



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:15 pm GMT

PDB ID : 1K3W  
Title : Crystal structure of a trapped reaction intermediate of the DNA Repair Enzyme Endonuclease VIII with DNA  
Authors : Golan, G.; Zharkov, D.O.; Gilboa, R.; Fernandes, A.S.; Kycia, J.H.; Gerchman, S.E.; Rieger, R.A.; Grollman, A.P.; Shoham, G.  
Deposited on : 2001-10-04  
Resolution : 1.42 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (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

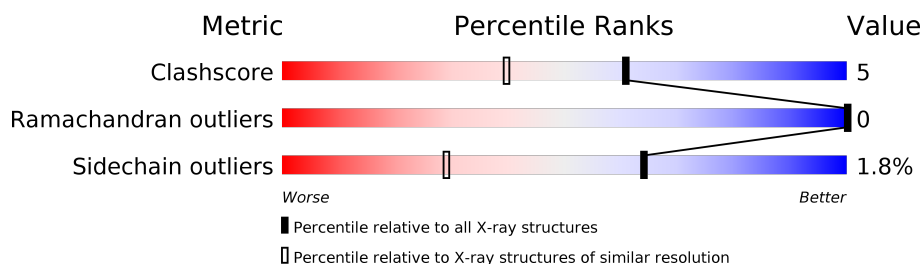
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.42 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	1955 (1.44-1.40)
Ramachandran outliers	110173	1908 (1.44-1.40)
Sidechain outliers	110143	1907 (1.44-1.40)

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  $\geq 3$ , 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	13	
2	C	13	
3	A	262	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2874 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(\*GP\*GP\*CP\*TP\*TP\*CP\*AP\*TP\*CP\*CP\*TP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			

- 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	11	Total	C	N	O	P	0	0	0
			221	103	46	61	11			

- Molecule 3 is a protein called Endonuclease VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	254	Total	C	N	O	S	0	8	0
			2080	1325	378	372	5			

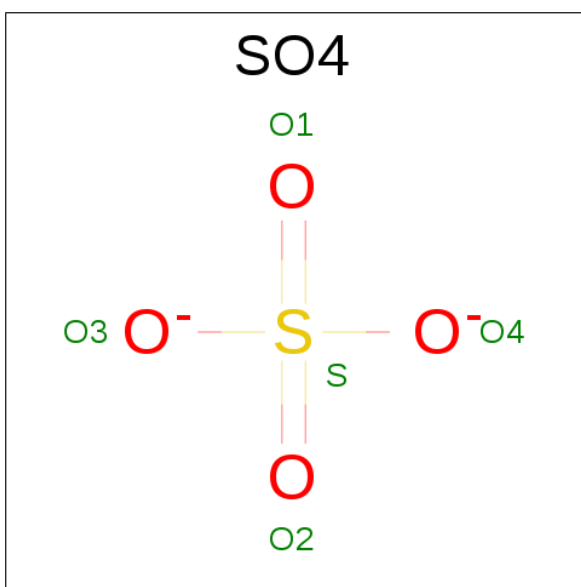
There are 2 discrepancies between the modelled and reference sequences:

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: O<sub>4</sub>S).



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		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	364	Total	O	0	0
			364	364		
6	B	14	Total	O	0	0
			14	14		
6	C	19	Total	O	0	0
			19	19		

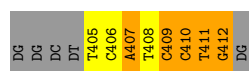
### 3 Residue-property plots [i](#)

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.

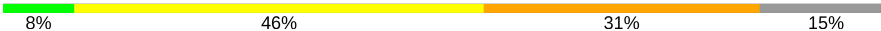
Note EDS was not executed.

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

Chain B: 



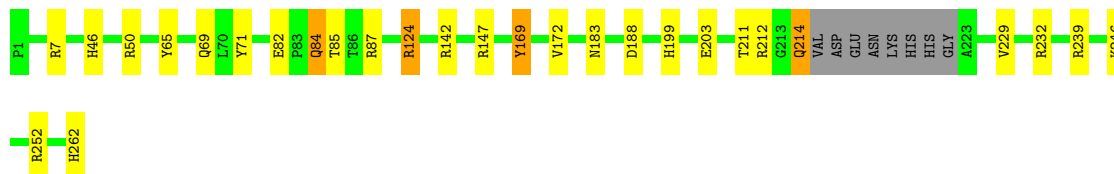
- Molecule 2: 5'-D(\*CP\*CP\*AP\*GP\*GP\*AP\*(PED)P\*GP\*AP\*AP\*GP\*CP\*C)-3'

Chain C: 



- Molecule 3: Endonuclease VIII

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.03Å 76.03Å 164.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.42	Depositor
% Data completeness (in resolution range)	95.2 (10.00-1.42)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.165 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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, 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	2.99	10/177 (5.6%)	5.11	51/270 (18.9%)
2	C	2.03	11/236 (4.7%)	5.37	85/360 (23.6%)
3	A	0.64	0/2162	1.31	23/2930 (0.8%)
All	All	1.15	21/2575 (0.8%)	2.51	159/3560 (4.5%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	DT	C5-C7	17.53	1.60	1.50
1	B	405	DT	C5-C7	16.62	1.60	1.50
1	B	408	DT	C5-C7	14.75	1.58	1.50
1	B	411	DT	C2-N3	10.29	1.46	1.37
1	B	405	DT	C2-N3	7.58	1.43	1.37
2	C	431	DG	O3'-P	-7.47	1.52	1.61
1	B	412	DG	C5-C4	6.94	1.43	1.38
1	B	408	DT	C2-N3	6.85	1.43	1.37
2	C	428	DG	N3-C4	6.42	1.40	1.35
1	B	412	DG	C5-C6	5.87	1.48	1.42
2	C	424	DG	C5-C4	5.72	1.42	1.38
1	B	412	DG	C6-N1	5.71	1.43	1.39
2	C	424	DG	N3-C4	5.62	1.39	1.35
2	C	425	DG	C5-C4	5.61	1.42	1.38
2	C	424	DG	C5-C6	5.51	1.47	1.42
2	C	428	DG	C5-C4	5.15	1.42	1.38
2	C	425	DG	C6-N1	5.14	1.43	1.39
2	C	431	DG	N3-C4	5.07	1.39	1.35
2	C	425	DG	N3-C4	5.06	1.39	1.35
1	B	412	DG	N3-C4	5.05	1.39	1.35
2	C	431	DG	C5-C6	5.03	1.47	1.42

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	DG	N3-C4-C5	-20.42	118.39	128.60
1	B	412	DG	N7-C8-N9	19.65	122.92	113.10
2	C	431	DG	N7-C8-N9	19.26	122.73	113.10
1	B	412	DG	C8-N9-C4	-19.23	98.71	106.40
2	C	425	DG	N7-C8-N9	18.03	122.11	113.10
1	B	409	DC	C2-N3-C4	17.66	128.73	119.90
2	C	424	DG	N7-C8-N9	17.56	121.88	113.10
1	B	409	DC	N3-C4-C5	-17.55	114.88	121.90
2	C	422	DC	N3-C4-C5	-17.37	114.95	121.90
1	B	412	DG	C2-N3-C4	17.32	120.56	111.90
2	C	422	DC	O4'-C4'-C3'	-17.25	95.65	106.00
2	C	423	DA	O4'-C1'-N9	17.10	119.97	108.00
2	C	431	DG	OP1-P-O3'	16.96	142.52	105.20
1	B	405	DT	C6-C5-C7	-16.44	113.03	122.90
2	C	431	DG	C8-N9-C4	-15.90	100.04	106.40
1	B	410	DC	C2-N3-C4	15.85	127.82	119.90
2	C	425	DG	C8-N9-C4	-15.53	100.19	106.40
2	C	422	DC	C2-N3-C4	15.50	127.65	119.90
2	C	425	DG	N3-C4-C5	-15.29	120.95	128.60
2	C	431	DG	N3-C4-C5	-15.03	121.09	128.60
1	B	411	DT	P-O3'-C3'	14.80	137.46	119.70
2	C	429	DA	N1-C2-N3	-14.54	122.03	129.30
2	C	424	DG	N3-C4-C5	-14.52	121.34	128.60
2	C	424	DG	C8-N9-C4	-14.34	100.66	106.40
2	C	425	DG	C2-N3-C4	13.92	118.86	111.90
2	C	432	DC	C2-N3-C4	13.56	126.68	119.90
1	B	406	DC	C2-N3-C4	13.50	126.65	119.90
1	B	411	DT	C2-N3-C4	-13.44	119.14	127.20
2	C	428	DG	N7-C8-N9	13.01	119.61	113.10
2	C	424	DG	C2-N3-C4	12.92	118.36	111.90
1	B	412	DG	C6-N1-C2	-12.83	117.40	125.10
2	C	431	DG	C2-N3-C4	12.79	118.30	111.90
1	B	409	DC	N3-C2-O2	12.63	130.74	121.90
2	C	431	DG	C5-N7-C8	-12.59	98.01	104.30
2	C	429	DA	C6-N1-C2	12.58	126.14	118.60
1	B	411	DT	C6-C5-C7	-12.21	115.58	122.90
3	A	239	ARG	NE-CZ-NH2	-12.05	114.28	120.30
2	C	431	DG	C6-N1-C2	-11.48	118.21	125.10
2	C	428	DG	N3-C4-C5	-11.42	122.89	128.60
1	B	410	DC	N3-C4-C5	-11.39	117.34	121.90
1	B	412	DG	C5-C6-N1	11.32	117.16	111.50
2	C	424	DG	C5-N7-C8	-11.32	98.64	104.30
2	C	423	DA	P-O3'-C3'	11.22	133.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	DC	N3-C4-C5	-11.22	117.41	121.90
2	C	432	DC	N3-C4-C5	-11.18	117.43	121.90
1	B	412	DG	N3-C4-N9	11.15	132.69	126.00
2	C	428	DG	C8-N9-C4	-11.10	101.96	106.40
2	C	431	DG	C5-C6-N1	10.89	116.94	111.50
2	C	425	DG	C5-N7-C8	-10.81	98.90	104.30
2	C	424	DG	C5-C6-N1	10.62	116.81	111.50
1	B	412	DG	C5-N7-C8	-10.28	99.16	104.30
2	C	424	DG	C6-N1-C2	-10.06	119.07	125.10
2	C	431	DG	N3-C4-N9	9.76	131.86	126.00
2	C	425	DG	C5-C6-N1	9.72	116.36	111.50
2	C	424	DG	N3-C4-N9	9.70	131.82	126.00
1	B	405	DT	C4-C5-C7	9.64	124.78	119.00
2	C	424	DG	C5-C6-O6	-9.57	122.86	128.60
2	C	428	DG	C5-C6-N1	9.53	116.27	111.50
2	C	430	DA	O4'-C1'-N9	9.50	114.65	108.00
2	C	431	DG	C5-C6-O6	-9.38	122.97	128.60
2	C	425	DG	C6-N1-C2	-9.14	119.62	125.10
1	B	406	DC	N3-C2-O2	9.12	128.29	121.90
2	C	432	DC	N3-C2-O2	9.11	128.27	121.90
1	B	411	DT	C4-C5-C6	9.03	123.42	118.00
2	C	422	DC	N3-C2-O2	8.89	128.12	121.90
2	C	429	DA	O4'-C1'-N9	-8.85	101.81	108.00
2	C	425	DG	N3-C4-N9	8.82	131.29	126.00
1	B	412	DG	N9-C4-C5	8.79	108.92	105.40
2	C	428	DG	C2-N3-C4	8.79	116.29	111.90
2	C	428	DG	C5-N7-C8	-8.78	99.91	104.30
3	A	169	TYR	CB-CG-CD1	8.66	126.20	121.00
1	B	409	DC	N3-C4-N4	8.57	124.00	118.00
1	B	405	DT	C2-N3-C4	-8.41	122.15	127.20
1	B	410	DC	N1-C2-N3	-8.38	113.33	119.20
3	A	142	ARG	NE-CZ-NH1	8.36	124.48	120.30
3	A	252	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	410	DC	N3-C4-N4	8.33	123.83	118.00
3	A	65	TYR	CB-CG-CD1	8.30	125.98	121.00
1	B	411	DT	C5-C6-N1	-8.24	118.76	123.70
2	C	428	DG	C6-N1-C2	-8.12	120.22	125.10
2	C	426	DA	O4'-C4'-C3'	-8.12	101.13	106.00
1	B	411	DT	N1-C2-N3	7.99	119.39	114.60
3	A	169	TYR	CG-CD1-CE1	7.92	127.64	121.30
3	A	239	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	410	DC	P-O3'-C3'	7.87	129.15	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	425	DG	C5-C6-O6	-7.82	123.91	128.60
2	C	429	DA	C5-C6-N1	-7.74	113.83	117.70
2	C	428	DG	O4'-C1'-N9	-7.72	102.60	108.00
2	C	422	DC	C6-N1-C1'	7.59	129.91	120.80
2	C	429	DA	O4'-C1'-C2'	-7.57	99.85	105.90
2	C	422	DC	C1'-O4'-C4'	-7.56	102.54	110.10
1	B	408	DT	N3-C2-O2	-7.54	117.78	122.30
1	B	411	DT	O4'-C1'-N1	7.48	113.23	108.00
2	C	422	DC	C4'-C3'-C2'	-7.43	96.42	103.10
1	B	408	DT	C2-N3-C4	-7.38	122.77	127.20
2	C	431	DG	C8-N9-C1'	7.28	136.46	127.00
1	B	409	DC	N1-C2-N3	-7.26	114.12	119.20
1	B	407	DA	O4'-C1'-N9	7.22	113.06	108.00
2	C	424	DG	C8-N9-C1'	7.21	136.37	127.00
2	C	426	DA	C5-C6-N1	-7.00	114.20	117.70
1	B	405	DT	C4-C5-C6	6.97	122.18	118.00
2	C	423	DA	C5-C6-N1	-6.97	114.22	117.70
1	B	408	DT	O4'-C1'-N1	-6.93	103.15	108.00
3	A	252	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	409	DC	O4'-C1'-N1	-6.91	103.17	108.00
3	A	183	ASN	O-C-N	-6.82	111.79	122.70
1	B	411	DT	N3-C2-O2	-6.79	118.22	122.30
2	C	423	DA	C6-N1-C2	6.73	122.64	118.60
2	C	422	DC	C2-N1-C1'	-6.67	111.46	118.80
2	C	428	DG	C5-C6-O6	-6.62	124.63	128.60
3	A	71	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	C	426	DA	C4-C5-C6	6.56	120.28	117.00
2	C	432	DC	N1-C2-N3	-6.45	114.69	119.20
1	B	406	DC	N1-C2-N3	-6.41	114.71	119.20
1	B	407	DA	C5-N7-C8	6.34	107.07	103.90
1	B	405	DT	C5-C6-N1	-6.33	119.90	123.70
1	B	409	DC	N1-C2-O2	-6.30	115.12	118.90
2	C	432	DC	N3-C4-N4	6.28	122.39	118.00
1	B	406	DC	N3-C4-N4	6.25	122.37	118.00
3	A	142	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	C	428	DG	N3-C4-N9	6.21	129.72	126.00
2	C	423	DA	C4'-C3'-C2'	-6.18	97.54	103.10
1	B	408	DT	P-O3'-C3'	6.07	126.98	119.70
2	C	429	DA	C1'-O4'-C4'	-6.05	104.05	110.10
2	C	422	DC	C5-C4-N4	6.05	124.44	120.20
1	B	407	DA	C4-C5-C6	6.05	120.02	117.00
3	A	124[A]	ARG	CD-NE-CZ	6.03	132.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	124[B]	ARG	CD-NE-CZ	6.03	132.05	123.60
2	C	425	DG	O4'-C1'-N9	-5.94	103.84	108.00
3	A	82	GLU	OE1-CD-OE2	5.90	130.38	123.30
2	C	425	DG	N9-C4-C5	5.88	107.75	105.40
1	B	409	DC	OP2-P-O3'	5.87	118.11	105.20
2	C	431	DG	O3'-P-O5'	-5.86	92.87	104.00
2	C	425	DG	C8-N9-C1'	5.84	134.59	127.00
2	C	423	DA	O4'-C4'-C3'	-5.81	102.17	104.50
2	C	422	DC	N1-C2-O2	-5.78	115.43	118.90
1	B	412	DG	N1-C6-O6	-5.74	116.46	119.90
3	A	124[A]	ARG	NE-CZ-NH2	-5.57	117.52	120.30
3	A	124[B]	ARG	NE-CZ-NH2	-5.57	117.52	120.30
3	A	50	ARG	NE-CZ-NH2	5.56	123.08	120.30
2	C	423	DA	N1-C2-N3	-5.51	126.55	129.30
3	A	87	ARG	NE-CZ-NH2	-5.49	117.55	120.30
3	A	7	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	C	430	DA	C4-C5-C6	5.31	119.65	117.00
2	C	431	DG	OP2-P-O3'	-5.28	93.59	105.20
1	B	410	DC	OP2-P-O3'	5.27	116.80	105.20
2	C	430	DA	P-O5'-C5'	-5.24	112.52	120.90
3	A	212[A]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
3	A	212[B]	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	C	423	DA	C5-C6-N6	5.21	127.87	123.70
2	C	431	DG	N1-C2-N3	5.21	127.03	123.90
2	C	426	DA	C6-C5-N7	-5.16	128.69	132.30
2	C	429	DA	C8-N9-C4	5.11	107.84	105.80
2	C	423	DA	OP1-P-O3'	5.05	116.32	105.20
1	B	405	DT	P-O5'-C5'	-5.05	112.82	120.90
3	A	147	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	A	232	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	407	DA	N7-C8-N9	-5.04	111.28	113.80
2	C	431	DG	O4'-C1'-C2'	5.02	109.92	105.90

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	B	160	0	92	5	0
2	C	221	0	119	5	0
3	A	2080	0	2078	14	0
4	A	1	0	0	0	0
5	A	15	0	0	0	0
6	A	364	0	0	7	0
6	B	14	0	0	1	0
6	C	19	0	0	0	0
All	All	2874	0	2289	24	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 5.

All (24) 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:C:431:DG:H2''	2:C:432:DC:H5''	1.24	1.17
3:A:211:THR:HA	3:A:214:GLN:HG3	1.67	0.75
2:C:431:DG:C2'	2:C:432:DC:H5''	2.11	0.72
1:B:411:DT:H2''	1:B:412:DG:O5'	1.96	0.65
1:B:410:DC:H1'	1:B:411:DT:H5'	1.78	0.64
3:A:199:HIS:HE1	6:A:688:HOH:O	1.82	0.62
2:C:431:DG:H2''	2:C:432:DC:C5'	2.16	0.60
3:A:262:HIS:HD2	6:A:664:HOH:O	1.83	0.59
3:A:211:THR:CA	3:A:214:GLN:HG3	2.35	0.56
3:A:246:LYS:HE2	6:A:840:HOH:O	2.04	0.56
3:A:188:ASP:HB2	6:A:797:HOH:O	2.05	0.56
3:A:262:HIS:HE1	6:A:670:HOH:O	1.90	0.53
1:B:407:DA:H8	6:B:962:HOH:O	1.92	0.53
3:A:46[B]:HIS:HD2	6:A:830:HOH:O	1.93	0.51
2:C:422:DC:H1'	2:C:423:DA:N7	2.27	0.50
2:C:422:DC:H2'	2:C:422:DC:O5'	2.14	0.48
1:B:409:DC:H2''	1:B:410:DC:O5'	2.14	0.48
3:A:172:VAL:CG1	3:A:229:VAL:HG23	2.44	0.47
3:A:199:HIS:HD2	3:A:203:GLU:OE2	1.99	0.44
1:B:410:DC:H2'	1:B:410:DC:H6	1.56	0.42
3:A:84[B]:GLN:HG2	3:A:85:THR:N	2.34	0.41
3:A:124[B]:ARG:HD2	3:A:124[B]:ARG:HH11	1.74	0.40
3:A:124[B]:ARG:NH2	6:A:821:HOH:O	2.54	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	258/262 (98%)	252 (98%)	6 (2%)	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	227/226 (100%)	222 (98%)	5 (2%)	57	20

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

Mol	Chain	Res	Type
3	A	69	GLN
3	A	84[A]	GLN
3	A	84[B]	GLN
3	A	169	TYR
3	A	214	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	12	ASN
3	A	68	ASN
3	A	133	ASN

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Mol	Chain	Res	Type
3	A	199	HIS
3	A	262	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
5	SO4	A	551	-	4,4,4	0.29	0	6,6,6	0.69	0
5	SO4	A	552	-	4,4,4	0.26	0	6,6,6	0.34	0
5	SO4	A	553	-	4,4,4	0.22	0	6,6,6	0.37	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
5	SO4	A	551	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	552	-	-	0/0/0/0	0/0/0/0
5	SO4	A	553	-	-	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.

No monomer is involved in short contacts.

## 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.