



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:52 AM UTC

PDB ID : 4WHT / pdb_00004wht
Title : Structure of the Hepatitis C virus envelope glycoprotein E2 antigenic region
412-423 bound to the broadly neutralizing antibody 3/11, P1 crystal form
Authors : Krey, T.; Rey, F.A.
Deposited on : 2014-09-23
Resolution : 2.22 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

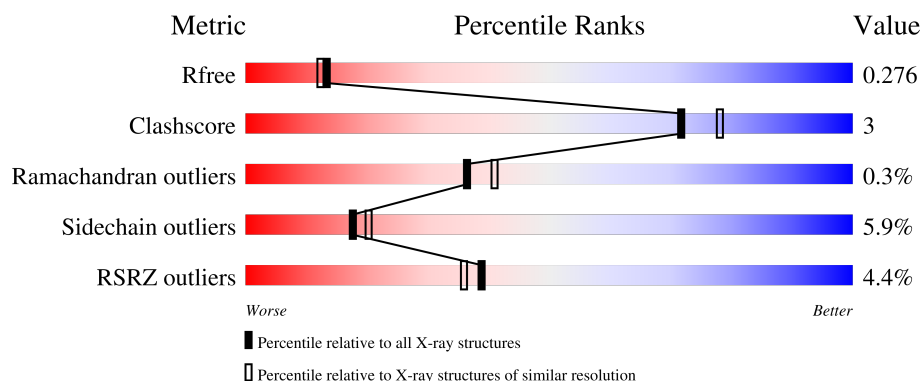
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 ≥ 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	252	72%10%18%
1	C	252	2% 67%13%19%
1	E	252	2% 72%10%17%
1	G	252	% 71%11%18%
1	I	252	% 68%13%19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	252	
1	M	252	
1	O	252	
1	Q	252	
1	S	252	
1	U	252	
1	X	252	
2	B	220	
2	D	220	
2	F	220	
2	H	220	
2	J	220	
2	L	220	
2	N	220	
2	P	220	
2	R	220	
2	T	220	
2	V	220	
2	Y	220	
3	a	12	
3	c	12	
3	e	12	
3	g	12	
3	i	12	
3	k	12	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	m	12	
3	o	12	
3	q	12	
3	s	12	
3	u	12	
3	x	12	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40099 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 of the Fab fragment derived from neutralizing antibody 3/11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1565	988	264	306	7			
1	C	205	Total	C	N	O	S	0	0	0
			1554	982	262	303	7			
1	E	208	Total	C	N	O	S	0	0	0
			1570	991	265	307	7			
1	G	207	Total	C	N	O	S	0	0	0
			1567	989	264	307	7			
1	I	205	Total	C	N	O	S	0	0	0
			1550	980	261	302	7			
1	K	204	Total	C	N	O	S	0	0	0
			1546	978	260	301	7			
1	M	204	Total	C	N	O	S	0	0	0
			1546	978	260	301	7			
1	O	205	Total	C	N	O	S	0	0	0
			1550	980	261	302	7			
1	Q	206	Total	C	N	O	S	0	0	0
			1557	984	262	304	7			
1	S	204	Total	C	N	O	S	0	0	0
			1546	978	260	301	7			
1	U	205	Total	C	N	O	S	0	0	0
			1554	982	262	303	7			
1	X	199	Total	C	N	O	S	0	0	0
			1495	945	250	293	7			

- Molecule 2 is a protein called Light chain of the Fab fragment derived from neutralizing antibody 3/11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	D	216	Total	C	N	O	S	0	0	0
			1642	1018	275	342	7			
2	F	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	H	216	Total	C	N	O	S	0	0	0
			1640	1017	274	342	7			
2	L	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	N	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	P	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	R	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	T	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	V	212	Total	C	N	O	S	0	0	0
			1615	1004	270	334	7			
2	Y	210	Total	C	N	O	S	0	0	0
			1591	987	266	331	7			

- Molecule 3 is a protein called Epitope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	c	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	e	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	g	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	i	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	k	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	m	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	o	11	Total	C	N	O	0	0	0
			88	55	17	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	q	10	Total	C	N	O	0	0	0
			80	51	15	14			
3	s	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	u	10	Total	C	N	O	0	0	0
			80	51	15	14			
3	x	12	Total	C	N	O	0	0	0
			97	60	19	18			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	C	44	Total	O	0	0
			44	44		
4	E	34	Total	O	0	0
			34	34		
4	G	29	Total	O	0	0
			29	29		
4	I	31	Total	O	0	0
			31	31		
4	J	55	Total	O	0	0
			55	55		
4	K	13	Total	O	0	0
			13	13		
4	M	18	Total	O	0	0
			18	18		
4	O	26	Total	O	0	0
			26	26		
4	Q	20	Total	O	0	0
			20	20		
4	S	27	Total	O	0	0
			27	27		
4	U	14	Total	O	0	0
			14	14		
4	X	42	Total	O	0	0
			42	42		
4	B	47	Total	O	0	0
			47	47		
4	D	62	Total	O	0	0
			62	62		

Continued on next page...

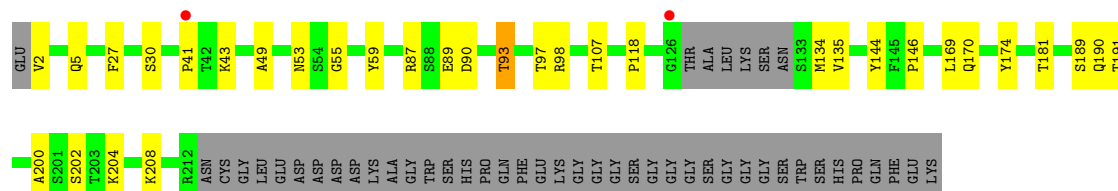
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	48	Total 48	O 48	0	0
4	H	51	Total 51	O 51	0	0
4	L	46	Total 46	O 46	0	0
4	N	24	Total 24	O 24	0	0
4	P	57	Total 57	O 57	0	0
4	R	29	Total 29	O 29	0	0
4	T	32	Total 32	O 32	0	0
4	V	21	Total 21	O 21	0	0
4	Y	40	Total 40	O 40	0	0
4	a	1	Total 1	O 1	0	0
4	s	1	Total 1	O 1	0	0

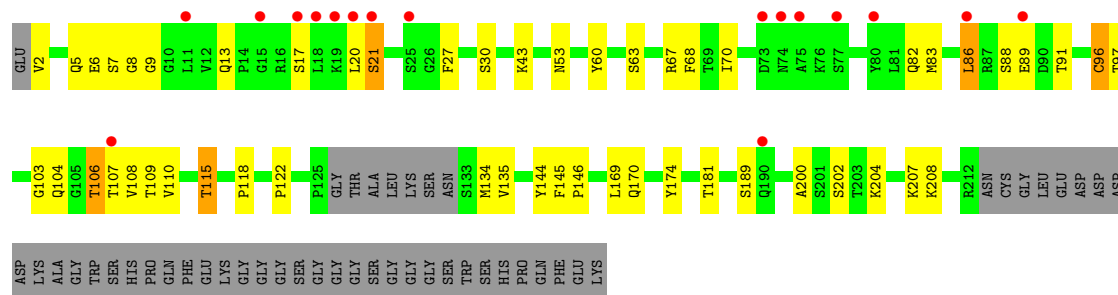
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



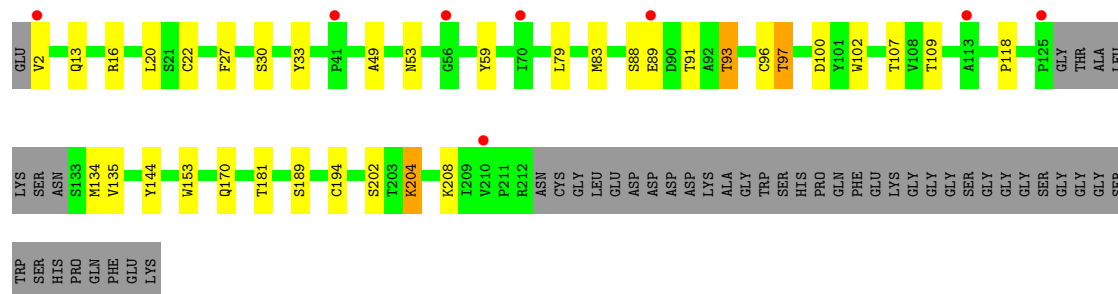
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

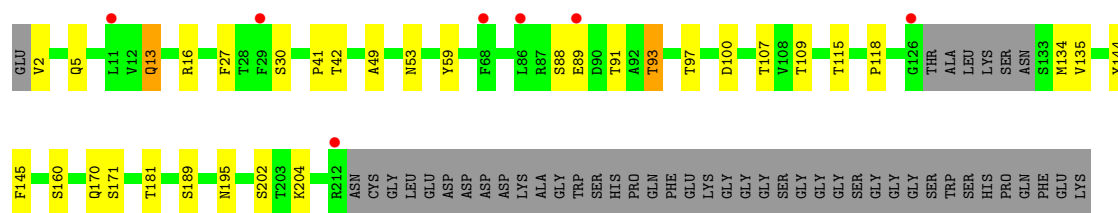


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

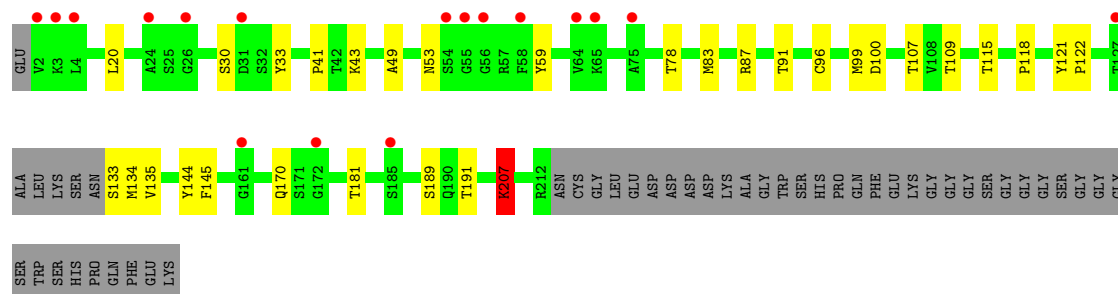


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

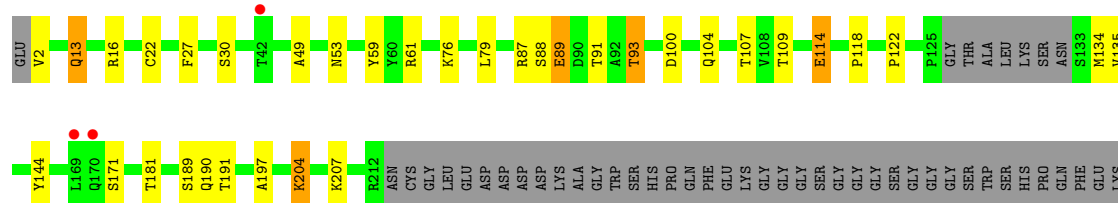




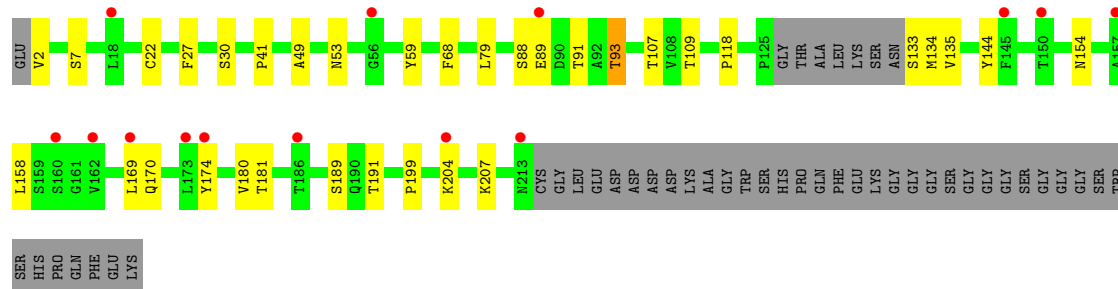
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

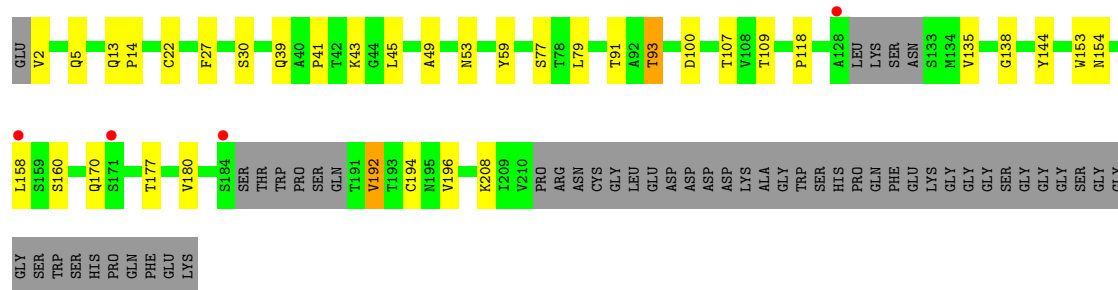


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11





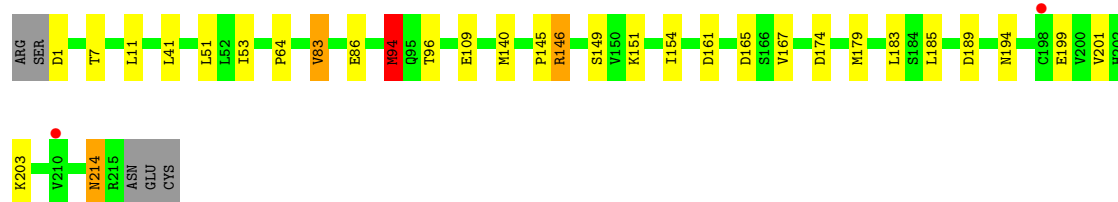
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain J: 85% 11% ..



- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain B: 84% 12% ..



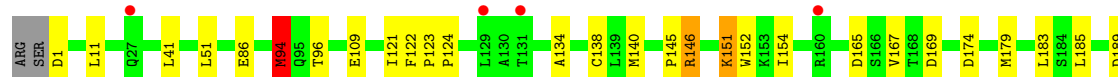
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

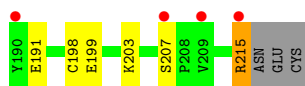
Chain D: 82% 14% ..



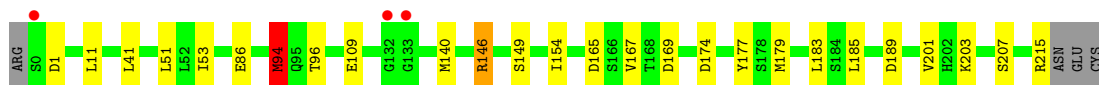
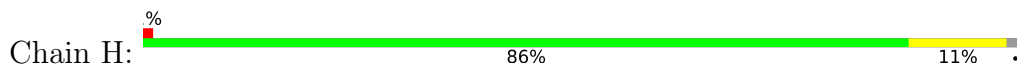
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain F: 82% 14% ..

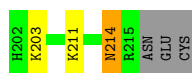
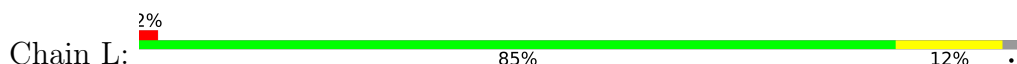




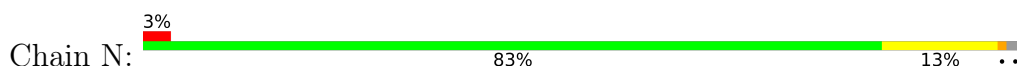
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



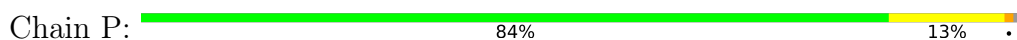
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



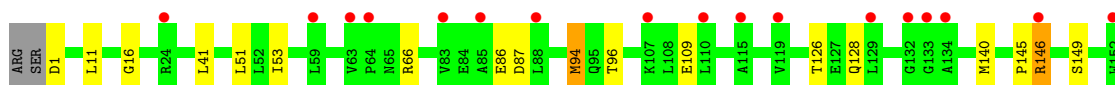
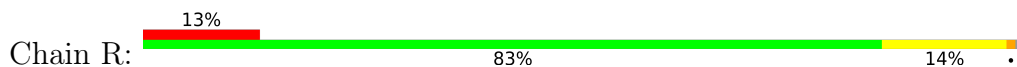
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

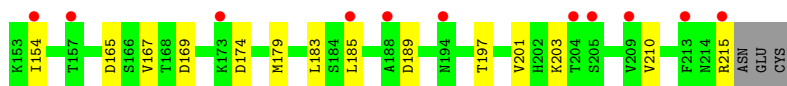


- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

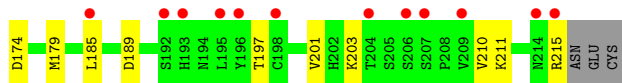
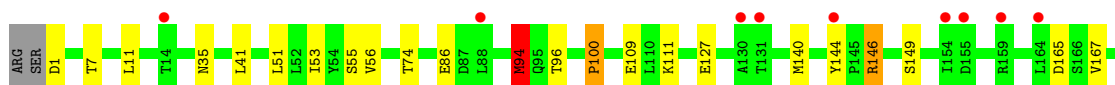
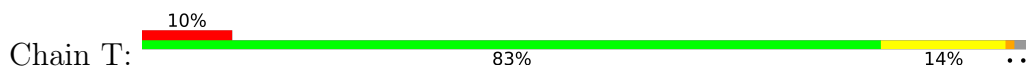


- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

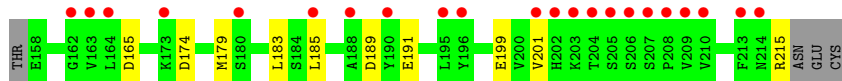
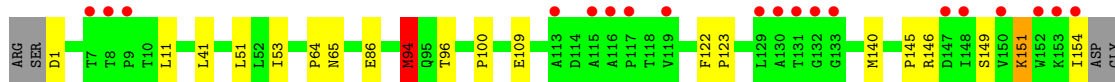
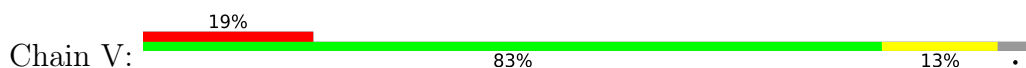




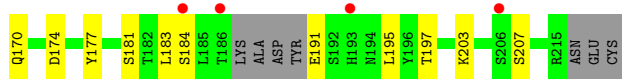
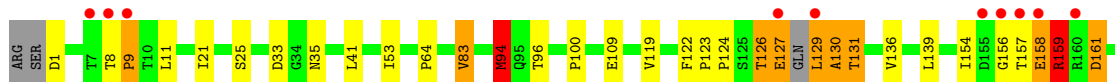
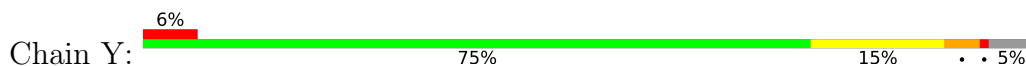
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



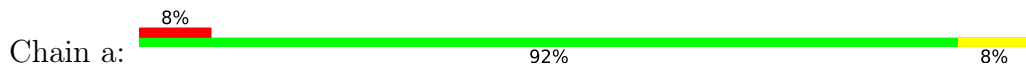
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



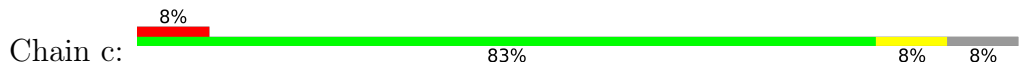
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

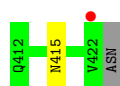


- Molecule 3: Epitope peptide

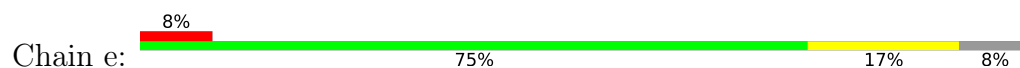


- Molecule 3: Epitope peptide





- Molecule 3: Epitope peptide

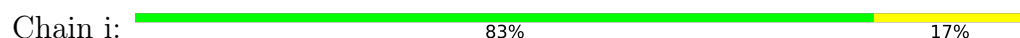


- Molecule 3: Epitope peptide

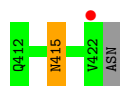
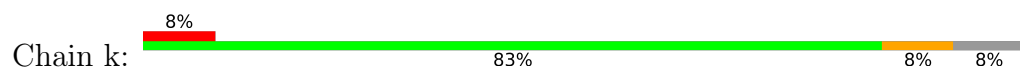


There are no outlier residues recorded for this chain.

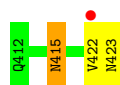
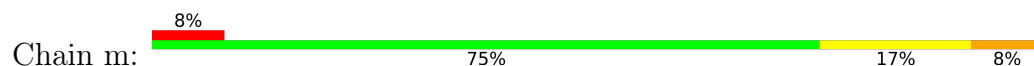
- Molecule 3: Epitope peptide



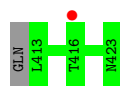
- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide

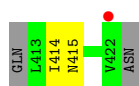


- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide





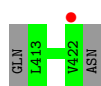
- Molecule 3: Epitope peptide

Chain s: 83% 8% 8%



- Molecule 3: Epitope peptide

Chain u: 8% 83% 17%



- Molecule 3: Epitope peptide

Chain x: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.79Å 128.22Å 163.63Å 88.79° 94.36° 96.15°	Depositor
Resolution (Å)	32.50 – 2.22 32.50 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.4 (32.50-2.22) 95.4 (32.50-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.209 , 0.243 0.234 , 0.276	Depositor DCC
R_{free} test set	12380 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	40099	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

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	0.83	0/1603	1.20	6/2188 (0.3%)
1	C	0.83	1/1592 (0.1%)	1.20	6/2173 (0.3%)
1	E	0.83	0/1608	1.19	9/2195 (0.4%)
1	G	0.82	1/1605 (0.1%)	1.20	6/2190 (0.3%)
1	I	0.80	0/1588	1.22	7/2167 (0.3%)
1	K	0.83	0/1584	1.22	7/2162 (0.3%)
1	M	0.77	0/1584	1.17	6/2162 (0.3%)
1	O	0.79	0/1588	1.19	6/2167 (0.3%)
1	Q	0.78	0/1595	1.17	5/2177 (0.2%)
1	S	0.85	0/1584	1.20	8/2162 (0.4%)
1	U	0.79	0/1592	1.21	4/2173 (0.2%)
1	X	0.90	0/1528	1.27	5/2082 (0.2%)
2	B	0.89	1/1664 (0.1%)	1.21	9/2264 (0.4%)
2	D	0.87	0/1672	1.25	14/2275 (0.6%)
2	F	0.83	1/1664 (0.1%)	1.20	5/2264 (0.2%)
2	H	0.86	1/1670 (0.1%)	1.19	3/2272 (0.1%)
2	J	0.82	0/1664	1.17	3/2264 (0.1%)
2	L	0.84	1/1664 (0.1%)	1.17	5/2264 (0.2%)
2	N	0.74	0/1664	1.17	7/2264 (0.3%)
2	P	0.79	1/1664 (0.1%)	1.19	6/2264 (0.3%)
2	R	0.77	0/1664	1.17	7/2264 (0.3%)
2	T	0.83	1/1664 (0.1%)	1.22	4/2264 (0.2%)
2	V	0.80	1/1644 (0.1%)	1.17	8/2235 (0.4%)
2	Y	0.99	2/1618 (0.1%)	1.41	17/2199 (0.8%)
3	a	0.75	0/99	1.16	0/135
3	c	0.75	0/91	1.38	2/124 (1.6%)
3	e	0.95	0/91	1.35	1/124 (0.8%)
3	g	0.92	0/99	1.33	0/135
3	i	0.80	0/99	1.40	1/135 (0.7%)
3	k	0.85	0/91	1.45	2/124 (1.6%)
3	m	0.76	0/99	1.46	2/135 (1.5%)
3	o	0.69	0/90	1.16	0/123
3	q	0.78	0/82	1.34	0/112
3	s	0.84	0/91	1.31	0/124

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	u	0.74	0/82	1.25	0/112
3	x	1.11	0/99	1.52	0/135
All	All	0.83	11/40080 (0.0%)	1.21	171/54609 (0.3%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	94	MET	SD-CE	-7.78	1.60	1.79
2	B	94	MET	SD-CE	-7.60	1.60	1.79
2	H	94	MET	SD-CE	-7.33	1.61	1.79
2	L	94	MET	SD-CE	-7.10	1.61	1.79
2	V	94	MET	SD-CE	-6.96	1.62	1.79

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	160	SER	N-CA-C	8.69	120.37	111.07
1	I	55	GLY	N-CA-C	8.55	126.67	115.47
1	X	93	THR	CB-CA-C	7.92	122.79	109.80
2	Y	130	ALA	CA-C-N	7.76	136.37	121.54
2	Y	130	ALA	C-N-CA	7.76	136.37	121.54

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	1565	0	1536	7	0
1	C	1554	0	1526	15	0
1	E	1570	0	1541	8	0
1	G	1567	0	1538	7	0
1	I	1550	0	1523	11	0
1	K	1546	0	1520	21	0
1	M	1546	0	1520	14	0
1	O	1550	0	1523	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1557	0	1530	10	0
1	S	1546	0	1520	13	0
1	U	1554	0	1526	11	0
1	X	1495	0	1472	13	0
2	B	1634	0	1593	8	0
2	D	1642	0	1599	15	0
2	F	1634	0	1593	12	0
2	H	1640	0	1598	7	0
2	J	1634	0	1593	10	0
2	L	1634	0	1593	8	0
2	N	1634	0	1593	11	0
2	P	1634	0	1593	12	0
2	R	1634	0	1593	11	0
2	T	1634	0	1593	12	0
2	V	1615	0	1578	8	0
2	Y	1591	0	1552	10	0
3	a	97	0	88	0	0
3	c	89	0	82	0	0
3	e	89	0	82	0	0
3	g	97	0	88	0	0
3	i	97	0	88	0	0
3	k	89	0	82	1	0
3	m	97	0	88	1	0
3	o	88	0	80	0	0
3	q	80	0	74	2	0
3	s	89	0	82	1	0
3	u	80	0	74	0	0
3	x	97	0	88	0	0
4	A	38	0	0	0	0
4	B	47	0	0	0	0
4	C	44	0	0	2	0
4	D	62	0	0	1	0
4	E	34	0	0	0	0
4	F	48	0	0	0	0
4	G	29	0	0	0	0
4	H	51	0	0	0	0
4	I	31	0	0	0	0
4	J	55	0	0	0	0
4	K	13	0	0	0	0
4	L	46	0	0	0	0
4	M	18	0	0	1	0
4	N	24	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	26	0	0	0	0
4	P	57	0	0	0	0
4	Q	20	0	0	0	0
4	R	29	0	0	1	0
4	S	27	0	0	1	0
4	T	32	0	0	1	0
4	U	14	0	0	1	0
4	V	21	0	0	0	0
4	X	42	0	0	0	0
4	Y	40	0	0	0	0
4	a	1	0	0	0	0
4	s	1	0	0	0	0
All	All	40099	0	38342	254	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 3.

The worst 5 of 254 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:M:97:THR:HG21	1:M:102:TRP:CE3	2.13	0.83
2:D:94:MET:HE3	2:D:96:THR:HG23	1.59	0.81
1:C:202:SER:HB3	1:I:208:LYS:HB3	1.65	0.76
2:Y:94:MET:HE3	2:Y:96:THR:HG23	1.70	0.73
2:J:44:ARG:NH1	2:J:86:GLU:O	2.23	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	203/252 (81%)	195 (96%)	8 (4%)	0	100	100
1	C	201/252 (80%)	195 (97%)	6 (3%)	0	100	100
1	E	204/252 (81%)	197 (97%)	7 (3%)	0	100	100
1	G	203/252 (81%)	197 (97%)	4 (2%)	2 (1%)	12	11
1	I	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	24	26
1	K	200/252 (79%)	194 (97%)	6 (3%)	0	100	100
1	M	200/252 (79%)	196 (98%)	4 (2%)	0	100	100
1	O	201/252 (80%)	196 (98%)	5 (2%)	0	100	100
1	Q	202/252 (80%)	199 (98%)	2 (1%)	1 (0%)	24	26
1	S	200/252 (79%)	196 (98%)	4 (2%)	0	100	100
1	U	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	24	26
1	X	193/252 (77%)	189 (98%)	2 (1%)	2 (1%)	12	11
2	B	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	D	214/220 (97%)	208 (97%)	4 (2%)	2 (1%)	14	13
2	F	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	H	214/220 (97%)	212 (99%)	2 (1%)	0	100	100
2	J	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	L	213/220 (97%)	210 (99%)	3 (1%)	0	100	100
2	N	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	P	213/220 (97%)	206 (97%)	7 (3%)	0	100	100
2	R	213/220 (97%)	206 (97%)	7 (3%)	0	100	100
2	T	213/220 (97%)	207 (97%)	6 (3%)	0	100	100
2	V	208/220 (94%)	203 (98%)	5 (2%)	0	100	100
2	Y	204/220 (93%)	186 (91%)	12 (6%)	6 (3%)	3	1
3	a	10/12 (83%)	10 (100%)	0	0	100	100
3	c	9/12 (75%)	9 (100%)	0	0	100	100
3	e	9/12 (75%)	9 (100%)	0	0	100	100
3	g	10/12 (83%)	10 (100%)	0	0	100	100
3	i	10/12 (83%)	10 (100%)	0	0	100	100
3	k	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
3	m	10/12 (83%)	10 (100%)	0	0	100	100
3	o	9/12 (75%)	8 (89%)	1 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	q	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
3	s	9/12 (75%)	9 (100%)	0	0	100	100
3	u	8/12 (67%)	8 (100%)	0	0	100	100
3	x	10/12 (83%)	10 (100%)	0	0	100	100
All	All	5064/5808 (87%)	4926 (97%)	123 (2%)	15 (0%)	36	41

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	7	THR
2	D	215	ARG
2	Y	159	ARG
1	G	125	PRO
1	X	160	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	176/208 (85%)	168 (96%)	8 (4%)	24	31
1	C	175/208 (84%)	167 (95%)	8 (5%)	24	30
1	E	176/208 (85%)	169 (96%)	7 (4%)	28	36
1	G	176/208 (85%)	168 (96%)	8 (4%)	24	31
1	I	174/208 (84%)	166 (95%)	8 (5%)	24	30
1	K	174/208 (84%)	161 (92%)	13 (8%)	12	13
1	M	174/208 (84%)	164 (94%)	10 (6%)	18	21
1	O	174/208 (84%)	163 (94%)	11 (6%)	16	18
1	Q	175/208 (84%)	165 (94%)	10 (6%)	18	21
1	S	174/208 (84%)	163 (94%)	11 (6%)	16	18
1	U	175/208 (84%)	164 (94%)	11 (6%)	16	18
1	X	167/208 (80%)	158 (95%)	9 (5%)	20	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	191/196 (97%)	178 (93%)	13 (7%)	14	16
2	D	192/196 (98%)	183 (95%)	9 (5%)	23	29
2	F	191/196 (97%)	179 (94%)	12 (6%)	16	18
2	H	192/196 (98%)	180 (94%)	12 (6%)	16	18
2	J	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	L	191/196 (97%)	179 (94%)	12 (6%)	16	18
2	N	191/196 (97%)	181 (95%)	10 (5%)	21	25
2	P	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	R	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	T	191/196 (97%)	178 (93%)	13 (7%)	14	16
2	V	189/196 (96%)	179 (95%)	10 (5%)	20	24
2	Y	187/196 (95%)	163 (87%)	24 (13%)	4	3
3	a	11/11 (100%)	10 (91%)	1 (9%)	9	8
3	c	10/11 (91%)	10 (100%)	0	100	100
3	e	10/11 (91%)	9 (90%)	1 (10%)	7	7
3	g	11/11 (100%)	11 (100%)	0	100	100
3	i	11/11 (100%)	10 (91%)	1 (9%)	9	8
3	k	10/11 (91%)	10 (100%)	0	100	100
3	m	11/11 (100%)	9 (82%)	2 (18%)	2	1
3	o	10/11 (91%)	10 (100%)	0	100	100
3	q	9/11 (82%)	9 (100%)	0	100	100
3	s	10/11 (91%)	10 (100%)	0	100	100
3	u	9/11 (82%)	9 (100%)	0	100	100
3	x	11/11 (100%)	11 (100%)	0	100	100
All	All	4501/4980 (90%)	4234 (94%)	267 (6%)	18	20

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	86	GLU
2	Y	1	ASP
2	Y	203	LYS
1	S	93	THR
1	S	13	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	35	ASN
2	Y	50	GLN
1	U	13	GLN
1	S	170	GLN
2	Y	98	HIS

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 oligosaccharides 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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	207/252 (82%)	0.20	1 (0%) 87 86	21, 35, 49, 66	0
1	C	205/252 (81%)	0.13	5 (2%) 59 57	20, 32, 51, 80	0
1	E	208/252 (82%)	0.39	6 (2%) 53 51	21, 37, 57, 79	0
1	G	207/252 (82%)	0.44	2 (0%) 79 78	22, 41, 62, 84	0
1	I	205/252 (81%)	0.23	2 (0%) 79 78	23, 36, 52, 69	0
1	K	204/252 (80%)	0.88	17 (8%) 17 15	28, 48, 71, 93	0
1	M	204/252 (80%)	0.77	8 (3%) 43 40	29, 46, 63, 78	0
1	O	205/252 (81%)	0.51	7 (3%) 48 45	23, 40, 61, 75	0
1	Q	206/252 (81%)	0.85	17 (8%) 17 15	25, 46, 73, 84	0
1	S	204/252 (80%)	0.18	3 (1%) 72 70	18, 34, 55, 78	0
1	U	205/252 (81%)	0.89	14 (6%) 23 20	24, 49, 73, 103	0
1	X	199/252 (78%)	0.13	4 (2%) 65 63	18, 34, 54, 87	0
2	B	215/220 (97%)	0.22	2 (0%) 81 79	18, 35, 59, 74	0
2	D	216/220 (98%)	0.12	3 (1%) 73 72	18, 31, 55, 87	0
2	F	215/220 (97%)	0.26	8 (3%) 45 42	20, 34, 62, 90	0
2	H	216/220 (98%)	0.13	3 (1%) 73 72	18, 35, 56, 69	0
2	J	215/220 (97%)	0.14	1 (0%) 87 86	18, 33, 56, 75	0
2	L	215/220 (97%)	0.31	4 (1%) 66 64	22, 39, 57, 68	0
2	N	215/220 (97%)	0.77	7 (3%) 49 46	30, 49, 68, 80	0
2	P	215/220 (97%)	0.23	1 (0%) 87 86	23, 37, 61, 75	0
2	R	215/220 (97%)	1.09	28 (13%) 7 5	30, 54, 78, 88	0
2	T	215/220 (97%)	0.77	21 (9%) 13 10	21, 44, 76, 90	0
2	V	212/220 (96%)	1.10	41 (19%) 3 2	27, 52, 88, 106	0
2	Y	210/220 (95%)	0.26	14 (6%) 24 21	15, 33, 72, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	a	12/12 (100%)	0.11	1 (8%) 17 15	23, 31, 50, 79	0
3	c	11/12 (91%)	0.28	1 (9%) 15 12	25, 28, 51, 52	0
3	e	11/12 (91%)	0.38	1 (9%) 15 12	23, 30, 56, 56	0
3	g	12/12 (100%)	0.05	0 100 100	26, 30, 46, 48	0
3	i	12/12 (100%)	0.16	0 100 100	30, 34, 50, 65	0
3	k	11/12 (91%)	0.70	1 (9%) 15 12	24, 36, 58, 59	0
3	m	12/12 (100%)	1.01	1 (8%) 17 15	39, 47, 69, 78	0
3	o	11/12 (91%)	0.75	1 (9%) 15 12	34, 43, 59, 61	0
3	q	10/12 (83%)	1.10	1 (10%) 12 10	42, 50, 56, 68	0
3	s	11/12 (91%)	0.21	0 100 100	27, 32, 45, 48	0
3	u	10/12 (83%)	0.63	1 (10%) 12 10	32, 37, 40, 54	0
3	x	12/12 (100%)	0.11	0 100 100	23, 29, 57, 59	0
All	All	5168/5808 (88%)	0.46	227 (4%) 39 36	15, 40, 67, 106	0

The worst 5 of 227 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	75	ALA	5.1
1	G	126	GLY	5.0
3	e	422	VAL	4.4
2	V	209	VAL	4.4
1	U	157	ALA	4.2

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 oligosaccharides 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.