Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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:

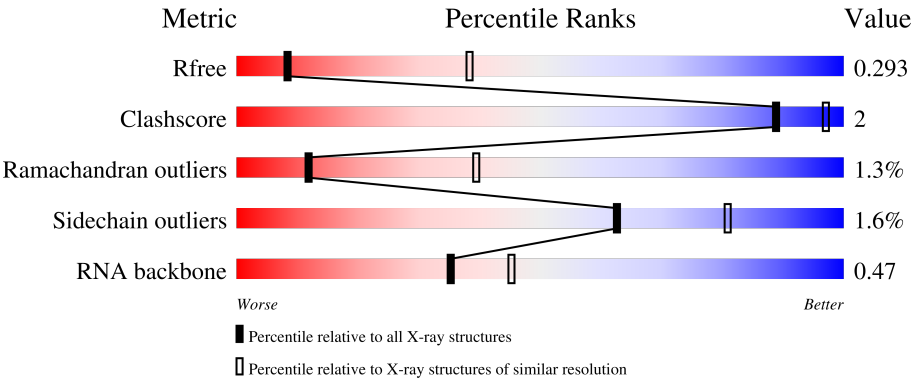
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 >=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 <=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% •

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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%

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Mol	Chain	Length	Quality of chain
1	BN	245	
1	BO	245	
1	BP	245	
1	BQ	245	
1	BR	245	
2	Aa	36	
2	Ag	36	
2	Am	36	
2	Ba	36	
2	Bg	36	
2	Bm	36	

2 Entry composition (i)

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

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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.

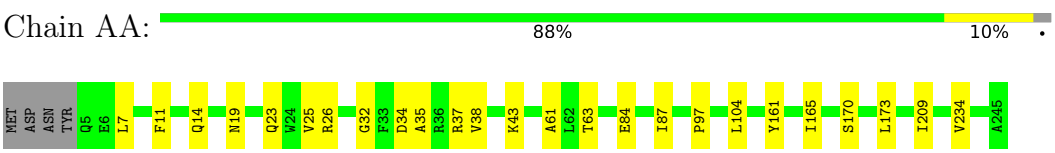
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Aa	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ag	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Am	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ba	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bg	36	Total	C	N	O	P	0	0	0
			720	324	72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

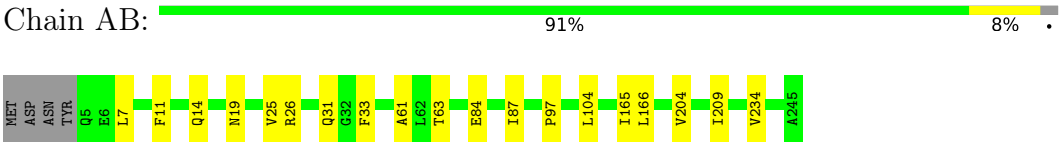
• Molecule 1: Nucleocapsid protein

Chain AA:



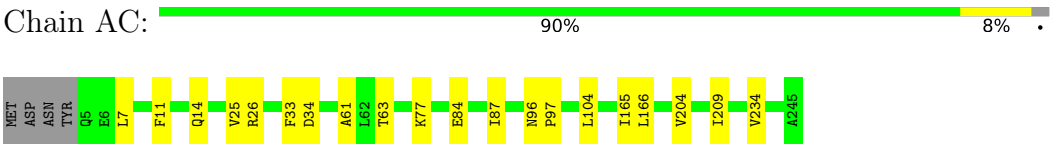
• Molecule 1: Nucleocapsid protein

Chain AB:



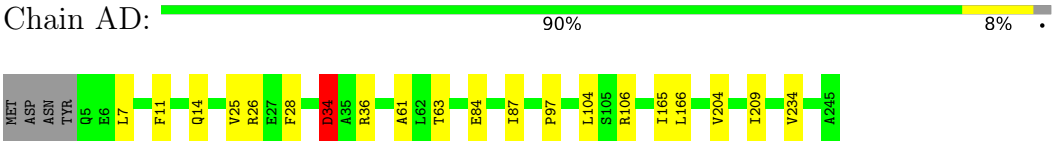
• Molecule 1: Nucleocapsid protein

Chain AC:



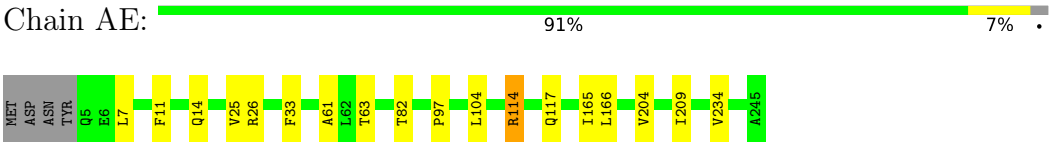
• Molecule 1: Nucleocapsid protein

Chain AD:



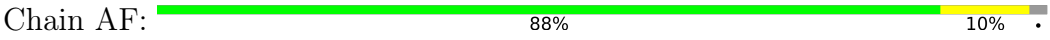
• Molecule 1: Nucleocapsid protein

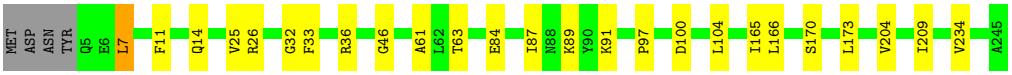
Chain AE:



• Molecule 1: Nucleocapsid protein

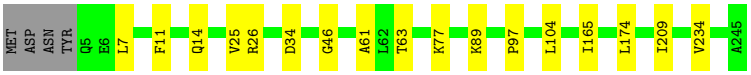
Chain AF:





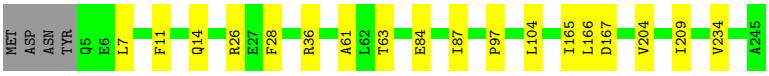
• Molecule 1: Nucleocapsid protein

Chain AG:



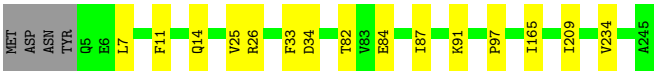
• Molecule 1: Nucleocapsid protein

Chain AH:



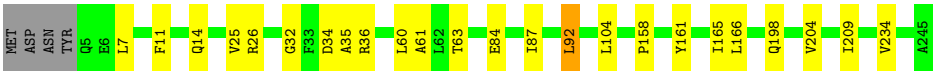
• Molecule 1: Nucleocapsid protein

Chain AI:



• Molecule 1: Nucleocapsid protein

Chain AJ:

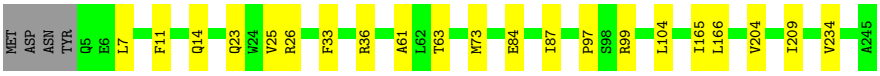


• Molecule 1: Nucleocapsid protein

Chain AK:

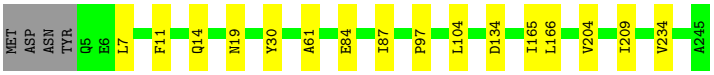
• Molecule 1: Nucleocapsid protein

Chain AL:



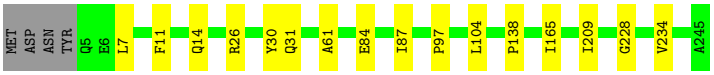
• Molecule 1: Nucleocapsid protein

Chain AM:



• Molecule 1: Nucleocapsid protein

Chain AN:



• Molecule 1: Nucleocapsid protein

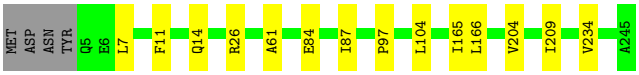
Chain AO:

• Molecule 1: Nucleocapsid protein

Chain AP:

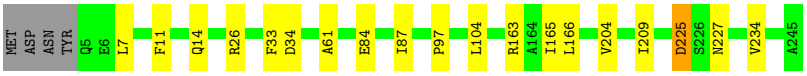
• Molecule 1: Nucleocapsid protein

Chain AQ:



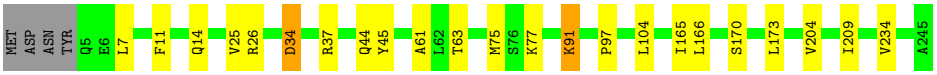
• Molecule 1: Nucleocapsid protein

Chain AR:



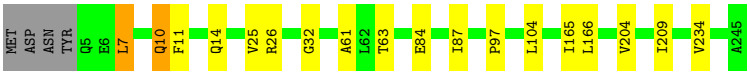
• Molecule 1: Nucleocapsid protein

Chain BA:



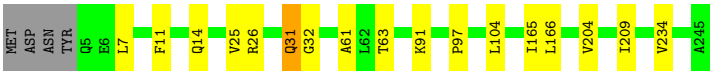
• Molecule 1: Nucleocapsid protein

Chain BB:



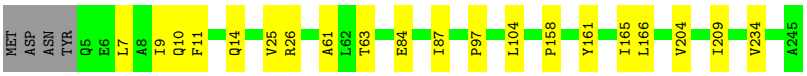
• Molecule 1: Nucleocapsid protein

Chain BC:



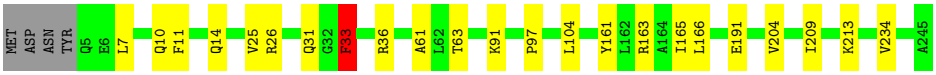
• Molecule 1: Nucleocapsid protein

Chain BD:



• Molecule 1: Nucleocapsid protein

Chain BE:

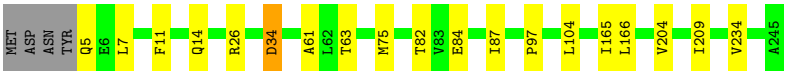


• Molecule 1: Nucleocapsid protein

Chain BF:

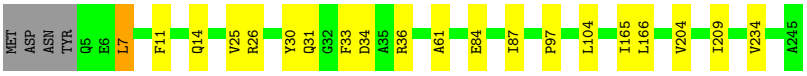
• Molecule 1: Nucleocapsid protein

Chain BG:



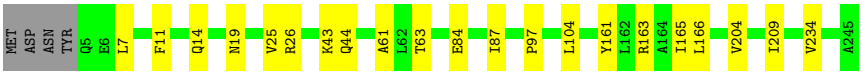
• Molecule 1: Nucleocapsid protein

Chain BH:



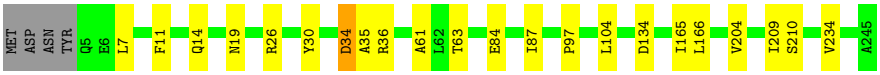
• Molecule 1: Nucleocapsid protein

Chain BI:



• Molecule 1: Nucleocapsid protein

Chain BJ:

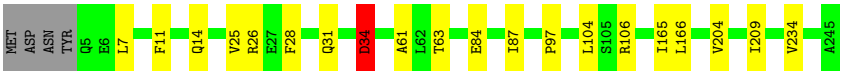


• Molecule 1: Nucleocapsid protein

Chain BK:

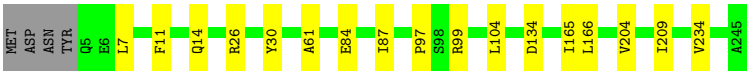
• Molecule 1: Nucleocapsid protein

Chain BL:



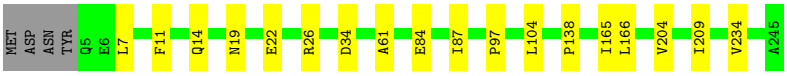
• Molecule 1: Nucleocapsid protein

Chain BM:



• Molecule 1: Nucleocapsid protein

Chain BN:

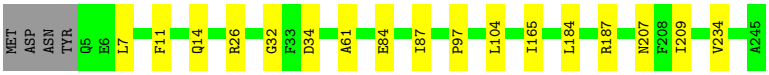


• Molecule 1: Nucleocapsid protein

Chain BO:

• Molecule 1: Nucleocapsid protein

Chain BP:

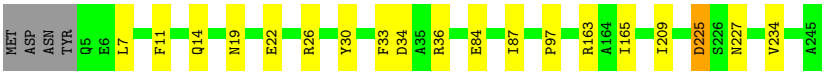


• Molecule 1: Nucleocapsid protein

Chain BQ:

• Molecule 1: Nucleocapsid protein

Chain BR:



• Molecule 2: 35-mer poly(U) RNA

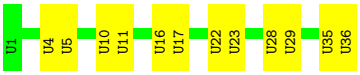
Chain Aa:

• Molecule 2: 35-mer poly(U) RNA

Chain Ag:

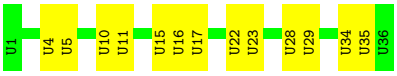
• Molecule 2: 35-mer poly(U) RNA

Chain Am:



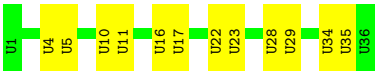
• Molecule 2: 35-mer poly(U) RNA

Chain Ba:



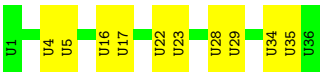
• Molecule 2: 35-mer poly(U) RNA

Chain Bg:



• Molecule 2: 35-mer poly(U) RNA

Chain Bm:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.83 (at 3.40Å)	Xtriage
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^2)	58.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.316 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	72072	wwPDB-VP
Average B, all atoms (Å^2)	73.0	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 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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

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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.

All (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
1:BO:33:PHE:HE1	1:BO:35:ALA:HB3	1.51	0.74
1:AK:10:GLN:HE21	1:AP:207:ASN:HD22	1.36	0.71
1:BH:36:ARG:HG3	1:BO:19:ASN:HD21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:25:VAL:HG23	1:AH:63:THR:HG21	1.79	0.63
1:AG:77:LYS:HB2	1:AL:99:ARG:HH22	1.63	0.63
1:BA:77:LYS:HB2	1:BF:99:ARG:HH22	1.64	0.62
1:BD:10:GLN:HB3	1:BI:19:ASN:ND2	2.13	0.61
1:BA:25:VAL:HG23	1:BB:63:THR:HG21	1.82	0.60
1:AK:25:VAL:HG23	1:AL:63:THR:HG21	1.85	0.59
1:AR:227:ASN:ND2	1:BN:138:PRO:HB3	2.18	0.59
1:AQ:165:ILE:HD13	1:AQ:234:VAL:HG11	1.85	0.58
1:BF:36:ARG:HH21	1:BF:207:ASN:HD21	1.51	0.57
1:BE:25:VAL:HG23	1:BF:63:THR:HG21	1.84	0.57
1:AJ:158:PRO:HD2	1:AJ:161:TYR:HD2	1.69	0.57
1:BR:165:ILE:HD13	1:BR:234:VAL:HG11	1.87	0.57
1:BP:165:ILE:HD13	1:BP:234:VAL:HG11	1.87	0.56
1:AI:25:VAL:HG23	1:AJ:63:THR:HG21	1.85	0.56
1:BH:25:VAL:HG23	1:BI:63:THR:HG21	1.87	0.56
1:AB:165:ILE:HD13	1:AB:234:VAL:HG11	1.88	0.56
1:BB:165:ILE:HD13	1:BB:234:VAL:HG11	1.88	0.56
1:BD:165:ILE:HD13	1:BD:234:VAL:HG11	1.88	0.56
1:BG:165:ILE:HD13	1:BG:234:VAL:HG11	1.88	0.56
1:BM:165:ILE:HD13	1:BM:234:VAL:HG11	1.88	0.56
1:BO:165:ILE:HD13	1:BO:234:VAL:HG11	1.88	0.56
1:BN:165:ILE:HD13	1:BN:234:VAL:HG11	1.88	0.56
1:AM:165:ILE:HD13	1:AM:234:VAL:HG11	1.87	0.55
1:BE:165:ILE:HD13	1:BE:234:VAL:HG11	1.88	0.55
1:BH:165:ILE:HD13	1:BH:234:VAL:HG11	1.88	0.55
1:BL:165:ILE:HD13	1:BL:234:VAL:HG11	1.88	0.55
1:AI:165:ILE:HD13	1:AI:234:VAL:HG11	1.88	0.55
1:AJ:165:ILE:HD13	1:AJ:234:VAL:HG11	1.88	0.55
1:AK:165:ILE:HD13	1:AK:234:VAL:HG11	1.88	0.55
1:AP:165:ILE:HD13	1:AP:234:VAL:HG11	1.88	0.55
1:BI:165:ILE:HD13	1:BI:234:VAL:HG11	1.88	0.55
1:AD:165:ILE:HD13	1:AD:234:VAL:HG11	1.89	0.55
1:AH:165:ILE:HD13	1:AH:234:VAL:HG11	1.89	0.55
1:AR:165:ILE:HD13	1:AR:234:VAL:HG11	1.88	0.55
1:BI:25:VAL:HG23	1:BJ:63:THR:HG21	1.89	0.55
1:AC:165:ILE:HD13	1:AC:234:VAL:HG11	1.88	0.55
1:AE:165:ILE:HD13	1:AE:234:VAL:HG11	1.88	0.55
1:BA:165:ILE:HD13	1:BA:234:VAL:HG11	1.88	0.55
1:BQ:165:ILE:HD13	1:BQ:234:VAL:HG11	1.88	0.55
1:BC:165:ILE:HD13	1:BC:234:VAL:HG11	1.88	0.55
1:BG:5:GLN:HG2	1:BH:36:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BQ:19:ASN:HA	1:BQ:22:GLU:HB2	1.89	0.54
1:AN:165:ILE:HD13	1:AN:234:VAL:HG11	1.88	0.54
1:BK:165:ILE:HD13	1:BK:234:VAL:HG11	1.89	0.54
1:AA:165:ILE:HD13	1:AA:234:VAL:HG11	1.88	0.54
1:AF:165:ILE:HD13	1:AF:234:VAL:HG11	1.88	0.54
1:AL:165:ILE:HD13	1:AL:234:VAL:HG11	1.88	0.53
1:BJ:165:ILE:HD13	1:BJ:234:VAL:HG11	1.89	0.53
1:AE:25:VAL:HG23	1:AF:63:THR:HG21	1.91	0.53
1:AA:25:VAL:HG23	1:AB:63:THR:HG21	1.90	0.53
1:AC:77:LYS:HG3	1:BD:84:GLU:OE1	2.09	0.53
1:AN:138:PRO:HB3	1:BR:227:ASN:ND2	2.25	0.52
1:BQ:198:GLN:HB2	1:BQ:199:PRO:HD3	1.91	0.52
1:AN:138:PRO:HG2	1:BR:225:ASP:CG	2.29	0.52
1:AL:36:ARG:HE	1:AP:19:ASN:CB	2.23	0.52
1:BE:11:PHE:HA	1:BE:14:GLN:HE21	1.74	0.52
1:BI:11:PHE:HA	1:BI:14:GLN:HE21	1.74	0.52
1:AI:11:PHE:HA	1:AI:14:GLN:HE21	1.75	0.52
1:AO:11:PHE:HA	1:AO:14:GLN:HE21	1.75	0.52
1:AR:11:PHE:HA	1:AR:14:GLN:HE21	1.75	0.52
1:BO:33:PHE:CE1	1:BO:35:ALA:HB3	2.39	0.52
1:BA:11:PHE:HA	1:BA:14:GLN:HE21	1.75	0.52
1:BC:25:VAL:HG23	1:BD:63:THR:HG21	1.92	0.52
1:AQ:11:PHE:HA	1:AQ:14:GLN:HE21	1.75	0.52
1:BH:11:PHE:HA	1:BH:14:GLN:HE21	1.75	0.52
1:BP:11:PHE:HA	1:BP:14:GLN:HE21	1.75	0.52
1:BR:11:PHE:HA	1:BR:14:GLN:HE21	1.75	0.52
1:BJ:11:PHE:HA	1:BJ:14:GLN:HE21	1.75	0.51
1:BC:11:PHE:HA	1:BC:14:GLN:HE21	1.76	0.51
1:AG:46:GLY:HA2	1:AG:89:LYS:HE2	1.91	0.51
1:BF:11:PHE:HA	1:BF:14:GLN:HE21	1.76	0.51
1:AH:11:PHE:HA	1:AH:14:GLN:HE21	1.76	0.51
1:AM:11:PHE:HA	1:AM:14:GLN:HE21	1.76	0.51
1:BB:11:PHE:HA	1:BB:14:GLN:HE21	1.76	0.51
1:AB:11:PHE:HA	1:AB:14:GLN:HE21	1.76	0.51
1:AP:11:PHE:HA	1:AP:14:GLN:HE21	1.75	0.51
1:BQ:11:PHE:HA	1:BQ:14:GLN:HE21	1.75	0.51
1:AE:11:PHE:HA	1:AE:14:GLN:HE21	1.76	0.51
1:AK:11:PHE:HA	1:AK:14:GLN:HE21	1.75	0.51
1:BD:11:PHE:HA	1:BD:14:GLN:HE21	1.75	0.51
1:BL:11:PHE:HA	1:BL:14:GLN:HE21	1.75	0.50
1:AA:11:PHE:HA	1:AA:14:GLN:HE21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:225:ASP:CG	1:BN:138:PRO:HG2	2.32	0.50
1:AC:11:PHE:HA	1:AC:14:GLN:HE21	1.75	0.50
1:AF:11:PHE:HA	1:AF:14:GLN:HE21	1.75	0.50
1:BG:11:PHE:HA	1:BG:14:GLN:HE21	1.75	0.50
1:BK:11:PHE:HA	1:BK:14:GLN:HE21	1.75	0.50
1:AG:11:PHE:HA	1:AG:14:GLN:HE21	1.75	0.50
1:BF:170:SER:HA	1:BF:173:LEU:HD12	1.93	0.50
1:BO:11:PHE:HA	1:BO:14:GLN:HE21	1.76	0.50
1:AO:165:ILE:HD13	1:AO:234:VAL:HG11	1.93	0.50
1:AH:166:LEU:HD21	1:AH:204:VAL:HG21	1.93	0.50
1:AP:19:ASN:HA	1:AP:22:GLU:HB2	1.94	0.50
1:AJ:158:PRO:HD2	1:AJ:161:TYR:CD2	2.46	0.50
1:AJ:11:PHE:HA	1:AJ:14:GLN:HE21	1.76	0.49
1:AD:11:PHE:HA	1:AD:14:GLN:HE21	1.77	0.49
1:AL:11:PHE:HA	1:AL:14:GLN:HE21	1.76	0.49
1:BM:11:PHE:HA	1:BM:14:GLN:HE21	1.76	0.49
1:BN:11:PHE:HA	1:BN:14:GLN:HE21	1.76	0.49
1:AN:11:PHE:HA	1:AN:14:GLN:HE21	1.77	0.49
1:BP:184:LEU:HD23	1:BP:187:ARG:HD2	1.94	0.49
1:AE:114:ARG:HA	1:AE:117:GLN:HE21	1.78	0.49
1:BG:75:MET:N	1:BL:31:GLN:HB2	2.28	0.48
1:AG:165:ILE:HD13	1:AG:234:VAL:HG11	1.95	0.48
1:BE:33:PHE:HE2	1:BE:36:ARG:HD2	1.78	0.48
1:AJ:25:VAL:HG23	1:AK:63:THR:HG21	1.96	0.48
1:BN:19:ASN:HA	1:BN:22:GLU:HB2	1.96	0.48
1:AF:170:SER:HA	1:AF:173:LEU:HD12	1.95	0.48
1:BE:191:GLU:OE2	1:BF:186:GLY:HA2	2.13	0.48
1:AI:91:LYS:HE2	1:BK:96:ASN:O	2.14	0.47
1:BK:25:VAL:HG23	1:BL:63:THR:HG21	1.97	0.47
1:AA:170:SER:HA	1:AA:173:LEU:HD12	1.96	0.47
1:AC:25:VAL:HG23	1:AD:63:THR:HG21	1.96	0.47
1:BA:63:THR:HG21	1:BF:25:VAL:HG23	1.97	0.46
1:AQ:166:LEU:HD21	1:AQ:204:VAL:HG21	1.97	0.46
1:BD:166:LEU:HD21	1:BD:204:VAL:HG21	1.98	0.46
1:BN:61:ALA:HB2	1:BN:104:LEU:HB3	1.98	0.46
1:BQ:208:PHE:HD2	1:BQ:209:ILE:HG13	1.81	0.46
1:AD:25:VAL:HG23	1:AE:63:THR:HG21	1.97	0.46
1:BL:34:ASP:HB3	1:BL:106:ARG:HG2	1.97	0.46
1:AF:46:GLY:HA2	1:AF:89:LYS:HE2	1.97	0.46
1:AN:61:ALA:HB2	1:AN:104:LEU:HB3	1.99	0.46
1:AB:166:LEU:HD21	1:AB:204:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:166:LEU:HD21	1:AJ:204:VAL:HG21	1.99	0.45
1:AL:166:LEU:HD21	1:AL:204:VAL:HG21	1.98	0.45
1:AO:61:ALA:HB2	1:AO:104:LEU:HB3	1.98	0.45
1:BD:158:PRO:HD2	1:BD:161:TYR:HD2	1.80	0.45
1:AR:166:LEU:HD21	1:AR:204:VAL:HG21	1.98	0.45
1:BI:163:ARG:NE	1:BJ:134:ASP:HB3	2.31	0.45
1:AF:166:LEU:HD21	1:AF:204:VAL:HG21	1.98	0.45
1:BE:163:ARG:HD3	1:BF:135:GLY:HA2	1.98	0.45
1:AM:61:ALA:HB2	1:AM:104:LEU:HB3	1.99	0.45
1:BA:170:SER:HA	1:BA:173:LEU:HD12	1.99	0.45
1:AO:197:THR:O	1:AO:201:ASN:ND2	2.50	0.45
1:BG:61:ALA:HB2	1:BG:104:LEU:HB3	1.99	0.45
1:BM:166:LEU:HD21	1:BM:204:VAL:HG21	1.99	0.45
1:BO:61:ALA:HB2	1:BO:104:LEU:HB3	1.99	0.45
1:BF:31:GLN:CD	1:BF:99:ARG:HB2	2.36	0.45
1:BI:61:ALA:HB2	1:BI:104:LEU:HB3	1.99	0.45
1:BM:61:ALA:HB2	1:BM:104:LEU:HB3	1.99	0.45
1:AJ:61:ALA:HB2	1:AJ:104:LEU:HB3	1.99	0.45
1:AO:161:TYR:HB3	1:AO:230:PRO:HD3	1.99	0.45
1:BB:166:LEU:HD21	1:BB:204:VAL:HG21	1.99	0.45
1:BD:84:GLU:HA	1:BD:87:ILE:HD12	1.98	0.44
1:AD:34:ASP:OD1	1:AD:106:ARG:HD3	2.17	0.44
1:AP:61:ALA:HB2	1:AP:104:LEU:HB3	1.99	0.44
1:BH:84:GLU:HA	1:BH:87:ILE:HD12	1.99	0.44
1:BC:61:ALA:HB2	1:BC:104:LEU:HB3	1.99	0.44
1:BF:61:ALA:HB2	1:BF:104:LEU:HB3	1.99	0.44
1:BP:61:ALA:HB2	1:BP:104:LEU:HB3	1.99	0.44
1:AE:61:ALA:HB2	1:AE:104:LEU:HB3	1.99	0.44
1:AQ:61:ALA:HB2	1:AQ:104:LEU:HB3	2.00	0.44
1:AR:61:ALA:HB2	1:AR:104:LEU:HB3	1.99	0.44
1:BB:25:VAL:HG23	1:BC:63:THR:HG21	1.98	0.44
1:BE:61:ALA:HB2	1:BE:104:LEU:HB3	1.99	0.44
1:BQ:61:ALA:HB2	1:BQ:104:LEU:HB3	2.00	0.44
1:AH:61:ALA:HB2	1:AH:104:LEU:HB3	2.00	0.44
1:AR:84:GLU:HA	1:AR:87:ILE:HD12	2.00	0.44
1:BH:61:ALA:HB2	1:BH:104:LEU:HB3	1.99	0.44
1:AK:84:GLU:HA	1:AK:87:ILE:HD12	1.99	0.44
1:BG:166:LEU:HD21	1:BG:204:VAL:HG21	2.00	0.44
1:AC:84:GLU:HA	1:AC:87:ILE:HD12	2.00	0.44
1:AF:61:ALA:HB2	1:AF:104:LEU:HB3	2.00	0.44
1:AJ:84:GLU:HA	1:AJ:87:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:166:LEU:HD21	1:BA:204:VAL:HG21	1.99	0.44
1:AB:25:VAL:HG23	1:AC:63:THR:HG21	2.00	0.44
1:AF:91:LYS:HE2	1:BA:45:TYR:CE1	2.52	0.44
1:AG:63:THR:HG21	1:AL:25:VAL:HG23	1.98	0.44
1:BG:82:THR:HB	1:BL:28:PHE:HE1	1.82	0.44
1:BH:166:LEU:HD21	1:BH:204:VAL:HG21	1.99	0.44
1:BJ:166:LEU:HD21	1:BJ:204:VAL:HG21	2.00	0.44
1:AF:84:GLU:HA	1:AF:87:ILE:HD12	2.00	0.44
1:BB:61:ALA:HB2	1:BB:104:LEU:HB3	2.00	0.44
1:BJ:61:ALA:HB2	1:BJ:104:LEU:HB3	1.99	0.44
1:BK:61:ALA:HB2	1:BK:104:LEU:HB3	1.99	0.44
1:AA:61:ALA:HB2	1:AA:104:LEU:HB3	2.00	0.43
1:BA:61:ALA:HB2	1:BA:104:LEU:HB3	1.99	0.43
1:AL:61:ALA:HB2	1:AL:104:LEU:HB3	2.00	0.43
1:BH:7:LEU:HD21	1:BI:43:LYS:HZ1	1.83	0.43
1:BL:166:LEU:HD21	1:BL:204:VAL:HG21	1.99	0.43
1:BO:161:TYR:HB3	1:BO:230:PRO:HD3	2.00	0.43
1:AK:61:ALA:HB2	1:AK:104:LEU:HB3	1.99	0.43
1:BD:61:ALA:HB2	1:BD:104:LEU:HB3	2.00	0.43
1:AB:61:ALA:HB2	1:AB:104:LEU:HB3	2.00	0.43
1:BB:7:LEU:O	1:BB:10:GLN:HG2	2.18	0.43
1:BB:84:GLU:HA	1:BB:87:ILE:HD12	2.01	0.43
1:AG:61:ALA:HB2	1:AG:104:LEU:HB3	2.00	0.43
1:AO:84:GLU:HA	1:AO:87:ILE:HD12	1.99	0.43
1:BC:166:LEU:HD21	1:BC:204:VAL:HG21	2.00	0.43
1:BE:166:LEU:HD21	1:BE:204:VAL:HG21	2.00	0.43
1:BG:84:GLU:HA	1:BG:87:ILE:HD12	1.99	0.43
1:BJ:84:GLU:HA	1:BJ:87:ILE:HD12	2.00	0.43
1:AB:84:GLU:HA	1:AB:87:ILE:HD12	2.00	0.43
1:AC:61:ALA:HB2	1:AC:104:LEU:HB3	2.00	0.43
1:AH:84:GLU:HA	1:AH:87:ILE:HD12	2.01	0.43
1:AP:166:LEU:HD21	1:AP:204:VAL:HG21	2.00	0.43
1:BF:84:GLU:HA	1:BF:87:ILE:HD12	2.01	0.43
1:BL:61:ALA:HB2	1:BL:104:LEU:HB3	2.00	0.43
1:AH:28:PHE:HE1	1:AI:82:THR:HB	1.84	0.43
1:AP:84:GLU:HA	1:AP:87:ILE:HD12	2.01	0.43
1:AC:166:LEU:HD21	1:AC:204:VAL:HG21	1.99	0.43
1:AJ:92:LEU:HD21	1:AJ:104:LEU:HG	2.01	0.43
1:AM:166:LEU:HD21	1:AM:204:VAL:HG21	2.00	0.43
1:BR:33:PHE:HB3	1:BR:34:ASP:H	1.57	0.43
1:BK:84:GLU:HA	1:BK:87:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BL:84:GLU:HA	1:BL:87:ILE:HD12	2.01	0.42
1:AI:84:GLU:HA	1:AI:87:ILE:HD12	2.01	0.42
1:BA:45:TYR:CE1	1:BA:91:LYS:HG2	2.54	0.42
1:BI:84:GLU:HA	1:BI:87:ILE:HD12	2.01	0.42
1:BJ:34:ASP:O	1:BJ:36:ARG:N	2.44	0.42
1:BK:166:LEU:HD21	1:BK:204:VAL:HG21	2.00	0.42
1:BR:84:GLU:HA	1:BR:87:ILE:HD12	2.01	0.42
1:AL:84:GLU:HA	1:AL:87:ILE:HD12	2.01	0.42
1:AN:84:GLU:HA	1:AN:87:ILE:HD12	2.01	0.42
1:BD:9:ILE:HD13	1:BE:213:LYS:HD3	2.00	0.42
1:BQ:84:GLU:HA	1:BQ:87:ILE:HD12	2.02	0.42
1:BI:166:LEU:HD21	1:BI:204:VAL:HG21	2.01	0.42
1:AD:166:LEU:HD21	1:AD:204:VAL:HG21	2.00	0.42
1:AJ:60:LEU:HD23	1:AJ:104:LEU:HD21	2.01	0.42
1:BM:134:ASP:HB3	1:BR:163:ARG:NH2	2.35	0.42
1:AA:63:THR:HG21	1:AF:25:VAL:HG23	2.01	0.42
1:AM:84:GLU:HA	1:AM:87:ILE:HD12	2.01	0.42
1:BF:165:ILE:HD13	1:BF:234:VAL:HG11	2.00	0.42
1:BN:84:GLU:HA	1:BN:87:ILE:HD12	2.01	0.42
1:BO:84:GLU:HA	1:BO:87:ILE:HD12	2.01	0.42
1:AD:61:ALA:HB2	1:AD:104:LEU:HB3	2.00	0.42
1:AA:84:GLU:HA	1:AA:87:ILE:HD12	2.01	0.42
1:AL:73:MET:CE	1:BI:44:GLN:HG3	2.50	0.42
1:AQ:84:GLU:HA	1:AQ:87:ILE:HD12	2.01	0.41
1:AD:84:GLU:HA	1:AD:87:ILE:HD12	2.01	0.41
1:AL:23:GLN:OE1	1:AP:14:GLN:HG2	2.20	0.41
1:BM:84:GLU:HA	1:BM:87:ILE:HD12	2.01	0.41
1:AE:166:LEU:HD21	1:AE:204:VAL:HG21	2.01	0.41
1:BP:84:GLU:HA	1:BP:87:ILE:HD12	2.01	0.41
1:BA:75:MET:O	1:BF:31:GLN:NE2	2.52	0.41
1:AA:43:LYS:HZ1	1:AF:7:LEU:HD21	1.84	0.41
1:AJ:34:ASP:O	1:AJ:36:ARG:N	2.54	0.41
1:AC:96:ASN:O	1:BC:91:LYS:HE2	2.20	0.41
1:AD:28:PHE:HE1	1:AE:82:THR:HB	1.86	0.41
1:AA:23:GLN:NE2	1:AK:50:TRP:HE1	2.19	0.41
1:AK:41:LEU:HB3	1:AK:102:LEU:HD11	2.03	0.41
1:AM:134:ASP:HB3	1:AR:163:ARG:NH2	2.36	0.41
1:BD:25:VAL:HG23	1:BE:63:THR:HG21	2.02	0.40
1:BN:166:LEU:HD21	1:BN:204:VAL:HG21	2.02	0.40
1:BC:31:GLN:HG3	1:BC:32:GLY:H	1.86	0.40
1:BO:33:PHE:CE2	1:BO:206:SER:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BG:63:THR:HG21	1:BL:25:VAL:HG23	2.02	0.40
1:BQ:166:LEU:HD21	1:BQ:204:VAL:HG21	2.02	0.40
1:BR:19:ASN:HA	1:BR:22:GLU:HB2	2.04	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	AD	34	ASP

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Mol	Chain	Res	Type
1	AP	31	GLN
1	BE	33	PHE
1	BF	31	GLN
1	BG	34	ASP
1	BJ	30	TYR
1	BN	34	ASP
1	BQ	31	GLN
1	AA	35	ALA
1	AB	33	PHE
1	AC	33	PHE
1	AC	34	ASP
1	AI	33	PHE
1	AP	35	ALA
1	AR	34	ASP
1	BJ	209	ILE
1	BP	34	ASP
1	BQ	209	ILE
1	AA	209	ILE
1	AB	209	ILE
1	AC	209	ILE
1	AD	209	ILE
1	AE	209	ILE
1	AF	32	GLY
1	AF	209	ILE
1	AG	209	ILE
1	AH	209	ILE
1	AI	209	ILE
1	AJ	32	GLY
1	AJ	209	ILE
1	AK	209	ILE
1	AL	33	PHE
1	AL	209	ILE
1	AM	209	ILE
1	AN	209	ILE
1	AO	209	ILE
1	AP	209	ILE
1	AQ	209	ILE
1	AR	33	PHE
1	AR	209	ILE
1	BA	209	ILE
1	BB	209	ILE
1	BC	209	ILE

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Mol	Chain	Res	Type
1	BD	209	ILE
1	BE	209	ILE
1	BF	209	ILE
1	BG	209	ILE
1	BH	30	TYR
1	BH	209	ILE
1	BI	209	ILE
1	BJ	34	ASP
1	BJ	35	ALA
1	BK	209	ILE
1	BL	209	ILE
1	BM	209	ILE
1	BN	209	ILE
1	BO	209	ILE
1	BP	32	GLY
1	BP	209	ILE
1	BQ	33	PHE
1	BR	209	ILE
1	AG	34	ASP
1	AK	35	ALA
1	AN	30	TYR
1	AN	228	GLY
1	BH	31	GLN
1	BK	31	GLN
1	BL	34	ASP
1	AB	31	GLN
1	BR	36	ARG
1	BB	32	GLY
1	BF	32	GLY
1	AA	97	PRO
1	AB	97	PRO
1	AC	97	PRO
1	AD	97	PRO
1	AE	97	PRO
1	AF	97	PRO
1	AG	97	PRO
1	AI	97	PRO
1	AK	97	PRO
1	AL	97	PRO
1	AM	97	PRO
1	AN	97	PRO
1	AO	97	PRO

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Mol	Chain	Res	Type
1	AP	97	PRO
1	AQ	97	PRO
1	AR	97	PRO
1	BA	97	PRO
1	BB	97	PRO
1	BC	97	PRO
1	BD	97	PRO
1	BE	97	PRO
1	BF	97	PRO
1	BG	97	PRO
1	BH	97	PRO
1	BI	97	PRO
1	BJ	97	PRO
1	BK	97	PRO
1	BL	97	PRO
1	BM	97	PRO
1	BN	97	PRO
1	BO	97	PRO
1	BP	97	PRO
1	BQ	97	PRO
1	BR	97	PRO
1	AH	97	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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	7	LEU
1	AA	19	ASN
1	AA	26	ARG
1	AB	7	LEU
1	AB	19	ASN
1	AB	26	ARG
1	AC	7	LEU
1	AC	26	ARG
1	AD	7	LEU
1	AD	26	ARG
1	AD	34	ASP
1	AD	36	ARG
1	AE	7	LEU
1	AE	26	ARG
1	AE	33	PHE
1	AE	114	ARG
1	AF	7	LEU
1	AF	26	ARG
1	AF	33	PHE
1	AF	36	ARG
1	AF	100	ASP
1	AG	7	LEU
1	AG	26	ARG
1	AG	174	LEU
1	AH	7	LEU
1	AH	26	ARG
1	AH	36	ARG
1	AH	167	ASP
1	AI	7	LEU
1	AI	26	ARG
1	AI	34	ASP
1	AJ	7	LEU
1	AJ	26	ARG
1	AJ	92	LEU
1	AJ	198	GLN
1	AK	7	LEU
1	AK	26	ARG
1	AK	44	GLN
1	AK	195	THR
1	AK	197	THR
1	AL	7	LEU
1	AL	26	ARG
1	AM	7	LEU

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Mol	Chain	Res	Type
1	AM	19	ASN
1	AM	30	TYR
1	AN	7	LEU
1	AN	26	ARG
1	AN	31	GLN
1	AO	7	LEU
1	AO	26	ARG
1	AP	7	LEU
1	AP	26	ARG
1	AQ	7	LEU
1	AQ	26	ARG
1	AR	7	LEU
1	AR	26	ARG
1	AR	225	ASP
1	BA	7	LEU
1	BA	26	ARG
1	BA	34	ASP
1	BA	44	GLN
1	BA	91	LYS
1	BB	7	LEU
1	BB	10	GLN
1	BB	26	ARG
1	BC	7	LEU
1	BC	26	ARG
1	BD	7	LEU
1	BD	26	ARG
1	BE	7	LEU
1	BE	26	ARG
1	BE	31	GLN
1	BE	33	PHE
1	BE	91	LYS
1	BF	7	LEU
1	BF	26	ARG
1	BF	36	ARG
1	BG	7	LEU
1	BG	26	ARG
1	BG	34	ASP
1	BH	7	LEU
1	BH	26	ARG
1	BH	33	PHE
1	BI	7	LEU
1	BI	26	ARG

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Mol	Chain	Res	Type
1	BJ	7	LEU
1	BJ	19	ASN
1	BJ	26	ARG
1	BJ	210	SER
1	BK	7	LEU
1	BK	26	ARG
1	BK	31	GLN
1	BL	7	LEU
1	BL	26	ARG
1	BL	34	ASP
1	BM	7	LEU
1	BM	26	ARG
1	BM	99	ARG
1	BN	7	LEU
1	BN	26	ARG
1	BO	7	LEU
1	BO	26	ARG
1	BO	160	ASP
1	BP	7	LEU
1	BP	26	ARG
1	BQ	7	LEU
1	BQ	26	ARG
1	BQ	199	PRO
1	BR	7	LEU
1	BR	26	ARG
1	BR	30	TYR
1	BR	225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	19	ASN
1	AA	23	GLN
1	AA	211	HIS
1	AB	14	GLN
1	AC	14	GLN
1	AC	198	GLN
1	AC	205	ASN
1	AD	14	GLN
1	AD	205	ASN
1	AD	211	HIS
1	AE	14	GLN

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Mol	Chain	Res	Type
1	AE	117	GLN
1	AE	198	GLN
1	AF	14	GLN
1	AF	19	ASN
1	AF	31	GLN
1	AF	183	ASN
1	AF	211	HIS
1	AG	14	GLN
1	AG	88	ASN
1	AG	175	GLN
1	AH	14	GLN
1	AH	205	ASN
1	AH	211	HIS
1	AI	44	GLN
1	AI	211	HIS
1	AJ	14	GLN
1	AJ	211	HIS
1	AK	14	GLN
1	AK	198	GLN
1	AK	211	HIS
1	AL	14	GLN
1	AL	183	ASN
1	AM	211	HIS
1	AN	31	GLN
1	AN	211	HIS
1	AO	19	ASN
1	AO	201	ASN
1	AO	211	HIS
1	AP	31	GLN
1	AP	207	ASN
1	AP	211	HIS
1	AQ	14	GLN
1	AQ	211	HIS
1	AR	227	ASN
1	BA	14	GLN
1	BA	198	GLN
1	BA	211	HIS
1	BB	14	GLN
1	BB	205	ASN
1	BB	211	HIS
1	BC	14	GLN
1	BC	44	GLN

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Mol	Chain	Res	Type
1	BC	211	HIS
1	BD	14	GLN
1	BD	31	GLN
1	BD	211	HIS
1	BE	14	GLN
1	BE	198	GLN
1	BE	211	HIS
1	BF	14	GLN
1	BF	31	GLN
1	BF	205	ASN
1	BF	211	HIS
1	BG	14	GLN
1	BG	211	HIS
1	BH	14	GLN
1	BH	19	ASN
1	BH	211	HIS
1	BI	14	GLN
1	BI	19	ASN
1	BI	211	HIS
1	BJ	14	GLN
1	BJ	211	HIS
1	BK	14	GLN
1	BK	198	GLN
1	BK	211	HIS
1	BL	14	GLN
1	BL	211	HIS
1	BM	211	HIS
1	BN	211	HIS
1	BO	19	ASN
1	BO	211	HIS
1	BP	207	ASN
1	BP	211	HIS
1	BQ	198	GLN
1	BR	169	HIS
1	BR	211	HIS
1	BR	227	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Aa	30/36 (83%)	13 (43%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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

All (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
2	Aa	16	U
2	Aa	17	U
2	Aa	22	U
2	Aa	23	U
2	Aa	28	U
2	Aa	29	U
2	Aa	34	U
2	Aa	35	U
2	Ag	3	U
2	Ag	6	U
2	Ag	10	U
2	Ag	11	U
2	Ag	14	U
2	Ag	16	U
2	Ag	17	U
2	Ag	22	U
2	Ag	23	U
2	Ag	28	U
2	Ag	29	U
2	Ag	34	U
2	Ag	35	U
2	Am	4	U
2	Am	5	U
2	Am	10	U
2	Am	11	U
2	Am	16	U
2	Am	17	U

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Mol	Chain	Res	Type
2	Am	22	U
2	Am	23	U
2	Am	28	U
2	Am	29	U
2	Am	35	U
2	Am	36	U
2	Ba	4	U
2	Ba	5	U
2	Ba	10	U
2	Ba	11	U
2	Ba	15	U
2	Ba	16	U
2	Ba	17	U
2	Ba	22	U
2	Ba	23	U
2	Ba	28	U
2	Ba	29	U
2	Ba	34	U
2	Ba	35	U
2	Bg	4	U
2	Bg	5	U
2	Bg	10	U
2	Bg	11	U
2	Bg	16	U
2	Bg	17	U
2	Bg	22	U
2	Bg	23	U
2	Bg	28	U
2	Bg	29	U
2	Bg	34	U
2	Bg	35	U
2	Bm	4	U
2	Bm	5	U
2	Bm	16	U
2	Bm	17	U
2	Bm	22	U
2	Bm	23	U
2	Bm	28	U
2	Bm	29	U
2	Bm	34	U
2	Bm	35	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

All 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
1	Bg	24:U	O3'	25:U	P	5.79
1	Aa	24:U	O3'	25:U	P	5.69
1	Bg	18:U	O3'	19:U	P	5.49
1	Ag	18:U	O3'	19:U	P	5.47
1	Bg	6:U	O3'	7:U	P	5.47
1	Aa	18:U	O3'	19:U	P	5.42

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Aa	30:U	O3'	31:U	P	5.38
1	Ag	30:U	O3'	31:U	P	5.37
1	Ba	6:U	O3'	7:U	P	5.33
1	Ba	30:U	O3'	31:U	P	5.31
1	Aa	12:U	O3'	13:U	P	5.26
1	Am	30:U	O3'	31:U	P	5.15
1	Bm	30:U	O3'	31:U	P	5.13
1	Bg	12:U	O3'	13:U	P	5.02
1	Aa	6:U	O3'	7:U	P	4.92
1	Bg	30:U	O3'	31:U	P	4.78
1	Bm	12:U	O3'	13:U	P	4.76
1	Bm	18:U	O3'	19:U	P	4.74
1	Ba	18:U	O3'	19:U	P	4.73
1	Am	12:U	O3'	13:U	P	4.71
1	Am	24:U	O3'	25:U	P	4.61
1	Bm	24:U	O3'	25:U	P	4.56
1	Am	6:U	O3'	7:U	P	4.54
1	Am	18:U	O3'	19:U	P	4.53
1	Bm	6:U	O3'	7:U	P	4.51

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.