



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

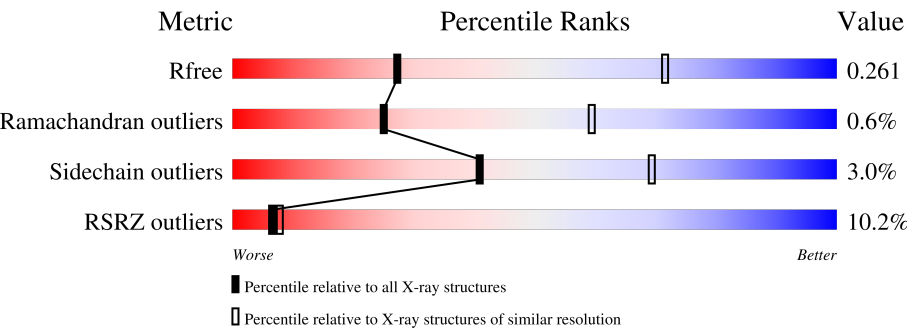
# 1 Overall quality at a glance i

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>

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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

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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			

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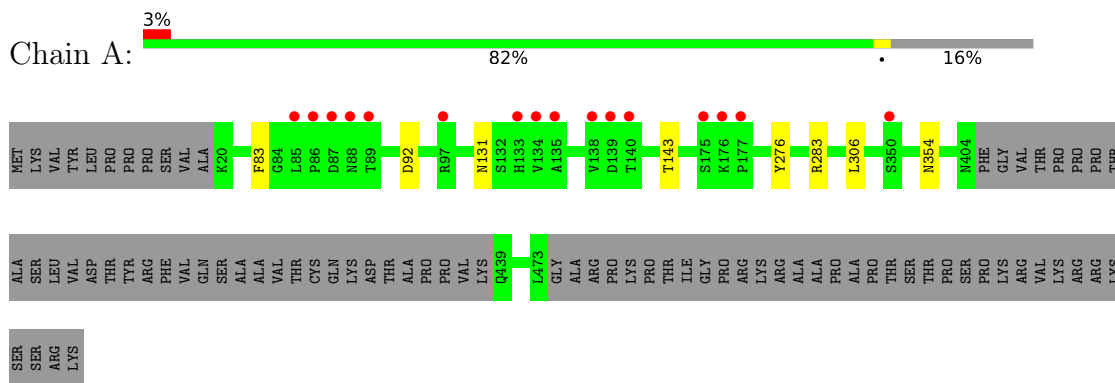
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	221	Total	C	N	O	S	0	0	0
			1666	1059	267	331	9			
3	T	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	N	219	Total	C	N	O	S	0	0	0
			1652	1049	265	329	9			
3	d	221	Total	C	N	O	S	0	0	0
			1666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

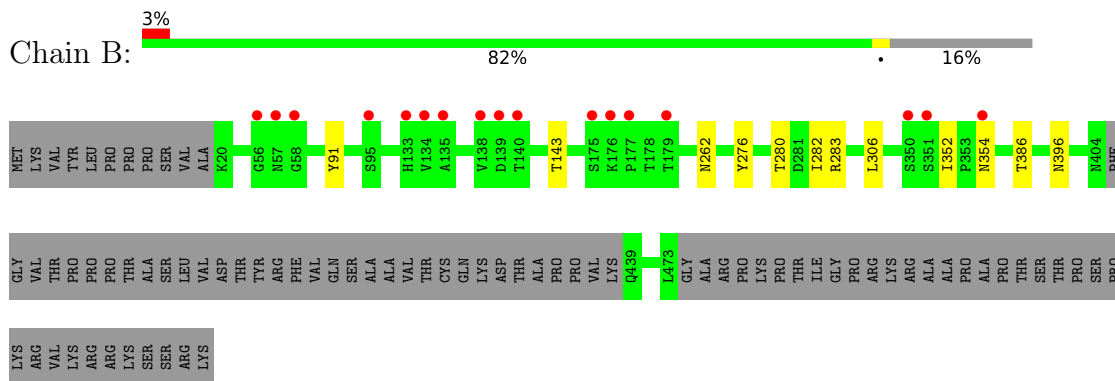
### 3 Residue-property plots [i](#)

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.

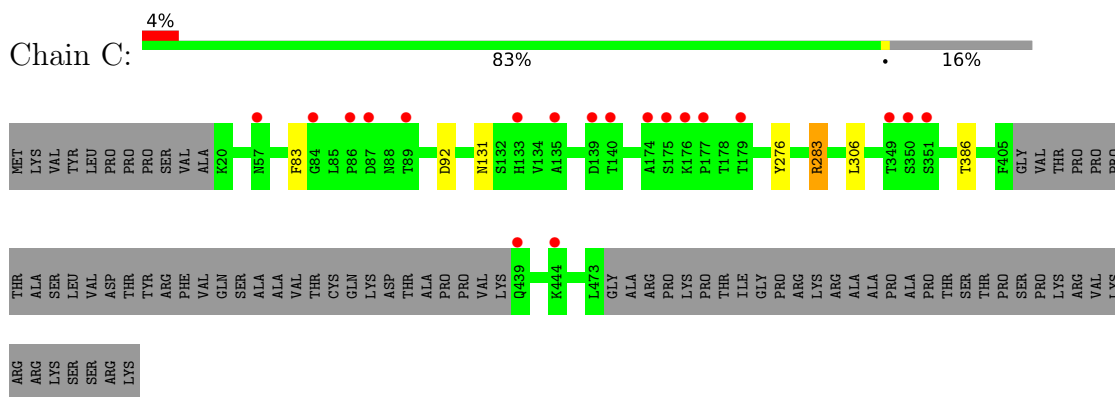
- Molecule 1: Major capsid protein L1




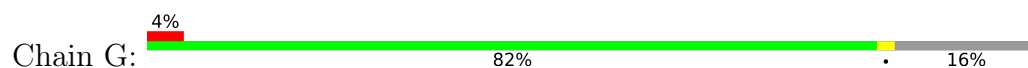
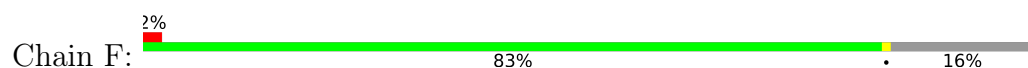
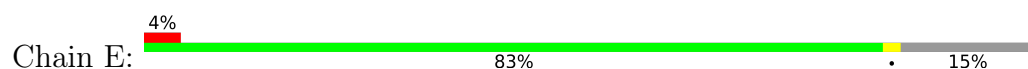
- Molecule 1: Major capsid protein L1



- Molecule 1: Major capsid protein L1

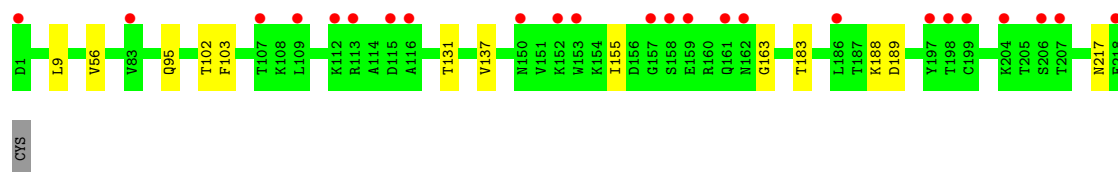


- Chain D:  3% 82% 16%

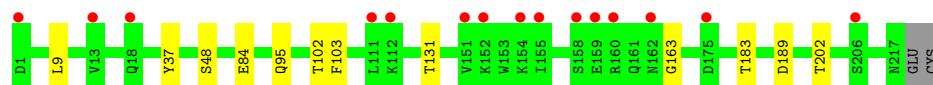




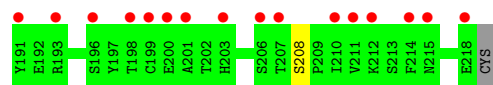
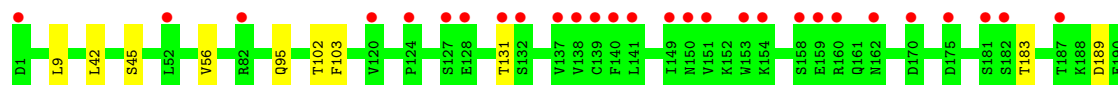
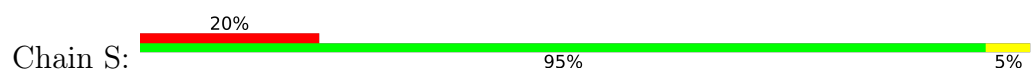




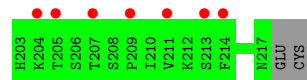
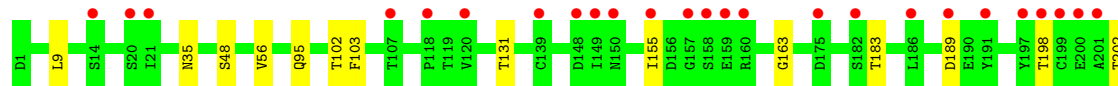
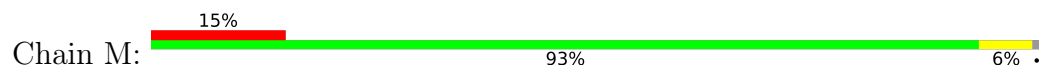
- Molecule 2: light chains of Fab fragment of antibody 28F10



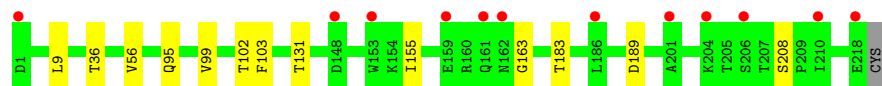
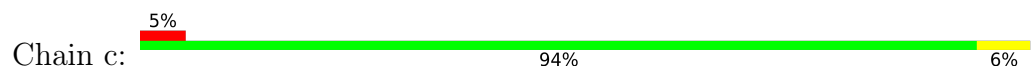
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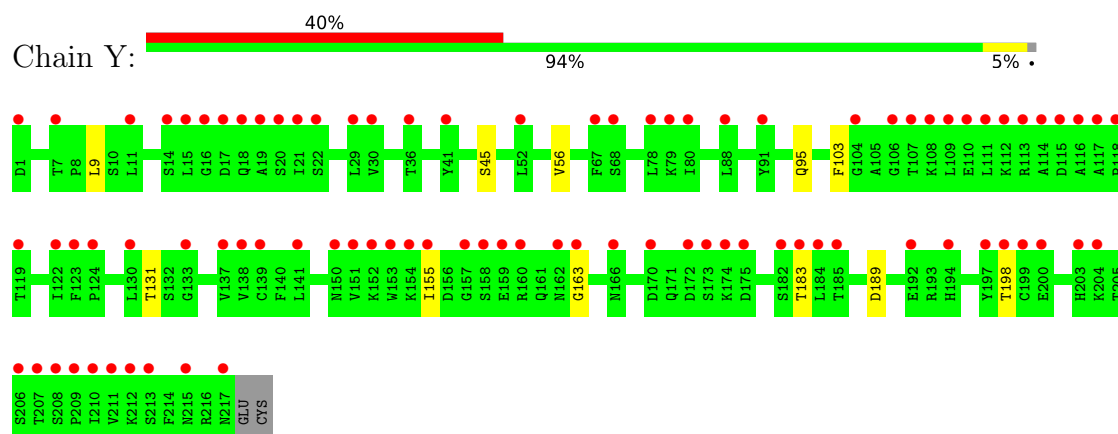
- Molecule 2: light chains of Fab fragment of antibody 28F10



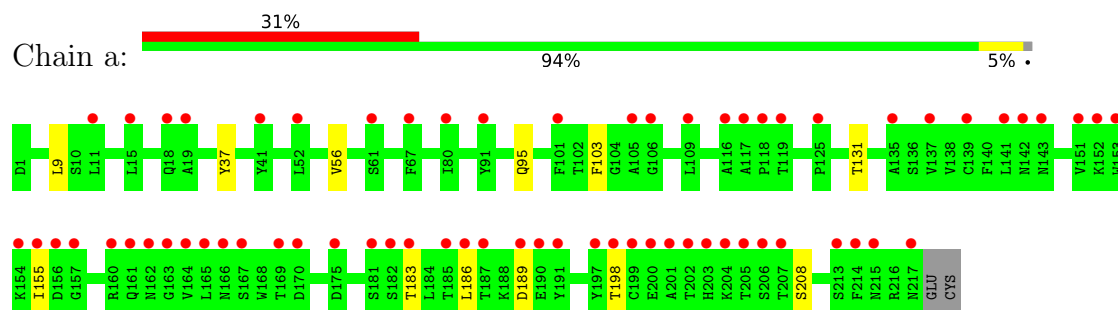
- Molecule 2: light chains of Fab fragment of antibody 28F10



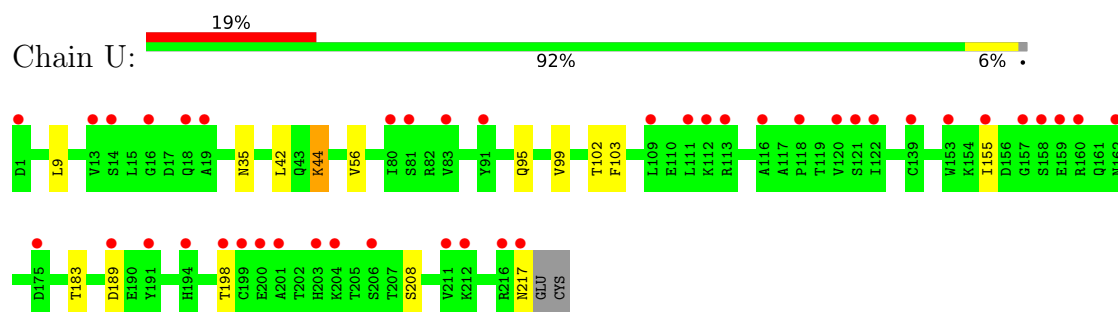
- Molecule 2: light chains of Fab fragment of antibody 28F10



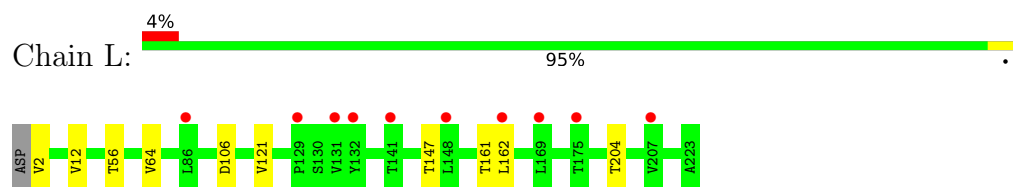
- Molecule 2: light chains of Fab fragment of antibody 28F10



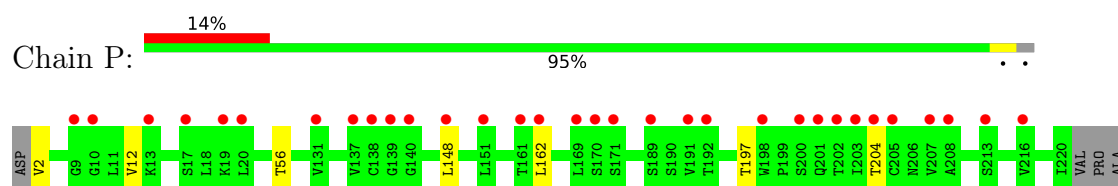
- Molecule 2: light chains of Fab fragment of antibody 28F10



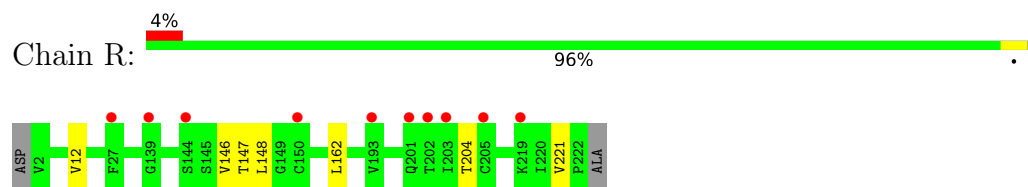
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



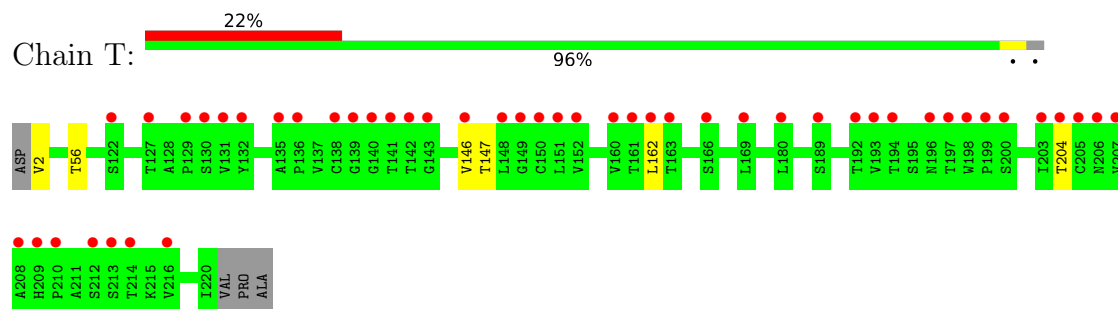
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



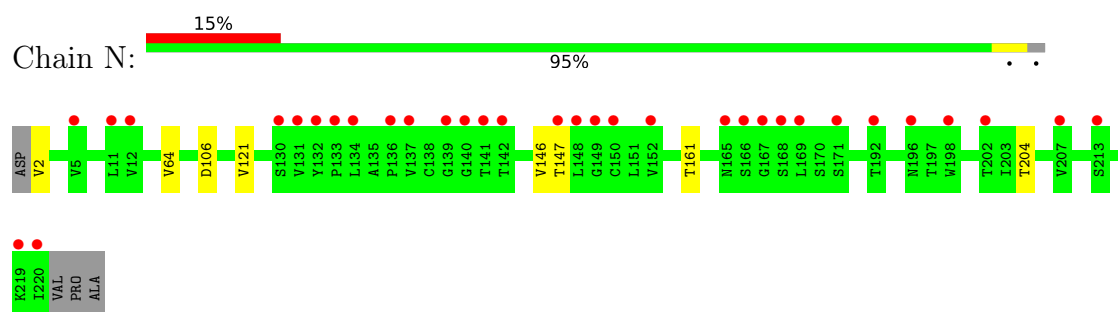
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



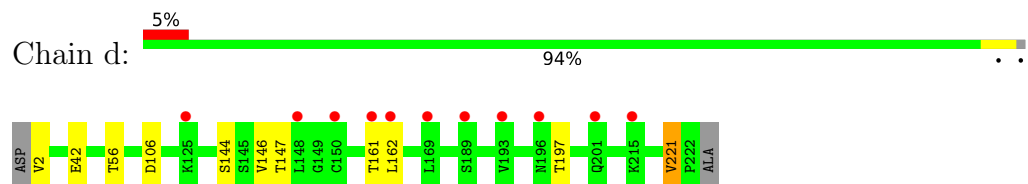
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



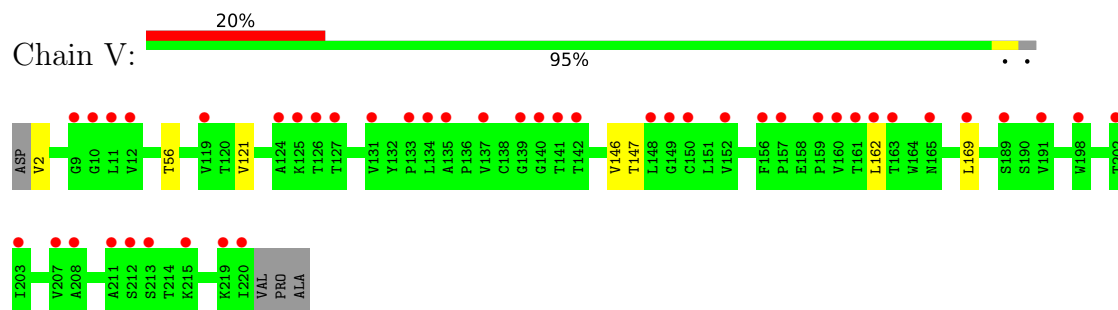
- Molecule 3: heavy chain of Fab fragment of antibody 28F10



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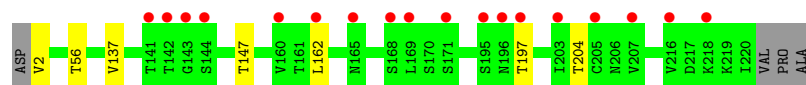


- Molecule 3: heavy chain of Fab fragment of antibody 28F10

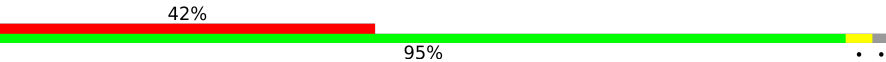


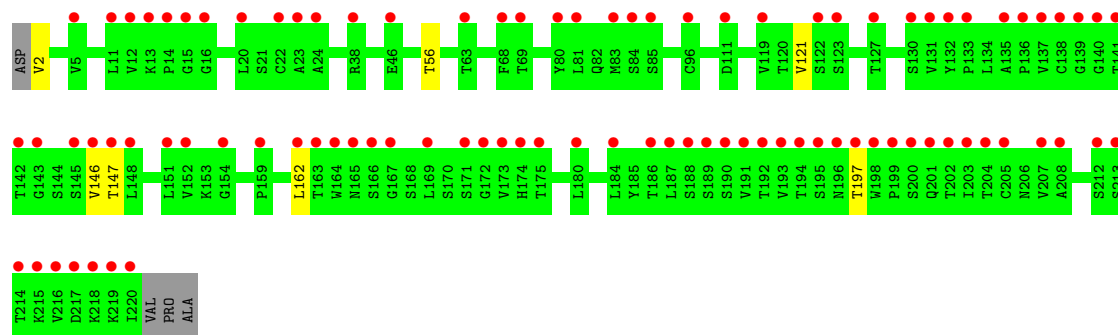
- Molecule 3: heavy chain of Fab fragment of antibody 28F10

Chain X: 

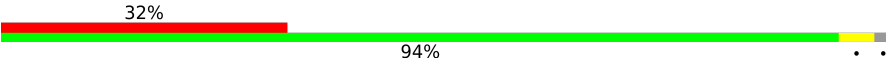


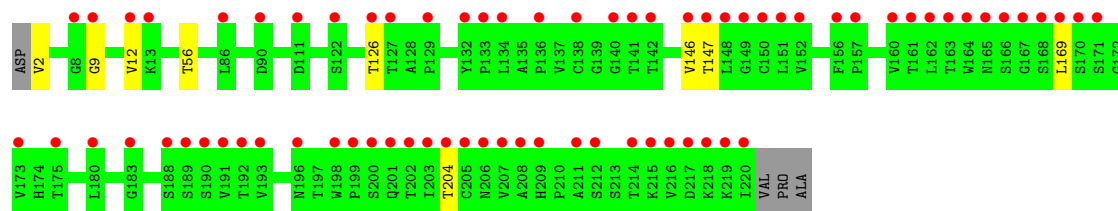
• Molecule 3: heavy chain of Fab fragment of antibody 28F10

Chain Z: 



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

Chain b: 



## 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

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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

All (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
1	E	405	PHE
3	R	221	VAL
3	d	221	VAL
2	W	45	SER
3	X	137	VAL
1	A	131	ASN
1	B	354	ASN
1	C	131	ASN
1	B	282	ILE
1	G	387	GLU
1	H	131	ASN
1	H	403	TRP
1	I	131	ASN
3	N	106	ASP

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Mol	Chain	Res	Type
1	A	354	ASN
1	G	131	ASN
1	G	354	ASN
1	I	387	GLU
2	K	45	SER
3	L	106	ASP
3	d	106	ASP
3	V	169	LEU
2	Y	45	SER
3	b	169	LEU
2	U	44	LYS
2	c	208	SER
2	a	208	SER
2	O	163	GLY
2	Q	163	GLY
2	c	163	GLY
1	I	282	ILE
2	K	163	GLY
2	O	56	VAL
2	S	56	VAL
2	M	163	GLY
3	N	64	VAL
2	c	56	VAL
2	Y	56	VAL
2	Y	163	GLY
2	a	56	VAL
2	U	56	VAL
1	G	282	ILE
2	K	56	VAL
2	S	208	SER
2	M	56	VAL
2	W	163	GLY
2	U	208	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	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
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

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	PHE
1	A	143	THR
1	A	276	TYR
1	A	283	ARG
1	A	306	LEU
1	B	91	TYR
1	B	143	THR
1	B	262	ASN
1	B	276	TYR
1	B	280	THR
1	B	283	ARG
1	B	306	LEU
1	B	352	ILE
1	B	396	ASN
1	C	83	PHE
1	C	276	TYR
1	C	283	ARG
1	C	306	LEU
1	D	83	PHE
1	D	91	TYR
1	D	143	THR
1	D	262	ASN
1	D	276	TYR
1	D	280	THR
1	D	283	ARG
1	D	306	LEU
1	D	405	PHE
1	E	83	PHE
1	E	91	TYR
1	E	143	THR
1	E	262	ASN
1	E	280	THR
1	E	306	LEU
1	E	407	VAL
1	E	471	LEU
1	F	83	PHE
1	F	276	TYR
1	F	280	THR
1	F	306	LEU
1	F	405	PHE
1	G	83	PHE
1	G	91	TYR
1	G	143	THR

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Mol	Chain	Res	Type
1	G	262	ASN
1	G	280	THR
1	G	306	LEU
1	H	91	TYR
1	H	262	ASN
1	H	283	ARG
1	H	306	LEU
1	I	83	PHE
1	I	91	TYR
1	I	143	THR
1	I	262	ASN
1	I	276	TYR
1	I	280	THR
1	I	283	ARG
1	I	306	LEU
1	I	396	ASN
1	J	143	THR
1	J	262	ASN
1	J	280	THR
1	J	282	ILE
1	J	306	LEU
2	K	9	LEU
2	K	37	TYR
2	K	95	GLN
2	K	103	PHE
2	K	131	THR
2	K	183	THR
2	K	186	LEU
2	K	189	ASP
3	L	2	VAL
3	L	12	VAL
3	L	56	THR
3	L	64	VAL
3	L	121	VAL
3	L	147	THR
3	L	161	THR
3	L	162	LEU
3	L	204	THR
2	O	9	LEU
2	O	95	GLN
2	O	102	THR
2	O	103	PHE

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Mol	Chain	Res	Type
2	O	131	THR
2	O	137	VAL
2	O	155	ILE
2	O	183	THR
2	O	189	ASP
3	P	2	VAL
3	P	12	VAL
3	P	56	THR
3	P	148	LEU
3	P	162	LEU
3	P	197	THR
3	P	204	THR
2	Q	9	LEU
2	Q	37	TYR
2	Q	48	SER
2	Q	95	GLN
2	Q	102	THR
2	Q	103	PHE
2	Q	131	THR
2	Q	183	THR
2	Q	189	ASP
2	Q	202	THR
3	R	12	VAL
3	R	146	VAL
3	R	147	THR
3	R	148	LEU
3	R	162	LEU
3	R	204	THR
2	S	9	LEU
2	S	42	LEU
2	S	45	SER
2	S	95	GLN
2	S	102	THR
2	S	103	PHE
2	S	131	THR
2	S	183	THR
2	S	189	ASP
3	T	2	VAL
3	T	56	THR
3	T	146	VAL
3	T	147	THR
3	T	162	LEU

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Mol	Chain	Res	Type
3	T	204	THR
2	M	9	LEU
2	M	35	ASN
2	M	48	SER
2	M	95	GLN
2	M	102	THR
2	M	103	PHE
2	M	131	THR
2	M	155	ILE
2	M	183	THR
2	M	189	ASP
2	M	198	THR
2	M	202	THR
3	N	2	VAL
3	N	121	VAL
3	N	146	VAL
3	N	147	THR
3	N	161	THR
3	N	204	THR
2	c	9	LEU
2	c	36	THR
2	c	95	GLN
2	c	99	VAL
2	c	102	THR
2	c	103	PHE
2	c	131	THR
2	c	155	ILE
2	c	183	THR
2	c	189	ASP
3	d	2	VAL
3	d	42	GLU
3	d	56	THR
3	d	146	VAL
3	d	147	THR
3	d	161	THR
3	d	162	LEU
3	d	197	THR
3	d	221	VAL
3	V	2	VAL
3	V	56	THR
3	V	121	VAL
3	V	146	VAL

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Mol	Chain	Res	Type
3	V	147	THR
3	V	162	LEU
2	W	9	LEU
2	W	45	SER
2	W	95	GLN
2	W	102	THR
2	W	103	PHE
2	W	155	ILE
2	W	183	THR
2	W	189	ASP
3	X	2	VAL
3	X	56	THR
3	X	147	THR
3	X	162	LEU
3	X	197	THR
3	X	204	THR
2	Y	9	LEU
2	Y	95	GLN
2	Y	103	PHE
2	Y	131	THR
2	Y	155	ILE
2	Y	183	THR
2	Y	189	ASP
2	Y	198	THR
3	Z	2	VAL
3	Z	56	THR
3	Z	121	VAL
3	Z	146	VAL
3	Z	147	THR
3	Z	162	LEU
3	Z	197	THR
2	a	9	LEU
2	a	37	TYR
2	a	95	GLN
2	a	103	PHE
2	a	131	THR
2	a	155	ILE
2	a	183	THR
2	a	186	LEU
2	a	189	ASP
2	a	198	THR
3	b	2	VAL

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Mol	Chain	Res	Type
3	b	12	VAL
3	b	56	THR
3	b	126	THR
3	b	146	VAL
3	b	147	THR
3	b	204	THR
2	U	9	LEU
2	U	35	ASN
2	U	42	LEU
2	U	44	LYS
2	U	95	GLN
2	U	99	VAL
2	U	102	THR
2	U	103	PHE
2	U	155	ILE
2	U	183	THR
2	U	189	ASP
2	U	198	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	HIS
1	B	326	HIS
1	C	404	ASN
1	E	270	GLN
1	E	326	HIS
1	F	404	ASN
1	F	472	GLN
1	H	133	HIS
1	H	326	HIS
1	J	326	HIS
1	J	327	ASN
3	L	181	GLN
3	R	181	GLN
2	W	203	HIS
2	Y	31	HIS
2	U	47	GLN

### 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

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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

All (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
2	Y	123	PHE	10.2
2	Y	112	LYS	10.2
2	Y	211	VAL	9.7
2	a	198	THR	9.3
3	b	150	CYS	9.1
2	Y	139	CYS	8.8
2	Y	182	SER	8.7
3	T	132	TYR	8.4
2	Y	208	SER	8.4
3	b	216	VAL	7.9
2	Y	212	LYS	7.8
3	Z	135	ALA	7.8
2	Y	151	VAL	7.7
1	C	133	HIS	7.7
2	S	191	TYR	7.7
2	Y	118	PRO	7.6
3	b	203	ILE	7.5
1	E	133	HIS	7.4
3	b	161	THR	7.4
2	a	153	TRP	7.3
3	V	10	GLY	7.3
2	a	213	SER	7.3
3	Z	193	VAL	7.2
2	Y	209	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
3	T	140	GLY	7.2
1	I	134	VAL	7.1
2	O	206	SER	7.0
3	Z	217	ASP	7.0
2	O	158	SER	7.0
2	Y	19	ALA	7.0
3	b	219	LYS	7.0
2	Y	124	PRO	6.9
2	Y	207	THR	6.9
2	Y	150	ASN	6.8
2	S	160	ARG	6.8
1	H	133	HIS	6.8
1	H	86	PRO	6.8
3	Z	200	SER	6.8
2	a	201	ALA	6.8
3	Z	188	SER	6.8
3	Z	141	THR	6.7
1	C	139	ASP	6.7
2	Y	111	LEU	6.7
3	Z	148	LEU	6.5
3	V	219	LYS	6.5
2	a	155	ILE	6.5
1	A	86	PRO	6.4
1	C	351	SER	6.4
2	S	153	TRP	6.3
3	Z	216	VAL	6.2
3	Z	192	THR	6.2
3	T	141	THR	6.2
3	b	193	VAL	6.1
3	b	200	SER	6.1
3	Z	147	THR	6.1
2	Y	184	LEU	6.1
3	b	208	ALA	6.0
2	Y	154	LYS	6.0
3	T	169	LEU	5.9
3	T	162	LEU	5.9
3	b	162	LEU	5.9
3	b	149	GLY	5.9
3	T	139	GLY	5.9
1	H	141	LYS	5.8
3	Z	152	VAL	5.8
1	I	177	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
2	S	162	ASN	5.8
2	a	109	LEU	5.7
3	b	205	CYS	5.7
3	Z	198	TRP	5.6
2	a	151	VAL	5.6
2	Y	109	LEU	5.6
1	I	133	HIS	5.6
2	Q	1	ASP	5.6
3	T	193	VAL	5.6
1	H	134	VAL	5.5
1	I	135	ALA	5.5
1	I	86	PRO	5.5
3	T	216	VAL	5.5
1	D	133	HIS	5.5
2	U	18	GLN	5.5
2	a	118	PRO	5.4
1	J	134	VAL	5.4
3	V	9	GLY	5.4
2	Y	116	ALA	5.4
3	Z	214	THR	5.4
1	E	57	ASN	5.4
2	Y	183	THR	5.3
1	H	139	ASP	5.3
3	b	202	THR	5.3
3	b	198	TRP	5.3
1	F	139	ASP	5.3
3	V	140	GLY	5.3
1	E	175	SER	5.3
1	H	439	GLN	5.3
2	Y	15	LEU	5.2
2	U	13	VAL	5.2
1	I	175	SER	5.2
1	B	175	SER	5.2
2	U	160	ARG	5.2
3	b	141	THR	5.2
3	N	149	GLY	5.2
1	D	177	PRO	5.1
3	V	208	ALA	5.1
1	F	177	PRO	5.1
2	Y	185	THR	5.1
3	V	11	LEU	5.0
2	Y	20	SER	5.0

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Mol	Chain	Res	Type	RSRZ
3	N	171	SER	5.0
2	Y	206	SER	5.0
1	J	177	PRO	5.0
3	Z	166	SER	5.0
1	H	138	VAL	5.0
1	F	141	LYS	5.0
3	V	165	ASN	5.0
3	Z	81	LEU	5.0
2	a	187	THR	5.0
3	b	189	SER	4.9
3	Z	142	THR	4.9
3	T	152	VAL	4.9
2	U	199	CYS	4.9
1	F	140	THR	4.9
2	a	214	PHE	4.9
2	a	91	TYR	4.9
2	S	182	SER	4.9
3	V	141	THR	4.9
3	Z	13	LYS	4.9
3	b	192	THR	4.9
2	S	139	CYS	4.9
3	Z	146	VAL	4.8
2	a	217	ASN	4.8
2	Y	67	PHE	4.8
1	G	133	HIS	4.8
2	Y	159	GLU	4.8
3	Z	213	SER	4.8
1	C	140	THR	4.8
2	Y	175	ASP	4.8
2	S	154	LYS	4.8
1	H	135	ALA	4.8
3	b	127	THR	4.8
3	N	150	CYS	4.7
3	b	204	THR	4.7
3	Z	136	PRO	4.7
2	a	199	CYS	4.7
3	V	133	PRO	4.7
3	b	148	LEU	4.7
1	B	58	GLY	4.7
1	D	85	LEU	4.7
2	S	211	VAL	4.7
2	a	182	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	a	203	HIS	4.6
1	E	177	PRO	4.6
3	b	163	THR	4.6
3	b	142	THR	4.6
2	S	198	THR	4.6
1	G	177	PRO	4.6
2	Q	206	SER	4.6
2	S	158	SER	4.6
2	O	152	LYS	4.5
2	a	164	VAL	4.5
3	Z	167	GLY	4.5
3	b	90	ASP	4.5
2	a	154	LYS	4.5
3	L	141	THR	4.5
3	b	215	LYS	4.5
2	Y	157	GLY	4.5
1	D	134	VAL	4.5
1	J	351	SER	4.5
2	U	198	THR	4.4
3	Z	191	VAL	4.4
1	A	133	HIS	4.4
1	H	177	PRO	4.4
1	F	135	ALA	4.4
2	Y	29	LEU	4.4
3	Z	162	LEU	4.4
1	B	140	THR	4.4
3	b	166	SER	4.4
3	P	138	CYS	4.4
1	B	133	HIS	4.4
1	I	351	SER	4.4
3	T	203	ILE	4.4
1	B	134	VAL	4.4
3	T	163	THR	4.4
3	b	129	PRO	4.4
2	a	156	ASP	4.3
3	T	208	ALA	4.3
1	G	174	ALA	4.3
3	T	161	THR	4.3
3	N	148	LEU	4.3
3	V	220	ILE	4.3
3	b	165	ASN	4.3
2	a	202	THR	4.3

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Mol	Chain	Res	Type	RSRZ
2	U	162	ASN	4.3
3	N	131	VAL	4.3
3	P	10	GLY	4.3
3	Z	38	ARG	4.3
3	V	150	CYS	4.3
3	b	13	LYS	4.3
3	b	211	ALA	4.3
3	b	190	SER	4.2
3	X	196	ASN	4.2
1	I	140	THR	4.2
2	Y	106	GLY	4.2
3	P	207	VAL	4.2
3	T	214	THR	4.2
2	Y	41	TYR	4.2
2	a	161	GLN	4.2
2	a	181	SER	4.2
3	Z	122	SER	4.2
2	Y	122	ILE	4.2
2	a	160	ARG	4.2
3	T	138	CYS	4.2
1	B	135	ALA	4.1
3	R	150	CYS	4.1
3	T	205	CYS	4.1
1	A	139	ASP	4.1
1	E	134	VAL	4.1
3	V	162	LEU	4.1
3	Z	205	CYS	4.1
2	a	186	LEU	4.1
2	Y	163	GLY	4.1
2	a	162	ASN	4.1
1	H	140	THR	4.1
3	N	165	ASN	4.1
3	b	207	VAL	4.0
2	U	118	PRO	4.0
1	A	134	VAL	4.0
3	Z	187	LEU	4.0
3	T	146	VAL	4.0
3	N	136	PRO	4.0
3	b	146	VAL	4.0
3	Z	180	LEU	4.0
3	Z	194	THR	4.0
1	J	133	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
3	V	160	VAL	4.0
1	C	87	ASP	4.0
3	Z	16	GLY	3.9
1	B	179	THR	3.9
1	C	179	THR	3.9
3	T	160	VAL	3.9
1	A	350	SER	3.9
3	T	131	VAL	3.9
2	a	165	LEU	3.9
3	b	201	GLN	3.9
3	b	164	TRP	3.9
3	Z	138	CYS	3.9
3	Z	208	ALA	3.9
2	Y	174	LYS	3.9
3	Z	219	LYS	3.9
3	V	161	THR	3.9
3	V	203	ILE	3.9
3	Z	127	THR	3.9
1	A	175	SER	3.9
2	M	197	TYR	3.9
3	b	167	GLY	3.9
2	a	139	CYS	3.9
3	Z	123	SER	3.8
2	Y	115	ASP	3.8
3	b	170	SER	3.8
3	Z	169	LEU	3.8
3	Z	159	PRO	3.8
2	Y	162	ASN	3.8
2	Q	112	LYS	3.8
1	E	56	GLY	3.8
3	b	168	SER	3.8
3	b	171	SER	3.8
3	Z	196	ASN	3.8
2	U	158	SER	3.8
2	Y	155	ILE	3.8
2	a	206	SER	3.8
2	a	135	ALA	3.7
2	a	125	PRO	3.7
3	X	203	ILE	3.7
3	Z	151	LEU	3.7
1	A	135	ALA	3.7
1	G	57	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
3	V	156	PHE	3.7
1	B	177	PRO	3.7
3	Z	165	ASN	3.7
3	b	214	THR	3.7
1	C	177	PRO	3.7
3	Z	137	VAL	3.7
1	D	57	ASN	3.7
3	T	213	SER	3.7
1	B	139	ASP	3.7
3	Z	220	ILE	3.7
1	G	134	VAL	3.7
2	S	124	PRO	3.6
3	b	180	LEU	3.6
3	Z	15	GLY	3.6
3	Z	11	LEU	3.6
1	G	86	PRO	3.6
3	P	208	ALA	3.6
3	T	142	THR	3.6
3	T	192	THR	3.6
3	N	137	VAL	3.6
3	Z	130	SER	3.6
3	b	122	SER	3.6
3	T	151	LEU	3.6
2	M	213	SER	3.6
2	Y	119	THR	3.6
1	E	90	VAL	3.6
1	E	135	ALA	3.6
2	c	162	ASN	3.6
3	V	207	VAL	3.6
3	Z	218	LYS	3.6
2	M	155	ILE	3.6
1	C	86	PRO	3.5
1	H	179	THR	3.5
2	M	199	CYS	3.5
2	a	137	VAL	3.5
3	T	210	PRO	3.5
2	U	139	CYS	3.5
3	Z	199	PRO	3.5
2	M	204	LYS	3.5
2	a	11	LEU	3.5
3	V	191	VAL	3.5
1	A	177	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	a	189	ASP	3.5
2	O	204	LYS	3.5
1	D	140	THR	3.5
3	P	192	THR	3.5
3	T	135	ALA	3.5
3	b	191	VAL	3.5
1	H	85	LEU	3.5
3	N	140	GLY	3.5
2	a	169	THR	3.5
2	O	113	ARG	3.5
1	H	178	THR	3.4
3	b	133	PRO	3.4
3	Z	22	CYS	3.4
3	N	134	LEU	3.4
2	a	207	THR	3.4
2	U	120	VAL	3.4
3	N	198	TRP	3.4
2	a	204	LYS	3.4
2	a	15	LEU	3.4
3	Z	203	ILE	3.4
2	a	101	PHE	3.4
3	b	140	GLY	3.4
2	Y	14	SER	3.4
1	C	350	SER	3.4
3	X	141	THR	3.4
2	c	148	ASP	3.4
2	U	19	ALA	3.4
2	S	215	ASN	3.4
3	Z	154	GLY	3.4
1	E	179	THR	3.4
1	G	350	SER	3.4
3	P	200	SER	3.4
2	K	142	ASN	3.3
3	T	204	THR	3.3
3	Z	175	THR	3.3
2	Y	114	ALA	3.3
1	J	352	ILE	3.3
2	a	197	TYR	3.3
1	F	179	THR	3.3
1	J	350	SER	3.3
3	R	203	ILE	3.3
1	J	179	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	N	130	SER	3.3
2	S	200	GLU	3.3
3	Z	202	THR	3.3
3	Z	173	VAL	3.3
3	N	168	SER	3.3
3	V	126	THR	3.3
3	Z	139	GLY	3.3
2	a	152	LYS	3.3
3	b	173	VAL	3.3
2	Q	159	GLU	3.3
3	L	207	VAL	3.3
3	Z	197	THR	3.3
3	b	175	THR	3.3
2	S	203	HIS	3.3
2	Y	141	LEU	3.3
2	Y	153	TRP	3.3
2	Y	133	GLY	3.3
2	a	61	SER	3.2
3	T	198	TRP	3.2
3	Z	145	SER	3.2
1	I	87	ASP	3.2
1	E	85	LEU	3.2
1	D	179	THR	3.2
3	R	144	SER	3.2
1	D	141	LYS	3.2
3	T	212	SER	3.2
3	T	127	THR	3.2
1	F	133	HIS	3.2
3	V	148	LEU	3.2
2	S	201	ALA	3.2
2	Y	91	TYR	3.2
1	B	95	SER	3.2
3	T	189	SER	3.2
2	M	139	CYS	3.2
1	G	135	ALA	3.2
2	Y	1	ASP	3.2
2	Y	215	ASN	3.2
3	T	194	THR	3.2
2	U	203	HIS	3.1
3	Z	207	VAL	3.1
2	U	191	TYR	3.1
2	M	148	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	Y	210	ILE	3.1
1	I	57	ASN	3.1
2	S	137	VAL	3.1
2	U	121	SER	3.1
3	V	149	GLY	3.1
3	N	202	THR	3.1
3	Z	23	ALA	3.1
2	Y	78	LEU	3.1
3	R	219	LYS	3.1
2	Y	117	ALA	3.1
2	Y	152	LYS	3.1
1	I	56	GLY	3.1
2	Y	18	GLN	3.1
2	U	155	ILE	3.1
2	K	210	ILE	3.1
1	J	139	ASP	3.1
3	Z	46	GLU	3.1
3	Z	215	LYS	3.1
2	Y	11	LEU	3.1
3	V	211	ALA	3.1
2	c	161	GLN	3.1
3	Z	140	GLY	3.1
2	Y	88	LEU	3.1
2	O	162	ASN	3.0
2	M	158	SER	3.0
2	U	175	ASP	3.0
2	S	218	GLU	3.0
2	Y	213	SER	3.0
2	S	212	LYS	3.0
2	c	153	TRP	3.0
2	O	207	THR	3.0
2	c	218	GLU	3.0
2	Y	203	HIS	3.0
3	T	143	GLY	3.0
2	O	83	VAL	3.0
3	Z	119	VAL	3.0
3	V	169	LEU	3.0
1	C	84	GLY	3.0
3	Z	204	THR	3.0
2	Q	155	ILE	3.0
3	P	203	ILE	3.0
3	L	162	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	87	ASP	3.0
2	Y	172	ASP	3.0
1	B	351	SER	3.0
3	P	139	GLY	3.0
3	V	202	THR	3.0
1	E	139	ASP	3.0
1	H	350	SER	3.0
2	M	149	ILE	3.0
1	A	85	LEU	3.0
2	U	14	SER	3.0
3	d	148	LEU	3.0
2	Q	111	LEU	3.0
3	T	196	ASN	3.0
2	a	185	THR	3.0
2	M	186	LEU	2.9
2	c	201	ALA	2.9
2	a	19	ALA	2.9
2	a	142	ASN	2.9
2	a	163	GLY	2.9
3	P	205	CYS	2.9
1	B	350	SER	2.9
2	S	210	ILE	2.9
2	a	183	THR	2.9
3	N	207	VAL	2.9
2	Y	17	ASP	2.9
3	X	218	LYS	2.9
2	a	157	GLY	2.9
1	C	57	ASN	2.9
2	Y	158	SER	2.9
3	R	201	GLN	2.9
3	P	137	VAL	2.9
2	Y	200	GLU	2.9
1	G	87	ASP	2.9
2	Y	21	ILE	2.9
3	b	152	VAL	2.9
3	Z	80	TYR	2.9
3	Z	132	TYR	2.9
3	N	141	THR	2.9
1	E	86	PRO	2.9
1	G	175	SER	2.9
2	U	206	SER	2.9
3	P	202	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	116	GLY	2.9
1	G	90	VAL	2.9
1	F	136	SER	2.9
1	J	175	SER	2.9
3	P	17	SER	2.9
1	A	140	THR	2.9
2	a	205	THR	2.9
2	U	111	LEU	2.9
2	a	41	TYR	2.9
2	S	128	GLU	2.9
3	Z	189	SER	2.9
1	C	349	THR	2.9
2	O	109	LEU	2.9
3	L	86	LEU	2.9
3	P	148	LEU	2.9
3	T	207	VAL	2.9
1	D	175	SER	2.9
3	N	196	ASN	2.9
3	Z	20	LEU	2.9
3	N	167	GLY	2.9
3	b	188	SER	2.8
2	M	157	GLY	2.8
2	U	81	SER	2.8
2	a	200	GLU	2.8
3	d	125	LYS	2.8
1	D	135	ALA	2.8
2	a	215	ASN	2.8
2	a	119	THR	2.8
2	Y	138	VAL	2.8
1	G	89	THR	2.8
2	Y	80	ILE	2.8
3	Z	5	VAL	2.8
3	Z	96	CYS	2.8
1	G	351	SER	2.8
2	M	214	PHE	2.8
3	b	147	THR	2.8
3	R	205	CYS	2.8
1	I	174	ALA	2.8
2	S	175	ASP	2.8
2	O	157	GLY	2.8
2	U	153	TRP	2.8
3	R	193	VAL	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	138	VAL	2.8
2	a	190	GLU	2.8
2	a	170	ASP	2.8
1	I	176	LYS	2.8
3	T	166	SER	2.8
3	X	169	LEU	2.8
2	Y	107	THR	2.8
3	N	219	LYS	2.8
2	M	200	GLU	2.7
3	P	170	SER	2.7
2	O	218	GLU	2.7
3	b	151	LEU	2.7
2	O	116	ALA	2.7
2	a	166	ASN	2.7
1	A	87	ASP	2.7
2	Y	16	GLY	2.7
3	Z	131	VAL	2.7
3	V	139	GLY	2.7
2	U	201	ALA	2.7
2	S	206	SER	2.7
3	T	148	LEU	2.7
2	O	198	THR	2.7
2	U	1	ASP	2.7
3	V	142	THR	2.7
1	I	181	VAL	2.7
2	Y	130	LEU	2.7
3	R	202	THR	2.7
1	D	176	LYS	2.7
3	b	199	PRO	2.7
3	Z	111	ASP	2.7
3	Z	164	TRP	2.7
3	N	192	THR	2.7
3	Z	12	VAL	2.7
1	H	89	THR	2.7
3	T	180	LEU	2.7
2	Y	68	SER	2.6
2	M	209	PRO	2.6
3	T	129	PRO	2.6
2	c	159	GLU	2.6
3	Z	84	SER	2.6
2	Y	170	ASP	2.6
3	Z	133	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	S	120	VAL	2.6
3	P	191	VAL	2.6
1	J	85	LEU	2.6
1	C	174	ALA	2.6
2	U	113	ARG	2.6
1	D	86	PRO	2.6
2	U	83	VAL	2.6
3	V	131	VAL	2.6
3	b	8	GLY	2.6
2	O	197	TYR	2.6
3	T	209	HIS	2.6
2	c	210	ILE	2.6
2	S	199	CYS	2.6
2	Y	7	THR	2.6
3	V	212	SER	2.6
3	X	171	SER	2.6
2	Q	151	VAL	2.6
2	c	204	LYS	2.6
3	Z	143	GLY	2.6
1	J	86	PRO	2.6
2	S	193	ARG	2.6
2	M	160	ARG	2.6
2	c	206	SER	2.6
2	U	189	ASP	2.6
2	U	91	TYR	2.5
3	Z	172	GLY	2.5
2	Q	175	ASP	2.5
3	V	163	THR	2.5
3	X	205	CYS	2.5
2	a	105	ALA	2.5
3	d	189	SER	2.5
3	V	189	SER	2.5
2	Q	162	ASN	2.5
2	S	127	SER	2.5
3	N	220	ILE	2.5
2	S	187	THR	2.5
2	M	191	TYR	2.5
3	b	196	ASN	2.5
3	R	27	PHE	2.5
2	Y	194	HIS	2.5
2	a	18	GLN	2.5
3	N	169	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	b	217	ASP	2.5
3	b	132	TYR	2.5
1	G	83	PHE	2.5
1	G	172	GLY	2.5
3	X	162	LEU	2.5
1	D	139	ASP	2.5
2	U	194	HIS	2.5
3	d	201	GLN	2.5
2	S	214	PHE	2.5
2	a	117	ALA	2.5
3	L	169	LEU	2.5
3	N	12	VAL	2.5
2	Q	154	LYS	2.5
1	G	173	THR	2.5
3	b	126	THR	2.5
2	M	120	VAL	2.5
2	a	116	ALA	2.5
2	a	191	TYR	2.5
3	d	162	LEU	2.5
3	d	169	LEU	2.5
2	O	115	ASP	2.5
2	M	211	VAL	2.5
1	C	176	LYS	2.5
2	M	14	SER	2.5
1	J	100	TRP	2.4
1	I	20	LYS	2.4
3	b	12	VAL	2.4
3	b	218	LYS	2.4
1	J	135	ALA	2.4
3	b	136	PRO	2.4
1	H	176	LYS	2.4
2	S	132	SER	2.4
2	a	141	LEU	2.4
2	U	211	VAL	2.4
3	b	160	VAL	2.4
3	b	138	CYS	2.4
1	I	350	SER	2.4
3	X	207	VAL	2.4
2	Q	158	SER	2.4
3	Z	85	SER	2.4
2	U	116	ALA	2.4
2	S	159	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	161	THR	2.4
3	P	216	VAL	2.4
3	N	152	VAL	2.4
3	d	193	VAL	2.4
2	Y	173	SER	2.4
3	P	213	SER	2.4
2	S	138	VAL	2.4
3	Z	190	SER	2.4
1	C	135	ALA	2.4
1	B	354	ASN	2.4
3	T	197	THR	2.4
3	V	159	PRO	2.4
3	Z	24	ALA	2.4
1	C	175	SER	2.4
3	V	137	VAL	2.4
1	E	381	LYS	2.4
3	P	131	VAL	2.4
3	T	122	SER	2.4
1	I	179	THR	2.4
2	M	107	THR	2.4
2	W	175	ASP	2.4
2	U	212	LYS	2.4
2	Y	110	GLU	2.3
3	T	136	PRO	2.3
3	Z	184	LEU	2.3
3	d	161	THR	2.3
2	O	153	TRP	2.3
3	V	124	ALA	2.3
1	B	57	ASN	2.3
2	Y	160	ARG	2.3
2	M	150	ASN	2.3
2	M	175	ASP	2.3
2	M	189	ASP	2.3
2	Y	113	ARG	2.3
3	V	213	SER	2.3
3	X	168	SER	2.3
3	b	157	PRO	2.3
2	O	161	GLN	2.3
3	V	135	ALA	2.3
3	b	169	LEU	2.3
3	N	5	VAL	2.3
3	R	139	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	T	130	SER	2.3
2	Q	152	LYS	2.3
3	P	201	GLN	2.3
1	B	176	LYS	2.3
3	L	175	THR	2.3
3	b	111	ASP	2.3
3	V	125	LYS	2.3
1	E	83	PHE	2.3
2	a	143	ASN	2.3
3	Z	68	PHE	2.3
3	b	206	ASN	2.3
3	b	183	GLY	2.3
1	E	176	LYS	2.3
2	c	186	LEU	2.3
2	U	109	LEU	2.3
3	L	148	LEU	2.3
3	Z	212	SER	2.3
3	b	86	LEU	2.3
2	Q	18	GLN	2.3
3	N	147	THR	2.3
3	Z	186	THR	2.3
2	a	80	ILE	2.3
1	E	180	VAL	2.3
2	S	140	PHE	2.3
3	X	195	SER	2.3
3	P	13	LYS	2.3
3	P	19	LYS	2.3
2	U	159	GLU	2.3
1	J	176	LYS	2.3
2	S	151	VAL	2.3
2	a	167	SER	2.3
3	T	200	SER	2.3
2	U	200	GLU	2.2
3	P	140	GLY	2.2
2	Q	160	ARG	2.2
2	S	141	LEU	2.2
3	P	204	THR	2.2
3	X	216	VAL	2.2
2	Q	13	VAL	2.2
3	V	157	PRO	2.2
3	P	9	GLY	2.2
3	P	171	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	LYS	2.2
2	O	112	LYS	2.2
2	Y	52	LEU	2.2
1	B	56	GLY	2.2
2	O	159	GLU	2.2
3	N	132	TYR	2.2
3	V	198	TRP	2.2
3	b	209	HIS	2.2
2	S	131	THR	2.2
2	Y	166	ASN	2.2
2	M	201	ALA	2.2
2	a	106	GLY	2.2
3	N	11	LEU	2.2
2	S	196	SER	2.2
3	Z	195	SER	2.2
3	b	212	SER	2.2
2	U	122	ILE	2.2
2	c	1	ASP	2.2
2	Y	79	LYS	2.2
1	F	86	PRO	2.2
2	U	16	GLY	2.2
2	S	207	THR	2.2
2	U	217	ASN	2.2
3	P	169	LEU	2.2
3	d	150	CYS	2.2
3	N	166	SER	2.2
2	Y	197	TYR	2.2
1	A	97	ARG	2.2
2	a	67	PHE	2.2
1	H	180	VAL	2.2
1	D	87	ASP	2.2
1	G	139	ASP	2.2
2	M	118	PRO	2.2
3	P	151	LEU	2.2
1	E	88	ASN	2.2
1	B	138	VAL	2.2
1	D	84	GLY	2.2
1	J	66	SER	2.2
2	a	52	LEU	2.2
3	P	189	SER	2.2
1	I	180	VAL	2.2
2	Y	217	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	b	9	GLY	2.2
1	H	351	SER	2.2
2	Y	192	GLU	2.2
1	A	89	THR	2.2
3	d	196	ASN	2.2
3	X	142	THR	2.2
3	Z	174	HIS	2.2
1	F	351	SER	2.1
3	Z	201	GLN	2.1
2	O	199	CYS	2.1
3	Z	83	MET	2.1
2	O	107	THR	2.1
2	M	207	THR	2.1
3	T	206	ASN	2.1
1	G	141	LYS	2.1
1	G	176	LYS	2.1
3	N	139	GLY	2.1
2	M	198	THR	2.1
3	X	144	SER	2.1
2	a	175	ASP	2.1
1	A	88	ASN	2.1
1	F	352	ILE	2.1
2	S	149	ILE	2.1
3	Z	63	THR	2.1
3	Z	69	THR	2.1
1	C	439	GLN	2.1
2	S	82	ARG	2.1
2	M	20	SER	2.1
2	U	112	LYS	2.1
3	T	199	PRO	2.1
1	C	89	THR	2.1
1	C	444	LYS	2.1
3	Z	14	PRO	2.1
3	V	152	VAL	2.1
2	O	150	ASN	2.1
2	U	157	GLY	2.1
3	V	134	LEU	2.1
3	L	131	VAL	2.1
2	O	186	LEU	2.1
2	S	52	LEU	2.1
3	P	20	LEU	2.1
3	P	198	TRP	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	36	THR	2.1
3	L	129	PRO	2.1
2	S	181	SER	2.1
2	M	21	ILE	2.1
1	E	84	GLY	2.1
2	Y	104	GLY	2.1
2	U	204	LYS	2.1
3	d	215	LYS	2.1
3	P	162	LEU	2.1
2	S	150	ASN	2.1
3	X	165	ASN	2.1
1	I	187	PRO	2.1
3	X	160	VAL	2.1
3	N	213	SER	2.1
2	Y	108	LYS	2.0
3	V	215	LYS	2.0
3	V	119	VAL	2.0
3	Z	163	THR	2.0
3	Z	171	SER	2.0
3	V	12	VAL	2.0
1	G	88	ASN	2.0
2	U	80	ILE	2.0
3	N	133	PRO	2.0
2	S	170	ASP	2.0
2	M	182	SER	2.0
2	Y	137	VAL	2.0
3	b	134	LEU	2.0
3	b	156	PHE	2.0
2	Y	22	SER	2.0
1	F	138	VAL	2.0
2	Y	30	VAL	2.0
2	Y	204	LYS	2.0
2	U	216	ARG	2.0
1	I	349	THR	2.0
3	N	142	THR	2.0
1	J	189	GLU	2.0
2	O	1	ASP	2.0
2	S	1	ASP	2.0
1	G	84	GLY	2.0
3	X	143	GLY	2.0
2	M	159	GLU	2.0
2	M	205	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	V	127	THR	2.0
3	X	197	THR	2.0
3	L	132	TYR	2.0

## 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.