



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 AM GMT

PDB ID : 3QDM  
Title : The complex between TCR DMF4 and human Class I MHC HLA-A2 with the bound MART-1(26-35)(A27L) decameric peptide  
Authors : Borbulevych, O.Y.; Baker, B.M.  
Deposited on : 2011-01-18  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

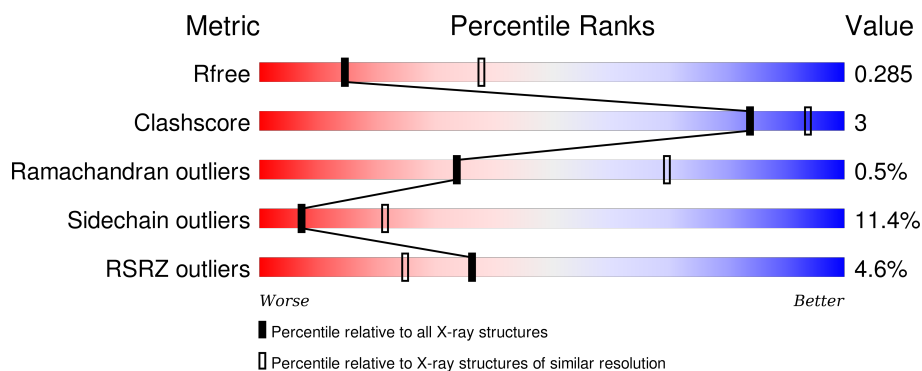
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	 3% 88% 11% .
2	B	100	 2% 92% 7% .
3	C	10	 80% 20%
4	D	195	 9% 79% 19% ..
5	E	242	 4% 82% 16% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6635 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	0	0
			2247	1403	409	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	10	Total	C	N	O	0	0	0
			69	45	10	14			

- Molecule 4 is a protein called DMF4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	1	0
			1513	950	245	309	9			

- Molecule 5 is a protein called DMF4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1930	1209	339	376	6			

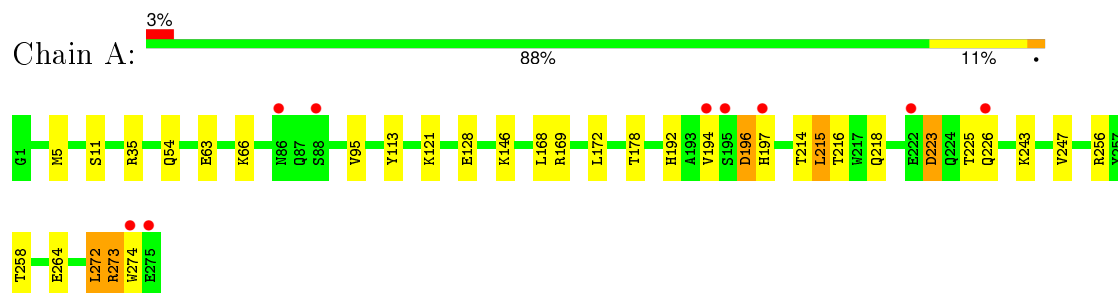
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	B	6	Total 6	O 6	0	0
6	C	1	Total 1	O 1	0	0
6	D	7	Total 7	O 7	0	0
6	E	5	Total 5	O 5	0	0

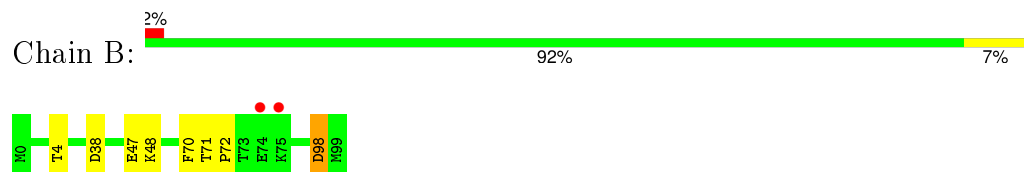
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

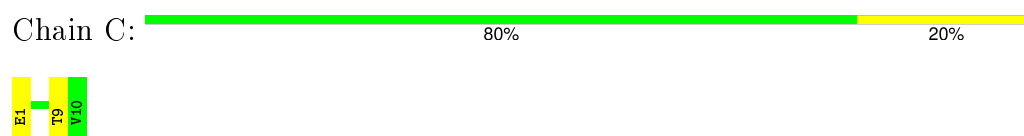
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



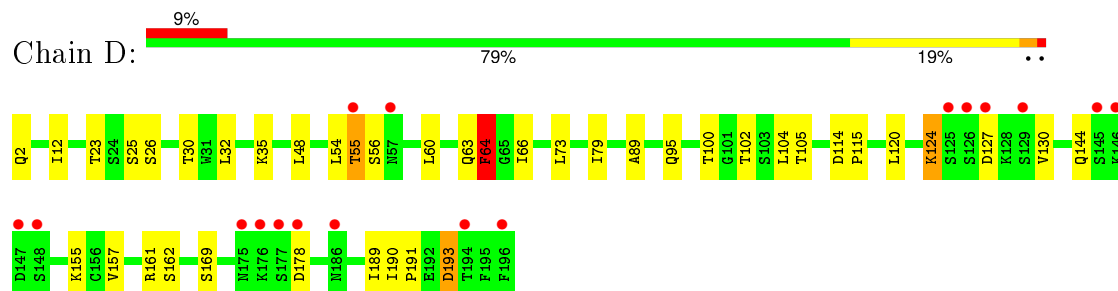
- Molecule 2: Beta-2-microglobulin



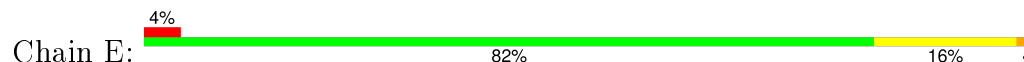
- Molecule 3: MART-1(27-35) peptide

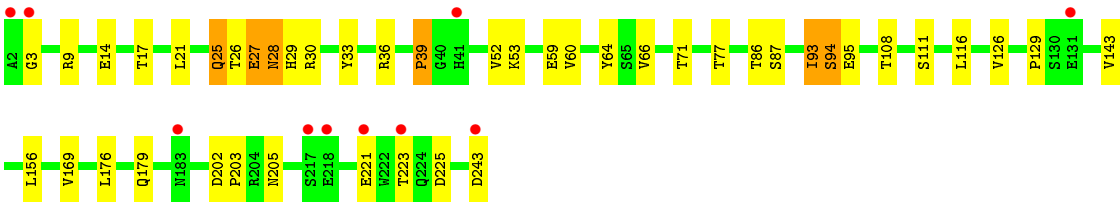


- Molecule 4: DMF4 alpha chain



- Molecule 5: DMF4 beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.01Å 69.75Å 227.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.80) 93.0 (19.81-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.211 , 0.284 0.213 , 0.285	Depositor DCC
$R_{free}$ test set	1064 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21056 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.53	0/2312	0.71	1/3137 (0.0%)
2	B	0.46	0/868	0.65	0/1169
3	C	0.62	0/68	1.00	0/90
4	D	0.52	0/1549	0.77	1/2101 (0.0%)
5	E	0.53	0/1983	0.72	0/2699
All	All	0.52	0/6780	0.72	2/9196 (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
1	A	0	1
4	D	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	LEU	CA-CB-CG	5.61	128.20	115.30
4	D	64	PHE	CB-CG-CD2	5.18	124.43	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	GLN	Peptide
4	D	55	THR	Peptide
4	D	56	SER	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	2247	0	2096	10	0
2	B	843	0	812	2	0
3	C	69	0	79	0	0
4	D	1513	0	1428	10	0
5	E	1930	0	1819	19	0
6	A	14	0	0	0	0
6	B	6	0	0	0	0
6	C	1	0	0	0	0
6	D	7	0	0	0	0
6	E	5	0	0	0	0
All	All	6635	0	6234	38	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 3.

All (38) 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:196:ASP:N	1:A:196:ASP:OD1	2.14	0.77
5:E:30:ARG:NH2	5:E:95:GLU:OE2	2.23	0.72
1:A:223:ASP:OD2	1:A:223:ASP:N	2.24	0.70
4:D:178:ASP:N	4:D:178:ASP:OD1	2.41	0.53
5:E:33:TYR:HE2	5:E:94:SER:HB2	1.77	0.50
5:E:25:GLN:NE2	5:E:28:ASN:O	2.47	0.48
5:E:14:GLU:HB3	5:E:116:LEU:HG	1.95	0.48
5:E:202:ASP:OD2	5:E:205:ASN:ND2	2.46	0.48
4:D:32:LEU:HB2	4:D:89:ALA:HB3	1.96	0.47
1:A:63:GLU:OE1	1:A:66:LYS:NZ	2.38	0.47
4:D:120:LEU:HD22	5:E:129:PRO:HA	1.97	0.47
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.97	0.46
5:E:36:ARG:NH1	5:E:64:TYR:OH	2.46	0.46
4:D:48:LEU:HD13	4:D:64:PHE:HB2	1.98	0.45
5:E:86:THR:HG23	5:E:111:SER:HA	1.98	0.45
1:A:215:LEU:HD22	1:A:243:LYS:HD3	1.98	0.45
5:E:59:GLU:H	5:E:59:GLU:HG2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:ARG:HD3	5:E:93:ILE:HG23	2.00	0.44
4:D:124:LYS:HA	4:D:124:LYS:HD2	1.49	0.44
5:E:30:ARG:HE	5:E:30:ARG:HB3	1.54	0.44
5:E:27:GLU:H	5:E:27:GLU:HG2	1.33	0.44
4:D:114:ASP:HA	4:D:115:PRO:HD2	1.66	0.43
4:D:48:LEU:HD23	4:D:54:LEU:HB2	2.01	0.43
4:D:115:PRO:HB2	4:D:193:ASP:HB3	2.01	0.43
5:E:93:ILE:HG21	5:E:93:ILE:HD13	1.43	0.42
4:D:130:VAL:HG11	5:E:143:VAL:HG21	2.00	0.42
5:E:30:ARG:HB2	5:E:94:SER:O	2.20	0.41
5:E:27:GLU:O	5:E:28:ASN:HB2	2.20	0.41
1:A:146:LYS:HB3	1:A:146:LYS:HE3	1.44	0.41
5:E:202:ASP:HA	5:E:203:PRO:HD3	1.83	0.41
1:A:169:ARG:HA	1:A:172:LEU:HD12	2.03	0.41
1:A:258:THR:HG22	1:A:273:ARG:HB3	2.03	0.41
5:E:21:LEU:HD22	5:E:108:THR:HG21	2.03	0.41
4:D:190:ILE:HG12	4:D:190:ILE:H	1.69	0.41
1:A:218:GLN:HA	1:A:223:ASP:HA	2.02	0.41
5:E:52:VAL:HG12	5:E:53:LYS:HG3	2.03	0.40
2:B:71:THR:HA	2:B:72:PRO:HD2	1.93	0.40
1:A:192:HIS:NE2	2:B:98:ASP:O	2.55	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	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	194/195 (100%)	173 (89%)	20 (10%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	240/242 (99%)	231 (96%)	6 (2%)	3 (1%)	15	44
All	All	813/822 (99%)	771 (95%)	38 (5%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	191	PRO
5	E	28	ASN
5	E	3	GLY
5	E	39	PRO

### 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	231/231 (100%)	209 (90%)	22 (10%)	11	30
2	B	96/95 (101%)	90 (94%)	6 (6%)	22	53
3	C	7/7 (100%)	5 (71%)	2 (29%)	0	1
4	D	173/172 (101%)	144 (83%)	29 (17%)	2	8
5	E	212/212 (100%)	189 (89%)	23 (11%)	8	23
All	All	719/717 (100%)	637 (89%)	82 (11%)	7	21

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	ARG
1	A	54	GLN
1	A	95	VAL
1	A	113	TYR
1	A	121	LYS
1	A	128	GLU
1	A	178	THR

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Mol	Chain	Res	Type
1	A	194	VAL
1	A	196	ASP
1	A	197	HIS
1	A	214	THR
1	A	215	LEU
1	A	216	THR
1	A	223	ASP
1	A	225	THR
1	A	247	VAL
1	A	256	ARG
1	A	264	GLU
1	A	272	LEU
1	A	273	ARG
1	A	274	TRP
2	B	4	THR
2	B	38	ASP
2	B	47	GLU
2	B	48	LYS
2	B	70	PHE
2	B	98	ASP
3	C	1	GLU
3	C	9	THR
4	D	2	GLN
4	D	12	ILE
4	D	23	THR
4	D	25	SER
4	D	26	SER
4	D	30	THR
4	D	35	LYS
4	D	55	THR
4	D	60	LEU
4	D	63	GLN
4	D	64	PHE
4	D	66	ILE
4	D	73	LEU
4	D	79	ILE
4	D	95	GLN
4	D	100	THR
4	D	102	THR
4	D	104	LEU
4	D	105	THR
4	D	124	LYS

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Mol	Chain	Res	Type
4	D	127	ASP
4	D	144	GLN
4	D	155	LYS
4	D	157	VAL
4	D	161	ARG
4	D	162	SER
4	D	169	SER
4	D	189	ILE
4	D	193	ASP
5	E	9	ARG
5	E	17	THR
5	E	25	GLN
5	E	26	THR
5	E	27	GLU
5	E	29	HIS
5	E	39	PRO
5	E	60	VAL
5	E	66	VAL
5	E	71	THR
5	E	77	THR
5	E	87	SER
5	E	93	ILE
5	E	94	SER
5	E	126	VAL
5	E	156	LEU
5	E	169	VAL
5	E	176	LEU
5	E	179	GLN
5	E	221	GLU
5	E	223	THR
5	E	225	ASP
5	E	243	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
4	D	2	GLN
4	D	95	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 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 [i](#)

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%)	-0.07	9 (3%) 50 38	18, 43, 82, 111	0
2	B	100/100 (100%)	-0.02	2 (2%) 68 58	27, 43, 78, 90	0
3	C	10/10 (100%)	-0.36	0 100 100	29, 32, 37, 44	0
4	D	195/195 (100%)	0.45	17 (8%) 13 6	30, 56, 106, 119	0
5	E	242/242 (100%)	-0.04	10 (4%) 41 29	26, 45, 73, 87	0
All	All	822/822 (100%)	0.07	38 (4%) 36 25	18, 46, 86, 119	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	2	ALA	9.7
1	A	275	GLU	7.2
4	D	176	LYS	7.1
4	D	57	ASN	5.1
4	D	178	ASP	5.0
4	D	186	ASN	4.6
5	E	243	ASP	4.4
4	D	175	ASN	4.4
4	D	125	SER	4.2
4	D	55	THR	4.2
4	D	126	SER	4.1
4	D	146	LYS	3.8
4	D	127	ASP	3.7
4	D	147	ASP	3.3
1	A	226	GLN	3.3
5	E	3	GLY	3.3
4	D	148	SER	3.3
4	D	129	SER	3.0
4	D	196	PHE	2.9
5	E	217	SER	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	223	THR	2.8
4	D	177	SER	2.8
1	A	194	VAL	2.8
4	D	145	SER	2.7
5	E	131	GLU	2.7
2	B	75	LYS	2.7
2	B	74	GLU	2.7
1	A	86	ASN	2.7
1	A	197	HIS	2.3
5	E	41	HIS	2.3
5	E	221	GLU	2.3
1	A	195	SER	2.3
1	A	274	TRP	2.3
4	D	194	THR	2.3
5	E	183	ASN	2.2
5	E	218	GLU	2.1
1	A	222	GLU	2.1
1	A	88	SER	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 carbohydrates 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.