



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:07 am BST

PDB ID : 3EPI  
Title : Structure of Human DNA Polymerase Iota complexed with N2-ethylguanine and incoming TTP  
Authors : Pence, M.G.  
Deposited on : 2008-09-29  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

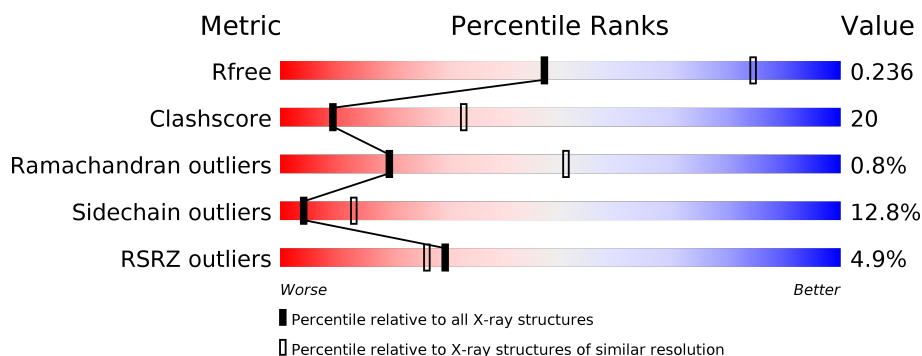
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	<div> <div>5%</div> <div>64%</div> <div>17%</div> <div>6%</div> <div>11%</div> </div>
2	B	18	<div> <div>33%</div> <div>6%</div> <div>61%</div> </div>
2	C	18	<div> <div>6%</div> <div>33%</div> <div>6%</div> <div>56%</div> </div>

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
2	DOC	B	13	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3290 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 iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2905	1832	507	545	21			

- Molecule 2 is a DNA chain called 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			142	67	29	39	7			
2	C	8	Total	C	N	O	P	0	0	0
			168	80	30	50	8			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

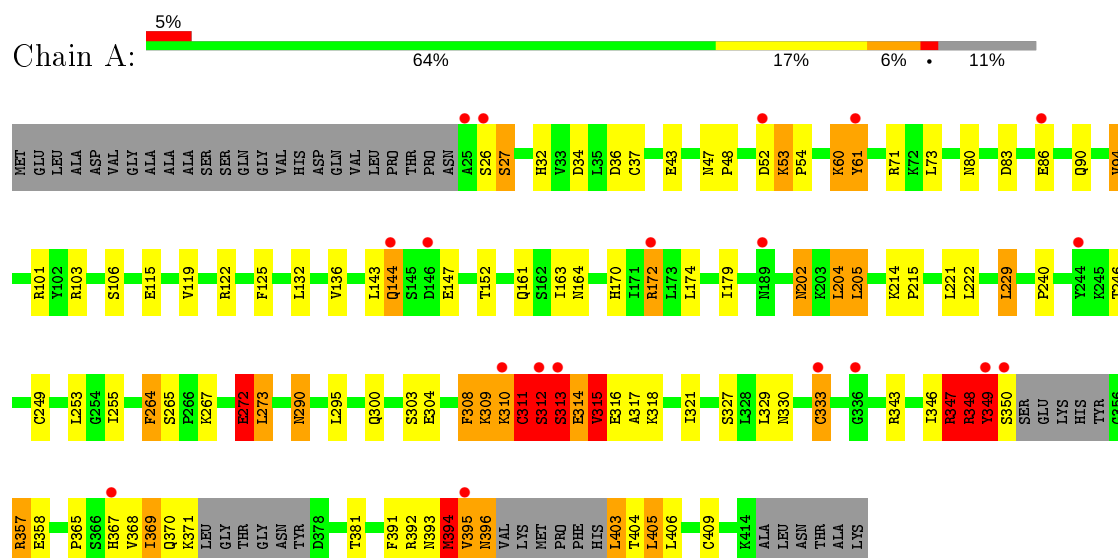
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	2	Total	O	0	0
			2	2		
5	C	5	Total	O	0	0
			5	5		

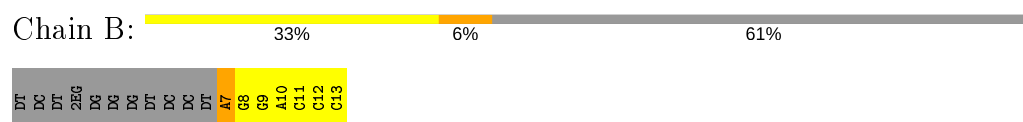
### 3 Residue-property plots [i](#)

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.

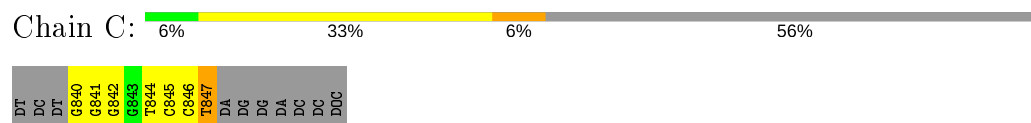
- Molecule 1: DNA polymerase iota



- Molecule 2: 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'



- Molecule 2: 5'-D(\*DTP\*DCP\*DTP\*(2EG)P\*DGP\*DGP\*DGP\*DTP\*DCP\*DCP\*DTP\*DAP\*DGP\*DGP\*DAP\*DCP\*DCP\*(DOC))-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.64Å 98.64Å 202.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (14.99-2.90) 99.9 (14.99-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.236 , 0.282 0.250 , 0.236	Depositor DCC
$R_{free}$ test set	667 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, 2EG, DOC

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	0.53	0/2944	0.76	3/3972 (0.1%)
2	B	1.65	6/139 (4.3%)	1.42	2/212 (0.9%)
2	C	1.60	8/160 (5.0%)	1.95	11/245 (4.5%)
All	All	0.71	14/3243 (0.4%)	0.91	16/4429 (0.4%)

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	A	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	846	DC	O3'-P	-7.86	1.51	1.61
2	C	847	DT	C2-O2	-7.46	1.16	1.22
2	B	7	DA	C6-N1	-6.54	1.30	1.35
2	B	7	DA	N3-C4	-6.36	1.31	1.34
2	C	847	DT	N3-C4	-6.34	1.33	1.38
2	C	847	DT	C2-N3	-5.62	1.33	1.37
2	C	847	DT	C3'-O3'	5.48	1.51	1.44
2	B	7	DA	C2-N3	-5.38	1.28	1.33
2	C	847	DT	P-OP1	-5.33	1.39	1.49
2	C	847	DT	C4-O4	-5.26	1.18	1.23
2	B	7	DA	N7-C5	-5.25	1.36	1.39
2	C	847	DT	C4-C5	-5.25	1.40	1.45
2	B	7	DA	C5-C4	-5.24	1.35	1.38
2	B	7	DA	P-O5'	-5.17	1.54	1.59



All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	DA	O4'-C1'-N9	12.37	116.66	108.00
2	C	847	DT	C6-C5-C7	9.99	128.89	122.90
2	C	847	DT	C4-C5-C7	-9.26	113.44	119.00
2	C	847	DT	O4'-C1'-N1	9.00	114.30	108.00
2	C	847	DT	C5-C4-O4	-8.37	119.04	124.90
2	C	847	DT	N1-C2-N3	7.50	119.10	114.60
2	C	847	DT	N3-C2-O2	-7.46	117.83	122.30
2	C	847	DT	C6-N1-C2	-7.43	117.58	121.30
2	C	847	DT	N3-C4-O4	6.68	123.91	119.90
2	C	846	DC	P-O3'-C3'	6.47	127.46	119.70
2	C	847	DT	C4'-C3'-O3'	6.29	125.44	109.70
2	C	847	DT	N1-C1'-C2'	6.21	124.39	112.60
1	A	348	ARG	N-CA-C	5.67	126.31	111.00
1	A	290	ASN	N-CA-CB	5.22	119.99	110.60
2	B	7	DA	N9-C4-C5	5.17	107.87	105.80
1	A	272	GLU	N-CA-CB	-5.10	101.42	110.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	LYS	Peptide
1	A	311	CYS	Peptide
1	A	312	SER	Peptide
1	A	313	SER	Peptide
1	A	314	GLU	Peptide
1	A	315	VAL	Peptide
1	A	316	GLU	Peptide
1	A	347	ARG	Peptide
1	A	348	ARG	Peptide
1	A	349	TYR	Peptide
1	A	370	GLN	Peptide
1	A	394	MET	Peptide
1	A	395	VAL	Peptide

## 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	2905	0	2955	89	0
2	B	142	0	78	19	5
2	C	168	0	95	23	5
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	62	0	0	1	0
5	B	2	0	0	0	0
5	C	5	0	0	2	0
All	All	3290	0	3128	122	5

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 20.

All (122) 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:A:403:LEU:N	1:A:403:LEU:HD13	1.56	1.14
1:A:349:TYR:CD1	1:A:350:SER:CB	2.30	1.13
2:C:840:2EG:H2'	2:C:841:DG:OP1	1.35	1.09
1:A:349:TYR:CG	1:A:350:SER:CB	2.41	1.04
2:B:11:DC:H2''	2:B:12:DC:H5'	1.39	1.03
1:A:315:VAL:HA	1:A:317:ALA:H	1.17	1.03
2:C:844:DT:C2'	2:C:845:DC:H5'	1.89	1.02
1:A:310:LYS:O	1:A:311:CYS:HB3	1.60	1.01
2:C:844:DT:H2''	2:C:845:DC:H5'	1.41	1.00
2:C:840:2EG:C2'	2:C:841:DG:OP1	2.01	0.99
2:C:841:DG:H1'	2:C:842:DG:O4'	1.62	0.99
1:A:403:LEU:N	1:A:403:LEU:CD1	2.30	0.95
1:A:369:ILE:O	1:A:371:LYS:HD2	1.67	0.94
2:B:13:DOC:C2	2:C:841:DG:H22	1.82	0.93
2:B:11:DC:C2'	2:B:12:DC:H5'	1.97	0.93
2:B:7:DA:N6	2:C:847:DT:O4	2.08	0.87
1:A:315:VAL:HA	1:A:317:ALA:N	1.93	0.84
1:A:310:LYS:NZ	1:A:310:LYS:HB2	1.95	0.81
2:C:840:2EG:H4'	2:C:841:DG:OP1	1.81	0.81
2:B:13:DOC:C4	2:C:841:DG:H1	1.95	0.80
1:A:346:ILE:O	1:A:357:ARG:HB2	1.82	0.80
2:C:841:DG:H2''	2:C:842:DG:O5'	1.83	0.78
1:A:314:GLU:O	1:A:315:VAL:HG23	1.83	0.77
1:A:369:ILE:O	1:A:371:LYS:CD	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:DG:H2''	2:B:9:DG:OP2	1.86	0.76
2:C:847:DT:H71	5:C:66:HOH:O	1.85	0.76
1:A:80:ASN:HB2	1:A:83:ASP:HB2	1.69	0.75
2:B:13:DOC:N3	2:C:841:DG:N2	2.34	0.75
1:A:310:LYS:HD3	1:A:311:CYS:N	2.03	0.74
1:A:310:LYS:O	1:A:311:CYS:CB	2.34	0.74
1:A:349:TYR:CB	1:A:350:SER:CB	2.68	0.71
1:A:202:ASN:ND2	1:A:205:LEU:H	1.88	0.71
1:A:52:ASP:O	1:A:53:LYS:HG2	1.90	0.71
1:A:144:GLN:HG3	1:A:147:GLU:HG2	1.74	0.69
1:A:396:ASN:C	1:A:396:ASN:OD1	2.30	0.69
1:A:106:SER:OG	1:A:122:ARG:NH2	2.23	0.69
2:C:840:2EG:C4'	2:C:841:DG:OP1	2.32	0.69
1:A:310:LYS:HD3	1:A:311:CYS:H	1.54	0.69
1:A:310:LYS:CD	1:A:311:CYS:N	2.58	0.66
1:A:52:ASP:O	1:A:52:ASP:OD2	2.14	0.65
2:B:7:DA:H2''	2:B:8:DG:OP2	1.96	0.65
1:A:313:SER:HA	1:A:314:GLU:HG3	1.78	0.64
1:A:347:ARG:HD3	1:A:404:THR:OG1	1.97	0.64
1:A:318:LYS:O	1:A:321:ILE:N	2.31	0.63
1:A:329:LEU:O	1:A:333:CYS:HB2	1.99	0.63
2:C:847:DT:C7	5:C:66:HOH:O	2.43	0.63
1:A:310:LYS:CG	1:A:311:CYS:N	2.63	0.62
2:C:844:DT:H2'	2:C:845:DC:H5'	1.81	0.62
1:A:365:PRO:HB2	1:A:368:VAL:HG22	1.82	0.62
1:A:308:PHE:O	1:A:309:LYS:HB3	1.99	0.61
2:B:8:DG:H1'	2:B:9:DG:H5'	1.82	0.61
1:A:349:TYR:HB2	1:A:350:SER:CB	2.30	0.61
1:A:43:GLU:OE2	1:A:101:ARG:NH2	2.34	0.60
1:A:310:LYS:HZ2	1:A:310:LYS:HB2	1.64	0.60
1:A:144:GLN:NE2	5:A:476:HOH:O	2.21	0.59
1:A:314:GLU:C	1:A:315:VAL:HG23	2.23	0.59
1:A:347:ARG:HD2	1:A:405:LEU:HB2	1.85	0.59
1:A:221:LEU:HD22	1:A:229:LEU:HD12	1.85	0.58
1:A:347:ARG:HG2	1:A:348:ARG:N	2.09	0.58
2:B:13:DOC:N3	2:C:841:DG:C2	2.71	0.58
1:A:348:ARG:NH1	1:A:358:GLU:OE1	2.37	0.58
1:A:164:ASN:H	1:A:170:HIS:CD2	2.23	0.57
1:A:202:ASN:C	1:A:202:ASN:HD22	2.08	0.57
1:A:202:ASN:HD21	1:A:205:LEU:H	1.53	0.57
2:C:842:DG:OP1	2:C:842:DG:H4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:H	1:A:170:HIS:HD2	1.53	0.56
1:A:347:ARG:HB2	1:A:357:ARG:HB3	1.87	0.56
1:A:144:GLN:CG	1:A:147:GLU:HG2	2.35	0.56
1:A:204:LEU:HD23	1:A:240:PRO:HG2	1.90	0.54
1:A:310:LYS:HZ3	1:A:310:LYS:HB2	1.68	0.54
2:B:10:DA:H2'	2:B:11:DC:C6	2.42	0.54
1:A:136:VAL:HG11	1:A:172:ARG:HB2	1.90	0.54
1:A:310:LYS:HG3	1:A:311:CYS:N	2.23	0.53
2:B:11:DC:C2'	2:B:12:DC:C5'	2.79	0.53
1:A:343:ARG:HB3	1:A:409:CYS:HB3	1.91	0.53
2:B:12:DC:H2'	2:B:13:DOC:O4'	2.09	0.53
1:A:396:ASN:O	1:A:396:ASN:OD1	2.29	0.51
1:A:346:ILE:HG22	1:A:406:LEU:HD23	1.92	0.51
1:A:249:CYS:O	1:A:253:LEU:HD13	2.11	0.50
1:A:315:VAL:HG13	1:A:318:LYS:HB3	1.94	0.50
1:A:214:LYS:HB2	1:A:215:PRO:HA	1.92	0.50
1:A:392:ARG:O	1:A:393:ASN:C	2.51	0.49
1:A:391:PHE:O	1:A:394:MET:HB2	2.13	0.49
1:A:300:GLN:HG2	2:C:844:DT:OP1	2.12	0.49
2:B:13:DOC:N4	2:C:841:DG:N1	2.49	0.48
1:A:132:LEU:HD22	1:A:179:ILE:HG21	1.94	0.48
1:A:53:LYS:HA	1:A:54:PRO:HD3	1.56	0.48
1:A:163:ILE:HG21	1:A:174:LEU:HD11	1.96	0.48
2:B:11:DC:H2'	2:B:12:DC:H5'	1.91	0.48
2:B:10:DA:C2'	2:B:11:DC:H5'	2.43	0.48
1:A:27:SER:HB3	1:A:172:ARG:NH2	2.29	0.47
1:A:272:GLU:HG3	1:A:272:GLU:O	2.15	0.47
1:A:312:SER:HA	1:A:313:SER:O	2.15	0.47
1:A:392:ARG:O	1:A:394:MET:N	2.49	0.46
1:A:308:PHE:O	1:A:309:LYS:CB	2.59	0.46
2:B:13:DOC:N4	2:C:841:DG:C6	2.69	0.45
1:A:255:ILE:HD11	1:A:264:PHE:CE2	2.51	0.45
1:A:144:GLN:HG2	1:A:147:GLU:OE2	2.17	0.45
1:A:369:ILE:O	1:A:371:LYS:HB2	2.17	0.45
1:A:308:PHE:HE1	1:A:403:LEU:O	2.01	0.44
2:B:10:DA:H2''	2:B:11:DC:H5'	1.99	0.44
1:A:300:GLN:CG	2:C:844:DT:OP1	2.66	0.44
1:A:265:SER:OG	1:A:267:LYS:HG2	2.18	0.44
1:A:90:GLN:HG3	1:A:90:GLN:O	2.17	0.43
1:A:52:ASP:C	1:A:52:ASP:OD2	2.57	0.43
1:A:47:ASN:HA	1:A:48:PRO:HD2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HB2	1:A:358:GLU:H	1.55	0.43
1:A:144:GLN:CG	1:A:147:GLU:CG	2.97	0.42
1:A:144:GLN:HG3	1:A:147:GLU:CG	2.48	0.42
2:C:841:DG:N3	2:C:842:DG:H1'	2.35	0.42
1:A:32:HIS:CE1	1:A:34:ASP:HB2	2.55	0.42
1:A:311:CYS:O	1:A:312:SER:HB2	2.19	0.42
1:A:303:SER:O	1:A:304:GLU:HG3	2.20	0.42
1:A:161:GLN:OE1	1:A:222:LEU:HB2	2.20	0.41
1:A:60:LYS:HB3	1:A:61:TYR:H	1.52	0.41
1:A:103:ARG:HG3	1:A:125:PHE:CZ	2.54	0.41
1:A:36:ASP:O	1:A:37:CYS:C	2.59	0.41
1:A:43:GLU:HG3	1:A:94:VAL:HG21	2.02	0.41
2:B:11:DC:H2'	2:B:12:DC:C6	2.55	0.41
1:A:246:THR:HG23	1:A:273:LEU:HD22	2.03	0.41
2:C:844:DT:C2'	2:C:845:DC:C5'	2.79	0.41
1:A:329:LEU:O	1:A:333:CYS:N	2.55	0.40

All (5) 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:B:7:DA:OP2	2:C:847:DT:O3'[12_544]	0.58	1.62
2:B:7:DA:P	2:C:847:DT:O3'[12_544]	0.94	1.26
2:B:7:DA:OP2	2:C:847:DT:C3'[12_544]	1.27	0.93
2:B:7:DA:OP1	2:C:847:DT:O3'[12_544]	1.91	0.29
2:B:7:DA:O5'	2:C:847:DT:O3'[12_544]	2.14	0.06

## 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	365/420 (87%)	338 (93%)	24 (7%)	3 (1%)	19 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	VAL
1	A	394	MET
1	A	311	CYS

### 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	329/376 (88%)	287 (87%)	42 (13%)	4 13

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	27	SER
1	A	53	LYS
1	A	60	LYS
1	A	61	TYR
1	A	71	ARG
1	A	73	LEU
1	A	86	GLU
1	A	94	VAL
1	A	115	GLU
1	A	119	VAL
1	A	143	LEU
1	A	144	GLN
1	A	152	THR
1	A	172	ARG
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	229	LEU
1	A	264	PHE
1	A	272	GLU
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	290	ASN
1	A	295	LEU
1	A	308	PHE
1	A	310	LYS
1	A	311	CYS
1	A	312	SER
1	A	313	SER
1	A	327	SER
1	A	330	ASN
1	A	333	CYS
1	A	347	ARG
1	A	349	TYR
1	A	357	ARG
1	A	367	HIS
1	A	369	ILE
1	A	381	THR
1	A	395	VAL
1	A	396	ASN
1	A	403	LEU
1	A	405	LEU

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

Mol	Chain	Res	Type
1	A	58	GLN
1	A	170	HIS
1	A	202	ASN
1	A	262	GLN
1	A	412	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
2	DOC	B	13	2	14,19,20	1.42	2 (14%)	13,26,29	2.26	4 (30%)
2	2EG	C	840	2	21,26,27	1.82	6 (28%)	20,37,40	2.54	6 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	B	13	2	-	2/4/18/19	0/2/2/2
2	2EG	C	840	2	-	0/6/24/25	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	DOC	C6-N1	3.75	1.40	1.35
2	C	840	2EG	O4'-C1'	-3.65	1.34	1.42
2	C	840	2EG	P-O5'	-3.33	1.53	1.62
2	B	13	DOC	C4-N3	2.99	1.40	1.35
2	C	840	2EG	C6-C5	-2.97	1.36	1.41
2	C	840	2EG	C1'-N9	-2.42	1.42	1.49
2	C	840	2EG	C5-C4	-2.23	1.35	1.40
2	C	840	2EG	C5'-C4'	2.15	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	840	2EG	C2-N3-C4	7.82	124.16	115.28
2	B	13	DOC	C4'-O4'-C1'	-6.04	104.10	109.81
2	C	840	2EG	C2'-C3'-C4'	-4.05	94.33	102.76
2	C	840	2EG	N3-C2-N1	-3.61	120.53	126.23
2	C	840	2EG	N2-C2-N1	3.50	123.24	117.19
2	B	13	DOC	C2-N3-C4	3.48	119.87	116.34
2	B	13	DOC	O4'-C1'-C2'	-2.30	104.18	106.67
2	C	840	2EG	C3'-C2'-C1'	2.22	108.10	102.54
2	B	13	DOC	N4-C4-N3	2.17	119.91	116.49
2	C	840	2EG	C2'-C1'-N9	2.00	118.89	114.27



There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	13	DOC	O4'-C4'-C5'-O5'
2	B	13	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	13	DOC	7	0
2	C	840	2EG	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
4	PO4	A	422	-	4,4,4	0.77	0	6,6,6	0.40	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 [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	373/420 (88%)	0.03	19 (5%) 28 24	4, 14, 23, 35	4 (1%)
2	B	6/18 (33%)	0.32	0 100 100	11, 12, 18, 21	0
2	C	7/18 (38%)	0.10	0 100 100	9, 11, 14, 16	0
All	All	386/456 (84%)	0.04	19 (4%) 29 26	4, 14, 23, 35	4 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	5.1
1	A	333	CYS	3.7
1	A	350	SER	3.6
1	A	367	HIS	3.1
1	A	52	ASP	3.0
1	A	312	SER	3.0
1	A	61	TYR	2.7
1	A	244	TYR	2.7
1	A	26	SER	2.6
1	A	349	TYR	2.5
1	A	313	SER	2.5
1	A	395	VAL	2.5
1	A	146	ASP	2.4
1	A	172	ARG	2.4
1	A	336	GLY	2.3
1	A	144	GLN	2.3
1	A	310	LYS	2.2
1	A	86	GLU	2.2
1	A	189	ASN	2.1

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2EG	C	840	24/25	0.85	0.32	21,26,31,32	0
2	DOC	B	13	18/19	0.93	0.22	13,16,17,17	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	A	421	1/1	0.95	0.06	15,15,15,15	0
4	PO4	A	422	5/5	0.96	0.27	32,32,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.