
4	D	175	SER	2.9
1	A	217	TRP	2.9
5	E	38	TYR	2.8
5	E	4	ILE	2.8
2	B	0	MET	2.8
4	D	88	CYS	2.8
4	D	86	TYR	2.8
4	D	9	PRO	2.7
4	D	181	ALA	2.7
5	E	95	ALA	2.6
1	A	197	HIS	2.6
5	E	226	GLN	2.6
5	E	224	TRP	2.6
4	D	191	ILE	2.6
5	E	126	VAL	2.6
5	E	227	ASP	2.6
4	D	131	VAL	2.6
5	E	122	PHE	2.6
5	E	233	THR	2.6
4	D	148	ASP	2.5
5	E	153	PRO	2.5
5	E	152	TYR	2.5
5	E	143	THR	2.5
5	E	25	ARG	2.4
5	E	142	ALA	2.4
5	E	36	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	119	TYR	2.4
5	E	10	ALA	2.4
4	D	8	GLY	2.4
4	D	183	ALA	2.4
4	D	127	SER	2.4
1	A	203	CYS	2.3
5	E	147	LEU	2.3
2	B	75	LYS	2.3
4	D	166	PHE	2.2
5	E	121	VAL	2.2
1	A	274	TRP	2.2
4	D	40	GLY	2.2
5	E	144	LEU	2.2
5	E	157	GLU	2.2
5	E	179	LYS	2.2
5	E	202	TRP	2.2
5	E	27	THR	2.2
5	E	146	CYS	2.1
1	A	160	LEU	2.1
1	A	95	VAL	2.1
5	E	225	THR	2.1
3	C	4	ILE	2.1
4	D	128	ASP	2.1
1	A	99	TYR	2.1
1	A	6	ARG	2.1
1	A	226	GLN	2.0
4	D	73	LEU	2.0
1	A	86	ASN	2.0
5	E	235	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.