



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 09:12 PM EDT

PDB ID : 6S3D  
Title : Structure of D25 Fab in complex with scaffold S0\_2.126  
Authors : Cramer, J.T.; Krey, T.  
Deposited on : 2019-06-25  
Resolution : 3.00 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	:	2.37.1
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

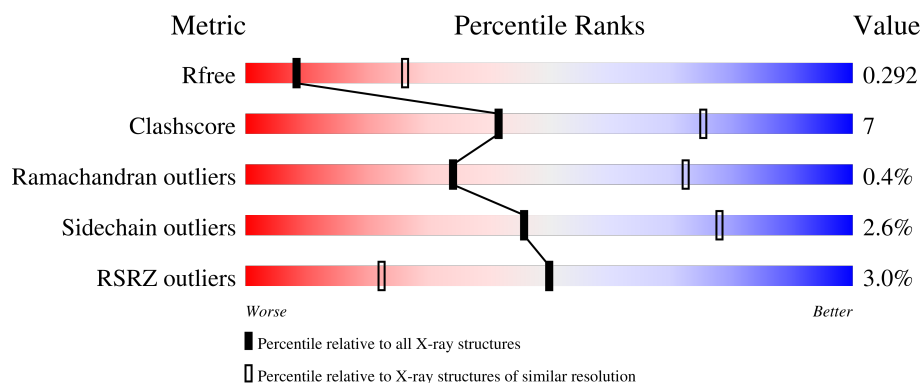
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	241	<div> <div>5%</div> <div> <div>75%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	241	<div> <div>2%</div> <div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>
1	E	241	<div> <div>3%</div> <div> <div>73%</div> <div>16%</div> <div>11%</div> </div> </div>
1	H	241	<div> <div>4%</div> <div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	225	<div> <div>3%</div> <div> <div>79%</div> <div>14%</div> <div>•</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	225	<div><div><div></div><div></div><div></div></div><div>3%75%16%8%</div></div>
2	F	225	<div><div><div></div><div></div><div></div></div><div>%76%15%8%</div></div>
2	L	225	<div><div><div></div><div></div><div></div></div><div>3%77%16%6%</div></div>
3	M	71	<div><div><div></div><div></div><div></div></div><div>%62%21%17%</div></div>
3	N	71	<div><div><div></div><div></div><div></div></div><div>%62%20%18%</div></div>
3	O	71	<div><div><div></div><div></div><div></div></div><div>%62%17%17%</div></div>
3	P	71	<div><div><div></div><div></div><div></div></div><div>56%25%18%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14439 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1572	1002	259	304	7			
1	C	215	Total	C	N	O	S	0	0	0
			1601	1020	265	309	7			
1	E	215	Total	C	N	O	S	0	0	0
			1590	1012	264	307	7			
1	H	212	Total	C	N	O	S	0	0	0
			1581	1006	261	307	7			

- Molecule 2 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1580	991	260	324	5			
2	D	206	Total	C	N	O	S	0	0	0
			1570	986	260	319	5			
2	F	206	Total	C	N	O	S	0	0	0
			1553	972	256	320	5			
2	L	211	Total	C	N	O	S	0	0	0
			1585	992	261	327	5			

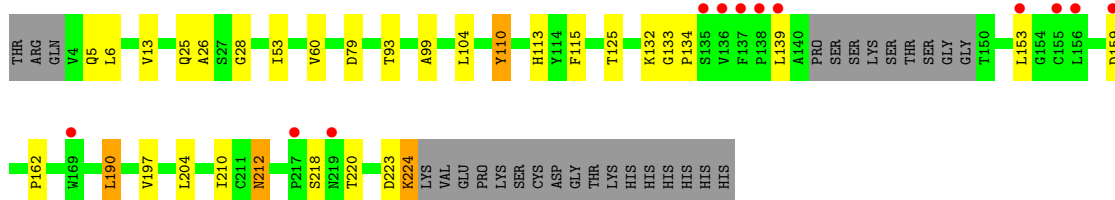
- Molecule 3 is a protein called S0\_2.126.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	59	Total	C	N	O	S	0	0	0
			444	277	77	85	5			
3	N	58	Total	C	N	O	S	0	0	0
			456	284	80	87	5			
3	O	59	Total	C	N	O	S	0	0	0
			452	280	79	88	5			
3	P	58	Total	C	N	O	S	0	0	0
			455	282	82	87	4			

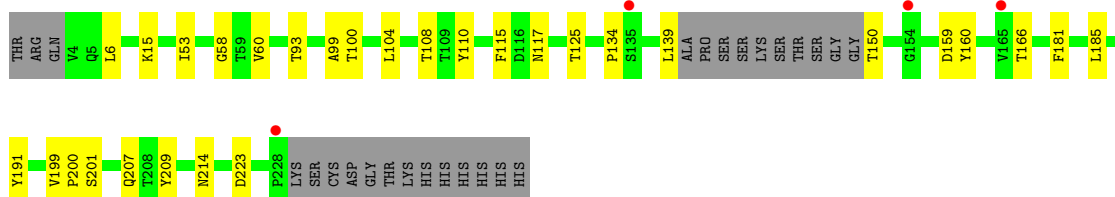
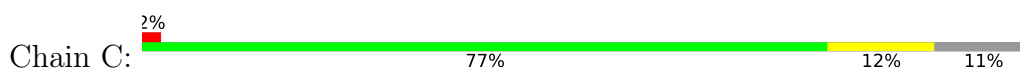
### 3 Residue-property plots [i](#)

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.

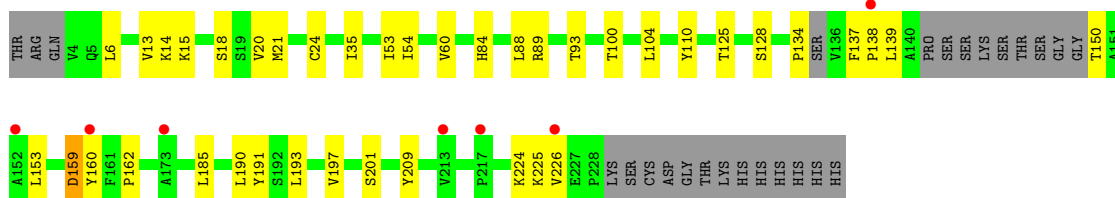
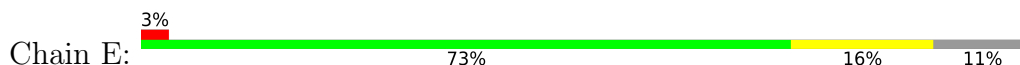
#### • Molecule 1: Heavy Chain



#### • Molecule 1: Heavy Chain

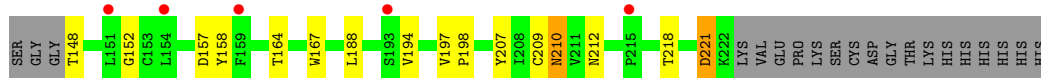


#### • Molecule 1: Heavy Chain

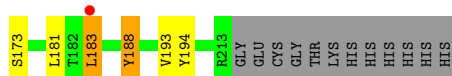
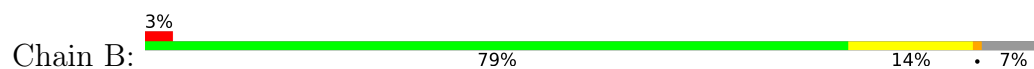


#### • Molecule 1: Heavy Chain

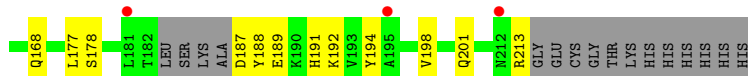
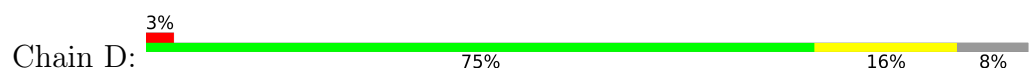




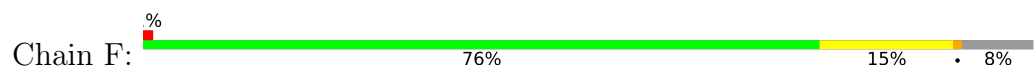
• Molecule 2: Light Chain



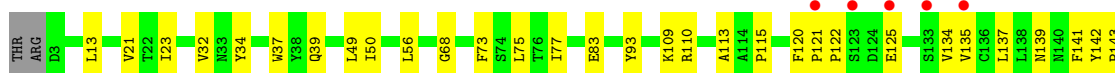
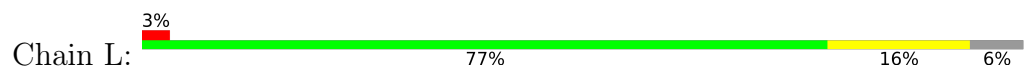
• Molecule 2: Light Chain



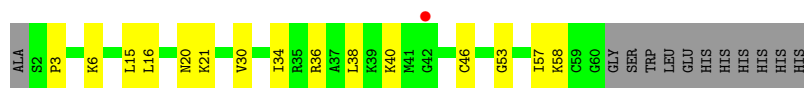
• Molecule 2: Light Chain



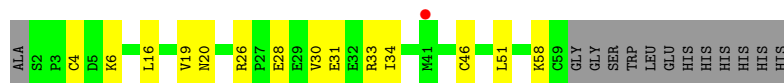
• Molecule 2: Light Chain



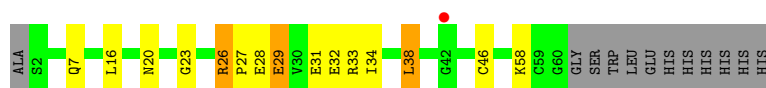
## • Molecule 3: S0\_2.126



## • Molecule 3: S0\_2.126



## • Molecule 3: S0\_2.126



## • Molecule 3: S0\_2.126



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.27Å 126.98Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 3.00 49.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.09-3.00) 99.7 (49.09-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.269 , 0.292 0.270 , 0.292	Depositor DCC
$R_{free}$ test set	2542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	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 88.81 % 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 4.2895e-08. 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	0.28	0/1612	0.55	0/2211
1	C	0.27	0/1642	0.53	0/2250
1	E	0.33	0/1629	0.58	0/2232
1	H	0.26	0/1621	0.53	0/2221
2	B	0.28	0/1612	0.51	0/2199
2	D	0.30	0/1600	0.53	0/2175
2	F	0.28	0/1583	0.51	0/2158
2	L	0.28	0/1617	0.50	0/2206
3	M	0.36	0/447	0.53	0/596
3	N	0.33	0/460	0.51	0/612
3	O	0.41	0/456	0.70	0/609
3	P	0.30	0/459	0.55	0/612
All	All	0.30	0/14738	0.54	0/20081

There are no bond length outliers.

There are no bond angle outliers.

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	1572	0	1525	21	0
1	C	1601	0	1562	15	0
1	E	1590	0	1539	23	0
1	H	1581	0	1546	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1580	0	1503	19	0
2	D	1570	0	1502	28	0
2	F	1553	0	1454	22	0
2	L	1585	0	1506	24	0
3	M	444	0	440	11	0
3	N	456	0	470	7	0
3	O	452	0	451	11	0
3	P	455	0	463	9	0
All	All	14439	0	13961	199	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 7.

The worst 5 of 199 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)
3:O:26:ARG:O	3:O:29:GLU:HB2	1.54	1.08
1:E:159:ASP:HB3	1:E:190:LEU:HD22	1.55	0.87
3:O:28:GLU:HA	3:O:31:GLU:HG3	1.62	0.79
1:E:14:LYS:HG3	1:E:20:VAL:HG12	1.68	0.74
3:O:26:ARG:CZ	3:O:28:GLU:HB2	2.18	0.74

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	208/241 (86%)	199 (96%)	8 (4%)	1 (0%)	29	68
1	C	211/241 (88%)	200 (95%)	11 (5%)	0	100	100
1	E	209/241 (87%)	201 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	208/241 (86%)	201 (97%)	6 (3%)	1 (0%)	29	68
2	B	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	29	68
2	D	198/225 (88%)	192 (97%)	5 (2%)	1 (0%)	29	68
2	F	198/225 (88%)	192 (97%)	5 (2%)	1 (0%)	29	68
2	L	209/225 (93%)	203 (97%)	5 (2%)	1 (0%)	29	68
3	M	57/71 (80%)	54 (95%)	2 (4%)	1 (2%)	8	37
3	N	56/71 (79%)	51 (91%)	5 (9%)	0	100	100
3	O	57/71 (80%)	53 (93%)	3 (5%)	1 (2%)	8	37
3	P	56/71 (79%)	51 (91%)	5 (9%)	0	100	100
All	All	1873/2148 (87%)	1794 (96%)	71 (4%)	8 (0%)	34	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	32	VAL
3	O	23	GLY
2	D	32	VAL
2	B	32	VAL
2	L	32	VAL

### 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	173/205 (84%)	169 (98%)	4 (2%)	50	80
1	C	178/205 (87%)	172 (97%)	6 (3%)	37	72
1	E	174/205 (85%)	170 (98%)	4 (2%)	50	80
1	H	177/205 (86%)	172 (97%)	5 (3%)	43	77
2	B	177/198 (89%)	172 (97%)	5 (3%)	43	77
2	D	177/198 (89%)	176 (99%)	1 (1%)	86	95
2	F	172/198 (87%)	168 (98%)	4 (2%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	177/198 (89%)	174 (98%)	3 (2%)	60	85
3	M	47/63 (75%)	46 (98%)	1 (2%)	53	82
3	N	52/63 (82%)	51 (98%)	1 (2%)	57	84
3	O	50/63 (79%)	45 (90%)	5 (10%)	7	29
3	P	51/63 (81%)	48 (94%)	3 (6%)	19	54
All	All	1605/1864 (86%)	1563 (97%)	42 (3%)	46	78

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	221	ASP
3	O	29	GLU
2	L	56	LEU
3	M	46	CYS
3	O	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	139	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	212/241 (87%)	0.21	12 (5%) 23 8	46, 89, 135, 169	0
1	C	215/241 (89%)	0.21	4 (1%) 66 37	51, 100, 165, 200	0
1	E	215/241 (89%)	0.15	7 (3%) 46 20	46, 101, 160, 194	0
1	H	212/241 (87%)	0.22	9 (4%) 36 14	50, 103, 190, 249	0
2	B	210/225 (93%)	0.01	6 (2%) 51 23	52, 84, 159, 176	0
2	D	206/225 (91%)	0.00	7 (3%) 45 19	36, 80, 149, 166	0
2	F	206/225 (91%)	-0.02	3 (1%) 73 46	50, 85, 189, 230	0
2	L	211/225 (93%)	0.03	7 (3%) 46 20	46, 86, 172, 190	0
3	M	59/71 (83%)	0.02	1 (1%) 70 41	89, 130, 160, 163	0
3	N	58/71 (81%)	-0.05	1 (1%) 70 41	76, 113, 148, 156	0
3	O	59/71 (83%)	-0.03	1 (1%) 70 41	82, 131, 152, 168	0
3	P	58/71 (81%)	-0.13	0 100 100	74, 114, 141, 146	0
All	All	1921/2148 (89%)	0.08	58 (3%) 50 22	36, 95, 165, 249	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	138	PRO	6.2
1	A	138	PRO	5.5
2	D	123	SER	5.5
1	C	135	SER	4.9
2	L	123	SER	4.3

### 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.