



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2023 – 11:54 AM EDT

PDB ID : 5F3H  
Title : Structure of myostatin in complex with humanized RK35 antibody  
Authors : Parris, K.D.; Mosyak, L.  
Deposited on : 2015-12-02  
Resolution : 2.70 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 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 : 2.35.1  
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) : 2.35.1

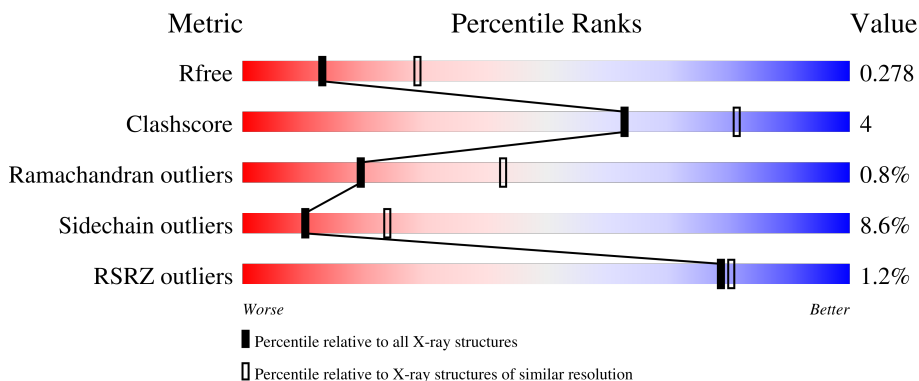
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	221	 80% 14% 6%
1	C	221	 82% 13% 5%
1	E	221	 79% 15% 5%
1	G	221	 80% 14% 6%
2	B	214	 86% 11% ..

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Mol	Chain	Length	Quality of chain
2	D	214	85% 12% ..
2	F	214	79% 18% ..
2	H	214	83% 14% ..
3	I	108	12% 71% 19% 6% .
3	J	108	4% 70% 20% 6% .
3	K	108	% 81% 16% ..
3	L	108	4% 75% 16% 5% ..

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15926 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 humanized RK35 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1535	C 969	N 254	O 305	S 7	0	0	0
1	C	211	Total 1564	C 986	N 259	O 312	S 7	0	0	0
1	E	211	Total 1579	C 995	N 264	O 313	S 7	0	1	0
1	G	208	Total 1547	C 975	N 257	O 308	S 7	0	0	0

- Molecule 2 is a protein called humanized RK35 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	Total 1620	C 1016	N 270	O 329	S 5	0	0	0
2	D	211	Total 1619	C 1015	N 270	O 329	S 5	0	0	0
2	F	211	Total 1619	C 1015	N 270	O 329	S 5	0	0	0
2	H	211	Total 1613	C 1009	N 271	O 328	S 5	0	0	0

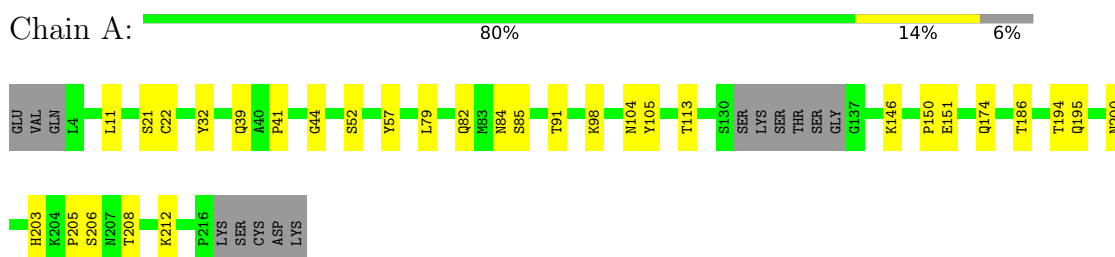
- Molecule 3 is a protein called Growth/differentiation factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	104	Total 802	C 511	N 134	O 145	S 12	0	0	0
3	J	104	Total 805	C 514	N 135	O 144	S 12	0	0	0
3	K	105	Total 821	C 524	N 136	O 149	S 12	0	0	0
3	L	104	Total 802	C 511	N 134	O 145	S 12	0	0	0

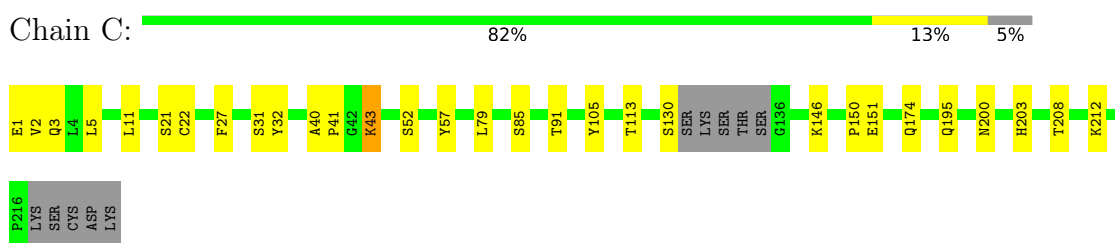
### 3 Residue-property plots [i](#)

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.

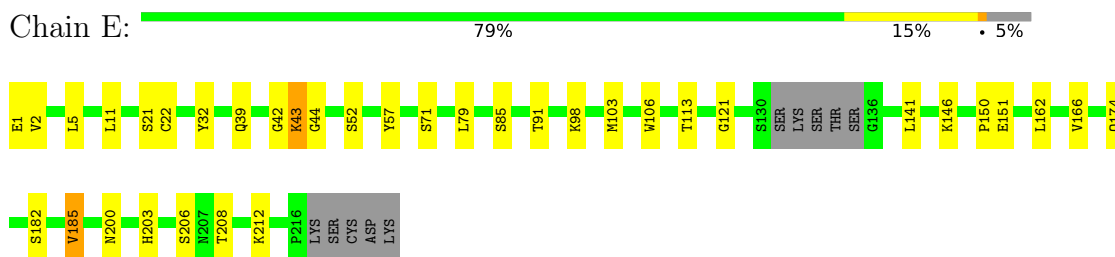
- Molecule 1: humanized RK35 antibody heavy chain



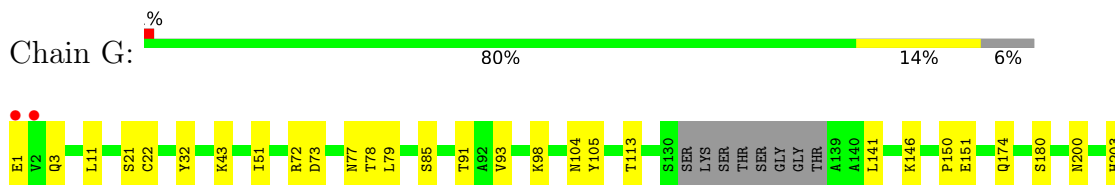
- Molecule 1: humanized RK35 antibody heavy chain



- Molecule 1: humanized RK35 antibody heavy chain



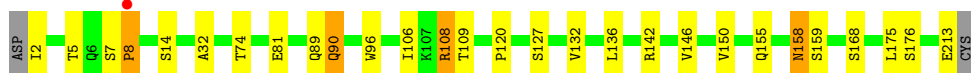
- Molecule 1: humanized RK35 antibody heavy chain





- Molecule 2: humanized RK35 antibody light chain

Chain B: 86% 11% ..



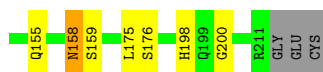
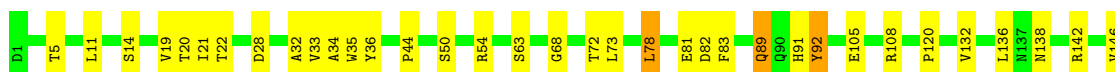
- Molecule 2: humanized RK35 antibody light chain

Chain D: 85% 12% ..



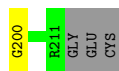
- Molecule 2: humanized RK35 antibody light chain

Chain F: 79% 18% ..



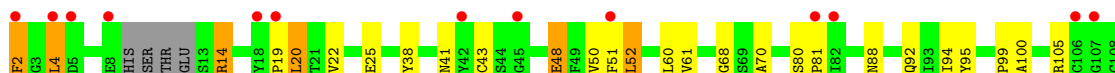
- Molecule 2: humanized RK35 antibody light chain

Chain H: 83% 14% ..



- Molecule 3: Growth/differentiation factor 8

Chain I: 12% 71% 19% 6% .




- Molecule 3: Growth/differentiation factor 8

Chain J:  4% 70% 20% 6% .




• Molecule 3: Growth/differentiation factor 8

Chain K:  % 81% 16% ..



• Molecule 3: Growth/differentiation factor 8

Chain L:  4% 75% 16% 5% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.14Å 80.92Å 101.40Å 88.33° 103.78° 92.40°	Depositor
Resolution (Å)	19.99 – 2.70 19.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	63.5 (19.99-2.70) 63.6 (19.87-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.71Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.218 , 0.270 0.230 , 0.278	Depositor DCC
$R_{free}$ test set	2045 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 7.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.082 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.62 % 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 8.3619e-03. 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	0.42	0/1572	0.71	0/2143
1	C	0.41	0/1601	0.71	0/2182
1	E	0.43	0/1616	0.76	0/2200
1	G	0.41	0/1583	0.73	0/2157
2	B	0.45	0/1658	0.76	2/2255 (0.1%)
2	D	0.42	0/1657	0.69	0/2254
2	F	0.46	0/1657	0.69	0/2254
2	H	0.44	0/1650	0.69	0/2243
3	I	0.48	0/826	0.70	0/1122
3	J	0.48	0/829	0.79	1/1124 (0.1%)
3	K	0.51	0/846	0.67	0/1148
3	L	0.47	0/826	0.75	0/1122
All	All	0.44	0/16321	0.72	3/22204 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	51	PHE	C-N-CA	7.08	139.40	121.70
2	B	127	SER	C-N-CA	5.88	134.65	122.30
2	B	127	SER	CA-C-N	5.64	127.49	116.20

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	1535	0	1490	12	0
1	C	1564	0	1519	8	0
1	E	1579	0	1542	15	0
1	G	1547	0	1510	8	0
2	B	1620	0	1554	10	0
2	D	1619	0	1558	8	0
2	F	1619	0	1558	25	0
2	H	1613	0	1553	13	0
3	I	802	0	734	14	0
3	J	805	0	745	13	0
3	K	821	0	753	9	0
3	L	802	0	734	13	0
All	All	15926	0	15250	134	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 4.

The worst 5 of 134 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:H:46:LEU:HD23	2:H:55:TYR:CB	1.96	0.96
2:F:50:SER:H	2:F:91:HIS:HE1	1.15	0.88
2:F:32:ALA:HB1	2:F:91:HIS:HB2	1.62	0.81
3:L:76:PRO:HB3	3:L:103:VAL:HG13	1.68	0.75
2:H:124:GLN:HE22	2:H:131:SER:HB2	1.53	0.71

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	203/221 (92%)	194 (96%)	7 (3%)	2 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	207/221 (94%)	199 (96%)	6 (3%)	2 (1%)	15	37
1	E	208/221 (94%)	198 (95%)	9 (4%)	1 (0%)	29	54
1	G	204/221 (92%)	189 (93%)	12 (6%)	3 (2%)	10	26
2	B	210/214 (98%)	192 (91%)	17 (8%)	1 (0%)	29	54
2	D	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
2	F	209/214 (98%)	197 (94%)	10 (5%)	2 (1%)	15	37
2	H	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
3	I	100/108 (93%)	91 (91%)	8 (8%)	1 (1%)	15	37
3	J	100/108 (93%)	90 (90%)	9 (9%)	1 (1%)	15	37
3	K	101/108 (94%)	95 (94%)	5 (5%)	1 (1%)	15	37
3	L	100/108 (93%)	91 (91%)	7 (7%)	2 (2%)	7	19
All	All	2060/2172 (95%)	1932 (94%)	112 (5%)	16 (1%)	19	43

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	PRO
1	E	43	LYS
1	G	43	LYS
1	G	77	ASN
3	J	52	LEU

### 5.3.2 Protein sidechains [i](#)

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	172/186 (92%)	163 (95%)	9 (5%)	23	49
1	C	175/186 (94%)	162 (93%)	13 (7%)	13	32
1	E	177/186 (95%)	165 (93%)	12 (7%)	16	36
1	G	174/186 (94%)	161 (92%)	13 (8%)	13	31
2	B	183/187 (98%)	167 (91%)	16 (9%)	10	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	184/187 (98%)	165 (90%)	19 (10%)	7	16
2	F	184/187 (98%)	167 (91%)	17 (9%)	9	21
2	H	183/187 (98%)	166 (91%)	17 (9%)	9	21
3	I	85/94 (90%)	74 (87%)	11 (13%)	4	10
3	J	86/94 (92%)	75 (87%)	11 (13%)	4	10
3	K	88/94 (94%)	83 (94%)	5 (6%)	20	44
3	L	85/94 (90%)	76 (89%)	9 (11%)	6	15
All	All	1776/1868 (95%)	1624 (91%)	152 (9%)	10	24

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	168	SER
3	L	4	LEU
3	I	20	LEU
3	J	39	LYS
3	L	92	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	199	GLN
3	L	41	ASN
3	I	41	ASN
3	J	57	HIS
2	D	138	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(Å <sup>2</sup> )	Q<0.9
1	A	207/221 (93%)	-0.47	0 <a href="#">100</a> <a href="#">100</a>	12, 28, 43, 69	0
1	C	211/221 (95%)	-0.48	0 <a href="#">100</a> <a href="#">100</a>	15, 29, 45, 55	0
1	E	211/221 (95%)	-0.48	0 <a href="#">100</a> <a href="#">100</a>	15, 29, 44, 91	0
1	G	208/221 (94%)	-0.26	2 (0%) <a href="#">82</a> <a href="#">83</a>	22, 41, 61, 78	0
2	B	212/214 (99%)	-0.50	1 (0%) <a href="#">91</a> <a href="#">92</a>	14, 31, 47, 60	0
2	D	211/214 (98%)	-0.47	0 <a href="#">100</a> <a href="#">100</a>	19, 34, 48, 60	0
2	F	211/214 (98%)	-0.46	0 <a href="#">100</a> <a href="#">100</a>	14, 33, 45, 60	0
2	H	211/214 (98%)	-0.36	0 <a href="#">100</a> <a href="#">100</a>	23, 40, 56, 63	0
3	I	104/108 (96%)	0.60	13 (12%) <a href="#">3</a> <a href="#">3</a>	38, 67, 102, 114	0
3	J	104/108 (96%)	0.09	4 (3%) <a href="#">40</a> <a href="#">39</a>	22, 51, 88, 99	0
3	K	105/108 (97%)	-0.07	1 (0%) <a href="#">82</a> <a href="#">83</a>	35, 58, 72, 92	0
3	L	104/108 (96%)	0.09	4 (3%) <a href="#">40</a> <a href="#">39</a>	26, 55, 81, 87	0
All	All	2099/2172 (96%)	-0.31	25 (1%) <a href="#">79</a> <a href="#">80</a>	12, 36, 69, 114	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	4	LEU	4.6
3	L	51	PHE	4.4
3	I	2	PHE	4.3
3	L	52	LEU	4.2
3	I	5	ASP	3.6

### 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.