



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:13 PM GMT

PDB ID : 4ZYP  
Title : Crystal Structure of Motavizumab and Quaternary-Specific RSV-Neutralizing Human Antibody AM14 in Complex with Prefusion RSV F Glycoprotein  
Authors : Gilman, M.S.A.; McLellan, J.S.  
Deposited on : 2015-05-21  
Resolution : 5.50 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  
<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

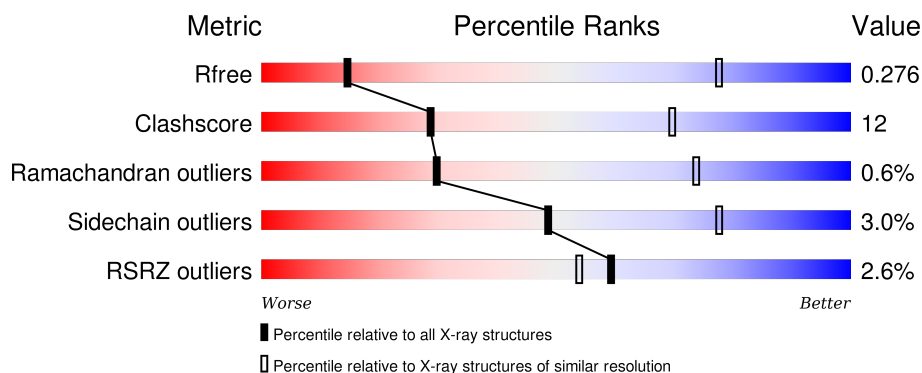
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 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.



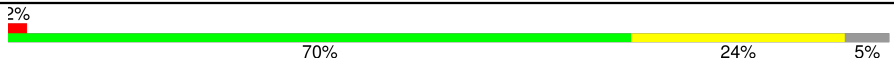









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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. 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	498	<div> <div></div> <div>61% 27% 10%</div> </div>
1	B	498	<div> <div></div> <div>61% 26% 10%</div> </div>
1	C	498	<div> <div></div> <div>59% 27% 10%</div> </div>
2	J	225	<div> <div></div> <div>64% 29% 5%</div> </div>
2	K	225	<div> <div></div> <div>62% 31% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	N	225	
3	L	213	
3	M	213	
3	O	213	
4	D	227	
4	F	227	
4	H	227	
5	E	215	
5	G	215	
5	I	215	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29990 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 Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			
1	B	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			
1	C	449	Total	C	N	O	S	0	0	0
			3482	2202	573	684	23			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ALA	PRO	conflict	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	GLU	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	PRO	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	PHE	deletion	UNP P03420
A	?	-	MET	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	TYR	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ALA	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	VAL	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
A	545	GLY	-	expression tag	UNP D9IEJ2
A	546	GLY	-	expression tag	UNP D9IEJ2
A	547	LEU	-	expression tag	UNP D9IEJ2
A	548	VAL	-	expression tag	UNP D9IEJ2
A	549	PRO	-	expression tag	UNP D9IEJ2
A	550	ARG	-	expression tag	UNP D9IEJ2
B	129	ALA	PRO	conflict	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	GLU	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	PRO	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	PHE	deletion	UNP P03420
B	?	-	MET	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	TYR	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	ALA	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	THR	deletion	UNP P03420
B	?	-	ASN	deletion	UNP P03420
B	?	-	VAL	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P03420
B	?	-	LEU	deletion	UNP P03420
B	?	-	SER	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	?	-	ARG	deletion	UNP P03420
B	?	-	LYS	deletion	UNP P03420
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
B	514	SER	-	linker	UNP P03420
B	515	ALA	-	linker	UNP P03420
B	516	ILE	-	linker	UNP P03420
B	517	GLY	-	linker	UNP P03420
B	545	GLY	-	expression tag	UNP D9IEJ2
B	546	GLY	-	expression tag	UNP D9IEJ2
B	547	LEU	-	expression tag	UNP D9IEJ2
B	548	VAL	-	expression tag	UNP D9IEJ2
B	549	PRO	-	expression tag	UNP D9IEJ2
B	550	ARG	-	expression tag	UNP D9IEJ2
C	129	ALA	PRO	conflict	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	GLU	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	PRO	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	PHE	deletion	UNP P03420
C	?	-	MET	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	TYR	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ASN	deletion	UNP P03420
C	?	-	ALA	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	UNP P03420
C	?	-	VAL	deletion	UNP P03420
C	?	-	THR	deletion	UNP P03420
C	?	-	LEU	deletion	UNP P03420
C	?	-	SER	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	?	-	ARG	deletion	UNP P03420
C	?	-	LYS	deletion	UNP P03420
C	155	CYS	SER	engineered mutation	UNP P03420
C	190	PHE	SER	engineered mutation	UNP P03420
C	207	LEU	VAL	engineered mutation	UNP P03420
C	290	CYS	SER	engineered mutation	UNP P03420
C	379	VAL	ILE	engineered mutation	UNP P03420
C	447	VAL	MET	engineered mutation	UNP P03420
C	514	SER	-	linker	UNP P03420
C	515	ALA	-	linker	UNP P03420
C	516	ILE	-	linker	UNP P03420
C	517	GLY	-	linker	UNP P03420
C	545	GLY	-	expression tag	UNP D9IEJ2
C	546	GLY	-	expression tag	UNP D9IEJ2
C	547	LEU	-	expression tag	UNP D9IEJ2
C	548	VAL	-	expression tag	UNP D9IEJ2
C	549	PRO	-	expression tag	UNP D9IEJ2
C	550	ARG	-	expression tag	UNP D9IEJ2

- Molecule 2 is a protein called Motavizumab antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			
2	K	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			
2	N	213	Total	C	N	O	S	0	0	0
			1626	1039	266	314	7			

- Molecule 3 is a protein called Motavizumab antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			
3	O	211	Total	C	N	O	S	0	0	0
			1611	1012	268	325	6			

- Molecule 4 is a protein called AM14 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	216	Total	C	N	O	S	0	0	0
			1636	1033	276	320	7			
4	H	216	Total	C	N	O	S	0	0	0
			1635	1033	276	319	7			
4	D	216	Total	C	N	O	S	0	0	0
			1636	1033	276	320	7			

- Molecule 5 is a protein called AM14 antibody light chain.

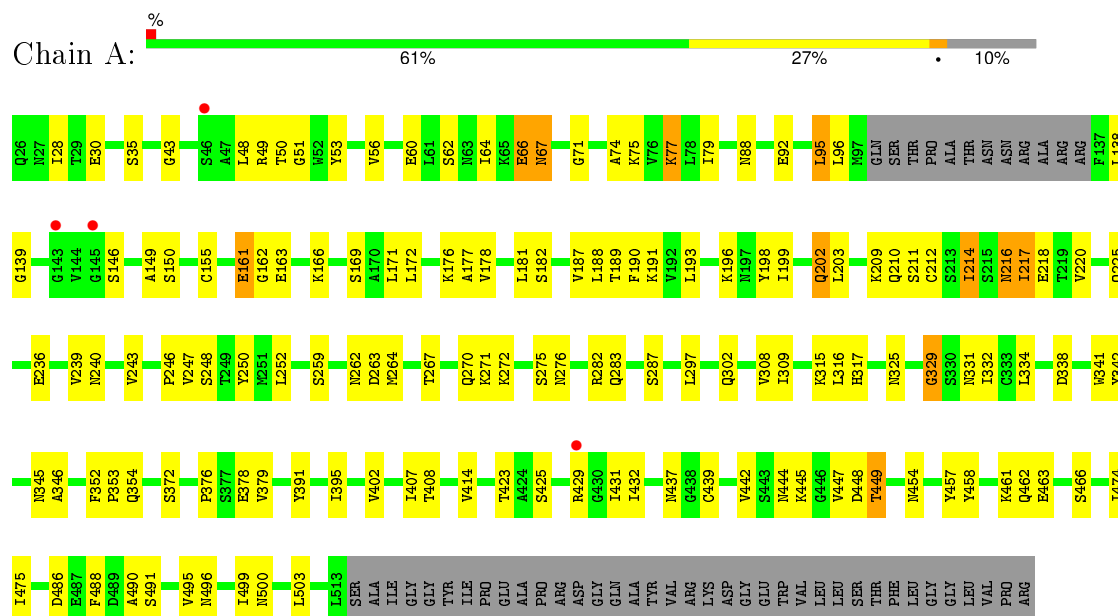
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			
5	I	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			
5	E	213	Total	C	N	O	S	0	0	0
			1642	1025	277	334	6			



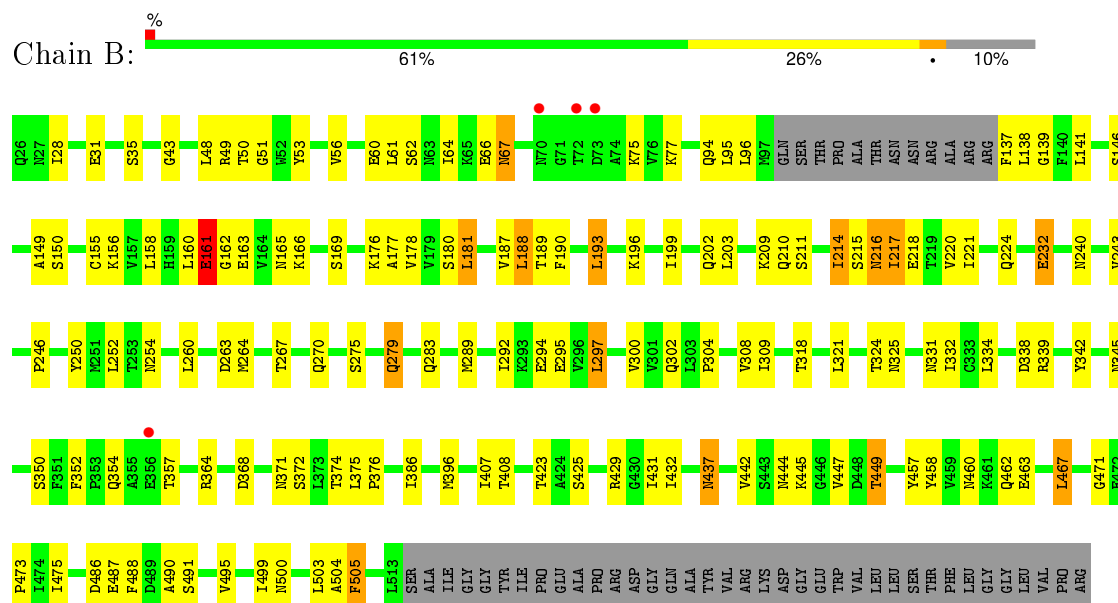
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

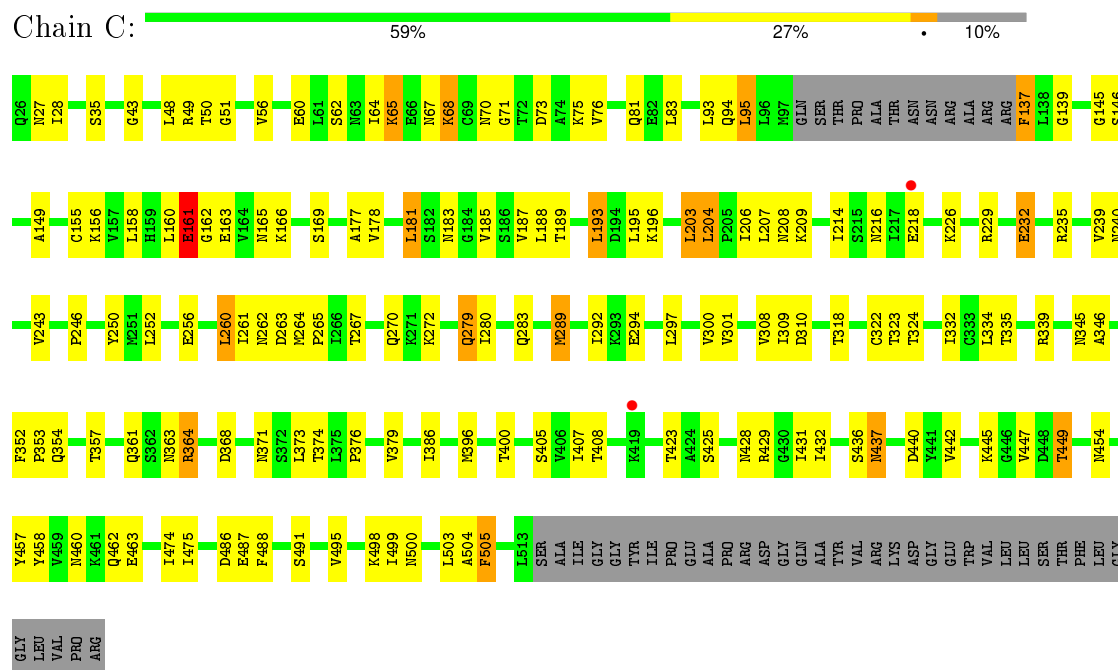
#### • Molecule 1: Fusion glycoprotein F0,Fibritin



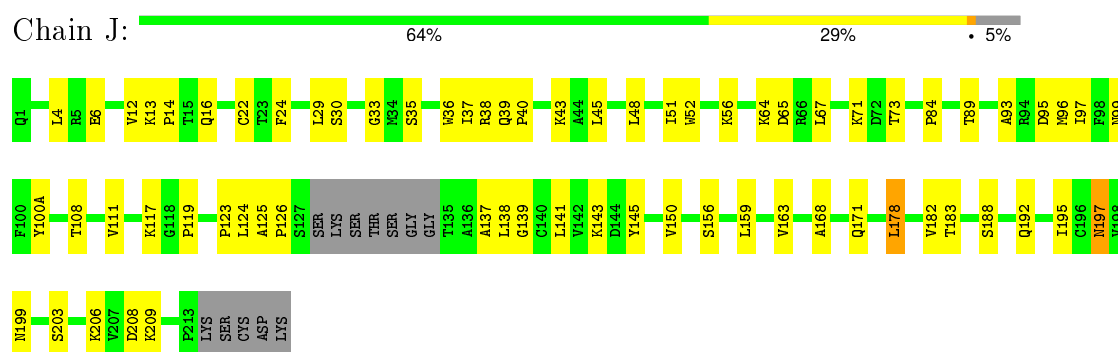
#### • Molecule 1: Fusion glycoprotein F0,Fibritin



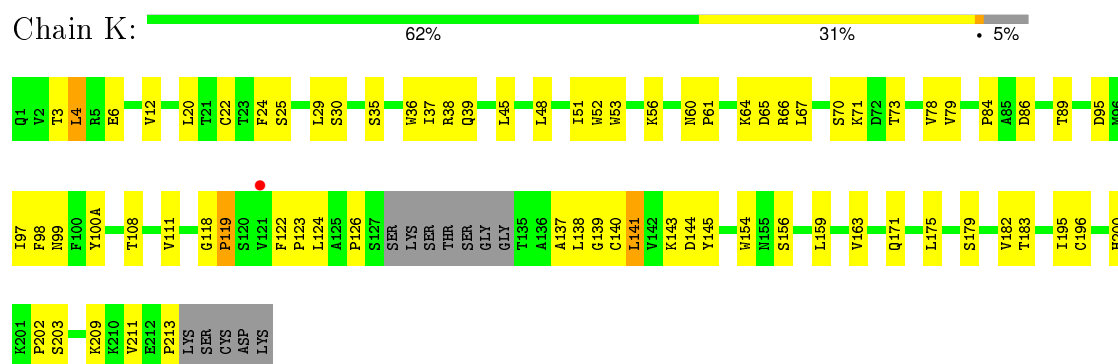
- Molecule 1: Fusion glycoprotein F0,Fibritin



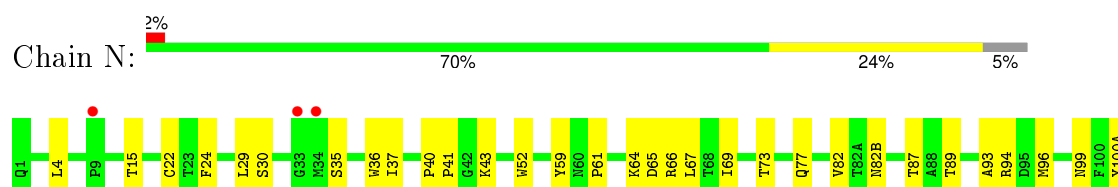
- Molecule 2: Motavizumab antibody Fab heavy chain



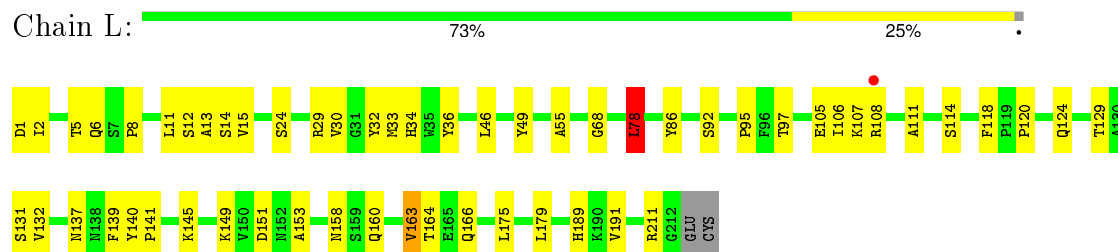
- Molecule 2: Motavizumab antibody Fab heavy chain



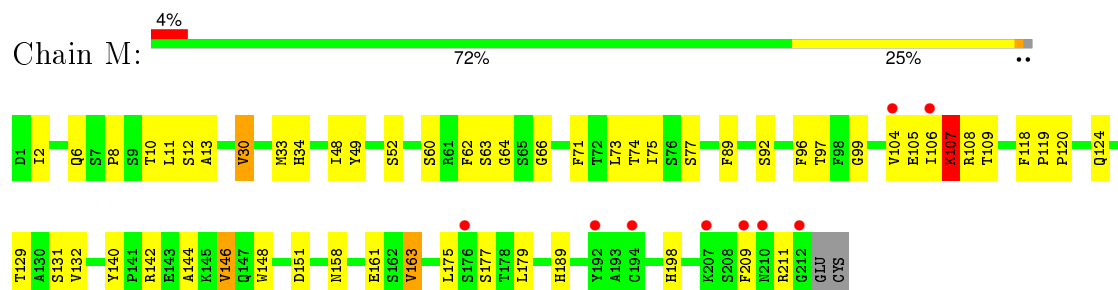
- Molecule 2: Motavizumab antibody Fab heavy chain



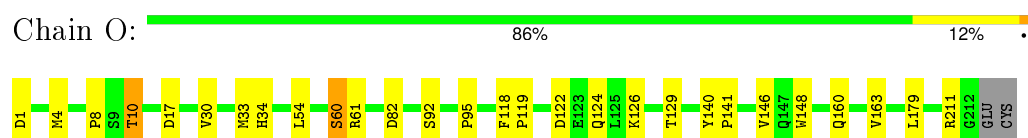
• Molecule 3: Motavizumab antibody light chain



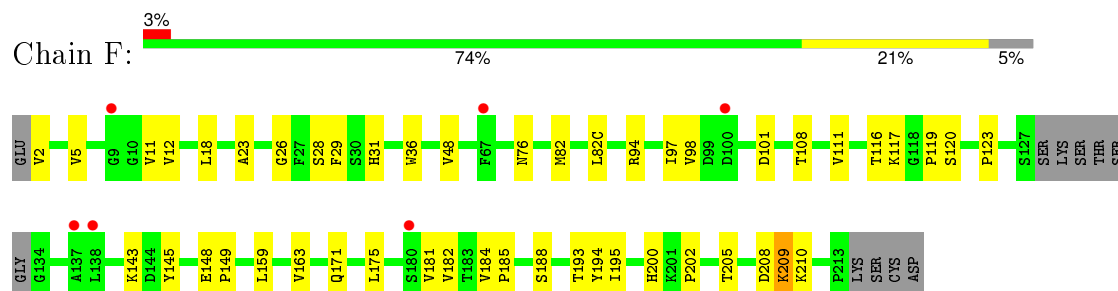
• Molecule 3: Motavizumab antibody light chain



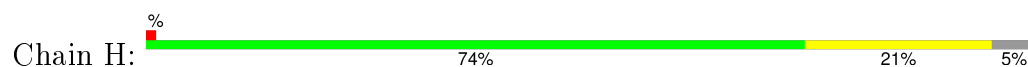
• Molecule 3: Motavizumab antibody light chain

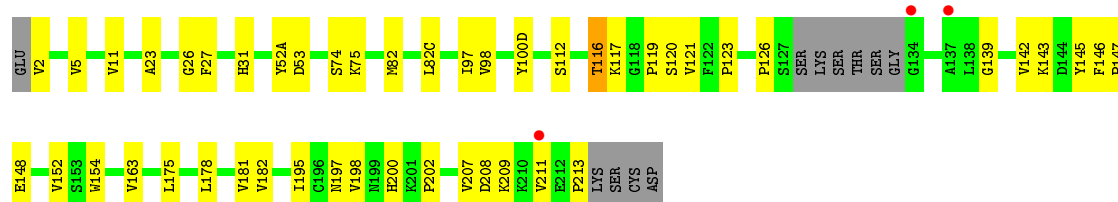


• Molecule 4: AM14 antibody Fab heavy chain

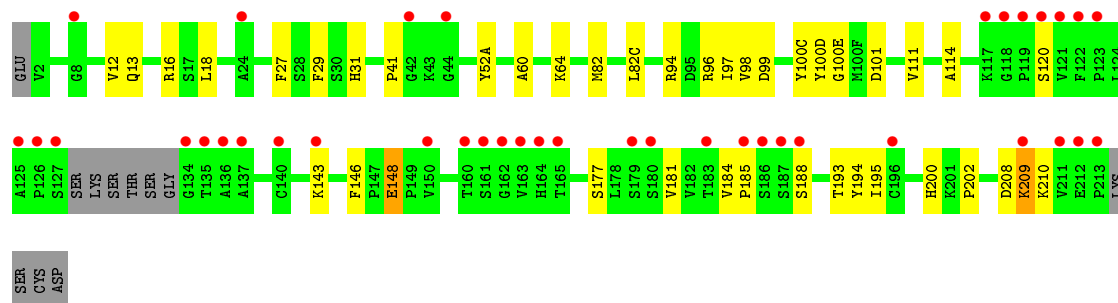
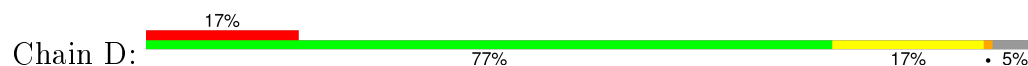


• Molecule 4: AM14 antibody Fab heavy chain

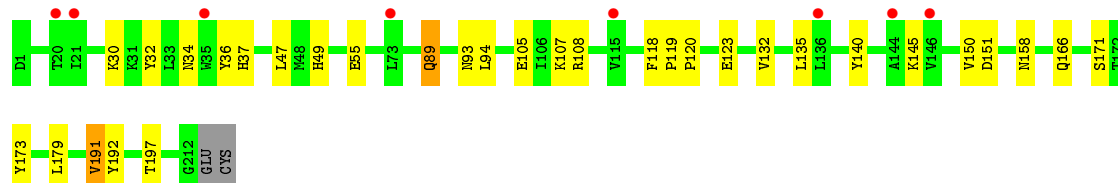
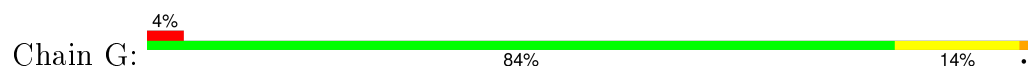




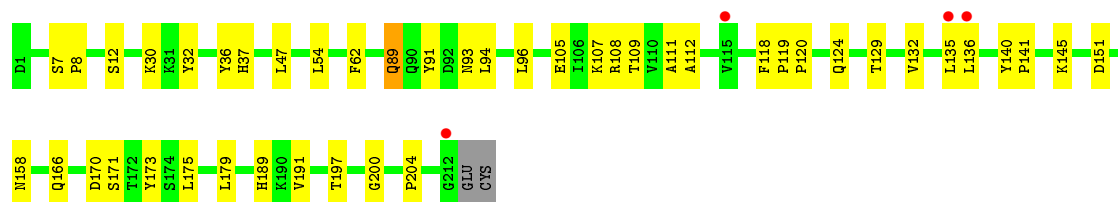
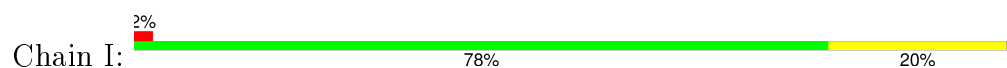
• Molecule 4: AM14 antibody Fab heavy chain



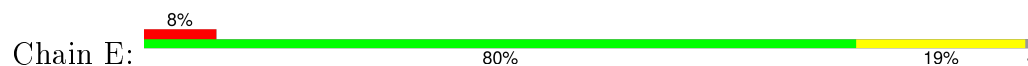
• Molecule 5: AM14 antibody light chain

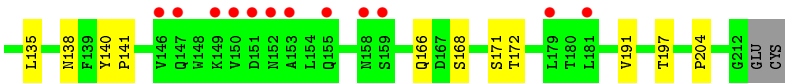


• Molecule 5: AM14 antibody light chain



• Molecule 5: AM14 antibody light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.38Å 210.29Å 118.20Å 90.00° 100.46° 90.00°	Depositor
Resolution (Å)	49.39 – 5.50 49.59 – 5.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.39-5.50) 97.2 (49.59-5.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 5.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.210 , 0.277 0.234 , 0.276	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	154.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 182.6	EDS
Estimated twinning fraction	0.056 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 17414 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	29990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	0.35	0/3532	0.67	1/4784 (0.0%)
1	B	0.34	0/3532	0.68	2/4784 (0.0%)
1	C	0.35	0/3532	0.71	1/4784 (0.0%)
2	J	0.40	0/1669	0.83	2/2283 (0.1%)
2	K	0.33	0/1669	0.73	1/2283 (0.0%)
2	N	0.29	0/1669	0.51	0/2283
3	L	0.34	0/1648	0.69	1/2235 (0.0%)
3	M	0.33	0/1648	0.71	1/2235 (0.0%)
3	O	0.29	0/1648	0.52	0/2235
4	D	0.28	0/1677	0.51	0/2286
4	F	0.28	0/1677	0.49	0/2286
4	H	0.31	0/1676	0.64	0/2285
5	E	0.33	0/1677	0.64	0/2277
5	G	0.26	0/1677	0.50	0/2277
5	I	0.30	0/1677	0.57	0/2277
All	All	0.33	0/30608	0.65	9/41594 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	107	LYS	N-CA-C	6.15	127.61	111.00
1	B	181	LEU	CA-CB-CG	-5.93	101.65	115.30
2	J	178	LEU	CA-CB-CG	5.85	128.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLY	N-CA-C	-5.50	99.34	113.10
1	B	188	LEU	CA-CB-CG	5.41	127.73	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	78	LEU	Mainchain

## 5.2 Too-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 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	3482	0	3526	107	0
1	B	3482	0	3526	96	0
1	C	3482	0	3526	114	0
2	J	1626	0	1610	55	0
2	K	1626	0	1610	62	0
2	N	1626	0	1610	37	0
3	L	1611	0	1564	45	1
3	M	1611	0	1564	52	0
3	O	1611	0	1564	19	1
4	D	1636	0	1579	28	0
4	F	1636	0	1579	30	0
4	H	1635	0	1576	34	0
5	E	1642	0	1597	35	0
5	G	1642	0	1597	20	0
5	I	1642	0	1597	31	0
All	All	29990	0	29625	686	1

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 12.

The worst 5 of 686 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:B:374:THR:HG21	1:C:454:ASN:H	1.33	0.93
1:B:28:ILE:HA	1:B:43:GLY:HA3	1.53	0.90
5:E:106:ILE:O	5:E:166:GLN:NE2	2.04	0.89
3:L:12:SER:O	3:L:107:LYS:NZ	2.06	0.89
4:H:75:LYS:NZ	3:M:77:SER:OG	2.05	0.88

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	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:LYS:NZ	3:O:17:ASP:OD1[2_645]	2.18	0.02

## 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	445/498 (89%)	410 (92%)	29 (6%)	6 (1%)	15	59
1	B	445/498 (89%)	410 (92%)	29 (6%)	6 (1%)	15	59
1	C	445/498 (89%)	411 (92%)	28 (6%)	6 (1%)	15	59
2	J	209/225 (93%)	192 (92%)	16 (8%)	1 (0%)	34	77
2	K	209/225 (93%)	193 (92%)	14 (7%)	2 (1%)	19	64
2	N	209/225 (93%)	196 (94%)	13 (6%)	0	100	100
3	L	209/213 (98%)	195 (93%)	13 (6%)	1 (0%)	34	77
3	M	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
3	O	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
4	D	212/227 (93%)	208 (98%)	4 (2%)	0	100	100
4	F	212/227 (93%)	208 (98%)	4 (2%)	0	100	100
4	H	212/227 (93%)	205 (97%)	7 (3%)	0	100	100
5	E	211/215 (98%)	202 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
5	I	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
All	All	3858/4134 (93%)	3633 (94%)	203 (5%)	22 (1%)	30	74

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	161	GLU
1	B	50	THR
1	B	161	GLU
1	C	50	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	410/448 (92%)	396 (97%)	14 (3%)	44	76
1	B	410/448 (92%)	382 (93%)	28 (7%)	20	57
1	C	410/448 (92%)	381 (93%)	29 (7%)	18	56
2	J	187/197 (95%)	184 (98%)	3 (2%)	70	88
2	K	187/197 (95%)	184 (98%)	3 (2%)	70	88
2	N	187/197 (95%)	183 (98%)	4 (2%)	61	85
3	L	183/185 (99%)	182 (100%)	1 (0%)	92	96
3	M	183/185 (99%)	179 (98%)	4 (2%)	60	83
3	O	183/185 (99%)	179 (98%)	4 (2%)	60	83
4	D	182/192 (95%)	179 (98%)	3 (2%)	70	88
4	F	182/192 (95%)	179 (98%)	3 (2%)	70	88
4	H	181/192 (94%)	178 (98%)	3 (2%)	68	88
5	E	189/191 (99%)	187 (99%)	2 (1%)	80	91
5	G	189/191 (99%)	187 (99%)	2 (1%)	80	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	189/191 (99%)	188 (100%)	1 (0%)	92	96
All	All	3452/3639 (95%)	3348 (97%)	104 (3%)	48	77

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	137	PHE
1	C	260	LEU
2	N	29	LEU
1	C	155	CYS
1	C	169	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	GLN
1	C	262	ASN
5	E	210	ASN
1	B	363	ASN
1	C	70	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 carbohydrates 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 ⓘ

### 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	449/498 (90%)	-0.08	4 (0%) 85 81	152, 187, 250, 286	0
1	B	449/498 (90%)	-0.25	4 (0%) 85 81	156, 197, 266, 334	0
1	C	449/498 (90%)	-0.32	2 (0%) 93 90	140, 186, 235, 255	0
2	J	213/225 (94%)	-0.20	0 100 100	148, 170, 197, 213	0
2	K	213/225 (94%)	-0.22	1 (0%) 91 88	164, 209, 288, 297	0
2	N	213/225 (94%)	0.00	4 (1%) 70 64	191, 238, 277, 289	0
3	L	211/213 (99%)	-0.24	1 (0%) 91 88	148, 195, 226, 253	0
3	M	211/213 (99%)	0.04	9 (4%) 39 35	177, 245, 273, 284	0
3	O	211/213 (99%)	-0.04	0 100 100	204, 239, 271, 298	0
4	D	216/227 (95%)	0.75	39 (18%) 2 6	193, 269, 359, 370	0
4	F	216/227 (95%)	0.02	6 (2%) 56 51	192, 234, 280, 287	0
4	H	216/227 (95%)	-0.08	3 (1%) 78 72	151, 183, 202, 211	0
5	E	213/215 (99%)	0.42	18 (8%) 13 16	221, 305, 367, 382	0
5	G	213/215 (99%)	0.14	8 (3%) 44 40	211, 250, 279, 297	0
5	I	213/215 (99%)	-0.15	4 (1%) 70 64	155, 191, 214, 231	0
All	All	3906/4134 (94%)	-0.05	103 (2%) 59 54	140, 208, 316, 382	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	121	VAL	7.0
4	D	120	SER	6.8
4	D	213	PRO	5.8
4	D	119	PRO	4.8
5	E	151	ASP	4.8

## 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.