



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:11 pm BST

PDB ID : 1R71  
Title : Crystal Structure of the DNA binding domain of KorB in complex with the operator DNA  
Authors : Khare, D.; Ziegelin, G.; Lanka, E.; Heinemann, U.  
Deposited on : 2003-10-17  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

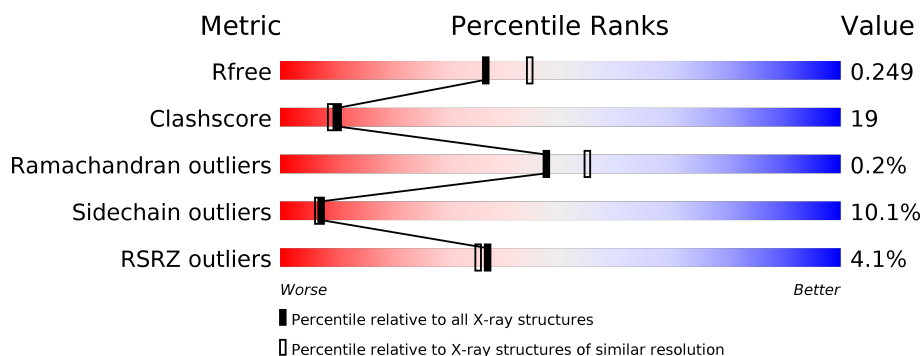
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	17	<div> <div>12%</div> <div>53%</div> <div>35%</div> </div>
1	G	17	<div> <div>47%</div> <div>53%</div> </div>
1	J	17	<div> <div>6%</div> <div>59%</div> <div>35%</div> </div>
1	K	17	<div> <div>47%</div> <div>53%</div> </div>
2	F	17	<div> <div>6%</div> <div>53%</div> <div>41%</div> </div>
2	H	17	<div> <div>18%</div> <div>65%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	17	
2	L	17	
3	A	178	
3	B	178	
3	C	178	
3	D	178	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6769 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 DNA chain called 5'-D(\*AP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*GP\*GP\*C P\*TP\*AP\*AP\*AP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	17	Total	Br	C	N	O	P	0	17	0
			349	1	167	66	99	16			
1	J	17	Total	Br	C	N	O	P	0	17	0
			349	1	167	66	99	16			
1	G	17	Total	Br	C	N	O	P	0	17	0
			349	1	167	66	99	16			
1	K	17	Total	Br	C	N	O	P	0	17	0
			349	1	167	66	99	16			

- Molecule 2 is a DNA chain called 5'-D(\*CP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*CP\*GP\*C P\*TP\*AP\*AP\*AP\*AP\*(BRU))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	17	Total	Br	C	N	O	P	0	17	0
			342	2	164	59	101	16			
2	F	17	Total	Br	C	N	O	P	0	17	0
			342	2	164	59	101	16			
2	L	17	Total	Br	C	N	O	P	0	17	0
			342	2	164	59	101	16			
2	H	17	Total	Br	C	N	O	P	0	17	0
			342	2	164	59	101	16			

- Molecule 3 is a protein called Transcriptional repressor protein korB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	114	Total	C	N	O	0	0	0
			912	573	159	180			
3	B	116	Total	C	N	O	0	0	0
			932	586	162	184			
3	C	112	Total	C	N	O	0	0	0
			894	563	157	174			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	115	Total	C	N	O	0	0	0
			920	577	161	182			

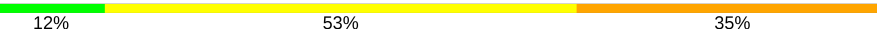
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	31	Total	O	0	0
			31	31		
4	I	21	Total	O	0	0
			21	21		
4	F	34	Total	O	0	0
			34	34		
4	J	24	Total	O	0	0
			24	24		
4	G	30	Total	O	0	0
			30	30		
4	L	23	Total	O	0	0
			23	23		
4	H	21	Total	O	0	0
			21	21		
4	K	24	Total	O	0	0
			24	24		
4	A	54	Total	O	0	0
			54	54		
4	B	29	Total	O	0	0
			29	29		
4	C	29	Total	O	0	0
			29	29		
4	D	27	Total	O	0	0
			27	27		

### 3 Residue-property plots

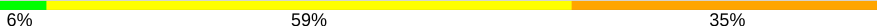
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 5'-D(\*AP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*GP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*G)-3'

Chain E: 



- Molecule 1: 5'-D(\*AP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*GP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*G)-3'

Chain J: 



- Molecule 1: 5'-D(\*AP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*GP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*G)-3'

Chain G: 



- Molecule 1: 5'-D(\*AP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*GP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*G)-3'

Chain K: 



- Molecule 2: 5'-D(\*CP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*CP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*(BRU))-3'

Chain I: 



- Molecule 2: 5'-D(\*CP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*CP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*(BRU))-3'

Chain F: 



- Molecule 2: 5'-D(\*CP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*CP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*(BRU))-3'

Chain L: 



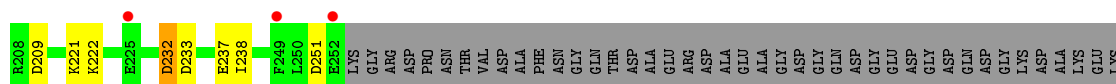
- Molecule 2: 5'-D(\*CP\*(BRU)P\*TP\*TP\*TP\*AP\*GP\*CP\*CP\*GP\*CP\*TP\*AP\*AP\*AP\*AP\*(BRU))-3'

Chain H: 



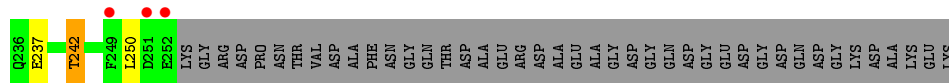
- Molecule 3: Transcriptional repressor protein korB

Chain A: 



- Molecule 3: Transcriptional repressor protein korB

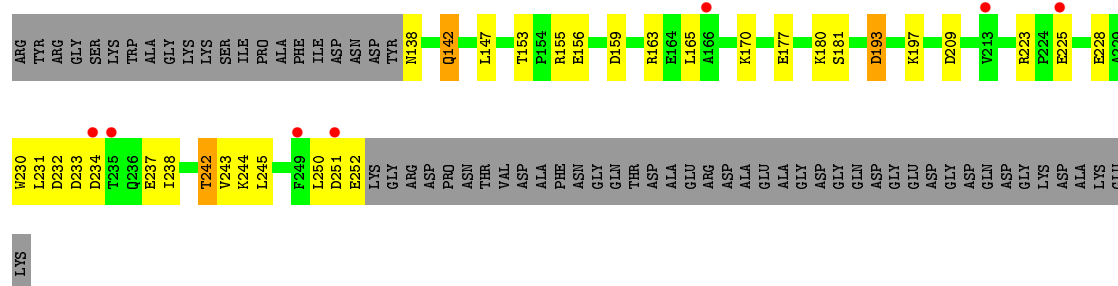
Chain B: 



- Molecule 3: Transcriptional repressor protein korB

Chain C: 

- Molecule 3: Transcriptional repressor protein korB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.44Å 110.44Å 160.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 27.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.20) 99.5 (27.61-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.195 , 0.250 0.202 , 0.249	Depositor DCC
$R_{free}$ test set	2911 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BRU

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	E	1.45	1/369 (0.3%)	2.29	26/566 (4.6%)
1	G	1.28	1/369 (0.3%)	2.11	24/566 (4.2%)
1	J	1.43	2/369 (0.5%)	2.22	22/566 (3.9%)
1	K	1.31	2/369 (0.5%)	2.32	30/566 (5.3%)
2	F	1.52	3/337 (0.9%)	2.17	18/515 (3.5%)
2	H	1.32	1/337 (0.3%)	2.11	14/515 (2.7%)
2	I	1.44	0/337	2.31	19/515 (3.7%)
2	L	1.38	1/337 (0.3%)	2.22	19/515 (3.7%)
3	A	0.80	0/923	0.90	4/1245 (0.3%)
3	B	0.70	0/944	0.82	1/1274 (0.1%)
3	C	0.70	0/905	0.91	5/1221 (0.4%)
3	D	0.80	0/931	0.89	3/1256 (0.2%)
All	All	1.08	11/6527 (0.2%)	1.64	185/9320 (2.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	10[A]	DG	C3'-O3'	-7.27	1.34	1.44
1	E	13[A]	DA	C3'-O3'	6.65	1.52	1.44
2	F	11[A]	DC	C1'-N1	5.99	1.57	1.49
2	F	11[A]	DC	C3'-O3'	5.40	1.50	1.44
2	L	7[B]	DG	N7-C5	5.21	1.42	1.39
1	J	10[B]	DG	N9-C4	5.18	1.42	1.38
1	K	9[B]	DG	N9-C4	-5.18	1.33	1.38
1	J	11[B]	DC	C3'-O3'	-5.16	1.37	1.44
2	F	9[A]	DC	C2-N3	5.13	1.39	1.35
1	K	12[B]	DT	C1'-N1	5.13	1.55	1.49
1	G	17[A]	DG	C8-N7	-5.03	1.27	1.30

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	7[B]	DG	O4'-C1'-N9	14.78	118.35	108.00
1	E	7[A]	DG	O4'-C1'-N9	13.47	117.43	108.00
2	F	3[A]	DT	O4'-C1'-N1	-11.98	99.62	108.00
1	G	7[A]	DG	O4'-C1'-N9	11.90	116.33	108.00
1	J	17[B]	DG	O4'-C4'-C3'	-11.84	98.90	106.00
2	F	7[A]	DG	O4'-C1'-N9	11.69	116.18	108.00
1	K	13[B]	DA	O4'-C1'-N9	-10.88	100.38	108.00
1	J	7[B]	DG	O4'-C1'-N9	10.68	115.47	108.00
1	J	17[B]	DG	C1'-O4'-C4'	-10.40	99.70	110.10
2	H	7[A]	DG	O4'-C1'-N9	10.34	115.24	108.00
1	E	10[A]	DG	O4'-C4'-C3'	-10.25	99.85	106.00
2	H	3[A]	DT	O4'-C1'-N1	-9.97	101.02	108.00
1	E	17[A]	DG	C1'-O4'-C4'	-9.93	100.17	110.10
1	E	17[A]	DG	O4'-C4'-C3'	-9.85	100.09	106.00
1	K	7[B]	DG	O4'-C1'-N9	9.84	114.89	108.00
2	L	7[B]	DG	O4'-C1'-N9	9.79	114.85	108.00
2	H	4[A]	DT	O4'-C1'-N1	-9.49	101.36	108.00
2	L	9[B]	DC	O4'-C1'-C2'	-9.40	98.38	105.90
1	K	3[B]	DT	O4'-C1'-N1	-9.33	101.47	108.00
1	K	17[B]	DG	O4'-C4'-C3'	-8.92	100.65	106.00
2	L	11[B]	DC	O4'-C4'-C3'	-8.83	100.70	106.00
2	F	11[A]	DC	P-O3'-C3'	8.74	130.19	119.70
2	L	5[B]	DT	O4'-C1'-N1	-8.73	101.89	108.00
2	I	14[B]	DA	P-O5'-C5'	-8.59	107.16	120.90
1	K	9[B]	DG	N3-C4-C5	8.57	132.89	128.60
1	J	13[B]	DA	O4'-C1'-N9	-8.52	102.04	108.00
1	E	3[A]	DT	N3-C4-O4	8.46	124.98	119.90
2	H	9[A]	DC	C1'-O4'-C4'	-8.45	101.65	110.10
2	I	9[B]	DC	P-O3'-C3'	8.40	129.78	119.70
1	K	9[B]	DG	N1-C6-O6	8.38	124.93	119.90
2	L	5[B]	DT	C5-C4-O4	-8.35	119.06	124.90
2	F	13[A]	DA	O4'-C1'-N9	-8.31	102.18	108.00
1	G	12[A]	DT	N3-C4-O4	8.17	124.81	119.90
1	K	9[B]	DG	N3-C4-N9	-8.15	121.11	126.00
2	F	7[A]	DG	O4'-C1'-C2'	-7.98	99.52	105.90
2	L	5[B]	DT	N3-C4-O4	7.90	124.64	119.90
2	H	10[A]	DG	O4'-C1'-N9	7.89	113.52	108.00
2	I	11[B]	DC	P-O3'-C3'	7.87	129.15	119.70
1	K	10[B]	DG	C2-N3-C4	7.87	115.83	111.90
2	L	9[B]	DC	N1-C2-O2	7.73	123.54	118.90
1	J	1[B]	DA	O4'-C1'-N9	-7.58	102.69	108.00
1	E	16[A]	DA	O4'-C1'-N9	-7.56	102.71	108.00
1	K	1[B]	DA	O4'-C1'-N9	-7.51	102.74	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	17[B]	DG	C1'-O4'-C4'	-7.42	102.68	110.10
2	F	9[A]	DC	N3-C4-N4	7.41	123.19	118.00
1	E	17[A]	DG	C4'-C3'-C2'	-7.35	96.48	103.10
1	J	4[B]	DT	C6-C5-C7	-7.32	118.51	122.90
2	I	1[B]	DC	N3-C4-C5	-7.24	119.00	121.90
1	G	17[A]	DG	O4'-C4'-C3'	-7.18	101.63	104.50
2	F	5[A]	DT	P-O3'-C3'	7.16	128.29	119.70
1	K	10[B]	DG	C5-C6-O6	-7.15	124.31	128.60
1	K	12[B]	DT	N3-C4-O4	7.09	124.16	119.90
1	K	9[B]	DG	N3-C2-N2	-7.08	114.94	119.90
2	F	1[A]	DC	O4'-C1'-N1	-7.07	103.05	108.00
2	I	1[B]	DC	C2-N3-C4	7.06	123.43	119.90
1	K	5[B]	DT	O4'-C1'-N1	-7.04	103.07	108.00
2	I	5[B]	DT	O4'-C1'-N1	-7.03	103.08	108.00
1	G	13[A]	DA	O4'-C1'-N9	-7.00	103.10	108.00
2	F	3[A]	DT	C6-C5-C7	-6.94	118.73	122.90
1	K	9[B]	DG	O4'-C1'-N9	-6.91	103.16	108.00
1	G	17[A]	DG	N9-C4-C5	-6.91	102.64	105.40
1	K	9[B]	DG	N1-C2-N2	6.87	122.38	116.20
1	J	1[B]	DA	O4'-C4'-C3'	-6.84	101.76	104.50
1	E	6[A]	DA	P-O3'-C3'	6.77	127.83	119.70
1	J	4[B]	DT	O4'-C1'-N1	-6.76	103.27	108.00
1	J	14[B]	DA	P-O3'-C3'	6.75	127.80	119.70
2	H	5[A]	DT	O4'-C1'-N1	-6.65	103.34	108.00
2	I	16[B]	DA	N1-C6-N6	6.63	122.58	118.60
1	E	4[A]	DT	O4'-C1'-N1	-6.61	103.38	108.00
1	J	4[B]	DT	C4-C5-C7	6.61	122.96	119.00
2	I	10[B]	DG	C5-C6-O6	-6.59	124.64	128.60
3	C	159	ASP	CB-CG-OD2	6.59	124.23	118.30
1	E	3[A]	DT	O4'-C1'-N1	-6.54	103.42	108.00
2	L	1[B]	DC	O4'-C1'-N1	-6.52	103.44	108.00
1	E	16[A]	DA	P-O3'-C3'	6.50	127.50	119.70
1	G	17[A]	DG	C1'-O4'-C4'	-6.50	103.60	110.10
1	E	5[A]	DT	P-O3'-C3'	6.47	127.47	119.70
1	G	7[A]	DG	C1'-O4'-C4'	-6.43	103.67	110.10
1	K	10[B]	DG	N3-C4-C5	-6.43	125.38	128.60
3	D	234	ASP	CB-CG-OD2	6.39	124.05	118.30
2	H	5[A]	DT	N3-C4-O4	6.38	123.73	119.90
1	K	11[B]	DC	C1'-O4'-C4'	-6.38	103.72	110.10
3	A	141	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	4[A]	DT	N3-C2-O2	-6.33	118.50	122.30
1	G	1[A]	DA	O4'-C1'-N9	-6.24	103.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	232	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	13[A]	DA	O4'-C1'-N9	-6.20	103.66	108.00
2	L	9[B]	DC	N3-C2-O2	-6.18	117.58	121.90
1	E	7[A]	DG	O4'-C1'-C2'	-6.14	100.98	105.90
3	C	232	ASP	CB-CG-OD2	6.12	123.80	118.30
1	J	3[B]	DT	C6-C5-C7	-6.11	119.23	122.90
1	E	4[A]	DT	N3-C4-O4	6.05	123.53	119.90
1	J	11[B]	DC	C1'-O4'-C4'	-6.04	104.06	110.10
1	E	5[A]	DT	N3-C4-O4	6.01	123.50	119.90
1	G	14[A]	DA	P-O3'-C3'	5.99	126.89	119.70
2	F	7[A]	DG	C1'-O4'-C4'	-5.98	104.12	110.10
2	I	13[B]	DA	O4'-C1'-N9	-5.98	103.81	108.00
1	G	10[A]	DG	O4'-C1'-N9	5.97	112.18	108.00
2	H	13[A]	DA	O4'-C1'-N9	-5.95	103.84	108.00
1	J	10[B]	DG	C2-N3-C4	5.92	114.86	111.90
1	J	10[B]	DG	P-O3'-C3'	5.90	126.78	119.70
1	E	1[A]	DA	O4'-C1'-N9	-5.88	103.88	108.00
3	A	233	ASP	CB-CG-OD2	5.87	123.58	118.30
2	F	7[A]	DG	P-O3'-C3'	5.86	126.74	119.70
1	G	11[A]	DC	OP1-P-OP2	5.85	128.38	119.60
1	G	12[A]	DT	C5-C4-O4	-5.84	120.81	124.90
1	J	3[B]	DT	C4-C5-C7	5.81	122.48	119.00
1	K	13[B]	DA	N9-C1'-C2'	5.79	123.60	112.60
2	I	10[B]	DG	C2-N3-C4	5.78	114.79	111.90
2	I	16[B]	DA	C3'-C2'-C1'	-5.75	95.60	102.50
2	L	3[B]	DT	O4'-C1'-N1	-5.71	104.01	108.00
1	G	15[A]	DA	P-O5'-C5'	-5.68	111.81	120.90
2	I	3[B]	DT	O4'-C1'-N1	-5.68	104.02	108.00
1	J	3[B]	DT	O4'-C1'-N1	-5.67	104.03	108.00
2	F	9[A]	DC	C5-C4-N4	-5.66	116.24	120.20
1	K	10[B]	DG	P-O3'-C3'	5.66	126.49	119.70
2	L	15[B]	DA	P-O3'-C3'	5.65	126.47	119.70
1	G	17[A]	DG	C8-N9-C4	5.61	108.64	106.40
2	I	15[B]	DA	P-O3'-C3'	5.60	126.42	119.70
1	J	6[B]	DA	O4'-C1'-N9	-5.58	104.10	108.00
2	I	5[B]	DT	C4-C5-C7	5.57	122.34	119.00
1	J	15[B]	DA	P-O3'-C3'	5.54	126.35	119.70
1	K	3[B]	DT	P-O3'-C3'	5.54	126.34	119.70
2	H	16[A]	DA	C1'-O4'-C4'	-5.53	104.57	110.10
1	G	3[A]	DT	O4'-C1'-C2'	-5.52	101.48	105.90
1	G	17[A]	DG	N3-C4-C5	5.52	131.36	128.60
1	E	11[A]	DC	C1'-O4'-C4'	-5.49	104.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	17[A]	DG	N1-C6-O6	5.48	123.19	119.90
2	L	8[B]	DC	O4'-C1'-C2'	-5.47	101.52	105.90
1	K	17[B]	DG	O4'-C1'-N9	-5.45	104.18	108.00
3	B	232	ASP	CB-CG-OD2	5.44	123.20	118.30
1	E	4[A]	DT	N1-C1'-C2'	5.40	122.86	112.60
2	I	8[B]	DC	O4'-C1'-N1	-5.38	104.23	108.00
1	K	7[B]	DG	P-O3'-C3'	5.38	126.16	119.70
2	H	5[A]	DT	C5-C4-O4	-5.37	121.14	124.90
1	E	16[A]	DA	N9-C1'-C2'	5.37	122.80	112.60
1	K	3[B]	DT	C5-C4-O4	-5.36	121.15	124.90
3	C	251	ASP	CB-CG-OD2	5.36	123.12	118.30
3	C	141	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	3[A]	DT	C5-C4-O4	-5.33	121.17	124.90
2	H	14[A]	DA	O4'-C1'-N9	-5.32	104.27	108.00
2	L	6[B]	DA	C8-N9-C4	-5.32	103.67	105.80
1	K	9[B]	DG	C5-C6-O6	-5.31	125.41	128.60
2	I	12[B]	DT	C3'-C2'-C1'	-5.30	96.14	102.50
2	F	12[A]	DT	C4-C5-C7	5.29	122.17	119.00
2	F	8[A]	DC	C6-N1-C2	-5.29	118.18	120.30
2	L	3[B]	DT	N1-C1'-C2'	5.27	122.61	112.60
2	F	5[A]	DT	O4'-C4'-C3'	5.26	109.16	106.00
2	F	3[A]	DT	C4-C5-C7	5.25	122.15	119.00
1	G	17[A]	DG	C4-C5-N7	5.25	112.90	110.80
3	C	194	LEU	CA-CB-CG	5.24	127.35	115.30
2	H	7[A]	DG	N1-C2-N2	5.24	120.91	116.20
1	G	9[A]	DG	C6-N1-C2	5.23	128.24	125.10
2	F	5[A]	DT	N3-C4-O4	5.23	123.04	119.90
1	K	10[B]	DG	C5-C6-N1	5.22	114.11	111.50
2	L	14[B]	DA	P-O3'-C3'	5.21	125.96	119.70
1	E	13[A]	DA	C4'-C3'-C2'	-5.20	98.42	103.10
2	L	1[B]	DC	C2-N1-C1'	5.20	124.52	118.80
1	G	4[A]	DT	N1-C2-O2	5.19	127.25	123.10
2	H	5[A]	DT	N1-C1'-C2'	5.17	122.42	112.60
2	L	7[B]	DG	N1-C6-O6	-5.17	116.80	119.90
1	E	12[A]	DT	C5-C4-O4	-5.16	121.29	124.90
2	I	1[B]	DC	O4'-C1'-C2'	-5.16	101.78	105.90
1	E	5[A]	DT	O4'-C1'-N1	-5.14	104.40	108.00
1	G	7[A]	DG	C3'-C2'-C1'	-5.14	96.33	102.50
2	F	11[A]	DC	C6-N1-C2	-5.13	118.25	120.30
2	L	13[B]	DA	O4'-C1'-N9	-5.12	104.42	108.00
2	I	16[B]	DA	O4'-C1'-N9	5.10	111.57	108.00
1	E	12[A]	DT	N3-C4-O4	5.10	122.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	232	ASP	CB-CG-OD2	5.09	122.88	118.30
1	K	12[B]	DT	O4'-C1'-N1	5.07	111.55	108.00
1	K	10[B]	DG	C6-N1-C2	-5.07	122.06	125.10
3	A	251	ASP	CB-CG-OD2	5.06	122.86	118.30
1	G	7[A]	DG	N3-C4-N9	-5.05	122.97	126.00
1	K	15[B]	DA	N9-C4-C5	5.05	107.82	105.80
1	J	12[B]	DT	O5'-P-OP1	5.04	116.75	110.70
1	J	5[B]	DT	C5-C4-O4	-5.03	121.38	124.90
2	L	9[B]	DC	C1'-O4'-C4'	-5.03	105.07	110.10
3	D	159	ASP	CB-CG-OD2	5.02	122.82	118.30
1	K	11[B]	DC	N1-C1'-C2'	5.02	122.14	112.60
1	G	17[A]	DG	C2-N3-C4	-5.02	109.39	111.90
1	J	12[B]	DT	N3-C4-O4	5.01	122.91	119.90
2	H	10[A]	DG	N1-C6-O6	5.01	122.91	119.90
1	J	10[B]	DG	N3-C4-C5	-5.01	126.09	128.60
1	E	12[A]	DT	O3'-P-O5'	-5.01	94.49	104.00

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	E	349	0	161	24	0
1	G	349	0	167	15	0
1	J	349	0	160	20	0
1	K	349	0	166	22	0
2	F	342	0	163	31	0
2	H	342	0	160	12	0
2	I	342	0	170	31	0
2	L	342	0	157	24	0
3	A	912	0	924	19	0
3	B	932	0	939	13	0
3	C	894	0	912	19	0
3	D	920	0	930	22	0
4	A	54	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	29	0	0	2	0
4	C	29	0	0	3	0
4	D	27	0	0	1	0
4	E	31	0	0	6	0
4	F	34	0	0	9	0
4	G	30	0	0	6	0
4	H	21	0	0	3	0
4	I	21	0	0	5	0
4	J	24	0	0	4	0
4	K	24	0	0	10	0
4	L	23	0	0	3	0
All	All	6769	0	5009	207	0

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 19.

All (207) 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)
2:L:17[B]:BRU:O3'	4:L:332:HOH:O	1.67	1.11
3:C:200:ASP:O	3:C:204:THR:HG22	1.49	1.11
2:I:1[B]:DC:H2''	2:I:2[B]:BRU:H5''	1.23	1.09
2:I:1[B]:DC:N4	1:J:17[B]:DG:O6	1.93	1.01
1:E:12[A]:DT:H2''	1:E:13[A]:DA:N7	1.75	1.01
2:I:1[B]:DC:H2''	2:I:2[B]:BRU:C5'	1.92	1.00
2:F:14[A]:DA:N7	4:F:33:HOH:O	1.93	0.99
1:G:7[A]:DG:N7	4:G:24:HOH:O	1.96	0.96
1:K:7[B]:DG:N7	4:K:33:HOH:O	1.98	0.94
3:A:148:GLN:HB2	4:A:332:HOH:O	1.74	0.88
2:I:1[B]:DC:N4	1:J:17[B]:DG:C6	2.43	0.87
2:I:15[B]:DA:N7	4:I:29:HOH:O	2.06	0.86
2:I:1[B]:DC:N3	1:J:17[B]:DG:N1	2.24	0.86
2:I:14[B]:DA:N7	4:I:22:HOH:O	2.10	0.84
2:F:16[A]:DA:N7	4:F:150:HOH:O	2.11	0.83
2:L:15[B]:DA:N3	4:L:80:HOH:O	2.11	0.82
2:I:6[B]:DA:OP2	4:I:26:HOH:O	1.97	0.81
2:F:10[A]:DG:N3	4:F:98:HOH:O	2.13	0.81
1:E:2[A]:BRU:BR	4:E:33:HOH:O	2.54	0.80
1:E:15[A]:DA:N3	4:E:26:HOH:O	2.15	0.80
1:K:3[B]:DT:O2	4:K:27:HOH:O	2.00	0.80
1:G:16[A]:DA:N7	4:G:34:HOH:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2[A]:BRU:BR	4:J:31:HOH:O	2.54	0.79
1:K:8[B]:DC:OP2	4:K:40:HOH:O	1.99	0.79
2:I:6[B]:DA:H8	4:I:26:HOH:O	1.68	0.76
2:L:16[B]:DA:N3	4:K:27:HOH:O	2.18	0.76
1:K:7[B]:DG:O6	4:K:23:HOH:O	2.04	0.75
2:I:1[B]:DC:N4	1:J:17[B]:DG:N1	2.33	0.75
1:E:10[A]:DG:N3	4:E:19:HOH:O	2.19	0.75
2:F:10[A]:DG:H1'	2:F:11[A]:DC:H5'	1.70	0.74
3:B:237:GLU:O	3:B:242:THR:HG21	1.87	0.74
2:H:2[A]:BRU:OP2	4:H:31:HOH:O	2.05	0.74
1:G:9[A]:DG:OP2	4:G:23:HOH:O	2.06	0.73
2:H:14[A]:DA:N3	4:H:20:HOH:O	2.21	0.73
1:E:12[A]:DT:O2	2:F:6[A]:DA:C2	2.43	0.72
2:H:2[A]:BRU:BR	4:K:37:HOH:O	2.64	0.71
1:E:14[A]:DA:N3	4:E:21:HOH:O	2.23	0.71
2:F:15[A]:DA:N7	4:F:133:HOH:O	2.21	0.71
3:A:197:LYS:NZ	3:A:232:ASP:OD1	2.23	0.71
2:I:8[B]:DC:OP2	4:I:21:HOH:O	2.08	0.71
1:G:14[A]:DA:N6	4:G:28:HOH:O	2.24	0.71
3:A:197:LYS:HE2	3:A:232:ASP:OD1	1.92	0.70
1:K:14[B]:DA:N7	4:K:22:HOH:O	2.24	0.70
2:H:2[A]:BRU:H2'	2:H:3[A]:DT:H71	1.73	0.70
2:L:4[B]:DT:C2	2:L:5[B]:DT:C5	2.80	0.70
2:H:11[A]:DC:H2''	2:H:12[A]:DT:O5'	1.91	0.69
2:I:4[B]:DT:H2'	2:I:5[B]:DT:H71	1.74	0.68
2:L:8[B]:DC:N4	1:K:10[B]:DG:O6	2.27	0.68
2:L:4[B]:DT:N3	2:L:5[B]:DT:C4	2.61	0.68
1:G:2[A]:BRU:H2''	1:G:3[A]:DT:O5'	1.93	0.67
1:E:15[A]:DA:H2''	1:E:16[A]:DA:O5'	1.94	0.67
2:I:2[B]:BRU:H2''	2:I:3[B]:DT:O5'	1.95	0.66
2:H:15[A]:DA:N3	4:H:21:HOH:O	2.27	0.66
2:I:1[B]:DC:C2'	2:I:2[B]:BRU:C5'	2.72	0.66
2:L:11[B]:DC:H2''	2:L:12[B]:DT:H5'	1.78	0.66
1:G:1[A]:DA:H2''	1:G:2[A]:BRU:H5''	1.77	0.66
2:I:1[B]:DC:N3	1:J:17[B]:DG:N2	2.43	0.66
2:F:12[A]:DT:H2'	3:A:181:SER:HB3	1.77	0.66
1:J:2[B]:BRU:C2'	1:J:3[B]:DT:H71	2.25	0.66
2:L:1[B]:DC:H2''	2:L:2[B]:BRU:O5'	1.95	0.66
2:I:1[B]:DC:O2	1:J:17[B]:DG:N2	2.28	0.66
1:E:10[A]:DG:N2	4:E:19:HOH:O	2.27	0.65
2:F:8[A]:DC:O2	4:F:67:HOH:O	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12[A]:DT:H2''	1:E:13[A]:DA:C5	2.32	0.65
1:K:12[B]:DT:H2'	3:D:181:SER:CB	2.26	0.65
2:H:10[A]:DG:H1'	2:H:11[A]:DC:H5'	1.78	0.65
2:L:4[B]:DT:C2	2:L:5[B]:DT:C6	2.85	0.65
2:F:14[A]:DA:N6	4:F:94:HOH:O	2.30	0.65
2:I:1[B]:DC:C4	1:J:17[B]:DG:N1	2.65	0.65
1:E:14[A]:DA:C2	2:F:5[A]:DT:O2	2.50	0.64
3:A:145:GLU:HA	4:A:332:HOH:O	1.97	0.64
1:G:12[A]:DT:H2'	3:C:181:SER:CB	2.28	0.64
3:D:230:TRP:HZ2	3:D:242:THR:HG23	1.62	0.64
3:D:230:TRP:CZ2	3:D:242:THR:HG23	2.33	0.64
3:A:197:LYS:CE	3:A:232:ASP:OD1	2.45	0.63
1:G:2[A]:BRU:H2'	1:G:3[A]:DT:H71	1.80	0.63
1:J:15[B]:DA:N3	4:J:20:HOH:O	2.28	0.63
2:I:13[B]:DA:H2''	2:I:14[B]:DA:O5'	1.98	0.62
3:C:143:VAL:HG12	4:C:315:HOH:O	2.00	0.62
1:E:12[A]:DT:O2	2:F:6[A]:DA:H2	1.82	0.62
3:C:144:ILE:H	3:C:144:ILE:HD12	1.65	0.62
3:A:143:VAL:HG11	3:A:160:PHE:CD1	2.35	0.61
1:E:12[A]:DT:H2''	1:E:13[A]:DA:C8	2.35	0.61
1:G:12[A]:DT:H2'	3:C:181:SER:HB3	1.83	0.61
3:D:238:ILE:HA	3:D:242:THR:HG21	1.82	0.61
1:E:14[A]:DA:H2''	1:E:15[A]:DA:O5'	2.01	0.61
3:D:138:ASN:O	3:D:142:GLN:HG2	2.00	0.60
2:I:1[B]:DC:C2	1:J:17[B]:DG:N2	2.69	0.60
3:B:184:PHE:O	3:B:188:HIS:HD2	1.84	0.60
3:C:144:ILE:N	3:C:144:ILE:HD12	2.16	0.60
3:D:153:THR:CG2	3:D:156:GLU:H	2.14	0.60
2:L:4[B]:DT:C4	2:L:5[B]:DT:C4	2.90	0.60
3:B:195:PRO:HG2	3:B:198:ILE:HD12	1.85	0.59
1:E:15[A]:DA:H1'	1:E:16[A]:DA:H5'	1.84	0.59
1:E:2[A]:BRU:C2'	1:E:3[A]:DT:H72	2.33	0.59
1:K:12[B]:DT:H2'	3:D:181:SER:HB3	1.84	0.59
2:F:5[A]:DT:H2''	2:F:6[A]:DA:H5'	1.84	0.58
2:I:15[B]:DA:N1	1:J:3[B]:DT:N3	2.46	0.58
3:D:153:THR:HG22	3:D:156:GLU:CG	2.33	0.58
2:F:2[A]:BRU:OP1	4:F:222:HOH:O	2.16	0.58
2:I:2[B]:BRU:N3	1:J:16[B]:DA:N1	2.36	0.58
3:C:158:ALA:HB1	3:C:192:LEU:HD13	1.84	0.58
2:F:11[A]:DC:H2'	2:F:12[A]:DT:C6	2.39	0.57
2:L:15[B]:DA:N1	1:K:3[B]:DT:N3	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1[B]:DC:O2	1:K:17[B]:DG:N2	2.30	0.56
2:H:14[A]:DA:H2''	2:H:15[A]:DA:O5'	2.04	0.56
2:L:11[B]:DC:H2''	2:L:12[B]:DT:C5'	2.35	0.55
3:D:193:ASP:CG	3:D:193:ASP:O	2.45	0.55
3:B:230:TRP:HZ2	3:B:242:THR:HG23	1.72	0.55
2:I:1[B]:DC:N3	1:J:17[B]:DG:C2	2.75	0.55
1:G:8[A]:DC:OP2	4:G:35:HOH:O	2.18	0.55
1:J:9[B]:DG:OP2	4:J:19:HOH:O	2.18	0.55
2:L:1[B]:DC:N3	1:K:17[B]:DG:N1	2.55	0.55
3:D:153:THR:HG23	3:D:156:GLU:H	1.71	0.54
3:B:142:GLN:HG3	3:D:163:ARG:HH12	1.72	0.54
1:E:15[A]:DA:C6	1:E:16[A]:DA:C5	2.94	0.54
2:F:3[A]:DT:H2'	3:B:186:THR:HG21	1.88	0.54
1:E:12[A]:DT:C2	2:F:6[A]:DA:N1	2.76	0.53
2:F:5[A]:DT:C2'	2:F:6[A]:DA:H5'	2.38	0.53
3:C:153:THR:HB	3:C:154:PRO:HD2	1.89	0.53
3:D:223:ARG:HD2	3:D:250:LEU:HB3	1.90	0.52
2:F:2[A]:BRU:H6	4:J:26:HOH:O	2.08	0.52
1:G:4[A]:DT:O2	2:H:15[A]:DA:C2	2.62	0.52
2:H:1[A]:DC:H6	2:H:1[A]:DC:HO5'	1.57	0.52
2:I:12[B]:DT:H2'	3:B:181:SER:CB	2.39	0.52
3:B:205:GLY:O	3:B:208:ARG:HD2	2.08	0.52
3:C:200:ASP:O	3:C:204:THR:CG2	2.42	0.52
3:D:153:THR:HG22	3:D:156:GLU:HG3	1.91	0.52
3:A:190:THR:O	3:A:194:LEU:HD13	2.10	0.51
3:C:140:ALA:O	3:C:144:ILE:CD1	2.59	0.51
4:K:29:HOH:O	3:D:180:LYS:HE2	2.09	0.51
3:A:158:ALA:HB1	3:A:192:LEU:HD13	1.93	0.51
2:I:9[B]:DC:N4	1:J:9[B]:DG:O6	2.43	0.51
4:F:265:HOH:O	1:J:7[B]:DG:H8	1.93	0.51
1:K:9[B]:DG:H2'	3:D:209:ASP:CG	2.31	0.50
1:E:10[A]:DG:O5'	1:E:10[A]:DG:H2'	2.11	0.50
3:D:155:ARG:HD3	4:D:319:HOH:O	2.11	0.50
3:C:150:ASN:HA	4:C:322:HOH:O	2.11	0.50
2:F:3[A]:DT:H71	3:B:182:PRO:HB2	1.94	0.50
2:L:4[B]:DT:C4	2:L:5[B]:DT:O4	2.65	0.49
2:L:1[B]:DC:O5'	2:L:1[B]:DC:H6	1.94	0.49
2:F:12[A]:DT:H2'	3:A:181:SER:CB	2.42	0.49
1:E:15[A]:DA:N6	1:E:16[A]:DA:C6	2.80	0.49
1:E:12[A]:DT:O2	2:F:6[A]:DA:N1	2.46	0.49
1:K:10[B]:DG:H2''	1:K:11[B]:DC:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10[A]:DG:H2''	2:F:11[A]:DC:O5'	2.12	0.48
2:I:7[B]:DG:H4'	2:I:8[B]:DC:H5'	1.94	0.48
2:I:5[B]:DT:N3	1:J:13[B]:DA:N1	2.61	0.48
2:F:11[A]:DC:C2'	2:F:12[A]:DT:C6	2.97	0.48
2:F:7[A]:DG:H2''	2:F:8[A]:DC:C6	2.49	0.47
3:A:147:LEU:O	3:A:147:LEU:HD22	2.14	0.47
2:F:16[A]:DA:C2'	2:F:17[A]:BRU:BR	3.18	0.47
2:I:11[B]:DC:H2'	2:I:12[B]:DT:C6	2.50	0.47
3:B:148:GLN:HG2	4:B:307:HOH:O	2.15	0.47
1:E:10[A]:DG:OP1	4:E:45:HOH:O	2.20	0.46
2:L:4[B]:DT:H2''	2:L:5[B]:DT:OP2	2.15	0.46
2:L:4[B]:DT:C5	2:L:5[B]:DT:H73	2.50	0.46
2:I:3[B]:DT:H2'	3:A:186:THR:HG21	1.95	0.46
2:L:4[B]:DT:N3	2:L:5[B]:DT:C5	2.84	0.46
2:F:11[A]:DC:H2'	2:F:12[A]:DT:C5	2.51	0.46
1:G:9[A]:DG:H2''	1:G:10[A]:DG:O5'	2.16	0.46
1:G:10[A]:DG:H2''	1:G:11[A]:DC:O5'	2.16	0.46
3:C:230:TRP:CD2	3:C:246:LEU:HD22	2.52	0.45
2:H:10[A]:DG:H2''	2:H:11[A]:DC:O5'	2.15	0.45
3:C:233:ASP:OD1	3:C:235:THR:OG1	2.33	0.45
1:K:6[B]:DA:H8	4:K:30:HOH:O	1.98	0.45
1:E:14[A]:DA:C2	2:F:5[A]:DT:C2	3.05	0.45
2:L:15[B]:DA:H2''	2:L:16[B]:DA:O5'	2.17	0.45
2:L:2[B]:BRU:OP1	4:L:60:HOH:O	2.20	0.45
3:A:164:GLU:OE1	3:A:177:GLU:OE2	2.35	0.44
2:I:4[B]:DT:N3	1:J:14[B]:DA:N1	2.66	0.44
1:J:9[B]:DG:H2'	3:A:209:ASP:CG	2.38	0.44
3:D:237:GLU:O	3:D:242:THR:HG21	2.17	0.44
1:J:9[B]:DG:H2'	3:A:209:ASP:OD2	2.18	0.43
2:I:1[B]:DC:C2'	2:I:2[B]:BRU:H5'	2.46	0.43
1:G:8[A]:DC:H2''	1:G:9[A]:DG:O5'	2.19	0.43
1:K:12[B]:DT:P	3:D:180:LYS:HD3	2.59	0.43
2:L:4[B]:DT:C6	2:L:5[B]:DT:C7	3.02	0.43
2:I:12[B]:DT:H2'	3:B:181:SER:HB3	2.00	0.42
3:D:153:THR:CG2	3:D:156:GLU:HG3	2.49	0.42
1:E:1[A]:DA:H5'	1:E:1[A]:DA:C8	2.53	0.42
3:C:206:ARG:NH2	3:C:231:LEU:O	2.47	0.42
1:K:16[B]:DA:H2''	1:K:17[B]:DG:O5'	2.19	0.42
3:A:139:GLU:OE1	3:A:143:VAL:HG23	2.19	0.42
1:G:5[A]:DT:H2''	1:G:6[A]:DA:C8	2.53	0.42
2:L:8[B]:DC:N4	1:K:10[B]:DG:C6	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5[B]:DT:OP1	3:C:247:ARG:NH2	2.51	0.42
1:K:4[B]:DT:H2''	1:K:5[B]:DT:OP2	2.20	0.41
3:A:207:VAL:HG22	3:A:238:ILE:HG21	2.02	0.41
3:D:242:THR:HG22	3:D:243:VAL:N	2.34	0.41
3:B:147:LEU:HA	3:B:147:LEU:HD23	1.86	0.41
3:A:153:THR:HB	3:A:154:PRO:HD2	2.03	0.41
4:G:44:HOH:O	3:C:180:LYS:NZ	2.48	0.41
3:C:223:ARG:HG3	3:C:250:LEU:HD13	2.01	0.41
1:K:12[B]:DT:OP2	3:D:180:LYS:HD3	2.20	0.41
4:B:317:HOH:O	3:D:142:GLN:CB	2.68	0.41
1:E:15[A]:DA:C6	1:E:16[A]:DA:C6	3.09	0.41
2:F:14[A]:DA:H2'	4:F:204:HOH:O	2.20	0.41
2:F:16[A]:DA:C2	2:F:17[A]:BRU:N3	2.89	0.41
1:K:2[B]:BRU:OP1	4:K:28:HOH:O	2.22	0.41
3:B:230:TRP:CZ2	3:B:242:THR:HG23	2.52	0.41
3:C:140:ALA:O	3:C:144:ILE:HD12	2.20	0.41
3:A:188:HIS:O	3:A:191:LEU:HB2	2.20	0.40
2:F:1[A]:DC:H2'	2:F:2[A]:BRU:C6	2.51	0.40
3:C:167:LYS:NZ	4:C:320:HOH:O	2.53	0.40
2:L:3[B]:DT:N3	1:K:15[B]:DA:N1	2.69	0.40
2:H:1[A]:DC:O5'	2:H:1[A]:DC:H6	2.04	0.40

There are no symmetry-related clashes.

## 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	
3	A	112/178 (63%)	110 (98%)	2 (2%)	0	100	100
3	B	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
3	C	110/178 (62%)	107 (97%)	3 (3%)	0	100	100
3	D	113/178 (64%)	109 (96%)	3 (3%)	1 (1%)	17	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	449/712 (63%)	438 (98%)	10 (2%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	233	ASP

### 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
3	A	99/147 (67%)	91 (92%)	8 (8%)	11 12
3	B	101/147 (69%)	93 (92%)	8 (8%)	12 12
3	C	97/147 (66%)	88 (91%)	9 (9%)	9 8
3	D	100/147 (68%)	85 (85%)	15 (15%)	3 2
All	All	397/588 (68%)	357 (90%)	40 (10%)	7 7

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	147	LEU
3	A	152	LEU
3	A	191	LEU
3	A	192	LEU
3	A	194	LEU
3	A	221	LYS
3	A	222	LYS
3	A	237	GLU
3	B	139	GLU
3	B	150	ASN
3	B	152	LEU
3	B	196	GLU
3	B	208	ARG
3	B	235	THR

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Mol	Chain	Res	Type
3	B	242	THR
3	B	250	LEU
3	C	165	LEU
3	C	176	LYS
3	C	177	GLU
3	C	191	LEU
3	C	192	LEU
3	C	194	LEU
3	C	204	THR
3	C	237	GLU
3	C	251	ASP
3	D	142	GLN
3	D	147	LEU
3	D	165	LEU
3	D	170	LYS
3	D	177	GLU
3	D	193	ASP
3	D	197	LYS
3	D	225	GLU
3	D	228	GLU
3	D	231	LEU
3	D	242	THR
3	D	244	LYS
3	D	245	LEU
3	D	251	ASP
3	D	252	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	148	GLN
3	B	142	GLN
3	B	188	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	BRU	G	2[A]	1,2	15,21,22	2.39	2 (13%)	17,30,33	2.12	4 (23%)
2	BRU	H	17[A]	1,2	15,21,22	2.06	1 (6%)	17,30,33	2.47	5 (29%)
2	BRU	F	2[A]	1,2	15,21,22	2.30	2 (13%)	17,30,33	2.12	3 (17%)
1	BRU	J	2[B]	1	15,21,22	2.41	2 (13%)	17,30,33	2.37	4 (23%)
2	BRU	I	2[B]	2	15,21,22	2.70	2 (13%)	17,30,33	2.18	3 (17%)
2	BRU	H	2[A]	1,2	15,21,22	2.36	1 (6%)	17,30,33	2.40	3 (17%)
2	BRU	I	17[B]	2	15,21,22	1.82	1 (6%)	17,30,33	2.52	4 (23%)
2	BRU	L	17[B]	2	15,21,22	1.88	1 (6%)	17,30,33	2.33	5 (29%)
1	BRU	E	2[A]	1,2	15,21,22	2.23	1 (6%)	17,30,33	2.08	5 (29%)
1	BRU	K	2[B]	1	15,21,22	2.58	2 (13%)	17,30,33	2.26	4 (23%)
2	BRU	L	2[B]	2	15,21,22	2.10	3 (20%)	17,30,33	2.27	7 (41%)
2	BRU	F	17[A]	1,2	15,21,22	2.23	1 (6%)	17,30,33	2.22	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BRU	G	2[A]	1,2	-	2/4/21/22	0/2/2/2
2	BRU	H	17[A]	1,2	-	2/4/21/22	0/2/2/2
2	BRU	F	2[A]	1,2	-	2/4/21/22	0/2/2/2
1	BRU	J	2[B]	1	-	1/4/21/22	0/2/2/2
2	BRU	I	2[B]	2	-	2/4/21/22	0/2/2/2
2	BRU	H	2[A]	1,2	-	1/4/21/22	0/2/2/2
2	BRU	I	17[B]	2	-	0/4/21/22	0/2/2/2
2	BRU	L	17[B]	2	-	2/4/21/22	0/2/2/2
1	BRU	E	2[A]	1,2	-	1/4/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BRU	K	2[B]	1	-	1/4/21/22	0/2/2/2
2	BRU	L	2[B]	2	-	3/4/21/22	0/2/2/2
2	BRU	F	17[A]	1,2	-	3/4/21/22	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2[B]	BRU	C4-C5	9.82	1.51	1.38
1	K	2[B]	BRU	C4-C5	9.44	1.50	1.38
2	H	2[A]	BRU	C4-C5	8.72	1.49	1.38
1	J	2[B]	BRU	C4-C5	8.71	1.49	1.38
1	G	2[A]	BRU	C4-C5	8.66	1.49	1.38
2	F	2[A]	BRU	C4-C5	8.42	1.49	1.38
2	F	17[A]	BRU	C4-C5	8.11	1.48	1.38
1	E	2[A]	BRU	C4-C5	7.83	1.48	1.38
2	H	17[A]	BRU	C4-C5	7.49	1.48	1.38
2	L	2[B]	BRU	C4-C5	6.80	1.47	1.38
2	L	17[B]	BRU	C4-C5	6.79	1.47	1.38
2	I	17[B]	BRU	C4-C5	6.57	1.46	1.38
2	I	2[B]	BRU	C2-N3	-3.07	1.32	1.38
1	J	2[B]	BRU	C2-N3	-2.77	1.32	1.38
2	L	2[B]	BRU	C2-N3	-2.51	1.33	1.38
2	L	2[B]	BRU	C1'-N1	-2.35	1.42	1.49
1	G	2[A]	BRU	C2-N3	-2.25	1.33	1.38
2	F	2[A]	BRU	C2-N3	-2.12	1.34	1.38
1	K	2[B]	BRU	C2-N3	-2.03	1.34	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	2[B]	BRU	C4-N3-C2	7.35	121.35	115.14
2	H	2[A]	BRU	C4-N3-C2	7.25	121.26	115.14
2	I	2[B]	BRU	C4-N3-C2	7.01	121.06	115.14
2	F	17[A]	BRU	C4-N3-C2	6.98	121.04	115.14
2	I	17[B]	BRU	C4-N3-C2	6.47	120.61	115.14
2	F	2[A]	BRU	C4-N3-C2	6.43	120.57	115.14
1	K	2[B]	BRU	C4-N3-C2	6.26	120.42	115.14
2	H	17[A]	BRU	C4-N3-C2	5.84	120.07	115.14
1	G	2[A]	BRU	C4-N3-C2	5.80	120.04	115.14
2	L	2[B]	BRU	C4-N3-C2	5.64	119.90	115.14
1	E	2[A]	BRU	C4-N3-C2	5.11	119.45	115.14
2	L	17[B]	BRU	C4-N3-C2	5.01	119.37	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	17[B]	BRU	BR-C5-C4	-4.91	114.04	121.50
2	H	2[A]	BRU	C5-C4-N3	-4.89	117.78	123.64
1	G	2[A]	BRU	C5-C4-N3	-4.84	117.84	123.64
1	E	2[A]	BRU	C5-C4-N3	-4.63	118.10	123.64
2	I	17[B]	BRU	BR-C5-C4	-4.63	114.48	121.50
2	H	17[A]	BRU	BR-C5-C4	-4.52	114.64	121.50
2	H	17[A]	BRU	C5-C4-N3	-4.17	118.65	123.64
2	F	2[A]	BRU	C5-C4-N3	-4.07	118.77	123.64
2	L	17[B]	BRU	C5-C4-N3	-4.02	118.83	123.64
2	I	17[B]	BRU	C5-C4-N3	-3.93	118.93	123.64
2	I	17[B]	BRU	BR-C5-C6	3.88	126.16	117.31
1	K	2[B]	BRU	C2'-C1'-N1	3.67	122.73	114.27
2	H	17[A]	BRU	BR-C5-C6	3.66	125.64	117.31
1	J	2[B]	BRU	C5-C4-N3	-3.54	119.40	123.64
2	L	2[B]	BRU	C5-C4-N3	-3.53	119.41	123.64
1	K	2[B]	BRU	C5-C4-N3	-3.39	119.58	123.64
2	L	2[B]	BRU	O4'-C1'-C2'	3.38	112.63	106.25
2	L	17[B]	BRU	BR-C5-C6	3.30	124.82	117.31
2	F	17[A]	BRU	BR-C5-C6	3.14	124.47	117.31
2	I	2[B]	BRU	C2'-C1'-N1	3.02	121.23	114.27
1	J	2[B]	BRU	C2'-C1'-N1	2.89	120.93	114.27
2	L	2[B]	BRU	C2'-C1'-N1	2.86	120.87	114.27
2	F	2[A]	BRU	C2'-C1'-N1	2.78	120.67	114.27
2	H	17[A]	BRU	C2'-C1'-N1	-2.75	107.93	114.27
2	I	2[B]	BRU	C5-C4-N3	-2.64	120.48	123.64
2	H	2[A]	BRU	C2'-C1'-N1	2.59	120.24	114.27
1	E	2[A]	BRU	O3'-C3'-C2'	-2.53	101.85	110.90
2	F	17[A]	BRU	C2'-C1'-N1	-2.47	108.57	114.27
1	G	2[A]	BRU	C3'-C2'-C1'	2.47	108.73	102.54
1	G	2[A]	BRU	C2'-C1'-N1	2.43	119.87	114.27
1	E	2[A]	BRU	C2'-C3'-C4'	2.38	107.73	102.76
2	L	2[B]	BRU	C6-N1-C1'	2.38	124.58	119.24
1	K	2[B]	BRU	C2'-C3'-C4'	2.28	107.51	102.76
1	E	2[A]	BRU	C2'-C1'-N1	2.20	119.34	114.27
2	L	2[B]	BRU	C2'-C3'-C4'	2.14	107.21	102.76
2	F	17[A]	BRU	C5-C4-N3	-2.13	121.09	123.64
2	L	2[B]	BRU	O3'-C3'-C2'	-2.11	103.34	110.90
1	J	2[B]	BRU	C6-N1-C1'	2.06	123.86	119.24
2	L	17[B]	BRU	O4'-C4'-C5'	2.01	115.98	109.37

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	2[A]	BRU	O4'-C1'-N1-C6
2	H	17[A]	BRU	O4'-C1'-N1-C6
2	F	2[A]	BRU	O4'-C1'-N1-C6
1	J	2[B]	BRU	O4'-C1'-N1-C6
2	I	2[B]	BRU	O4'-C1'-N1-C6
2	H	2[A]	BRU	O4'-C1'-N1-C6
2	L	17[B]	BRU	O4'-C1'-N1-C6
1	E	2[A]	BRU	O4'-C1'-N1-C6
1	K	2[B]	BRU	O4'-C1'-N1-C6
2	L	2[B]	BRU	O4'-C1'-N1-C6
2	F	17[A]	BRU	O4'-C1'-N1-C6
2	F	17[A]	BRU	C3'-C4'-C5'-O5'
2	F	17[A]	BRU	O4'-C4'-C5'-O5'
2	H	17[A]	BRU	O4'-C4'-C5'-O5'
2	L	17[B]	BRU	O4'-C4'-C5'-O5'
1	G	2[A]	BRU	O4'-C4'-C5'-O5'
2	L	2[B]	BRU	C3'-C4'-C5'-O5'
2	L	2[B]	BRU	O4'-C4'-C5'-O5'
2	F	2[A]	BRU	O4'-C4'-C5'-O5'
2	I	2[B]	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	2[A]	BRU	3	0
2	F	2[A]	BRU	4	0
1	J	2[B]	BRU	1	0
2	I	2[B]	BRU	6	0
2	H	2[A]	BRU	3	0
2	L	17[B]	BRU	1	0
1	E	2[A]	BRU	2	0
1	K	2[B]	BRU	1	0
2	L	2[B]	BRU	2	0
2	F	17[A]	BRU	2	0

## 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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	16/17 (94%)	-0.76	0 100 100	24, 27, 33, 34	16 (100%)
1	G	16/17 (94%)	-0.79	0 100 100	22, 30, 43, 46	16 (100%)
1	J	16/17 (94%)	-0.78	0 100 100	18, 26, 32, 34	16 (100%)
1	K	16/17 (94%)	-0.79	0 100 100	20, 27, 38, 43	16 (100%)
2	F	15/17 (88%)	-0.72	0 100 100	20, 25, 36, 37	15 (100%)
2	H	15/17 (88%)	-0.78	0 100 100	25, 28, 37, 41	15 (100%)
2	I	15/17 (88%)	-0.76	0 100 100	17, 27, 33, 43	15 (100%)
2	L	15/17 (88%)	-0.72	0 100 100	21, 28, 35, 37	15 (100%)
3	A	114/178 (64%)	-0.04	4 (3%) 44 42	25, 43, 77, 96	0
3	B	116/178 (65%)	0.29	7 (6%) 21 20	28, 58, 87, 103	0
3	C	112/178 (62%)	0.23	6 (5%) 25 24	32, 56, 89, 100	0
3	D	115/178 (64%)	0.17	7 (6%) 21 20	29, 52, 88, 104	0
All	All	581/848 (68%)	-0.03	24 (4%) 37 35	17, 46, 85, 104	124 (21%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	225	GLU	5.3
3	B	137	TYR	4.6
3	B	252	GLU	4.2
3	C	249	PHE	4.0
3	B	166	ALA	3.4
3	B	249	PHE	3.3
3	D	234	ASP	3.3
3	A	252	GLU	3.3
3	D	249	PHE	3.1
3	D	251	ASP	2.8
3	A	225	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	166	ALA	2.7
3	C	228	GLU	2.7
3	D	225	GLU	2.6
3	C	224	PRO	2.5
3	D	235	THR	2.4
3	A	147	LEU	2.4
3	D	213	VAL	2.4
3	A	249	PHE	2.3
3	C	251	ASP	2.3
3	C	142	GLN	2.1
3	B	251	ASP	2.1
3	B	196	GLU	2.1
3	B	225	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BRU	H	17[A]	20/21	0.96	0.10	31,38,43,50	20
2	BRU	F	17[A]	20/21	0.96	0.10	29,38,42,49	20
2	BRU	H	2[A]	20/21	0.97	0.10	19,29,41,47	20
2	BRU	I	17[B]	20/21	0.97	0.09	24,32,36,45	20
2	BRU	L	17[B]	20/21	0.97	0.10	24,34,39,50	20
1	BRU	K	2[B]	20/21	0.97	0.11	22,32,37,39	20
2	BRU	F	2[A]	20/21	0.97	0.12	19,29,38,44	20
1	BRU	E	2[A]	20/21	0.98	0.11	12,20,30,32	20
1	BRU	J	2[B]	20/21	0.98	0.11	18,27,35,36	20
2	BRU	L	2[B]	20/21	0.98	0.10	18,31,36,42	20
1	BRU	G	2[A]	20/21	0.98	0.10	20,31,37,38	20
2	BRU	I	2[B]	20/21	0.99	0.10	24,33,40,40	20

## 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.