



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 04:01 PM EDT

PDB ID : 4V9E  
Title : Crystal Structure of Rift Valley Fever Virus Nucleocapsid Protein Hexamer Bound to Single-stranded RNA.  
Authors : Raymond, D.D.; Smith, J.L.  
Deposited on : 2012-09-19  
Resolution : 3.40 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>.

---

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 : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

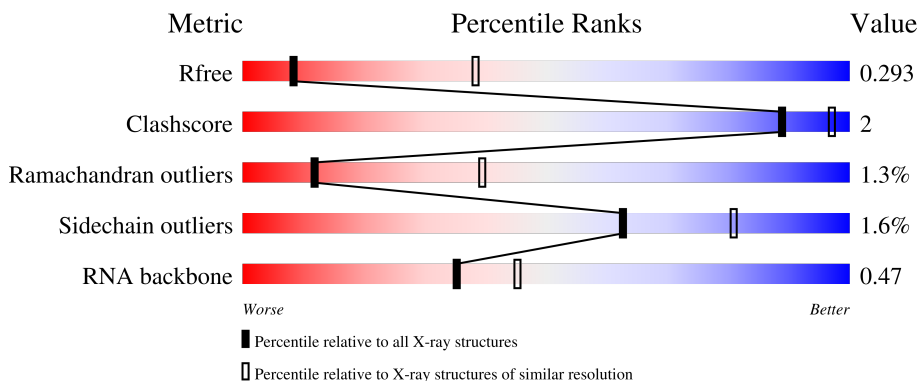
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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.





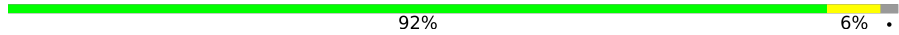



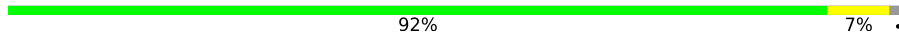
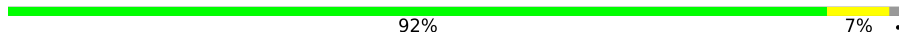


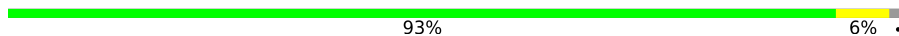














Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RNA backbone	3102	1006 (3.84-2.96)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	245	88% 10% .
1	AB	245	91% 8% .
1	AC	245	90% 8% .
1	AD	245	90% 8% .
1	AE	245	91% 7% .
1	AF	245	88% 10% .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	AG	245	 91% 7%
1	AH	245	 91% 7%
1	AI	245	 92% 6%
1	AJ	245	 89% 9%
1	AK	245	 89% 9%
1	AL	245	 90% 9%
1	AM	245	 92% 7%
1	AN	245	 92% 7%
1	AO	245	 92% 7%
1	AP	245	 91% 8%
1	AQ	245	 93% 6%
1	AR	245	 91% 7%
1	BA	245	 89% 9%
1	BB	245	 91% 7%
1	BC	245	 91% 7%
1	BD	245	 90% 8%
1	BE	245	 89% 9%
1	BF	245	 89% 9%
1	BG	245	 91% 7%
1	BH	245	 90% 8%
1	BI	245	 90% 9%
1	BJ	245	 89% 9%
1	BK	245	 91% 7%
1	BL	245	 90% 8%
1	BM	245	 91% 7%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	BN	245	 91% 7% .
1	BO	245	 91% 8% .
1	BP	245	 91% 7% .
1	BQ	245	 90% 8% ..
1	BR	245	 91% 7% .
2	Aa	36	 64% 36%
2	Ag	36	 64% 36%
2	Am	36	 67% 33%
2	Ba	36	 64% 36%
2	Bg	36	 67% 33%
2	Bm	36	 72% 28%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 72072 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	241	1882	1188	339	343	12	0	0	0
1	AB	241	1882	1188	339	343	12	0	0	0
1	AC	241	1882	1188	339	343	12	0	0	0
1	AD	241	1882	1188	339	343	12	0	0	0
1	AE	241	1882	1188	339	343	12	0	0	0
1	AF	241	1882	1188	339	343	12	0	0	0
1	AG	241	1882	1188	339	343	12	0	0	0
1	AH	241	1882	1188	339	343	12	0	0	0
1	AI	241	1882	1188	339	343	12	0	0	0
1	AJ	241	1882	1188	339	343	12	0	0	0
1	AK	241	1882	1188	339	343	12	0	0	0
1	AL	241	1882	1188	339	343	12	0	0	0
1	AM	241	1882	1188	339	343	12	0	0	0
1	AN	241	1882	1188	339	343	12	0	0	0
1	AO	241	1882	1188	339	343	12	0	0	0
1	AP	241	1882	1188	339	343	12	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	AR	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BA	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BB	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BC	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BD	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BE	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BF	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BG	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BH	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BI	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BJ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BK	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BL	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BM	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BN	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BO	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BP	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BQ	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			
1	BR	241	Total	C	N	O	S	0	0	0
			1882	1188	339	343	12			

- Molecule 2 is a RNA chain called 35-mer poly(U) RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Aa	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ag	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Am	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ba	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bg	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bm	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			

### 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. 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: Nucleocapsid protein

Chain AA: 



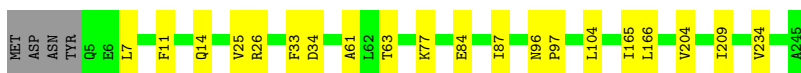
- Molecule 1: Nucleocapsid protein

Chain AB: 



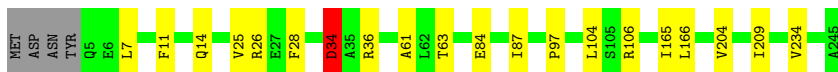
- Molecule 1: Nucleocapsid protein

Chain AC: 



- Molecule 1: Nucleocapsid protein

Chain AD: 




- Molecule 1: Nucleocapsid protein

Chain AE: 



- Molecule 1: Nucleocapsid protein

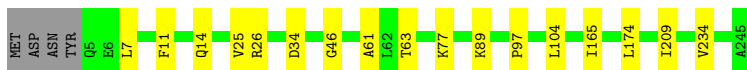
Chain AF: 





- Molecule 1: Nucleocapsid protein

Chain AG: 91% 7%



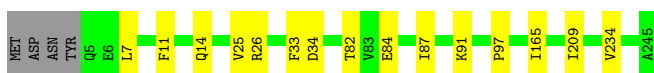
- Molecule 1: Nucleocapsid protein

Chain AH: 91% 7%



- Molecule 1: Nucleocapsid protein

Chain AI: 92% 6%



- Molecule 1: Nucleocapsid protein

Chain AJ: 89% 9%



- Molecule 1: Nucleocapsid protein

Chain AK: 89% 9%



- Molecule 1: Nucleocapsid protein

Chain AL: 90% 9%



- Molecule 1: Nucleocapsid protein

Chain AM: 92% 7%



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



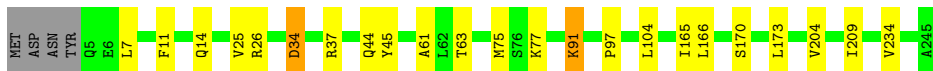
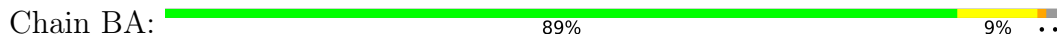
- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



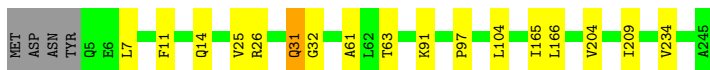
- Molecule 1: Nucleocapsid protein





- Molecule 1: Nucleocapsid protein

Chain BC: 91% 7%



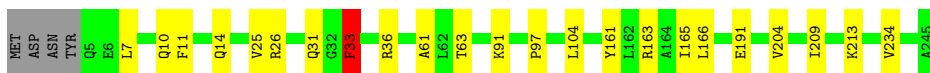
- Molecule 1: Nucleocapsid protein

Chain BD: 90% 8%



- Molecule 1: Nucleocapsid protein

Chain BE: 89% 9%



- Molecule 1: Nucleocapsid protein

Chain BF: 89% 9%



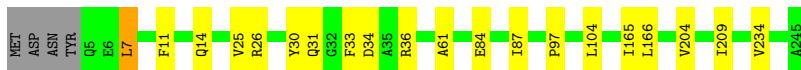
- Molecule 1: Nucleocapsid protein

Chain BG: 91% 7%



- Molecule 1: Nucleocapsid protein

Chain BH: 90% 8%

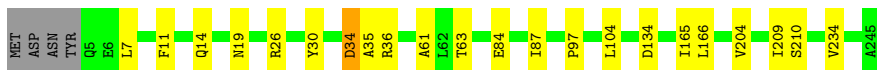
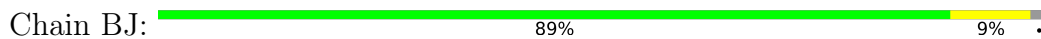


- Molecule 1: Nucleocapsid protein

Chain BI: 90% 9%



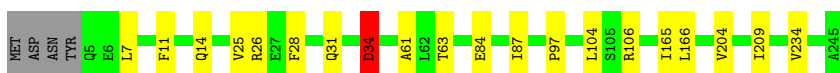
- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



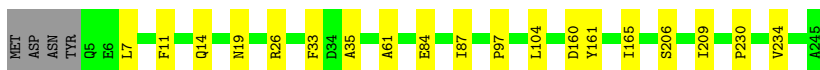
- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein





- Molecule 1: Nucleocapsid protein



- Molecule 1: Nucleocapsid protein



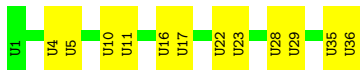
- Molecule 2: 35-mer poly(U) RNA



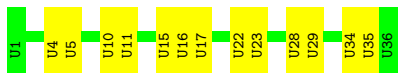
- Molecule 2: 35-mer poly(U) RNA



- Molecule 2: 35-mer poly(U) RNA



- Molecule 2: 35-mer poly(U) RNA



- Molecule 2: 35-mer poly(U) RNA





- Molecule 2: 35-mer poly(U) RNA

Chain Bm:   
72% 28%

A horizontal bar chart for Chain Bm showing 72% green and 28% yellow segments.



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.66Å 173.33Å 172.90Å 119.95° 99.34° 90.12°	Depositor
Resolution (Å)	57.42 – 3.40 57.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (57.42-3.40) 93.9 (57.42-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.40Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.225 , 0.240 0.283 , 0.293	Depositor DCC
$R_{free}$ test set	5935 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtrriage
Anisotropy	0.679	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.316 for -h,k,-k-l	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	72072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	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 21.66 % 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 6.6968e-03.*

<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	AA	0.40	0/1918	0.53	0/2586
1	AB	0.40	0/1918	0.53	0/2586
1	AC	0.40	0/1918	0.53	0/2586
1	AD	0.39	0/1918	0.54	0/2586
1	AE	0.40	0/1918	0.53	0/2586
1	AF	0.40	0/1918	0.53	0/2586
1	AG	0.40	0/1918	0.54	0/2586
1	AH	0.39	0/1918	0.53	0/2586
1	AI	0.40	0/1918	0.53	0/2586
1	AJ	0.40	0/1918	0.56	0/2586
1	AK	0.39	0/1918	0.53	0/2586
1	AL	0.40	0/1918	0.53	0/2586
1	AM	0.39	0/1918	0.53	0/2586
1	AN	0.40	0/1918	0.53	0/2586
1	AO	0.40	0/1918	0.53	0/2586
1	AP	0.40	0/1918	0.53	0/2586
1	AQ	0.40	0/1918	0.53	0/2586
1	AR	0.40	0/1918	0.53	0/2586
1	BA	0.40	0/1918	0.53	0/2586
1	BB	0.40	0/1918	0.53	0/2586
1	BC	0.40	0/1918	0.54	0/2586
1	BD	0.39	0/1918	0.55	0/2586
1	BE	0.40	0/1918	0.53	0/2586
1	BF	0.39	0/1918	0.53	0/2586
1	BG	0.40	0/1918	0.53	0/2586
1	BH	0.40	0/1918	0.54	0/2586
1	BI	0.40	0/1918	0.53	0/2586
1	BJ	0.40	0/1918	0.54	0/2586
1	BK	0.39	0/1918	0.52	0/2586
1	BL	0.39	0/1918	0.52	0/2586
1	BM	0.40	0/1918	0.53	0/2586
1	BN	0.39	0/1918	0.53	0/2586
1	BO	0.40	0/1918	0.54	0/2586
1	BP	0.40	0/1918	0.53	0/2586



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BQ	0.40	0/1918	0.53	0/2586
1	BR	0.40	0/1918	0.54	0/2586
2	Aa	1.10	0/786	0.92	0/1200
2	Ag	1.11	0/786	0.94	0/1200
2	Am	1.12	0/786	0.92	0/1200
2	Ba	1.11	0/786	0.93	0/1200
2	Bg	1.09	0/786	0.92	0/1200
2	Bm	1.11	0/786	0.92	0/1200
All	All	0.47	0/73764	0.57	0/100296

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	AA	1882	0	1906	11	1
1	AB	1882	0	1906	7	0
1	AC	1882	0	1906	9	0
1	AD	1882	0	1906	9	0
1	AE	1882	0	1906	8	0
1	AF	1882	0	1906	11	0
1	AG	1882	0	1906	7	0
1	AH	1882	0	1906	7	0
1	AI	1882	0	1906	6	0
1	AJ	1882	0	1906	12	0
1	AK	1882	0	1906	9	1
1	AL	1882	0	1906	11	0
1	AM	1882	0	1906	6	0
1	AN	1882	0	1906	6	0
1	AO	1882	0	1906	6	0
1	AP	1882	0	1906	9	0
1	AQ	1882	0	1906	5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AR	1882	0	1906	8	0
1	BA	1882	0	1906	12	0
1	BB	1882	0	1906	8	0
1	BC	1882	0	1906	8	0
1	BD	1882	0	1906	12	0
1	BE	1882	0	1906	11	1
1	BF	1882	0	1906	13	0
1	BG	1882	0	1906	9	0
1	BH	1882	0	1906	9	0
1	BI	1882	0	1906	12	1
1	BJ	1882	0	1906	8	0
1	BK	1882	0	1906	7	0
1	BL	1882	0	1906	10	0
1	BM	1882	0	1906	6	0
1	BN	1882	0	1906	8	0
1	BO	1882	0	1906	9	0
1	BP	1882	0	1906	6	0
1	BQ	1882	0	1906	8	0
1	BR	1882	0	1906	8	0
2	Aa	720	0	366	0	0
2	Ag	720	0	366	0	0
2	Am	720	0	366	0	0
2	Ba	720	0	366	0	0
2	Bg	720	0	366	0	0
2	Bm	720	0	366	0	0
All	All	72072	0	70812	257	2

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 2.

The worst 5 of 257 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)
1:BD:10:GLN:HB3	1:BI:19:ASN:HD21	1.35	0.91
1:BA:34:ASP:HB2	1:BA:37:ARG:HB3	1.63	0.81
1:AA:34:ASP:HB3	1:AA:37:ARG:HB3	1.66	0.77
1:BE:10:GLN:HE21	1:BP:207:ASN:HD22	1.35	0.75
1:AA:34:ASP:HB2	1:AA:38:VAL:HG23	1.68	0.74

All (2) 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)
1:AK:161:TYR:OH	1:BI:161:TYR:OH[1_455]	1.89	0.31
1:AA:161:TYR:OH	1:BE:161:TYR:OH[1_455]	1.91	0.29

## 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	AA	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	9	34
1	AB	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	9	34
1	AC	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	9	34
1	AD	239/245 (98%)	225 (94%)	11 (5%)	3 (1%)	12	39
1	AE	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	19	51
1	AF	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	12	39
1	AG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	12	39
1	AH	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	19	51
1	AI	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	12	39
1	AJ	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	12	39
1	AK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	12	39
1	AL	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	12	39
1	AM	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	19	51
1	AN	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	9	34
1	AO	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	19	51
1	AP	239/245 (98%)	225 (94%)	10 (4%)	4 (2%)	9	34
1	AQ	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	19	51
1	AR	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	9	34
1	BA	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	19	51
1	BB	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	12	39

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BC	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	12	39
1	BD	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	19	51
1	BE	239/245 (98%)	222 (93%)	14 (6%)	3 (1%)	12	39
1	BF	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	9	34
1	BG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	12	39
1	BH	239/245 (98%)	223 (93%)	11 (5%)	5 (2%)	7	30
1	BI	239/245 (98%)	226 (95%)	11 (5%)	2 (1%)	19	51
1	BJ	239/245 (98%)	224 (94%)	10 (4%)	5 (2%)	7	30
1	BK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	12	39
1	BL	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	12	39
1	BM	239/245 (98%)	228 (95%)	8 (3%)	3 (1%)	12	39
1	BN	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	12	39
1	BO	239/245 (98%)	224 (94%)	13 (5%)	2 (1%)	19	51
1	BP	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	9	34
1	BQ	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	9	34
1	BR	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	12	39
All	All	8604/8820 (98%)	8131 (94%)	361 (4%)	112 (1%)	12	39

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AJ	35	ALA
1	BC	31	GLN
1	BH	34	ASP
1	BM	30	TYR
1	AA	32	GLY

### 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	AA	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AB	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AC	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	AD	194/198 (98%)	190 (98%)	4 (2%)	53	76
1	AE	194/198 (98%)	190 (98%)	4 (2%)	53	76
1	AF	194/198 (98%)	189 (97%)	5 (3%)	46	72
1	AG	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AH	194/198 (98%)	190 (98%)	4 (2%)	53	76
1	AI	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AJ	194/198 (98%)	190 (98%)	4 (2%)	53	76
1	AK	194/198 (98%)	189 (97%)	5 (3%)	46	72
1	AL	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	AM	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AN	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	AO	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	AP	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	AQ	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	AR	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BA	194/198 (98%)	189 (97%)	5 (3%)	46	72
1	BB	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BC	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	BD	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	BE	194/198 (98%)	189 (97%)	5 (3%)	46	72
1	BF	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BG	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BH	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BI	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	BJ	194/198 (98%)	190 (98%)	4 (2%)	53	76
1	BK	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BL	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BM	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BN	194/198 (98%)	192 (99%)	2 (1%)	76	88

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BO	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BP	194/198 (98%)	192 (99%)	2 (1%)	76	88
1	BQ	194/198 (98%)	191 (98%)	3 (2%)	65	82
1	BR	194/198 (98%)	190 (98%)	4 (2%)	53	76
All	All	6984/7128 (98%)	6872 (98%)	112 (2%)	62	81

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	7	LEU
1	BR	30	TYR
1	BE	31	GLN
1	BR	26	ARG
1	BN	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	BE	14	GLN
1	BI	211	HIS
1	BE	211	HIS
1	BG	211	HIS
1	BK	198	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Aa	30/36 (83%)	13 (43%)	0
2	Ag	30/36 (83%)	13 (43%)	0
2	Am	30/36 (83%)	12 (40%)	0
2	Ba	30/36 (83%)	13 (43%)	0
2	Bg	30/36 (83%)	12 (40%)	0
2	Bm	30/36 (83%)	10 (33%)	0
All	All	180/216 (83%)	73 (40%)	0

5 of 73 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Aa	4	U
2	Aa	5	U
2	Aa	10	U
2	Aa	11	U
2	Aa	14	U

There are no RNA pucker outliers to report.

#### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	Ag	5
2	Ba	5
2	Bg	5
2	Aa	5
2	Am	5
2	Bm	5

The worst 5 of 30 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ag	12:U	O3'	13:U	P	7.07
1	Ba	12:U	O3'	13:U	P	6.29
1	Ag	6:U	O3'	7:U	P	6.03
1	Ag	24:U	O3'	25:U	P	5.86
1	Ba	24:U	O3'	25:U	P	5.80



## 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.