



Full wwPDB X-ray Structure Validation Report

Jun 16, 2014 – 06:02 PM BST

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

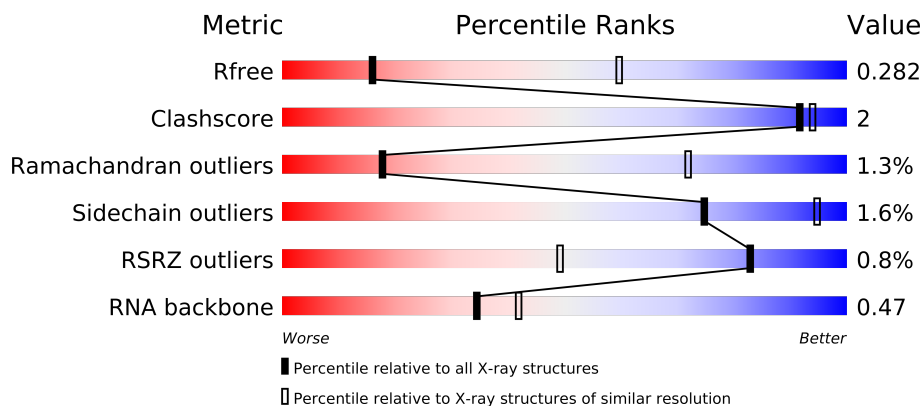
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AB	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AC	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AD	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AE	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AF	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AG	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AH	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AI	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AJ	245	<div><div></div><div></div><div></div><div></div><div></div></div>
1	AK	245	<div><div></div><div></div><div></div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	AL	245	
1	AM	245	
1	AN	245	
1	AO	245	
1	AP	245	
1	AQ	245	
1	AR	245	
1	BA	245	
1	BB	245	
1	BC	245	
1	BD	245	
1	BE	245	
1	BF	245	
1	BG	245	
1	BH	245	
1	BI	245	
1	BJ	245	
1	BK	245	
1	BL	245	
1	BM	245	
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

There are 2 unique types of molecules in this entry. The entry contains 72072 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

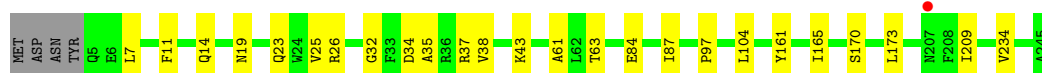
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Aa	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ag	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Am	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Ba	36	Total	C	N	O	P	0	0	0
			720	324	72	288	36			
2	Bg	36	Total	C	N	O	P	0	0	0
			720	324	72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

3 Residue-property plots

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

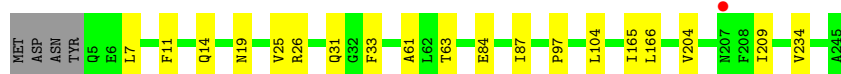
- Molecule 1: Nucleocapsid protein

Chain AA: 



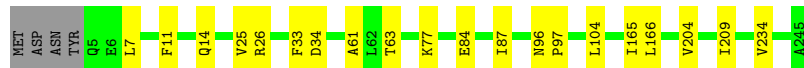
- Molecule 1: Nucleocapsid protein

Chain AB: 



- Molecule 1: Nucleocapsid protein

Chain AC: 



- Molecule 1: Nucleocapsid protein

Chain AD: 



- Molecule 1: Nucleocapsid protein

Chain AE: 



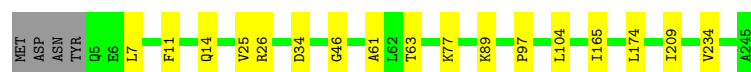
- Molecule 1: Nucleocapsid protein

Chain AF: 



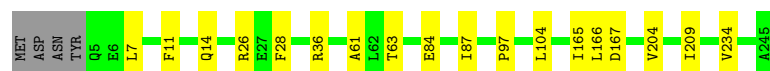
- Molecule 1: Nucleocapsid protein

Chain AG: 



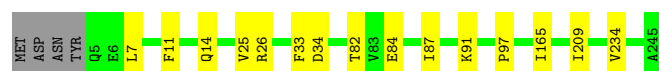
- Molecule 1: Nucleocapsid protein

Chain AH: 



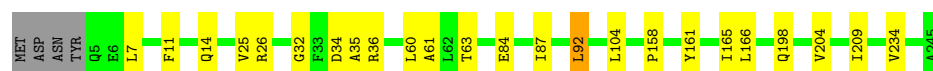
- Molecule 1: Nucleocapsid protein

Chain AI: 



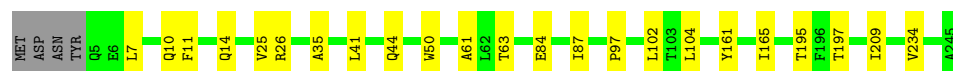
- Molecule 1: Nucleocapsid protein

Chain AJ: 



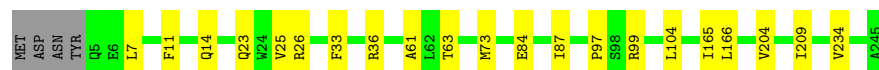
- Molecule 1: Nucleocapsid protein

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: 



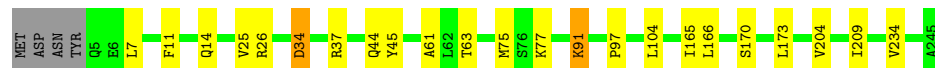
- Molecule 1: Nucleocapsid protein

Chain AR: 



- Molecule 1: Nucleocapsid protein

Chain BA: 



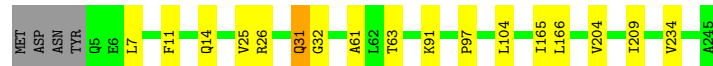
- Molecule 1: Nucleocapsid protein

Chain BB: 



- Molecule 1: Nucleocapsid protein

Chain BC: 



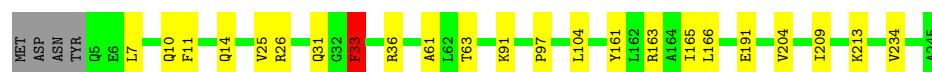
- Molecule 1: Nucleocapsid protein

Chain BD: 



- Molecule 1: Nucleocapsid protein

Chain BE: 



- Molecule 1: Nucleocapsid protein

Chain BF: 



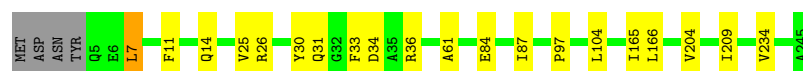
- Molecule 1: Nucleocapsid protein

Chain BG: 



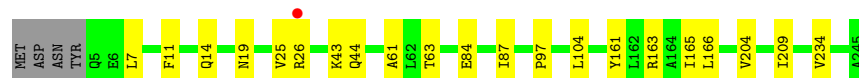
- Molecule 1: Nucleocapsid protein

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: 



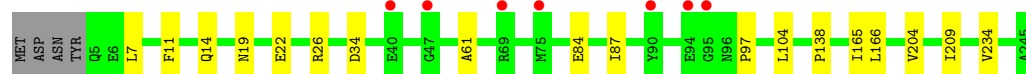
- Molecule 1: Nucleocapsid protein

Chain BM: 



- Molecule 1: Nucleocapsid protein

Chain BN: 



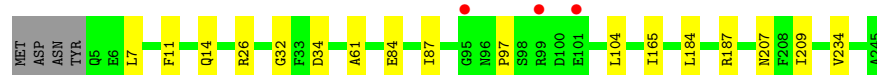
- Molecule 1: Nucleocapsid protein

Chain BO: 



- Molecule 1: Nucleocapsid protein

Chain BP: 



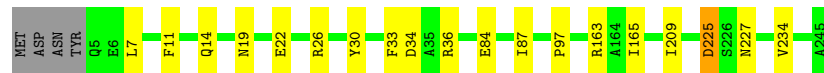
- Molecule 1: Nucleocapsid protein

Chain BQ: 



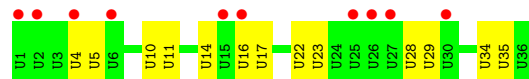
- Molecule 1: Nucleocapsid protein

Chain BR: 



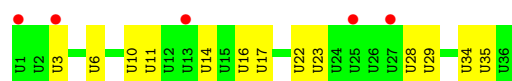
- Molecule 2: 35-mer poly(U) RNA

Chain Aa: 



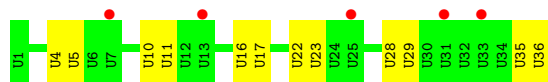
- Molecule 2: 35-mer poly(U) RNA

Chain Ag: 



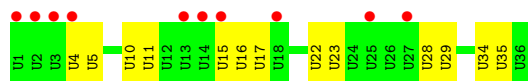
- Molecule 2: 35-mer poly(U) RNA

Chain Am: 



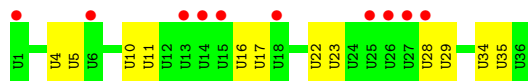
- Molecule 2: 35-mer poly(U) RNA

Chain Ba: 



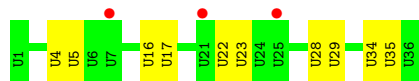
- Molecule 2: 35-mer poly(U) RNA

Chain Bg: 



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

Chain Bm: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.225 , 0.240 0.278 , 0.282	Depositor DCC
R_{free} test set	5935 reflections (5.30%)	DCC
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 , 36.2	EDS
Estimated twinning fraction	0.316 for -h,k,-k-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 117932 reflections	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.*

¹Intensities estimated from amplitudes.

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	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AP	1882	0	1906	9	0
1	AQ	1882	0	1906	5	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (257) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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: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:BG:165:ILE:HD13	1:BG: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: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: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:BI:165:ILE:HD13	1:BI:234:VAL:HG11	1.88	0.55
1:AH:165:ILE:HD13	1:AH:234:VAL:HG11	1.89	0.55
1:AD:165:ILE:HD13	1:AD: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:AE:165:ILE:HD13	1:AE:234:VAL:HG11	1.88	0.55
1:BQ:165:ILE:HD13	1:BQ:234:VAL:HG11	1.88	0.55
1:AC:165:ILE:HD13	1:AC:234:VAL:HG11	1.88	0.55
1:BA:165:ILE:HD13	1:BA: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
1:BQ:19:ASN:HA	1:BQ:22:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:AF:165:ILE:HD13	1:AF:234:VAL:HG11	1.88	0.54
1:AA:165:ILE:HD13	1:AA: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:BO:33:PHE:CE1	1:BO:35:ALA:HB3	2.39	0.52
1:AO:11:PHE:HA	1:AO:14:GLN:HE21	1.75	0.52
1:AI:11:PHE:HA	1:AI:14:GLN:HE21	1.75	0.52
1:AR:11:PHE:HA	1:AR:14:GLN:HE21	1.75	0.52
1:BC:25:VAL:HG23	1:BD:63:THR:HG21	1.92	0.52
1:BA:11:PHE:HA	1:BA:14:GLN:HE21	1.75	0.52
1:BH:11:PHE:HA	1:BH:14:GLN:HE21	1.75	0.52
1:AQ:11:PHE:HA	1:AQ: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:BF:11:PHE:HA	1:BF:14:GLN:HE21	1.76	0.51
1:AG:46:GLY:HA2	1:AG:89:LYS:HE2	1.91	0.51
1:AM:11:PHE:HA	1:AM:14:GLN:HE21	1.76	0.51
1:AH:11:PHE:HA	1:AH:14:GLN:HE21	1.76	0.51
1:BB:11:PHE:HA	1:BB: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:AB:11:PHE:HA	1:AB:14:GLN:HE21	1.76	0.51
1:AE:11:PHE:HA	1:AE:14:GLN:HE21	1.76	0.51
1:BD:11:PHE:HA	1:BD:14:GLN:HE21	1.75	0.51
1:AK:11:PHE:HA	1:AK:14:GLN:HE21	1.75	0.51
1:BL:11:PHE:HA	1:BL:14:GLN:HE21	1.75	0.50
1:AR:225:ASP:CG	1:BN:138:PRO:HG2	2.32	0.50
1:AA:11:PHE:HA	1:AA:14:GLN:HE21	1.76	0.50
1:AF:11:PHE:HA	1:AF:14:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BG:11:PHE:HA	1:BG:14:GLN:HE21	1.75	0.50
1:AC:11:PHE:HA	1:AC: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:BO:11:PHE:HA	1:BO:14:GLN:HE21	1.76	0.50
1:BF:170:SER:HA	1:BF:173:LEU:HD12	1.93	0.50
1:AO:165:ILE:HD13	1:AO:234:VAL:HG11	1.93	0.50
1:AP:19:ASN:HA	1:AP:22:GLU:HB2	1.94	0.50
1:AH:166:LEU:HD21	1:AH:204:VAL:HG21	1.93	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:BK:25:VAL:HG23	1:BL:63:THR:HG21	1.97	0.47
1:AI:91:LYS:HE2	1:BK:96:ASN:O	2.14	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:BQ:208:PHE:HD2	1:BQ:209:ILE:HG13	1.81	0.46
1:BN:61:ALA:HB2	1:BN:104:LEU:HB3	1.98	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:AN:61:ALA:HB2	1:AN:104:LEU:HB3	1.99	0.46
1:AF:46:GLY:HA2	1:AF:89:LYS:HE2	1.97	0.46
1:AJ:166:LEU:HD21	1:AJ:204:VAL:HG21	1.99	0.45
1:AB:166:LEU:HD21	1:AB:204:VAL:HG21	1.99	0.45
1:AO:61:ALA:HB2	1:AO:104:LEU:HB3	1.98	0.45
1:AL:166:LEU:HD21	1:AL:204:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:BE:163:ARG:HD3	1:BF:135:GLY:HA2	1.98	0.45
1:AF:166:LEU:HD21	1:AF:204:VAL:HG21	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: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:AO:197:THR:O	1:AO:201:ASN:ND2	2.50	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:BH:84:GLU:HA	1:BH:87:ILE:HD12	1.99	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: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: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:BQ:61:ALA:HB2	1:BQ:104:LEU:HB3	2.00	0.44
1:AE:61:ALA:HB2	1:AE:104:LEU:HB3	1.99	0.44
1:BE:61:ALA:HB2	1:BE:104:LEU:HB3	1.99	0.44
1:AQ:61:ALA:HB2	1:AQ:104:LEU:HB3	2.00	0.44
1:BH:61:ALA:HB2	1:BH:104:LEU:HB3	1.99	0.44
1:AR:84:GLU:HA	1:AR:87:ILE:HD12	2.00	0.44
1:AH:61:ALA:HB2	1:AH:104:LEU:HB3	2.00	0.44
1:BG:166:LEU:HD21	1:BG:204:VAL:HG21	2.00	0.44
1:AK:84:GLU:HA	1:AK:87:ILE:HD12	1.99	0.44
1:BA:166:LEU:HD21	1:BA:204:VAL:HG21	1.99	0.44
1:AJ:84:GLU:HA	1:AJ:87:ILE:HD12	2.00	0.44
1:AF:61:ALA:HB2	1:AF:104:LEU:HB3	2.00	0.44
1:AC:84:GLU:HA	1:AC:87:ILE:HD12	2.00	0.44
1:AG:63:THR:HG21	1:AL:25:VAL:HG23	1.98	0.44
1:AF:91:LYS:HE2	1:BA:45:TYR:CE1	2.52	0.44
1:BH:166:LEU:HD21	1:BH:204:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BG:82:THR:HB	1:BL:28:PHE:HE1	1.82	0.44
1:AB:25:VAL:HG23	1:AC:63:THR:HG21	2.00	0.44
1:BJ:166:LEU:HD21	1:BJ:204:VAL:HG21	2.00	0.44
1:BJ:61:ALA:HB2	1:BJ:104:LEU:HB3	1.99	0.44
1:BB:61:ALA:HB2	1:BB:104:LEU:HB3	2.00	0.44
1:BK:61:ALA:HB2	1:BK:104:LEU:HB3	1.99	0.44
1:AF:84:GLU:HA	1:AF:87:ILE:HD12	2.00	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: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:AL:61:ALA:HB2	1:AL:104:LEU:HB3	2.00	0.43
1:BO:161:TYR:HB3	1:BO:230:PRO:HD3	2.00	0.43
1:BD:61:ALA:HB2	1:BD:104:LEU:HB3	2.00	0.43
1:AK:61:ALA:HB2	1:AK:104:LEU:HB3	1.99	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:BC:166:LEU:HD21	1:BC: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:BE:166:LEU:HD21	1:BE:204:VAL:HG21	2.00	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:AC:61:ALA:HB2	1:AC:104:LEU:HB3	2.00	0.43
1:AB:84:GLU:HA	1:AB:87:ILE:HD12	2.00	0.43
1:BL:61:ALA:HB2	1:BL:104:LEU:HB3	2.00	0.43
1:BF:84:GLU:HA	1:BF:87:ILE:HD12	2.01	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:AP:84:GLU:HA	1:AP:87:ILE:HD12	2.01	0.43
1:AH:28:PHE:HE1	1:AI:82:THR:HB	1.84	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:AC:166:LEU:HD21	1:AC:204:VAL:HG21	1.99	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
1:BL:84:GLU:HA	1:BL:87:ILE:HD12	2.01	0.42
1:BA:45:TYR:CE1	1:BA:91:LYS:HG2	2.54	0.42
1:BJ:34:ASP:O	1:BJ:36:ARG:N	2.44	0.42
1:AI:84:GLU:HA	1:AI:87:ILE:HD12	2.01	0.42
1:BI:84:GLU:HA	1:BI:87:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:BR:84:GLU:HA	1:BR:87:ILE:HD12	2.01	0.42
1:BK:166:LEU:HD21	1:BK:204:VAL:HG21	2.00	0.42
1:AL:84:GLU:HA	1:AL:87:ILE:HD12	2.01	0.42
1:BQ:84:GLU:HA	1:BQ:87:ILE:HD12	2.02	0.42
1:BD:9:ILE:HD13	1:BE:213:LYS:HD3	2.00	0.42
1:AN:84:GLU:HA	1:AN:87:ILE:HD12	2.01	0.42
1:BI:166:LEU:HD21	1:BI:204:VAL:HG21	2.01	0.42
1:AJ:60:LEU:HD23	1:AJ:104:LEU:HD21	2.01	0.42
1:AD:166:LEU:HD21	1:AD:204:VAL:HG21	2.00	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:BO:84:GLU:HA	1:BO: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: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:AL:23:GLN:OE1	1:AP:14:GLN:HG2	2.20	0.41
1:AD:84:GLU:HA	1:AD:87:ILE:HD12	2.01	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:AD:28:PHE:HE1	1:AE:82:THR:HB	1.86	0.41
1:AC:96:ASN:O	1:BC:91:LYS:HE2	2.20	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:AA:23:GLN:NE2	1:AK:50:TRP:HE1	2.19	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:BO:33:PHE:CE2	1:BO:206:SER:HB2	2.56	0.40
1:BC:31:GLN:HG3	1:BC:32:GLY:H	1.86	0.40
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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	14	66
1	AB	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	14	66
1	AC	239/245 (98%)	227 (95%)	8 (3%)	4 (2%)	14	66
1	AD	239/245 (98%)	225 (94%)	11 (5%)	3 (1%)	18	72
1	AE	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	27	81
1	AF	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	18	72
1	AG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	18	72
1	AH	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	27	81
1	AI	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	18	72
1	AJ	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	18	72
1	AK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	18	72
1	AL	239/245 (98%)	224 (94%)	12 (5%)	3 (1%)	18	72
1	AM	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	27	81
1	AN	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	14	66
1	AO	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	27	81
1	AP	239/245 (98%)	225 (94%)	10 (4%)	4 (2%)	14	66
1	AQ	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	27	81
1	AR	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	14	66
1	BA	239/245 (98%)	225 (94%)	12 (5%)	2 (1%)	27	81
1	BB	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	18	72
1	BC	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	18	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BD	239/245 (98%)	229 (96%)	8 (3%)	2 (1%)	27	81
1	BE	239/245 (98%)	222 (93%)	14 (6%)	3 (1%)	18	72
1	BF	239/245 (98%)	226 (95%)	9 (4%)	4 (2%)	14	66
1	BG	239/245 (98%)	227 (95%)	9 (4%)	3 (1%)	18	72
1	BH	239/245 (98%)	223 (93%)	11 (5%)	5 (2%)	11	61
1	BI	239/245 (98%)	226 (95%)	11 (5%)	2 (1%)	27	81
1	BJ	239/245 (98%)	224 (94%)	10 (4%)	5 (2%)	11	61
1	BK	239/245 (98%)	229 (96%)	7 (3%)	3 (1%)	18	72
1	BL	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	18	72
1	BM	239/245 (98%)	228 (95%)	8 (3%)	3 (1%)	18	72
1	BN	239/245 (98%)	226 (95%)	10 (4%)	3 (1%)	18	72
1	BO	239/245 (98%)	224 (94%)	13 (5%)	2 (1%)	27	81
1	BP	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	14	66
1	BQ	239/245 (98%)	224 (94%)	11 (5%)	4 (2%)	14	66
1	BR	239/245 (98%)	223 (93%)	13 (5%)	3 (1%)	18	72
All	All	8604/8820 (98%)	8131 (94%)	361 (4%)	112 (1%)	18	72

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	76	95
1	AB	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	AC	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	AD	194/198 (98%)	190 (98%)	4 (2%)	66	93
1	AE	194/198 (98%)	190 (98%)	4 (2%)	66	93
1	AF	194/198 (98%)	189 (97%)	5 (3%)	59	91
1	AG	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	AH	194/198 (98%)	190 (98%)	4 (2%)	66	93
1	AI	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	AJ	194/198 (98%)	190 (98%)	4 (2%)	66	93
1	AK	194/198 (98%)	189 (97%)	5 (3%)	59	91
1	AL	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	AM	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	AN	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	AO	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	AP	194/198 (98%)	192 (99%)	2 (1%)	85	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AQ	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	AR	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BA	194/198 (98%)	189 (97%)	5 (3%)	59	91
1	BB	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BC	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	BD	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	BE	194/198 (98%)	189 (97%)	5 (3%)	59	91
1	BF	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BG	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BH	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BI	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	BJ	194/198 (98%)	190 (98%)	4 (2%)	66	93
1	BK	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BL	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BM	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BN	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	BO	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BP	194/198 (98%)	192 (99%)	2 (1%)	85	96
1	BQ	194/198 (98%)	191 (98%)	3 (2%)	76	95
1	BR	194/198 (98%)	190 (98%)	4 (2%)	66	93
All	All	6984/7128 (98%)	6872 (98%)	112 (2%)	75	95

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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

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
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

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Mol	Chain	Res	Type
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	241/245 (98%)	0.07	1 (0%) 90 68	33, 69, 98, 112	0
1	AB	241/245 (98%)	0.14	1 (0%) 90 68	47, 80, 111, 142	0
1	AC	241/245 (98%)	0.01	0 100 100	32, 62, 87, 109	0
1	AD	241/245 (98%)	0.03	0 100 100	29, 66, 96, 113	0
1	AE	241/245 (98%)	0.03	0 100 100	28, 58, 89, 103	0
1	AF	241/245 (98%)	0.06	0 100 100	24, 62, 93, 116	0
1	AG	241/245 (98%)	-0.02	0 100 100	23, 57, 85, 109	0
1	AH	241/245 (98%)	-0.02	0 100 100	20, 62, 87, 103	0
1	AI	241/245 (98%)	-0.02	0 100 100	27, 59, 87, 98	0
1	AJ	241/245 (98%)	-0.01	0 100 100	24, 63, 90, 105	0
1	AK	241/245 (98%)	0.04	0 100 100	35, 66, 88, 112	0
1	AL	241/245 (98%)	0.07	0 100 100	33, 66, 93, 109	0
1	AM	241/245 (98%)	0.18	2 (0%) 83 49	34, 77, 118, 129	0
1	AN	241/245 (98%)	0.30	3 (1%) 75 39	33, 82, 138, 152	0
1	AO	241/245 (98%)	0.13	1 (0%) 90 68	33, 69, 98, 109	0
1	AP	241/245 (98%)	0.08	3 (1%) 75 39	22, 67, 100, 123	0
1	AQ	241/245 (98%)	-0.00	0 100 100	28, 63, 95, 112	0
1	AR	241/245 (98%)	0.03	1 (0%) 90 68	27, 65, 99, 114	0
1	BA	241/245 (98%)	0.06	0 100 100	32, 65, 91, 108	0
1	BB	241/245 (98%)	0.07	0 100 100	30, 65, 98, 111	0
1	BC	241/245 (98%)	0.08	0 100 100	40, 65, 92, 105	0
1	BD	241/245 (98%)	0.12	0 100 100	40, 69, 95, 107	0
1	BE	241/245 (98%)	0.15	0 100 100	48, 71, 93, 108	0
1	BF	241/245 (98%)	0.15	0 100 100	26, 72, 99, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BG	241/245 (98%)	0.09	0 100 100	22, 63, 95, 109	0
1	BH	241/245 (98%)	0.10	0 100 100	30, 65, 96, 114	0
1	BI	241/245 (98%)	0.16	1 (0%) 90 68	35, 74, 101, 114	0
1	BJ	241/245 (98%)	0.20	1 (0%) 90 68	46, 81, 108, 144	0
1	BK	241/245 (98%)	0.15	0 100 100	37, 68, 94, 115	0
1	BL	241/245 (98%)	0.14	0 100 100	39, 70, 97, 112	0
1	BM	241/245 (98%)	0.24	3 (1%) 75 39	39, 78, 114, 124	0
1	BN	241/245 (98%)	0.34	7 (2%) 49 21	46, 86, 133, 146	0
1	BO	241/245 (98%)	0.12	1 (0%) 90 68	35, 70, 102, 121	0
1	BP	241/245 (98%)	0.13	3 (1%) 75 39	24, 70, 102, 123	0
1	BQ	241/245 (98%)	0.07	0 100 100	37, 64, 98, 109	0
1	BR	241/245 (98%)	0.11	0 100 100	28, 71, 101, 119	0
2	Aa	36/36 (100%)	1.36	10 (27%) 1 1	77, 88, 154, 155	0
2	Ag	36/36 (100%)	0.99	5 (13%) 4 2	71, 98, 151, 151	0
2	Am	36/36 (100%)	1.24	5 (13%) 4 2	105, 125, 146, 147	0
2	Ba	36/36 (100%)	1.34	10 (27%) 1 1	77, 96, 174, 175	0
2	Bg	36/36 (100%)	1.43	10 (27%) 1 1	84, 97, 152, 152	0
2	Bm	36/36 (100%)	1.20	3 (8%) 11 5	109, 126, 131, 133	0
All	All	8892/9036 (98%)	0.13	71 (0%) 83 49	20, 69, 106, 175	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Aa	27	U	6.3
2	Ba	15	U	4.9
2	Ag	1	U	4.8
2	Aa	1	U	4.6
1	BM	95	GLY	4.5
2	Bg	25	U	4.5
2	Bg	27	U	4.4
2	Bg	13	U	4.2
2	Ba	3	U	4.2
2	Am	7	U	4.1
2	Ag	27	U	4.1
1	BP	95	GLY	3.9
2	Ba	1	U	3.9

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Mol	Chain	Res	Type	RSRZ
1	AN	95	GLY	3.8
2	Ba	27	U	3.8
2	Ba	25	U	3.8
2	Aa	25	U	3.7
1	AN	92	LEU	3.6
2	Aa	4	U	3.6
2	Bg	1	U	3.5
2	Am	31	U	3.4
2	Ag	25	U	3.4
1	BJ	95	GLY	3.4
2	Bm	21	U	3.3
1	AO	94	GLU	3.3
2	Bg	6	U	3.2
2	Bm	25	U	3.1
2	Aa	30	U	3.1
2	Bg	15	U	3.1
1	AR	101	GLU	2.9
2	Ba	2	U	2.9
2	Bg	18	U	2.9
1	AN	40	GLU	2.9
2	Aa	15	U	2.9
2	Bm	7	U	2.8
1	BN	94	GLU	2.7
2	Bg	28	U	2.7
2	Am	33	U	2.7
1	BN	75	MET	2.7
2	Ba	4	U	2.6
2	Ag	3	U	2.6
2	Am	25	U	2.6
1	BI	26	ARG	2.6
2	Ba	13	U	2.6
1	AP	32	GLY	2.6
2	Am	13	U	2.6
1	BN	69	ARG	2.6
1	BN	90	TYR	2.5
1	BM	14	GLN	2.5
1	BN	95	GLY	2.4
2	Ag	13	U	2.4
2	Ba	18	U	2.4
1	BM	16	VAL	2.4
1	AP	100	ASP	2.4
1	BN	47	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	Bg	26	U	2.3
1	BN	40	GLU	2.3
2	Aa	6	U	2.3
1	AA	207	ASN	2.3
1	AM	100	ASP	2.3
1	BO	99	ARG	2.2
1	BP	99	ARG	2.2
2	Bg	14	U	2.2
1	BP	101	GLU	2.2
2	Aa	2	U	2.1
2	Aa	26	U	2.1
2	Ba	14	U	2.1
2	Aa	16	U	2.1
1	AB	207	ASN	2.0
1	AM	40	GLU	2.0
1	AP	97	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.