Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 10:40 AM EDT

PDB ID	:	4DL2
Title	:	Human DNA polymerase eta inserting dCMPNPP opposite CG template (GG0a)
Authors	:	Zhao, Y.; Biertumpfel, C.; Gregory, M.; Hua, Y.; Hanaoka, F.; Yang, W.
Deposited on	:	2012-02-05
Resolution	:	2.15 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

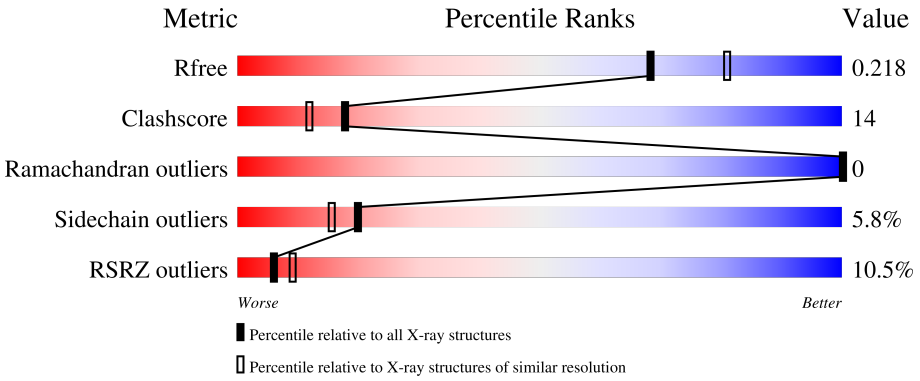
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	10% 74% 21%
2	T	12	25% 58% 42%
3	P	9	44% 56%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4126 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
			Total	C	N	O	S			
1	A	428	3380	2121	605	628	26	0	8	0

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(*AP*CP*GP*GP*CP*TP*CP*AP*CP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	12	266	125	49	79	13	0	2	1

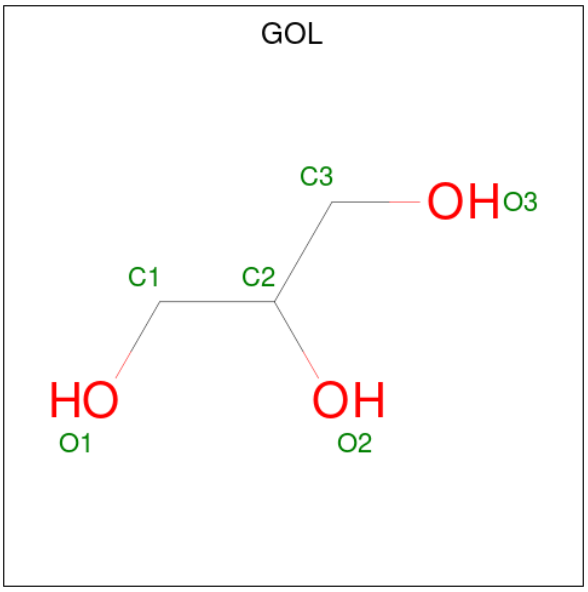
- Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*GP*TP*GP*TP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	9	214	100	44	60	10	0	2	1

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

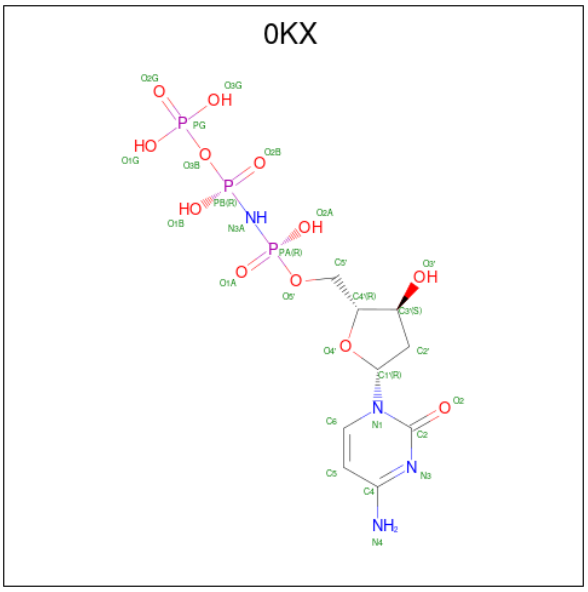
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- 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	P	1	Total	C	N	O	P	0	0
			28	9	4	12	3		

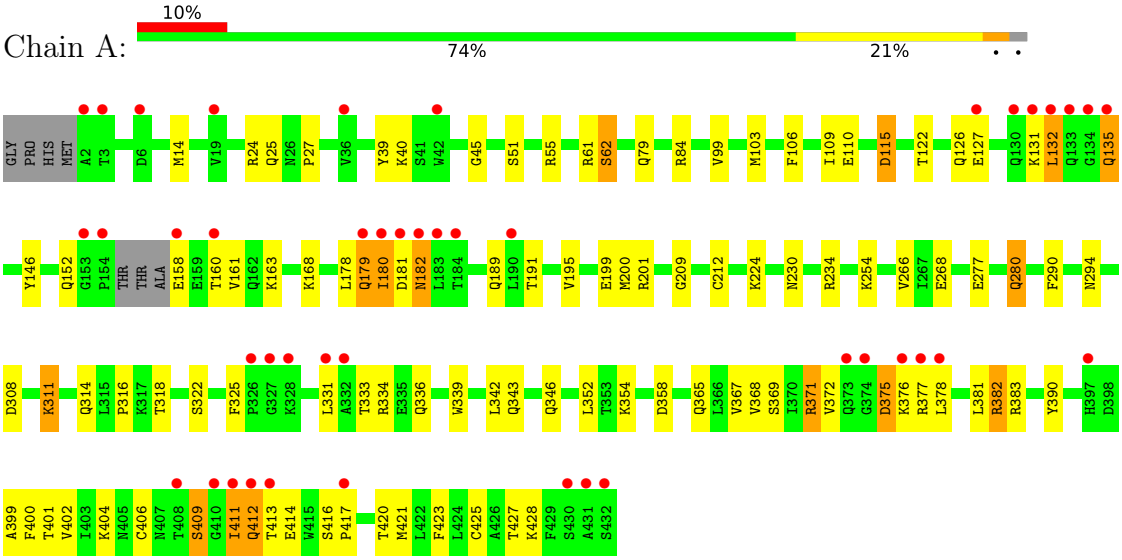
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total	O	0	0
			189	189		
7	T	14	Total	O	0	0
			14	14		
7	P	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 2: DNA (5'-D(*AP*CP*GP*GP*CP*TP*CP*AP*CP*AP*CP*T)-3')

• Molecule 3: DNA (5'-D(*TP*AP*GP*TP*GP*TP*GP*AP*G)-3')

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	97.86Å 97.86Å 80.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15 19.44 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.15) 99.5 (19.44-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.193 , 0.222 0.187 , 0.218	Depositor DCC
R_{free} test set	1832 reflections (7.69%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4126	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 0KX, 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	0.24	0/3461	0.42	0/4669
2	T	0.60	0/297	0.89	1/457 (0.2%)
3	P	0.40	0/240	0.86	0/369
All	All	0.30	0/3998	0.51	1/5495 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	6	DT	P-O3'-C3'	5.12	125.84	119.70

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	3380	0	3436	89	0
2	T	266	0	146	16	0
3	P	214	0	114	4	0
4	A	2	0	0	0	0
5	A	18	0	24	2	0
6	P	28	0	15	3	0
7	A	189	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	15	0	0	0	0
7	T	14	0	0	0	0
All	All	4126	0	3735	103	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 14.

All (103) 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:62:SER:HB2	2:T:3[B]:DG:C2	1.98	0.99
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.26	0.97
1:A:382:ARG:HH11	1:A:382:ARG:CG	1.81	0.93
1:A:322:SER:HB3	1:A:423:PHE:HD1	1.33	0.92
2:T:3[B]:DG:N3	2:T:3[B]:DG:H2'	1.84	0.90
2:T:2:DC:H4'	2:T:3[B]:DG:OP1	1.71	0.88
1:A:372:VAL:HB	1:A:417:PRO:HG2	1.65	0.77
1:A:382:ARG:HG2	1:A:382:ARG:NH1	1.96	0.77
1:A:383:ARG:HB3	1:A:402:VAL:CG1	2.15	0.76
1:A:409:SER:OG	1:A:411:ILE:HD12	1.88	0.73
1:A:371:ARG:NH2	1:A:375:ASP:O	2.23	0.71
1:A:84:ARG:NH1	7:A:751:HOH:O	2.23	0.70
1:A:158:GLU:O	1:A:161:VAL:HG22	1.92	0.70
1:A:381:LEU:HD22	1:A:406:CYS:SG	2.32	0.69
1:A:122:THR:O	1:A:126:GLN:HG2	1.93	0.68
1:A:322:SER:HB3	1:A:423:PHE:CD1	2.24	0.67
2:T:2:DC:C4'	2:T:3[B]:DG:OP1	2.44	0.65
1:A:412:GLN:HG2	1:A:412:GLN:O	1.96	0.65
1:A:62:SER:HB2	2:T:3[B]:DG:N1	2.12	0.64
1:A:383:ARG:HB3	1:A:402:VAL:HG11	1.80	0.62
2:T:7:DC:H2"	2:T:8:DA:H5'	1.82	0.62
1:A:181:ASP:OD1	1:A:182:ASN:N	2.34	0.60
2:T:3[B]:DG:N3	2:T:3[B]:DG:C2'	2.60	0.59
1:A:61[B]:ARG:HG3	2:T:3[B]:DG:O6	2.03	0.58
1:A:99:VAL:HG12	1:A:103[A]:MET:CE	2.33	0.58
1:A:131:LYS:NZ	7:A:784:HOH:O	2.36	0.58
1:A:62:SER:HA	2:T:3[B]:DG:C5	2.38	0.58
2:T:7:DC:H2'	2:T:8:DA:C8	2.38	0.58
1:A:423:PHE:CZ	1:A:425:CYS:HB2	2.39	0.57
1:A:25:GLN:O	1:A:27:PRO:HD3	2.04	0.57
1:A:308:ASP:OD2	1:A:311:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:SER:HB3	1:A:423:PHE:HB3	1.87	0.56
1:A:179:GLN:CG	1:A:181:ASP:OD1	2.53	0.56
2:T:2:DC:H5"	2:T:3[A]:DG:OP1	2.04	0.56
1:A:318:THR:HG22	1:A:427:THR:HG22	1.88	0.55
1:A:371:ARG:HG2	1:A:420:THR:OG1	2.06	0.55
1:A:381:LEU:HD11	1:A:383:ARG:CZ	2.36	0.55
1:A:62:SER:O	1:A:62:SER:OG	2.23	0.55
1:A:368:VAL:HG21	1:A:399:ALA:HA	1.90	0.54
1:A:39:TYR:O	1:A:45:GLY:HA2	2.08	0.54
1:A:382:ARG:HB3	3:P:4:DT:OP2	2.08	0.53
1:A:376:LYS:HG2	1:A:376:LYS:O	2.10	0.52
1:A:230:ASN:O	1:A:234:ARG:HB2	2.11	0.51
1:A:371:ARG:HB3	1:A:421:MET:HB3	1.93	0.50
1:A:371:ARG:HD3	1:A:378:LEU:O	2.11	0.50
1:A:40:LYS:HD3	1:A:79:GLN:OE1	2.11	0.50
1:A:325:PHE:CD2	1:A:331:LEU:HD21	2.47	0.50
1:A:99:VAL:HG12	1:A:103[A]:MET:HE2	1.92	0.49
1:A:371:ARG:NH2	1:A:377:ARG:O	2.45	0.49
1:A:61[B]:ARG:HH12	6:P:10:0KX:H5	1.61	0.49
1:A:110:GLU:HB2	1:A:311:LYS:O	2.13	0.49
1:A:334:ARG:HG3	1:A:400:PHE:CZ	2.48	0.49
1:A:383:ARG:CB	1:A:402:VAL:CG1	2.89	0.49
1:A:24:ARG:HB2	5:A:505:GOL:O2	2.12	0.49
1:A:209:GLY:O	5:A:505:GOL:H31	2.13	0.49
1:A:106:PHE:CG	1:A:200[B]:MET:HG2	2.48	0.49
1:A:106:PHE:CD1	1:A:200[B]:MET:HG2	2.47	0.48
1:A:189:GLN:OE1	7:A:619:HOH:O	2.20	0.48
1:A:109:ILE:HD11	1:A:314:GLN:HG2	1.95	0.48
1:A:99:VAL:HG12	1:A:103[A]:MET:HE1	1.95	0.48
1:A:381:LEU:HD11	1:A:383:ARG:NH1	2.28	0.48
6:P:10:0KX:O5'	6:P:10:0KX:H15	2.14	0.48
1:A:14:MET:HG2	1:A:115:ASP:O	2.13	0.48
1:A:179:GLN:HG3	1:A:181:ASP:OD1	2.15	0.47
1:A:352:LEU:HB3	1:A:390:TYR:CE1	2.49	0.47
1:A:354:LYS:NZ	1:A:358:ASP:OD2	2.41	0.47
6:P:10:0KX:H7	6:P:10:0KX:O2B	2.15	0.47
1:A:277:GLU:O	1:A:280:GLN:HG3	2.15	0.47
1:A:382:ARG:CG	1:A:382:ARG:NH1	2.51	0.47
1:A:266:VAL:HA	1:A:290:PHE:CZ	2.51	0.46
3:P:5:DG:C8	3:P:6:DT:H72	2.51	0.46
1:A:201:ARG:HG2	1:A:212:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TRP:O	1:A:343:GLN:HG2	2.16	0.45
1:A:365:GLN:OE1	1:A:428:LYS:HE2	2.16	0.45
2:T:2:DC:H4'	2:T:3[A]:DG:OP1	2.16	0.45
1:A:195:VAL:O	1:A:199:GLU:HG3	2.17	0.45
1:A:336:GLN:HG2	7:A:699:HOH:O	2.16	0.45
1:A:416:SER:HA	1:A:417:PRO:C	2.38	0.44
1:A:51:SER:O	1:A:55:ARG:HG3	2.16	0.44
1:A:290:PHE:O	1:A:294:ASN:HB2	2.18	0.44
1:A:411:ILE:HD13	1:A:414:GLU:HB2	2.00	0.44
1:A:342:LEU:O	1:A:346:GLN:HG3	2.18	0.44
1:A:103[B]:MET:HG2	1:A:200[B]:MET:CE	2.48	0.44
1:A:180:ILE:H	1:A:180:ILE:HG13	1.46	0.43
1:A:224:LYS:HE2	3:P:9[B]:DG:OP1	2.18	0.43
1:A:411:ILE:O	1:A:412:GLN:HB3	2.17	0.43
1:A:178:LEU:HD11	1:A:191:THR:OG1	2.18	0.43
2:T:2:DC:C4'	2:T:3[A]:DG:OP1	2.66	0.43
3:P:3:DG:H2"	3:P:4:DT:O5'	2.18	0.43
1:A:333:THR:OG1	1:A:336:GLN:HB2	2.19	0.43
1:A:146:TYR:OH	1:A:163:LYS:HG2	2.18	0.42
1:A:401:THR:O	1:A:404:LYS:HG2	2.19	0.42
1:A:371:ARG:HD2	1:A:377:ARG:O	2.20	0.42
1:A:254:LYS:HD3	1:A:254:LYS:HA	1.78	0.42
1:A:409:SER:CB	1:A:416:SER:OG	2.67	0.42
1:A:200[A]:MET:HE2	1:A:200[A]:MET:HB2	1.86	0.42
1:A:381:LEU:CD2	1:A:406:CYS:SG	3.05	0.42
2:T:2:DC:C5'	2:T:3[A]:DG:OP1	2.67	0.42
1:A:316:PRO:HA	2:T:8:DA:OP1	2.20	0.41
1:A:62:SER:CB	2:T:3[B]:DG:N1	2.82	0.41
1:A:132:LEU:HB2	1:A:135:GLN:HB3	2.02	0.41
1:A:135:GLN:O	1:A:180:ILE:HG21	2.21	0.41
1:A:367:VAL:HG11	1:A:382:ARG:NE	2.36	0.41

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	432/435 (99%)	424 (98%)	8 (2%)	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	373/372 (100%)	352 (94%)	21 (6%)	21 16

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	115	ASP
1	A	127	GLU
1	A	132	LEU
1	A	135	GLN
1	A	152	GLN
1	A	160	THR
1	A	168	LYS
1	A	179	GLN
1	A	180	ILE
1	A	182	ASN
1	A	268	GLU
1	A	280	GLN
1	A	311	LYS
1	A	371	ARG
1	A	375	ASP
1	A	382	ARG
1	A	409	SER
1	A	411	ILE
1	A	412	GLN
1	A	413	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.26	0
5	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.28	0
6	0KX	P	10	4	28,29,29	2.73	10 (35%)	40,45,45	1.38	5 (12%)

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	GOL	A	504	-	-	3/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	506	-	-	2/4/4/4	-
6	0KX	P	10	4	-	4/19/34/34	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	10	0KX	PA-O1A	10.58	1.63	1.46
6	P	10	0KX	O3'-C3'	-4.39	1.34	1.43
6	P	10	0KX	O2-C2	-3.88	1.16	1.23
6	P	10	0KX	C5'-C4'	-2.54	1.43	1.51
6	P	10	0KX	PG-O3G	-2.42	1.45	1.54
6	P	10	0KX	PA-N3A	2.41	1.69	1.63
6	P	10	0KX	C2-N1	-2.39	1.34	1.40
6	P	10	0KX	C2'-C3'	-2.12	1.47	1.52
6	P	10	0KX	C3'-C4'	-2.11	1.47	1.53
6	P	10	0KX	C4-N4	2.08	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	10	0KX	O4'-C1'-N1	3.45	114.03	107.86
6	P	10	0KX	O2A-PA-O1A	-2.46	104.76	109.92
6	P	10	0KX	O2A-PA-O5'	2.41	113.28	106.75
6	P	10	0KX	C2'-C1'-N1	-2.39	108.27	113.77
6	P	10	0KX	O2-C2-N3	-2.18	118.79	122.33

There are no chirality outliers.

All (11) torsion outliers are listed below:

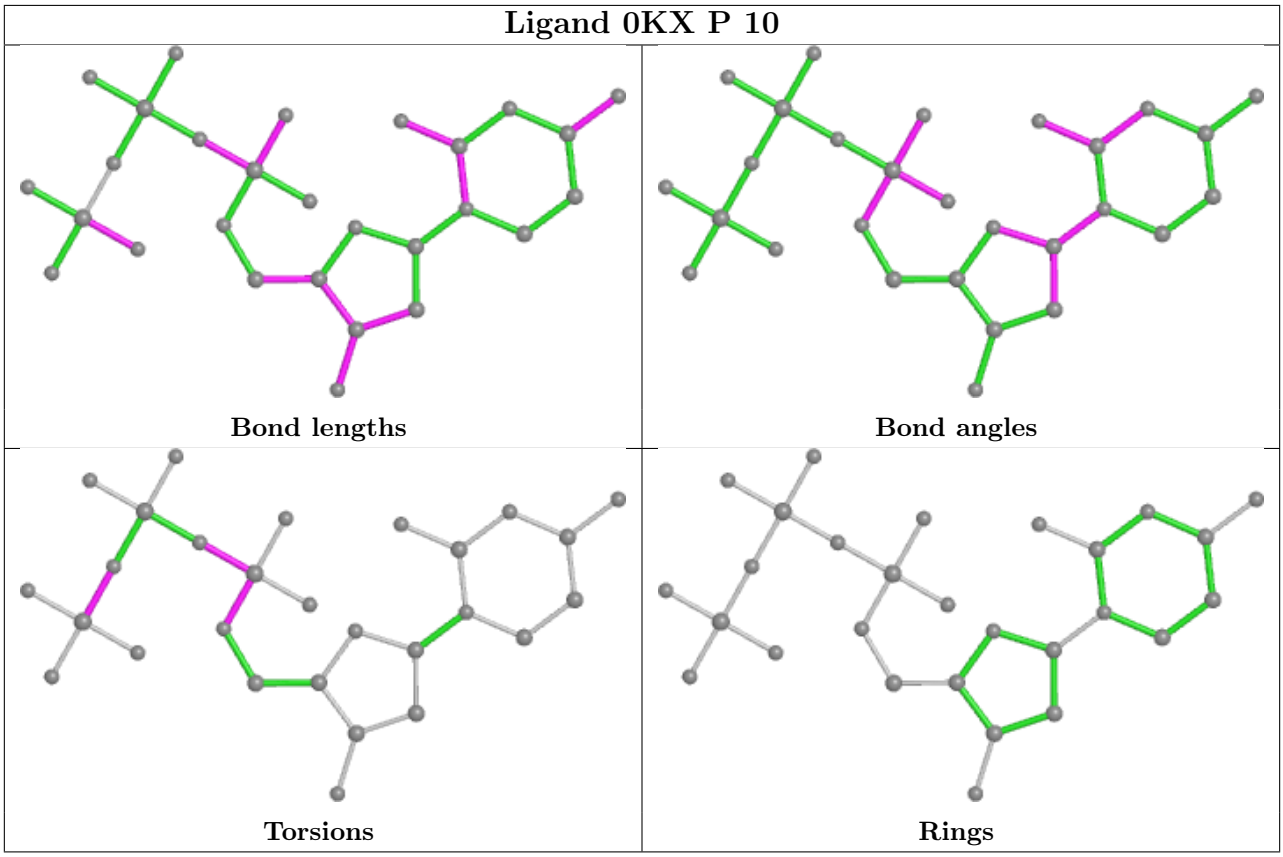
Mol	Chain	Res	Type	Atoms
5	A	504	GOL	O1-C1-C2-C3
5	A	505	GOL	O1-C1-C2-O2
5	A	505	GOL	O1-C1-C2-C3
5	A	506	GOL	O1-C1-C2-C3
6	P	10	0KX	PB-O3B-PG-O3G
6	P	10	0KX	PB-N3A-PA-O1A
5	A	504	GOL	O1-C1-C2-O2
5	A	506	GOL	O1-C1-C2-O2
6	P	10	0KX	C5'-O5'-PA-O2A
6	P	10	0KX	PB-N3A-PA-O5'
5	A	504	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	GOL	2	0
6	P	10	0KX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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^{th} 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	428/435 (98%)	0.56	44 (10%) 6 9	12, 24, 54, 83	0
2	T	12/12 (100%)	1.50	3 (25%) 0 0	27, 30, 68, 91	0
3	P	9/9 (100%)	-0.13	0 100 100	22, 27, 36, 48	0
All	All	449/456 (98%)	0.57	47 (10%) 6 9	12, 24, 54, 91	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	3[A]	DG	7.8
2	T	1	DA	7.4
1	A	412	GLN	6.1
1	A	133	GLN	5.9
1	A	411	ILE	5.7
1	A	181	ASP	5.3
1	A	131	LYS	5.1
1	A	179	GLN	4.9
1	A	2	ALA	4.9
2	T	2	DC	4.7
1	A	134	GLY	4.2
1	A	410	GLY	4.1
1	A	182	ASN	3.9
1	A	328	LYS	3.9
1	A	408	THR	3.7
1	A	327	GLY	3.6
1	A	431	ALA	3.5
1	A	36	VAL	3.3
1	A	432	SER	3.3
1	A	180	ILE	3.3
1	A	184	THR	3.2
1	A	3	THR	3.2
1	A	160	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	376	LYS	3.0
1	A	130	GLN	3.0
1	A	158	GLU	2.9
1	A	378	LEU	2.9
1	A	135	GLN	2.9
1	A	19	VAL	2.8
1	A	417	PRO	2.8
1	A	183	LEU	2.6
1	A	373	GLN	2.6
1	A	413	THR	2.6
1	A	153	GLY	2.6
1	A	132	LEU	2.5
1	A	190	LEU	2.5
1	A	374	GLY	2.5
1	A	42	TRP	2.5
1	A	397	HIS	2.4
1	A	331	LEU	2.3
1	A	332	ALA	2.3
1	A	326	PRO	2.3
1	A	127	GLU	2.3
1	A	154	PRO	2.3
1	A	430	SER	2.2
1	A	6	ASP	2.2
1	A	377	ARG	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

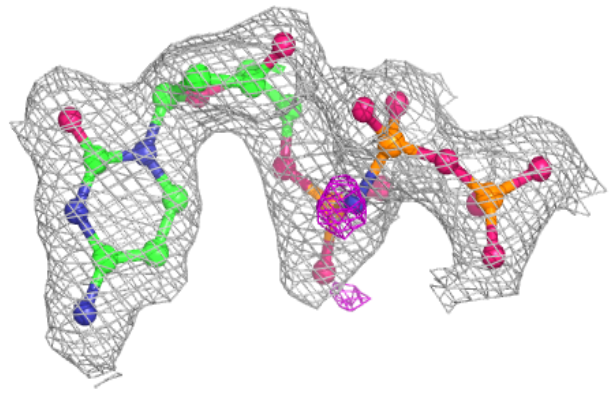
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

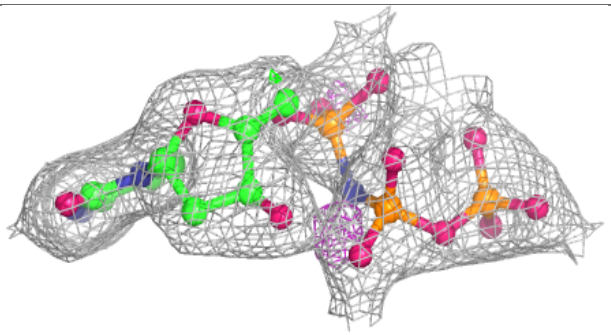
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	503	1/1	0.88	0.09	18,18,18,18	0
5	GOL	A	505	6/6	0.89	0.20	28,31,33,34	0
5	GOL	A	506	6/6	0.89	0.24	32,34,39,40	0
5	GOL	A	504	6/6	0.94	0.12	15,18,23,23	0
6	0KX	P	10	28/28	0.95	0.12	12,16,20,21	0
4	MG	A	502	1/1	0.96	0.08	14,14,14,14	0

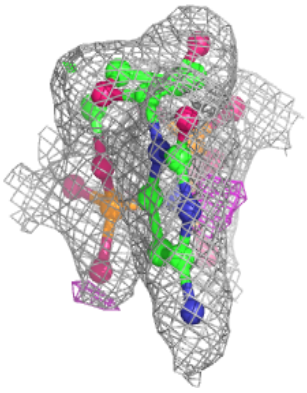
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 0KX P 10:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.