



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:19 pm GMT

PDB ID : 2EA0
Title : Crystal structure of the DNA repair enzyme endonuclease-VIII (Nei) from E. coli in complex with AP-site containing DNA substrate
Authors : Golan, G.; Zharov, D.O.; Grollman, A.P.; Shoham, G.
Deposited on : 2007-01-29
Resolution : 1.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

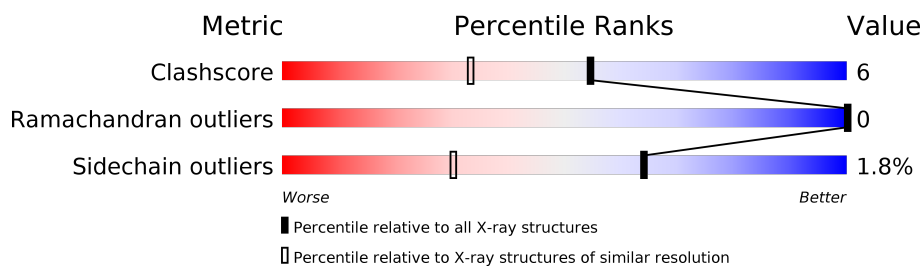
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	12	
2	C	12	
3	A	262	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	511	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3023 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(P*GP*GP*CP*TP*TP*CP*AP*TP*CP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			243	116	40	75	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			240	112	49	67	12			

- Molecule 3 is a protein called Endonuclease VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	254	Total	C	N	O	S	0	15	0
			2096	1338	378	375	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



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

- Molecule 7 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	34	Total	O	0	0
			34	34		
7	C	18	Total	O	0	0
			18	18		
7	A	360	Total	O	0	0
			360	360		

3 Residue-property plots [i](#)

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.

Note EDS was not executed.

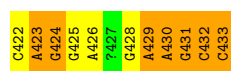
- Molecule 1: 5'-D(P*GP*GP*CP*TP*TP*CP*AP*TP*CP*CP*TP*G)-3'

Chain B: 




- Molecule 2: 5'-D(P*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 is therefore incomplete.

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.18Å 76.18Å 164.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.40	Depositor
% Data completeness (in resolution range)	95.8 (30.00-1.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.160 , 0.204	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3023	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PED, GOL, ZN, 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	3.14	16/270 (5.9%)	5.86	101/414 (24.4%)
2	C	1.97	6/257 (2.3%)	5.73	107/392 (27.3%)
3	A	0.68	0/2217	1.25	20/3006 (0.7%)
All	All	1.31	22/2744 (0.8%)	2.89	228/3812 (6.0%)

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
2	C	1	0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	DG	O3'-P	18.25	1.83	1.61
1	B	404	DT	C5-C7	18.21	1.60	1.50
1	B	411	DT	C5-C7	16.45	1.59	1.50
1	B	405	DT	C5-C7	16.27	1.59	1.50
1	B	408	DT	C5-C7	14.69	1.58	1.50
1	B	411	DT	C2-N3	9.98	1.45	1.37
1	B	404	DT	C2-N3	7.82	1.44	1.37
1	B	402	DG	C5-C4	6.80	1.43	1.38
1	B	412	DG	C5-C4	6.62	1.43	1.38
1	B	405	DT	C2-N3	6.58	1.43	1.37
1	B	408	DT	C2-N3	6.53	1.43	1.37
2	C	430	DA	O3'-P	-6.14	1.53	1.61
1	B	401	DG	C5-C4	5.86	1.42	1.38
2	C	425	DG	N3-C4	5.79	1.39	1.35
1	B	401	DG	C5-C6	5.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	429	DA	C3'-O3'	-5.60	1.36	1.44
2	C	424	DG	C5-C4	5.54	1.42	1.38
1	B	402	DG	N3-C4	5.53	1.39	1.35
1	B	412	DG	C5-C6	5.51	1.47	1.42
2	C	424	DG	C5-C6	5.41	1.47	1.42
2	C	425	DG	C6-N1	5.11	1.43	1.39
1	B	412	DG	C6-N1	5.04	1.43	1.39

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	DG	N3-C4-C5	-22.43	117.39	128.60
2	C	429	DA	OP2-P-O3'	22.16	153.95	105.20
2	C	424	DG	N7-C8-N9	21.70	123.95	113.10
1	B	402	DG	N7-C8-N9	21.44	123.82	113.10
1	B	412	DG	N7-C8-N9	20.95	123.57	113.10
1	B	402	DG	C8-N9-C4	-20.02	98.39	106.40
1	B	401	DG	N7-C8-N9	19.68	122.94	113.10
2	C	425	DG	N7-C8-N9	19.62	122.91	113.10
1	B	409	DC	N3-C4-C5	-19.24	114.20	121.90
1	B	412	DG	C8-N9-C4	-18.97	98.81	106.40
2	C	428	DG	N7-C8-N9	18.86	122.53	113.10
1	B	412	DG	N3-C4-C5	-18.81	119.19	128.60
1	B	402	DG	C2-N3-C4	18.59	121.20	111.90
1	B	410	DC	OP1-P-O3'	-18.45	64.61	105.20
1	B	409	DC	C2-N3-C4	18.31	129.06	119.90
2	C	433	DC	C2-N3-C4	18.21	129.00	119.90
2	C	425	DG	C8-N9-C4	-17.94	99.22	106.40
2	C	424	DG	C8-N9-C4	-17.93	99.23	106.40
2	C	431	DG	N7-C8-N9	17.17	121.69	113.10
1	B	402	DG	O4'-C1'-N9	17.10	119.97	108.00
2	C	424	DG	N3-C4-C5	-17.02	120.09	128.60
1	B	401	DG	C8-N9-C4	-16.93	99.63	106.40
2	C	422	DC	N3-C4-C5	-16.73	115.21	121.90
2	C	422	DC	C2-N3-C4	16.69	128.25	119.90
1	B	403	DC	C2-N3-C4	16.28	128.04	119.90
1	B	406	DC	N3-C4-C5	-16.26	115.40	121.90
1	B	411	DT	C6-C5-C7	-15.44	113.63	122.90
2	C	433	DC	N3-C4-C5	-15.41	115.74	121.90
2	C	424	DG	C5-N7-C8	-15.35	96.63	104.30
2	C	431	DG	C8-N9-C4	-15.34	100.26	106.40
1	B	403	DC	N3-C4-C5	-15.06	115.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	DC	C2-N3-C4	14.78	127.29	119.90
1	B	401	DG	N3-C4-C5	-14.49	121.36	128.60
1	B	401	DG	C2-N3-C4	14.42	119.11	111.90
2	C	432	DC	O3'-P-O5'	14.38	131.32	104.00
1	B	402	DG	N3-C4-N9	14.16	134.50	126.00
3	A	239	ARG	NE-CZ-NH2	-14.14	113.23	120.30
2	C	430	DA	OP2-P-O3'	-14.08	74.22	105.20
2	C	429	DA	P-O3'-C3'	14.03	136.53	119.70
2	C	425	DG	N3-C4-C5	-13.98	121.61	128.60
2	C	428	DG	C5-N7-C8	-13.92	97.34	104.30
1	B	411	DT	OP1-P-O3'	-13.88	74.67	105.20
2	C	428	DG	C8-N9-C4	-13.75	100.90	106.40
1	B	412	DG	C2-N3-C4	13.65	118.72	111.90
2	C	422	DC	OP1-P-O3'	13.48	134.85	105.20
1	B	402	DG	C6-N1-C2	-13.46	117.03	125.10
2	C	432	DC	C2-N3-C4	13.33	126.56	119.90
1	B	402	DG	C5-C6-N1	13.27	118.14	111.50
1	B	402	DG	C5-N7-C8	-13.17	97.72	104.30
1	B	401	DG	C5-N7-C8	-13.06	97.77	104.30
1	B	412	DG	C6-N1-C2	-12.82	117.41	125.10
1	B	412	DG	C5-N7-C8	-12.57	98.01	104.30
2	C	424	DG	C2-N3-C4	12.43	118.11	111.90
3	A	169	TYR	CB-CG-CD1	12.39	128.43	121.00
1	B	411	DT	C2-N3-C4	-12.37	119.78	127.20
2	C	424	DG	C6-N1-C2	-12.31	117.71	125.10
1	B	410	DC	N3-C4-C5	-12.23	117.01	121.90
2	C	431	DG	C5-N7-C8	-11.84	98.38	104.30
2	C	425	DG	C5-N7-C8	-11.60	98.50	104.30
1	B	405	DT	C6-C5-C7	-11.56	115.97	122.90
2	C	430	DA	P-O3'-C3'	11.53	133.53	119.70
1	B	410	DC	C2-N3-C4	11.50	125.65	119.90
1	B	401	DG	P-O3'-C3'	-11.46	105.95	119.70
1	B	412	DG	N3-C4-N9	11.27	132.76	126.00
2	C	430	DA	OP1-P-OP2	-11.22	102.77	119.60
2	C	424	DG	N3-C4-N9	11.18	132.71	126.00
2	C	425	DG	C2-N3-C4	10.79	117.29	111.90
1	B	405	DT	C5-C6-N1	-10.74	117.25	123.70
2	C	423	DA	OP1-P-O3'	-10.68	81.72	105.20
1	B	402	DG	P-O3'-C3'	-10.56	107.02	119.70
1	B	404	DT	N1-C1'-C2'	10.56	132.67	112.60
2	C	424	DG	C5-C6-O6	-10.47	122.32	128.60
2	C	424	DG	C5-C6-N1	10.43	116.72	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	428	DG	C2-N3-C4	10.35	117.08	111.90
2	C	431	DG	N3-C4-C5	-10.30	123.45	128.60
2	C	429	DA	P-O5'-C5'	-10.28	104.45	120.90
2	C	432	DC	N3-C4-C5	-10.28	117.79	121.90
1	B	405	DT	C6-N1-C2	10.26	126.43	121.30
1	B	412	DG	C5-C6-N1	10.08	116.54	111.50
1	B	402	DG	O3'-P-O5'	-10.07	84.86	104.00
3	A	239	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	C	423	DA	O4'-C4'-C3'	-9.88	100.07	106.00
2	C	431	DG	C2-N3-C4	9.79	116.80	111.90
1	B	411	DT	C4-C5-C6	9.72	123.83	118.00
1	B	408	DT	N3-C2-O2	-9.57	116.56	122.30
2	C	429	DA	N1-C2-N3	-9.45	124.58	129.30
2	C	432	DC	N1-C2-O2	9.45	124.57	118.90
2	C	422	DC	OP2-P-O3'	-9.35	84.64	105.20
2	C	429	DA	C4'-C3'-O3'	9.34	133.05	109.70
1	B	404	DT	C2-N3-C4	-9.20	121.68	127.20
1	B	405	DT	O4'-C1'-N1	-9.19	101.56	108.00
2	C	426	DA	O4'-C4'-C3'	-9.08	100.55	106.00
1	B	401	DG	C5-C6-O6	-9.04	123.18	128.60
2	C	431	DG	C5-C6-N1	9.03	116.02	111.50
1	B	401	DG	C5-C6-N1	9.02	116.01	111.50
2	C	428	DG	N3-C4-C5	-8.99	124.10	128.60
1	B	405	DT	C2-N3-C4	-8.85	121.89	127.20
1	B	411	DT	C5-C6-N1	-8.84	118.40	123.70
2	C	432	DC	OP2-P-O3'	-8.76	85.94	105.20
1	B	410	DC	OP2-P-O3'	8.73	124.40	105.20
2	C	423	DA	N1-C2-N3	-8.69	124.95	129.30
2	C	428	DG	C5-C6-N1	8.67	115.84	111.50
1	B	408	DT	O4'-C1'-N1	-8.64	101.95	108.00
2	C	429	DA	O4'-C1'-N9	8.60	114.02	108.00
1	B	401	DG	O4'-C4'-C3'	-8.56	100.86	106.00
1	B	402	DG	C5-C6-O6	-8.43	123.54	128.60
1	B	404	DT	C4-C5-C6	8.33	123.00	118.00
3	A	124[A]	ARG	NE-CZ-NH1	-8.32	116.14	120.30
3	A	124[B]	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	401	DG	N3-C4-N9	8.27	130.96	126.00
1	B	404	DT	N3-C2-O2	-8.25	117.35	122.30
1	B	404	DT	C6-C5-C7	-8.23	117.96	122.90
2	C	430	DA	N1-C2-N3	-8.20	125.20	129.30
2	C	431	DG	O4'-C1'-N9	-8.07	102.35	108.00
2	C	433	DC	O4'-C4'-C3'	-8.02	101.19	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	DA	C4-C5-C6	7.98	120.99	117.00
1	B	406	DC	N3-C4-N4	7.98	123.59	118.00
2	C	429	DA	OP1-P-O3'	-7.91	87.81	105.20
2	C	429	DA	C2-N3-C4	7.90	114.55	110.60
2	C	422	DC	N3-C2-O2	7.84	127.39	121.90
2	C	422	DC	C5-C6-N1	7.80	124.90	121.00
2	C	422	DC	O4'-C1'-N1	7.77	113.44	108.00
1	B	411	DT	N3-C2-O2	-7.73	117.66	122.30
1	B	401	DG	C6-N1-C2	-7.69	120.49	125.10
3	A	169	TYR	CG-CD1-CE1	7.66	127.43	121.30
1	B	410	DC	N3-C4-N4	7.65	123.35	118.00
1	B	403	DC	C5-C6-N1	7.59	124.80	121.00
1	B	408	DT	C5-C6-N1	-7.59	119.15	123.70
2	C	428	DG	C6-N1-C2	-7.55	120.57	125.10
2	C	425	DG	C6-N1-C2	-7.55	120.57	125.10
3	A	232	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	C	433	DC	C5-C6-N1	7.45	124.72	121.00
1	B	409	DC	OP2-P-O3'	7.39	121.46	105.20
2	C	430	DA	C2-N3-C4	7.34	114.27	110.60
1	B	411	DT	N1-C2-N3	7.29	118.98	114.60
1	B	412	DG	N1-C2-N3	7.28	128.27	123.90
1	B	404	DT	N1-C2-N3	7.23	118.94	114.60
3	A	65	TYR	CB-CG-CD1	7.16	125.30	121.00
2	C	432	DC	O4'-C1'-N1	7.12	112.99	108.00
2	C	433	DC	N1-C2-N3	-7.12	114.21	119.20
2	C	431	DG	C8-N9-C1'	7.10	136.23	127.00
2	C	428	DG	C5-C6-O6	-7.07	124.36	128.60
1	B	412	DG	C5-C6-O6	-7.05	124.37	128.60
2	C	424	DG	P-O3'-C3'	7.03	128.13	119.70
2	C	425	DG	N9-C4-C5	7.02	108.21	105.40
2	C	424	DG	N1-C2-N3	6.98	128.09	123.90
2	C	425	DG	N3-C4-N9	6.97	130.18	126.00
2	C	433	DC	N3-C4-N4	6.97	122.88	118.00
3	A	171	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	C	425	DG	C8-N9-C1'	6.92	135.99	127.00
2	C	422	DC	C6-N1-C2	-6.91	117.54	120.30
1	B	401	DG	C4'-C3'-C2'	-6.91	96.88	103.10
2	C	432	DC	P-O5'-C5'	-6.90	109.86	120.90
1	B	403	DC	N3-C4-N4	6.89	122.83	118.00
2	C	431	DG	C6-N1-C2	-6.80	121.02	125.10
1	B	402	DG	N9-C4-C5	6.79	108.12	105.40
2	C	422	DC	N3-C4-N4	6.75	122.73	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	DT	C4-C5-C6	6.66	122.00	118.00
2	C	433	DC	C4'-C3'-C2'	-6.66	97.10	103.10
2	C	432	DC	N3-C4-N4	6.63	122.64	118.00
1	B	412	DG	N9-C4-C5	6.61	108.05	105.40
1	B	408	DT	C4-C5-C6	6.60	121.96	118.00
1	B	412	DG	O5'-P-OP1	6.54	118.55	110.70
2	C	429	DA	N9-C4-C5	-6.54	103.18	105.80
1	B	403	DC	O4'-C1'-C2'	-6.53	100.68	105.90
2	C	430	DA	C4'-C3'-O3'	6.52	126.01	109.70
1	B	408	DT	C2-N3-C4	-6.34	123.40	127.20
3	A	87	ARG	NE-CZ-NH1	-6.30	117.15	120.30
2	C	425	DG	C5-C6-N1	6.25	114.63	111.50
1	B	406	DC	O4'-C1'-N1	-6.23	103.64	108.00
3	A	147	ARG	NE-CZ-NH1	-6.23	117.19	120.30
2	C	424	DG	C8-N9-C1'	6.22	135.09	127.00
1	B	406	DC	N3-C2-O2	6.19	126.23	121.90
2	C	432	DC	N1-C2-N3	-6.18	114.87	119.20
2	C	431	DG	C5-C6-O6	-6.18	124.89	128.60
2	C	432	DC	P-O3'-C3'	-6.13	112.34	119.70
3	A	252	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	401	DG	C8-N9-C1'	6.10	134.93	127.00
1	B	409	DC	N1-C2-N3	-6.03	114.98	119.20
2	C	430	DA	O4'-C1'-N9	6.01	112.20	108.00
2	C	424	DG	OP2-P-O3'	-6.00	92.01	105.20
1	B	406	DC	O4'-C1'-C2'	-5.93	101.16	105.90
1	B	409	DC	N3-C4-N4	5.90	122.13	118.00
1	B	411	DT	C4-C5-C7	5.89	122.53	119.00
3	A	90	ARG	CG-CD-NE	5.86	124.09	111.80
2	C	429	DA	C8-N9-C4	5.85	108.14	105.80
1	B	401	DG	OP1-P-O3'	-5.83	92.37	105.20
2	C	431	DG	OP2-P-O3'	-5.73	92.60	105.20
1	B	402	DG	OP1-P-O3'	5.71	117.76	105.20
1	B	401	DG	N9-C4-C5	5.71	107.68	105.40
1	B	403	DC	N1-C2-N3	-5.64	115.25	119.20
1	B	407	DA	C6-C5-N7	-5.64	128.35	132.30
1	B	404	DT	C5-C6-N1	-5.62	120.33	123.70
2	C	429	DA	C1'-O4'-C4'	-5.59	104.51	110.10
2	C	423	DA	N9-C1'-C2'	5.58	123.19	112.60
2	C	429	DA	N3-C4-N9	5.56	131.85	127.40
1	B	410	DC	P-O3'-C3'	5.54	126.34	119.70
3	A	71	TYR	CB-CG-CD1	5.50	124.30	121.00
2	C	426	DA	N1-C2-N3	-5.49	126.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	424	DG	C4-C5-N7	5.48	112.99	110.80
1	B	409	DC	N3-C2-O2	5.46	125.72	121.90
2	C	425	DG	O5'-P-OP1	5.44	117.23	110.70
1	B	407	DA	N3-C4-C5	-5.43	123.00	126.80
2	C	429	DA	C4-C5-N7	5.42	113.41	110.70
1	B	403	DC	P-O5'-C5'	-5.42	112.22	120.90
2	C	431	DG	N9-C4-C5	5.42	107.57	105.40
1	B	403	DC	N1-C2-O2	5.42	122.15	118.90
2	C	423	DA	C6-N1-C2	5.42	121.85	118.60
3	A	232	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	C	431	DG	O4'-C1'-C2'	5.34	110.17	105.90
3	A	78	ASP	CB-CG-OD1	5.32	123.09	118.30
3	A	131	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	412	DG	C8-N9-C1'	5.31	133.90	127.00
2	C	426	DA	C5-C6-N1	-5.29	115.06	117.70
1	B	405	DT	OP2-P-O3'	5.28	116.83	105.20
2	C	426	DA	C4-C5-C6	5.27	119.63	117.00
1	B	409	DC	P-O5'-C5'	-5.22	112.55	120.90
2	C	429	DA	C3'-C2'-C1'	-5.22	96.24	102.50
3	A	75[A]	ARG	NE-CZ-NH2	-5.21	117.69	120.30
3	A	75[B]	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	C	433	DC	N3-C2-O2	5.18	125.53	121.90
1	B	402	DG	N1-C2-N2	-5.18	111.54	116.20
2	C	423	DA	C2-N3-C4	5.15	113.17	110.60
2	C	431	DG	OP1-P-OP2	5.12	127.28	119.60
2	C	429	DA	O4'-C1'-C2'	-5.09	101.83	105.90
1	B	405	DT	C4-C5-C7	5.06	122.04	119.00
2	C	425	DG	C5-C6-O6	-5.03	125.58	128.60
3	A	71	TYR	CB-CG-CD2	-5.02	117.99	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	429	DA	C3'

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	B	243	0	137	4	0
2	C	240	0	130	8	1
3	A	2096	0	2100	18	0
4	A	20	0	0	1	0
4	C	5	0	0	0	0
5	A	1	0	0	0	0
6	A	6	0	7	6	0
7	A	360	0	0	4	0
7	B	34	0	0	2	0
7	C	18	0	0	1	0
All	All	3023	0	2374	30	1

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 6.

All (30) 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:A:147:ARG:HH21	6:A:511:GOL:H32	1.18	1.02
3:A:187:LYS:HD2	4:A:553:SO4:O3	1.88	0.72
1:B:405:DT:H5''	7:B:989:HOH:O	1.91	0.70
3:A:112:ARG:H	3:A:115:GLN:HE21	1.41	0.69
3:A:112:ARG:H	3:A:115:GLN:NE2	1.98	0.61
3:A:147:ARG:HE	6:A:511:GOL:C1	2.13	0.61
2:C:433:DC:H4'	2:C:433:DC:OP1	2.06	0.54
7:C:996:HOH:O	3:A:231:HIS:HE1	1.93	0.52
3:A:231:HIS:HD2	7:A:984:HOH:O	1.91	0.52
2:C:423:DA:OP2	2:C:423:DA:C8	2.62	0.52
1:B:401:DG:H2''	1:B:402:DG:C8	2.47	0.50
7:B:682:HOH:O	6:A:511:GOL:H11	2.12	0.48
3:A:147:ARG:NH2	6:A:511:GOL:H32	2.04	0.48
3:A:147:ARG:HE	6:A:511:GOL:H12	1.79	0.48
3:A:140[B]:LYS:HG3	3:A:198:ALA:CB	2.44	0.47
3:A:172:VAL:CG1	3:A:229:VAL:HG23	2.44	0.47
2:C:431:DG:H2''	2:C:432:DC:O5'	2.14	0.47
2:C:429:DA:H4'	2:C:430:DA:OP1	2.15	0.46
3:A:262:HIS:HE1	7:A:995:HOH:O	1.99	0.45
3:A:60:ASN:O	3:A:61:ASP:HB2	2.17	0.44
1:B:402:DG:H1	2:C:432:DC:H42	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:DA:H8	2:C:423:DA:OP2	2.01	0.44
3:A:177[B]:GLN:NE2	7:A:641:HOH:O	2.50	0.43
1:B:401:DG:H2'	1:B:401:DG:H5''	1.63	0.43
3:A:190:ASN:OD1	3:A:193[A]:GLN:HG3	2.19	0.42
3:A:147:ARG:NE	6:A:511:GOL:O1	2.49	0.41
2:C:423:DA:H1'	2:C:424:DG:C8	2.56	0.41
3:A:193[B]:GLN:NE2	7:A:763:HOH:O	2.53	0.41
3:A:144:LEU:HD11	3:A:194:LEU:CD2	2.51	0.40
2:C:433:DC:C4'	2:C:433:DC:OP1	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:433:DC:O2	2:C:433:DC:O2[6_553]	1.69	0.51

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	266/262 (102%)	257 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	233/226 (103%)	228 (98%)	5 (2%)	59 23

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	69	GLN
3	A	124[A]	ARG
3	A	124[B]	ARG
3	A	169	TYR
3	A	231	HIS

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	68	ASN
3	A	115	GLN
3	A	231	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	0.63	0	5,5,5	0.62	0
4	SO4	A	551	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	A	553	-	4,4,4	0.19	0	6,6,6	0.37	0
4	SO4	A	554	-	4,4,4	0.32	0	6,6,6	0.86	0
4	SO4	A	555	-	4,4,4	0.37	0	6,6,6	0.32	0
4	SO4	C	552	-	4,4,4	0.17	0	6,6,6	0.21	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
4	SO4	A	551	-	-	0/0/0/0	0/0/0/0
4	SO4	A	553	-	-	0/0/0/0	0/0/0/0
4	SO4	A	554	-	-	0/0/0/0	0/0/0/0
4	SO4	A	555	-	-	0/0/0/0	0/0/0/0
4	SO4	C	552	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	511	GOL	6	0
4	A	553	SO4	1	0

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.