



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:41 AM UTC

PDB ID : 6NCA / pdb\_00006nca  
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

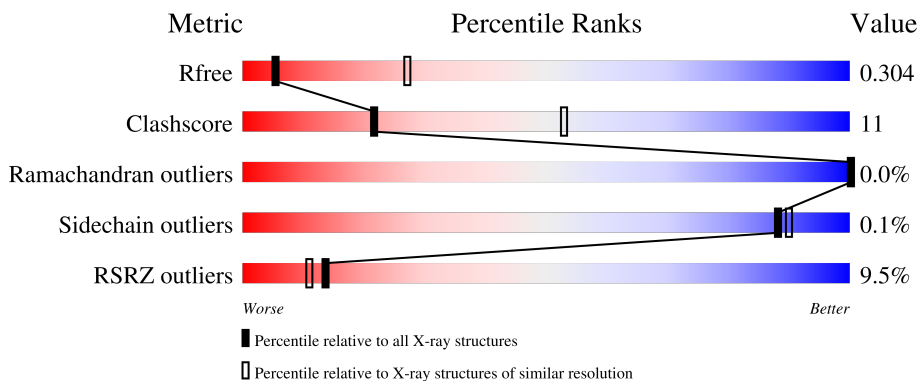
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (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	 22% (red), 56% (green), 44% (yellow)
1	2	9	 67% (green), 33% (yellow)
1	3	9	 33% (red), 33% (orange), 67% (yellow)
1	4	9	 56% (green), 44% (yellow)
1	5	9	 33% (red), 67% (green), 33% (yellow)

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Mol	Chain	Length	Quality of chain
1	6	9	11% 78% 22%
1	7	9	44% 100%
1	8	9	22% 78% 22%
1	U	9	44% 56%
1	V	9	22% 44% 56%
1	W	9	22% 67% 33%
1	X	9	22% 44% 56%
1	Y	9	22% 89% 11%
1	Z	9	44% 56%
1	u	9	11% 67% 33%
1	v	9	11% 56% 44%
1	w	9	22% 78% 22%
1	x	9	11% 78% 22%
1	y	9	11% 78% 22%
1	z	9	11% 89% 11%
2	A	275	12% 76% 24%
2	B	275	10% 71% 29%
2	C	275	16% 67% 33%
2	D	275	6% 75% 25%
2	E	275	14% 70% 30%
2	F	275	12% 68% 32%
2	G	275	11% 65% 35%
2	H	275	8% 63% 37%
2	I	275	5% 71% 29%
2	J	275	5% 74% 26%

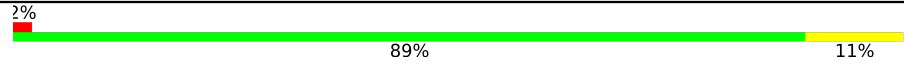
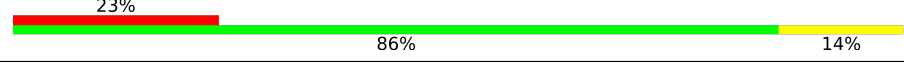
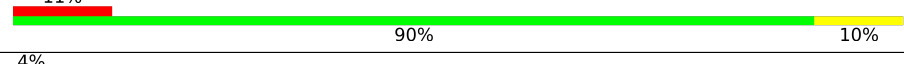


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Mol	Chain	Length	Quality of chain
2	K	275	9% 70% 30%
2	L	275	5% 73% 27%
2	M	275	9% 78% 22%
2	N	275	6% 72% 28%
2	O	275	11% 73% 27%
2	P	275	8% 65% 35%
2	Q	275	12% 73% 27%
2	R	275	12% 63% 37%
2	S	275	7% 73% 27%
2	T	275	5% 77% 23%
3	a	100	14% 80% 20%
3	b	100	3% 76% 24%
3	c	100	20% 73% 27%
3	d	100	3% 82% 18%
3	e	100	20% 85% 14%
3	f	100	16% 87% 13%
3	g	100	16% 78% 22%
3	h	100	5% 87% 13%
3	i	100	3% 88% 12%
3	j	100	3% 83% 17%
3	k	100	11% 83% 17%
3	l	100	8% 87% 12%
3	m	100	12% 86% 14%
3	n	100	2% 89% 11%
3	o	100	15% 85% 15%

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Mol	Chain	Length	Quality of chain
3	p	100	 2% 89% 11%
3	q	100	 23% 86% 14%
3	r	100	 11% 90% 10%
3	s	100	 4% 84% 16%
3	t	100	 2% 85% 15%

## 2 Entry composition [i](#)

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
			Total	C	N	O			
1	Y	9	76	52	11	13	0	0	0
1	u	9	76	52	11	13	0	0	0
1	z	9	76	52	11	13	0	0	0
1	y	9	76	52	11	13	0	0	0
1	8	9	76	52	11	13	0	0	0
1	w	9	76	52	11	13	0	0	0
1	4	9	76	52	11	13	0	0	0
1	3	9	76	52	11	13	0	0	0
1	W	9	76	52	11	13	0	0	0
1	6	9	76	52	11	13	0	0	0
1	x	9	76	52	11	13	0	0	0
1	5	9	76	52	11	13	0	0	0
1	X	9	76	52	11	13	0	0	0
1	v	9	76	52	11	13	0	0	0
1	2	9	76	52	11	13	0	0	0
1	U	9	76	52	11	13	0	0	0

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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
			Total	C	N	O	S			
3	p	100	837	533	141	159	4	5	0	0
3	q	100	837	533	141	159	4	5	0	0
3	r	100	837	533	141	159	4	5	0	0
3	i	100	837	533	141	159	4	5	0	0
3	t	100	837	533	141	159	4	5	0	0
3	e	100	837	533	141	159	4	5	0	0

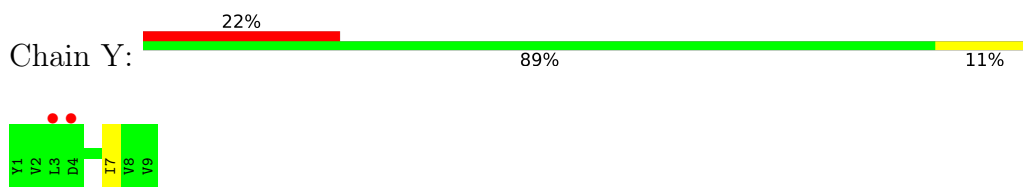
There are 20 discrepancies between the modelled and reference sequences:

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

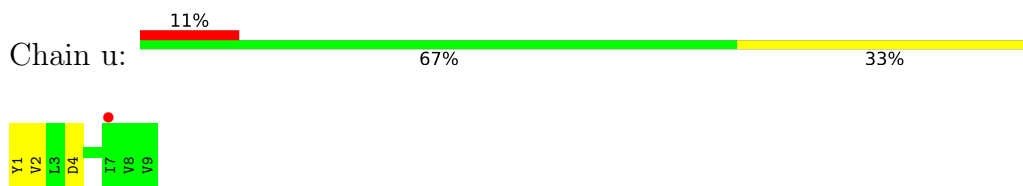
### 3 Residue-property plots [i](#)

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.

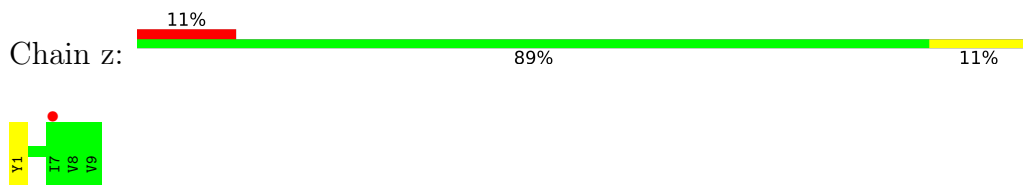
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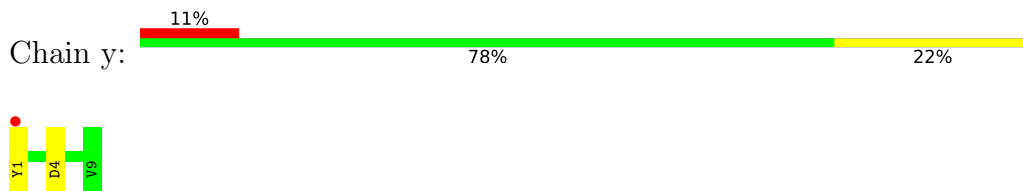
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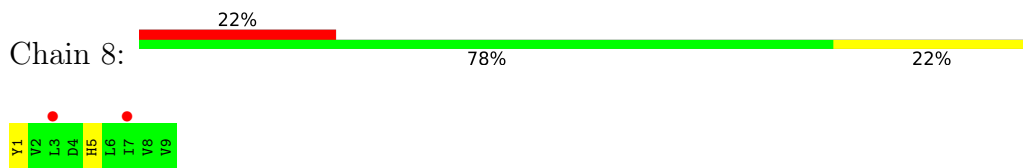
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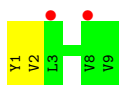
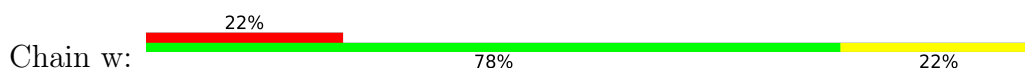
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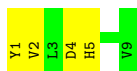
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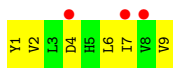
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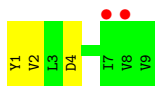
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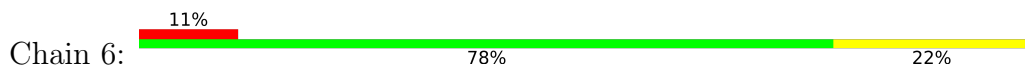
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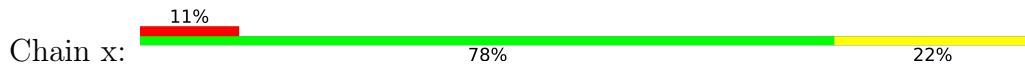
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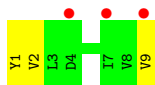
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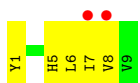
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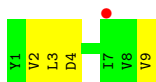
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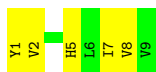
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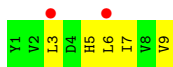
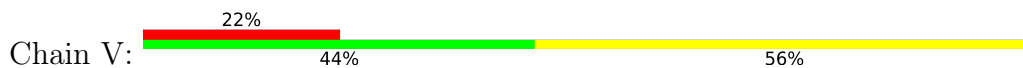
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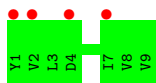
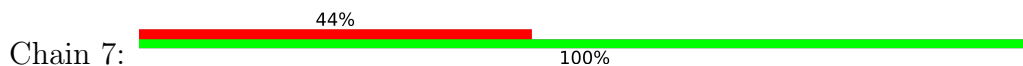
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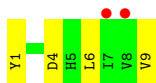
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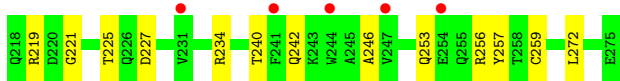
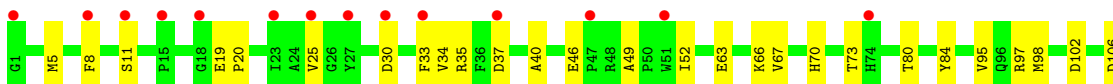
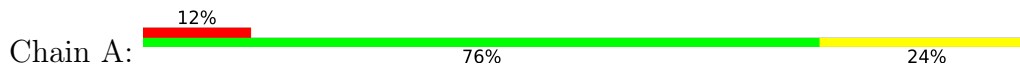
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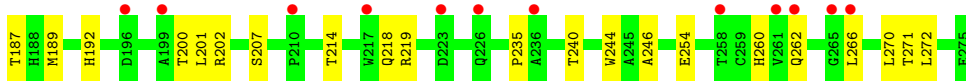
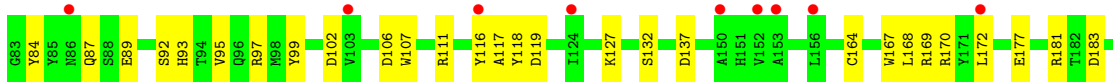
- Molecule 1: Replication and transcription activator



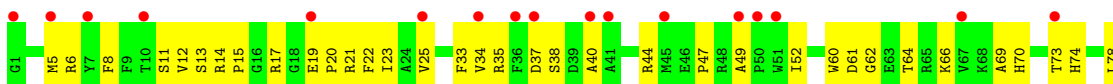
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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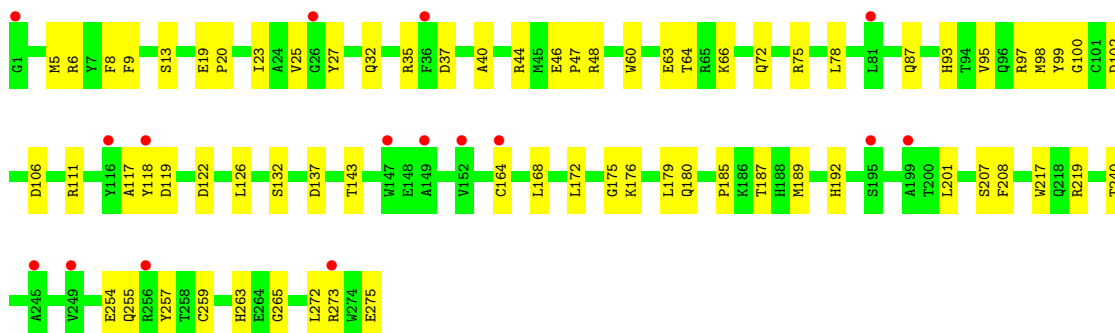
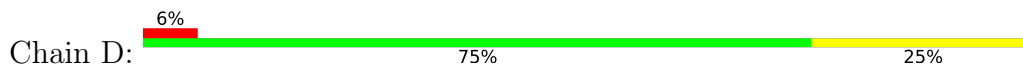


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

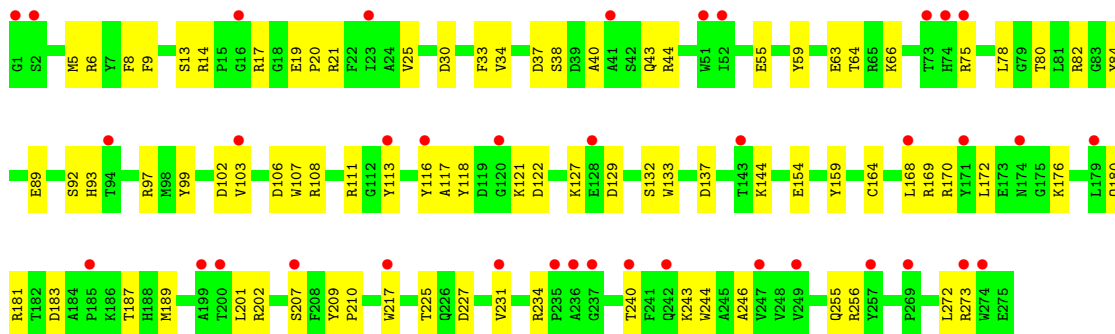




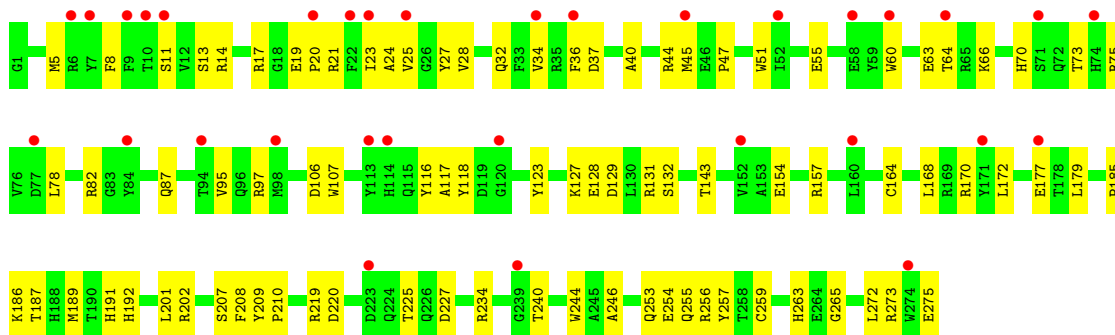
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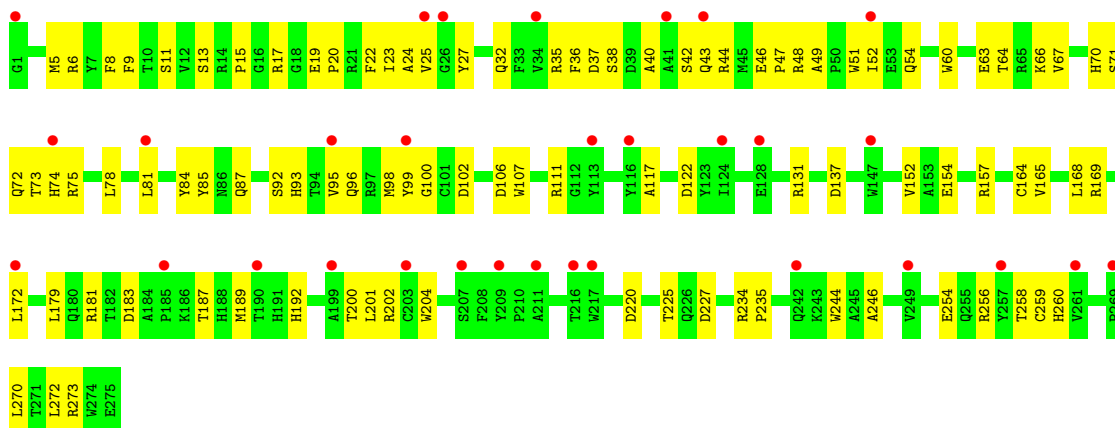


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

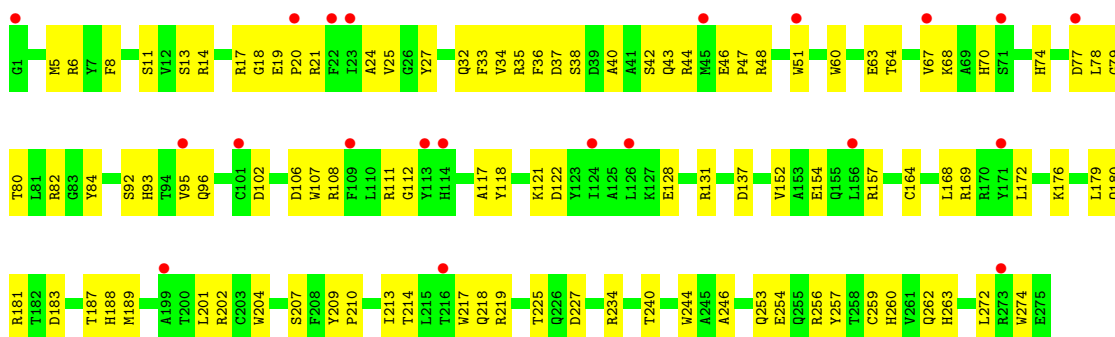


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

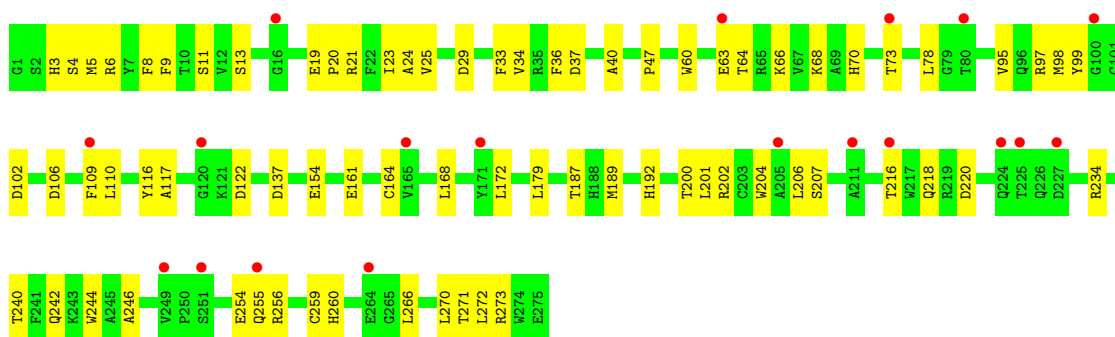
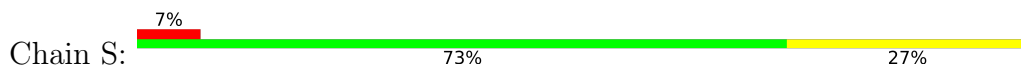




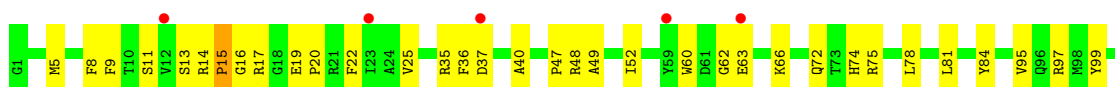
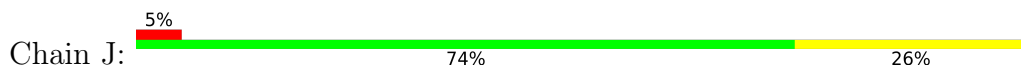
• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

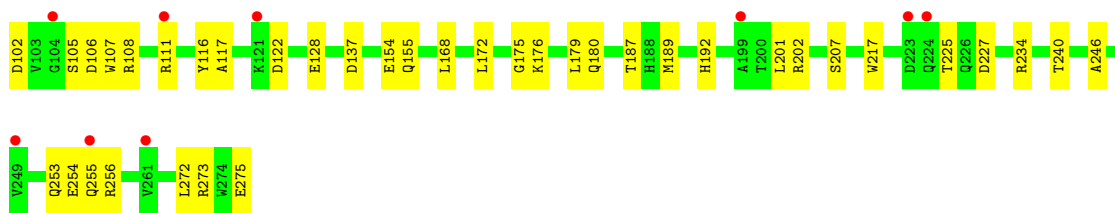


• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

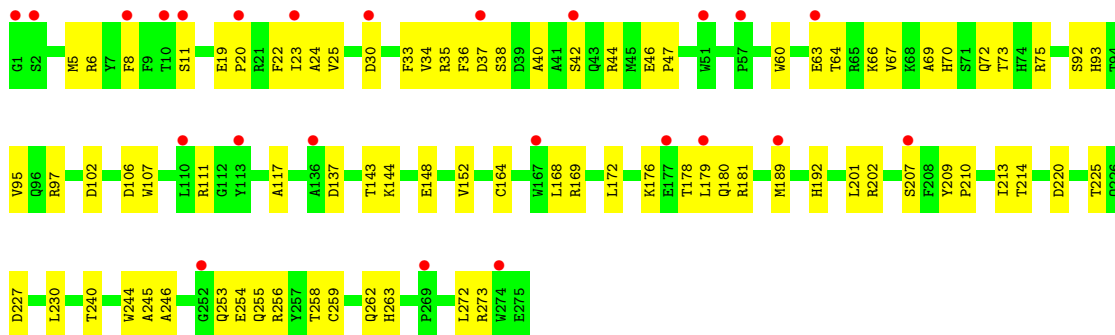


• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

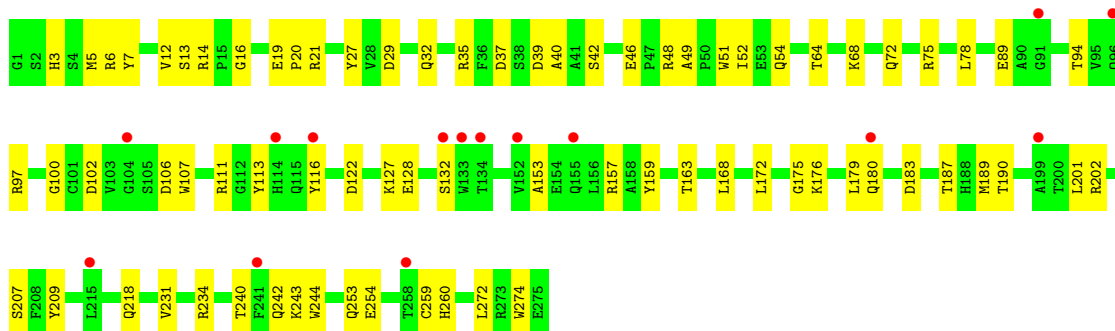




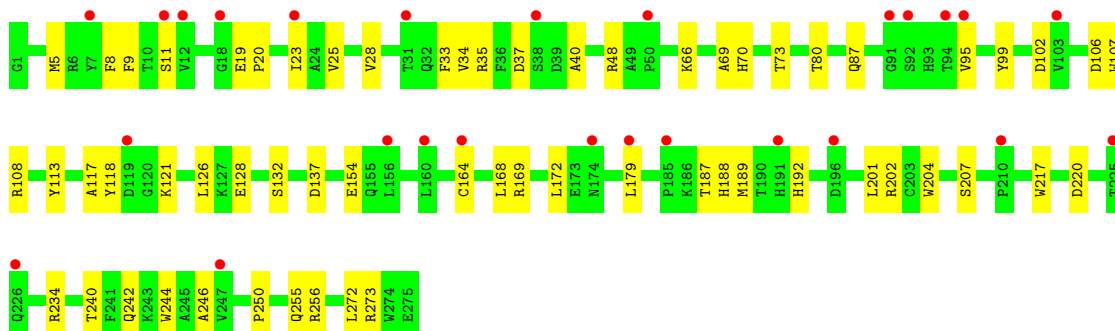
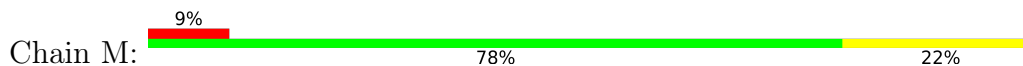
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



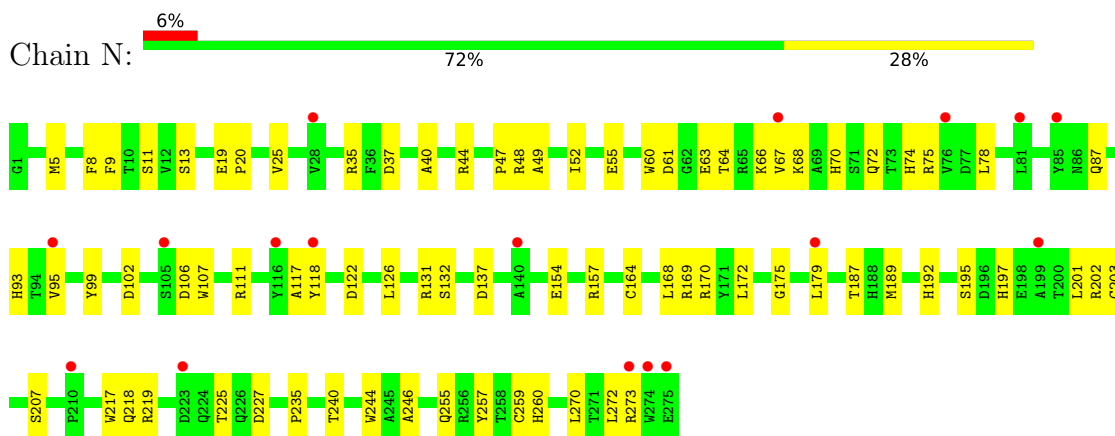
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



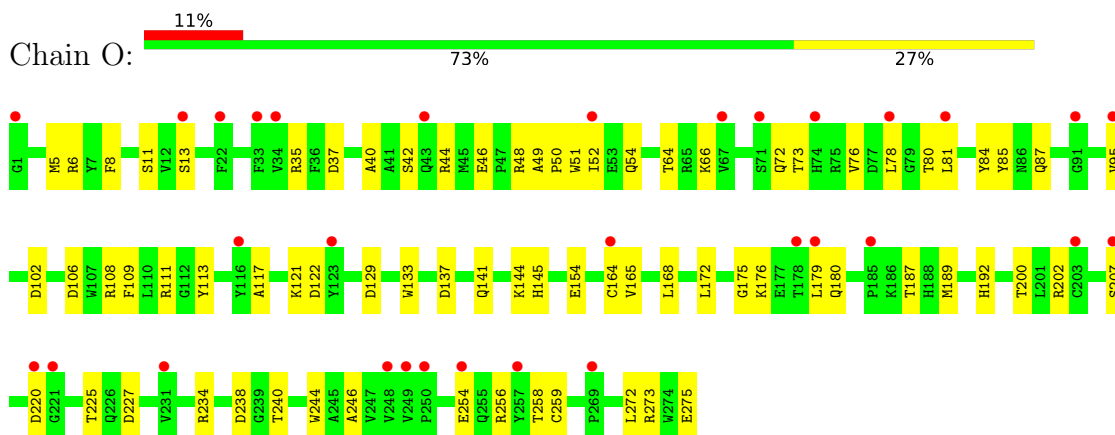
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



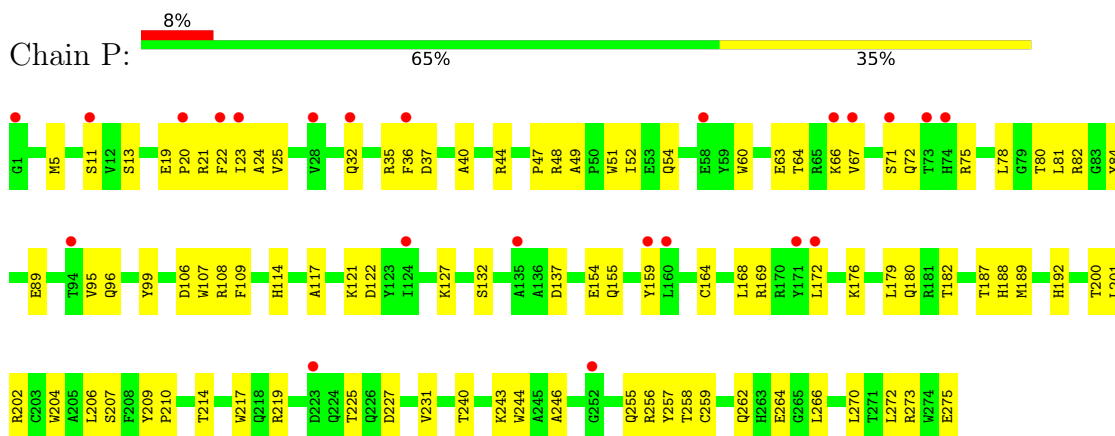
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



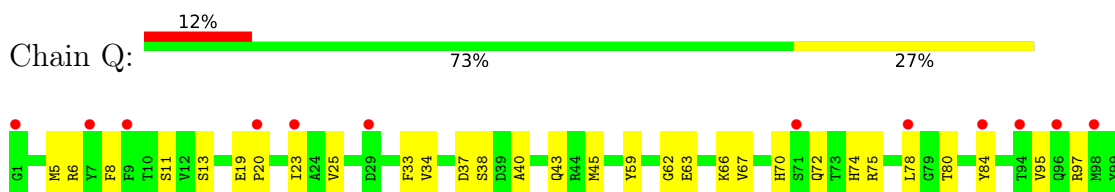
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

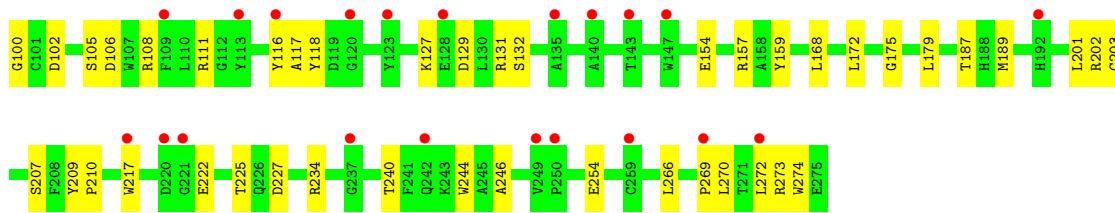


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

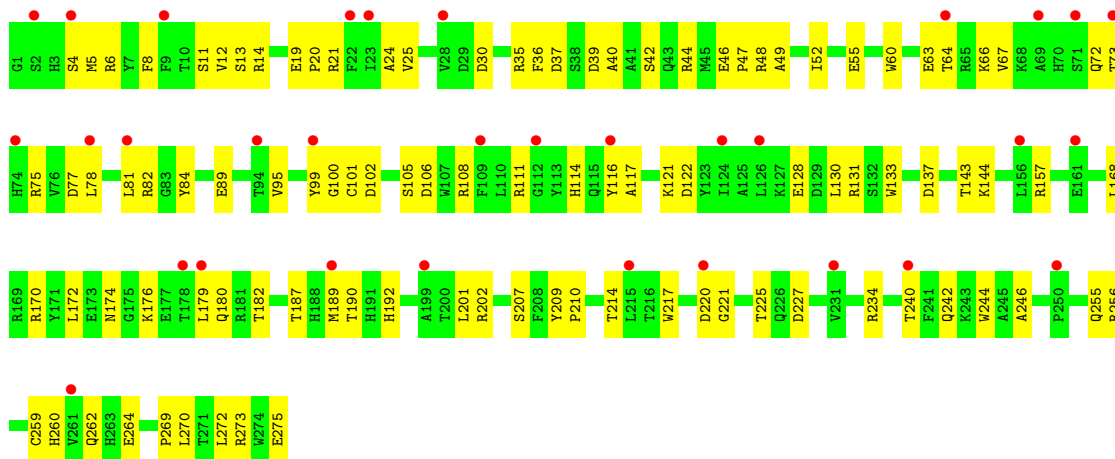


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

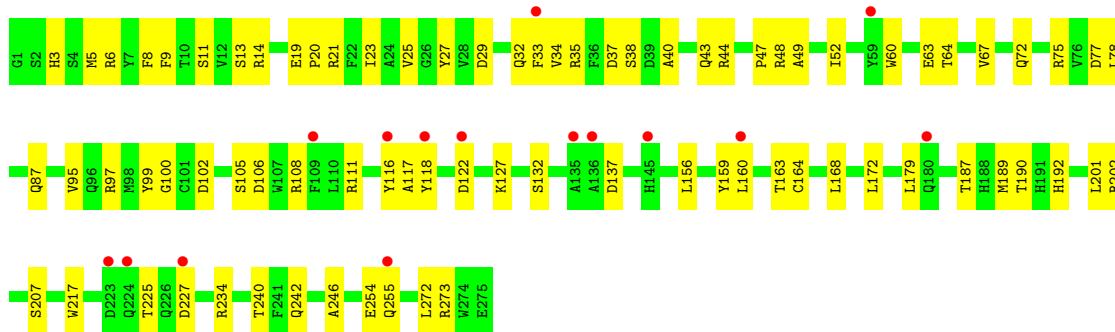




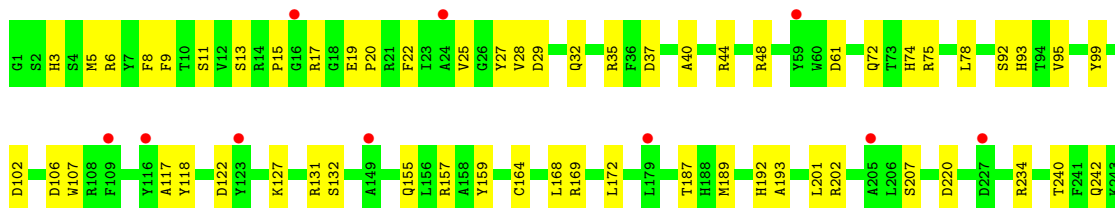
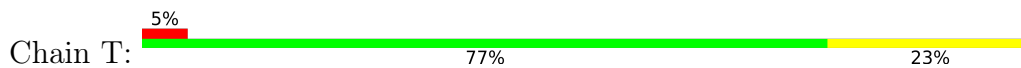
• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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

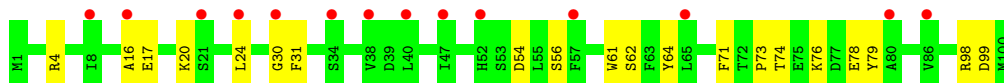
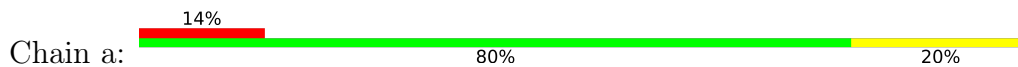


• Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

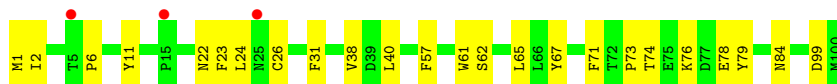
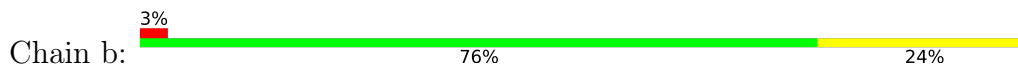




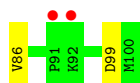
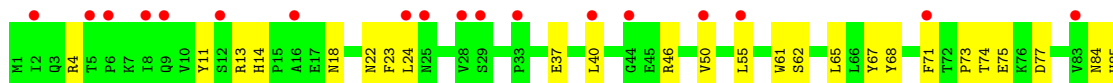
- Molecule 3: Beta-2-microglobulin



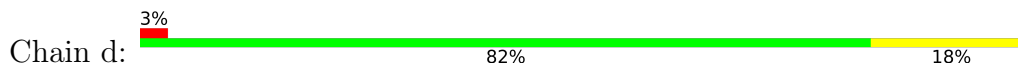
- Molecule 3: Beta-2-microglobulin



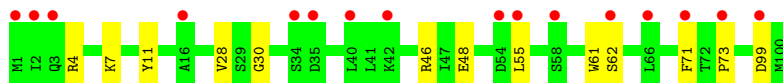
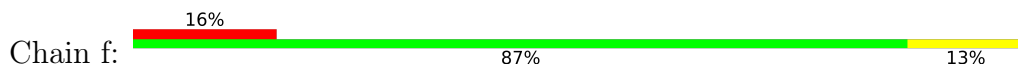
- Molecule 3: Beta-2-microglobulin



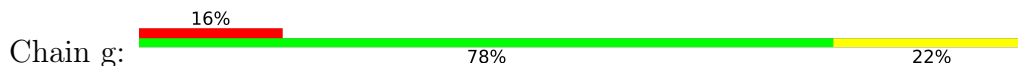
- Molecule 3: Beta-2-microglobulin

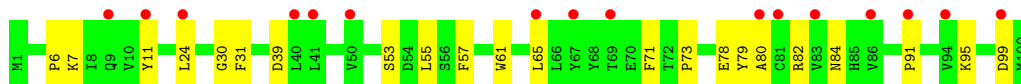


- Molecule 3: Beta-2-microglobulin

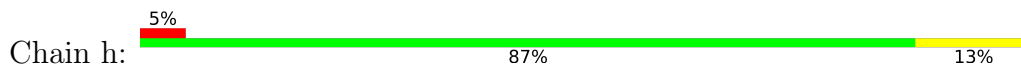


- Molecule 3: Beta-2-microglobulin

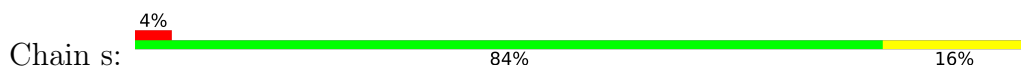




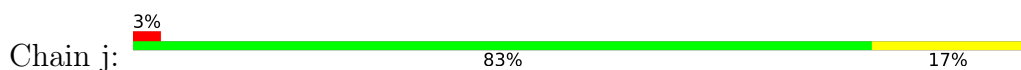
- Molecule 3: Beta-2-microglobulin



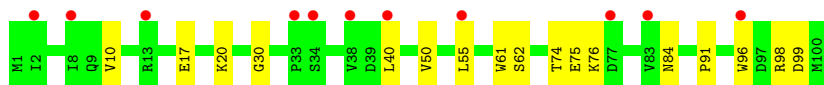
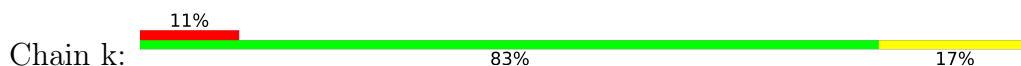
- Molecule 3: Beta-2-microglobulin



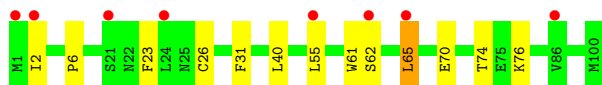
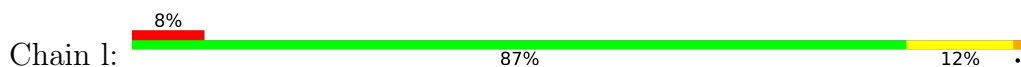
- Molecule 3: Beta-2-microglobulin



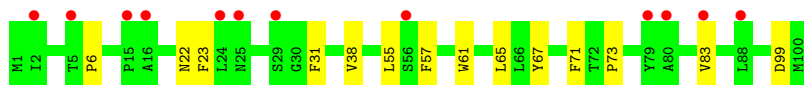
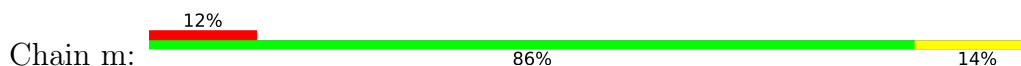
- Molecule 3: Beta-2-microglobulin



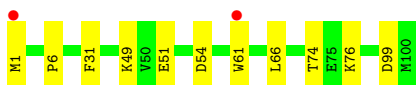
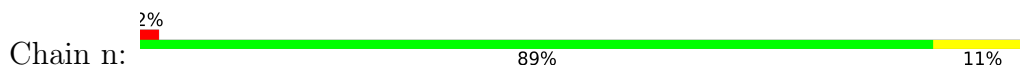
- Molecule 3: Beta-2-microglobulin



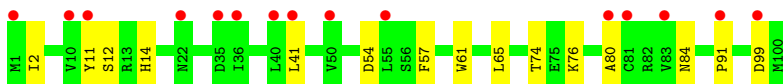
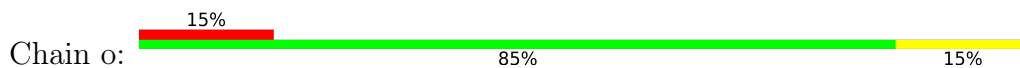
- Molecule 3: Beta-2-microglobulin



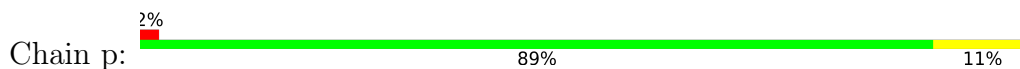
- Molecule 3: Beta-2-microglobulin



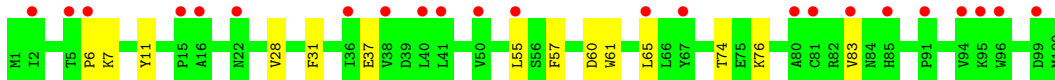
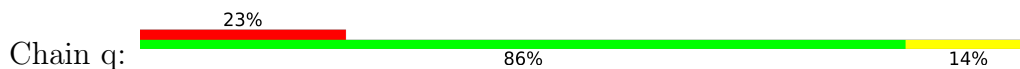
- Molecule 3: Beta-2-microglobulin



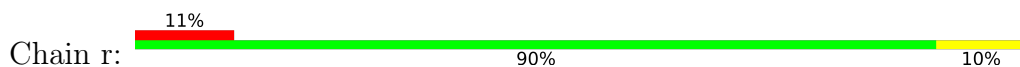
- Molecule 3: Beta-2-microglobulin



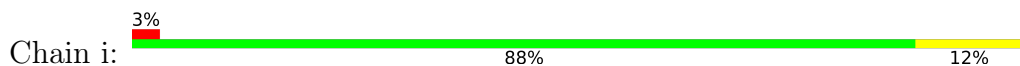
- Molecule 3: Beta-2-microglobulin



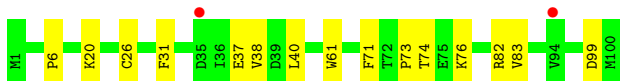
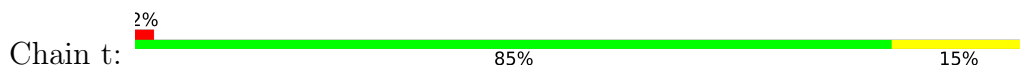
- Molecule 3: Beta-2-microglobulin



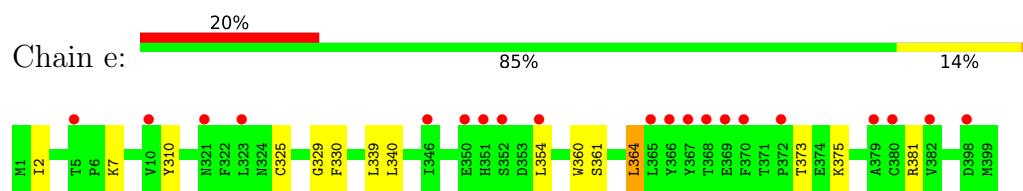
- Molecule 3: Beta-2-microglobulin



- 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 , 0.304	Depositor DCC
$R_{free}$ test set	1516 reflections (0.69%)	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	0.15	0/77	0.48	0/104
1	2	0.12	0/77	0.44	0/104
1	3	0.19	0/77	0.50	0/104
1	4	0.16	0/77	0.56	0/104
1	5	0.20	0/77	0.61	0/104
1	6	0.19	0/77	0.69	0/104
1	7	0.12	0/77	0.45	0/104
1	8	0.16	0/77	0.56	0/104
1	U	0.17	0/77	0.49	0/104
1	V	0.20	0/77	0.59	0/104
1	W	0.12	0/77	0.42	0/104
1	X	0.16	0/77	0.46	0/104
1	Y	0.14	0/77	0.43	0/104
1	Z	0.17	0/77	0.54	0/104
1	u	0.15	0/77	0.42	0/104
1	v	0.14	0/77	0.43	0/104
1	w	0.15	0/77	0.48	0/104
1	x	0.17	0/77	0.39	0/104
1	y	0.13	0/77	0.36	0/104
1	z	0.12	0/77	0.46	0/104
2	A	0.18	0/2312	0.48	0/3137
2	B	0.13	0/2312	0.42	0/3137
2	C	0.16	0/2312	0.45	0/3137
2	D	0.14	0/2312	0.42	0/3137
2	E	0.14	0/2312	0.40	0/3137
2	F	0.14	0/2312	0.44	0/3137
2	G	0.14	0/2312	0.44	0/3137
2	H	0.13	0/2312	0.44	0/3137
2	I	0.13	0/2312	0.41	0/3137
2	J	0.13	0/2312	0.43	0/3137
2	K	0.15	0/2312	0.45	0/3137
2	L	0.13	0/2312	0.42	0/3137
2	M	0.13	0/2312	0.43	0/3137
2	N	0.13	0/2312	0.42	0/3137

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	O	0.14	0/2312	0.44	0/3137
2	P	0.13	0/2312	0.43	0/3137
2	Q	0.15	0/2312	0.42	0/3137
2	R	0.15	0/2312	0.44	0/3137
2	S	0.13	0/2312	0.41	0/3137
2	T	0.13	0/2312	0.41	0/3137
3	a	0.16	0/860	0.47	0/1162
3	b	0.14	0/860	0.44	0/1162
3	c	0.17	0/860	0.53	0/1162
3	d	0.14	0/860	0.43	0/1162
3	e	0.13	0/860	0.42	0/1162
3	f	0.14	0/860	0.46	0/1162
3	g	0.16	0/860	0.46	0/1162
3	h	0.14	0/860	0.42	0/1162
3	i	0.14	0/860	0.44	0/1162
3	j	0.14	0/860	0.42	0/1162
3	k	0.15	0/860	0.45	0/1162
3	l	0.13	0/860	0.43	0/1162
3	m	0.14	0/860	0.43	0/1162
3	n	0.14	0/860	0.41	0/1162
3	o	0.13	0/860	0.46	0/1162
3	p	0.13	0/860	0.42	0/1162
3	q	0.14	0/860	0.45	0/1162
3	r	0.14	0/860	0.44	0/1162
3	s	0.13	0/860	0.43	0/1162
3	t	0.14	0/860	0.42	0/1162
All	All	0.14	0/64980	0.44	0/88060

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 [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	76	0	82	5	0
1	2	76	0	82	2	0
1	3	76	0	82	8	0
1	4	76	0	82	6	0
1	5	76	0	82	5	0
1	6	76	0	82	2	0
1	7	76	0	82	0	0
1	8	76	0	82	2	0
1	U	76	0	82	6	0
1	V	76	0	82	5	0
1	W	76	0	82	6	0
1	X	76	0	82	9	0
1	Y	76	0	82	1	0
1	Z	76	0	82	8	0
1	u	76	0	82	4	0
1	v	76	0	82	4	0
1	w	76	0	82	4	0
1	x	76	0	82	3	0
1	y	76	0	82	3	0
1	z	76	0	82	1	0
2	A	2247	0	2096	50	2
2	B	2247	0	2096	57	0
2	C	2247	0	2096	64	0
2	D	2247	0	2096	49	2
2	E	2247	0	2096	62	0
2	F	2247	0	2096	69	1
2	G	2247	0	2096	73	0
2	H	2247	0	2096	74	0
2	I	2247	0	2096	55	0
2	J	2247	0	2096	57	0
2	K	2247	0	2096	60	0
2	L	2247	0	2096	45	1
2	M	2247	0	2096	44	1
2	N	2247	0	2096	60	0
2	O	2247	0	2096	64	0
2	P	2247	0	2096	65	0
2	Q	2247	0	2096	62	0
2	R	2247	0	2096	84	0
2	S	2247	0	2096	46	0
2	T	2247	0	2096	44	0
3	a	837	0	803	17	0
3	b	837	0	803	17	1
3	c	837	0	803	21	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	837	0	803	14	0
3	e	837	0	803	11	0
3	f	837	0	803	10	0
3	g	837	0	803	17	0
3	h	837	0	803	15	0
3	i	837	0	803	12	0
3	j	837	0	803	14	0
3	k	837	0	803	11	0
3	l	837	0	803	8	0
3	m	837	0	803	9	0
3	n	837	0	803	12	0
3	o	837	0	803	11	0
3	p	837	0	803	8	0
3	q	837	0	803	11	0
3	r	837	0	803	12	0
3	s	837	0	803	13	1
3	t	837	0	803	13	0
All	All	63200	0	59620	1309	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1309 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:170:ARG:CZ	2:R:174:ASN:HD21	1.58	1.16
2:R:170:ARG:NH2	2:R:174:ASN:ND2	1.92	1.16
2:E:181:ARG:NH1	2:E:183:ASP:OD2	1.78	1.14
2:E:102:ASP:OD2	2:E:111:ARG:NH1	1.84	1.09
2:R:55:GLU:OE2	2:R:170:ARG:NH2	1.86	1.08

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:84:ASN:OD1	2:L:176:LYS:NZ[1_565]	2.00	0.20
2:A:221:GLY:O	2:D:111:ARG:NH2[1_455]	2.08	0.12
2:F:275:GLU:OXT	3:s:20:LYS:NZ[2_455]	2.08	0.12
2:A:108:ARG:NH2	2:D:275:GLU:OE2[1_455]	2.15	0.05
3:c:46:ARG:NH2	2:M:128:GLU:OE2[1_565]	2.15	0.05

## 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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	60
2	I	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	J	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	60
2	K	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	L	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	30	60
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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%)	9 (100%)	0	100	100
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%)	9 (100%)	0	100	100
1	6	9/9 (100%)	9 (100%)	0	100	100
1	7	9/9 (100%)	9 (100%)	0	100	100
1	8	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%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	9 (100%)	0	100	100
1	z	9/9 (100%)	9 (100%)	0	100	100
2	A	231/231 (100%)	231 (100%)	0	100	100
2	B	231/231 (100%)	231 (100%)	0	100	100
2	C	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	D	231/231 (100%)	231 (100%)	0	100	100
2	E	231/231 (100%)	231 (100%)	0	100	100
2	F	231/231 (100%)	231 (100%)	0	100	100
2	G	231/231 (100%)	231 (100%)	0	100	100
2	H	231/231 (100%)	231 (100%)	0	100	100
2	I	231/231 (100%)	231 (100%)	0	100	100
2	J	231/231 (100%)	231 (100%)	0	100	100
2	K	231/231 (100%)	231 (100%)	0	100	100
2	L	231/231 (100%)	231 (100%)	0	100	100
2	M	231/231 (100%)	231 (100%)	0	100	100
2	N	231/231 (100%)	231 (100%)	0	100	100
2	O	231/231 (100%)	231 (100%)	0	100	100
2	P	231/231 (100%)	231 (100%)	0	100	100
2	Q	231/231 (100%)	231 (100%)	0	100	100
2	R	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	S	231/231 (100%)	230 (100%)	1 (0%)	84	84
2	T	231/231 (100%)	231 (100%)	0	100	100
3	a	95/95 (100%)	95 (100%)	0	100	100
3	b	95/95 (100%)	95 (100%)	0	100	100
3	c	95/95 (100%)	95 (100%)	0	100	100
3	d	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	f	95/95 (100%)	95 (100%)	0	100	100
3	g	95/95 (100%)	95 (100%)	0	100	100
3	h	95/95 (100%)	95 (100%)	0	100	100
3	i	95/95 (100%)	95 (100%)	0	100	100
3	j	95/95 (100%)	95 (100%)	0	100	100
3	k	95/95 (100%)	95 (100%)	0	100	100
3	l	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	m	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	n	95/95 (100%)	95 (100%)	0	100	100
3	o	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	p	95/95 (100%)	95 (100%)	0	100	100
3	q	95/95 (100%)	94 (99%)	1 (1%)	65	76
3	r	95/95 (100%)	95 (100%)	0	100	100
3	s	95/95 (100%)	95 (100%)	0	100	100
3	t	95/95 (100%)	95 (100%)	0	100	100
All	All	6700/6700 (100%)	6692 (100%)	8 (0%)	88	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	364	LEU
2	R	73	THR
3	o	65	LEU
3	m	65	LEU
3	q	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	54	GLN
3	r	14	HIS
2	O	218	GLN
2	Q	141	GLN
2	T	96	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	1.36	2 (22%) 2 2	58, 65, 74, 78	0
1	2	9/9 (100%)	1.17	0 100 100	45, 52, 60, 64	0
1	3	9/9 (100%)	1.67	3 (33%) 1 1	39, 42, 49, 56	0
1	4	9/9 (100%)	1.22	0 100 100	45, 50, 63, 66	0
1	5	9/9 (100%)	1.91	3 (33%) 1 1	52, 56, 59, 64	0
1	6	9/9 (100%)	1.01	1 (11%) 10 9	44, 50, 56, 66	0
1	7	9/9 (100%)	1.81	4 (44%) 0 0	39, 45, 49, 64	0
1	8	9/9 (100%)	1.25	2 (22%) 2 2	31, 36, 49, 54	0
1	U	9/9 (100%)	1.35	0 100 100	58, 62, 70, 72	0
1	V	9/9 (100%)	1.55	2 (22%) 2 2	62, 73, 86, 96	0
1	W	9/9 (100%)	1.63	2 (22%) 2 2	42, 45, 54, 57	0
1	X	9/9 (100%)	1.67	2 (22%) 2 2	44, 52, 64, 70	0
1	Y	9/9 (100%)	1.38	2 (22%) 2 2	36, 46, 52, 60	0
1	Z	9/9 (100%)	1.35	0 100 100	68, 69, 79, 84	0
1	u	9/9 (100%)	1.36	1 (11%) 10 9	53, 58, 65, 69	0
1	v	9/9 (100%)	0.95	1 (11%) 10 9	51, 55, 61, 61	0
1	w	9/9 (100%)	1.62	2 (22%) 2 2	52, 57, 68, 72	0
1	x	9/9 (100%)	1.32	1 (11%) 10 9	44, 49, 60, 63	0
1	y	9/9 (100%)	1.33	1 (11%) 10 9	32, 39, 49, 51	0
1	z	9/9 (100%)	1.57	1 (11%) 10 9	55, 57, 72, 76	0
2	A	275/275 (100%)	1.11	33 (12%) 9 7	36, 74, 90, 98	5 (1%)
2	B	275/275 (100%)	1.01	27 (9%) 13 10	24, 62, 76, 84	5 (1%)
2	C	275/275 (100%)	1.22	45 (16%) 4 4	39, 83, 98, 106	5 (1%)
2	D	275/275 (100%)	0.91	16 (5%) 29 19	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%)	1.13	38 (13%) 6 5	27, 61, 82, 98	5 (1%)
2	F	275/275 (100%)	1.16	32 (11%) 9 8	28, 58, 79, 93	5 (1%)
2	G	275/275 (100%)	1.04	31 (11%) 10 8	27, 64, 84, 102	5 (1%)
2	H	275/275 (100%)	0.94	21 (7%) 20 14	22, 52, 71, 94	5 (1%)
2	I	275/275 (100%)	0.85	15 (5%) 30 21	15, 40, 58, 78	5 (1%)
2	J	275/275 (100%)	0.87	14 (5%) 33 22	17, 38, 54, 74	5 (1%)
2	K	275/275 (100%)	1.13	24 (8%) 16 12	35, 78, 95, 103	5 (1%)
2	L	275/275 (100%)	0.95	15 (5%) 30 21	27, 58, 75, 84	4 (1%)
2	M	275/275 (100%)	0.98	26 (9%) 14 11	31, 70, 88, 106	5 (1%)
2	N	275/275 (100%)	0.92	17 (6%) 26 18	23, 53, 77, 87	5 (1%)
2	O	275/275 (100%)	1.09	31 (11%) 10 8	22, 53, 80, 91	5 (1%)
2	P	275/275 (100%)	0.96	23 (8%) 17 13	17, 47, 67, 85	5 (1%)
2	Q	275/275 (100%)	1.09	33 (12%) 9 7	25, 61, 84, 100	5 (1%)
2	R	275/275 (100%)	1.12	32 (11%) 9 8	24, 51, 73, 88	5 (1%)
2	S	275/275 (100%)	0.92	19 (6%) 23 16	20, 44, 64, 89	4 (1%)
2	T	275/275 (100%)	0.71	13 (4%) 36 24	16, 37, 54, 74	4 (1%)
3	a	100/100 (100%)	1.26	14 (14%) 6 5	32, 85, 100, 108	1 (1%)
3	b	100/100 (100%)	0.87	3 (3%) 52 35	20, 55, 72, 80	1 (1%)
3	c	100/100 (100%)	1.45	20 (20%) 3 2	30, 88, 106, 114	1 (1%)
3	d	100/100 (100%)	0.80	3 (3%) 52 35	19, 51, 70, 76	1 (1%)
3	e	100/100 (100%)	1.40	20 (20%) 3 2	22, 72, 98, 102	1 (1%)
3	f	100/100 (100%)	1.23	16 (16%) 5 4	22, 58, 70, 80	1 (1%)
3	g	100/100 (100%)	1.30	16 (16%) 5 4	26, 76, 89, 94	1 (1%)
3	h	100/100 (100%)	0.78	5 (5%) 34 23	21, 44, 61, 74	1 (1%)
3	i	100/100 (100%)	0.65	3 (3%) 52 35	11, 31, 49, 57	1 (1%)
3	j	100/100 (100%)	0.59	3 (3%) 52 35	12, 31, 50, 59	1 (1%)
3	k	100/100 (100%)	1.23	11 (11%) 10 9	28, 88, 101, 109	1 (1%)
3	l	100/100 (100%)	1.01	8 (8%) 18 14	17, 54, 73, 81	1 (1%)
3	m	100/100 (100%)	1.09	12 (12%) 9 7	25, 72, 91, 101	1 (1%)
3	n	100/100 (100%)	0.89	2 (2%) 65 46	15, 54, 73, 86	1 (1%)
3	o	100/100 (100%)	1.33	15 (15%) 5 5	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%)	0.76	2 (2%) 65 46	16, 40, 62, 76	1 (1%)
3	q	100/100 (100%)	1.46	23 (23%) 2 2	30, 78, 93, 97	1 (1%)
3	r	100/100 (100%)	1.12	11 (11%) 10 9	20, 49, 72, 92	1 (1%)
3	s	100/100 (100%)	0.76	4 (4%) 42 28	13, 35, 56, 62	1 (1%)
3	t	100/100 (100%)	0.66	2 (2%) 65 46	14, 32, 49, 57	1 (1%)
All	All	7680/7680 (100%)	1.02	728 (9%) 14 11	11, 57, 88, 114	117 (1%)

The worst 5 of 728 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	1	GLY	7.1
2	Q	1	GLY	6.5
2	O	249	VAL	6.3
3	e	368	THR	6.0
2	G	1	GLY	5.3

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.