



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2020 – 12:04 PM EST

PDB ID : 6WL4  
Title : preTCRbeta-pMHC complex crystal structure  
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Deposited on : 2020-04-18  
Resolution : 3.60 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.

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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	:	2.15.1
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)	:	2.15.1

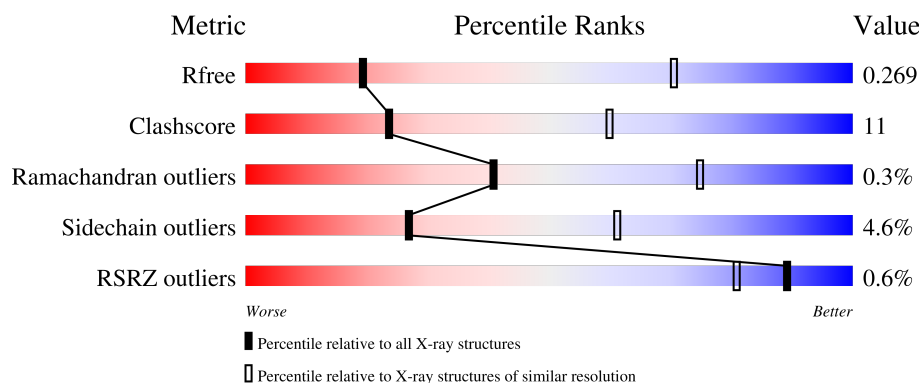
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	185	<div> <div>74%</div> <div>20%</div> <div>...</div> </div>
1	D	185	<div> <div>76%</div> <div>18%</div> <div>..</div> </div>
1	G	185	<div> <div>63%</div> <div>29%</div> <div>..</div> </div>
2	B	8	<div> <div>75%</div> <div>25%</div> </div>
2	E	8	<div> <div>63%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	8	<div><div></div><div>88%</div><div>13%</div></div>
3	C	239	<div><div></div><div>67%</div><div>31%</div><div>..</div></div>
3	F	239	<div><div></div><div>71%</div><div>27%</div><div>.</div></div>
3	I	239	<div><div>3%</div><div></div><div>74%</div><div>21%</div><div>.</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10281 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 H-2 class I histocompatibility antigen, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1446	904	256	280	6			
1	D	177	Total	C	N	O	S	0	0	0
			1439	900	255	278	6			
1	G	177	Total	C	N	O	S	0	0	0
			1439	900	255	278	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	CYS	ARG	engineered mutation	UNP P01901
A	121	GLN	CYS	engineered mutation	UNP P01901
D	62	CYS	ARG	engineered mutation	UNP P01901
D	121	GLN	CYS	engineered mutation	UNP P01901
G	62	CYS	ARG	engineered mutation	UNP P01901
G	121	GLN	CYS	engineered mutation	UNP P01901

- Molecule 2 is a protein called ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			68	44	12	12			
2	E	8	Total	C	N	O	0	0	0
			68	44	12	12			
2	H	8	Total	C	N	O	0	0	0
			68	44	12	12			

- Molecule 3 is a protein called N15 preTCR beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1913	1206	341	358	8			

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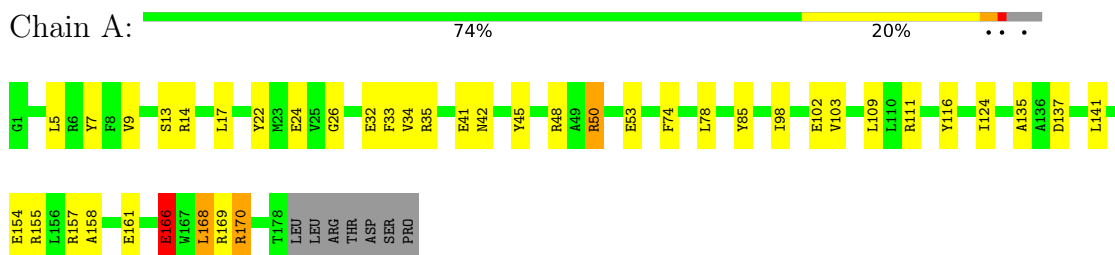
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	238	Total	C	N	O	S	0	0	0
			1919	1209	342	360	8			
3	I	238	Total	C	N	O	S	0	0	0
			1921	1210	342	361	8			

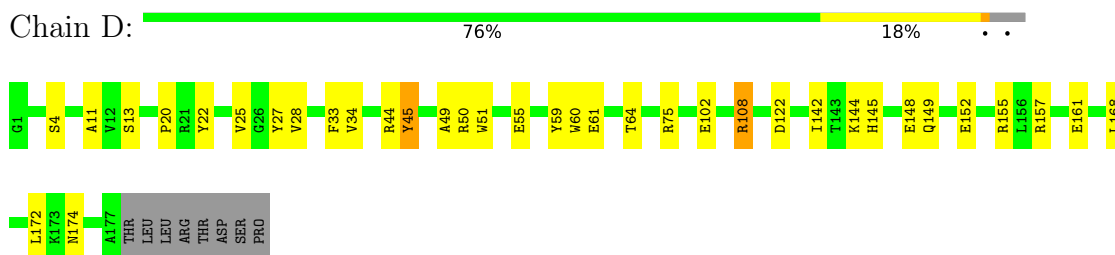
### 3 Residue-property plots [i](#)

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.

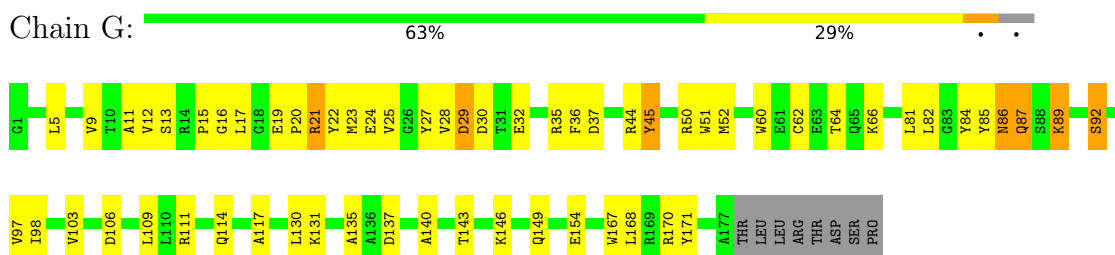
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



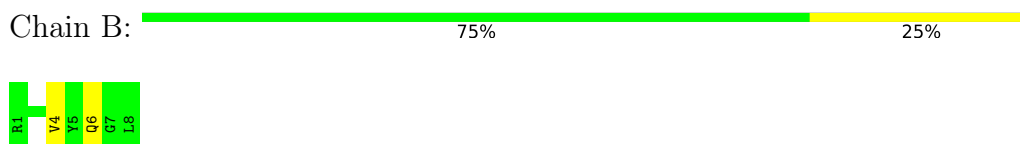
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



- Molecule 2: ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU




- Molecule 2: ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU

Chain E:  63% 38%



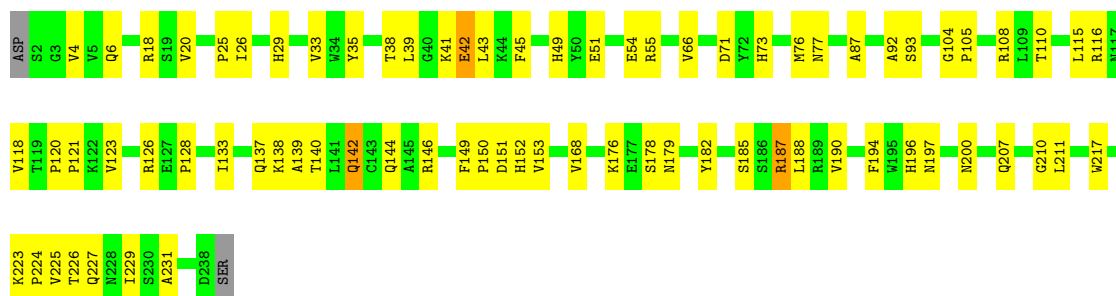
- Molecule 2: ARG-GLY-TYR-VAL-TYR-GLN-GLY-LEU

Chain H:  88% 13%



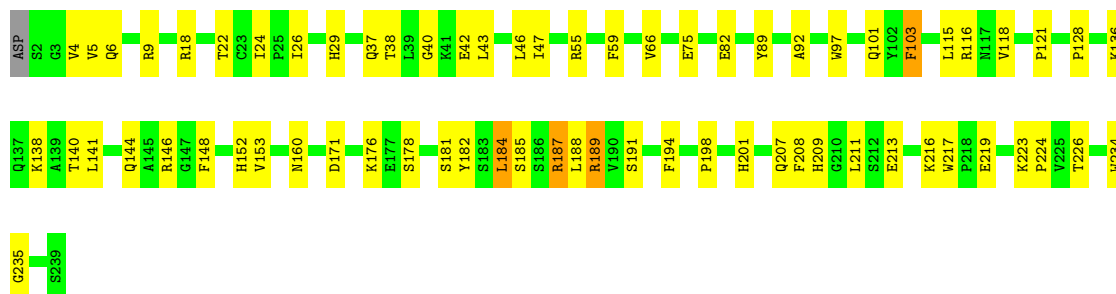
- Molecule 3: N15 preTCR beta

Chain C:  67% 31% ..



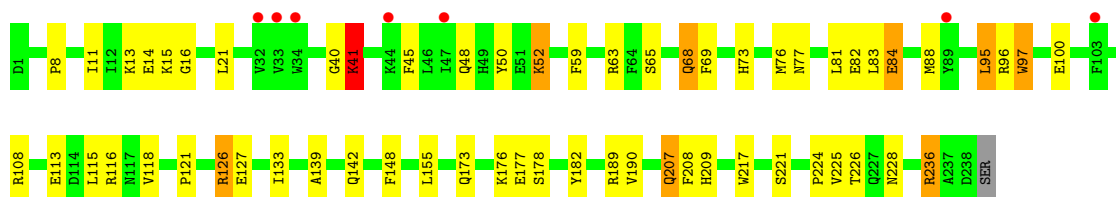
- Molecule 3: N15 preTCR beta

Chain F:  71% 27% .



- Molecule 3: N15 preTCR beta

Chain I:  3% 74% 21% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.55Å 110.55Å 316.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 3.60 49.44 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.44-3.60) 99.1 (49.44-3.60)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.226 , 0.269 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	1130 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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	0.29	0/1481	0.49	1/2003 (0.0%)
1	D	0.24	0/1474	0.43	0/1993
1	G	0.25	0/1474	0.46	0/1993
2	B	0.26	0/69	0.47	0/90
2	E	0.24	0/69	0.40	0/90
2	H	0.22	0/69	0.36	0/90
3	C	0.24	0/1967	0.42	0/2664
3	F	0.31	0/1973	0.47	0/2672
3	I	0.25	0/1975	0.46	0/2675
All	All	0.27	0/10551	0.45	1/14270 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLU	CB-CA-C	-5.12	100.16	110.40

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	1446	0	1360	36	0
1	D	1439	0	1353	27	0
1	G	1439	0	1353	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	68	0	67	2	0
2	E	68	0	67	3	0
2	H	68	0	67	1	0
3	C	1913	0	1828	51	0
3	F	1919	0	1833	45	0
3	I	1921	0	1835	38	0
All	All	10281	0	9763	224	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 11.

The worst 5 of 224 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:G:86:ASN:ND2	1:G:86:ASN:O	2.06	0.88
3:F:187:ARG:HG2	3:F:187:ARG:HH11	1.39	0.87
1:A:5:LEU:HB2	1:A:168:LEU:HD22	1.57	0.86
1:A:5:LEU:CB	1:A:168:LEU:HD22	2.05	0.86
3:I:95:LEU:O	3:I:95:LEU:HD12	1.84	0.77

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	176/185 (95%)	169 (96%)	7 (4%)	0	100	100
1	D	175/185 (95%)	164 (94%)	11 (6%)	0	100	100
1	G	175/185 (95%)	166 (95%)	8 (5%)	1 (1%)	25	64
2	B	6/8 (75%)	6 (100%)	0	0	100	100
2	E	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
3	C	235/239 (98%)	224 (95%)	10 (4%)	1 (0%)	34	71
3	F	236/239 (99%)	223 (94%)	13 (6%)	0	100	100
3	I	236/239 (99%)	221 (94%)	13 (6%)	2 (1%)	19	59
All	All	1251/1296 (96%)	1183 (95%)	64 (5%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	41	LYS
3	I	68	GLN
1	G	16	GLY
3	C	42	GLU

### 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	147/154 (96%)	140 (95%)	7 (5%)	25	60
1	D	146/154 (95%)	142 (97%)	4 (3%)	44	73
1	G	146/154 (95%)	136 (93%)	10 (7%)	16	50
2	B	6/6 (100%)	6 (100%)	0	100	100
2	E	6/6 (100%)	6 (100%)	0	100	100
2	H	6/6 (100%)	6 (100%)	0	100	100
3	C	210/212 (99%)	204 (97%)	6 (3%)	42	72
3	F	211/212 (100%)	201 (95%)	10 (5%)	26	61
3	I	211/212 (100%)	198 (94%)	13 (6%)	18	53
All	All	1089/1116 (98%)	1039 (95%)	50 (5%)	27	61

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	187	ARG
1	G	21	ARG
3	I	155	LEU
3	F	189	ARG
3	F	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	HIS
3	C	196	HIS
3	C	200	ASN
1	G	86	ASN

### 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(Å²)	Q<0.9	
1	A	178/185 (96%)	-0.40	0	100	100	57, 90, 124, 166	0
1	D	177/185 (95%)	-0.29	0	100	100	66, 103, 146, 168	0
1	G	177/185 (95%)	-0.16	0	100	100	89, 129, 178, 186	0
2	B	8/8 (100%)	-0.02	0	100	100	82, 98, 125, 126	0
2	E	8/8 (100%)	0.24	0	100	100	83, 104, 115, 123	0
2	H	8/8 (100%)	0.09	0	100	100	120, 125, 145, 146	0
3	C	237/239 (99%)	-0.40	0	100	100	56, 85, 137, 158	0
3	F	238/239 (99%)	-0.38	0	100	100	59, 90, 130, 151	0
3	I	238/239 (99%)	-0.01	7 (2%)	51	35	78, 129, 168, 190	0
All	All	1269/1296 (97%)	-0.27	7 (0%)	89	81	56, 103, 158, 190	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	34	TRP	4.4
3	I	33	VAL	3.5
3	I	32	VAL	2.8
3	I	47	ILE	2.6
3	I	44	LYS	2.4

### 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.