



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 01:44 PM EDT

PDB ID : 6NCA  
Title : HLA-A2 (A\*02:01) bound to a peptide from the Epstein-Barr virus BRLF1 protein  
Authors : Stern, L.J.; Selin, L.K.; Song, I.Y.  
Deposited on : 2018-12-11  
Resolution : 3.30 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)

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>.

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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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

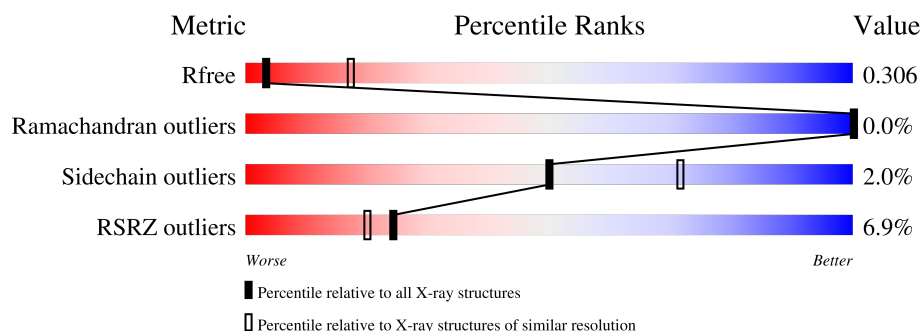
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	164625	1085 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	1	9	
1	2	9	
1	3	9	
1	4	9	
1	5	9	
1	6	9	

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Mol	Chain	Length	Quality of chain
1	7	9	<div> <div>44%</div> <div>100%</div> </div>
1	8	9	<div> <div>22%</div> <div>89%</div> <div>11%</div> </div>
1	U	9	<div> <div>100%</div> </div>
1	V	9	<div> <div>11%</div> <div>89%</div> <div>11%</div> </div>
1	W	9	<div> <div>22%</div> <div>100%</div> </div>
1	X	9	<div> <div>22%</div> <div>100%</div> </div>
1	Y	9	<div> <div>11%</div> <div>100%</div> </div>
1	Z	9	<div> <div>100%</div> </div>
1	u	9	<div> <div>11%</div> <div>100%</div> </div>
1	v	9	<div> <div>100%</div> </div>
1	w	9	<div> <div>22%</div> <div>100%</div> </div>
1	x	9	<div> <div>11%</div> <div>100%</div> </div>
1	y	9	<div> <div>11%</div> <div>89%</div> <div>11%</div> </div>
1	z	9	<div> <div>11%</div> <div>100%</div> </div>
2	A	275	<div> <div>5%</div> <div>98%</div> </div>
2	B	275	<div> <div>7%</div> <div>99%</div> </div>
2	C	275	<div> <div>12%</div> <div>99%</div> </div>
2	D	275	<div> <div>4%</div> <div>97%</div> </div>
2	E	275	<div> <div>12%</div> <div>99%</div> </div>
2	F	275	<div> <div>9%</div> <div>97%</div> </div>
2	G	275	<div> <div>7%</div> <div>98%</div> </div>
2	H	275	<div> <div>4%</div> <div>97%</div> </div>
2	I	275	<div> <div>4%</div> <div>99%</div> </div>
2	J	275	<div> <div>2%</div> <div>98%</div> </div>
2	K	275	<div> <div>7%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	275	
2	M	275	
2	N	275	
2	O	275	
2	P	275	
2	Q	275	
2	R	275	
2	S	275	
2	T	275	
3	a	100	
3	b	100	
3	c	100	
3	d	100	
3	e	100	
3	f	100	
3	g	100	
3	h	100	
3	i	100	
3	j	100	
3	k	100	
3	l	100	
3	m	100	
3	n	100	
3	o	100	
3	p	100	

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Mol	Chain	Length	Quality of chain
3	q	100	<div><div></div><div>17%</div><div></div><div>98%</div><div></div></div>
3	r	100	<div><div></div><div>6%</div><div></div><div>99%</div><div></div></div>
3	s	100	<div><div></div><div>3%</div><div></div><div>95%</div><div>5%</div></div>
3	t	100	<div><div></div><div>%</div><div></div><div>98%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 63200 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 Replication and transcription activator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Y	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	u	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	z	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	y	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	8	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	w	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	4	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	3	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	W	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	6	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	x	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	5	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	X	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	v	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	2	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	U	9	Total	C	N	O	0	0	0
			76	52	11	13			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Z	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	V	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	7	9	Total	C	N	O	0	0	0
			76	52	11	13			
1	1	9	Total	C	N	O	0	0	0
			76	52	11	13			

- Molecule 2 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	B	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	C	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	D	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	E	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	F	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	G	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	H	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	S	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			
2	J	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	K	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	L	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			
2	M	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	N	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	O	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	Q	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	R	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	I	275	Total	C	N	O	S	21	0	0
			2247	1403	409	426	9			
2	T	275	Total	C	N	O	S	17	0	0
			2247	1403	409	426	9			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	b	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	c	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	d	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	f	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	g	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	h	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	s	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	j	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	k	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	l	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	m	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	n	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			
3	o	100	Total	C	N	O	S	5	0	0
			837	533	141	159	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	p	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	q	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	r	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	i	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	t	100	Total 837	C 533	N 141	O 159	S 4	5	0	0
3	e	100	Total 837	C 533	N 141	O 159	S 4	5	0	0

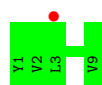
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	-	initiating methionine	UNP P61769
b	1	MET	-	initiating methionine	UNP P61769
c	1	MET	-	initiating methionine	UNP P61769
d	1	MET	-	initiating methionine	UNP P61769
f	1	MET	-	initiating methionine	UNP P61769
g	1	MET	-	initiating methionine	UNP P61769
h	1	MET	-	initiating methionine	UNP P61769
s	1	MET	-	initiating methionine	UNP P61769
j	1	MET	-	initiating methionine	UNP P61769
k	1	MET	-	initiating methionine	UNP P61769
l	1	MET	-	initiating methionine	UNP P61769
m	1	MET	-	initiating methionine	UNP P61769
n	1	MET	-	initiating methionine	UNP P61769
o	1	MET	-	initiating methionine	UNP P61769
p	1	MET	-	initiating methionine	UNP P61769
q	1	MET	-	initiating methionine	UNP P61769
r	1	MET	-	initiating methionine	UNP P61769
i	1	MET	-	initiating methionine	UNP P61769
t	1	MET	-	initiating methionine	UNP P61769
e	1	MET	-	initiating methionine	UNP P61769

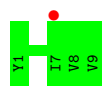
### 3 Residue-property plots

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.

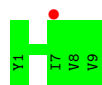
- Molecule 1: Replication and transcription activator



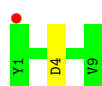
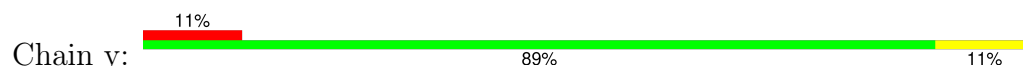
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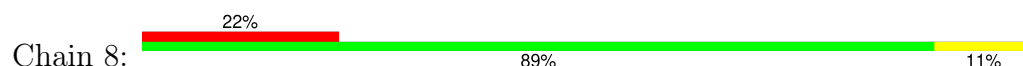
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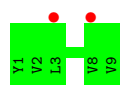
- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator

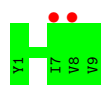


- Molecule 1: Replication and transcription activator

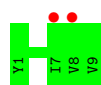


There are no outlier residues recorded for this chain.

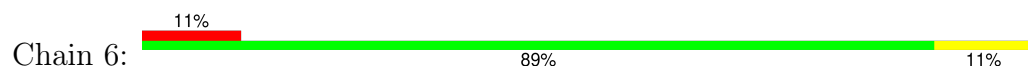
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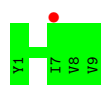
- Molecule 1: Replication and transcription activator



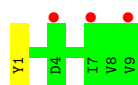
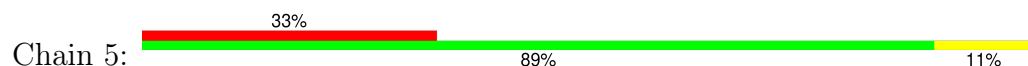
- Molecule 1: Replication and transcription activator



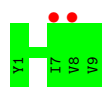
- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator



There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator



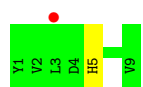
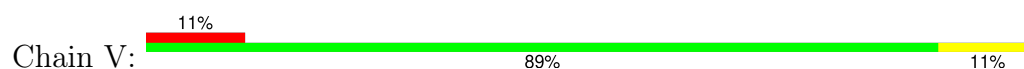
There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

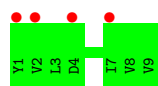
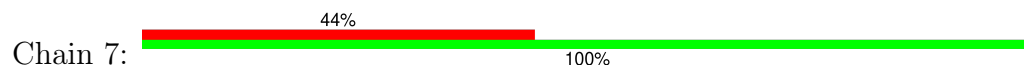


There are no outlier residues recorded for this chain.

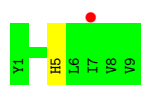
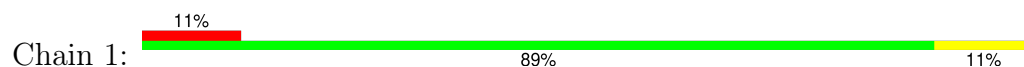
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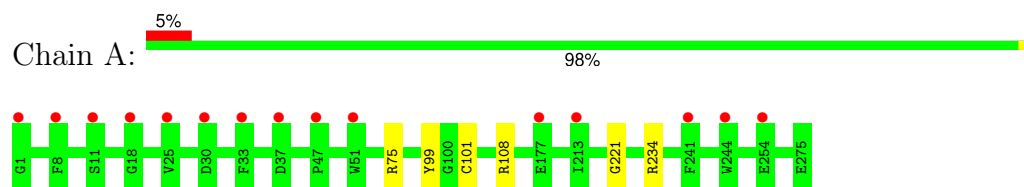
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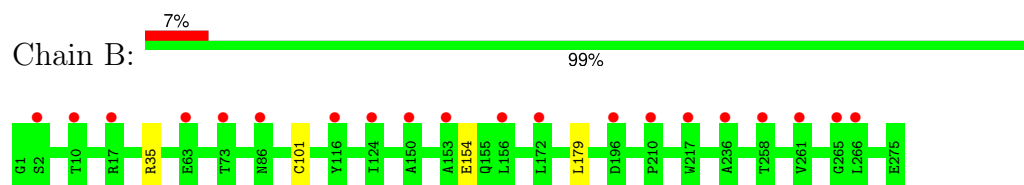
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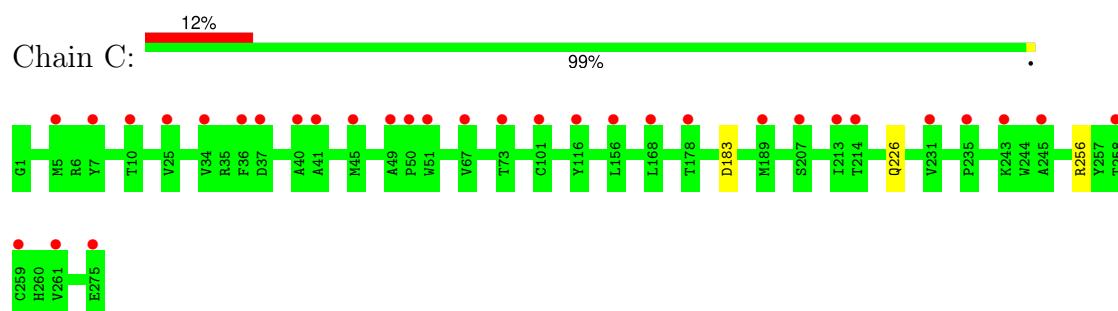
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



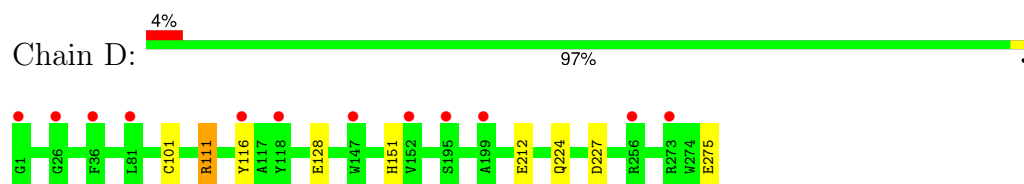
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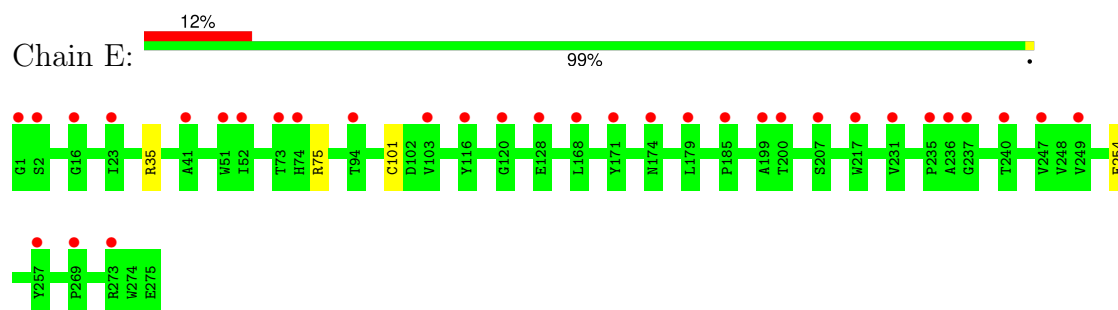
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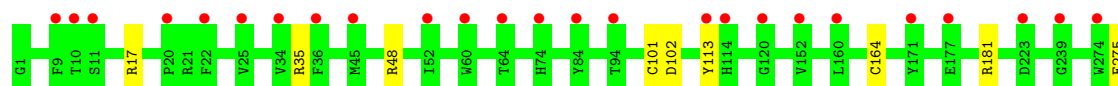


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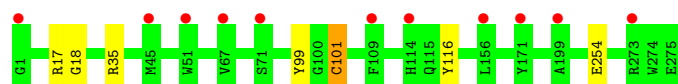




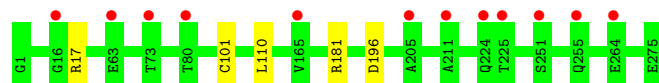
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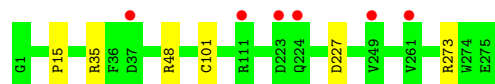
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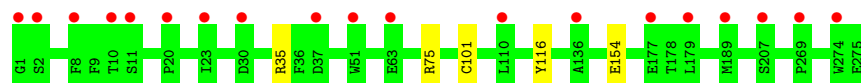
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



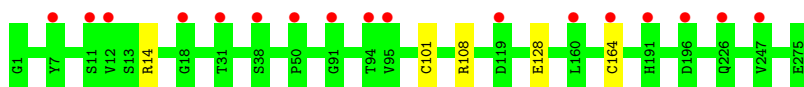
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



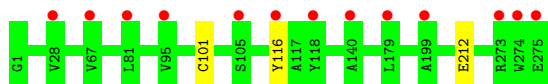
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



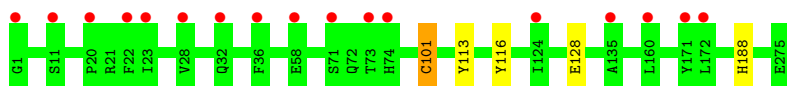
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



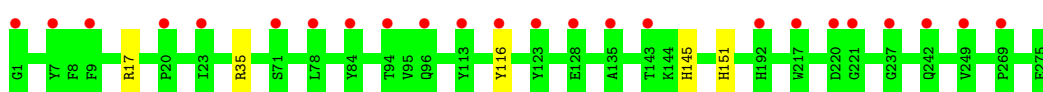
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



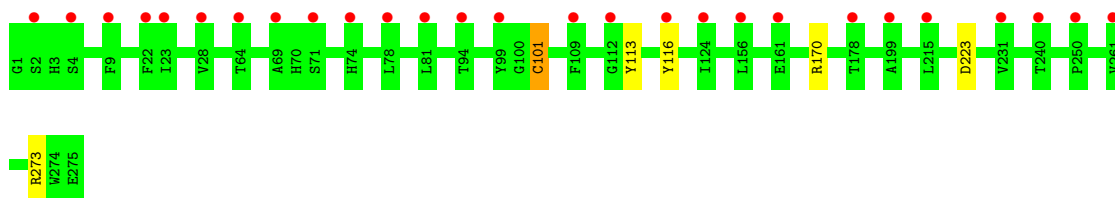
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

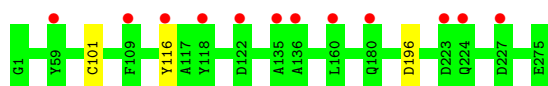


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

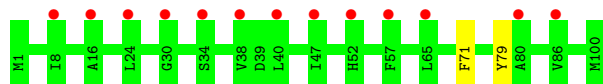




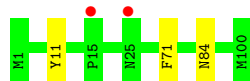
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



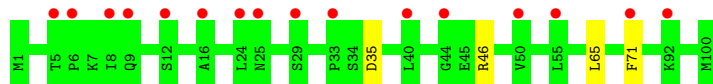
- Molecule 3: Beta-2-microglobulin



- Molecule 3: Beta-2-microglobulin



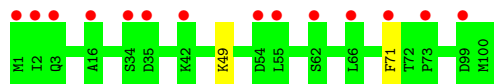
- Molecule 3: Beta-2-microglobulin



- Molecule 3: Beta-2-microglobulin

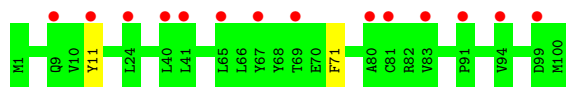


- Molecule 3: Beta-2-microglobulin

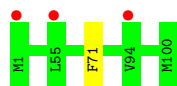


- Molecule 3: Beta-2-microglobulin





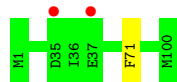
- Molecule 3: Beta-2-microglobulin



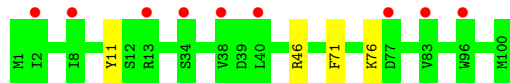
- Molecule 3: Beta-2-microglobulin



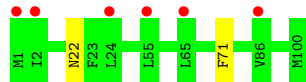
- Molecule 3: Beta-2-microglobulin



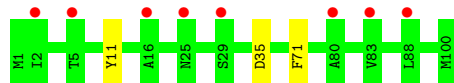
- Molecule 3: Beta-2-microglobulin



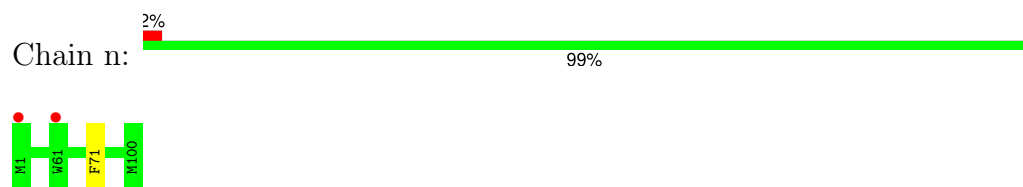
- Molecule 3: Beta-2-microglobulin



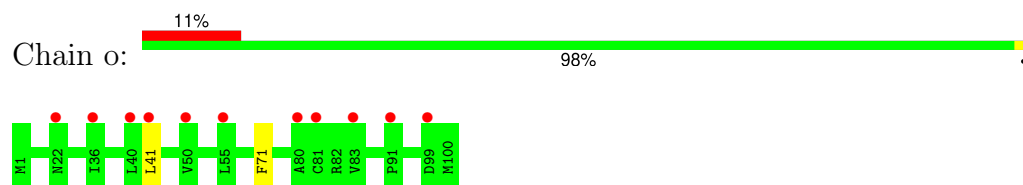
- Molecule 3: Beta-2-microglobulin



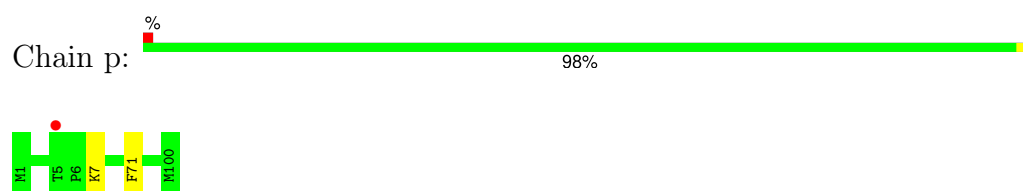
## ● Molecule 3: Beta-2-microglobulin



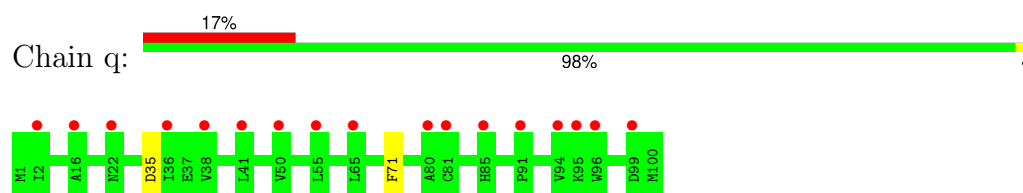
## ● Molecule 3: Beta-2-microglobulin



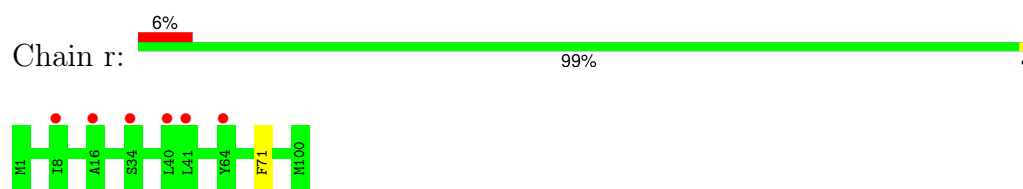
## ● Molecule 3: Beta-2-microglobulin



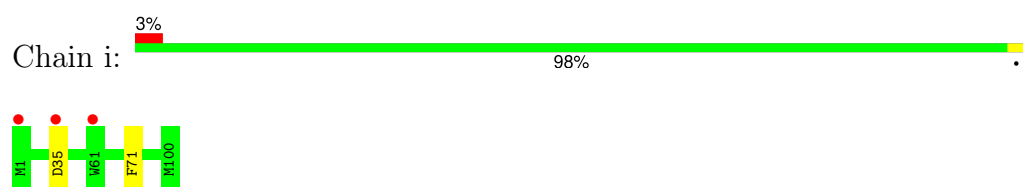
## ● Molecule 3: Beta-2-microglobulin



## ● Molecule 3: Beta-2-microglobulin

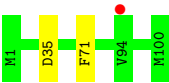


## ● Molecule 3: Beta-2-microglobulin

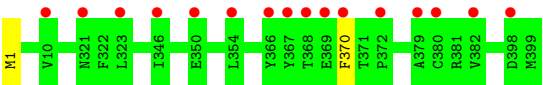


## ● Molecule 3: Beta-2-microglobulin





● Molecule 3: Beta-2-microglobulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.91Å 100.17Å 292.41Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	111.42 – 3.30 111.42 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (111.42-3.30) 92.6 (111.42-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.285 , 0.303 0.285 , 0.306	Depositor DCC
$R_{free}$ test set	164152 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtrriage
Anisotropy	0.437	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	63200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7800e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	1	0.22	0/77	0.57	0/104
1	2	0.21	0/77	0.49	0/104
1	3	0.24	0/77	0.58	0/104
1	4	0.25	0/77	0.54	0/104
1	5	0.30	0/77	0.69	0/104
1	6	0.27	0/77	0.69	0/104
1	7	0.23	0/77	0.54	0/104
1	8	0.22	0/77	0.64	0/104
1	U	0.21	0/77	0.57	0/104
1	V	0.24	0/77	0.75	0/104
1	W	0.20	0/77	0.52	0/104
1	X	0.21	0/77	0.55	0/104
1	Y	0.19	0/77	0.55	0/104
1	Z	0.24	0/77	0.61	0/104
1	u	0.21	0/77	0.48	0/104
1	v	0.26	0/77	0.59	0/104
1	w	0.24	0/77	0.66	0/104
1	x	0.23	0/77	0.48	0/104
1	y	0.22	0/77	0.50	0/104
1	z	0.20	0/77	0.52	0/104
2	A	0.30	0/2312	0.54	1/3137 (0.0%)
2	B	0.25	0/2312	0.48	0/3137
2	C	0.27	0/2312	0.50	0/3137
2	D	0.26	0/2312	0.49	0/3137
2	E	0.25	0/2312	0.48	0/3137
2	F	0.26	0/2312	0.51	1/3137 (0.0%)
2	G	0.25	0/2312	0.49	0/3137
2	H	0.25	0/2312	0.51	1/3137 (0.0%)
2	I	0.24	0/2312	0.49	0/3137
2	J	0.25	0/2312	0.49	0/3137
2	K	0.26	0/2312	0.51	0/3137
2	L	0.25	0/2312	0.48	0/3137
2	M	0.25	0/2312	0.50	1/3137 (0.0%)
2	N	0.25	0/2312	0.50	0/3137

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	O	0.25	0/2312	0.51	0/3137
2	P	0.25	0/2312	0.50	1/3137 (0.0%)
2	Q	0.26	0/2312	0.48	0/3137
2	R	0.26	0/2312	0.51	1/3137 (0.0%)
2	S	0.24	0/2312	0.49	0/3137
2	T	0.24	0/2312	0.48	0/3137
3	a	0.26	0/860	0.51	0/1162
3	b	0.26	0/860	0.50	0/1162
3	c	0.25	0/860	0.57	1/1162 (0.1%)
3	d	0.26	0/860	0.50	0/1162
3	e	0.24	0/860	0.47	0/1162
3	f	0.24	0/860	0.51	0/1162
3	g	0.25	0/860	0.50	0/1162
3	h	0.25	0/860	0.49	0/1162
3	i	0.25	0/860	0.49	0/1162
3	j	0.26	0/860	0.49	0/1162
3	k	0.26	0/860	0.51	0/1162
3	l	0.25	0/860	0.48	0/1162
3	m	0.25	0/860	0.47	0/1162
3	n	0.24	0/860	0.48	0/1162
3	o	0.25	0/860	0.50	0/1162
3	p	0.25	0/860	0.49	0/1162
3	q	0.25	0/860	0.51	0/1162
3	r	0.24	0/860	0.48	0/1162
3	s	0.25	0/860	0.50	0/1162
3	t	0.26	0/860	0.49	0/1162
All	All	0.25	0/64980	0.50	7/88060 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	65	LEU	CB-CG-CD2	-6.77	99.50	111.00
2	A	75	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	P	101	CYS	CA-CB-SG	-5.19	104.67	114.00
2	H	101	CYS	CA-CB-SG	-5.17	104.70	114.00
2	M	164	CYS	CA-CB-SG	-5.11	104.80	114.00
2	F	164	CYS	CA-CB-SG	-5.07	104.87	114.00
2	R	101	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	7/9 (78%)	7 (100%)	0	0	100	100
1	2	7/9 (78%)	7 (100%)	0	0	100	100
1	3	7/9 (78%)	7 (100%)	0	0	100	100
1	4	7/9 (78%)	7 (100%)	0	0	100	100
1	5	7/9 (78%)	7 (100%)	0	0	100	100
1	6	7/9 (78%)	7 (100%)	0	0	100	100
1	7	7/9 (78%)	7 (100%)	0	0	100	100
1	8	7/9 (78%)	7 (100%)	0	0	100	100
1	U	7/9 (78%)	7 (100%)	0	0	100	100
1	V	7/9 (78%)	7 (100%)	0	0	100	100
1	W	7/9 (78%)	7 (100%)	0	0	100	100
1	X	7/9 (78%)	7 (100%)	0	0	100	100
1	Y	7/9 (78%)	7 (100%)	0	0	100	100
1	Z	7/9 (78%)	7 (100%)	0	0	100	100
1	u	7/9 (78%)	7 (100%)	0	0	100	100
1	v	7/9 (78%)	7 (100%)	0	0	100	100
1	w	7/9 (78%)	7 (100%)	0	0	100	100
1	x	7/9 (78%)	7 (100%)	0	0	100	100
1	y	7/9 (78%)	7 (100%)	0	0	100	100
1	z	7/9 (78%)	7 (100%)	0	0	100	100
2	A	273/275 (99%)	262 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	C	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	D	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	E	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
2	F	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	G	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	H	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	61
2	I	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	J	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	61
2	K	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	L	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	61
2	M	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	N	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	O	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	P	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	Q	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	R	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
2	S	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	T	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
3	a	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	b	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	c	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	d	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	e	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	f	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	g	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	h	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	i	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	j	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	k	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	l	98/100 (98%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	m	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	n	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	o	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	p	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	q	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	r	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	s	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	t	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
All	All	7560/7680 (98%)	7335 (97%)	222 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	16	GLY
2	H	18	GLY
2	J	15	PRO

### 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	1	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	2	9/9 (100%)	9 (100%)	0	100	100
1	3	9/9 (100%)	9 (100%)	0	100	100
1	4	9/9 (100%)	9 (100%)	0	100	100
1	5	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	6	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	7	9/9 (100%)	9 (100%)	0	100	100
1	8	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	U	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	W	9/9 (100%)	9 (100%)	0	100	100
1	X	9/9 (100%)	9 (100%)	0	100	100
1	Y	9/9 (100%)	9 (100%)	0	100	100
1	Z	9/9 (100%)	9 (100%)	0	100	100
1	u	9/9 (100%)	9 (100%)	0	100	100
1	v	9/9 (100%)	9 (100%)	0	100	100
1	w	9/9 (100%)	9 (100%)	0	100	100
1	x	9/9 (100%)	9 (100%)	0	100	100
1	y	9/9 (100%)	8 (89%)	1 (11%)	5	19
1	z	9/9 (100%)	9 (100%)	0	100	100
2	A	231/231 (100%)	228 (99%)	3 (1%)	65	79
2	B	231/231 (100%)	227 (98%)	4 (2%)	56	74
2	C	231/231 (100%)	228 (99%)	3 (1%)	65	79
2	D	231/231 (100%)	223 (96%)	8 (4%)	31	58
2	E	231/231 (100%)	227 (98%)	4 (2%)	56	74
2	F	231/231 (100%)	224 (97%)	7 (3%)	36	62
2	G	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	H	231/231 (100%)	225 (97%)	6 (3%)	41	66
2	I	231/231 (100%)	228 (99%)	3 (1%)	65	79
2	J	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	K	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	L	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	M	231/231 (100%)	228 (99%)	3 (1%)	65	79
2	N	231/231 (100%)	228 (99%)	3 (1%)	65	79
2	O	231/231 (100%)	229 (99%)	2 (1%)	75	85
2	P	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	Q	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	R	231/231 (100%)	225 (97%)	6 (3%)	41	66
2	S	231/231 (100%)	226 (98%)	5 (2%)	47	69
2	T	231/231 (100%)	228 (99%)	3 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	b	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	c	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	d	95/95 (100%)	94 (99%)	1 (1%)	70	82
3	e	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	f	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	g	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	h	95/95 (100%)	94 (99%)	1 (1%)	70	82
3	i	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	j	95/95 (100%)	94 (99%)	1 (1%)	70	82
3	k	95/95 (100%)	91 (96%)	4 (4%)	25	53
3	l	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	m	95/95 (100%)	92 (97%)	3 (3%)	34	61
3	n	95/95 (100%)	94 (99%)	1 (1%)	70	82
3	o	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	p	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	q	95/95 (100%)	93 (98%)	2 (2%)	48	70
3	r	95/95 (100%)	94 (99%)	1 (1%)	70	82
3	s	95/95 (100%)	91 (96%)	4 (4%)	25	53
3	t	95/95 (100%)	93 (98%)	2 (2%)	48	70
All	All	6700/6700 (100%)	6564 (98%)	136 (2%)	50	71

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	4	ASP
1	8	5	HIS
1	6	1	TYR
1	5	1	TYR
1	V	5	HIS
2	A	99	TYR
2	A	101	CYS
2	A	234	ARG
3	a	71	PHE
3	a	79	TYR

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Mol	Chain	Res	Type
2	B	35	ARG
2	B	101	CYS
2	B	154	GLU
2	B	179	LEU
3	b	11	TYR
3	b	71	PHE
2	C	183	ASP
2	C	226	GLN
2	C	256	ARG
3	c	35	ASP
3	c	71	PHE
2	D	101	CYS
2	D	111	ARG
2	D	116	TYR
2	D	128	GLU
2	D	151	HIS
2	D	212	GLU
2	D	224	GLN
2	D	227	ASP
3	d	71	PHE
2	E	35	ARG
2	E	75	ARG
2	E	101	CYS
2	E	254	GLU
2	F	17	ARG
2	F	35	ARG
2	F	48	ARG
2	F	101	CYS
2	F	102	ASP
2	F	113	TYR
2	F	181	ARG
3	f	49	LYS
3	f	71	PHE
2	G	54	GLN
2	G	101	CYS
2	G	116	TYR
2	G	223	ASP
2	G	227	ASP
3	g	11	TYR
3	g	71	PHE
2	H	17	ARG
2	H	35	ARG

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Mol	Chain	Res	Type
2	H	99	TYR
2	H	101	CYS
2	H	116	TYR
2	H	254	GLU
3	h	71	PHE
2	S	17	ARG
2	S	101	CYS
2	S	110	LEU
2	S	181	ARG
2	S	196	ASP
3	s	22	ASN
3	s	35	ASP
3	s	62	SER
3	s	71	PHE
2	J	35	ARG
2	J	48	ARG
2	J	101	CYS
2	J	227	ASP
2	J	273	ARG
3	j	71	PHE
2	K	35	ARG
2	K	75	ARG
2	K	101	CYS
2	K	116	TYR
2	K	154	GLU
3	k	11	TYR
3	k	46	ARG
3	k	71	PHE
3	k	76	LYS
2	L	21	ARG
2	L	154	GLU
2	L	223	ASP
2	L	227	ASP
2	L	234	ARG
3	l	22	ASN
3	l	71	PHE
2	M	14	ARG
2	M	101	CYS
2	M	108	ARG
3	m	11	TYR
3	m	35	ASP
3	m	71	PHE

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Mol	Chain	Res	Type
2	N	101	CYS
2	N	116	TYR
2	N	212	GLU
3	n	71	PHE
2	O	101	CYS
2	O	151	HIS
3	o	41	LEU
3	o	71	PHE
2	P	101	CYS
2	P	113	TYR
2	P	116	TYR
2	P	128	GLU
2	P	188	HIS
3	p	7	LYS
3	p	71	PHE
2	Q	17	ARG
2	Q	35	ARG
2	Q	116	TYR
2	Q	145	HIS
2	Q	151	HIS
3	q	35	ASP
3	q	71	PHE
2	R	101	CYS
2	R	113	TYR
2	R	116	TYR
2	R	170	ARG
2	R	223	ASP
2	R	273	ARG
3	r	71	PHE
2	I	101	CYS
2	I	116	TYR
2	I	196	ASP
3	i	35	ASP
3	i	71	PHE
2	T	101	CYS
2	T	116	TYR
2	T	196	ASP
3	t	35	ASP
3	t	71	PHE
1	1	5	HIS
3	e	1	MET
3	e	370	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	5	HIS
1	2	5	HIS
1	7	5	HIS
2	A	70	HIS
2	A	192	HIS
2	N	155	GLN
2	O	54	GLN
2	O	188	HIS
2	P	188	HIS
2	R	174	ASN
2	I	192	HIS
2	T	155	GLN
2	T	192	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, 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	1	9/9 (100%)	1.21	1 (11%) 12 11	58, 65, 74, 78	0
1	2	9/9 (100%)	1.03	0 100 100	45, 52, 60, 64	0
1	3	9/9 (100%)	1.53	2 (22%) 3 2	39, 42, 49, 56	0
1	4	9/9 (100%)	1.07	0 100 100	45, 50, 63, 66	0
1	5	9/9 (100%)	1.76	3 (33%) 1 1	52, 56, 59, 64	0
1	6	9/9 (100%)	0.86	1 (11%) 12 11	44, 50, 56, 66	0
1	7	9/9 (100%)	1.66	4 (44%) 1 0	39, 45, 49, 64	0
1	8	9/9 (100%)	1.10	2 (22%) 3 2	31, 36, 49, 54	0
1	U	9/9 (100%)	1.20	0 100 100	58, 62, 70, 72	0
1	V	9/9 (100%)	1.40	1 (11%) 12 11	62, 73, 86, 96	0
1	W	9/9 (100%)	1.49	2 (22%) 3 2	42, 45, 54, 57	0
1	X	9/9 (100%)	1.52	2 (22%) 3 2	44, 52, 64, 70	0
1	Y	9/9 (100%)	1.23	1 (11%) 12 11	36, 46, 52, 60	0
1	Z	9/9 (100%)	1.20	0 100 100	68, 69, 79, 84	0
1	u	9/9 (100%)	1.21	1 (11%) 12 11	53, 58, 65, 69	0
1	v	9/9 (100%)	0.81	0 100 100	51, 55, 61, 61	0
1	w	9/9 (100%)	1.47	2 (22%) 3 2	52, 57, 68, 72	0
1	x	9/9 (100%)	1.17	1 (11%) 12 11	44, 49, 60, 63	0
1	y	9/9 (100%)	1.18	1 (11%) 12 11	32, 39, 49, 51	0
1	z	9/9 (100%)	1.42	1 (11%) 12 11	55, 57, 72, 76	0
2	A	275/275 (100%)	0.96	15 (5%) 32 25	36, 74, 90, 98	5 (1%)
2	B	275/275 (100%)	0.86	20 (7%) 22 19	24, 62, 76, 84	5 (1%)
2	C	275/275 (100%)	1.06	32 (11%) 11 11	39, 83, 98, 106	5 (1%)
2	D	275/275 (100%)	0.76	12 (4%) 39 30	26, 56, 75, 98	5 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	E	275/275 (100%)	0.97	33 (12%)	10	10	27, 61, 82, 98	5 (1%)
2	F	275/275 (100%)	1.01	25 (9%)	16	15	28, 58, 79, 93	5 (1%)
2	G	275/275 (100%)	0.89	19 (6%)	24	20	27, 64, 84, 102	5 (1%)
2	H	275/275 (100%)	0.79	11 (4%)	43	32	22, 52, 71, 94	5 (1%)
2	I	275/275 (100%)	0.69	12 (4%)	39	30	15, 40, 58, 78	5 (1%)
2	J	275/275 (100%)	0.72	6 (2%)	62	47	17, 38, 54, 74	5 (1%)
2	K	275/275 (100%)	0.98	19 (6%)	24	20	35, 78, 95, 103	5 (1%)
2	L	275/275 (100%)	0.80	8 (2%)	54	40	27, 58, 75, 84	4 (1%)
2	M	275/275 (100%)	0.83	17 (6%)	28	22	31, 70, 88, 106	5 (1%)
2	N	275/275 (100%)	0.77	13 (4%)	37	28	23, 53, 77, 87	5 (1%)
2	O	275/275 (100%)	0.94	22 (8%)	20	18	22, 53, 80, 91	5 (1%)
2	P	275/275 (100%)	0.81	17 (6%)	28	22	17, 47, 67, 85	5 (1%)
2	Q	275/275 (100%)	0.94	24 (8%)	17	16	25, 61, 84, 100	5 (1%)
2	R	275/275 (100%)	0.97	27 (9%)	14	14	24, 51, 73, 88	5 (1%)
2	S	275/275 (100%)	0.77	12 (4%)	39	30	20, 44, 64, 89	4 (1%)
2	T	275/275 (100%)	0.56	10 (3%)	46	34	16, 37, 54, 74	4 (1%)
3	a	100/100 (100%)	1.11	13 (13%)	9	9	32, 85, 100, 108	1 (1%)
3	b	100/100 (100%)	0.72	2 (2%)	64	50	20, 55, 72, 80	1 (1%)
3	c	100/100 (100%)	1.30	16 (16%)	6	5	30, 88, 106, 114	1 (1%)
3	d	100/100 (100%)	0.65	2 (2%)	64	50	19, 51, 70, 76	1 (1%)
3	e	100/100 (100%)	1.25	16 (16%)	6	5	22, 72, 98, 102	1 (1%)
3	f	100/100 (100%)	1.07	14 (14%)	7	8	22, 58, 70, 80	1 (1%)
3	g	100/100 (100%)	1.14	14 (14%)	7	8	26, 76, 89, 94	1 (1%)
3	h	100/100 (100%)	0.63	3 (3%)	52	39	21, 44, 61, 74	1 (1%)
3	i	100/100 (100%)	0.50	3 (3%)	52	39	11, 31, 49, 57	1 (1%)
3	j	100/100 (100%)	0.44	2 (2%)	64	50	12, 31, 50, 59	1 (1%)
3	k	100/100 (100%)	1.08	9 (9%)	17	15	28, 88, 101, 109	1 (1%)
3	l	100/100 (100%)	0.86	6 (6%)	29	23	17, 54, 73, 81	1 (1%)
3	m	100/100 (100%)	0.93	8 (8%)	20	18	25, 72, 91, 101	1 (1%)
3	n	100/100 (100%)	0.74	2 (2%)	64	50	15, 54, 73, 86	1 (1%)
3	o	100/100 (100%)	1.17	11 (11%)	12	11	21, 69, 82, 93	1 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	p	100/100 (100%)	0.61	1 (1%) 79 68	16, 40, 62, 76	1 (1%)
3	q	100/100 (100%)	1.31	17 (17%) 5 4	30, 78, 93, 97	1 (1%)
3	r	100/100 (100%)	0.97	6 (6%) 29 23	20, 49, 72, 92	1 (1%)
3	s	100/100 (100%)	0.61	3 (3%) 52 39	13, 35, 56, 62	1 (1%)
3	t	100/100 (100%)	0.51	1 (1%) 79 68	14, 32, 49, 57	1 (1%)
All	All	7680/7680 (100%)	0.87	528 (6%) 24 20	11, 57, 88, 114	117 (1%)

All (528) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	1	GLY	6.9
2	Q	1	GLY	6.3
2	O	249	VAL	6.2
3	e	368	THR	5.9
2	G	1	GLY	5.1
2	L	116	TYR	5.1
2	D	199	ALA	4.8
3	g	80	ALA	4.7
3	q	81	CYS	4.7
2	F	34	VAL	4.6
2	Q	78	LEU	4.5
2	E	1	GLY	4.4
2	C	34	VAL	4.4
2	N	81	LEU	4.3
2	I	116	TYR	4.2
2	E	23	ILE	4.1
2	T	116	TYR	4.1
2	E	249	VAL	4.0
3	g	94	VAL	4.0
2	M	94	THR	4.0
2	F	45	MET	3.9
3	q	41	LEU	3.9
3	m	16	ALA	3.9
2	K	11	SER	3.8
3	a	8	ILE	3.8
3	g	81	CYS	3.8
2	N	116	TYR	3.8
2	M	11	SER	3.7
3	l	86	VAL	3.7
2	Q	128	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	128	GLU	3.7
3	q	80	ALA	3.6
3	o	41	LEU	3.6
2	F	113	TYR	3.6
2	P	171	TYR	3.6
2	F	20	PRO	3.6
3	e	323	LEU	3.5
2	F	36	PHE	3.5
2	R	261	VAL	3.5
3	j	35	ASP	3.5
3	q	55	LEU	3.4
2	Q	217	TRP	3.4
2	C	245	ALA	3.4
2	K	177	GLU	3.4
3	g	41	LEU	3.4
3	r	41	LEU	3.4
3	e	398	ASP	3.4
2	Q	23	ILE	3.3
2	C	261	VAL	3.3
2	M	95	VAL	3.3
2	E	217	TRP	3.3
3	n	1	MET	3.3
3	o	81	CYS	3.3
3	q	16	ALA	3.2
2	A	30	ASP	3.2
2	L	199	ALA	3.2
2	Q	94	THR	3.2
2	C	37	ASP	3.2
3	e	366	TYR	3.2
3	e	354	LEU	3.2
3	i	61	TRP	3.2
1	5	4	ASP	3.1
2	Q	249	VAL	3.1
2	R	124	ILE	3.1
2	Q	123	TYR	3.1
2	H	114	HIS	3.1
2	A	37	ASP	3.1
1	V	3	LEU	3.1
2	L	104	GLY	3.1
3	e	346	ILE	3.1
3	e	372	PRO	3.1
2	A	1	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	o	22	ASN	3.0
2	P	74	HIS	3.0
3	c	50	VAL	3.0
1	5	7	ILE	3.0
2	N	118	TYR	3.0
2	P	71	SER	3.0
2	Q	71	SER	3.0
1	3	7	ILE	3.0
2	O	221	GLY	3.0
2	D	81	LEU	3.0
2	T	179	LEU	3.0
2	C	214	THR	3.0
2	F	74	HIS	2.9
2	O	74	HIS	2.9
2	F	171	TYR	2.9
2	C	40	ALA	2.9
2	S	205	ALA	2.9
2	O	178	THR	2.9
3	l	1	MET	2.9
2	C	259	CYS	2.9
2	P	124	ILE	2.9
2	B	261	VAL	2.9
2	B	266	LEU	2.9
3	k	40	LEU	2.9
2	D	36	PHE	2.9
2	H	109	PHE	2.9
2	T	227	ASP	2.9
2	Q	96	GLN	2.9
2	F	22	PHE	2.9
3	e	370	PHE	2.9
2	R	74	HIS	2.9
3	f	1	MET	2.9
3	l	55	LEU	2.9
2	E	171	TYR	2.9
2	E	236	ALA	2.8
3	f	55	LEU	2.8
2	S	165	VAL	2.8
2	K	207	SER	2.8
2	N	28	VAL	2.8
2	O	248	VAL	2.8
2	P	28	VAL	2.8
2	I	223	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	y	1	TYR	2.8
2	F	52	ILE	2.8
3	e	379	ALA	2.8
2	R	231	VAL	2.8
3	g	9	GLN	2.8
2	R	2	SER	2.8
2	B	153	ALA	2.8
3	h	1	MET	2.8
2	C	231	VAL	2.8
2	K	30	ASP	2.8
3	i	35	ASP	2.8
2	K	136	ALA	2.8
3	b	25	ASN	2.8
2	K	10	THR	2.8
2	F	120	GLY	2.8
2	P	1	GLY	2.8
2	A	241	PHE	2.8
2	F	9	PHE	2.8
2	K	20	PRO	2.8
2	H	71	SER	2.8
2	R	71	SER	2.8
3	c	29	SER	2.8
2	O	254	GLU	2.8
2	R	109	PHE	2.8
2	P	20	PRO	2.7
2	E	199	ALA	2.7
3	m	2	ILE	2.7
2	E	269	PRO	2.7
2	N	199	ALA	2.7
2	F	223	ASP	2.7
3	s	35	ASP	2.7
3	q	99	ASP	2.7
2	E	120	GLY	2.7
2	R	199	ALA	2.7
2	B	156	LEU	2.7
2	E	116	TYR	2.7
2	Q	84	TYR	2.7
2	E	207	SER	2.7
2	G	34	VAL	2.7
3	m	25	ASN	2.7
2	S	225	THR	2.7
2	P	135	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	55	LEU	2.7
2	M	12	VAL	2.7
3	q	38	VAL	2.7
3	e	350	GLU	2.7
2	O	52	ILE	2.7
3	f	73	PRO	2.7
2	C	49	ALA	2.7
2	R	81	LEU	2.7
3	f	3	GLN	2.7
2	C	5	MET	2.7
2	H	67	VAL	2.7
3	m	83	VAL	2.7
2	D	273	ARG	2.7
2	T	205	ALA	2.6
3	k	83	VAL	2.6
2	D	118	TYR	2.6
3	g	67	TYR	2.6
2	C	275	GLU	2.6
2	K	37	ASP	2.6
2	M	38	SER	2.6
2	I	160	LEU	2.6
3	c	40	LEU	2.6
3	o	40	LEU	2.6
2	R	64	THR	2.6
1	7	2	VAL	2.6
2	O	95	VAL	2.6
2	C	213	ILE	2.6
3	c	71	PHE	2.6
3	o	55	LEU	2.6
2	E	185	PRO	2.6
2	F	11	SER	2.6
2	G	190	THR	2.6
2	A	51	TRP	2.6
1	8	7	ILE	2.6
1	X	7	ILE	2.6
2	R	22	PHE	2.6
2	T	109	PHE	2.6
3	a	24	LEU	2.6
2	B	210	PRO	2.6
1	w	8	VAL	2.6
2	C	10	THR	2.6
2	J	261	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	q	2	ILE	2.6
2	O	257	TYR	2.6
2	Q	7	TYR	2.6
2	O	250	PRO	2.6
3	c	6	PRO	2.6
2	O	203	CYS	2.6
2	I	227	ASP	2.6
3	c	8	ILE	2.5
3	s	93	ILE	2.5
2	C	36	PHE	2.5
2	G	81	LEU	2.5
2	H	1	GLY	2.5
3	c	16	ALA	2.5
1	u	7	ILE	2.5
2	Q	192	HIS	2.5
2	M	164	CYS	2.5
3	c	12	SER	2.5
3	o	36	ILE	2.5
3	d	1	MET	2.5
2	F	177	GLU	2.5
2	R	161	GLU	2.5
3	o	50	VAL	2.5
3	k	2	ILE	2.5
2	M	91	GLY	2.5
2	G	211	ALA	2.5
2	P	22	PHE	2.5
2	A	244	TRP	2.5
3	k	34	SER	2.5
3	q	96	TRP	2.5
3	f	35	ASP	2.5
2	Q	116	TYR	2.5
3	a	16	ALA	2.5
3	r	64	TYR	2.5
2	C	189	MET	2.5
2	H	45	MET	2.5
2	G	261	VAL	2.5
3	r	8	ILE	2.4
2	E	74	HIS	2.4
2	B	265	GLY	2.4
2	Q	242	GLN	2.4
3	c	44	GLY	2.4
3	g	91	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	w	3	LEU	2.4
2	R	78	LEU	2.4
2	R	9	PHE	2.4
2	C	243	LYS	2.4
2	P	32	GLN	2.4
2	T	149	ALA	2.4
3	o	80	ALA	2.4
2	K	2	SER	2.4
2	O	13	SER	2.4
2	R	28	VAL	2.4
2	T	59	TYR	2.4
3	o	83	VAL	2.4
3	q	50	VAL	2.4
1	7	4	ASP	2.4
2	E	235	PRO	2.4
1	W	7	ILE	2.4
1	7	7	ILE	2.4
2	B	17	ARG	2.4
2	O	179	LEU	2.4
3	c	24	LEU	2.4
3	f	2	ILE	2.4
3	g	24	LEU	2.4
2	B	10	THR	2.4
2	C	258	THR	2.4
2	E	94	THR	2.4
2	Q	143	THR	2.4
2	K	189	MET	2.4
3	t	94	VAL	2.4
3	r	34	SER	2.4
2	K	110	LEU	2.4
2	M	160	LEU	2.4
3	k	8	ILE	2.4
3	l	24	LEU	2.4
2	A	8	PHE	2.4
2	M	191	HIS	2.4
2	C	73	THR	2.4
2	F	64	THR	2.4
2	H	199	ALA	2.4
2	K	51	TRP	2.4
2	Q	135	ALA	2.4
3	a	38	VAL	2.4
2	S	224	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	257	TYR	2.4
2	M	7	TYR	2.4
3	b	15	PRO	2.4
3	m	29	SER	2.4
2	K	8	PHE	2.4
3	f	71	PHE	2.4
3	a	30	GLY	2.4
3	f	16	ALA	2.4
1	5	9	VAL	2.4
2	G	242	GLN	2.4
2	I	118	TYR	2.3
3	c	33	PRO	2.3
3	d	93	ILE	2.3
2	C	207	SER	2.3
2	R	4	SER	2.3
2	B	86	ASN	2.3
3	e	369	GLU	2.3
2	B	150	ALA	2.3
3	k	38	VAL	2.3
3	m	80	ALA	2.3
2	D	256	ARG	2.3
2	F	60	TRP	2.3
2	L	215	LEU	2.3
2	E	52	ILE	2.3
2	L	180	GLN	2.3
2	G	116	TYR	2.3
2	B	2	SER	2.3
2	A	177	GLU	2.3
2	A	254	GLU	2.3
1	X	8	VAL	2.3
2	L	114	HIS	2.3
2	Q	221	GLY	2.3
2	I	136	ALA	2.3
3	e	10	VAL	2.3
2	P	160	LEU	2.3
2	R	240	THR	2.3
3	g	40	LEU	2.3
3	g	65	LEU	2.3
3	m	5	THR	2.3
2	P	23	ILE	2.3
2	K	269	PRO	2.3
2	D	116	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	116	TYR	2.3
2	P	36	PHE	2.3
2	N	105	SER	2.3
2	Q	220	ASP	2.3
2	S	16	GLY	2.3
2	J	111	ARG	2.3
2	K	1	GLY	2.3
3	a	52	HIS	2.3
3	q	95	LYS	2.3
2	G	124	ILE	2.3
3	l	2	ILE	2.3
2	B	73	THR	2.3
2	C	178	THR	2.3
2	E	73	THR	2.3
3	c	5	THR	2.3
2	J	224	GLN	2.3
2	O	116	TYR	2.3
3	a	57	PHE	2.3
2	C	45	MET	2.3
2	N	273	ARG	2.3
2	B	236	ALA	2.3
2	E	2	SER	2.3
2	G	26	GLY	2.3
2	J	249	VAL	2.3
2	N	140	ALA	2.3
3	h	94	VAL	2.3
3	q	94	VAL	2.3
2	J	223	ASP	2.3
3	a	65	LEU	2.3
2	K	23	ILE	2.3
2	B	258	THR	2.3
2	F	10	THR	2.3
2	O	269	PRO	2.3
2	G	43	GLN	2.3
2	Q	237	GLY	2.3
2	T	16	GLY	2.3
3	a	80	ALA	2.3
2	C	168	LEU	2.3
2	E	179	LEU	2.3
2	K	179	LEU	2.3
2	N	275	GLU	2.3
3	h	55	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	52	ILE	2.2
2	D	147	TRP	2.2
2	E	51	TRP	2.2
2	C	101	CYS	2.2
2	M	50	PRO	2.2
2	O	123	TYR	2.2
1	3	8	VAL	2.2
2	D	1	GLY	2.2
2	R	112	GLY	2.2
2	L	134	THR	2.2
2	H	273	ARG	2.2
2	O	43	GLN	2.2
1	W	8	VAL	2.2
2	C	67	VAL	2.2
2	F	160	LEU	2.2
2	G	172	LEU	2.2
1	x	7	ILE	2.2
2	P	58	GLU	2.2
2	C	50	PRO	2.2
2	M	196	ASP	2.2
3	c	25	ASN	2.2
3	g	69	THR	2.2
2	O	164	CYS	2.2
3	c	9	GLN	2.2
3	e	382	VAL	2.2
2	B	172	LEU	2.2
2	C	156	LEU	2.2
2	D	26	GLY	2.2
2	A	11	SER	2.2
2	N	274	TRP	2.2
2	O	71	SER	2.2
2	Q	9	PHE	2.2
3	a	34	SER	2.2
2	B	196	ASP	2.2
3	f	99	ASP	2.2
2	R	94	THR	2.2
2	C	7	TYR	2.2
2	S	255	GLN	2.2
2	N	67	VAL	2.2
2	I	224	GLN	2.2
2	C	41	ALA	2.2
3	e	380	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	1	7	ILE	2.2
3	a	47	ILE	2.2
2	B	63	GLU	2.2
3	j	37	GLU	2.2
3	q	85	HIS	2.2
2	A	25	VAL	2.2
2	F	152	VAL	2.2
2	G	95	VAL	2.2
2	G	216	THR	2.2
2	G	249	VAL	2.2
3	m	88	LEU	2.2
2	G	74	HIS	2.1
2	C	51	TRP	2.1
3	q	91	PRO	2.1
2	E	103	VAL	2.1
2	S	251	SER	2.1
2	N	95	VAL	2.1
2	T	251	SER	2.1
3	r	40	LEU	2.1
2	P	73	THR	2.1
2	Q	113	TYR	2.1
2	R	69	ALA	2.1
2	I	180	GLN	2.1
2	A	18	GLY	2.1
2	I	109	PHE	2.1
2	S	63	GLU	2.1
2	K	63	GLU	2.1
2	A	47	PRO	2.1
2	R	250	PRO	2.1
2	H	51	TRP	2.1
2	R	156	LEU	2.1
3	l	65	LEU	2.1
3	f	62	SER	2.1
2	H	171	TYR	2.1
3	o	99	ASP	2.1
2	C	235	PRO	2.1
2	F	114	HIS	2.1
2	B	217	TRP	2.1
3	f	66	LEU	2.1
3	i	1	MET	2.1
3	k	96	TRP	2.1
2	E	240	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	258	THR	2.1
2	P	11	SER	2.1
2	B	116	TYR	2.1
2	N	179	LEU	2.1
2	R	215	LEU	2.1
1	6	9	VAL	2.1
2	E	247	VAL	2.1
2	K	274	TRP	2.1
3	r	16	ALA	2.1
2	A	213	ILE	2.1
2	E	273	ARG	2.1
3	q	36	ILE	2.1
1	7	1	TYR	2.1
2	C	116	TYR	2.1
2	F	239	GLY	2.1
2	G	257	TYR	2.1
2	R	178	THR	2.1
3	f	34	SER	2.1
3	g	11	TYR	2.1
3	s	62	SER	2.1
2	M	226	GLN	2.1
2	T	255	GLN	2.1
3	e	321	ASN	2.1
2	J	37	ASP	2.1
3	k	77	ASP	2.1
2	H	156	LEU	2.1
2	P	172	LEU	2.1
3	q	65	LEU	2.1
2	Q	20	PRO	2.1
2	G	128	GLU	2.1
2	E	41	ALA	2.0
2	S	211	ALA	2.0
3	k	13	ARG	2.0
2	E	200	THR	2.0
2	F	84	TYR	2.0
2	M	31	THR	2.0
2	R	99	TYR	2.0
2	I	59	TYR	2.0
3	e	367	TYR	2.0
1	Y	3	LEU	2.0
2	E	168	LEU	2.0
2	M	119	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	81	LEU	2.0
3	f	54	ASP	2.0
3	g	99	ASP	2.0
2	D	152	VAL	2.0
2	E	231	VAL	2.0
2	F	25	VAL	2.0
3	a	86	VAL	2.0
2	S	264	GLU	2.0
3	c	92	LYS	2.0
3	f	42	LYS	2.0
3	n	61	TRP	2.0
2	B	124	ILE	2.0
2	R	23	ILE	2.0
2	I	135	ALA	2.0
2	E	16	GLY	2.0
2	F	94	THR	2.0
2	S	73	THR	2.0
2	S	80	THR	2.0
3	p	5	THR	2.0
2	A	33	PHE	2.0
1	8	3	LEU	2.0
2	D	195	SER	2.0
3	a	40	LEU	2.0
2	E	174	ASN	2.0
3	q	22	ASN	2.0
2	C	25	VAL	2.0
2	M	247	VAL	2.0
2	O	231	VAL	2.0
2	I	122	ASP	2.0
3	g	83	VAL	2.0
2	Q	269	PRO	2.0
3	o	91	PRO	2.0
1	z	7	ILE	2.0
2	F	274	TRP	2.0
2	E	237	GLY	2.0
2	M	18	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [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.