



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:41 PM GMT

PDB ID : 1K3X
Title : Crystal structure of a trapped reaction intermediate of the DNA repair enzyme
Endonuclease VIII with Brominated-DNA
Authors : Golan, G.; Zharkov, D.O.; Gilboa, R.; Fernandes, A.S.; Kycia, J.H.; Gerch-
man, S.E.; Rieger, R.A.; Grollman, A.P.; Shoham, G.
Deposited on : 2001-10-04
Resolution : 1.25 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>

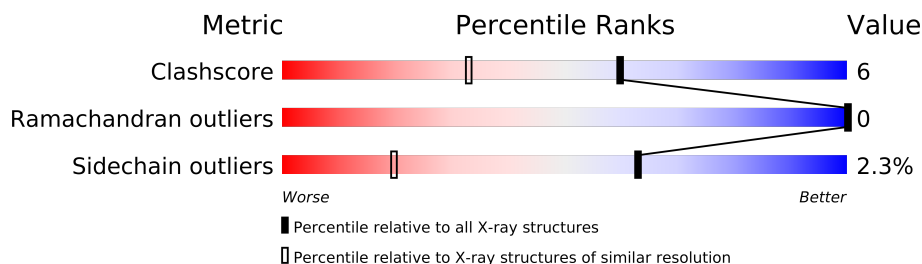
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.25 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))
Clashscore	79885	1125 (1.30-1.22)
Ramachandran outliers	78287	1075 (1.30-1.22)
Sidechain outliers	78261	1073 (1.30-1.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	13	
2	C	13	
3	A	262	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2998 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 DNA chain called 5'-D(*GP*GP*CP*(BRU)P*(BRU)P*CP*AP*(BRU)P*CP*CP*(BRU)P*GP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	10	Total	Br	C	N	O	P	0	0	0
			199	4	92	30	63	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			202	94	43	55	10			

- Molecule 3 is a protein called Endonuclease VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	8	0
			2059	1316	370	368	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	THR	PRO	SEE REMARK 999	UNP P50465
A	112	ARG	THR	SEE REMARK 999	UNP P50465

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

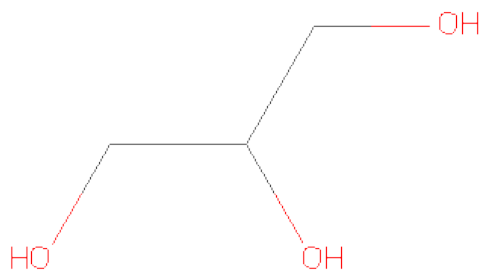
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0
6	A	1	Total 6	C 3	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	441	Total 441	O 441	0	0
7	B	24	Total 24	O 24	0	0
7	C	23	Total 23	O 23	0	0

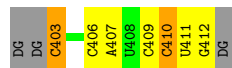
3 Residue-property plots

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.

Note EDS was not executed.

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

Chain B: 



- Molecule 2: 5'-D(*CP*CP*AP*GP*GP*AP*(PED)P*GP*AP*AP*GP*CP*C)-3'

Chain C: 



- Molecule 3: Endonuclease VIII

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 76.50Å 164.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.25	Depositor
% Data completeness (in resolution range)	97.4 (10.00-1.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.149 , 0.181	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2998	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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: PED, GOL, ZN, BRU, SO4

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	B	1.81	3/129 (2.3%)	5.89	44/188 (23.4%)
2	C	2.08	9/215 (4.2%)	6.05	92/328 (28.0%)
3	A	0.74	0/2136	1.29	21/2898 (0.7%)
All	All	1.01	12/2480 (0.5%)	2.62	157/3414 (4.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	DG	C5-C4	6.66	1.43	1.38
2	C	431	DG	C5-C4	6.30	1.42	1.38
2	C	431	DG	C5-C6	5.92	1.48	1.42
2	C	425	DG	C5-C6	5.47	1.47	1.42
2	C	431	DG	N3-C4	5.36	1.39	1.35
2	C	424	DG	C5-C6	5.32	1.47	1.42
2	C	424	DG	C5-C4	5.30	1.42	1.38
1	B	406	DC	N3-C4	5.29	1.37	1.33
2	C	425	DG	N3-C4	5.26	1.39	1.35
2	C	431	DG	P-O5'	5.17	1.65	1.59
1	B	412	DG	C5-C6	5.13	1.47	1.42
2	C	428	DG	C6-N1	5.04	1.43	1.39

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	430	DA	C6-N1-C2	24.49	133.30	118.60
1	B	412	DG	N3-C4-C5	-22.55	117.33	128.60
2	C	431	DG	N7-C8-N9	21.99	124.09	113.10
2	C	424	DG	N7-C8-N9	20.22	123.21	113.10
2	C	431	DG	C8-N9-C4	-20.20	98.32	106.40
1	B	412	DG	N7-C8-N9	20.20	123.20	113.10
1	B	403	DC	C2-N3-C4	19.85	129.82	119.90
2	C	429	DA	N1-C2-N3	-19.66	119.47	129.30
2	C	431	DG	N3-C4-C5	-19.54	118.83	128.60
2	C	424	DG	C8-N9-C4	-19.39	98.65	106.40
1	B	412	DG	C8-N9-C4	-19.13	98.75	106.40
2	C	422	DC	C2-N3-C4	19.04	129.42	119.90
1	B	403	DC	N3-C4-C5	-18.67	114.43	121.90
2	C	422	DC	N3-C4-C5	-18.46	114.52	121.90
2	C	430	DA	N1-C2-N3	-18.22	120.19	129.30
2	C	429	DA	C6-N1-C2	17.97	129.38	118.60
1	B	412	DG	C2-N3-C4	17.42	120.61	111.90
2	C	430	DA	C5-C6-N1	-16.88	109.26	117.70
1	B	409	DC	N3-C4-C5	-16.78	115.19	121.90
2	C	431	DG	C2-N3-C4	15.65	119.72	111.90
1	B	409	DC	C2-N3-C4	15.27	127.54	119.90
2	C	430	DA	N1-C6-N6	15.14	127.68	118.60
1	B	412	DG	C6-N1-C2	-15.13	116.02	125.10
2	C	425	DG	N7-C8-N9	15.11	120.66	113.10
1	B	407	DA	N1-C6-N6	-14.37	109.98	118.60
2	C	431	DG	C5-N7-C8	-14.24	97.18	104.30
2	C	425	DG	C8-N9-C4	-14.08	100.77	106.40
1	B	412	DG	N3-C4-N9	13.53	134.12	126.00
3	A	75	ARG	CD-NE-CZ	13.26	142.16	123.60
2	C	429	DA	C8-N9-C4	13.14	111.06	105.80
1	B	412	DG	C5-C6-N1	13.00	118.00	111.50
2	C	424	DG	C5-N7-C8	-12.95	97.83	104.30
1	B	410	DC	N3-C4-C5	-12.65	116.84	121.90
2	C	428	DG	C5-C6-O6	-12.61	121.04	128.60
1	B	410	DC	C2-N3-C4	12.44	126.12	119.90
2	C	428	DG	N7-C8-N9	12.18	119.19	113.10
2	C	424	DG	N3-C4-C5	-11.78	122.71	128.60
1	B	412	DG	C5-N7-C8	-11.75	98.43	104.30
1	B	406	DC	N3-C4-C5	-11.57	117.27	121.90
2	C	429	DA	C1'-O4'-C4'	-11.52	98.58	110.10
2	C	429	DA	N9-C4-C5	-11.35	101.26	105.80
1	B	409	DC	N3-C2-O2	11.28	129.80	121.90
2	C	431	DG	N3-C4-N9	11.26	132.75	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	429	DA	C5-C6-N1	-11.14	112.13	117.70
1	B	403	DC	C5-C6-N1	11.04	126.52	121.00
1	B	409	DC	O4'-C1'-N1	-11.01	100.29	108.00
2	C	429	DA	N7-C8-N9	-10.84	108.38	113.80
2	C	422	DC	N3-C2-O2	10.67	129.37	121.90
2	C	422	DC	C5-C6-N1	10.64	126.32	121.00
1	B	407	DA	C5-C6-N6	10.63	132.21	123.70
2	C	425	DG	N3-C4-C5	-10.51	123.35	128.60
3	A	75	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	C	429	DA	N1-C6-N6	10.32	124.79	118.60
2	C	428	DG	C5-N7-C8	-10.28	99.16	104.30
2	C	430	DA	N9-C4-C5	-10.22	101.71	105.80
2	C	424	DG	C6-N1-C2	-9.84	119.20	125.10
2	C	424	DG	C8-N9-C1'	9.73	139.65	127.00
2	C	425	DG	C5-N7-C8	-9.71	99.45	104.30
3	A	232	ARG	NE-CZ-NH1	9.70	125.15	120.30
2	C	431	DG	C6-N1-C2	-9.53	119.38	125.10
2	C	430	DA	P-O5'-C5'	-9.32	105.99	120.90
2	C	431	DG	C5-C6-N1	9.27	116.14	111.50
1	B	403	DC	N3-C4-N4	9.13	124.39	118.00
2	C	430	DA	OP1-P-OP2	8.88	132.93	119.60
2	C	430	DA	C4-C5-N7	8.84	115.12	110.70
2	C	422	DC	O4'-C4'-C3'	-8.77	100.74	106.00
3	A	239	ARG	NE-CZ-NH2	-8.39	116.11	120.30
2	C	424	DG	N1-C2-N3	8.37	128.92	123.90
2	C	424	DG	N9-C4-C5	8.28	108.71	105.40
2	C	428	DG	C8-N9-C4	-8.21	103.11	106.40
2	C	430	DA	C8-N9-C4	8.01	109.00	105.80
2	C	425	DG	C2-N3-C4	7.93	115.87	111.90
3	A	239	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	C	428	DG	C5-C6-N1	7.86	115.43	111.50
2	C	422	DC	C6-N1-C1'	7.86	130.23	120.80
1	B	409	DC	N1-C2-O2	-7.80	114.22	118.90
2	C	429	DA	O4'-C1'-C2'	-7.80	99.66	105.90
1	B	412	DG	N9-C4-C5	7.79	108.52	105.40
3	A	188	ASP	CB-CG-OD1	7.78	125.30	118.30
3	A	239	ARG	CD-NE-CZ	7.75	134.45	123.60
3	A	252	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	403	DC	C6-N1-C2	-7.52	117.29	120.30
2	C	431	DG	N9-C4-C5	7.50	108.40	105.40
2	C	422	DC	C6-N1-C2	-7.47	117.31	120.30
1	B	403	DC	O4'-C1'-C2'	-7.45	99.94	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	423	DA	O4'-C4'-C3'	-7.45	101.52	104.50
2	C	422	DC	O4'-C1'-N1	7.41	113.19	108.00
2	C	429	DA	C4-C5-N7	7.34	114.37	110.70
2	C	426	DA	C6-N1-C2	7.33	123.00	118.60
1	B	406	DC	C2-N3-C4	7.22	123.51	119.90
2	C	428	DG	C2-N3-C4	7.10	115.45	111.90
3	A	235	GLU	OE1-CD-OE2	-7.09	114.79	123.30
2	C	424	DG	C5-C6-N1	7.07	115.03	111.50
1	B	412	DG	N1-C2-N3	7.04	128.12	123.90
3	A	232	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	C	424	DG	N3-C2-N2	-6.98	115.01	119.90
2	C	426	DA	C5-C6-N1	-6.96	114.22	117.70
2	C	429	DA	O4'-C4'-C3'	-6.96	101.72	104.50
1	B	412	DG	C5-C6-O6	-6.89	124.46	128.60
1	B	407	DA	N3-C4-C5	-6.82	122.02	126.80
2	C	425	DG	C8-N9-C1'	6.82	135.87	127.00
1	B	403	DC	N3-C2-O2	6.81	126.67	121.90
2	C	428	DG	C4-C5-N7	6.81	113.52	110.80
2	C	430	DA	C6-C5-N7	-6.74	127.59	132.30
2	C	425	DG	C5-C6-O6	-6.68	124.59	128.60
1	B	403	DC	OP1-P-OP2	-6.63	109.66	119.60
2	C	429	DA	C4'-C3'-O3'	-6.59	93.22	109.70
2	C	424	DG	C2-N3-C4	6.54	115.17	111.90
2	C	422	DC	N1-C2-O2	-6.46	115.02	118.90
1	B	410	DC	N3-C4-N4	6.44	122.51	118.00
2	C	426	DA	N1-C2-N3	-6.42	126.09	129.30
1	B	407	DA	N9-C4-C5	6.42	108.37	105.80
1	B	407	DA	C2-N3-C4	6.42	113.81	110.60
2	C	429	DA	O4'-C1'-N9	-6.41	103.51	108.00
2	C	422	DC	C5-C4-N4	6.28	124.59	120.20
2	C	425	DG	O4'-C1'-N9	-6.24	103.63	108.00
3	A	226	ARG	NE-CZ-NH1	-6.23	117.19	120.30
2	C	425	DG	C6-N1-C2	-6.23	121.36	125.10
2	C	428	DG	C6-N1-C2	-6.15	121.41	125.10
1	B	409	DC	OP2-P-O3'	6.15	118.72	105.20
3	A	206	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	407	DA	C5-N7-C8	5.97	106.88	103.90
2	C	425	DG	N9-C4-C5	5.96	107.78	105.40
1	B	403	DC	N1-C2-N3	-5.96	115.03	119.20
2	C	428	DG	N1-C6-O6	5.94	123.47	119.90
2	C	422	DC	P-O3'-C3'	5.90	126.78	119.70
1	B	409	DC	O4'-C1'-C2'	-5.88	101.19	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	430	DA	N3-C4-C5	5.87	130.91	126.80
1	B	406	DC	OP1-P-O3'	5.80	117.97	105.20
2	C	422	DC	C2-N1-C1'	-5.76	112.46	118.80
1	B	407	DA	O5'-P-OP2	-5.76	100.52	105.70
3	A	233	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	409	DC	N3-C4-N4	5.67	121.97	118.00
2	C	423	DA	C6-C5-N7	-5.66	128.34	132.30
1	B	407	DA	C4-C5-N7	-5.64	107.88	110.70
1	B	410	DC	O5'-P-OP2	-5.57	100.68	105.70
2	C	430	DA	O3'-P-O5'	-5.56	93.44	104.00
2	C	431	DG	N1-C6-O6	-5.55	116.57	119.90
3	A	87	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	406	DC	N3-C2-O2	5.49	125.74	121.90
3	A	8	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	C	426	DA	O4'-C4'-C3'	-5.38	102.35	104.50
2	C	424	DG	O4'-C1'-N9	-5.37	104.24	108.00
2	C	431	DG	N1-C2-N2	-5.37	111.37	116.20
3	A	114	GLU	CA-CB-CG	5.35	125.18	113.40
2	C	422	DC	OP2-P-O3'	5.35	116.96	105.20
3	A	75	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	A	142	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	A	90	ARG	CG-CD-NE	5.27	122.87	111.80
2	C	423	DA	C4-C5-C6	5.26	119.63	117.00
2	C	422	DC	OP1-P-OP2	-5.24	111.74	119.60
2	C	422	DC	C4'-C3'-C2'	-5.23	98.39	103.10
3	A	188	ASP	CB-CG-OD2	-5.20	113.62	118.30
3	A	151	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	C	422	DC	N1-C2-N3	-5.17	115.58	119.20
2	C	429	DA	C2-N3-C4	5.08	113.14	110.60
2	C	424	DG	C5-C6-O6	-5.01	125.59	128.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	404	BRU	C4'

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	B	199	0	0	3	0
2	C	202	0	0	3	0
3	A	2059	0	0	6	0
4	A	1	0	0	0	0
5	A	25	0	0	1	0
6	A	24	0	0	1	0
7	A	441	0	0	1	0
7	B	24	0	0	1	0
7	C	23	0	0	0	0
All	All	2998	0	0	9	0

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 6.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:410:DC:C2'	1:B:411:BRU:BR	3.10	0.54
3:A:195:ASP:OD2	6:A:512:GOL:O2	2.30	0.50
2:C:430:DA:OP2	3:A:124[A]:ARG:NE	2.47	0.47
2:C:430:DA:OP2	3:A:124[A]:ARG:NH2	2.49	0.46
3:A:124[A]:ARG:NH2	7:A:644:HOH:O	2.50	0.45
1:B:403:DC:N4	7:B:995:HOH:O	2.49	0.45
3:A:140[B]:LYS:NZ	5:A:552:SO4:O3	2.50	0.45
3:A:78:ASP:OD1	3:A:98:LYS:NZ	2.54	0.40
1:B:403:DC:N4	2:C:430:DA:N6	2.70	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	257/262 (98%)	247 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	224/226 (99%)	218 (97%)	6 (3%)	57	14

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	PRO
3	A	69	GLN
3	A	123	GLN
3	A	124[A]	ARG
3	A	124[B]	ARG
3	A	169	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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	B	404	1,2	19,21,22	2.21	5 (26%)	22,30,33	3.62	7 (31%)
1	BRU	B	405	1,2	19,21,22	1.67	3 (15%)	22,30,33	3.15	6 (27%)
1	BRU	B	408	1,2	19,21,22	1.70	3 (15%)	22,30,33	2.46	5 (22%)
1	BRU	B	411	1,2	19,21,22	2.15	4 (21%)	22,30,33	1.78	7 (31%)

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	B	404	1,2	1/1/4/4	1/5/21/22	0/2/2/2
1	BRU	B	405	1,2	-	0/5/21/22	0/2/2/2
1	BRU	B	408	1,2	-	0/5/21/22	0/2/2/2
1	BRU	B	411	1,2	-	0/5/21/22	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	BRU	P-OP1	6.02	1.53	1.46
1	B	405	BRU	P-OP1	5.78	1.53	1.46
1	B	404	BRU	C4-C5	5.18	1.48	1.39
1	B	411	BRU	P-OP1	5.01	1.52	1.46
1	B	411	BRU	C2-N3	4.81	1.46	1.37
1	B	408	BRU	C4-C5	4.36	1.47	1.39
1	B	411	BRU	C4-C5	4.10	1.46	1.39
1	B	408	BRU	P-OP1	3.91	1.51	1.46
1	B	411	BRU	C4-N3	2.97	1.42	1.37
1	B	404	BRU	C2-N3	2.91	1.43	1.37
1	B	408	BRU	C2-N3	2.70	1.42	1.37
1	B	405	BRU	C4-C5	2.29	1.43	1.39
1	B	404	BRU	C2-N1	2.10	1.40	1.38
1	B	404	BRU	C6-N1	2.04	1.39	1.34
1	B	405	BRU	C2-N3	2.04	1.41	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	BRU	C6-N1-C2	10.36	125.34	122.41
1	B	404	BRU	BR-C5-C4	-10.21	101.55	120.11
1	B	404	BRU	BR-C5-C6	9.32	136.45	117.98
1	B	408	BRU	C6-N1-C2	-8.66	119.95	122.41
1	B	405	BRU	C5-C6-N1	-7.53	114.72	119.67
1	B	404	BRU	C6-N1-C2	5.64	124.01	122.41
1	B	405	BRU	O4'-C1'-N1	-4.76	98.73	107.68
1	B	408	BRU	C5-C6-N1	4.45	122.60	119.67
1	B	411	BRU	C6-N1-C1'	-3.94	109.57	119.33
1	B	404	BRU	O4'-C1'-N1	3.92	115.05	107.68
1	B	411	BRU	N3-C2-N1	3.34	118.76	115.97
1	B	408	BRU	O4'-C1'-N1	-3.24	101.60	107.68
1	B	408	BRU	N3-C2-N1	3.12	118.58	115.97
1	B	404	BRU	O3'-C3'-C2'	-2.94	99.70	110.78
1	B	405	BRU	BR-C5-C4	-2.82	114.98	120.11
1	B	411	BRU	C6-N1-C2	-2.67	121.65	122.41
1	B	404	BRU	O4'-C4'-C3'	-2.67	98.90	105.66
1	B	411	BRU	C4-N3-C2	-2.54	120.19	125.39
1	B	405	BRU	C6-C5-C4	2.36	127.20	118.50
1	B	404	BRU	O4'-C4'-C5'	2.34	117.71	109.36
1	B	411	BRU	O4'-C4'-C5'	2.30	117.58	109.36
1	B	411	BRU	O3'-C3'-C4'	-2.26	100.83	110.14
1	B	408	BRU	C2'-C1'-N1	2.10	119.54	114.08
1	B	405	BRU	C5-C4-N3	-2.07	112.80	116.70
1	B	411	BRU	C3'-C2'-C1'	-2.01	97.10	102.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	404	BRU	C4'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	404	BRU	P-O5'-C5'-C4'

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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
6	GOL	A	511	-	5,5,5	0.85	0	5,5,5	2.20	2 (40%)
6	GOL	A	512	-	5,5,5	0.44	0	5,5,5	0.95	0
6	GOL	A	513	-	5,5,5	0.94	0	5,5,5	1.30	1 (20%)
6	GOL	A	514	-	5,5,5	0.53	0	5,5,5	0.51	0
5	SO4	A	551	-	4,4,4	0.68	0	6,6,6	0.96	1 (16%)
5	SO4	A	552	-	4,4,4	0.72	0	6,6,6	0.45	0
5	SO4	A	553	-	4,4,4	0.47	0	6,6,6	0.49	0
5	SO4	A	554	-	4,4,4	0.20	0	6,6,6	0.16	0
5	SO4	A	555	-	4,4,4	0.51	0	6,6,6	0.71	0

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
6	GOL	A	511	-	-	0/4/4/4	0/0/0/0
6	GOL	A	512	-	-	0/4/4/4	0/0/0/0
6	GOL	A	513	-	-	0/4/4/4	0/0/0/0
6	GOL	A	514	-	-	0/4/4/4	0/0/0/0
5	SO4	A	551	-	-	0/0/0/0	0/0/0/0
5	SO4	A	552	-	-	0/0/0/0	0/0/0/0
5	SO4	A	553	-	-	0/0/0/0	0/0/0/0
5	SO4	A	554	-	-	0/0/0/0	0/0/0/0
5	SO4	A	555	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	GOL	O3-C3-C2	4.23	130.34	109.71
6	A	511	GOL	C3-C2-C1	-2.37	100.79	111.26
6	A	513	GOL	O3-C3-C2	2.35	121.16	109.71
5	A	551	SO4	O2-S-O1	2.14	116.60	109.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.