



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 11:39 PM EDT

PDB ID : 2XGQ  
Title : Structure of yeast DNA polymerase eta in complex with C8-N-acetyl-2-aminoanthracene containing DNA  
Authors : Schneider, S.; Schorr, S.; Carell, T.  
Deposited on : unknown  
Resolution : 2.70 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) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

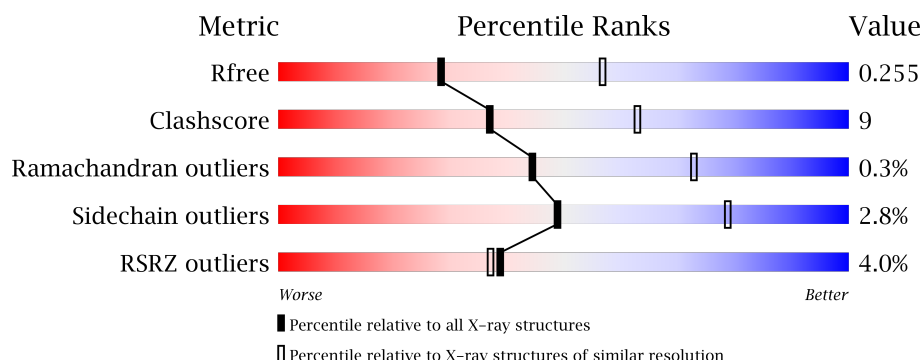
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	536	<div> <div>2%</div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div>
1	B	536	<div> <div>5%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
2	P	9	<div> <div>11%</div> <div>33%</div> <div>44%</div> <div>22%</div> </div>
2	Q	9	<div> <div>11%</div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
3	T	11	<div> <div>9%</div> <div>64%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
3	U	11	

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
3	8AG	T	5	X	-	-	-
3	8AG	U	5	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9079 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 protein called DNA POLYMERASE ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	47	1	1
			4064	2588	687	765	24			
1	B	512	Total	C	N	O	S	86	3	1
			4079	2598	689	767	25			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q04049
A	-21	ALA	-	expression tag	UNP Q04049
A	-20	SER	-	expression tag	UNP Q04049
A	-19	TRP	-	expression tag	UNP Q04049
A	-18	SER	-	expression tag	UNP Q04049
A	-17	HIS	-	expression tag	UNP Q04049
A	-16	PRO	-	expression tag	UNP Q04049
A	-15	GLN	-	expression tag	UNP Q04049
A	-14	PHE	-	expression tag	UNP Q04049
A	-13	GLU	-	expression tag	UNP Q04049
A	-12	LYS	-	expression tag	UNP Q04049
A	-11	GLY	-	expression tag	UNP Q04049
A	-10	ALA	-	expression tag	UNP Q04049
A	-9	SER	-	expression tag	UNP Q04049
A	-8	THR	-	expression tag	UNP Q04049
A	-7	SER	-	expression tag	UNP Q04049
A	-6	LEU	-	expression tag	UNP Q04049
A	-5	TYR	-	expression tag	UNP Q04049
A	-4	LYS	-	expression tag	UNP Q04049
A	-3	LYS	-	expression tag	UNP Q04049
A	-2	ALA	-	expression tag	UNP Q04049
A	-1	GLY	-	expression tag	UNP Q04049
A	0	ARG	-	expression tag	UNP Q04049
B	-22	MET	-	expression tag	UNP Q04049
B	-21	ALA	-	expression tag	UNP Q04049

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP Q04049
B	-19	TRP	-	expression tag	UNP Q04049
B	-18	SER	-	expression tag	UNP Q04049
B	-17	HIS	-	expression tag	UNP Q04049
B	-16	PRO	-	expression tag	UNP Q04049
B	-15	GLN	-	expression tag	UNP Q04049
B	-14	PHE	-	expression tag	UNP Q04049
B	-13	GLU	-	expression tag	UNP Q04049
B	-12	LYS	-	expression tag	UNP Q04049
B	-11	GLY	-	expression tag	UNP Q04049
B	-10	ALA	-	expression tag	UNP Q04049
B	-9	SER	-	expression tag	UNP Q04049
B	-8	THR	-	expression tag	UNP Q04049
B	-7	SER	-	expression tag	UNP Q04049
B	-6	LEU	-	expression tag	UNP Q04049
B	-5	TYR	-	expression tag	UNP Q04049
B	-4	LYS	-	expression tag	UNP Q04049
B	-3	LYS	-	expression tag	UNP Q04049
B	-2	ALA	-	expression tag	UNP Q04049
B	-1	GLY	-	expression tag	UNP Q04049
B	0	ARG	-	expression tag	UNP Q04049

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	9	Total	C	N	O	P	0	0	0
			188	90	39	51	8			
2	Q	9	Total	C	N	O	P	0	0	0
			188	90	39	51	8			

- Molecule 3 is a DNA chain called 5'-D(\*CP\*8AG\*CP\*TP\*CP\*AP\*TP\*CP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	11	Total	C	N	O	P	0	0	0
			233	120	38	65	10			
3	U	10	Total	C	N	O	P	0	0	0
			217	111	35	61	10			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total 4	Ca 4	0	0
4	A	3	Total 3	Ca 3	0	0

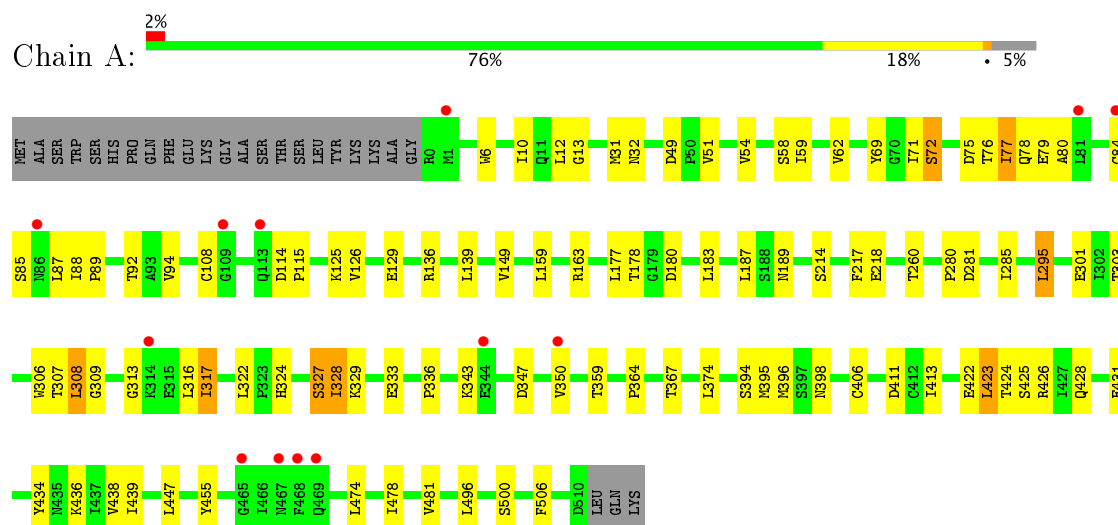
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total 45	O 45	0	0
5	B	54	Total 54	O 54	0	0
5	P	1	Total 1	O 1	0	0
5	Q	1	Total 1	O 1	0	0
5	T	2	Total 2	O 2	0	0

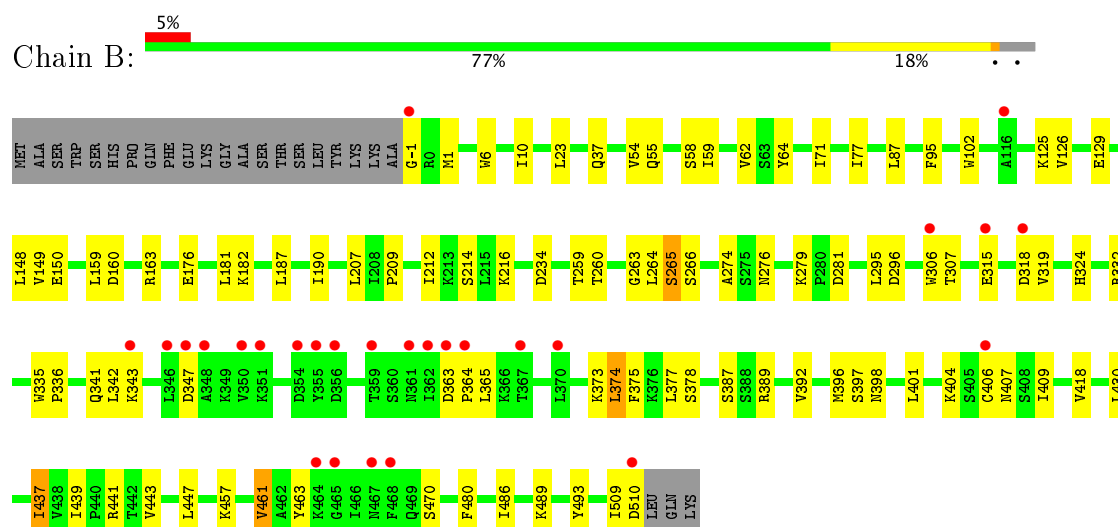
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: DNA POLYMERASE ETA



#### • Molecule 1: DNA POLYMERASE ETA

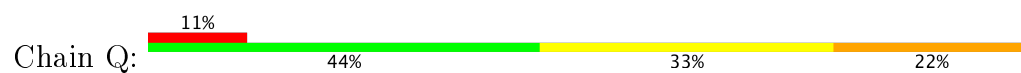


#### • Molecule 2: 5'-D(\*GP\*TP\*GP\*GP\*AP\*TP\*GP\*AP\*G)-3'

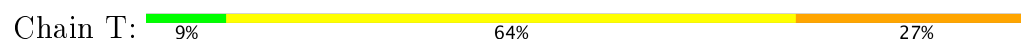




- Molecule 2: 5'-D(\*GP\*TP\*GP\*GP\*AP\*TP\*GP\*AP\*G)-3'



- Molecule 3: 5'-D(\*CP\*8AG\*CP\*TP\*CP\*AP\*TP\*CP\*CP\*AP\*C)-3'



- Molecule 3: 5'-D(\*CP\*8AG\*CP\*TP\*CP\*AP\*TP\*CP\*CP\*AP\*C)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.53Å 103.53Å 292.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 2.70 46.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.30-2.70) 99.6 (46.30-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.217 , 0.264 0.221 , 0.255	Depositor DCC
$R_{free}$ test set	2233 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 8AG

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	A	0.63	1/4145 (0.0%)	0.64	0/5589
1	B	0.62	0/4166	0.67	0/5616
2	P	2.38	2/212 (0.9%)	1.97	11/327 (3.4%)
2	Q	0.67	0/212	1.46	4/327 (1.2%)
3	T	2.26	1/213 (0.5%)	1.86	9/322 (2.8%)
3	U	1.11	0/196	1.63	4/298 (1.3%)
All	All	0.80	4/9144 (0.0%)	0.84	28/12479 (0.2%)

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
3	T	1	0
3	U	1	0
All	All	2	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	8	DG	C3'-O3'	-6.39	1.35	1.44
3	T	13	DA	C3'-O3'	-5.20	1.37	1.44
2	P	7	DG	C6-N1	-5.10	1.35	1.39
1	A	108	CYS	CB-SG	5.05	1.90	1.82

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	6	DC	O4'-C4'-C3'	-10.29	99.82	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	7	DG	O4'-C1'-N9	-9.95	101.04	108.00
3	U	14	DC	O4'-C4'-C3'	-8.85	100.69	106.00
2	P	6	DT	O4'-C1'-C2'	-8.25	99.30	105.90
3	T	14	DC	O4'-C4'-C3'	-7.31	101.58	104.50
2	Q	10	DT	O4'-C4'-C3'	-7.00	101.70	104.50
3	T	4	DC	C6-N1-C2	-6.90	117.54	120.30
2	Q	12	DA	O4'-C4'-C3'	-6.34	101.96	104.50
2	P	5	DG	O4'-C1'-C2'	-6.32	100.84	105.90
2	Q	11	DG	O4'-C1'-N9	6.27	112.39	108.00
3	T	6	DC	C4'-C3'-C2'	-6.25	97.47	103.10
3	T	9	DA	P-O3'-C3'	6.22	127.17	119.70
3	U	7	DT	N3-C4-O4	6.22	123.63	119.90
2	P	8	DG	O4'-C1'-N9	6.20	112.34	108.00
2	P	10	DT	C1'-O4'-C4'	-6.12	103.98	110.10
2	P	11	DG	O4'-C1'-C2'	-6.04	101.07	105.90
2	P	10	DT	O4'-C4'-C3'	-6.03	102.09	104.50
3	T	11	DC	O4'-C1'-N1	-5.95	103.83	108.00
3	T	14	DC	C1'-O4'-C4'	-5.84	104.26	110.10
2	P	7	DG	N1-C6-O6	-5.77	116.44	119.90
2	P	7	DG	C5-C6-O6	5.70	132.02	128.60
2	P	6	DT	C1'-O4'-C4'	-5.64	104.46	110.10
3	T	4	DC	N1-C1'-C2'	5.59	123.22	112.60
2	Q	7	DG	O4'-C1'-N9	-5.56	104.11	108.00
2	P	10	DT	N3-C4-O4	5.48	123.19	119.90
3	T	12	DC	O4'-C1'-N1	5.20	111.64	108.00
3	U	7	DT	C5-C4-O4	-5.13	121.31	124.90
3	T	7	DT	O4'-C1'-C2'	-5.12	101.81	105.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	T	5	8AG	C8
3	U	5	8AG	C8

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	A	4064	0	4115	68	0
1	B	4079	0	4134	68	0
2	P	188	0	101	1	0
2	Q	188	0	101	5	0
3	T	233	0	137	7	0
3	U	217	0	125	8	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
5	A	45	0	0	2	0
5	B	54	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	T	2	0	0	0	0
All	All	9079	0	8713	154	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 9.

All (154) 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)
1:B:404:LYS:HB3	1:B:407:ASN:OD1	1.19	1.35
1:A:125:LYS:NZ	1:A:398:ASN:O	1.64	1.27
1:B:276:ASN:OD1	1:B:279:LYS:NZ	1.76	1.17
1:B:176:GLU:HB3	1:B:182:LYS:HG2	1.35	1.06
2:Q:12:DA:C8	2:Q:12:DA:H5'	1.90	1.06
2:Q:12:DA:H8	2:Q:12:DA:H5'	1.21	1.03
1:B:404:LYS:CB	1:B:407:ASN:OD1	2.08	1.01
1:A:78:GLN:HA	1:A:78:GLN:OE1	1.71	0.88
1:A:333:GLU:O	1:A:336:PRO:HD3	1.86	0.76
3:T:4:DC:H2''	3:T:5:8AG:O2P	1.83	0.76
1:A:307:THR:O	1:A:307:THR:HG22	1.86	0.76
1:A:424:THR:O	1:A:428:GLN:HG2	1.85	0.75
3:U:6:DC:H2'	3:U:7:DT:C6	2.24	0.73
1:B:363:ASP:OD1	1:B:365:LEU:N	2.23	0.72
1:B:37:GLN:HE22	1:B:259:THR:H	1.38	0.72
2:P:6:DT:H2''	2:P:7:DG:N7	2.07	0.69
2:Q:12:DA:H2''	2:Q:13:DG:O5'	1.92	0.69
1:B:176:GLU:HB3	1:B:182:LYS:CG	2.18	0.68
1:B:125:LYS:HE2	1:B:398:ASN:O	1.93	0.68
1:A:76:THR:HG22	1:A:78:GLN:H	1.59	0.68
1:A:129:GLU:OE1	1:A:425:SER:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:O	1:A:75:ASP:HB2	1.94	0.67
1:B:437:ILE:HG22	1:B:510:ASP:N	2.09	0.67
1:B:58:SER:HB2	3:U:5:8AG:C45	2.25	0.66
1:B:489:LYS:HA	1:B:489:LYS:HE3	1.78	0.65
1:A:398:ASN:HD22	1:A:500:SER:HB3	1.64	0.62
3:U:5:8AG:H452	3:U:5:8AG:H31	1.81	0.62
1:B:401:LEU:HD13	1:B:406:CYS:HB2	1.82	0.61
1:B:209:PRO:O	1:B:212:ILE:HG22	2.00	0.61
1:B:363:ASP:C	1:B:363:ASP:OD1	2.39	0.61
1:A:94:VAL:HG12	1:A:126:VAL:HA	1.82	0.60
3:T:5:8AG:H2'1	3:T:6:DC:H5''	1.84	0.60
1:B:375:PHE:O	1:B:378:SER:OG	2.19	0.60
1:A:308:LEU:O	1:A:313:GLY:HA3	2.02	0.59
1:A:183:LEU:HD22	1:A:187:LEU:HD12	1.84	0.59
1:B:315:GLU:O	1:B:319:VAL:HG23	2.05	0.57
1:A:307:THR:CG2	1:A:307:THR:O	2.52	0.57
1:A:54:VAL:O	1:A:92:THR:HG23	2.04	0.57
3:U:5:8AG:N3	3:U:5:8AG:H2'2	2.20	0.57
1:A:177:LEU:HD23	1:A:214:SER:HB2	1.86	0.56
3:U:5:8AG:H2'1	3:U:6:DC:C6	2.40	0.56
1:B:396:MET:HG2	1:B:397:SER:N	2.19	0.56
3:U:5:8AG:C45	3:U:5:8AG:C31	2.85	0.55
1:B:-1:GLY:O	1:B:207:LEU:HD11	2.07	0.55
1:A:350:VAL:HG21	1:A:364:PRO:HB3	1.89	0.55
3:T:4:DC:HO5'	3:T:4:DC:H6	1.55	0.55
1:B:149:VAL:HG22	1:B:159:LEU:CD2	2.37	0.54
1:B:489:LYS:HE3	1:B:489:LYS:CA	2.36	0.54
1:A:317:ILE:HA	1:A:322:LEU:HD12	1.89	0.54
1:B:176:GLU:HA	1:B:182:LYS:HA	1.88	0.54
1:B:306:TRP:CZ3	2:Q:12:DA:H4'	2.43	0.53
1:B:181:LEU:HD12	1:B:182:LYS:H	1.72	0.53
1:A:189:ASN:HB3	5:A:2021:HOH:O	2.08	0.53
1:B:149:VAL:HG22	1:B:159:LEU:HD22	1.91	0.53
1:A:149:VAL:HG22	1:A:159:LEU:HD22	1.90	0.53
1:A:306:TRP:O	1:A:307:THR:HB	2.09	0.53
3:U:5:8AG:H452	3:U:5:8AG:C31	2.39	0.52
1:B:55:GLN:HG3	1:B:126:VAL:HG21	1.92	0.51
1:B:389:ARG:HG2	1:B:389:ARG:HH11	1.74	0.51
1:A:32:ASN:ND2	5:A:2002:HOH:O	1.96	0.51
1:B:437:ILE:O	1:B:437:ILE:CG2	2.54	0.51
1:A:13:GLY:O	1:A:163[A]:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ILE:O	1:B:489:LYS:HG2	2.10	0.50
1:A:58:SER:HB3	3:T:5:8AG:H452	1.92	0.50
1:B:176:GLU:HB2	1:B:181:LEU:O	2.11	0.50
1:B:363:ASP:OD1	1:B:364:PRO:N	2.44	0.50
1:A:301:GLU:OE1	1:A:327:SER:OG	2.29	0.50
1:B:148:LEU:HB3	1:B:160:ASP:HB3	1.93	0.49
1:A:406:CYS:HA	1:A:411:ASP:HB3	1.93	0.49
1:B:23:LEU:HD23	1:B:234:ASP:HA	1.94	0.49
1:A:6:TRP:O	1:A:10:ILE:HG12	2.13	0.49
1:B:1:MET:C	1:B:207:LEU:HD23	2.33	0.49
1:A:31:MET:HG2	1:A:260:THR:HG22	1.95	0.49
1:A:78:GLN:CA	1:A:78:GLN:OE1	2.50	0.49
1:A:396:MET:O	1:A:426:ARG:NH2	2.45	0.49
1:B:176:GLU:CB	1:B:182:LYS:HG2	2.25	0.48
1:A:413:ILE:HG23	1:A:478:ILE:HD11	1.95	0.48
1:A:69:TYR:CD1	1:A:84:CYS:SG	3.06	0.48
1:A:51:VAL:HA	1:A:88:ILE:O	2.13	0.48
1:A:303:THR:O	1:A:309:GLY:HA2	2.13	0.48
1:A:439:ILE:O	1:A:506:PHE:HA	2.14	0.47
1:B:343:LYS:O	1:B:347:ASP:OD1	2.31	0.47
1:A:114:ASP:C	1:A:114:ASP:OD1	2.52	0.47
1:A:71:ILE:CD1	1:A:87:LEU:HD13	2.44	0.47
1:B:401:LEU:HD13	1:B:406:CYS:CB	2.43	0.47
2:Q:11:DG:H2"	2:Q:12:DA:H5"	1.97	0.47
1:A:306:TRP:CE3	1:A:306:TRP:HA	2.49	0.47
3:T:4:DC:C2'	3:T:5:8AG:O2P	2.59	0.46
1:B:276:ASN:HA	1:B:279:LYS:HE3	1.97	0.46
1:A:406:CYS:SG	1:A:496:LEU:HD12	2.55	0.46
1:B:443:VAL:HG23	1:B:461:VAL:HG12	1.96	0.46
1:A:84:CYS:O	1:A:85:SER:HB2	2.15	0.46
1:A:347:ASP:O	1:A:350:VAL:HG12	2.15	0.46
1:B:437:ILE:HG22	1:B:437:ILE:O	2.16	0.45
1:A:76:THR:HG22	1:A:77:ILE:N	2.31	0.45
1:B:457:LYS:HG2	1:B:480:PHE:CG	2.51	0.45
1:B:64:TYR:OH	1:B:279:LYS:HD3	2.17	0.45
1:A:114:ASP:OD1	1:A:115:PRO:N	2.50	0.45
1:A:59:ILE:HG21	1:A:62:VAL:HG22	1.98	0.45
1:B:336:PRO:HD2	1:B:341:GLN:OE1	2.16	0.45
1:B:187:LEU:O	1:B:190:ILE:HG22	2.18	0.44
1:B:374:LEU:HD13	1:B:374:LEU:N	2.32	0.44
1:B:392:VAL:HG21	1:B:430:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG21	1:B:62:VAL:HG22	2.00	0.44
1:A:136:ARG:NH1	1:A:139:LEU:HD22	2.32	0.44
1:A:406:CYS:SG	1:A:406:CYS:O	2.75	0.44
1:A:343:LYS:HE3	1:A:367:THR:OG1	2.17	0.44
1:A:49:ASP:HB3	1:A:88:ILE:HD12	2.00	0.44
3:U:5:8AG:C36	3:U:6:DC:H4'	2.48	0.44
1:A:306:TRP:HE3	1:A:306:TRP:HA	1.83	0.44
1:A:76:THR:HB	1:A:79:GLU:HG3	1.98	0.44
1:A:217:PHE:HD2	1:A:285:ILE:HD13	1.83	0.43
1:A:474:LEU:HD23	1:A:474:LEU:C	2.39	0.43
1:B:263:GLY:HA3	1:B:274:ALA:HB3	2.00	0.43
1:B:447:LEU:HD12	1:B:447:LEU:C	2.39	0.43
1:A:434:TYR:O	1:A:436:LYS:HG3	2.18	0.43
1:A:59:ILE:HD11	1:A:80:ALA:HB2	2.00	0.43
1:A:71:ILE:CD1	1:A:87:LEU:CD1	2.96	0.43
3:T:5:8AG:H2'1	3:T:6:DC:C5'	2.48	0.43
1:A:447:LEU:HD11	1:A:455:TYR:HB2	1.99	0.43
1:A:280:PRO:O	1:A:281:ASP:C	2.56	0.43
1:A:329:LYS:HE2	1:A:333:GLU:OE1	2.19	0.43
1:B:187:LEU:HD21	1:B:212:ILE:HD13	2.00	0.42
1:B:296:ASP:OD2	1:B:332:ARG:NH2	2.48	0.42
1:B:437:ILE:CG2	1:B:509:ILE:HG13	2.49	0.42
1:B:102:TRP:NE1	1:B:129:GLU:OE2	2.36	0.42
1:B:181:LEU:HD12	1:B:182:LYS:N	2.34	0.42
1:B:374:LEU:N	1:B:374:LEU:CD1	2.82	0.42
1:B:373:LYS:O	1:B:377:LEU:HB2	2.19	0.42
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.90	0.42
1:A:76:THR:HG22	1:A:78:GLN:N	2.31	0.42
1:B:6:TRP:O	1:B:10:ILE:HG12	2.19	0.42
1:B:54:VAL:HG11	1:B:77:ILE:CD1	2.50	0.42
1:B:335:TRP:CE2	1:B:342:LEU:HD13	2.54	0.42
1:B:443:VAL:HG23	1:B:461:VAL:CG1	2.50	0.41
1:A:49:ASP:HB3	1:A:88:ILE:CD1	2.50	0.41
3:T:10:DT:H2''	3:T:11:DC:C6	2.56	0.41
1:B:437:ILE:HG22	1:B:509:ILE:CG1	2.51	0.41
1:A:149:VAL:HG22	1:A:159:LEU:CD2	2.50	0.41
1:B:260:THR:O	1:B:281:ASP:HA	2.20	0.41
1:B:318:ASP:C	1:B:318:ASP:OD1	2.59	0.41
1:B:439:ILE:HD11	1:B:463:TYR:CD2	2.55	0.41
1:A:328:ILE:HG13	1:A:328:ILE:O	2.18	0.41
1:A:178:THR:C	1:A:180:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:MET:HE3	1:A:506:PHE:CE1	2.56	0.41
1:B:95:PHE:CG	1:B:418:VAL:HG13	2.56	0.41
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.93	0.40
1:A:316:LEU:O	1:A:317:ILE:C	2.60	0.40
1:B:214:SER:O	1:B:216:LYS:NZ	2.53	0.40
1:B:71:ILE:CD1	1:B:87:LEU:HD13	2.50	0.40
1:A:218:GLU:O	1:A:285:ILE:HD11	2.21	0.40
1:A:431:GLU:HG2	1:A:438:VAL:HG23	2.03	0.40
1:B:150:GLU:HG3	1:B:387:SER:O	2.21	0.40
1:B:265:SER:OG	1:B:266:SER:N	2.52	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	
1	A	510/536 (95%)	492 (96%)	16 (3%)	2 (0%)	38	66
1	B	513/536 (96%)	504 (98%)	8 (2%)	1 (0%)	51	79
All	All	1023/1072 (95%)	996 (97%)	24 (2%)	3 (0%)	44	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	PRO
1	B	493	TYR
1	A	317	ILE



### 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	
1	A	458/478 (96%)	444 (97%)	14 (3%)	45	75
1	B	460/478 (96%)	448 (97%)	12 (3%)	51	81
All	All	918/956 (96%)	892 (97%)	26 (3%)	49	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	72	SER
1	A	77	ILE
1	A	295	LEU
1	A	308	LEU
1	A	324	HIS
1	A	327	SER
1	A	328	ILE
1	A	359	THR
1	A	374	LEU
1	A	394	SER
1	A	422	GLU
1	A	423	LEU
1	A	481	VAL
1	B	163	ARG
1	B	264	LEU
1	B	265	SER
1	B	295	LEU
1	B	307	THR
1	B	324	HIS
1	B	374	LEU
1	B	409	ILE
1	B	437	ILE
1	B	441	ARG
1	B	461	VAL
1	B	470	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	361	ASN
1	A	398	ASN
1	A	400	ASN
1	B	37	GLN
1	B	40	GLN
1	B	57	ASN
1	B	202	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
3	8AG	T	5	3	40,45,46	2.15	5 (12%)	51,67,70	1.59	6 (11%)
3	8AG	U	5	3	40,45,46	2.11	5 (12%)	51,67,70	1.54	10 (19%)

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
3	8AG	T	5	3	1/1/8/9	0/15/45/46	0/6/6/6
3	8AG	U	5	3	1/1/8/9	0/15/45/46	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	8AG	C8-N9	-7.67	1.32	1.47
3	U	5	8AG	C8-N9	-7.36	1.33	1.47
3	T	5	8AG	C34-C35	2.33	1.47	1.42
3	U	5	8AG	C34-C35	2.35	1.47	1.42
3	U	5	8AG	O6-C6	4.25	1.35	1.24
3	T	5	8AG	O6-C6	4.39	1.35	1.24
3	U	5	8AG	C6-C5	5.23	1.47	1.41
3	T	5	8AG	C6-C5	5.82	1.48	1.41
3	U	5	8AG	C2-N2	6.75	1.47	1.34
3	T	5	8AG	C2-N2	6.76	1.47	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8AG	C2'-C1'-N9	-6.18	107.24	115.59
3	T	5	8AG	C5-N7-C8	-4.39	102.97	108.90
3	U	5	8AG	C5-N7-C8	-3.98	103.52	108.90
3	U	5	8AG	C33-C32-N29	-3.27	116.28	119.40
3	U	5	8AG	C2'-C1'-N9	-3.23	111.22	115.59
3	T	5	8AG	C32-N29-C30	-2.45	119.51	121.55
3	U	5	8AG	O4'-C1'-N9	-2.38	105.83	108.65
3	U	5	8AG	N1-C2-N3	-2.07	122.09	125.45
3	U	5	8AG	C40-C38-C37	-2.05	118.64	122.00
3	T	5	8AG	C2-N3-C4	2.39	120.67	113.95
3	U	5	8AG	C31-C32-N29	2.44	122.92	120.12
3	U	5	8AG	C2-N3-C4	2.55	121.11	113.95
3	T	5	8AG	N3-C4-N9	2.82	131.50	126.75
3	T	5	8AG	C6-N1-C2	3.22	120.69	116.06
3	U	5	8AG	N3-C4-N9	3.29	132.30	126.75
3	U	5	8AG	C6-N1-C2	3.37	120.91	116.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	U	5	8AG	C8
3	T	5	8AG	C8

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	8AG	5	0
3	U	5	8AG	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	510/536 (95%)	0.14	13 (2%) 58 58	21, 42, 80, 127	9 (1%)
1	B	512/536 (95%)	0.21	27 (5%) 27 25	24, 40, 85, 148	22 (4%)
2	P	9/9 (100%)	0.23	1 (11%) 6 5	47, 50, 55, 64	0
2	Q	9/9 (100%)	0.73	1 (11%) 6 5	56, 63, 92, 106	0
3	T	10/11 (90%)	0.08	0 100 100	44, 54, 61, 99	0
3	U	9/11 (81%)	0.38	0 100 100	52, 65, 79, 102	0
All	All	1059/1112 (95%)	0.18	42 (3%) 39 37	21, 42, 84, 148	31 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	ASP	5.6
1	B	510	ASP	5.3
1	A	113	GLN	4.4
1	B	346	LEU	4.0
1	B	355	TYR	3.9
1	B	-1	GLY	3.5
1	A	467	ASN	3.5
1	B	465	GLY	3.3
1	B	347	ASP	3.3
1	B	359	THR	3.2
1	A	469	GLN	3.1
1	B	362	ILE	3.0
1	B	364	PRO	2.9
1	A	109	GLY	2.9
1	B	318	ASP	2.9
1	A	84	CYS	2.9
1	B	351	LYS	2.8
1	B	348	ALA	2.8
1	B	343	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	354	ASP	2.7
1	A	468	PHE	2.7
1	B	467	ASN	2.6
1	A	465	GLY	2.6
1	B	468	PHE	2.5
1	B	367	THR	2.5
2	P	5	DG	2.4
1	A	344	GLU	2.4
1	B	464	LYS	2.4
1	A	350	VAL	2.4
1	B	363	ASP	2.3
1	B	350	VAL	2.2
1	B	315	GLU	2.2
1	A	81	LEU	2.2
1	A	1	MET	2.1
1	B	361	ASN	2.1
1	A	314	LYS	2.1
2	Q	13	DG	2.1
1	B	370	LEU	2.1
1	B	406	CYS	2.1
1	B	116	ALA	2.1
1	A	86	ASN	2.1
1	B	306	TRP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	8AG	U	5	40/41	0.74	0.27	-	100,109,133,139	0
3	8AG	T	5	40/41	0.92	0.18	-	50,66,93,96	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	B	600	1/1	0.93	0.14	-0.97	68,68,68,68	0
4	CA	B	602	1/1	0.82	0.09	-2.77	70,70,70,70	0
4	CA	A	602	1/1	0.90	0.07	-	66,66,66,66	0
4	CA	A	601	1/1	0.78	0.11	-	81,81,81,81	0
4	CA	B	601	1/1	0.80	0.16	-	81,81,81,81	0
4	CA	A	600	1/1	0.85	0.09	-	78,78,78,78	0
4	CA	B	603	1/1	0.93	0.06	-	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.