



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:38 PM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

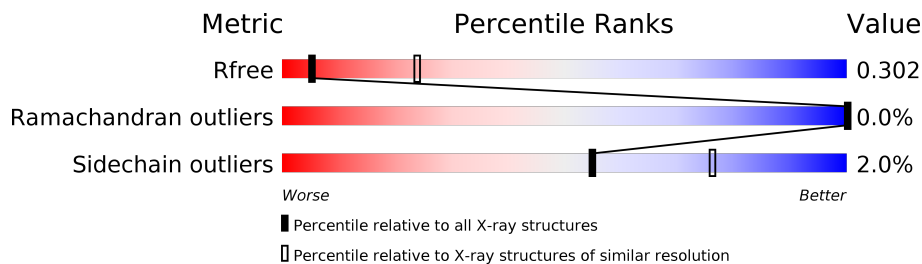
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.




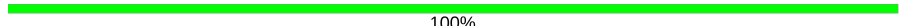

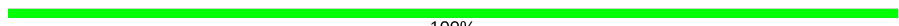













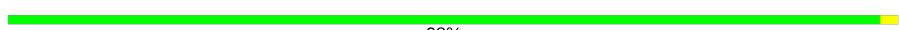
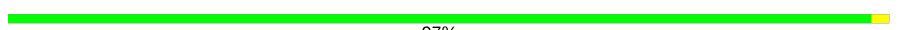
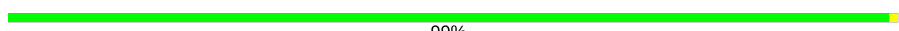

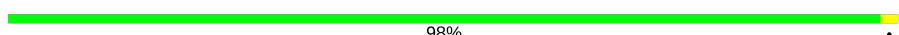
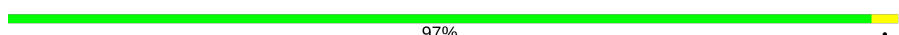
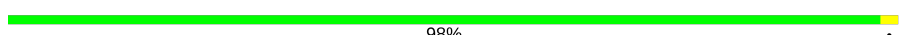
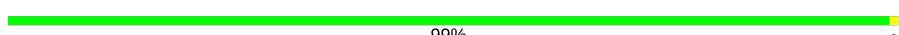
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 on 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	9	
1	2	9	
1	3	9	
1	4	9	
1	5	9	
1	6	9	
1	7	9	
1	8	9	
1	U	9	


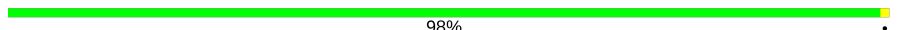
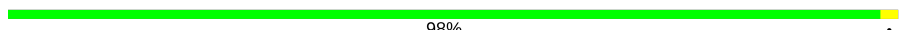
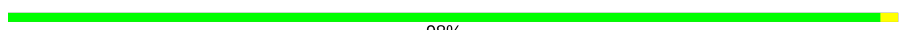











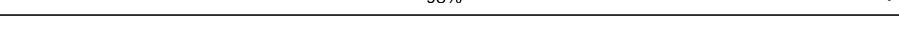
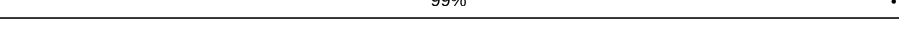
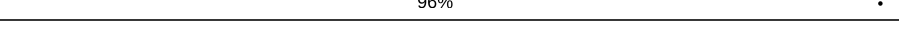
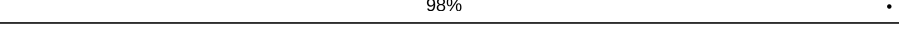
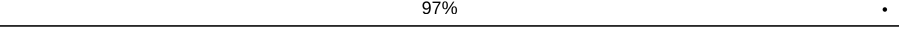
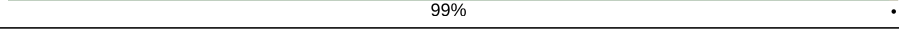
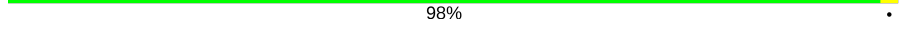
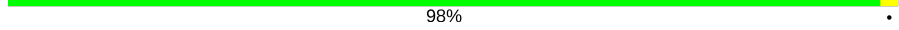
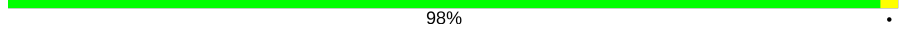
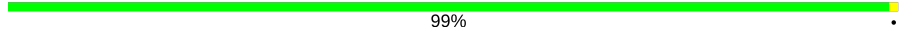
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Mol	Chain	Length	Quality of chain
1	V	9	 89% 11%
1	W	9	 100%
1	X	9	 100%
1	Y	9	 100%
1	Z	9	 100%
1	u	9	 100%
1	v	9	 100%
1	w	9	 100%
1	x	9	 100%
1	y	9	 89% 11%
1	z	9	 100%
2	A	275	 98% .
2	B	275	 99% .
2	C	275	 99% .
2	D	275	 97% .
2	E	275	 99% .
2	F	275	 97% .
2	G	275	 98% .
2	H	275	 97% .
2	I	275	 99% .
2	J	275	 98% .
2	K	275	 98% .
2	L	275	 97% .
2	M	275	 98% .
2	N	275	 99% .

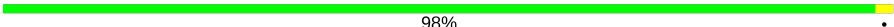
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Mol	Chain	Length	Quality of chain
2	O	275	 99%
2	P	275	 98%
2	Q	275	 98%
2	R	275	 98%
2	S	275	 98%
2	T	275	 99%
3	a	100	 98%
3	b	100	 97%
3	c	100	 96%
3	d	100	 99%
3	e	100	 98%
3	f	100	 98%
3	g	100	 98%
3	h	100	 99%
3	i	100	 98%
3	j	100	 99%
3	k	100	 96%
3	l	100	 98%
3	m	100	 97%
3	n	100	 99%
3	o	100	 98%
3	p	100	 98%
3	q	100	 98%
3	r	100	 99%
3	s	100	 95% 5%

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Mol	Chain	Length	Quality of chain
3	t	100	 98%

## 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
			Total	C	N	O			
1	Z	9	76	52	11	13	0	0	0
1	V	9	76	52	11	13	0	0	0
1	7	9	76	52	11	13	0	0	0
1	1	9	76	52	11	13	0	0	0

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

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

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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

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. 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. 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

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain u:  100%


There are no outlier residues recorded for this chain.

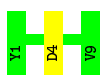
- Molecule 1: Replication and transcription activator

Chain z:  100%


There are no outlier residues recorded for this chain.

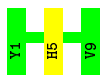
- Molecule 1: Replication and transcription activator

Chain y:  89% 11%



- Molecule 1: Replication and transcription activator

Chain 8:  89% 11%



- Molecule 1: Replication and transcription activator

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain 3:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain 6:  89% 11%



- Molecule 1: Replication and transcription activator

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain 5:  89% 11%



- Molecule 1: Replication and transcription activator

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Replication and transcription activator

Chain V:  89% 11%




- Molecule 1: Replication and transcription activator

Chain 7:  100%

There are no outlier residues recorded for this chain.

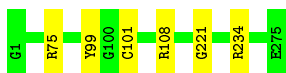
- Molecule 1: Replication and transcription activator

Chain 1:  89% 11%



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

Chain A:  98%



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

Chain B:  99%



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

Chain C:  99%



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

Chain D:  97%



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

Chain E:  99%



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

Chain F:  97%



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

Chain G:  98%



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

Chain H:  97%



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

Chain S:  98%



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

Chain J:  98%



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

Chain K:  98%



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

Chain L:  97%



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

Chain M:  98%



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

Chain N:  99%



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

Chain O:  99%



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

Chain P:  98%



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

Chain Q:  98%



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

Chain R:  98%



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

Chain I:  99%



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

Chain T:  99%



- Molecule 3: Beta-2-microglobulin

Chain a:  98%



- Molecule 3: Beta-2-microglobulin

Chain b:  97%



- Molecule 3: Beta-2-microglobulin

Chain c:  96%



- Molecule 3: Beta-2-microglobulin

Chain d:  99%



- Molecule 3: Beta-2-microglobulin

Chain f:  98%



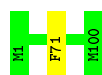
• Molecule 3: Beta-2-microglobulin

Chain g:  98%



• Molecule 3: Beta-2-microglobulin

Chain h:  99%



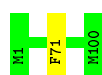
• Molecule 3: Beta-2-microglobulin

Chain s:  95% 5%



• Molecule 3: Beta-2-microglobulin

Chain j:  99%



• Molecule 3: Beta-2-microglobulin

Chain k:  96%



• Molecule 3: Beta-2-microglobulin

Chain l:  98%



• Molecule 3: Beta-2-microglobulin

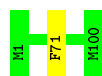


Chain m:  97%



• Molecule 3: Beta-2-microglobulin

Chain n:  99%



• Molecule 3: Beta-2-microglobulin

Chain o:  98%



• Molecule 3: Beta-2-microglobulin

Chain p:  98%



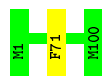
• Molecule 3: Beta-2-microglobulin

Chain q:  98%



• Molecule 3: Beta-2-microglobulin

Chain r:  99%



• Molecule 3: Beta-2-microglobulin

Chain i:  98%



• Molecule 3: Beta-2-microglobulin

Chain t:  98%



• Molecule 3: Beta-2-microglobulin

Chain e:  98%



## 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 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (111.42-3.30) 89.0 (111.42-3.00)	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 0.284 , 0.302	Depositor DCC
$R_{free}$ test set	1516 reflections (0.70%)	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 , 17.3	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	0.81	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

### 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.

All (7) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	34	66
2	I	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	J	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	34	66
2	K	273/275 (99%)	263 (96%)	10 (4%)	0	100	100
2	L	273/275 (99%)	264 (97%)	8 (3%)	1 (0%)	34	66
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 [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%)	8 (89%)	1 (11%)	6	23
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%)	6	23
1	6	9/9 (100%)	8 (89%)	1 (11%)	6	23
1	7	9/9 (100%)	9 (100%)	0	100	100
1	8	9/9 (100%)	8 (89%)	1 (11%)	6	23
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%)	6	23
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%)	6	23
1	z	9/9 (100%)	9 (100%)	0	100	100
2	A	231/231 (100%)	228 (99%)	3 (1%)	69	82
2	B	231/231 (100%)	227 (98%)	4 (2%)	60	78
2	C	231/231 (100%)	228 (99%)	3 (1%)	69	82
2	D	231/231 (100%)	223 (96%)	8 (4%)	36	64
2	E	231/231 (100%)	227 (98%)	4 (2%)	60	78
2	F	231/231 (100%)	224 (97%)	7 (3%)	41	68
2	G	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	H	231/231 (100%)	225 (97%)	6 (3%)	46	71
2	I	231/231 (100%)	228 (99%)	3 (1%)	69	82
2	J	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	K	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	L	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	M	231/231 (100%)	228 (99%)	3 (1%)	69	82
2	N	231/231 (100%)	228 (99%)	3 (1%)	69	82
2	O	231/231 (100%)	229 (99%)	2 (1%)	78	87
2	P	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	Q	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	R	231/231 (100%)	225 (97%)	6 (3%)	46	71
2	S	231/231 (100%)	226 (98%)	5 (2%)	52	74
2	T	231/231 (100%)	228 (99%)	3 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	b	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	c	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	d	95/95 (100%)	94 (99%)	1 (1%)	73	85
3	e	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	f	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	g	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	h	95/95 (100%)	94 (99%)	1 (1%)	73	85
3	i	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	j	95/95 (100%)	94 (99%)	1 (1%)	73	85
3	k	95/95 (100%)	91 (96%)	4 (4%)	30	60
3	l	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	m	95/95 (100%)	92 (97%)	3 (3%)	39	67
3	n	95/95 (100%)	94 (99%)	1 (1%)	73	85
3	o	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	p	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	q	95/95 (100%)	93 (98%)	2 (2%)	53	75
3	r	95/95 (100%)	94 (99%)	1 (1%)	73	85
3	s	95/95 (100%)	91 (96%)	4 (4%)	30	60
3	t	95/95 (100%)	93 (98%)	2 (2%)	53	75
All	All	6700/6700 (100%)	6564 (98%)	136 (2%)	55	76

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

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

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

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

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

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

Mol	Chain	Res	Type
1	y	5	HIS
1	2	5	HIS
1	7	5	HIS
2	A	70	HIS
2	A	192	HIS
2	N	155	GLN
2	O	54	GLN
2	O	188	HIS
2	P	188	HIS
2	R	174	ASN
2	I	192	HIS
2	T	155	GLN
2	T	192	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.