



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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-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

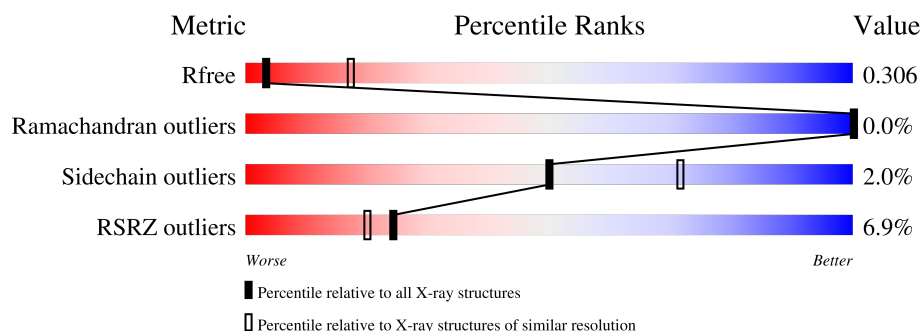
1 Overall quality at a glance ⓘ

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 ≥ 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	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	2	9	<div> <div></div> <div>100%</div> </div>
1	3	9	<div> <div>22%</div> <div> <div></div> <div>100%</div> </div> </div>
1	4	9	<div> <div></div> <div>100%</div> </div>
1	5	9	<div> <div>33%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	6	9	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
2	L	275	<div> <div>3%</div> <div>97%</div> </div>
2	M	275	<div> <div>6%</div> <div>98%</div> </div>
2	N	275	<div> <div>5%</div> <div>99%</div> </div>
2	O	275	<div> <div>8%</div> <div>99%</div> </div>
2	P	275	<div> <div>6%</div> <div>98%</div> </div>
2	Q	275	<div> <div>9%</div> <div>98%</div> </div>
2	R	275	<div> <div>10%</div> <div>98%</div> </div>
2	S	275	<div> <div>4%</div> <div>98%</div> </div>
2	T	275	<div> <div>4%</div> <div>99%</div> </div>
3	a	100	<div> <div>13%</div> <div>98%</div> </div>
3	b	100	<div> <div>2%</div> <div>97%</div> </div>
3	c	100	<div> <div>16%</div> <div>96%</div> </div>
3	d	100	<div> <div>2%</div> <div>99%</div> </div>
3	e	100	<div> <div>16%</div> <div>98%</div> </div>
3	f	100	<div> <div>14%</div> <div>98%</div> </div>
3	g	100	<div> <div>14%</div> <div>98%</div> </div>
3	h	100	<div> <div>3%</div> <div>99%</div> </div>
3	i	100	<div> <div>3%</div> <div>98%</div> </div>
3	j	100	<div> <div>2%</div> <div>99%</div> </div>
3	k	100	<div> <div>9%</div> <div>96%</div> </div>
3	l	100	<div> <div>6%</div> <div>98%</div> </div>
3	m	100	<div> <div>8%</div> <div>97%</div> </div>
3	n	100	<div> <div>2%</div> <div>99%</div> </div>
3	o	100	<div> <div>11%</div> <div>98%</div> </div>
3	p	100	<div> <div>%</div> <div>98%</div> </div>

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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 [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Replication and transcription activator



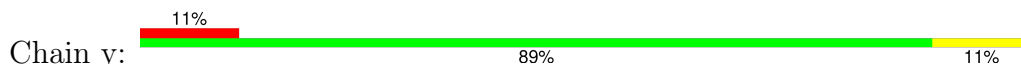
- Molecule 1: Replication and transcription activator



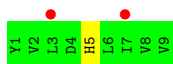
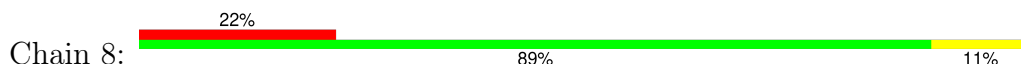
- Molecule 1: Replication and transcription activator



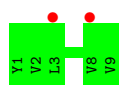
- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator

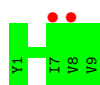


- Molecule 1: Replication and transcription activator

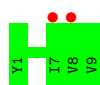


There are no outlier residues recorded for this chain.

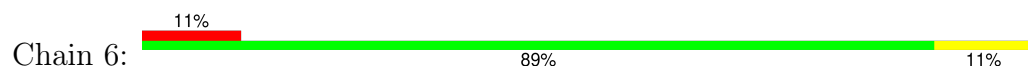
- Molecule 1: Replication and transcription activator



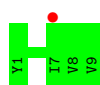
- Molecule 1: Replication and transcription activator



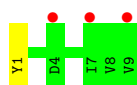
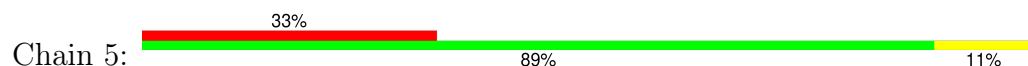
- Molecule 1: Replication and transcription activator



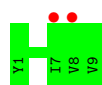
- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- Molecule 1: Replication and transcription activator



- 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



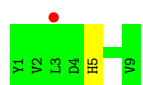
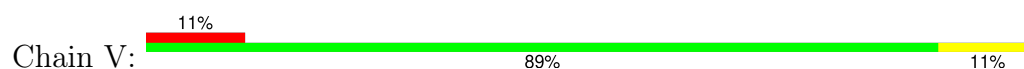
There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

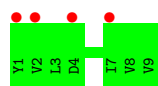
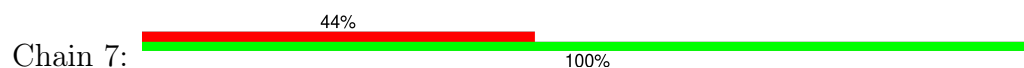


There are no outlier residues recorded for this chain.

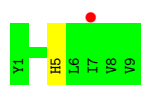
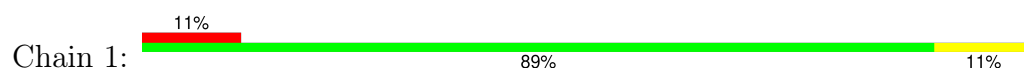
- Molecule 1: Replication and transcription activator



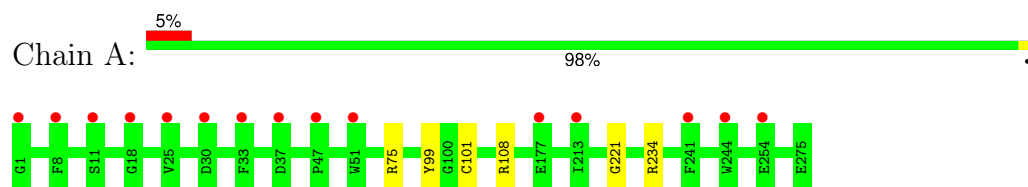
- Molecule 1: Replication and transcription activator



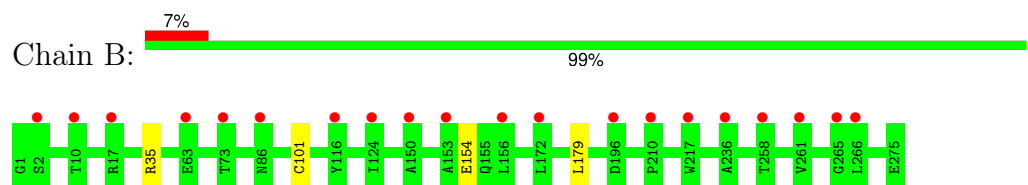
- Molecule 1: Replication and transcription activator



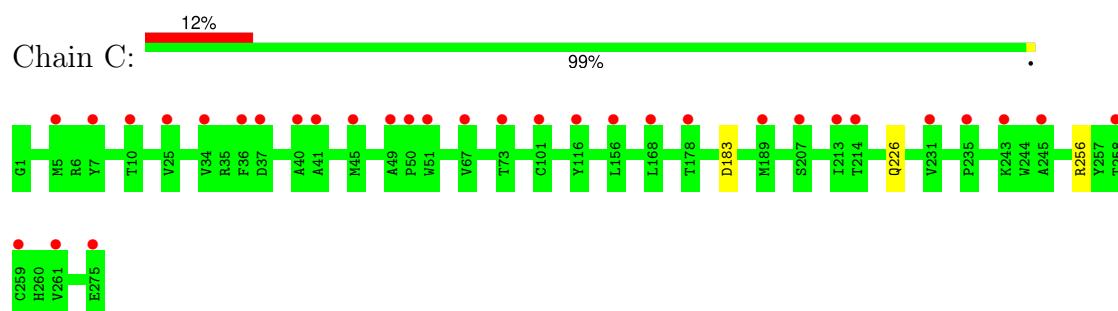
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



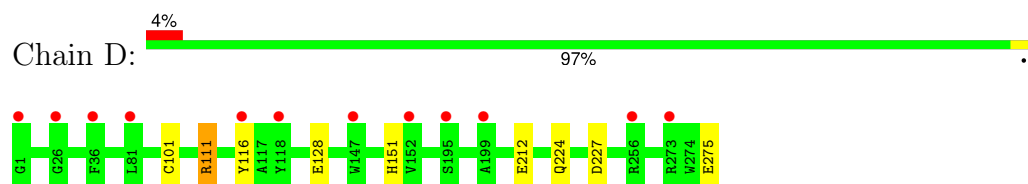
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



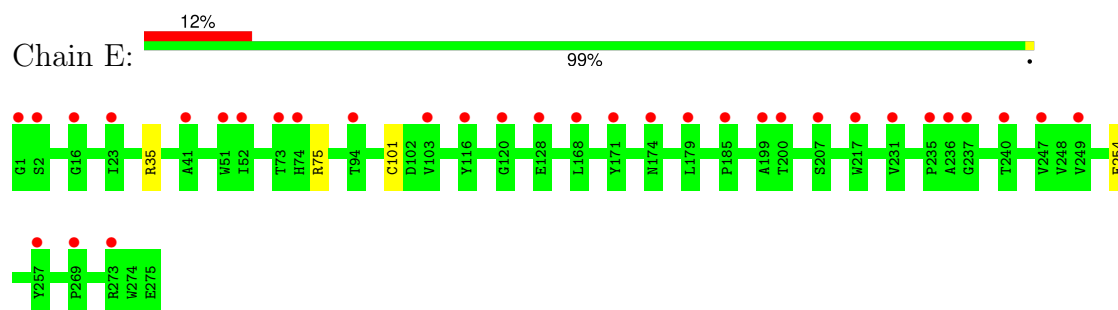
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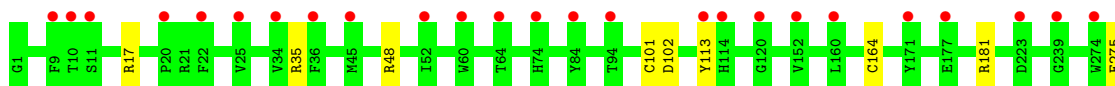


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

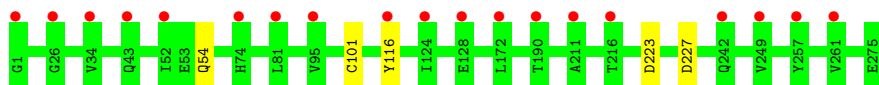


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

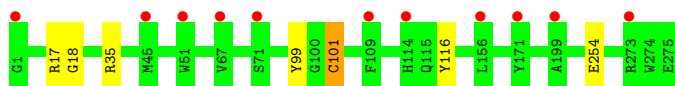




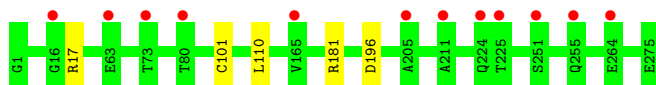
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



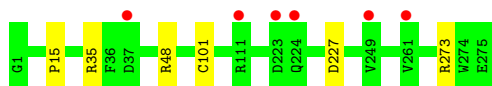
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



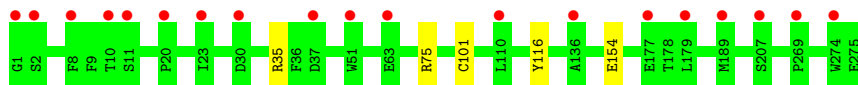
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



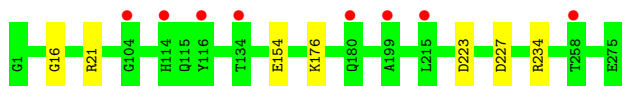
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



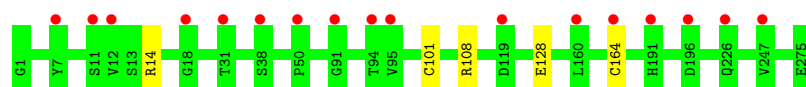
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



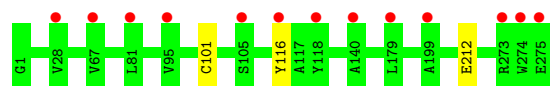
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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



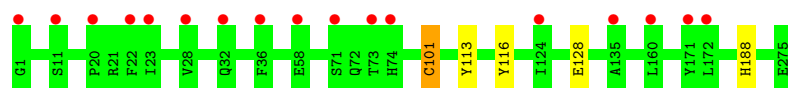
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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



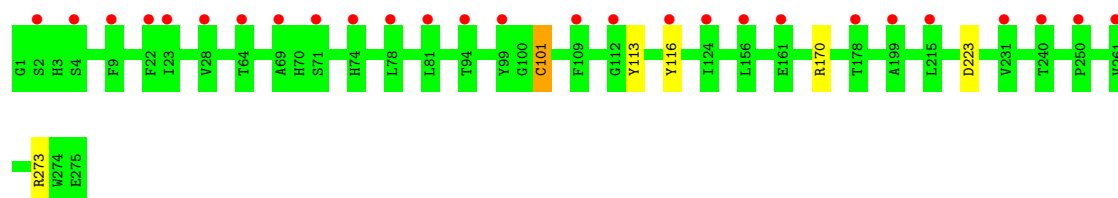
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



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

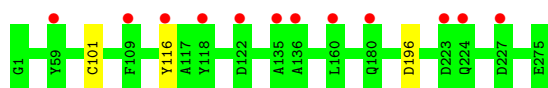


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

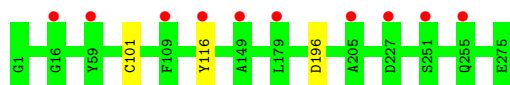


- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain

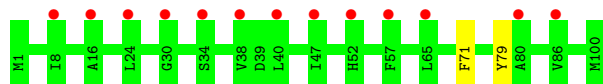




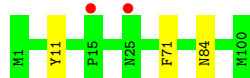
- Molecule 2: HLA class I histocompatibility antigen, A-2 alpha chain



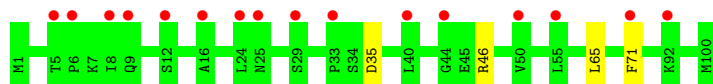
- Molecule 3: Beta-2-microglobulin



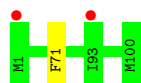
- Molecule 3: Beta-2-microglobulin



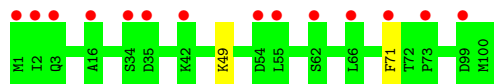
- Molecule 3: Beta-2-microglobulin



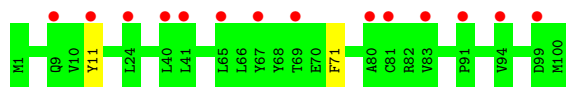
- Molecule 3: Beta-2-microglobulin



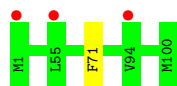
- Molecule 3: Beta-2-microglobulin



- Molecule 3: Beta-2-microglobulin



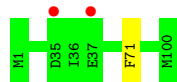
- Molecule 3: Beta-2-microglobulin



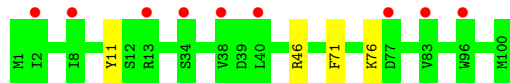
- Molecule 3: Beta-2-microglobulin



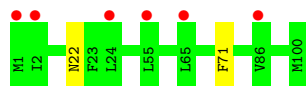
- Molecule 3: Beta-2-microglobulin



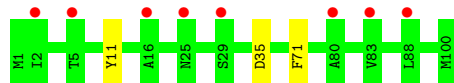
- Molecule 3: Beta-2-microglobulin



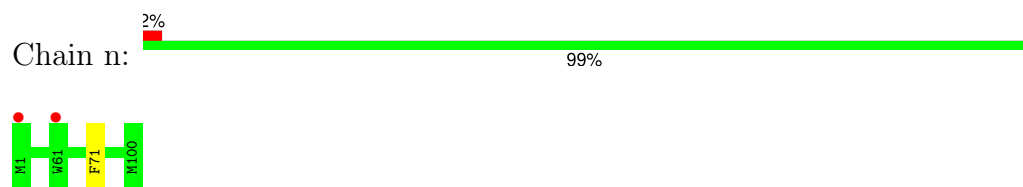
- Molecule 3: Beta-2-microglobulin



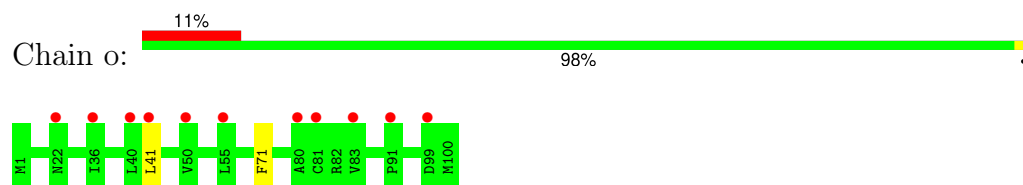
- Molecule 3: Beta-2-microglobulin



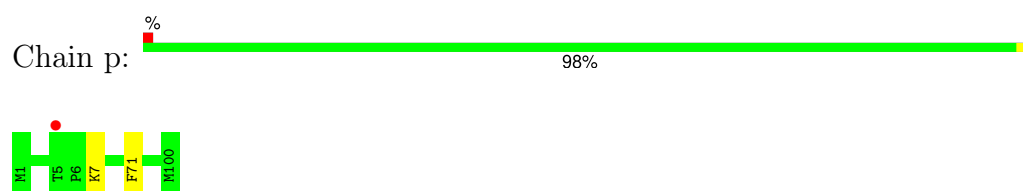
• Molecule 3: Beta-2-microglobulin



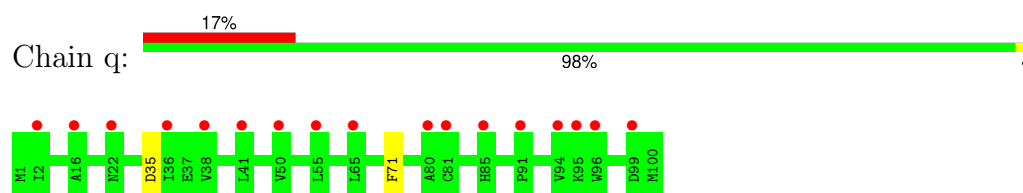
• Molecule 3: Beta-2-microglobulin



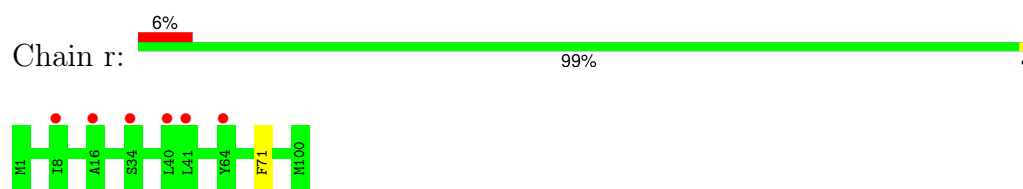
• Molecule 3: Beta-2-microglobulin



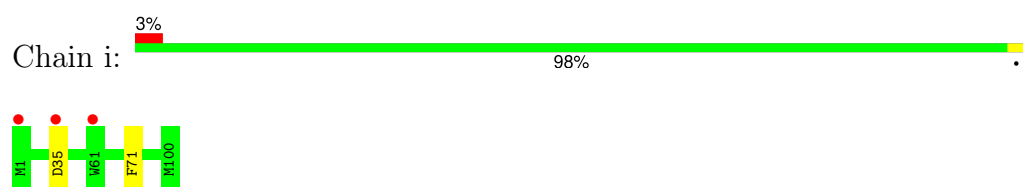
• Molecule 3: Beta-2-microglobulin



• Molecule 3: Beta-2-microglobulin

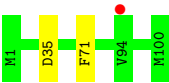


• Molecule 3: Beta-2-microglobulin

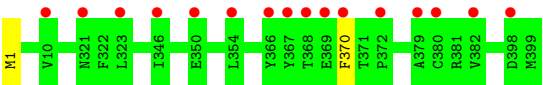


• Molecule 3: Beta-2-microglobulin





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.01Å)	Xtriage
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 ²)	39.6	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	63200	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	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.

The worst 5 of 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

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

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	q	71	PHE
2	R	170	ARG
2	T	196	ASP
3	g	11	TYR
2	G	227	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	188	HIS
2	P	188	HIS
2	T	192	HIS
2	I	192	HIS
2	T	155	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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(Å²)	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 ²)	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%)

The worst 5 of 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

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.