



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:18 am BST

PDB ID : 3KPR  
Title : Crystal Structure of the LC13 TCR in complex with HLA B\*4405 bound to EEYLKAWTF a mimotope  
Authors : Macdonald, W.A.; Chen, Z.; Gras, S.; Archbold, J.K.; Tynan, F.E.; Clements, C.S.; Bharadwaj, M.; Kjer-Nielsen, L.; Saunders, P.M.; Wilce, M.C.; Crawford, F.; Stadinsky, B.; Jackson, D.; Brooks, A.G.; Purcell, A.W.; Kappler, J.W.; Burrows, S.R.; Rossjohn, J.; McCluskey, J.  
Deposited on : 2009-11-16  
Resolution : 2.60 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](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 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

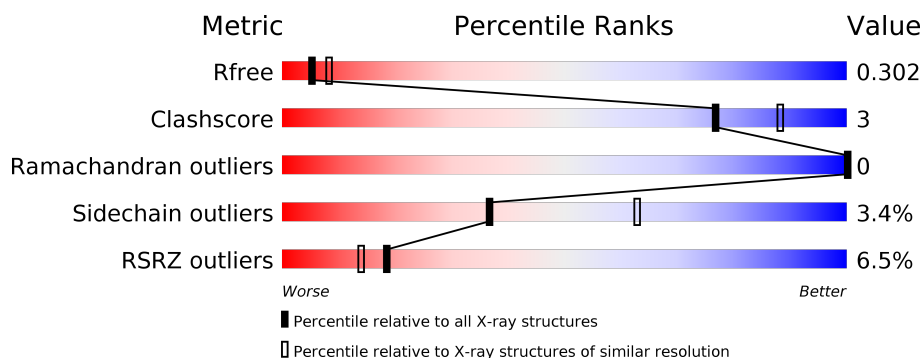
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	276	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
1	F	276	<div> <div>18%</div> <div>89%</div> <div>10%</div> </div>
2	B	99	<div> <div>7%</div> <div>92%</div> <div>8%</div> </div>
2	G	99	<div> <div>3%</div> <div>88%</div> <div>12%</div> </div>
3	C	9	<div> <div>78%</div> <div>22%</div> </div>
3	H	9	<div> <div>78%</div> <div>22%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	201	<div><div></div><div>5%</div><div>89%</div><div>10%</div></div>
4	I	201	<div><div></div><div>3%</div><div>90%</div><div>10%</div></div>
5	E	241	<div><div></div><div>2%</div><div>90%</div><div>10%</div></div>
5	J	241	<div><div></div><div>%</div><div>88%</div><div>11%</div><div>.</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13434 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, B-44 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			
1	F	276	Total	C	N	O	S	0	0	0
			2259	1408	407	437	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TYR	ASP	VARIANT	UNP P30481
F	116	TYR	ASP	VARIANT	UNP P30481

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called EEYLKAWTF, mimotope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			85	58	11	16			
3	H	9	Total	C	N	O	0	0	0
			85	58	11	16			

- Molecule 4 is a protein called LC13 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

- Molecule 5 is a protein called LC13 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			
5	J	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			

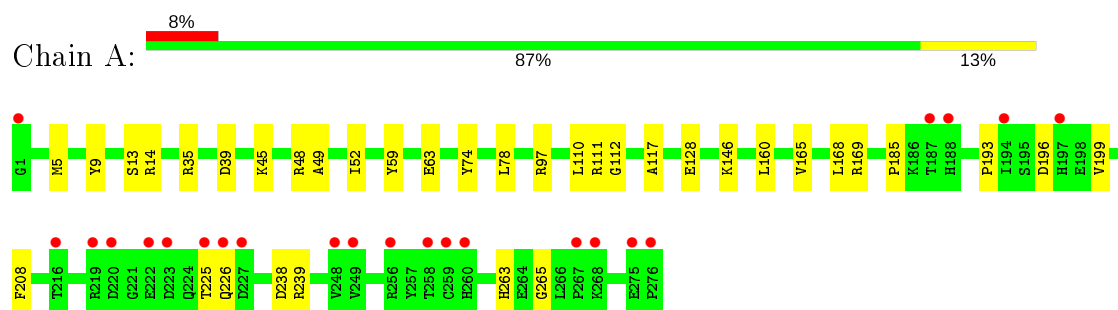
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	4	Total	O	0	0
			4	4		
6	C	1	Total	O	0	0
			1	1		
6	D	16	Total	O	0	0
			16	16		
6	E	19	Total	O	0	0
			19	19		
6	F	26	Total	O	0	0
			26	26		
6	G	10	Total	O	0	0
			10	10		
6	H	3	Total	O	0	0
			3	3		
6	I	9	Total	O	0	0
			9	9		
6	J	9	Total	O	0	0
			9	9		

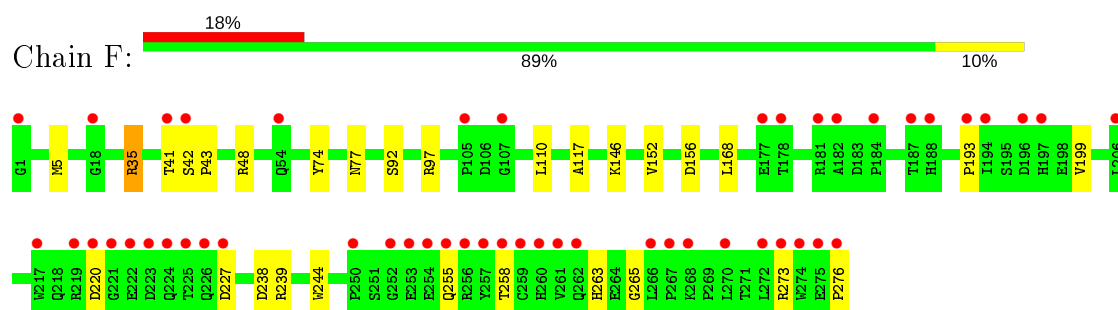
### 3 Residue-property plots [i](#)

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.

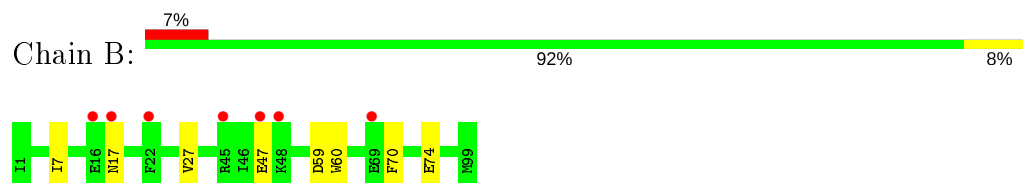
- Molecule 1: HLA class I histocompatibility antigen, B-44 alpha chain



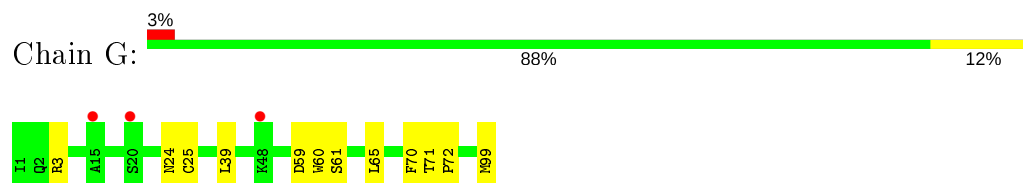
- Molecule 1: HLA class I histocompatibility antigen, B-44 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: EEYLKAWTF, mimotope peptide

Chain C:  78% 22%




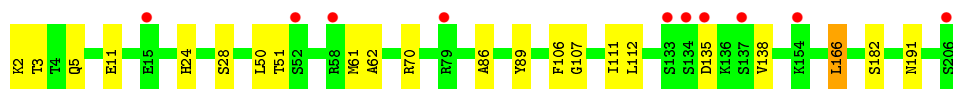
- Molecule 3: EEYLKAWTF, mimotope peptide

Chain H:  78% 22%




- Molecule 4: LC13 TCR alpha chain

Chain D:  5% 89% 10%




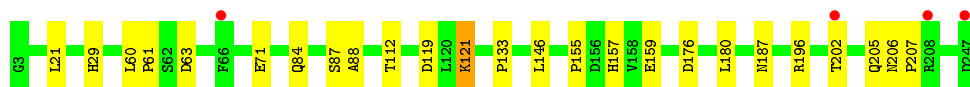
- Molecule 4: LC13 TCR alpha chain

Chain I:  3% 90% 10%




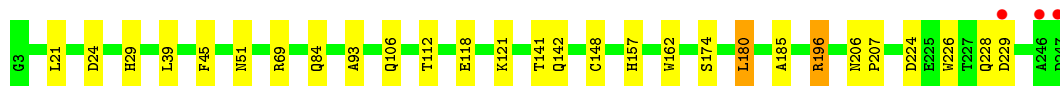
- Molecule 5: LC13 TCR beta chain

Chain E:  2% 90% 10%



- Molecule 5: LC13 TCR beta chain

Chain J:  88% 11% 1%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.12Å 53.22Å 143.20Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.60) 97.5 (49.31-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.219 , 0.279 0.257 , 0.302	Depositor DCC
$R_{free}$ test set	2538 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 38.6	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	0.89	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 33.06 % 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 8.4962e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.32	0/2320	0.48	0/3154
1	F	0.32	0/2320	0.48	0/3154
2	B	0.33	0/852	0.46	0/1152
2	G	0.33	0/852	0.46	0/1152
3	C	0.34	0/88	0.42	0/117
3	H	0.32	0/88	0.42	0/117
4	D	0.40	0/1603	0.57	1/2181 (0.0%)
4	I	0.33	0/1603	0.51	1/2181 (0.0%)
5	E	0.44	1/1971 (0.1%)	0.49	0/2681
5	J	0.41	0/1971	0.51	1/2681 (0.0%)
All	All	0.36	1/13668 (0.0%)	0.50	3/18570 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	159	GLU	CG-CD	-5.59	1.43	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	185	ALA	CB-CA-C	5.92	118.97	110.10
4	I	166	LEU	CA-CB-CG	5.38	127.68	115.30
4	D	166	LEU	CA-CB-CG	5.32	127.53	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	2259	0	2128	20	0
1	F	2259	0	2128	14	0
2	B	829	0	794	4	0
2	G	829	0	794	7	0
3	C	85	0	78	3	0
3	H	85	0	78	3	0
4	D	1567	0	1492	10	0
4	I	1567	0	1492	10	0
5	E	1919	0	1820	9	0
5	J	1919	0	1820	10	0
6	A	19	0	0	0	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	D	16	0	0	1	0
6	E	19	0	0	0	0
6	F	26	0	0	0	0
6	G	10	0	0	0	0
6	H	3	0	0	0	0
6	I	9	0	0	0	0
6	J	9	0	0	0	0
All	All	13434	0	12624	77	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.

The worst 5 of 77 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:59:TYR:HE1	3:C:1:GLU:HG2	1.56	0.70
1:A:263:HIS:CD2	1:A:265:GLY:H	2.16	0.64
4:D:51:THR:HG22	4:D:70:ARG:HD3	1.79	0.62
5:E:21:LEU:HD22	5:E:112:THR:HG21	1.81	0.62
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.81	0.61

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	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	F	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	G	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
4	I	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
5	E	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
5	J	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
All	All	1632/1652 (99%)	1565 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	237/237 (100%)	233 (98%)	4 (2%)	60	81
1	F	237/237 (100%)	230 (97%)	7 (3%)	41	67
2	B	94/94 (100%)	90 (96%)	4 (4%)	29	54
2	G	94/94 (100%)	93 (99%)	1 (1%)	73	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	180/180 (100%)	172 (96%)	8 (4%)	28	53
4	I	180/180 (100%)	174 (97%)	6 (3%)	38	64
5	E	207/207 (100%)	200 (97%)	7 (3%)	37	63
5	J	207/207 (100%)	195 (94%)	12 (6%)	20	40
All	All	1452/1452 (100%)	1403 (97%)	49 (3%)	37	63

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	187	ASN
1	F	156	ASP
5	J	180	LEU
1	F	42	SER
1	F	220	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	236	GLN
1	F	255	GLN
5	J	206	ASN
1	F	70	ASN
1	F	263	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	276/276 (100%)	0.52	23 (8%)	11 8	24, 36, 44, 50	1 (0%)
1	F	276/276 (100%)	0.81	50 (18%)	1 0	25, 35, 44, 49	1 (0%)
2	B	99/99 (100%)	0.61	7 (7%)	16 11	27, 35, 46, 47	0
2	G	99/99 (100%)	0.50	3 (3%)	50 43	29, 36, 43, 45	0
3	C	9/9 (100%)	0.35	0	100 100	31, 34, 37, 38	0
3	H	9/9 (100%)	0.41	0	100 100	33, 34, 37, 38	0
4	D	201/201 (100%)	0.52	10 (4%)	28 23	26, 36, 44, 57	0
4	I	201/201 (100%)	0.39	7 (3%)	44 36	28, 36, 46, 55	0
5	E	241/241 (100%)	0.23	4 (1%)	70 66	29, 36, 46, 54	0
5	J	241/241 (100%)	0.23	3 (1%)	79 76	28, 36, 44, 57	0
All	All	1652/1652 (100%)	0.47	107 (6%)	18 14	24, 36, 45, 57	2 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	134	SER	6.0
2	B	48	LYS	5.3
1	F	42	SER	4.7
1	A	197	HIS	4.4
4	D	154	LYS	4.2

### 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 [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.