



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 03:06 PM EDT

PDB ID : 5Y9F  
Title : Crystal structure of HPV59 pentamer in complex with the Fab fragment of antibody 28F10  
Authors : Li, S.W.; Li, Z.H.  
Deposited on : 2017-08-24  
Resolution : 3.35 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>.

---

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

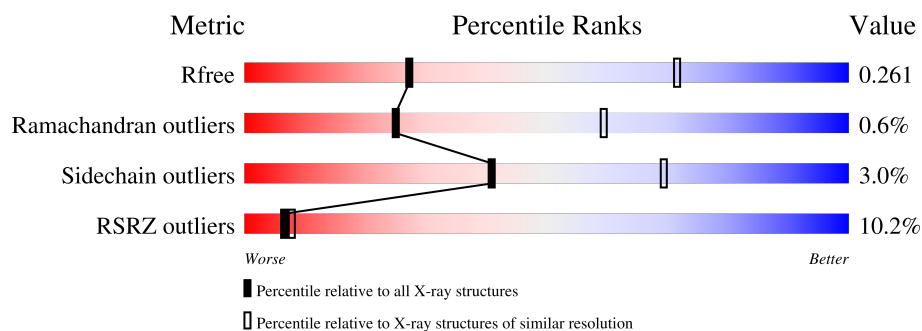
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	500	<div> <div>3%</div> <div>82%</div> <div>16%</div> </div>
1	B	500	<div> <div>3%</div> <div>82%</div> <div>16%</div> </div>
1	C	500	<div> <div>4%</div> <div>83%</div> <div>16%</div> </div>
1	D	500	<div> <div>3%</div> <div>82%</div> <div>16%</div> </div>
1	E	500	<div> <div>4%</div> <div>83%</div> <div>15%</div> </div>
1	F	500	<div> <div>2%</div> <div>83%</div> <div>16%</div> </div>
1	G	500	<div> <div>4%</div> <div>82%</div> <div>16%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	500	
1	I	500	
1	J	500	
2	K	219	
2	M	219	
2	O	219	
2	Q	219	
2	S	219	
2	U	219	
2	W	219	
2	Y	219	
2	a	219	
2	c	219	
3	L	223	
3	N	223	
3	P	223	
3	R	223	
3	T	223	
3	V	223	
3	X	223	
3	Z	223	
3	b	223	
3	d	223	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 66832 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	B	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	C	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	D	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	E	427	Total	C	N	O	S	0	0	0
			3384	2154	568	645	17			
1	F	421	Total	C	N	O	S	0	0	0
			3345	2128	562	638	17			
1	G	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	H	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	I	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			
1	J	420	Total	C	N	O	S	0	0	0
			3334	2119	561	637	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q81971
A	175	SER	CYS	engineered mutation	UNP Q81971
B	9	MET	-	initiating methionine	UNP Q81971
B	175	SER	CYS	engineered mutation	UNP Q81971
C	9	MET	-	initiating methionine	UNP Q81971
C	175	SER	CYS	engineered mutation	UNP Q81971
D	9	MET	-	initiating methionine	UNP Q81971
D	175	SER	CYS	engineered mutation	UNP Q81971
E	9	MET	-	initiating methionine	UNP Q81971

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	175	SER	CYS	engineered mutation	UNP Q81971
F	9	MET	-	initiating methionine	UNP Q81971
F	175	SER	CYS	engineered mutation	UNP Q81971
G	9	MET	-	initiating methionine	UNP Q81971
G	175	SER	CYS	engineered mutation	UNP Q81971
H	9	MET	-	initiating methionine	UNP Q81971
H	175	SER	CYS	engineered mutation	UNP Q81971
I	9	MET	-	initiating methionine	UNP Q81971
I	175	SER	CYS	engineered mutation	UNP Q81971
J	9	MET	-	initiating methionine	UNP Q81971
J	175	SER	CYS	engineered mutation	UNP Q81971

- Molecule 2 is a protein called light chains of Fab fragment of antibody 28F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	O	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	Q	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	S	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	M	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	c	218	Total	C	N	O	S	0	0	0
			1689	1054	288	341	6			
2	W	219	Total	C	N	O	S	0	0	0
			1695	1057	289	342	7			
2	Y	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	a	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			
2	U	217	Total	C	N	O	S	0	0	0
			1680	1049	287	338	6			

- Molecule 3 is a protein called heavy chain of Fab fragment of antibody 28F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	222	Total	C	N	O	S	0	0	0
			1671	1062	268	332	9			
3	P	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			

*Continued on next page...*

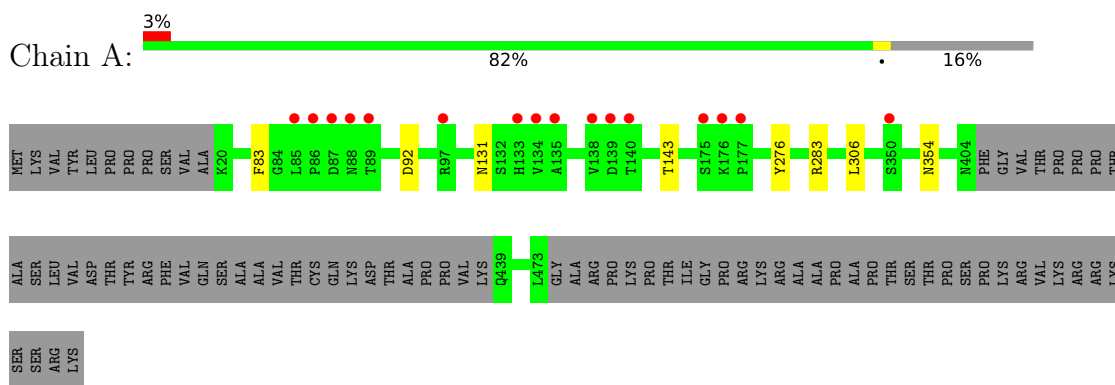
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	221	Total	C	N	O	S	0	0	0
			1666	1059	267	331	9			
3	T	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	N	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	d	221	Total	C	N	O	S	0	0	0
			1666	1059	267	331	9			
3	V	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	X	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	Z	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	b	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			

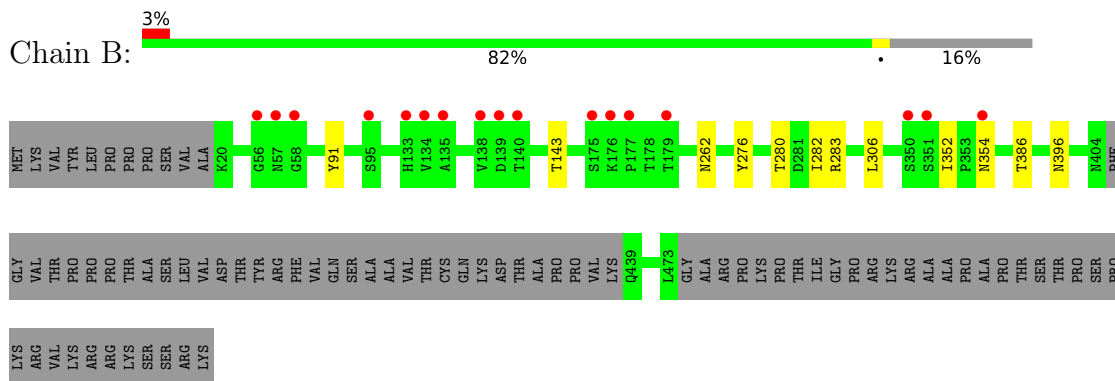
### 3 Residue-property plots [i](#)

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.

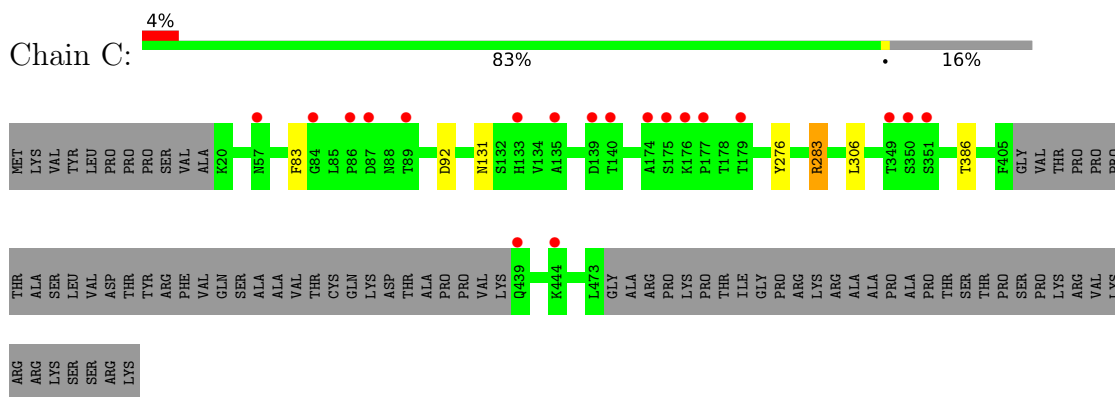
#### • Molecule 1: Major capsid protein L1



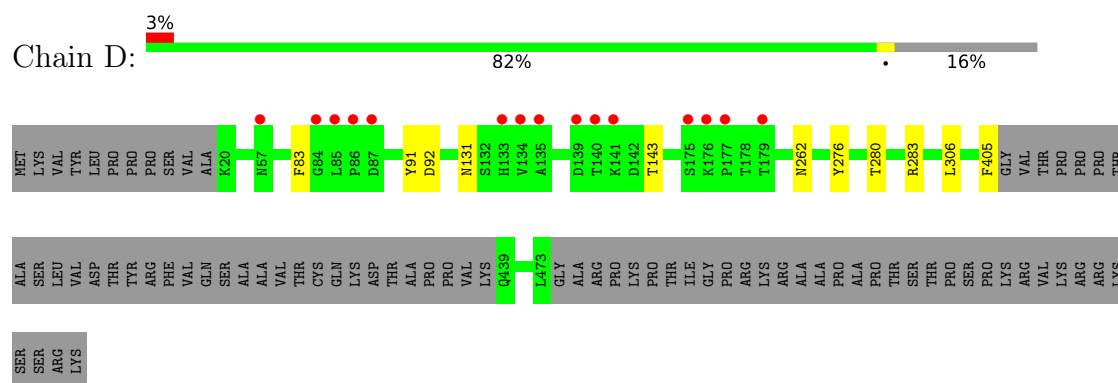
#### • Molecule 1: Major capsid protein L1



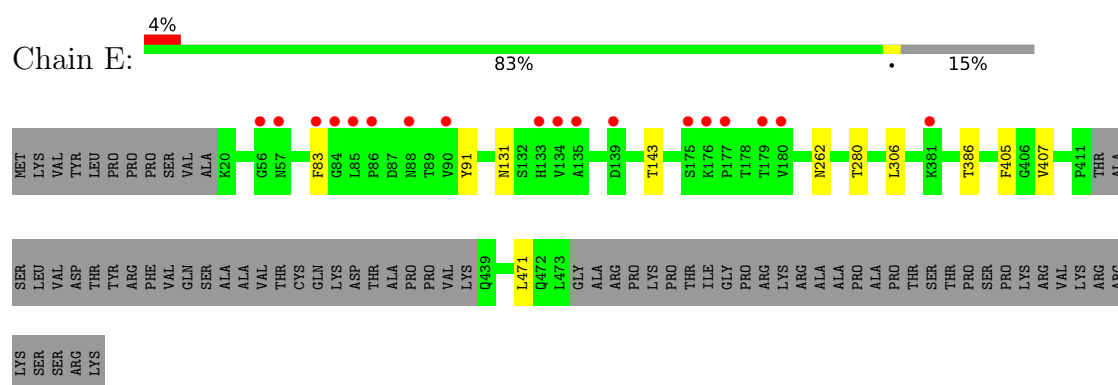
#### • Molecule 1: Major capsid protein L1



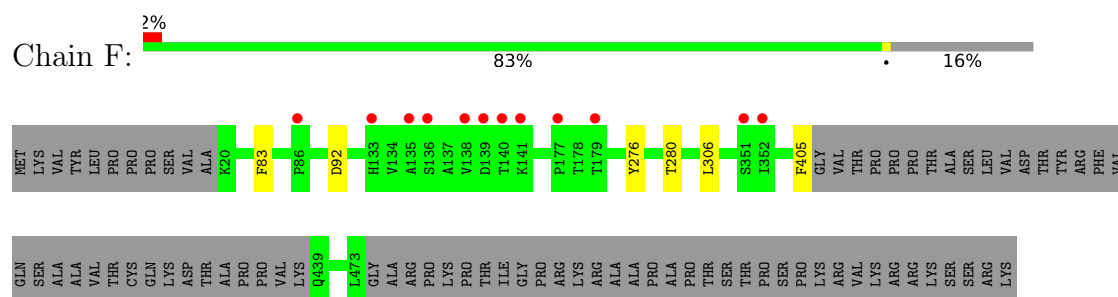
## • Molecule 1: Major capsid protein L1



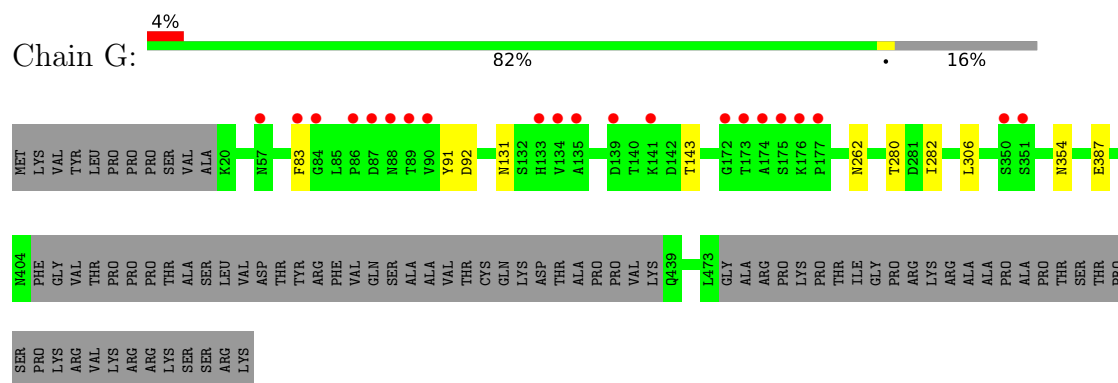
## • Molecule 1: Major capsid protein L1



## • Molecule 1: Major capsid protein L1



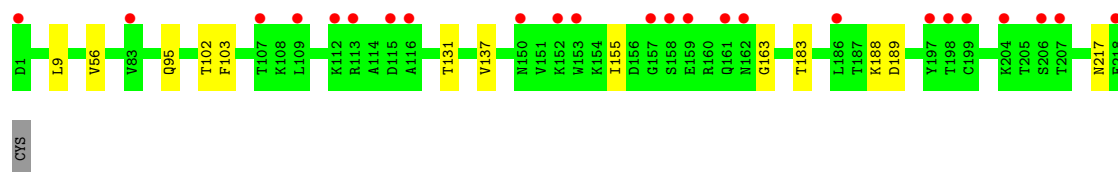
## • Molecule 1: Major capsid protein L1



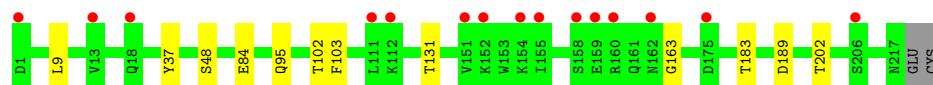
## • Molecule 1: Major capsid protein L1



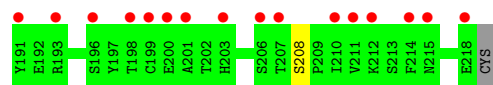
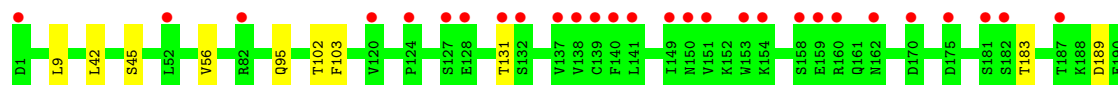
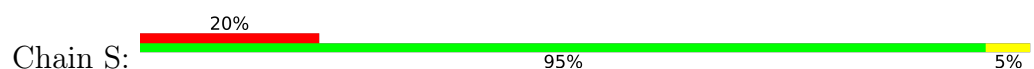




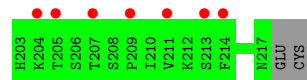
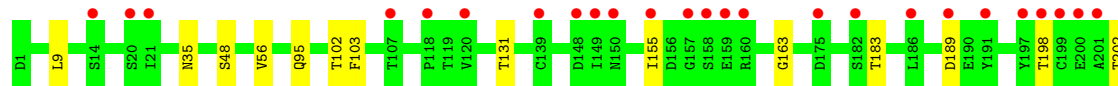
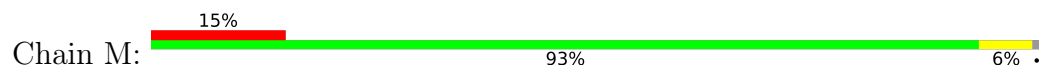
- Molecule 2: light chains of Fab fragment of antibody 28F10



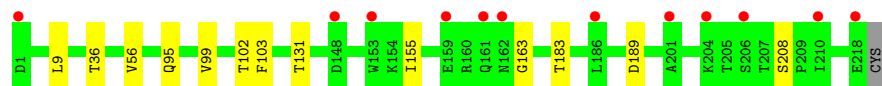
- Molecule 2: light chains of Fab fragment of antibody 28F10



- Molecule 2: light chains of Fab fragment of antibody 28F10



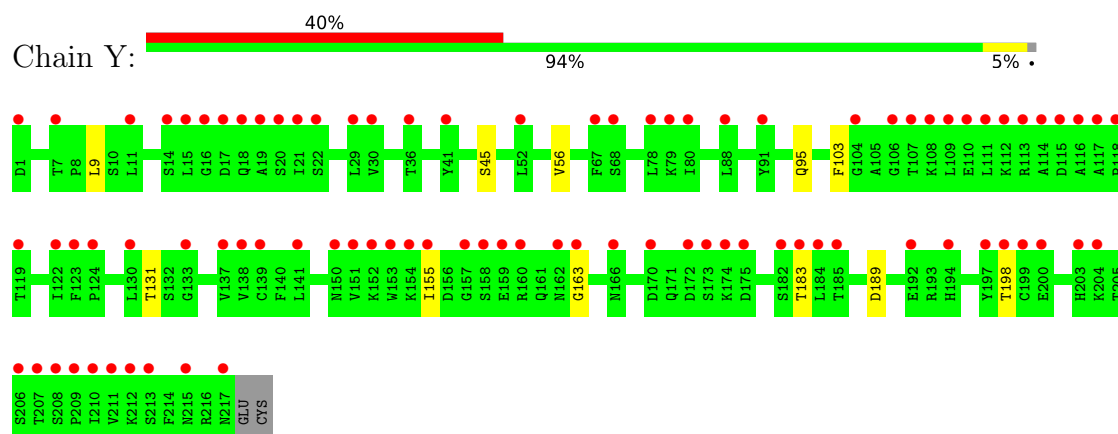
- Molecule 2: light chains of Fab fragment of antibody 28F10



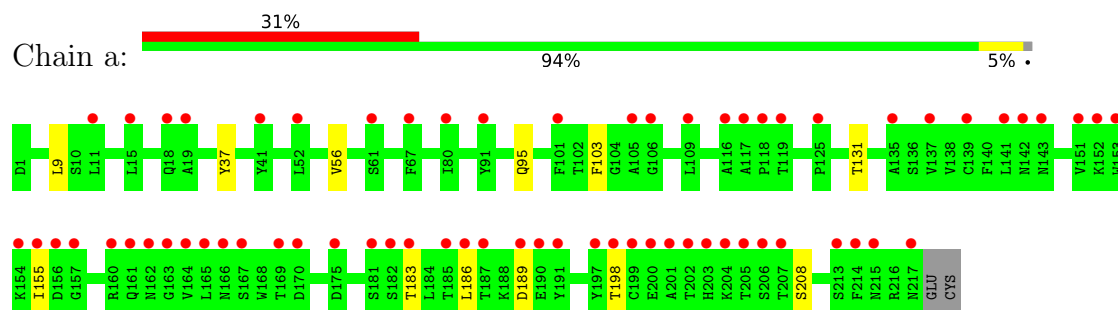
- Molecule 2: light chains of Fab fragment of antibody 28F10



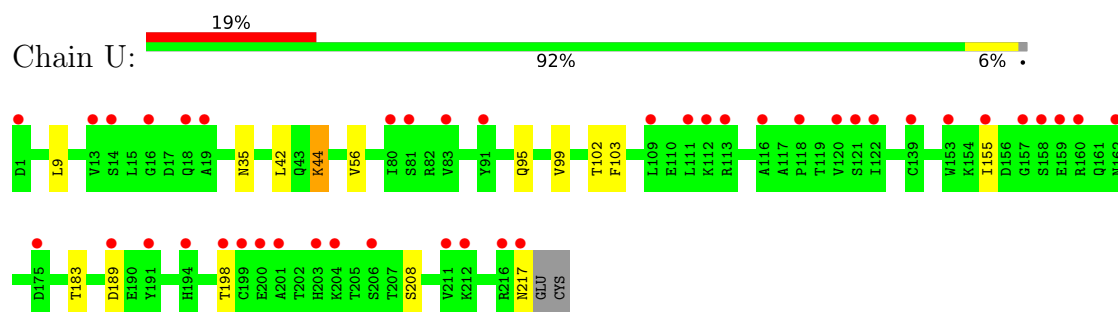
- Molecule 2: light chains of Fab fragment of antibody 28F10



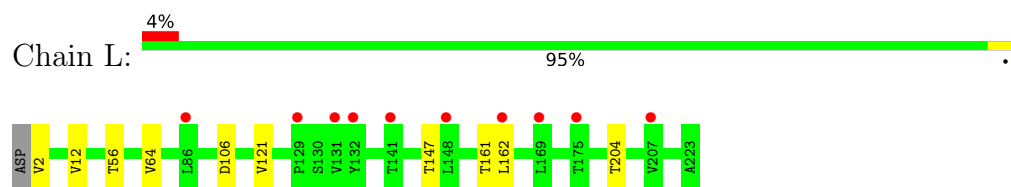
- Molecule 2: light chains of Fab fragment of antibody 28F10



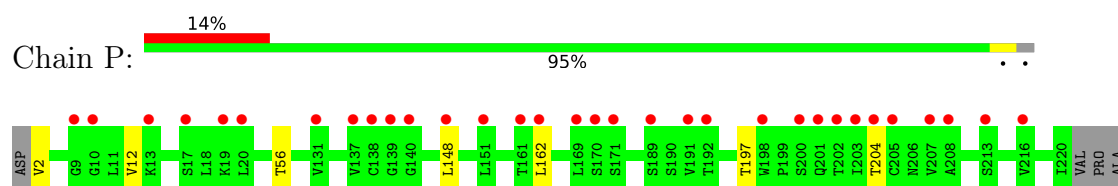
- Molecule 2: light chains of Fab fragment of antibody 28F10



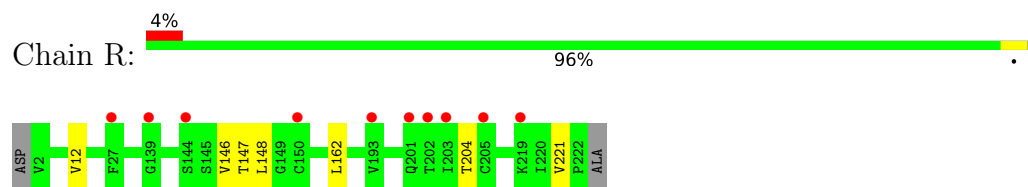
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



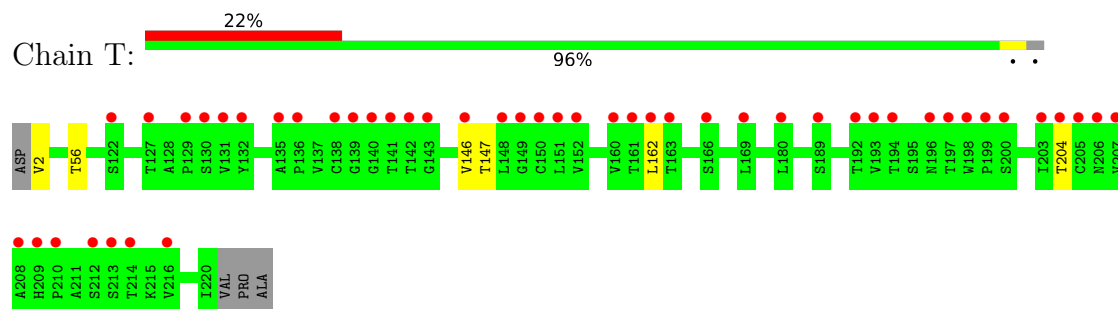
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



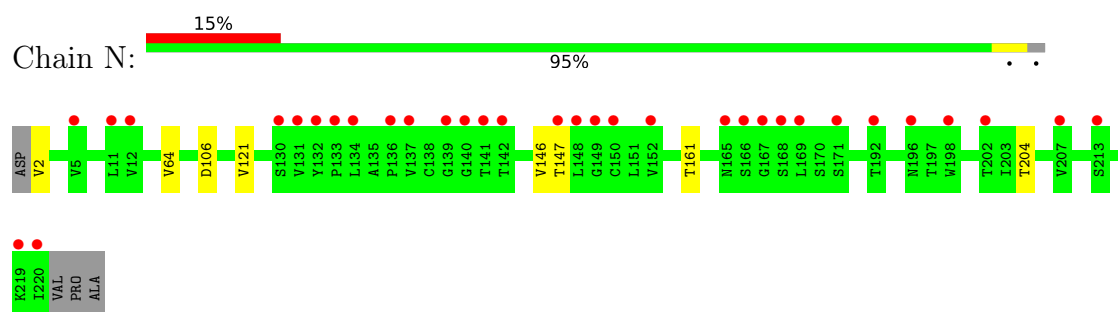
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



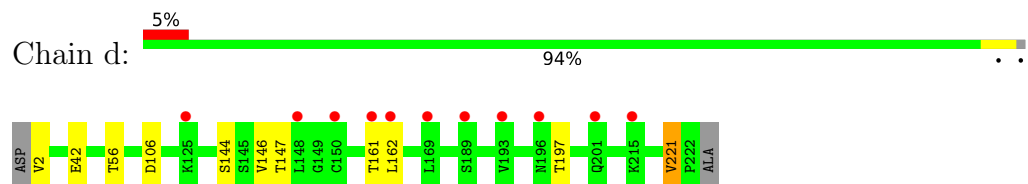
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



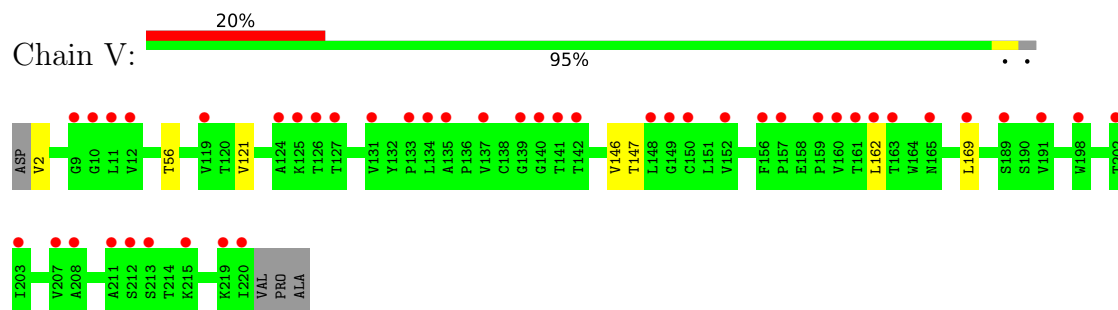
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



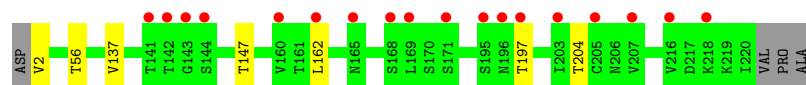
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



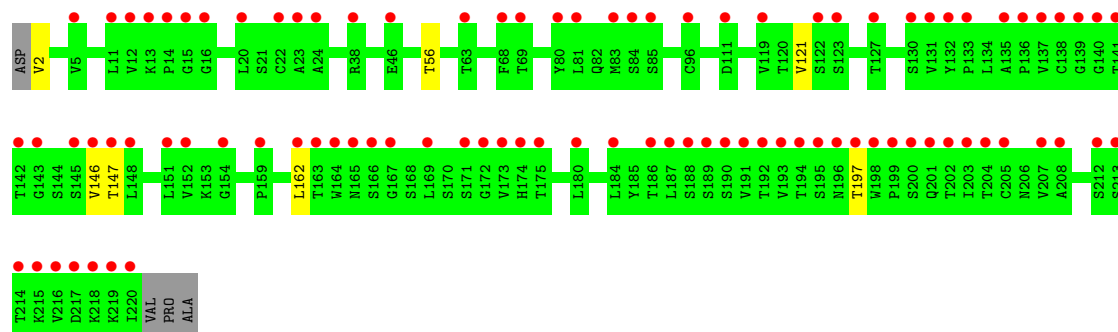
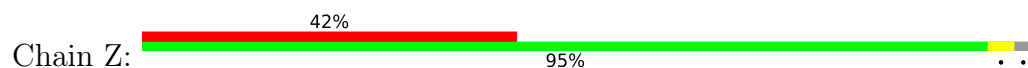
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



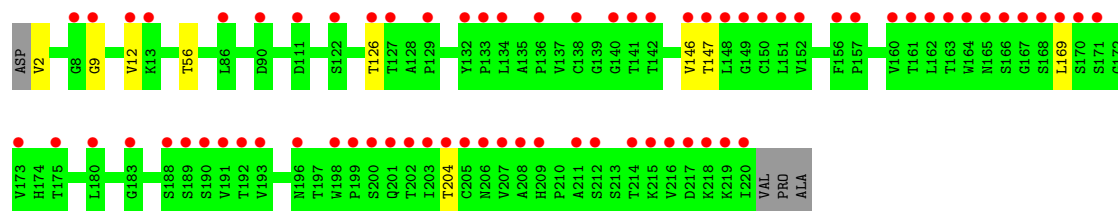
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



- Molecule 3: heavy chain of Fab fragment of antibody 28F10



- Molecule 3: heavy chain of Fab fragment of antibody 28F10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.27Å 417.23Å 134.94Å 90.00° 111.02° 90.00°	Depositor
Resolution (Å)	36.53 – 3.35 36.53 – 3.35	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.53-3.35) 94.1 (36.53-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.230 , 0.261 0.230 , 0.261	Depositor DCC
$R_{free}$ test set	8049 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	66832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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	0.25	0/3421	0.45	0/4656
1	B	0.25	0/3421	0.45	0/4656
1	C	0.25	0/3433	0.46	0/4672
1	D	0.26	0/3433	0.45	0/4672
1	E	0.26	0/3475	0.46	0/4733
1	F	0.25	0/3433	0.45	0/4672
1	G	0.25	0/3421	0.45	0/4656
1	H	0.25	0/3421	0.45	0/4656
1	I	0.25	0/3421	0.44	0/4656
1	J	0.25	0/3421	0.45	0/4656
2	K	0.30	0/1718	0.50	0/2331
2	M	0.26	0/1718	0.50	0/2331
2	O	0.26	0/1727	0.50	0/2343
2	Q	0.26	0/1718	0.49	0/2331
2	S	0.25	0/1727	0.49	0/2343
2	U	0.25	0/1718	0.49	0/2331
2	W	0.26	0/1733	0.50	0/2351
2	Y	0.25	0/1718	0.49	0/2331
2	a	0.25	0/1718	0.49	0/2331
2	c	0.26	0/1727	0.50	0/2343
3	L	0.27	0/1716	0.52	0/2344
3	N	0.25	0/1696	0.48	0/2315
3	P	0.26	0/1696	0.51	0/2315
3	R	0.26	0/1711	0.50	0/2337
3	T	0.25	0/1696	0.50	0/2315
3	V	0.25	0/1696	0.48	0/2315
3	X	0.25	0/1696	0.50	0/2315
3	Z	0.25	0/1696	0.50	0/2315
3	b	0.26	0/1696	0.50	0/2315
3	d	0.26	0/1711	0.51	0/2337
All	All	0.25	0/68532	0.48	0/93274

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	416/500 (83%)	386 (93%)	28 (7%)	2 (0%)	29	63
1	B	416/500 (83%)	388 (93%)	26 (6%)	2 (0%)	29	63
1	C	417/500 (83%)	386 (93%)	29 (7%)	2 (0%)	29	63
1	D	417/500 (83%)	389 (93%)	27 (6%)	1 (0%)	47	78
1	E	423/500 (85%)	390 (92%)	31 (7%)	2 (0%)	29	63
1	F	417/500 (83%)	390 (94%)	27 (6%)	0	100	100
1	G	416/500 (83%)	387 (93%)	25 (6%)	4 (1%)	15	49
1	H	416/500 (83%)	387 (93%)	27 (6%)	2 (0%)	29	63
1	I	416/500 (83%)	386 (93%)	27 (6%)	3 (1%)	22	56
1	J	416/500 (83%)	388 (93%)	27 (6%)	1 (0%)	47	78
2	K	215/219 (98%)	199 (93%)	13 (6%)	3 (1%)	11	40
2	M	215/219 (98%)	199 (93%)	14 (6%)	2 (1%)	17	51
2	O	216/219 (99%)	201 (93%)	12 (6%)	3 (1%)	11	40
2	Q	215/219 (98%)	200 (93%)	14 (6%)	1 (0%)	29	63
2	S	216/219 (99%)	201 (93%)	13 (6%)	2 (1%)	17	51
2	U	215/219 (98%)	200 (93%)	12 (6%)	3 (1%)	11	40
2	W	217/219 (99%)	202 (93%)	13 (6%)	2 (1%)	17	51

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Y	215/219 (98%)	201 (94%)	11 (5%)	3 (1%)	11	40
2	a	215/219 (98%)	201 (94%)	12 (6%)	2 (1%)	17	51
2	c	216/219 (99%)	201 (93%)	12 (6%)	3 (1%)	11	40
3	L	220/223 (99%)	207 (94%)	12 (6%)	1 (0%)	29	63
3	N	217/223 (97%)	203 (94%)	12 (6%)	2 (1%)	17	51
3	P	217/223 (97%)	204 (94%)	13 (6%)	0	100	100
3	R	219/223 (98%)	205 (94%)	13 (6%)	1 (0%)	29	63
3	T	217/223 (97%)	203 (94%)	14 (6%)	0	100	100
3	V	217/223 (97%)	203 (94%)	13 (6%)	1 (0%)	29	63
3	X	217/223 (97%)	202 (93%)	14 (6%)	1 (0%)	29	63
3	Z	217/223 (97%)	203 (94%)	14 (6%)	0	100	100
3	b	217/223 (97%)	202 (93%)	14 (6%)	1 (0%)	29	63
3	d	219/223 (98%)	204 (93%)	13 (6%)	2 (1%)	17	51
All	All	8502/9420 (90%)	7918 (93%)	532 (6%)	52 (1%)	25	59

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	283	ARG
1	J	282	ILE
2	O	217	ASN
1	D	131	ASN
1	E	131	ASN

### 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	376/444 (85%)	371 (99%)	5 (1%)	69	84
1	B	376/444 (85%)	367 (98%)	9 (2%)	49	74
1	C	377/444 (85%)	373 (99%)	4 (1%)	73	86

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	377/444 (85%)	368 (98%)	9 (2%)	49	74
1	E	382/444 (86%)	374 (98%)	8 (2%)	53	77
1	F	377/444 (85%)	372 (99%)	5 (1%)	69	84
1	G	376/444 (85%)	370 (98%)	6 (2%)	62	81
1	H	376/444 (85%)	372 (99%)	4 (1%)	73	86
1	I	376/444 (85%)	367 (98%)	9 (2%)	49	74
1	J	376/444 (85%)	371 (99%)	5 (1%)	69	84
2	K	195/197 (99%)	187 (96%)	8 (4%)	30	61
2	M	195/197 (99%)	183 (94%)	12 (6%)	18	49
2	O	196/197 (100%)	187 (95%)	9 (5%)	27	59
2	Q	195/197 (99%)	185 (95%)	10 (5%)	24	55
2	S	196/197 (100%)	187 (95%)	9 (5%)	27	59
2	U	195/197 (99%)	183 (94%)	12 (6%)	18	49
2	W	197/197 (100%)	189 (96%)	8 (4%)	30	61
2	Y	195/197 (99%)	187 (96%)	8 (4%)	30	61
2	a	195/197 (99%)	185 (95%)	10 (5%)	24	55
2	c	196/197 (100%)	186 (95%)	10 (5%)	24	55
3	L	189/190 (100%)	180 (95%)	9 (5%)	25	57
3	N	187/190 (98%)	181 (97%)	6 (3%)	39	68
3	P	187/190 (98%)	180 (96%)	7 (4%)	34	63
3	R	189/190 (100%)	183 (97%)	6 (3%)	39	68
3	T	187/190 (98%)	181 (97%)	6 (3%)	39	68
3	V	187/190 (98%)	181 (97%)	6 (3%)	39	68
3	X	187/190 (98%)	181 (97%)	6 (3%)	39	68
3	Z	187/190 (98%)	180 (96%)	7 (4%)	34	63
3	b	187/190 (98%)	180 (96%)	7 (4%)	34	63
3	d	189/190 (100%)	180 (95%)	9 (5%)	25	57
All	All	7600/8310 (92%)	7371 (97%)	229 (3%)	41	69

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	45	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	U	95	GLN
3	N	147	THR
2	U	42	LEU
3	Z	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	31	HIS
2	W	203	HIS
1	H	326	HIS
3	R	181	GLN
1	H	133	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 monosaccharides 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, 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	420/500 (84%)	0.05	16 (3%) 40 42	43, 63, 117, 149	0
1	B	420/500 (84%)	0.04	17 (4%) 38 40	39, 64, 123, 155	0
1	C	421/500 (84%)	0.07	19 (4%) 33 36	39, 56, 113, 177	0
1	D	421/500 (84%)	0.04	15 (3%) 42 45	35, 52, 117, 171	0
1	E	427/500 (85%)	0.08	18 (4%) 36 38	38, 54, 115, 154	0
1	F	421/500 (84%)	0.08	12 (2%) 51 54	44, 65, 124, 165	0
1	G	420/500 (84%)	0.17	21 (5%) 28 31	49, 71, 126, 157	0
1	H	420/500 (84%)	0.23	20 (4%) 30 33	51, 73, 136, 166	0
1	I	420/500 (84%)	0.17	20 (4%) 30 33	51, 71, 132, 182	0
1	J	420/500 (84%)	0.18	16 (3%) 40 42	46, 69, 126, 159	0
2	K	217/219 (99%)	0.07	2 (0%) 84 87	51, 81, 127, 138	0
2	M	217/219 (99%)	0.72	32 (14%) 2 2	77, 141, 191, 202	0
2	O	218/219 (99%)	0.72	24 (11%) 5 6	69, 133, 179, 196	0
2	Q	217/219 (99%)	0.40	15 (6%) 16 19	57, 105, 138, 165	0
2	S	218/219 (99%)	1.10	44 (20%) 1 1	69, 128, 219, 236	0
2	U	217/219 (99%)	0.89	42 (19%) 1 1	75, 137, 195, 209	0
2	W	219/219 (100%)	0.15	1 (0%) 91 93	65, 87, 114, 152	0
2	Y	217/219 (99%)	2.16	88 (40%) 0 0	113, 179, 223, 233	0
2	a	217/219 (99%)	1.53	67 (30%) 0 0	95, 158, 223, 232	0
2	c	218/219 (99%)	0.28	12 (5%) 25 27	62, 90, 140, 149	0
3	L	222/223 (99%)	0.31	10 (4%) 33 36	56, 90, 118, 183	0
3	N	219/223 (98%)	0.70	33 (15%) 2 2	57, 104, 176, 194	0
3	P	219/223 (98%)	0.68	32 (14%) 2 2	62, 111, 183, 222	0
3	R	221/223 (99%)	0.33	10 (4%) 33 36	47, 73, 145, 167	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	T	219/223 (98%)	1.13	48 (21%) 0 1	50, 110, 214, 229	0
3	V	219/223 (98%)	0.95	44 (20%) 1 1	72, 117, 206, 216	0
3	X	219/223 (98%)	0.40	18 (8%) 11 13	67, 91, 144, 198	0
3	Z	219/223 (98%)	2.07	93 (42%) 0 0	91, 157, 237, 259	0
3	b	219/223 (98%)	1.61	72 (32%) 0 0	73, 130, 224, 232	0
3	d	221/223 (99%)	0.30	11 (4%) 28 31	54, 84, 134, 179	0
All	All	8582/9420 (91%)	0.47	872 (10%) 6 8	35, 82, 200, 259	0

The worst 5 of 872 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	198	THR	13.1
3	T	149	GLY	12.3
3	b	220	ILE	12.0
2	Y	199	CYS	11.0
3	T	150	CYS	10.9

## 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.