



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DL5
Title : Human DNA polymerase eta inserting dCMPNPP opposite the 5'G of cisplatin crosslinked Gs (Pt-GG2).
Authors : Zhao, Y.; Biertumpfel, C.; Gregory, M.; Hanaoka, F.; Hua, Y.; Yang, W.
Deposited on : 2012-02-05
Resolution : 2.92 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

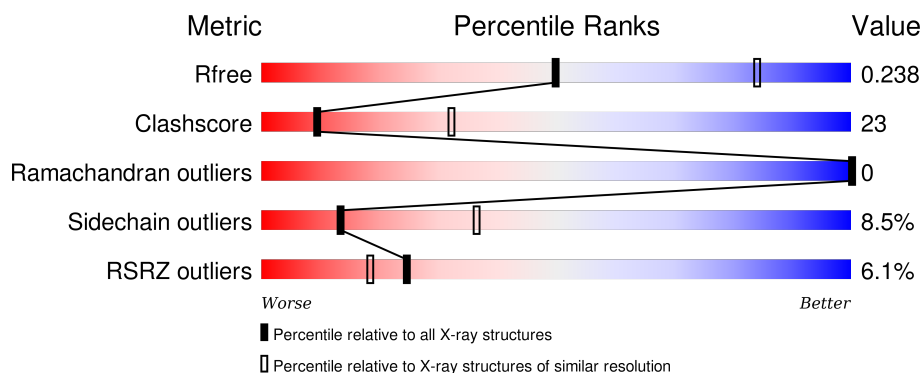
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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 ≥ 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	435	<div> <div>6%</div> <div>65%</div> <div>27%</div> <div>5%</div> </div>
2	T	12	<div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
3	P	9	<div> <div>11%</div> <div>22%</div> <div>56%</div> <div>22%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4038 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	424	Total	C	N	O	S	0	0	0
			3282	2054	593	613	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Y253
A	-1	PRO	-	EXPRESSION TAG	UNP Q9Y253
A	0	HIS	-	EXPRESSION TAG	UNP Q9Y253

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*CP*GP*GP*TP*CP*AP*CP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	9	0
			366	174	66	108	18			

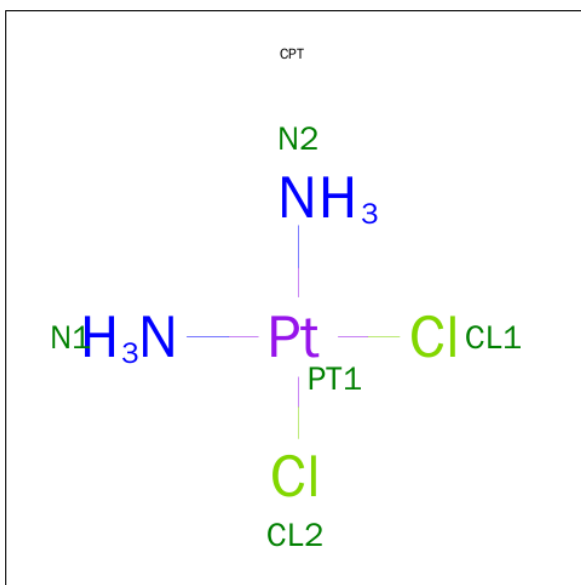
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*GP*TP*GP*TP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	P	0	9	0
			354	168	66	103	17			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

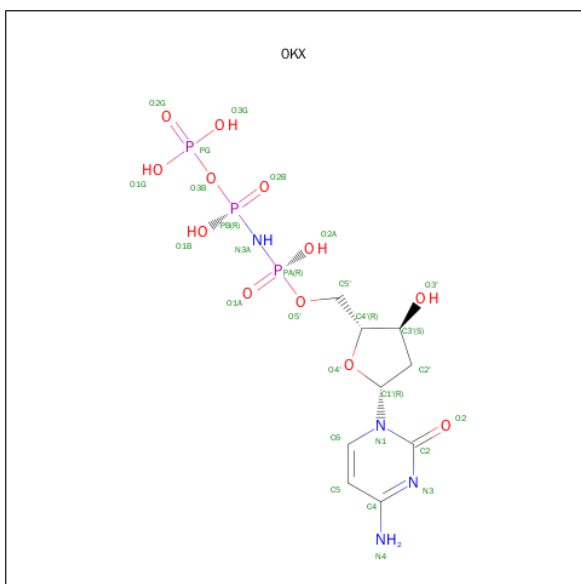
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		

- Molecule 5 is CISPLATIN (three-letter code: CPT) (formula: Cl₂H₆N₂Pt).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	T	1	Total	N	Pt		0	1
			6	4	2			

- Molecule 6 is 2'-DEOXY-5'-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]AMINO}PHOSPHORYL]CYTIDINE (three-letter code: 0KX) (formula: $C_9H_{17}N_4O_{12}P_3$).

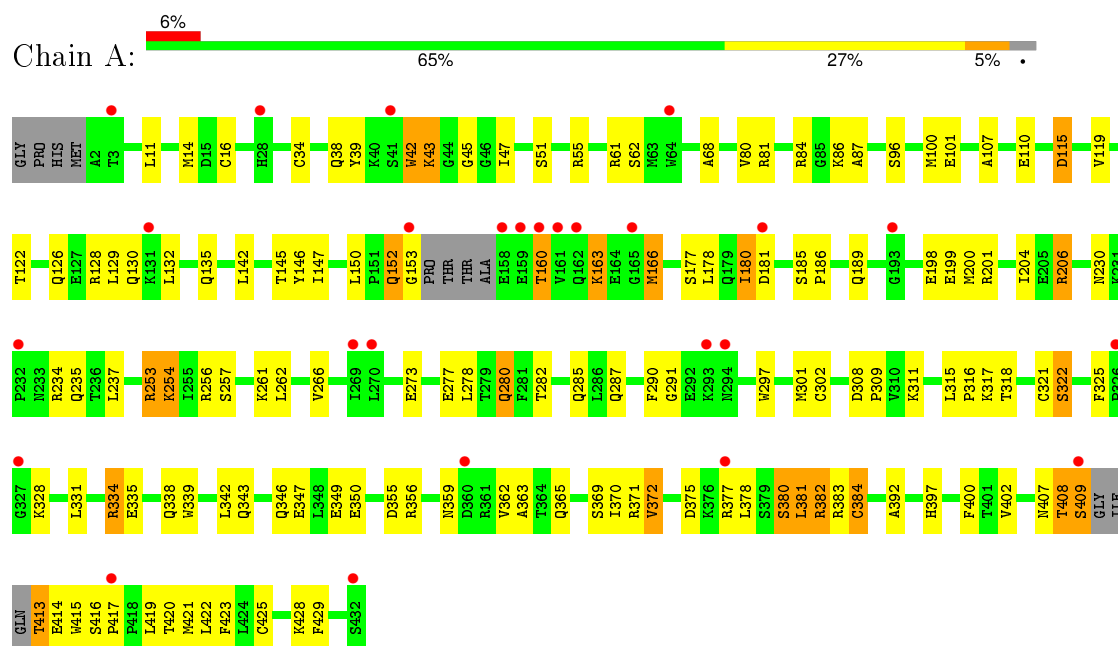


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	1
			28	9	4	12	3		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

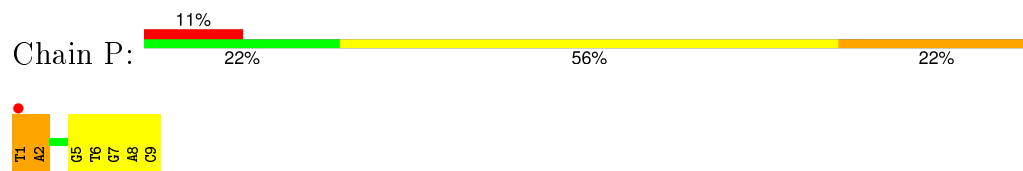
- Molecule 1: DNA polymerase eta



- Molecule 2: DNA (5'-D(*TP*AP*CP*GP*GP*TP*CP*AP*CP*AP*CP*T)-3')



- Molecule 3: DNA (5'-D(P*TP*AP*GP*TP*GP*TP*GP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	99.41 Å 99.41 Å 82.08 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.92 19.96 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.92) 99.7 (19.96-2.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.93 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.245 , 0.255 0.233 , 0.238	Depositor DCC
R_{free} test set	757 reflections (8.16%)	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.3	EDS
Estimated twinning fraction	0.065 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 10048 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4038	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 0KX, CPT, MG

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	0.31	0/3337	0.45	0/4506
2	T	1.47	12/408 (2.9%)	1.66	12/624 (1.9%)
3	P	0.99	4/395 (1.0%)	1.45	7/604 (1.2%)
All	All	0.62	16/4140 (0.4%)	0.82	19/5734 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1[B]	DT	N1-C2	5.93	1.42	1.38
2	T	5[A]	DG	P-OP1	-5.93	1.38	1.49
2	T	5[B]	DG	P-OP1	-5.93	1.38	1.49
2	T	4[A]	DG	C4'-O4'	-5.89	1.39	1.45
2	T	4[B]	DG	C4'-O4'	-5.89	1.39	1.45
2	T	4[A]	DG	C1'-N9	-5.87	1.39	1.47
2	T	4[B]	DG	C1'-N9	-5.87	1.39	1.47
2	T	5[A]	DG	C5'-C4'	-5.86	1.44	1.51
2	T	5[B]	DG	C5'-C4'	-5.86	1.44	1.51
2	T	5[A]	DG	C5-C6	5.81	1.48	1.42
2	T	5[B]	DG	C5-C6	5.81	1.48	1.42
3	P	1[B]	DT	C1'-N1	5.33	1.56	1.49
2	T	4[A]	DG	O4'-C1'	-5.16	1.36	1.42
2	T	4[B]	DG	O4'-C1'	-5.16	1.36	1.42
3	P	2[A]	DA	N9-C4	5.10	1.41	1.37
3	P	2[B]	DA	N9-C4	5.10	1.41	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1[B]	DT	N3-C2-O2	-6.82	118.21	122.30
3	P	1[B]	DT	C5-C4-O4	-6.53	120.33	124.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	4[A]	DG	C1'-O4'-C4'	-5.82	104.28	110.10
2	T	4[B]	DG	C1'-O4'-C4'	-5.82	104.28	110.10
2	T	4[A]	DG	C4-N9-C1'	-5.74	119.04	126.50
2	T	4[B]	DG	C4-N9-C1'	-5.74	119.04	126.50
2	T	5[A]	DG	C5-C6-N1	-5.69	108.66	111.50
2	T	5[B]	DG	C5-C6-N1	-5.69	108.66	111.50
3	P	1[B]	DT	C6-C5-C7	5.58	126.25	122.90
3	P	5[A]	DG	N3-C4-N9	-5.55	122.67	126.00
3	P	5[B]	DG	N3-C4-N9	-5.55	122.67	126.00
2	T	5[A]	DG	C8-N9-C1'	5.53	134.19	127.00
2	T	5[B]	DG	C8-N9-C1'	5.53	134.19	127.00
2	T	4[A]	DG	N3-C4-C5	5.34	131.27	128.60
2	T	4[B]	DG	N3-C4-C5	5.34	131.27	128.60
3	P	2[A]	DA	C8-N9-C4	-5.16	103.74	105.80
3	P	2[B]	DA	C8-N9-C4	-5.16	103.74	105.80
2	T	5[A]	DG	C8-N9-C4	-5.03	104.39	106.40
2	T	5[B]	DG	C8-N9-C4	-5.03	104.39	106.40

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	A	3282	0	3269	134	0
2	T	366	0	202	38	0
3	P	354	0	186	12	0
4	A	2	0	0	0	0
5	T	6	0	0	1	0
6	A	28	0	8	1	0
All	All	4038	0	3665	174	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 23.

All (174) 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:381:LEU:HD23	1:A:381:LEU:C	1.62	1.19
1:A:152:GLN:HG2	1:A:153:GLY:N	1.47	1.18
2:T:5[A]:DG:H2''	2:T:6[A]:DT:C5'	1.74	1.16
2:T:5[A]:DG:C2'	2:T:6[A]:DT:H5''	1.75	1.14
1:A:152:GLN:HG2	1:A:153:GLY:H	0.96	1.12
1:A:42:TRP:CZ3	1:A:43:LYS:HD3	1.85	1.10
1:A:371:ARG:HG2	1:A:420:THR:OG1	1.53	1.08
1:A:206:ARG:CG	1:A:206:ARG:HH21	1.71	1.03
1:A:277:GLU:O	1:A:280:GLN:HG3	1.59	1.02
2:T:5[A]:DG:H2''	2:T:6[A]:DT:H5''	0.99	0.99
2:T:6[B]:DT:H2''	2:T:7[B]:DC:H5''	1.46	0.96
1:A:152:GLN:CG	1:A:153:GLY:N	2.32	0.92
2:T:6[B]:DT:C2'	2:T:7[B]:DC:H5''	2.00	0.92
1:A:206:ARG:HG3	1:A:206:ARG:HH21	1.31	0.91
1:A:365:GLN:OE1	1:A:428:LYS:HE2	1.71	0.91
3:P:8[A]:DA:H2''	3:P:9[A]:DC:H5'	1.50	0.89
1:A:315:LEU:HD11	1:A:359:ASN:OD1	1.73	0.88
1:A:381:LEU:HD23	1:A:381:LEU:O	1.73	0.88
2:T:6[B]:DT:H2''	2:T:7[B]:DC:C5'	2.07	0.84
1:A:381:LEU:C	1:A:381:LEU:CD2	2.40	0.83
1:A:160:THR:HG22	1:A:166:MET:HG2	1.61	0.82
2:T:7[A]:DC:H2''	2:T:8[A]:DA:H5'	1.61	0.81
1:A:317:LYS:HB2	2:T:9[B]:DC:OP1	1.83	0.79
1:A:152:GLN:CG	1:A:153:GLY:H	1.89	0.78
3:P:8[A]:DA:H2''	3:P:9[A]:DC:C5'	2.12	0.78
1:A:381:LEU:HD23	1:A:382:ARG:N	2.00	0.75
2:T:9[B]:DC:H2''	2:T:10[B]:DA:H5'	1.68	0.75
1:A:180:ILE:H	1:A:180:ILE:CD1	2.00	0.74
1:A:315:LEU:CD1	1:A:359:ASN:CG	2.59	0.71
1:A:317:LYS:HB2	2:T:8[A]:DA:OP1	1.90	0.71
1:A:315:LEU:HD11	1:A:359:ASN:CG	2.11	0.71
1:A:206:ARG:HG2	1:A:206:ARG:HH21	1.56	0.70
2:T:8[B]:DA:H2'	2:T:9[B]:DC:C6	2.25	0.70
1:A:369:SER:HB3	1:A:423:PHE:HB3	1.72	0.70
2:T:7[A]:DC:C2'	2:T:8[A]:DA:H5'	2.21	0.69
1:A:206:ARG:CG	1:A:206:ARG:NH2	2.42	0.68
1:A:180:ILE:HD12	1:A:180:ILE:H	1.56	0.68
2:T:8[B]:DA:H2''	2:T:9[B]:DC:H5'	1.75	0.68
1:A:185:SER:O	1:A:189:GLN:HG3	1.94	0.68
1:A:253:ARG:HB3	1:A:253:ARG:HH11	1.57	0.68
1:A:383:ARG:HB3	1:A:402:VAL:CG1	2.24	0.68
1:A:334:ARG:HG3	1:A:335:GLU:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:5[A]:DG:C3'	2:T:6[A]:DT:H5''	2.23	0.67
1:A:253:ARG:CG	1:A:253:ARG:HH11	2.08	0.67
1:A:334:ARG:O	1:A:338:GLN:HG3	1.94	0.67
1:A:180:ILE:N	1:A:180:ILE:CD1	2.57	0.66
1:A:14:MET:HG2	1:A:115:ASP:O	1.97	0.65
2:T:4[B]:DG:O6	5:T:101[B]:CPT:N1	2.30	0.65
1:A:383:ARG:CB	1:A:402:VAL:CG1	2.75	0.64
1:A:180:ILE:HD13	1:A:181:ASP:N	2.11	0.64
2:T:5[A]:DG:C2	2:T:6[A]:DT:C2	2.87	0.63
1:A:84:ARG:NH2	1:A:350:GLU:OE1	2.32	0.63
1:A:254:LYS:HD2	1:A:254:LYS:N	2.13	0.63
1:A:355:ASP:OD1	1:A:359:ASN:ND2	2.32	0.62
1:A:146:TYR:OH	1:A:163:LYS:HD3	2.00	0.62
1:A:107:ALA:HB3	1:A:119:VAL:CG1	2.29	0.62
1:A:122:THR:O	1:A:126:GLN:HG2	1.99	0.62
1:A:38:GLN:NE2	2:T:4[A]:DG:H1'	2.16	0.61
1:A:372:VAL:HB	1:A:417:PRO:HG2	1.81	0.61
3:P:1[B]:DT:H73	3:P:1[B]:DT:OP2	2.00	0.61
1:A:371:ARG:HG2	1:A:420:THR:HG1	1.66	0.61
2:T:5[A]:DG:C2'	2:T:6[A]:DT:C5'	2.55	0.61
1:A:365:GLN:NE2	1:A:384:CYS:SG	2.74	0.60
1:A:317:LYS:N	2:T:9[B]:DC:OP1	2.34	0.60
1:A:128:ARG:HH22	1:A:199:GLU:CD	2.04	0.60
1:A:253:ARG:CB	1:A:253:ARG:HH11	2.15	0.60
1:A:322:SER:HB3	1:A:423:PHE:HD1	1.67	0.60
1:A:128:ARG:NH2	1:A:199:GLU:OE2	2.34	0.59
1:A:42:TRP:CE3	1:A:43:LYS:HD3	2.33	0.59
3:P:8[B]:DA:H2'	3:P:9[B]:DC:C6	2.37	0.59
1:A:423:PHE:CE2	1:A:425:CYS:HB2	2.38	0.59
1:A:38:GLN:HE22	2:T:5[B]:DG:H1'	1.66	0.58
1:A:371:ARG:HA	1:A:380:SER:HB2	1.84	0.58
1:A:180:ILE:HD13	1:A:181:ASP:H	1.68	0.57
1:A:253:ARG:HG2	1:A:253:ARG:NH1	2.18	0.57
1:A:206:ARG:HG2	1:A:206:ARG:NH2	2.16	0.57
1:A:383:ARG:HB3	1:A:402:VAL:HG11	1.86	0.56
2:T:5[A]:DG:N2	2:T:6[A]:DT:C2	2.73	0.56
1:A:180:ILE:N	1:A:180:ILE:HD13	2.20	0.56
2:T:5[B]:DG:H2''	2:T:6[B]:DT:O5'	2.05	0.56
1:A:407:ASN:OD1	1:A:408:THR:N	2.38	0.56
1:A:383:ARG:CB	1:A:402:VAL:HG11	2.36	0.56
1:A:423:PHE:CZ	1:A:425:CYS:HB2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:CG	1:A:253:ARG:NH1	2.67	0.55
1:A:338:GLN:HG2	1:A:400:PHE:CD2	2.41	0.55
1:A:38:GLN:NE2	2:T:5[B]:DG:H1'	2.22	0.55
1:A:80:VAL:HG11	1:A:87:ALA:HB1	1.87	0.55
1:A:38:GLN:HE22	2:T:4[A]:DG:H1'	1.72	0.54
1:A:206:ARG:HG3	1:A:206:ARG:NH2	2.10	0.54
2:T:4[A]:DG:H2''	2:T:5[A]:DG:O5'	2.08	0.53
1:A:317:LYS:N	2:T:8[A]:DA:OP1	2.41	0.53
1:A:34:CYS:HB3	1:A:51:SER:HB3	1.91	0.53
1:A:198:GLU:HG2	1:A:235:GLN:NE2	2.25	0.53
2:T:5[A]:DG:H2''	2:T:6[A]:DT:H5'	1.84	0.52
1:A:230:ASN:O	1:A:234:ARG:HB2	2.09	0.52
1:A:372:VAL:HG13	1:A:380:SER:CB	2.39	0.52
2:T:7[A]:DC:O2	3:P:7[A]:DG:N2	2.43	0.52
1:A:356:ARG:HD3	1:A:362:VAL:HG12	1.91	0.52
1:A:315:LEU:HD22	1:A:316:PRO:HD2	1.91	0.52
1:A:371:ARG:HB3	1:A:421:MET:HB3	1.91	0.52
1:A:339:TRP:O	1:A:343:GLN:HG2	2.10	0.51
1:A:277:GLU:O	1:A:280:GLN:CG	2.47	0.50
1:A:365:GLN:CD	1:A:428:LYS:HE2	2.31	0.50
2:T:11[B]:DC:H2''	2:T:12[B]:DT:O5'	2.11	0.49
3:P:9[B]:DC:O5'	3:P:9[B]:DC:H6	1.96	0.49
1:A:408:THR:O	1:A:409:SER:O	2.30	0.49
1:A:147:ILE:HG21	1:A:150:LEU:HD12	1.93	0.49
1:A:11:LEU:HD13	1:A:11:LEU:C	2.34	0.49
2:T:6[B]:DT:C3'	2:T:7[B]:DC:H5''	2.37	0.48
1:A:342:LEU:O	1:A:346:GLN:HG3	2.13	0.48
1:A:325:PHE:CD2	1:A:331:LEU:HD21	2.49	0.48
1:A:363:ALA:HB2	1:A:429:PHE:CE1	2.48	0.48
3:P:7[A]:DG:H2''	3:P:8[A]:DA:OP2	2.13	0.48
3:P:8[A]:DA:C2'	3:P:9[A]:DC:O5'	2.62	0.47
1:A:129:LEU:O	1:A:132:LEU:O	2.32	0.47
1:A:262:LEU:O	1:A:266:VAL:HG23	2.15	0.47
1:A:51:SER:O	1:A:55:ARG:HG3	2.14	0.47
1:A:282:THR:OG1	1:A:285:GLN:HG3	2.14	0.47
1:A:110:GLU:HB2	1:A:311:LYS:O	2.14	0.47
1:A:201:ARG:HD3	1:A:235:GLN:OE1	2.16	0.46
1:A:39:TYR:O	1:A:45:GLY:HA2	2.15	0.46
1:A:381:LEU:O	1:A:381:LEU:CD2	2.52	0.46
1:A:383:ARG:HB2	1:A:402:VAL:CG1	2.46	0.46
1:A:96:SER:O	1:A:100:MET:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD23	1:A:382:ARG:CA	2.45	0.46
1:A:407:ASN:ND2	1:A:415:TRP:HA	2.31	0.46
1:A:397:HIS:HD1	1:A:397:HIS:C	2.17	0.46
2:T:10[A]:DA:H2''	2:T:11[A]:DC:O5'	2.16	0.45
1:A:198:GLU:HG2	1:A:235:GLN:HE22	1.81	0.45
2:T:7[A]:DC:H2'	2:T:8[A]:DA:C8	2.51	0.45
2:T:6[B]:DT:C1'	2:T:7[B]:DC:H5''	2.46	0.45
2:T:8[A]:DA:H1'	2:T:9[A]:DC:H5'	1.98	0.45
1:A:200:MET:O	1:A:204:ILE:HG13	2.16	0.45
1:A:408:THR:OG1	1:A:408:THR:O	2.30	0.45
1:A:308:ASP:OD2	1:A:309:PRO:HD2	2.16	0.45
2:T:5[A]:DG:N2	2:T:6[A]:DT:O2	2.50	0.45
1:A:42:TRP:CZ3	1:A:43:LYS:CD	2.77	0.45
1:A:42:TRP:CH2	1:A:43:LYS:HD3	2.46	0.45
3:P:8[A]:DA:H2''	3:P:9[A]:DC:O5'	2.16	0.44
1:A:349:GLU:OE1	1:A:392:ALA:HB2	2.16	0.44
3:P:2[A]:DA:H8	3:P:2[A]:DA:OP2	2.00	0.44
1:A:415:TRP:HE1	1:A:419:LEU:HD21	1.83	0.44
1:A:377:ARG:O	1:A:378:LEU:C	2.55	0.44
1:A:413:THR:HG22	1:A:414:GLU:HG2	2.00	0.44
1:A:266:VAL:HA	1:A:290:PHE:CZ	2.51	0.44
1:A:261:LYS:NZ	3:P:6[A]:DT:OP1	2.31	0.44
1:A:287:GLN:O	1:A:291:GLY:N	2.50	0.44
1:A:278:LEU:HB2	1:A:302:CYS:CB	2.47	0.44
2:T:10[B]:DA:H2''	2:T:11[B]:DC:C5	2.53	0.43
1:A:375:ASP:OD2	1:A:380:SER:OG	2.33	0.43
1:A:61:ARG:O	1:A:62:SER:OG	2.29	0.43
1:A:61:ARG:O	1:A:62:SER:CB	2.65	0.43
1:A:142:LEU:HB3	1:A:145:THR:HB	2.00	0.42
1:A:318:THR:HA	1:A:429:PHE:HE2	1.83	0.42
2:T:4[A]:DG:H2'	2:T:5[A]:DG:H8	1.84	0.42
1:A:185:SER:HA	1:A:186:PRO:HD3	1.89	0.42
1:A:152:GLN:O	1:A:153:GLY:C	2.57	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.91	0.42
1:A:200:MET:HB2	1:A:200:MET:HE2	1.81	0.42
1:A:256:ARG:O	1:A:257:SER:OG	2.27	0.41
1:A:408:THR:HG23	1:A:416:SER:O	2.19	0.41
1:A:370:ILE:HG22	1:A:422:LEU:HD23	2.03	0.41
2:T:8[A]:DA:H2''	2:T:9[A]:DC:H5'	2.03	0.41
1:A:166:MET:HB3	1:A:166:MET:HE3	1.92	0.41
1:A:407:ASN:ND2	1:A:414:GLU:O	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:NZ	1:A:347:GLU:OE1	2.42	0.41
1:A:237:LEU:HD23	1:A:237:LEU:C	2.41	0.41
1:A:47:ILE:HD11	1:A:68:ALA:CB	2.51	0.41
1:A:297:TRP:O	1:A:301:MET:HB2	2.21	0.41
1:A:383:ARG:HB2	1:A:402:VAL:HG11	2.03	0.41
1:A:317:LYS:O	1:A:429:PHE:CD2	2.74	0.41
1:A:16:CYS:HA	6:A:503[A]:0KX:O1B	2.21	0.40
3:P:8[B]:DA:H2'	3:P:9[B]:DC:C5	2.55	0.40
1:A:42:TRP:CE3	1:A:43:LYS:CD	3.02	0.40

There are no symmetry-related clashes.

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	
1	A	418/435 (96%)	414 (99%)	4 (1%)	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	
1	A	351/372 (94%)	321 (92%)	30 (8%)	13	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	TRP
1	A	43	LYS
1	A	81	ARG
1	A	101	GLU
1	A	115	ASP
1	A	130	GLN
1	A	135	GLN
1	A	152	GLN
1	A	160	THR
1	A	163	LYS
1	A	166	MET
1	A	177	SER
1	A	180	ILE
1	A	206	ARG
1	A	253	ARG
1	A	254	LYS
1	A	273	GLU
1	A	280	GLN
1	A	321	CYS
1	A	322	SER
1	A	328	LYS
1	A	334	ARG
1	A	372	VAL
1	A	380	SER
1	A	381	LEU
1	A	382	ARG
1	A	384	CYS
1	A	408	THR
1	A	409	SER
1	A	413	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	135	GLN
1	A	179	GLN
1	A	365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are 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	$\# Z > 2$
6	0KX	A	503[A]	4	24,29,29	3.67	9 (37%)	33,45,45	1.94	11 (33%)
5	CPT	T	101[A]	2	0,2,4	0.00	-	0,1,6	0.00	-
5	CPT	T	101[B]	2	0,2,4	0.00	-	0,1,6	0.00	-

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	0KX	A	503[A]	4	-	0/13/34/34	0/2/2/2
5	CPT	T	101[A]	2	-	0/0/0/0	0/0/0/0
5	CPT	T	101[B]	2	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	503[A]	0KX	PB-O1B	-10.17	1.28	1.56
6	A	503[A]	0KX	PA-O1A	-10.15	1.34	1.46
6	A	503[A]	0KX	PB-O2B	-5.02	1.40	1.46
6	A	503[A]	0KX	PA-O2A	-4.15	1.45	1.56
6	A	503[A]	0KX	PG-O3G	-3.94	1.40	1.54
6	A	503[A]	0KX	O3'-C3'	-3.24	1.36	1.43
6	A	503[A]	0KX	O4'-C1'	-3.10	1.35	1.42
6	A	503[A]	0KX	PG-O1G	-3.08	1.43	1.54
6	A	503[A]	0KX	PG-O2G	-3.06	1.41	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	503[A]	0KX	O2B-PB-N3A	-3.91	105.90	111.90
6	A	503[A]	0KX	PG-O3B-PB	-2.79	123.30	132.67
6	A	503[A]	0KX	C2'-C3'-C4'	-2.57	97.44	102.77
6	A	503[A]	0KX	C5-C4-N3	-2.46	118.69	121.80
6	A	503[A]	0KX	C3'-C2'-C1'	2.19	107.67	102.40
6	A	503[A]	0KX	N4-C4-N3	2.21	120.53	116.50
6	A	503[A]	0KX	O5'-C5'-C4'	2.22	117.31	109.12
6	A	503[A]	0KX	O4'-C4'-C3'	2.33	111.52	105.67
6	A	503[A]	0KX	O3'-C3'-C2'	3.37	121.91	110.74
6	A	503[A]	0KX	C2-N3-C4	3.73	120.87	115.61
6	A	503[A]	0KX	O2A-PA-O1A	4.49	119.37	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503[A]	0KX	1	0
5	T	101[B]	CPT	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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	424/435 (97%)	0.47	26 (6%) 25 18	55, 80, 102, 113	0
2	T	9/12 (75%)	0.62	0 100 100	83, 85, 90, 91	0
3	P	9/9 (100%)	0.81	1 (11%) 7 4	81, 83, 94, 98	1 (11%)
All	All	442/456 (96%)	0.48	27 (6%) 25 18	55, 80, 102, 113	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	GLN	6.4
1	A	327	GLY	4.7
1	A	158	GLU	4.7
1	A	432	SER	4.2
1	A	160	THR	3.8
1	A	131	LYS	3.7
1	A	28	HIS	3.3
1	A	232	PRO	3.3
1	A	193	GLY	3.2
1	A	377	ARG	3.1
1	A	409	SER	3.1
3	P	1[B]	DT	2.8
1	A	270	LEU	2.7
1	A	360	ASP	2.7
1	A	326	PRO	2.7
1	A	159	GLU	2.5
1	A	64	TRP	2.5
1	A	269	ILE	2.5
1	A	293	LYS	2.5
1	A	294	ASN	2.5
1	A	3	THR	2.5
1	A	161	VAL	2.3
1	A	41	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	2.2
1	A	181	ASP	2.1
1	A	417	PRO	2.1
1	A	165	GLY	2.1

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

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

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. 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, 95th 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(\AA^2)	Q<0.9
4	MG	A	501[A]	1/1	0.88	0.28	1.38	67,67,67,67	1
4	MG	A	502[A]	1/1	0.42	0.23	0.42	71,71,71,71	1
6	0KX	A	503[A]	28/28	0.87	0.24	0.26	63,77,82,83	28
5	CPT	T	101[A]	3/5	0.98	0.17	-3.09	91,91,92,271	3
5	CPT	T	101[B]	3/5	0.98	0.17	-3.14	77,77,82,90	3

6.5 Other polymers [i](#)

There are no such residues in this entry.