



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 PM UTC

PDB ID : 1R71 / pdb_00001r71
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

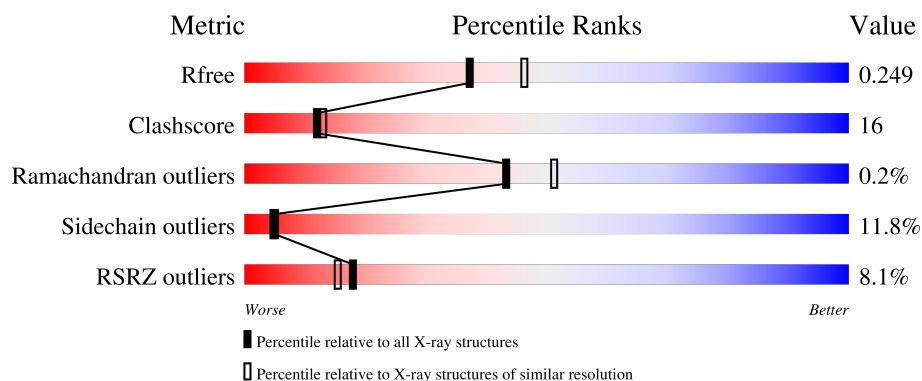
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	24% 59% 18%
1	G	17	24% 71% 6%
1	J	17	53% 29% 18%
1	K	17	24% 65% 12%
2	F	17	24% 35% 41%

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Mol	Chain	Length	Quality of chain
2	H	17	24% 65% 12%
2	I	17	18% 47% 35%
2	L	17	29% 47% 24%
3	A	178	4% 47% 14% • 36%
3	B	178	7% 50% 14% • 35%
3	C	178	9% 47% 15% • 37%
3	D	178	6% 45% 17% • 35%

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			

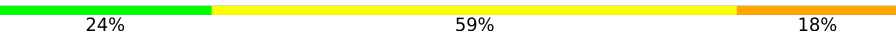
- Molecule 4 is water.

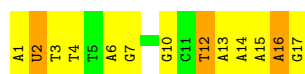
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	31	Total	O	0	0
			31	31		
4	I	21	Total	O	0	0
			21	21		
4	F	34	Total	O	0	0
			34	34		
4	J	24	Total	O	0	0
			24	24		
4	G	30	Total	O	0	0
			30	30		
4	L	23	Total	O	0	0
			23	23		
4	H	21	Total	O	0	0
			21	21		
4	K	24	Total	O	0	0
			24	24		
4	A	54	Total	O	0	0
			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 [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 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: 

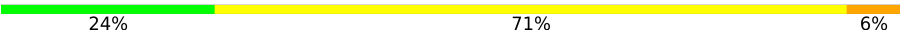


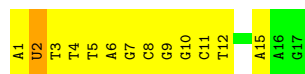
- Molecule 1: 5'-D(*AP*(BRU)P*TP*TP*TP*AP*GP*CP*GP*GP*CP*TP*AP*AP*AP*AP*G)-3'

Chain J: 

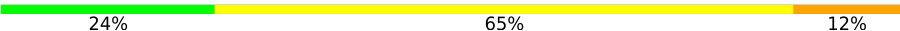


- Molecule 1: 5'-D(*AP*(BRU)P*TP*TP*TP*AP*GP*CP*GP*GP*CP*TP*AP*AP*AP*AP*G)-3'

Chain G: 

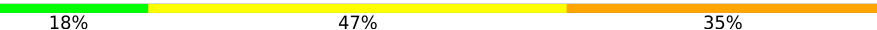


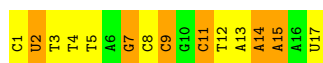
- Molecule 1: 5'-D(*AP*(BRU)P*TP*TP*TP*AP*GP*CP*GP*GP*CP*TP*AP*AP*AP*AP*G)-3'

Chain K: 

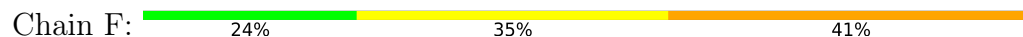


- Molecule 2: 5'-D(*CP*(BRU)P*TP*TP*TP*AP*GP*CP*CP*GP*CP*TP*AP*AP*AP*AP*(BRU))-3'

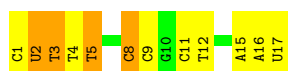
Chain I: 



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



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



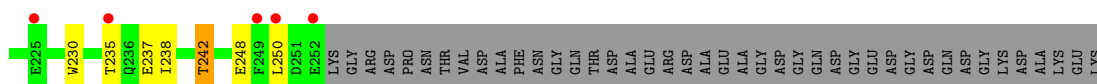
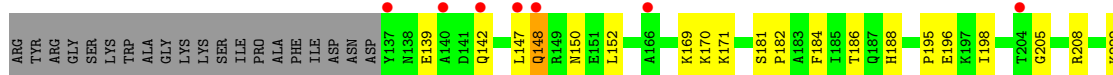
- Molecule 2: 5'-D(*CP*(BRU)P*TP*TP*TP*AP*GP*CP*CP*GP*CP*TP*AP*AP*AP*AP*(BRU))-3'



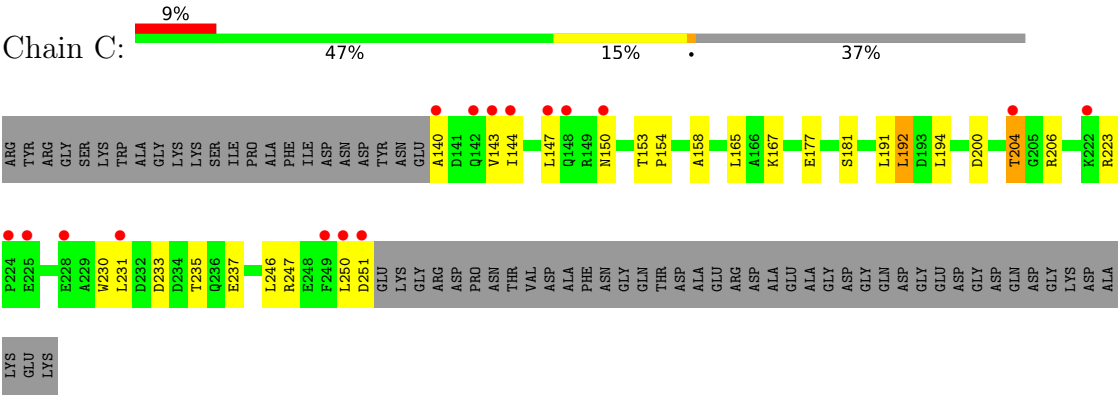
- Molecule 3: Transcriptional repressor protein korB



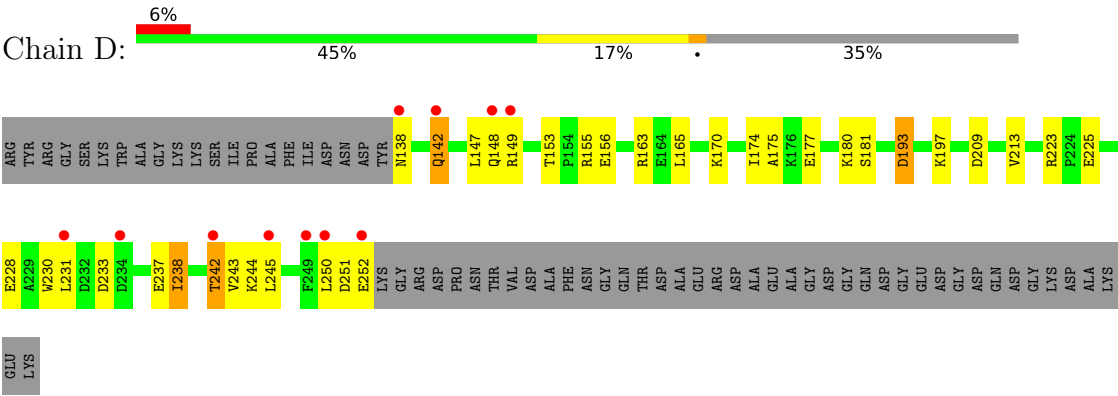
- Molecule 3: Transcriptional repressor protein korB



- Molecule 3: Transcriptional repressor protein korB



● 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, α , β , γ	110.44Å 110.44Å 160.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.20) 99.4 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	42.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/369	1.55	7/566 (1.2%)
1	G	0.58	0/369	1.36	2/566 (0.4%)
1	J	0.64	0/369	1.44	2/566 (0.4%)
1	K	0.60	0/369	1.48	4/566 (0.7%)
2	F	0.71	0/337	1.54	8/515 (1.6%)
2	H	0.61	0/337	1.48	5/515 (1.0%)
2	I	0.66	0/337	1.55	7/515 (1.4%)
2	L	0.63	0/337	1.48	5/515 (1.0%)
3	A	1.08	1/923 (0.1%)	1.01	1/1245 (0.1%)
3	B	0.89	0/944	0.97	0/1274
3	C	0.91	0/905	1.00	0/1221
3	D	1.07	2/931 (0.2%)	1.05	4/1256 (0.3%)
All	All	0.86	3/6527 (0.0%)	1.25	45/9320 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	189	VAL	C-O	-6.16	1.17	1.24
3	D	213	VAL	CA-CB	-6.04	1.47	1.54
3	D	149	ARG	CA-C	5.02	1.59	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	14[B]	DA	P-O5'-C5'	-8.56	107.16	120.00
3	D	149	ARG	N-CA-C	7.72	123.16	112.04
1	K	13[B]	DA	N9-C1'-C2'	6.74	123.60	113.50
1	J	17[B]	DG	C1'-O4'-C4'	-6.67	99.70	109.70
2	F	11[A]	DC	P-O3'-C3'	6.66	130.19	120.20
2	I	7[B]	DG	O4'-C1'-N9	6.63	118.35	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	9[B]	DC	P-O3'-C3'	6.38	129.78	120.20
1	E	17[A]	DG	C1'-O4'-C4'	-6.35	100.17	109.70
1	E	12[A]	DT	O3'-P-O5'	-6.34	94.49	104.00
1	E	4[A]	DT	N1-C1'-C2'	6.24	122.86	113.50
2	F	11[A]	DC	C2'-C3'-O3'	6.20	120.81	111.50
1	E	16[A]	DA	N9-C1'-C2'	6.20	122.80	113.50
3	A	251	ASP	N-CA-C	6.16	118.92	111.40
2	L	3[B]	DT	N1-C1'-C2'	6.07	122.61	113.50
1	E	7[A]	DG	O4'-C1'-N9	6.02	117.43	108.40
2	I	11[B]	DC	P-O3'-C3'	5.96	129.15	120.20
1	E	16[A]	DA	C2'-C3'-O3'	5.96	120.44	111.50
2	H	5[A]	DT	N1-C1'-C2'	5.95	122.42	113.50
2	F	3[A]	DT	O4'-C1'-N1	-5.86	99.62	108.40
2	F	10[A]	DG	C2'-C3'-O3'	-5.84	102.74	111.50
1	K	11[B]	DC	N1-C1'-C2'	5.76	122.14	113.50
2	L	8[B]	DC	N1-C1'-C2'	5.71	122.06	113.50
2	H	3[A]	DT	N1-C1'-C2'	5.60	121.90	113.50
2	H	7[A]	DG	O3'-P-O5'	-5.59	95.62	104.00
2	F	11[A]	DC	N1-C1'-C2'	5.57	121.85	113.50
2	F	3[A]	DT	N1-C1'-C2'	5.54	121.81	113.50
1	G	15[A]	DA	P-O5'-C5'	-5.46	111.81	120.00
2	L	5[B]	DT	N1-C1'-C2'	5.46	121.69	113.50
3	D	238	ILE	N-CA-C	5.42	114.55	106.85
2	F	5[A]	DT	P-O3'-C3'	5.39	128.29	120.20
2	I	15[B]	DA	C2'-C3'-O3'	5.37	119.56	111.50
2	H	9[A]	DC	C1'-O4'-C4'	-5.37	101.65	109.70
2	L	9[B]	DC	O4'-C1'-C2'	-5.35	98.38	106.40
1	K	13[B]	DA	O4'-C1'-N9	-5.34	100.38	108.40
1	G	7[A]	DG	O4'-C1'-N9	5.29	116.33	108.40
3	D	149	ARG	CA-C-N	5.21	131.08	121.70
3	D	149	ARG	C-N-CA	5.21	131.08	121.70
2	F	7[A]	DG	O4'-C1'-N9	5.19	116.18	108.40
2	I	11[B]	DC	N1-C1'-C2'	5.16	121.24	113.50
2	I	15[B]	DA	N9-C1'-C2'	5.15	121.23	113.50
2	H	4[A]	DT	N1-C1'-C2'	5.09	121.14	113.50
2	L	5[B]	DT	C4'-C3'-O3'	-5.09	102.37	110.00
1	E	6[A]	DA	P-O3'-C3'	5.09	127.83	120.20
1	J	14[B]	DA	P-O3'-C3'	5.07	127.80	120.20
1	K	3[B]	DT	C4'-C3'-O3'	-5.03	102.45	110.00

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	19	0
1	G	349	0	167	10	0
1	J	349	0	160	18	0
1	K	349	0	166	17	0
2	F	342	0	163	24	0
2	H	342	0	160	9	0
2	I	342	0	170	26	0
2	L	342	0	157	20	0
3	A	912	0	924	19	0
3	B	932	0	939	14	0
3	C	894	0	912	18	0
3	D	920	0	930	23	0
4	A	54	0	0	2	0
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	1	0
4	F	34	0	0	2	0
4	G	30	0	0	0	0
4	H	21	0	0	0	0
4	I	21	0	0	0	0
4	J	24	0	0	2	0
4	K	24	0	0	4	0
4	L	23	0	0	0	0
All	All	6769	0	5009	172	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 16.

All (172) 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)
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

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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:N7	1.75	1.01
2:I:1[B]:DC:H2''	2:I:2[B]:BRU:C5'	1.92	1.00
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:1[B]:DC:N3	1:J:17[B]:DG:N1	2.24	0.86
1:E:2[A]:BRU:BR	4:E:33:HOH:O	2.54	0.80
2:F:2[A]:BRU:BR	4:J:31:HOH:O	2.54	0.79
2:I:1[B]:DC:N4	1:J:17[B]:DG:N1	2.33	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
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
3:A:197:LYS:NZ	3:A:232:ASP:OD1	2.23	0.71
3:A:197:LYS:HE2	3:A:232:ASP:OD1	1.92	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: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
2:I:1[B]:DC:N3	1:J:17[B]:DG:N2	2.43	0.66
1:G:1[A]:DA:H2''	1:G:2[A]:BRU:H5''	1.77	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: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:L:4[B]:DT:C2	2:L:5[B]:DT:C6	2.85	0.65
2:H:10[A]:DG:H1'	2:H:11[A]:DC:H5'	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:13[B]:DA:H2''	2:I:14[B]:DA:O5'	1.98	0.62
1:E:12[A]:DT:O2	2:F:6[A]:DA:H2	1.82	0.62
3:C:143:VAL:HG12	4:C:315:HOH:O	2.00	0.62
3:C:144:ILE:HD12	3:C:144:ILE:H	1.65	0.62
1:E:12[A]:DT:H2''	1:E:13[A]:DA:C8	2.35	0.61
3:A:143:VAL:HG11	3:A:160:PHE:CD1	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:HD12	3:C:144:ILE:N	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:D:193:ASP:CG	3:D:193:ASP:O	2.45	0.60
1:E:15[A]:DA:H1'	1:E:16[A]:DA:H5'	1.84	0.59
3:B:195:PRO:HG2	3:B:198:ILE:HD12	1.85	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:I:15[B]:DA:N1	1:J:3[B]:DT:N3	2.46	0.58
2:F:5[A]:DT:H2''	2:F:6[A]:DA:H5'	1.84	0.58
3:D:153:THR:HG22	3:D:156:GLU:CG	2.33	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
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
1:K:9[B]:DG:H2'	3:D:209:ASP:CG	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:223:ARG:HD2	3:D:250:LEU:HB3	1.90	0.52
2:H:1[A]:DC:HO5'	2:H:1[A]:DC:H6	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
2:I:9[B]:DC:N4	1:J:9[B]:DG:O6	2.43	0.51
3:A:158:ALA:HB1	3:A:192:LEU:HD13	1.93	0.51
4:F:265:HOH:O	1:J:7[B]:DG:H8	1.93	0.51
1:E:10[A]:DG:H2'	1:E:10[A]:DG:O5'	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:H6	2:L:1[B]:DC:O5'	1.94	0.49
2:F:12[A]:DT:H2'	3:A:181:SER:CB	2.42	0.49
1:E:12[A]:DT:O2	2:F:6[A]:DA:N1	2.46	0.49
1:E:15[A]:DA:N6	1:E:16[A]:DA:C6	2.80	0.49
1:J:9[B]:DG:H2'	3:A:209:ASP:CG	2.38	0.49
1:K:10[B]:DG:H2''	1:K:11[B]:DC:O4'	2.12	0.48
2:I:7[B]:DG:H4'	2:I:8[B]:DC:H5'	1.94	0.48
2:F:10[A]:DG:H2''	2:F:11[A]:DC:O5'	2.12	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:HD22	3:A:147:LEU:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:10[A]:DG:H2''	2:H:11[A]:DC:O5'	2.15	0.45
3:C:230:TRP:CD2	3:C:246:LEU:HD22	2.52	0.45
1:K:6[B]:DA:H8	4:K:30:HOH:O	1.98	0.45
3:C:233:ASP:OD1	3:C:235:THR:OG1	2.33	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
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
3:B:170:LYS:O	3:B:171:LYS:C	2.60	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
2:L:4[B]:DT:C6	2:L:5[B]:DT:C7	3.02	0.43
1:K:12[B]:DT:P	3:D:180:LYS:HD3	2.59	0.43
1:E:1[A]:DA:C8	1:E:1[A]:DA:H5'	2.53	0.42
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:K:16[B]:DA:H2''	1:K:17[B]:DG:O5'	2.19	0.42
3:C:206:ARG:NH2	3:C:231:LEU:O	2.47	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
1:K:5[B]:DT:H72	4:K:20:HOH:O	2.20	0.42
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:HD23	3:B:147:LEU:HA	1.86	0.41
3:A:153:THR:HB	3:A:154:PRO:HD2	2.03	0.41
1:K:12[B]:DT:OP2	3:D:180:LYS:HD3	2.20	0.41
3:C:223:ARG:HG3	3:C:250:LEU:HD13	2.01	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
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:D:174:ILE:O	3:D:175:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1[A]:DC:H2'	2:F:2[A]:BRU:C6	2.51	0.40
3:A:188:HIS:O	3:A:191:LEU:HB2	2.20	0.40
2:L:3[B]:DT:N3	1:K:15[B]:DA:N1	2.69	0.40
3:C:167:LYS:NZ	4:C:320:HOH:O	2.53	0.40
2:H:1[A]:DC:H6	2:H:1[A]:DC:O5'	2.04	0.40

There are no symmetry-related clashes.

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	
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%)	14	14
All	All	449/712 (63%)	438 (98%)	10 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	233	ASP

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	
3	A	99/147 (67%)	89 (90%)	10 (10%)	7	7
3	B	101/147 (69%)	89 (88%)	12 (12%)	5	4
3	C	97/147 (66%)	88 (91%)	9 (9%)	8	9
3	D	100/147 (68%)	84 (84%)	16 (16%)	2	2
All	All	397/588 (68%)	350 (88%)	47 (12%)	5	5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	147	LEU
3	A	149	ARG
3	A	152	LEU
3	A	191	LEU
3	A	192	LEU
3	A	194	LEU
3	A	197	LYS
3	A	221	LYS
3	A	222	LYS
3	A	237	GLU
3	B	139	GLU
3	B	148	GLN
3	B	150	ASN
3	B	152	LEU
3	B	169	LYS
3	B	196	GLU
3	B	222	LYS
3	B	235	THR
3	B	238	ILE
3	B	242	THR
3	B	248	GLU
3	B	250	LEU
3	C	147	LEU
3	C	165	LEU
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

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Mol	Chain	Res	Type
3	D	148	GLN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	146	ASN
3	A	148	GLN
3	B	138	ASN
3	B	188	HIS
3	C	146	ASN
3	C	148	GLN
3	D	187	GLN

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
2	BRU	H	17[A]	1,2	18,21,22	1.30	2 (11%)	25,30,33	3.05	10 (40%)
2	BRU	H	2[A]	1,2	18,21,22	1.46	3 (16%)	25,30,33	2.33	8 (32%)
2	BRU	L	17[B]	2	18,21,22	1.53	4 (22%)	25,30,33	2.90	9 (36%)
2	BRU	F	17[A]	1,2	18,21,22	1.47	2 (11%)	25,30,33	2.71	9 (36%)
1	BRU	G	2[A]	1,2	18,21,22	1.45	5 (27%)	25,30,33	2.39	10 (40%)
2	BRU	F	2[A]	1,2	18,21,22	1.42	4 (22%)	25,30,33	2.42	7 (28%)
1	BRU	E	2[A]	1,2	18,21,22	1.62	2 (11%)	25,30,33	2.83	11 (44%)
2	BRU	L	2[B]	2	18,21,22	1.58	4 (22%)	25,30,33	2.96	14 (56%)
1	BRU	K	2[B]	1	18,21,22	1.58	5 (27%)	25,30,33	2.62	9 (36%)
2	BRU	I	17[B]	2	18,21,22	1.33	3 (16%)	25,30,33	2.73	8 (32%)
2	BRU	I	2[B]	2	18,21,22	1.62	4 (22%)	25,30,33	2.61	8 (32%)
1	BRU	J	2[B]	1	18,21,22	1.61	5 (27%)	25,30,33	2.34	8 (32%)

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
2	BRU	H	17[A]	1,2	-	1/7/21/22	0/2/2/2
2	BRU	H	2[A]	1,2	-	0/7/21/22	0/2/2/2
2	BRU	L	17[B]	2	-	1/7/21/22	0/2/2/2
2	BRU	F	17[A]	1,2	-	2/7/21/22	0/2/2/2
1	BRU	G	2[A]	1,2	-	1/7/21/22	0/2/2/2
2	BRU	F	2[A]	1,2	-	1/7/21/22	0/2/2/2
1	BRU	E	2[A]	1,2	-	0/7/21/22	0/2/2/2
2	BRU	L	2[B]	2	-	2/7/21/22	0/2/2/2
1	BRU	K	2[B]	1	-	0/7/21/22	0/2/2/2
2	BRU	I	17[B]	2	-	0/7/21/22	0/2/2/2
2	BRU	I	2[B]	2	-	0/7/21/22	0/2/2/2
1	BRU	J	2[B]	1	-	0/7/21/22	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2[A]	BRU	C6-N1	-4.40	1.30	1.38
1	J	2[B]	BRU	C4-N3	-3.93	1.31	1.38
2	L	2[B]	BRU	C6-N1	-3.80	1.31	1.38
2	I	2[B]	BRU	C2-N3	-3.38	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2[A]	BRU	C4-N3	-3.37	1.32	1.38
2	H	17[A]	BRU	C6-C5	3.21	1.40	1.34
2	I	2[B]	BRU	C4-N3	-3.20	1.32	1.38
2	L	17[B]	BRU	C2-N1	3.15	1.43	1.38
2	F	17[A]	BRU	C6-C5	3.05	1.40	1.34
2	H	2[A]	BRU	C4-N3	-3.04	1.33	1.38
1	J	2[B]	BRU	C2-N3	-3.03	1.32	1.38
2	I	2[B]	BRU	C4-C5	3.02	1.51	1.45
2	I	17[B]	BRU	C6-C5	3.01	1.40	1.34
2	F	2[A]	BRU	C4-N3	-2.92	1.33	1.38
1	K	2[B]	BRU	C2-N1	2.91	1.43	1.38
2	L	2[B]	BRU	C4-N3	-2.82	1.33	1.38
1	G	2[A]	BRU	C4-N3	-2.80	1.33	1.38
2	H	2[A]	BRU	C6-N1	-2.79	1.33	1.38
1	K	2[B]	BRU	C4-C5	2.78	1.50	1.45
2	L	17[B]	BRU	C4-N3	-2.76	1.33	1.38
1	K	2[B]	BRU	C6-C5	2.75	1.39	1.34
2	L	2[B]	BRU	C2-N3	-2.74	1.33	1.38
2	I	17[B]	BRU	C4-N3	-2.63	1.33	1.38
2	F	2[A]	BRU	C6-N1	-2.58	1.33	1.38
2	F	17[A]	BRU	C4-N3	-2.58	1.34	1.38
1	J	2[B]	BRU	C6-C5	2.51	1.39	1.34
2	I	2[B]	BRU	C6-C5	2.48	1.39	1.34
1	G	2[A]	BRU	C6-N1	-2.45	1.33	1.38
1	G	2[A]	BRU	C2-N3	-2.44	1.33	1.38
2	L	17[B]	BRU	C6-C5	2.44	1.39	1.34
1	G	2[A]	BRU	C2-N1	2.41	1.42	1.38
2	L	17[B]	BRU	O2-C2	2.38	1.27	1.23
2	H	2[A]	BRU	C4-C5	2.32	1.49	1.45
1	J	2[B]	BRU	C4-C5	2.31	1.49	1.45
2	F	2[A]	BRU	C2-N3	-2.30	1.34	1.38
1	G	2[A]	BRU	C4-C5	2.28	1.49	1.45
1	J	2[B]	BRU	C2-N1	2.27	1.42	1.38
2	L	2[B]	BRU	C1'-N1	-2.25	1.42	1.48
1	K	2[B]	BRU	C2-N3	-2.20	1.34	1.38
2	H	17[A]	BRU	C2-N1	2.19	1.41	1.38
1	K	2[B]	BRU	C6-N1	-2.15	1.34	1.38
2	F	2[A]	BRU	C4-C5	2.12	1.49	1.45
2	I	17[B]	BRU	C2-N3	-2.06	1.34	1.38

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	17[A]	BRU	O4-C4-C5	-7.35	116.43	125.80
2	F	17[A]	BRU	C5-C4-N3	6.73	121.09	113.34
2	L	17[B]	BRU	O4-C4-C5	-6.67	117.30	125.80
2	I	17[B]	BRU	O4-C4-C5	-6.58	117.41	125.80
1	G	2[A]	BRU	N3-C2-N1	6.37	123.19	114.89
2	I	2[B]	BRU	C5-C4-N3	6.21	120.48	113.34
2	F	17[A]	BRU	O4-C4-C5	-6.20	117.90	125.80
2	L	17[B]	BRU	N3-C2-N1	6.09	122.82	114.89
2	L	17[B]	BRU	C4-N3-C2	-6.08	119.37	127.34
2	H	17[A]	BRU	N3-C2-N1	6.04	122.76	114.89
1	E	2[A]	BRU	C4-N3-C2	-6.01	119.45	127.34
2	L	2[B]	BRU	C4-N3-C2	-5.67	119.90	127.34
2	I	17[B]	BRU	N3-C2-N1	5.64	122.23	114.89
1	G	2[A]	BRU	C4-N3-C2	-5.57	120.04	127.34
2	H	17[A]	BRU	C4-N3-C2	-5.54	120.07	127.34
2	L	2[B]	BRU	BR-C5-C4	5.47	124.31	118.02
1	K	2[B]	BRU	C5-C4-N3	5.42	119.58	113.34
1	E	2[A]	BRU	O4'-C1'-N1	5.40	117.45	107.86
1	J	2[B]	BRU	N3-C2-N1	5.40	121.91	114.89
2	L	2[B]	BRU	C5-C4-N3	5.28	119.41	113.34
1	K	2[B]	BRU	N3-C2-N1	5.28	121.76	114.89
1	K	2[B]	BRU	C4-N3-C2	-5.27	120.42	127.34
1	J	2[B]	BRU	C5-C4-N3	5.27	119.40	113.34
2	L	2[B]	BRU	O2-C2-N1	-5.26	115.95	122.80
1	E	2[A]	BRU	N3-C2-N1	5.20	121.66	114.89
2	F	2[A]	BRU	C4-N3-C2	-5.16	120.57	127.34
2	I	17[B]	BRU	C4-N3-C2	-5.13	120.61	127.34
2	F	2[A]	BRU	N3-C2-N1	5.01	121.41	114.89
2	H	2[A]	BRU	N3-C2-N1	5.00	121.40	114.89
1	E	2[A]	BRU	O2-C2-N1	-4.97	116.33	122.80
2	I	2[B]	BRU	N3-C2-N1	4.90	121.27	114.89
2	I	17[B]	BRU	C5-C4-N3	4.86	118.93	113.34
2	H	17[A]	BRU	O4'-C1'-N1	4.85	116.48	107.86
2	F	17[A]	BRU	C4-N3-C2	-4.81	121.04	127.34
2	I	2[B]	BRU	C4-N3-C2	-4.79	121.06	127.34
2	L	17[B]	BRU	C5-C4-N3	4.77	118.83	113.34
2	I	2[B]	BRU	BR-C5-C4	4.75	123.48	118.02
2	F	2[A]	BRU	C5-C4-N3	4.72	118.77	113.34
2	H	2[A]	BRU	C4-N3-C2	-4.64	121.26	127.34
2	H	17[A]	BRU	C5-C4-N3	4.61	118.65	113.34
2	F	17[A]	BRU	C6-C5-C4	-4.61	116.00	120.67
1	J	2[B]	BRU	C4-N3-C2	-4.57	121.35	127.34
2	I	2[B]	BRU	C6-C5-C4	-4.50	116.10	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2[A]	BRU	BR-C5-C4	4.39	123.08	118.02
1	K	2[B]	BRU	BR-C5-C4	4.22	122.88	118.02
2	H	17[A]	BRU	O2-C2-N1	-4.20	117.33	122.80
1	E	2[A]	BRU	C5-C4-N3	4.14	118.10	113.34
2	H	2[A]	BRU	BR-C5-C4	4.05	122.69	118.02
1	E	2[A]	BRU	BR-C5-C4	4.03	122.66	118.02
2	F	17[A]	BRU	N3-C2-N1	3.99	120.08	114.89
1	E	2[A]	BRU	O4-C4-C5	-3.97	120.74	125.80
2	H	2[A]	BRU	O2-C2-N1	-3.95	117.66	122.80
2	I	17[B]	BRU	BR-C5-C6	3.94	126.16	120.64
1	G	2[A]	BRU	C5-C4-N3	3.91	117.84	113.34
2	F	2[A]	BRU	O2-C2-N1	-3.90	117.71	122.80
2	H	2[A]	BRU	C5-C4-N3	3.86	117.78	113.34
2	L	2[B]	BRU	O4-C4-C5	-3.82	120.92	125.80
2	L	17[B]	BRU	O4'-C1'-N1	3.81	114.62	107.86
2	L	2[B]	BRU	N3-C2-N1	3.77	119.80	114.89
2	H	17[A]	BRU	BR-C5-C6	3.58	125.64	120.64
1	K	2[B]	BRU	C2'-C1'-N1	3.57	122.73	113.81
1	K	2[B]	BRU	C6-C5-C4	-3.53	117.09	120.67
2	L	17[B]	BRU	BR-C5-C4	-3.45	114.04	118.02
2	L	2[B]	BRU	O4'-C1'-C2'	3.42	112.63	106.25
1	K	2[B]	BRU	O4-C4-C5	-3.17	121.76	125.80
2	L	2[B]	BRU	C1'-N1-C2	-3.17	111.47	117.66
2	F	2[A]	BRU	O4-C4-C5	-3.15	121.78	125.80
2	I	17[B]	BRU	O2-C2-N1	-3.10	118.76	122.80
2	I	17[B]	BRU	BR-C5-C4	-3.08	114.48	118.02
1	J	2[B]	BRU	O2-C2-N3	-3.04	115.88	121.49
2	L	2[B]	BRU	BR-C5-C6	-3.03	116.40	120.64
2	L	17[B]	BRU	BR-C5-C6	2.98	124.82	120.64
2	H	2[A]	BRU	O4-C4-C5	-2.98	122.00	125.80
2	I	2[B]	BRU	C2'-C1'-N1	2.97	121.23	113.81
1	G	2[A]	BRU	BR-C5-C4	2.95	121.42	118.02
2	H	17[A]	BRU	BR-C5-C4	-2.94	114.64	118.02
1	J	2[B]	BRU	C2'-C1'-N1	2.85	120.93	113.81
2	L	2[B]	BRU	C2'-C1'-N1	2.82	120.87	113.81
2	H	2[A]	BRU	O4'-C1'-N1	2.76	112.75	107.86
2	F	2[A]	BRU	C2'-C1'-N1	2.74	120.67	113.81
2	F	17[A]	BRU	BR-C5-C6	2.74	124.47	120.64
2	L	17[B]	BRU	O2-C2-N1	-2.72	119.25	122.80
2	F	17[A]	BRU	O4'-C1'-N1	2.68	112.62	107.86
1	E	2[A]	BRU	BR-C5-C6	-2.63	116.97	120.64
1	J	2[B]	BRU	C6-C5-C4	-2.62	118.02	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2[A]	BRU	O3'-C3'-C2'	-2.60	101.85	110.88
2	I	17[B]	BRU	O4'-C1'-N1	2.57	112.43	107.86
2	H	2[A]	BRU	C2'-C1'-N1	2.57	120.24	113.81
1	G	2[A]	BRU	O2-C2-N3	-2.57	116.75	121.49
2	H	17[A]	BRU	O4-C4-N3	2.55	124.90	120.11
1	G	2[A]	BRU	C3'-C2'-C1'	2.51	108.73	102.60
2	I	2[B]	BRU	O4'-C1'-N1	-2.43	103.55	107.86
2	I	2[B]	BRU	O4-C4-N3	-2.43	115.55	120.11
1	E	2[A]	BRU	C2'-C3'-C4'	2.43	107.73	102.80
1	G	2[A]	BRU	C2'-C1'-N1	2.42	119.87	113.81
2	L	2[B]	BRU	C6-N1-C2	2.40	123.70	121.30
1	J	2[B]	BRU	BR-C5-C4	2.37	120.75	118.02
2	H	17[A]	BRU	C2'-C1'-N1	-2.35	107.93	113.81
1	G	2[A]	BRU	O4-C4-C5	-2.33	122.83	125.80
1	K	2[B]	BRU	O4'-C1'-N1	2.33	112.00	107.86
1	K	2[B]	BRU	C2'-C3'-C4'	2.32	107.51	102.80
2	L	2[B]	BRU	C1'-N1-C6	2.29	124.58	120.74
1	E	2[A]	BRU	C2'-C1'-N1	2.21	119.34	113.81
2	L	2[B]	BRU	C2'-C3'-C4'	2.17	107.21	102.80
1	G	2[A]	BRU	O4'-C1'-N1	-2.17	104.01	107.86
2	L	2[B]	BRU	O3'-C3'-C2'	-2.17	103.34	110.88
1	J	2[B]	BRU	O4-C4-N3	-2.13	116.11	120.11
1	G	2[A]	BRU	O2-C2-N1	-2.11	120.05	122.80
2	F	17[A]	BRU	C2'-C1'-N1	-2.10	108.57	113.81
2	L	17[B]	BRU	O4'-C4'-C5'	2.08	115.98	109.33
2	F	17[A]	BRU	C2'-C3'-C4'	2.00	106.86	102.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	17[A]	BRU	C3'-C4'-C5'-O5'
2	F	17[A]	BRU	O4'-C4'-C5'-O5'
2	L	17[B]	BRU	O4'-C4'-C5'-O5'
2	H	17[A]	BRU	O4'-C4'-C5'-O5'
2	L	2[B]	BRU	C3'-C4'-C5'-O5'
2	L	2[B]	BRU	O4'-C4'-C5'-O5'
1	G	2[A]	BRU	O4'-C4'-C5'-O5'
2	F	2[A]	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 20 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	E	16/17 (94%)	-0.68	0 100 100	12, 13, 17, 17	16 (100%)
1	G	16/17 (94%)	-0.54	0 100 100	11, 15, 21, 23	16 (100%)
1	J	16/17 (94%)	-0.74	0 100 100	9, 13, 16, 17	16 (100%)
1	K	16/17 (94%)	-0.61	0 100 100	10, 14, 19, 21	16 (100%)
2	F	15/17 (88%)	-0.70	0 100 100	10, 13, 18, 18	15 (100%)
2	H	15/17 (88%)	-0.53	0 100 100	12, 14, 19, 20	15 (100%)
2	I	15/17 (88%)	-0.83	0 100 100	8, 13, 17, 22	15 (100%)
2	L	15/17 (88%)	-0.73	0 100 100	11, 14, 17, 19	15 (100%)
3	A	114/178 (64%)	0.29	8 (7%) 22 19	25, 43, 77, 96	0
3	B	116/178 (65%)	0.78	12 (10%) 12 9	28, 58, 87, 103	0
3	C	112/178 (62%)	0.80	16 (14%) 6 4	32, 56, 89, 100	0
3	D	115/178 (64%)	0.66	11 (9%) 13 11	29, 52, 88, 104	0
All	All	581/848 (68%)	0.35	47 (8%) 18 15	8, 46, 85, 104	124 (21%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	ALA	8.0
3	B	137	TYR	4.1
3	B	235	THR	3.9
3	B	204	THR	3.5
3	A	142	GLN	3.3
3	C	144	ILE	3.3
3	C	143	VAL	3.3
3	D	234	ASP	3.2
3	C	251	ASP	3.2
3	D	252	GLU	3.2
3	C	147	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	250	LEU	3.1
3	C	249	PHE	3.1
3	D	138	ASN	2.9
3	C	150	ASN	2.9
3	C	228	GLU	2.9
3	A	252	GLU	2.9
3	B	249	PHE	2.8
3	A	147	LEU	2.8
3	C	225	GLU	2.8
3	C	204	THR	2.7
3	A	148	GLN	2.7
3	D	249	PHE	2.7
3	C	142	GLN	2.7
3	B	142	GLN	2.7
3	B	252	GLU	2.6
3	D	245	LEU	2.6
3	B	148	GLN	2.5
3	C	231	LEU	2.5
3	B	166	ALA	2.4
3	C	148	GLN	2.4
3	D	242	THR	2.3
3	D	142	GLN	2.3
3	D	148	GLN	2.3
3	B	140	ALA	2.3
3	A	144	ILE	2.3
3	D	149	ARG	2.2
3	A	139	GLU	2.2
3	B	225	GLU	2.2
3	C	222	LYS	2.2
3	C	224	PRO	2.2
3	A	140	ALA	2.2
3	B	147	LEU	2.1
3	A	225	GLU	2.1
3	B	250	LEU	2.0
3	D	231	LEU	2.0
3	D	250	LEU	2.0

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	BRU	I	17[B]	20/21	0.93	0.12	24,32,36,45	20
1	BRU	E	2[A]	20/21	0.94	0.09	12,20,30,32	20
2	BRU	F	2[A]	20/21	0.94	0.10	19,29,38,44	20
2	BRU	F	17[A]	20/21	0.94	0.10	29,38,42,49	20
2	BRU	L	17[B]	20/21	0.94	0.10	24,34,39,50	20
2	BRU	H	17[A]	20/21	0.94	0.12	31,38,43,50	20
2	BRU	H	2[A]	20/21	0.95	0.09	19,29,41,47	20
1	BRU	G	2[A]	20/21	0.95	0.10	20,31,37,38	20
1	BRU	J	2[B]	20/21	0.96	0.09	18,27,35,36	20
2	BRU	I	2[B]	20/21	0.96	0.09	24,33,40,40	20
2	BRU	L	2[B]	20/21	0.96	0.08	18,31,36,42	20
1	BRU	K	2[B]	20/21	0.96	0.09	22,32,37,39	20

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.