



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:29 AM EDT

PDB ID : 6EH9  
Title : HA1.7 Human T-Cell Receptor specific for Influenza virus epitope  
PKYVKQNTLKLAT presented by Human Leukocyte Antigen HLA-DR0101  
Authors : Rizkallah, P.J.; Cole, D.K.  
Deposited on : 2017-09-12  
Resolution : 2.49 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)	:	2.37.1

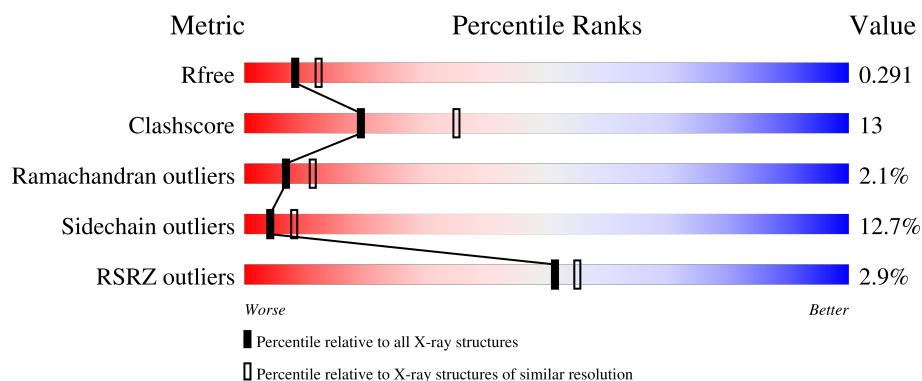
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	202	 4% 71% 23% 5%
2	B	241	 2% 68% 27% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3523 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 Human T Cell Receptor Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	2	0
			1585	1002	261	313	9			

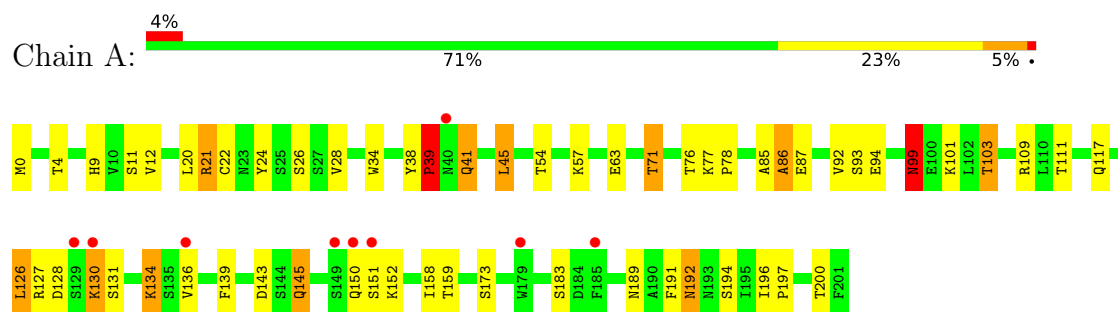
- Molecule 2 is a protein called Human T Cell Receptor Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1938	1227	332	370	9			

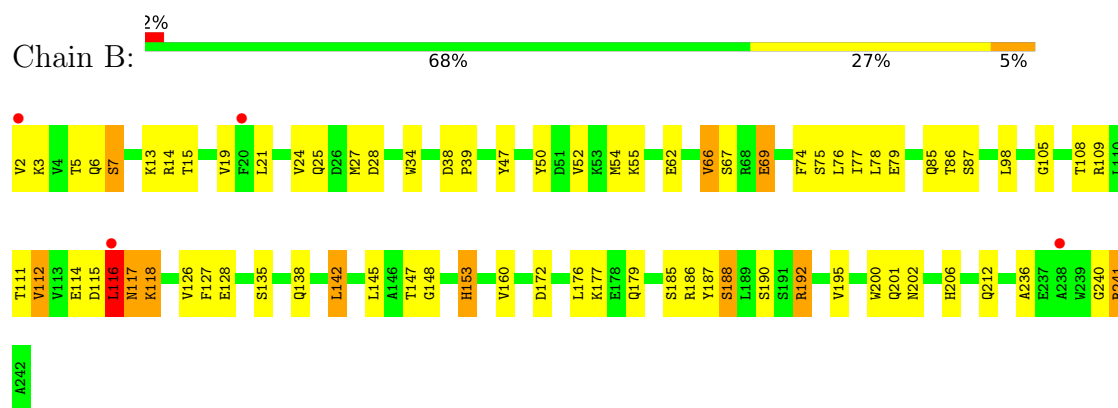
### 3 Residue-property plots

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: Human T Cell Receptor Alpha Chain



#### • Molecule 2: Human T Cell Receptor Beta Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.46Å 49.96Å 72.75Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	48.87 – 2.49 41.16 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.87-2.49) 98.3 (41.16-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.232 , 0.297 0.233 , 0.291	Depositor DCC
$R_{free}$ test set	881 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.72	1/1625 (0.1%)	0.88	1/2205 (0.0%)
2	B	0.63	0/1988	0.77	1/2696 (0.0%)
All	All	0.67	1/3613 (0.0%)	0.82	2/4901 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	GLU	CD-OE1	5.61	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LEU	CA-CB-CG	5.86	128.79	115.30
2	B	142	LEU	CA-CB-CG	5.19	127.25	115.30

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	A	1585	0	1524	46	0
2	B	1938	0	1865	53	0
All	All	3523	0	3389	89	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 13.

All (89) 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:116:LEU:HD13	2:B:116:LEU:O	1.78	0.84
1:A:9[B]:HIS:HD2	1:A:109[B]:ARG:O	1.61	0.84
1:A:109[B]:ARG:HH11	1:A:109[B]:ARG:HG2	1.43	0.84
1:A:0:MET:HB2	1:A:93:SER:C	1.98	0.82
1:A:0:MET:SD	1:A:0:MET:O	2.43	0.76
1:A:24:TYR:O	1:A:71:THR:HG23	1.86	0.76
1:A:0:MET:HG3	1:A:93:SER:HA	1.68	0.76
1:A:109[B]:ARG:HG2	1:A:109[B]:ARG:NH1	2.06	0.71
2:B:115:ASP:O	2:B:117:ASN:N	2.24	0.70
1:A:0:MET:HG2	1:A:92:VAL:HG13	1.75	0.69
1:A:128:ASP:O	1:A:134:LYS:HG2	1.93	0.69
1:A:0:MET:O	1:A:0:MET:CG	2.43	0.67
2:B:116:LEU:O	2:B:117:ASN:C	2.34	0.66
1:A:134:LYS:HG3	2:B:127:PHE:CD2	2.31	0.66
1:A:136:VAL:HG21	2:B:127:PHE:CD2	2.31	0.65
2:B:21:LEU:HD12	2:B:76:LEU:HD23	1.80	0.64
1:A:196:ILE:HD12	1:A:196:ILE:H	1.63	0.64
2:B:126:VAL:HG23	2:B:236:ALA:HB3	1.80	0.63
2:B:127:PHE:CE1	2:B:145:LEU:HD12	2.33	0.63
1:A:0:MET:HB3	1:A:94:GLU:CG	2.31	0.60
1:A:0:MET:HB3	1:A:94:GLU:HG2	1.81	0.60
1:A:9[B]:HIS:CD2	1:A:109[B]:ARG:O	2.51	0.60
1:A:126:LEU:HB3	2:B:128:GLU:O	2.01	0.60
1:A:128:ASP:HB2	2:B:127:PHE:HA	1.85	0.58
2:B:111:THR:OG1	2:B:153:HIS:CE1	2.60	0.54
2:B:147:THR:HA	2:B:188:SER:OG	2.07	0.54
2:B:172:ASP:OD1	2:B:192:ARG:NH2	2.41	0.54
2:B:111:THR:OG1	2:B:153:HIS:HE1	1.92	0.53
2:B:6:GLN:HE21	2:B:105:GLY:HA3	1.73	0.53
2:B:21:LEU:O	2:B:75:SER:HA	2.09	0.53
1:A:196:ILE:HG22	1:A:197:PRO:HD2	1.91	0.52
2:B:177:LYS:HD3	2:B:187:TYR:CE1	2.44	0.52
1:A:189:ASN:OD1	1:A:192:ASN:ND2	2.41	0.52
1:A:57:LYS:HE2	1:A:63:GLU:OE2	2.10	0.52
1:A:134:LYS:HG3	2:B:127:PHE:CE2	2.43	0.52
2:B:116:LEU:O	2:B:116:LEU:CD1	2.56	0.52
1:A:127:ARG:HG3	1:A:134:LYS:HB3	1.91	0.52
1:A:159:THR:HG21	2:B:190:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:O	1:A:39:PRO:C	2.49	0.51
1:A:38:TYR:HB2	1:A:41:GLN:HG2	1.91	0.51
2:B:62:GLU:H	2:B:62:GLU:CD	2.15	0.49
2:B:160:VAL:HA	2:B:206:HIS:O	2.13	0.49
1:A:127:ARG:HG3	1:A:134:LYS:CB	2.42	0.48
2:B:27:MET:O	2:B:28:ASP:HB3	2.14	0.48
2:B:148:GLY:HA2	2:B:186:ARG:HD2	1.96	0.48
2:B:13:LYS:O	2:B:112:VAL:HA	2.13	0.48
2:B:66:VAL:CG1	2:B:67:SER:N	2.77	0.47
2:B:47:TYR:HB3	2:B:66:VAL:HG21	1.96	0.47
2:B:69:GLU:N	2:B:69:GLU:OE2	2.48	0.47
1:A:0:MET:SD	1:A:103:THR:CG2	3.03	0.47
2:B:52:VAL:O	2:B:54:MET:HG2	2.16	0.46
1:A:99:ASN:O	2:B:50:TYR:CE1	2.69	0.46
2:B:38:ASP:O	2:B:39:PRO:C	2.53	0.46
1:A:26:SER:OG	1:A:28:VAL:O	2.23	0.46
2:B:118:LYS:O	2:B:118:LYS:HG3	2.15	0.46
1:A:11:SER:HA	1:A:111:THR:O	2.15	0.46
1:A:99:ASN:O	2:B:50:TYR:CZ	2.69	0.46
2:B:34:TRP:CD1	2:B:74:PHE:CD2	3.05	0.44
1:A:22:CYS:HB2	1:A:34:TRP:CZ2	2.52	0.44
1:A:145:GLN:HE21	1:A:145:GLN:N	2.16	0.44
2:B:47:TYR:CB	2:B:66:VAL:HG21	2.47	0.44
1:A:139:PHE:HB2	1:A:191:PHE:CE2	2.53	0.44
2:B:201:GLN:HA	2:B:241:ARG:O	2.18	0.44
1:A:0:MET:HE1	1:A:101:LYS:HG3	2.00	0.43
1:A:134:LYS:HG3	2:B:127:PHE:HD2	1.81	0.43
2:B:66:VAL:HG11	2:B:74:PHE:CZ	2.53	0.43
2:B:24:VAL:HG12	2:B:25:GLN:N	2.33	0.43
2:B:202:ASN:O	2:B:240:GLY:HA3	2.19	0.43
1:A:85:ALA:O	1:A:86:ALA:HB2	2.17	0.43
2:B:66:VAL:HG13	2:B:67:SER:N	2.34	0.43
2:B:2:VAL:HA	2:B:27:MET:SD	2.59	0.43
2:B:126:VAL:CG2	2:B:236:ALA:HB3	2.48	0.43
2:B:86:THR:HG23	2:B:111:THR:HA	2.01	0.43
1:A:151:SER:HB2	1:A:158:ILE:HD12	2.01	0.42
1:A:0:MET:HB2	1:A:93:SER:CA	2.48	0.42
2:B:6:GLN:O	2:B:7:SER:C	2.58	0.42
2:B:21:LEU:HB2	2:B:76:LEU:HB3	2.01	0.42
1:A:77:LYS:HA	1:A:78:PRO:HD3	1.91	0.42
2:B:66:VAL:CG1	2:B:74:PHE:CE1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:LEU:HD23	2:B:85:GLN:CD	2.41	0.42
1:A:71:THR:O	1:A:71:THR:CG2	2.68	0.41
1:A:127:ARG:HA	1:A:134:LYS:HB3	2.02	0.41
1:A:136:VAL:HG21	2:B:127:PHE:CE2	2.55	0.41
2:B:19:VAL:O	2:B:77:ILE:HA	2.21	0.41
2:B:200:TRP:O	2:B:240:GLY:HA2	2.21	0.41
1:A:0:MET:HB3	1:A:94:GLU:HG3	2.00	0.41
1:A:21:ARG:HA	1:A:21:ARG:HD2	1.89	0.40
2:B:66:VAL:HG11	2:B:74:PHE:CE1	2.57	0.40
2:B:14:ARG:NH1	2:B:114:GLU:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	202/202 (100%)	184 (91%)	12 (6%)	6 (3%)	4	6
2	B	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	12	21
All	All	441/443 (100%)	409 (93%)	23 (5%)	9 (2%)	7	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
2	B	116	LEU
1	A	194	SER
2	B	7	SER
2	B	117	ASN
1	A	130	LYS
1	A	131	SER
1	A	86	ALA

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Mol	Chain	Res	Type
1	A	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	181/180 (101%)	157 (87%)	24 (13%)	4	7
2	B	215/215 (100%)	189 (88%)	26 (12%)	5	9
All	All	396/395 (100%)	346 (87%)	50 (13%)	4	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	12	VAL
1	A	20	LEU
1	A	21	ARG
1	A	39	PRO
1	A	41	GLN
1	A	45	LEU
1	A	54	THR
1	A	71	THR
1	A	76	THR
1	A	99	ASN
1	A	103	THR
1	A	117	GLN
1	A	126	LEU
1	A	130	LYS
1	A	134	LYS
1	A	143	ASP
1	A	145	GLN
1	A	150	GLN
1	A	152	LYS
1	A	173	SER
1	A	183	SER

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	200	THR
2	B	3	LYS
2	B	5	THR
2	B	15	THR
2	B	55	LYS
2	B	66	VAL
2	B	69	GLU
2	B	79	GLU
2	B	87	SER
2	B	98	LEU
2	B	108	THR
2	B	109	ARG
2	B	112	VAL
2	B	116	LEU
2	B	118	LYS
2	B	135	SER
2	B	138	GLN
2	B	142	LEU
2	B	153	HIS
2	B	176	LEU
2	B	179	GLN
2	B	185	SER
2	B	188	SER
2	B	192	ARG
2	B	195	VAL
2	B	212	GLN
2	B	241	ARG

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

Mol	Chain	Res	Type
1	A	125	GLN
1	A	145	GLN
1	A	189	ASN
1	A	192	ASN
2	B	6	GLN
2	B	138	GLN
2	B	153	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 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<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	202/202 (100%)	0.30	9 (4%) 33 36	26, 58, 116, 143	0
2	B	241/241 (100%)	0.12	4 (1%) 70 72	32, 69, 105, 134	0
All	All	443/443 (100%)	0.20	13 (2%) 51 55	26, 65, 110, 143	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	SER	5.8
2	B	20	PHE	4.8
1	A	149	SER	3.5
1	A	130	LYS	3.4
1	A	150	GLN	3.0
1	A	136	VAL	2.9
1	A	185	PHE	2.9
2	B	238	ALA	2.8
1	A	40	ASN	2.8
1	A	151	SER	2.6
2	B	2	VAL	2.1
1	A	179	TRP	2.1
2	B	116	LEU	2.0

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.