



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:13 AM GMT

PDB ID : 4EVN  
Title : Crystal Structure of Fab CR6261 (somatic heavy chain with germline-reverted light chain)  
Authors : Whittle, J.R.R.  
Deposited on : 2012-04-26  
Resolution : 2.85 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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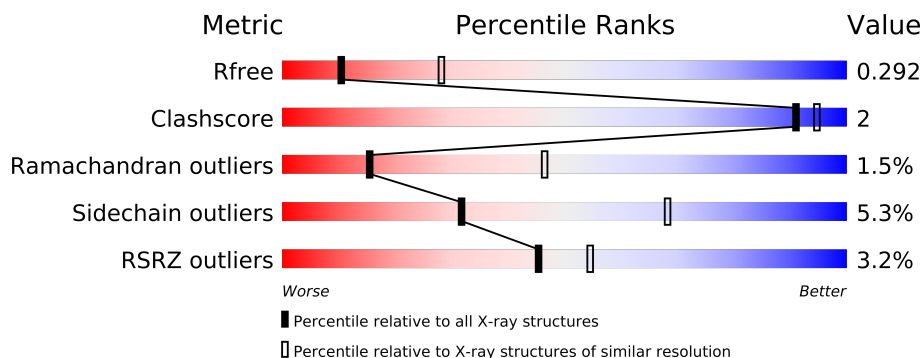
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.85 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))
$R_{free}$	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	242	
1	C	242	
1	E	242	
1	G	242	
1	I	242	
1	K	242	
1	M	242	
1	O	242	
2	B	217	
2	D	217	
2	F	217	
2	H	217	
2	J	217	
2	L	217	

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Mol	Chain	Length	Quality of chain
2	N	217	
2	P	217	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25293 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	C	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	E	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	G	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	I	221	Total	C	N	O	S	0	0	0
			1625	1029	269	318	9			
1	K	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	M	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			
1	O	221	Total	C	N	O	S	0	0	0
			1623	1028	268	318	9			

- Molecule 2 is a protein called Fab Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1541	972	251	314	4			
2	D	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	F	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	H	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	J	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	L	213	Total	C	N	O	S	0	0	0
			1540	970	251	315	4			

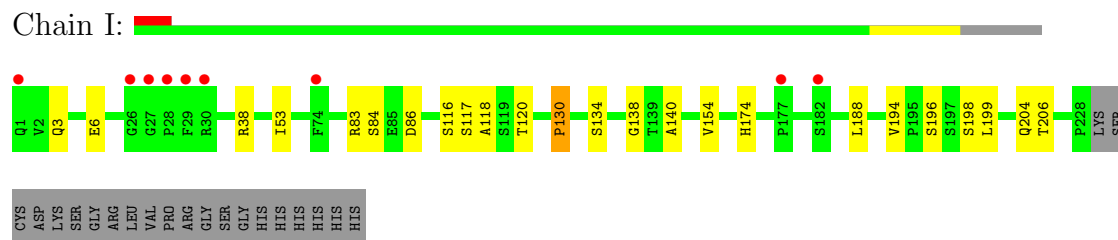
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	213	Total	C	N	O	S	0	0	0
			1537	969	250	314	4			
2	P	213	Total	C	N	O	S	0	0	0
			1539	970	251	314	4			

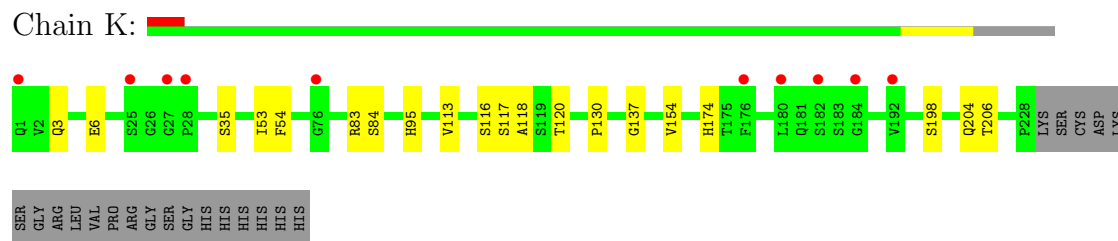


Chain I:



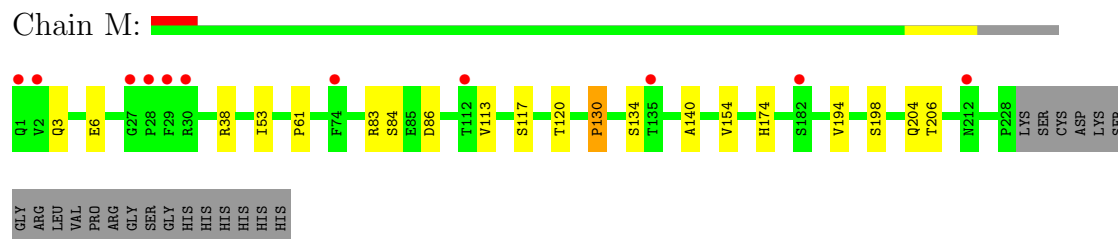
- Molecule 1: Fab Heavy Chain

Chain K:



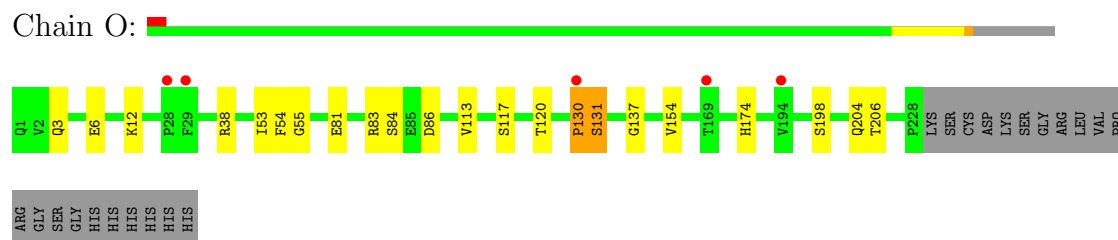
- Molecule 1: Fab Heavy Chain

Chain M:



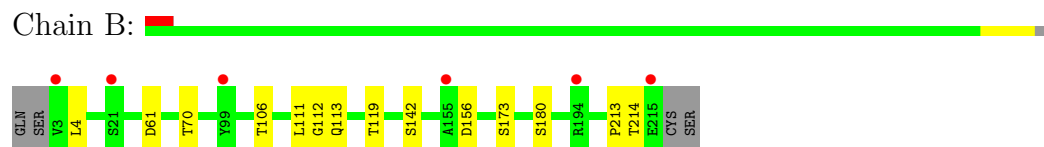
- Molecule 1: Fab Heavy Chain

Chain O:



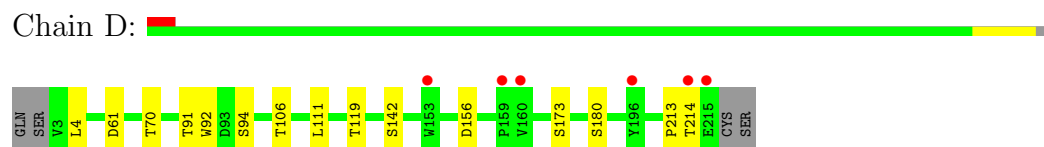
- Molecule 2: Fab Lambda Light Chain

Chain B:



- Molecule 2: Fab Lambda Light Chain

Chain D:



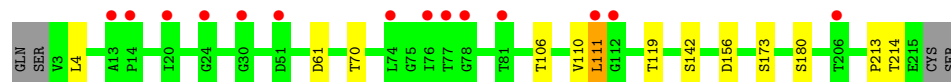
- Molecule 2: Fab Lambda Light Chain

Chain F: 



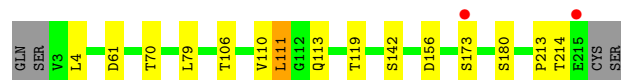
- Molecule 2: Fab Lambda Light Chain

Chain H: 



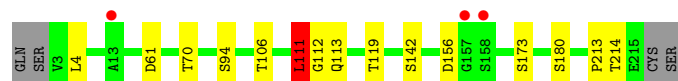
- Molecule 2: Fab Lambda Light Chain

Chain J: 



- Molecule 2: Fab Lambda Light Chain

Chain L: 



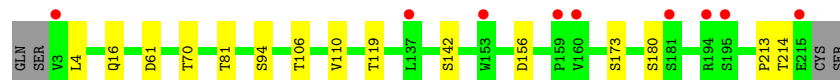
- Molecule 2: Fab Lambda Light Chain

Chain N: 



- Molecule 2: Fab Lambda Light Chain

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.11Å 159.27Å 176.44Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	55.01 – 2.85 176.44 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (55.01-2.85) 92.7 (176.44-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.230 , 0.293 0.228 , 0.292	Depositor DCC
$R_{free}$ test set	1946 reflections (2.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 24.2	EDS
Estimated twinning fraction	0.073 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 86892 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/1664	0.59	0/2270
1	C	0.53	1/1664 (0.1%)	0.62	0/2270
1	E	0.57	0/1666	0.66	0/2272
1	G	0.50	0/1664	0.61	0/2270
1	I	0.52	0/1666	0.63	0/2272
1	K	0.53	0/1664	0.66	0/2270
1	M	0.49	0/1664	0.57	0/2270
1	O	0.51	0/1664	0.62	0/2270
2	B	0.46	0/1580	0.60	1/2168 (0.0%)
2	D	0.48	0/1576	0.61	0/2164
2	F	0.46	0/1576	0.62	0/2164
2	H	0.42	0/1576	0.56	0/2164
2	J	0.44	0/1576	0.59	0/2164
2	L	0.43	0/1579	0.60	0/2168
2	N	0.43	0/1576	0.59	0/2164
2	P	0.45	0/1578	0.60	0/2166
All	All	0.48	1/25933 (0.0%)	0.61	1/35486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLN	CD-NE2	6.42	1.49	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	GLN	N-CA-C	-5.67	95.69	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1623	0	0	1	0
1	C	1623	0	0	3	0
1	E	1625	0	0	8	0
1	G	1623	0	0	6	0
1	I	1625	0	0	6	0
1	K	1623	0	0	4	0
1	M	1623	0	0	4	1
1	O	1623	0	0	7	0
2	B	1541	0	22	1	0
2	D	1537	0	22	4	0
2	F	1537	0	22	2	0
2	H	1537	0	22	1	0
2	J	1537	0	22	3	0
2	L	1540	0	22	3	0
2	N	1537	0	22	3	0
2	P	1539	0	22	3	1
All	All	25293	0	176	51	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:81:GLU:OE2	1:O:12:LYS:NZ	2.02	0.93
1:I:138:GLY:O	1:I:196:SER:N	2.06	0.89
2:D:94:SER:OG	2:N:94:SER:OG	1.97	0.82
1:E:217:ASN:ND2	1:O:55:GLY:O	2.13	0.82
1:E:12:LYS:NZ	1:O:81:GLU:OE2	2.26	0.68

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:61:PRO:O	2:P:16:GLN:NE2[2_555]	2.08	0.12

## 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	219/242 (90%)	211 (96%)	6 (3%)	2 (1%)	25	62
1	C	219/242 (90%)	210 (96%)	6 (3%)	3 (1%)	16	49
1	E	219/242 (90%)	207 (94%)	9 (4%)	3 (1%)	16	49
1	G	219/242 (90%)	207 (94%)	10 (5%)	2 (1%)	25	62
1	I	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	16	49
1	K	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	16	49
1	M	219/242 (90%)	209 (95%)	8 (4%)	2 (1%)	25	62
1	O	219/242 (90%)	208 (95%)	7 (3%)	4 (2%)	13	41
2	B	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	12	39
2	D	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	16	49
2	F	211/217 (97%)	201 (95%)	7 (3%)	3 (1%)	16	49
2	H	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	12	39
2	J	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	12	39
2	L	211/217 (97%)	199 (94%)	7 (3%)	5 (2%)	9	31
2	N	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	12	39
2	P	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	16	49
All	All	3440/3672 (94%)	3272 (95%)	116 (3%)	52 (2%)	15	46

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	PRO
2	J	111	LEU
2	L	111	LEU
2	N	111	LEU
2	B	214	THR

### 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	178/202 (88%)	166 (93%)	12 (7%)	23	54
1	C	178/202 (88%)	167 (94%)	11 (6%)	26	59
1	E	179/202 (89%)	168 (94%)	11 (6%)	26	59
1	G	178/202 (88%)	168 (94%)	10 (6%)	30	64
1	I	179/202 (89%)	169 (94%)	10 (6%)	30	64
1	K	178/202 (88%)	168 (94%)	10 (6%)	30	64
1	M	178/202 (88%)	168 (94%)	10 (6%)	30	64
1	O	178/202 (88%)	168 (94%)	10 (6%)	30	64
2	B	164/182 (90%)	156 (95%)	8 (5%)	35	72
2	D	163/182 (90%)	156 (96%)	7 (4%)	40	77
2	F	163/182 (90%)	156 (96%)	7 (4%)	40	77
2	H	163/182 (90%)	154 (94%)	9 (6%)	30	66
2	J	163/182 (90%)	156 (96%)	7 (4%)	40	77
2	L	164/182 (90%)	156 (95%)	8 (5%)	35	72
2	N	163/182 (90%)	155 (95%)	8 (5%)	35	72
2	P	164/182 (90%)	157 (96%)	7 (4%)	40	77
All	All	2733/3072 (89%)	2588 (95%)	145 (5%)	32	68

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	206	THR
1	I	154	VAL
1	O	120	THR
2	H	70	THR
2	H	173	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

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 ⓘ

### 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	221/242 (91%)	-0.04	7 (3%) 45 54	35, 65, 111, 200	0
1	C	221/242 (91%)	-0.02	6 (2%) 52 61	32, 60, 132, 231	0
1	E	221/242 (91%)	0.16	9 (4%) 35 42	24, 57, 123, 199	0
1	G	221/242 (91%)	0.18	9 (4%) 35 42	52, 75, 130, 200	0
1	I	221/242 (91%)	0.02	9 (4%) 35 42	38, 72, 122, 200	0
1	K	221/242 (91%)	0.18	10 (4%) 32 38	31, 64, 111, 198	0
1	M	221/242 (91%)	0.33	11 (4%) 28 33	48, 76, 133, 200	0
1	O	221/242 (91%)	0.04	5 (2%) 57 66	28, 68, 146, 199	0
2	B	213/217 (98%)	0.05	6 (2%) 50 60	38, 75, 107, 163	0
2	D	213/217 (98%)	-0.05	6 (2%) 50 60	30, 64, 104, 165	0
2	F	213/217 (98%)	-0.05	1 (0%) 88 92	31, 65, 105, 162	0
2	H	213/217 (98%)	0.42	14 (6%) 18 21	55, 92, 141, 207	0
2	J	213/217 (98%)	-0.13	2 (0%) 81 87	42, 76, 114, 161	0
2	L	213/217 (98%)	0.05	3 (1%) 72 80	34, 71, 118, 163	0
2	N	213/217 (98%)	-0.08	4 (1%) 64 72	40, 77, 113, 183	0
2	P	213/217 (98%)	0.03	9 (4%) 35 41	32, 73, 114, 164	0
All	All	3472/3672 (94%)	0.07	111 (3%) 45 54	24, 72, 123, 231	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	28	PRO	12.9
1	M	29	PHE	9.4
2	J	173	SER	7.6
1	I	26	GLY	6.5
1	C	136	SER	6.2

## 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 ⓘ

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.