



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 08:50 am BST

PDB ID : 1DEE  
Title : Structure of S. aureus protein A bound to a human IgM Fab  
Authors : Graille, M.; Stura, E.A.; Corper, A.L.; Sutton, B.J.; Taussig, M.J.; Charbonnier, J.B.; Silverman, G.J.  
Deposited on : 1999-11-15  
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.

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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	:	2.11
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

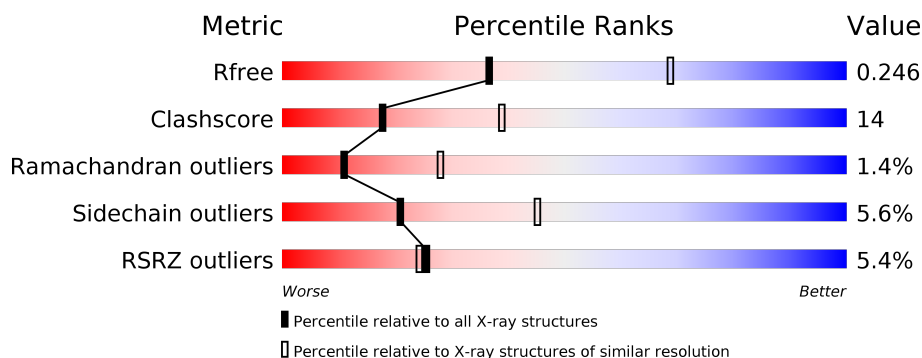
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 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	214	<div> <div></div> <div>71% 25% .</div> </div>
1	C	214	<div> <div>7%</div> <div>66% 32% .</div> </div>
1	E	214	<div> <div></div> <div>64% 34% .</div> </div>
2	B	223	<div> <div>5%</div> <div>68% 30% .</div> </div>
2	D	223	<div> <div>15%</div> <div>63% 35% .</div> </div>
2	F	223	<div> <div>5%</div> <div>67% 32% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	54	<div><div></div><div>6%</div><div>74%</div><div>19%</div><div>• 6%</div></div>
3	H	54	<div><div></div><div>6%</div><div>67%</div><div>28%</div><div>• •</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10859 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 IGM RF 2A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1640	1021	276	337	6			
1	C	214	Total	C	N	O	S	0	0	0
			1640	1021	276	337	6			
1	E	214	Total	C	N	O	S	0	0	0
			1640	1021	276	337	6			

- Molecule 2 is a protein called IGM RF 2A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1701	1071	290	333	7			
2	D	223	Total	C	N	O	S	0	0	0
			1701	1071	290	333	7			
2	F	223	Total	C	N	O	S	0	0	0
			1701	1071	290	333	7			

- Molecule 3 is a protein called IMMUNOGLOBULIN G BINDING PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	51	Total	C	N	O	S	0	0	0
			401	245	70	85	1			
3	H	54	Total	C	N	O	S	0	0	0
			425	261	74	89	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		

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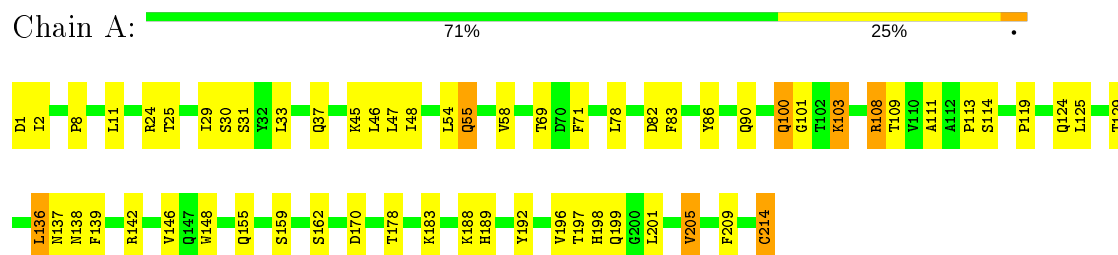
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O	0	0
			1	1		
4	F	2	Total	O	0	0
			2	2		

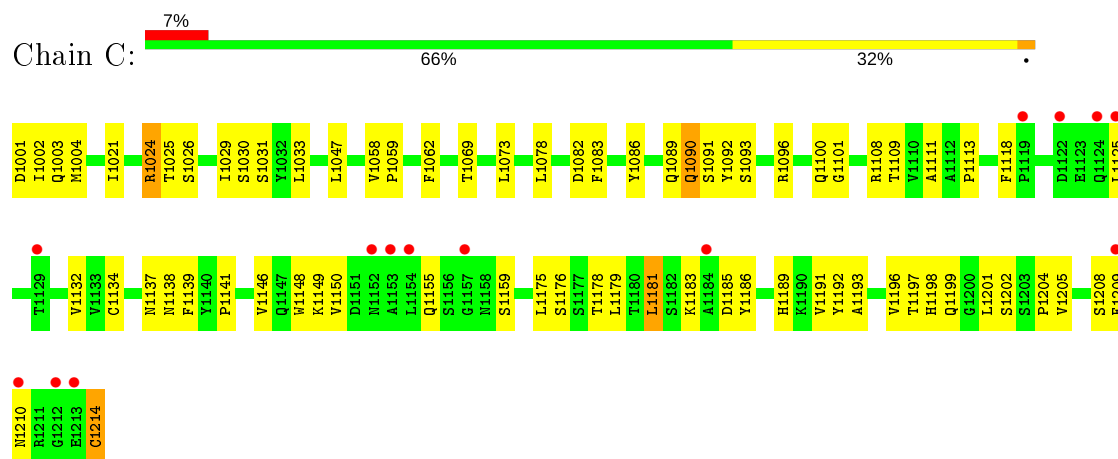
### 3 Residue-property plots

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.

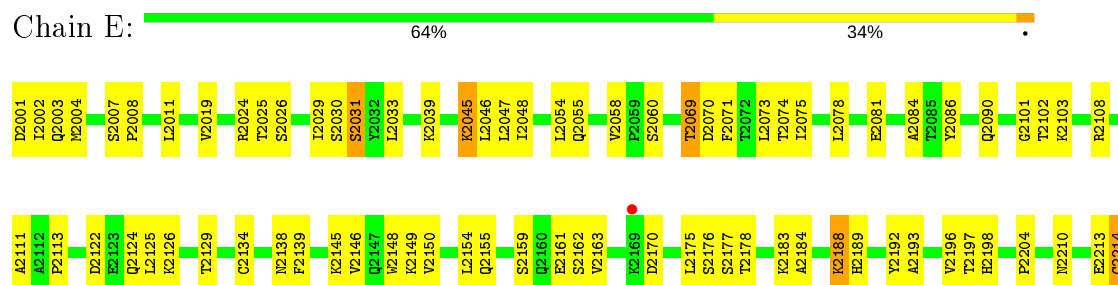
#### • Molecule 1: IGM RF 2A2



#### • Molecule 1: IGM RF 2A2

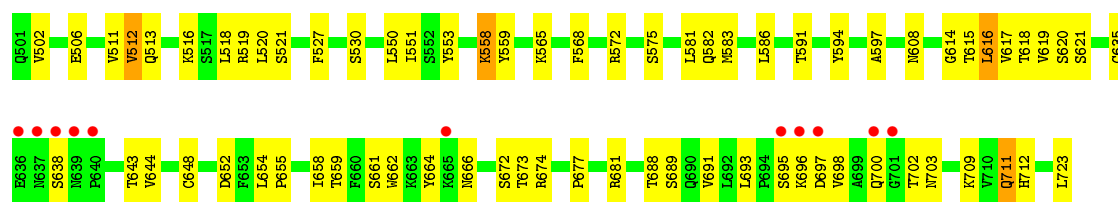


#### • Molecule 1: IGM RF 2A2

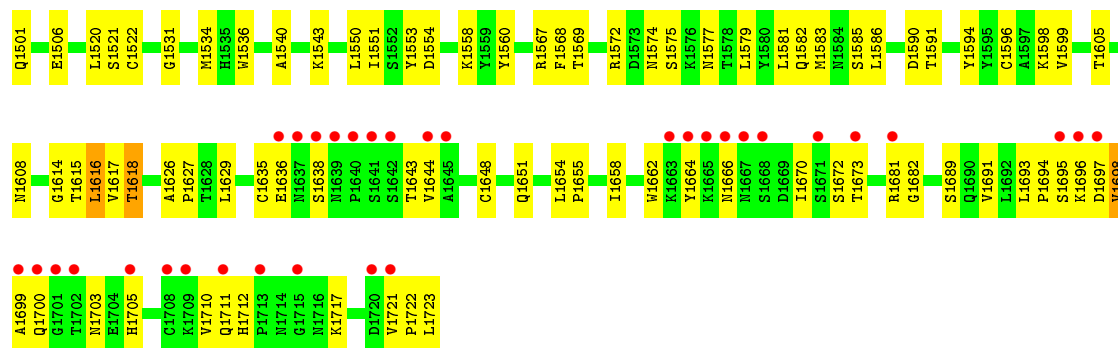


#### • Molecule 2: IGM RF 2A2





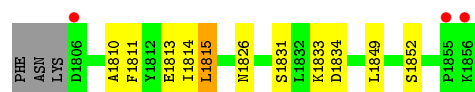
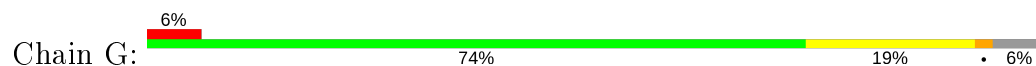
• Molecule 2: IGM RF 2A2



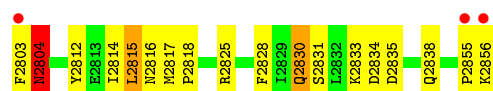
• Molecule 2: IGM RF 2A2



• Molecule 3: IMMUNOGLOBULIN G BINDING PROTEIN A



• Molecule 3: IMMUNOGLOBULIN G BINDING PROTEIN A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.52Å 78.91Å 163.24Å 90.00° 100.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 78.7 (19.96-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.217 , 0.281 0.192 , 0.246	Depositor DCC
$R_{free}$ test set	2328 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 65.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	0.44	0/1674	0.74	1/2270 (0.0%)
1	C	0.41	0/1674	0.69	0/2270
1	E	0.39	0/1674	0.70	1/2270 (0.0%)
2	B	0.41	0/1742	0.64	0/2367
2	D	0.40	0/1742	0.65	0/2367
2	F	0.37	0/1742	0.62	0/2367
3	G	0.34	0/406	0.55	0/545
3	H	0.36	0/431	0.61	0/579
All	All	0.40	0/11085	0.67	2/15035 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	CA-CB-CG	6.52	130.29	115.30
1	E	2011	LEU	CA-CB-CG	5.32	127.54	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	1640	0	1594	40	0
1	C	1640	0	1591	50	0
1	E	1640	0	1591	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1701	0	1648	49	0
2	D	1701	0	1648	51	0
2	F	1701	0	1648	47	0
3	G	401	0	385	8	0
3	H	425	0	402	14	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
All	All	10859	0	10507	288	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 14.

The worst 5 of 288 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:F:2569:THR:HG21	3:H:2831:SER:HA	1.53	0.89
1:C:1214:CYS:HG	2:D:1635:CYS:HG	1.10	0.86
1:E:2214:CYS:HG	2:F:2635:CYS:HG	1.21	0.85
2:F:2569:THR:HG22	2:F:2582:GLN:HB3	1.60	0.83
1:C:1146:VAL:HG12	1:C:1196:VAL:HG22	1.60	0.82

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	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17	40
1	C	212/214 (99%)	197 (93%)	13 (6%)	2 (1%)	17	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	212/214 (99%)	199 (94%)	10 (5%)	3 (1%)	11	28
2	B	221/223 (99%)	202 (91%)	16 (7%)	3 (1%)	11	28
2	D	221/223 (99%)	201 (91%)	16 (7%)	4 (2%)	8	21
2	F	221/223 (99%)	204 (92%)	13 (6%)	4 (2%)	8	21
3	G	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
3	H	52/54 (96%)	49 (94%)	2 (4%)	1 (2%)	8	20
All	All	1400/1419 (99%)	1301 (93%)	80 (6%)	19 (1%)	11	28

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	696	LYS
2	D	1696	LYS
2	F	2696	LYS
1	C	1031	SER
1	A	30	SER

### 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	189/189 (100%)	177 (94%)	12 (6%)	18	40
1	C	189/189 (100%)	181 (96%)	8 (4%)	30	58
1	E	189/189 (100%)	178 (94%)	11 (6%)	20	43
2	B	188/188 (100%)	176 (94%)	12 (6%)	17	39
2	D	188/188 (100%)	178 (95%)	10 (5%)	22	48
2	F	188/188 (100%)	181 (96%)	7 (4%)	34	63
3	G	45/48 (94%)	41 (91%)	4 (9%)	9	22
3	H	47/48 (98%)	43 (92%)	4 (8%)	10	24
All	All	1223/1227 (100%)	1155 (94%)	68 (6%)	21	45

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1202	SER
2	D	1618	THR
3	G	1849	LEU
1	C	1214	CYS
2	D	1577	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1138	ASN
2	D	1608	ASN
3	H	2808	GLN
1	C	1198	HIS
2	D	1577	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 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 ⓘ

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	214/214 (100%)	-0.68	0 <span>100</span> <span>100</span>	11, 30, 70, 91	0
1	C	214/214 (100%)	-0.13	14 (6%) <span>18</span> <span>17</span>	12, 40, 96, 109	0
1	E	214/214 (100%)	-0.54	1 (0%) <span>91</span> <span>92</span>	19, 45, 72, 99	0
2	B	223/223 (100%)	-0.30	11 (4%) <span>29</span> <span>28</span>	11, 31, 132, 163	0
2	D	223/223 (100%)	0.27	33 (14%) <span>2</span> <span>1</span>	12, 46, 135, 156	0
2	F	223/223 (100%)	-0.24	12 (5%) <span>25</span> <span>24</span>	17, 45, 124, 153	0
3	G	51/54 (94%)	-0.30	3 (5%) <span>22</span> <span>21</span>	17, 42, 113, 156	0
3	H	54/54 (100%)	-0.18	3 (5%) <span>24</span> <span>23</span>	27, 51, 80, 110	0
All	All	1416/1419 (99%)	-0.26	77 (5%) <span>25</span> <span>24</span>	11, 40, 106, 163	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2638	SER	9.9
3	G	1856	LYS	9.5
2	D	1638	SER	8.0
2	B	696	LYS	7.7
2	D	1699	ALA	7.4

### 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 carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.