



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K58
Title : Crystal structure of E.coli Pol II-normal DNA-dTTP ternary complex
Authors : Yang, W.; Wang, F.
Deposited on : 2009-10-06
Resolution : 2.05 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

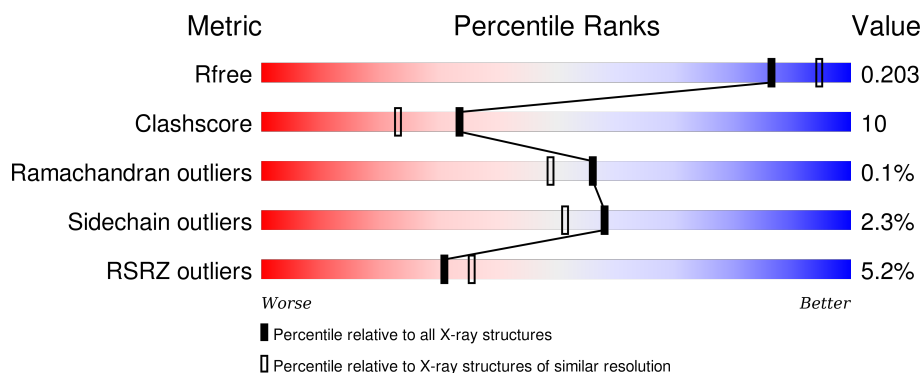
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	786	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
2	T	17	<div> <div>29%</div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
3	P	13	<div> <div>15%</div> <div>54%</div> <div>31%</div> <div>15%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7733 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	0	0
			6332	4036	1127	1144	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P21189
A	-1	PRO	-	EXPRESSION TAG	UNP P21189
A	0	HIS	-	EXPRESSION TAG	UNP P21189
A	335	ASN	ASP	ENGINEERED	UNP P21189

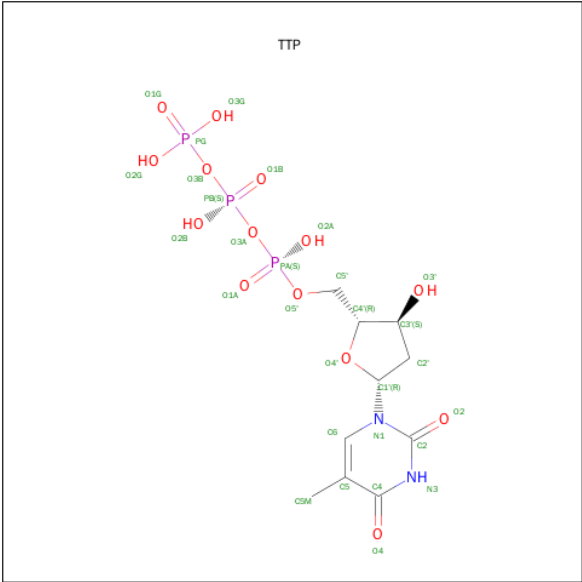
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*AP*AP*GP*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	17	Total	C	N	O	P	0	0	0
			347	166	68	97	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			262	126	48	76	12			

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	690	Total	O	0	0
			690	690		
6	T	46	Total	O	0	0
			46	46		
6	P	25	Total	O	0	0
			25	25		

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 ($RSRZ > 2$). 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 II



• Molecule 2: DNA (5'-D(*TP*AP*AP*GP*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.82Å 100.30Å 126.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 28.18 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.05) 89.5 (28.18-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.203 0.198 , 0.203	Depositor DCC
R_{free} test set	1445 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62952 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7733	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: DOC, MG, TTP

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	0.51	0/6501	0.72	3/8816 (0.0%)
2	T	0.86	0/390	1.26	5/600 (0.8%)
3	P	1.16	4/273 (1.5%)	1.08	1/420 (0.2%)
All	All	0.57	4/7164 (0.1%)	0.78	9/9836 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	904	DC	C3'-O3'	-7.67	1.33	1.44
3	P	904	DC	C4'-C3'	-6.67	1.45	1.52
3	P	904	DC	O3'-P	-6.29	1.53	1.61
3	P	904	DC	P-O5'	-6.04	1.53	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	814	DG	C1'-O4'-C4'	-6.72	103.38	110.10
1	A	509	ARG	NE-CZ-NH2	6.31	123.46	120.30
2	T	814	DG	OP2-P-O3'	6.12	118.67	105.20
2	T	814	DG	C3'-C2'-C1'	-6.11	95.17	102.50
1	A	509	ARG	NE-CZ-NH1	-6.08	117.26	120.30
2	T	818	DA	O4'-C4'-C3'	-5.27	102.39	104.50
1	A	149	PRO	N-CA-C	-5.24	98.47	112.10
2	T	814	DG	O4'-C1'-N9	5.15	111.60	108.00
3	P	902	DT	OP1-P-O3'	5.09	116.41	105.20

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	6332	0	6200	125	0
2	T	347	0	192	9	0
3	P	262	0	148	5	0
4	A	29	0	13	2	0
5	A	2	0	0	0	0
6	A	690	0	0	17	0
6	P	25	0	0	0	0
6	T	46	0	0	2	0
All	All	7733	0	6553	137	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 10.

All (137) 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:636:THR:HG22	1:A:649:GLN:OE1	1.44	1.14
1:A:288:PHE:CE1	1:A:300:LEU:HD11	1.83	1.13
1:A:288:PHE:CE1	1:A:300:LEU:CD1	2.44	1.00
1:A:256:ARG:HG2	1:A:256:ARG:NH1	1.61	1.00
1:A:256:ARG:CG	1:A:256:ARG:HH11	1.75	0.98
1:A:256:ARG:HG2	1:A:256:ARG:HH11	0.81	0.97
1:A:235:LYS:HG3	6:A:1351:HOH:O	1.65	0.97
1:A:298:GLN:HG2	1:A:303:GLU:O	1.63	0.97
1:A:288:PHE:HE1	1:A:300:LEU:CD1	1.80	0.95
1:A:294:GLU:OE2	1:A:305:LYS:HA	1.71	0.90
1:A:549:THR:HG22	6:A:1452:HOH:O	1.70	0.90
1:A:288:PHE:CZ	1:A:300:LEU:HD11	2.07	0.89
1:A:288:PHE:HE1	1:A:300:LEU:HD11	1.30	0.87
1:A:782:LEU:O	1:A:783:PHE:HB2	1.75	0.84
1:A:258:HIS:HB2	1:A:264:VAL:CG1	2.09	0.82
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.43	0.81
2:T:817:DC:H2''	2:T:818:DA:O4'	1.79	0.81
1:A:549:THR:HG23	6:A:1455:HOH:O	1.80	0.81
2:T:803:DA:H2	6:T:500:HOH:O	1.67	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:HG3	1:A:323:GLU:OE2	1.85	0.77
1:A:319:ARG:O	1:A:323:GLU:HG3	1.88	0.74
1:A:397:HIS:HB3	6:A:1322:HOH:O	1.87	0.73
1:A:258:HIS:HB2	1:A:264:VAL:HG12	1.72	0.72
1:A:581:LEU:HD12	1:A:588:SER:HB2	1.71	0.72
1:A:294:GLU:HG3	1:A:305:LYS:HG2	1.73	0.70
1:A:0:HIS:HB3	6:A:1360:HOH:O	1.90	0.70
1:A:298:GLN:HG3	1:A:305:LYS:HG3	1.74	0.69
1:A:303:GLU:OE2	1:A:334:LYS:NZ	2.23	0.69
1:A:388:ALA:HB1	1:A:509:ARG:HD2	1.75	0.69
1:A:260:PHE:CE1	1:A:261:LYS:HE3	2.29	0.68
1:A:379:PRO:O	1:A:383:ARG:HG2	1.93	0.68
1:A:479:GLU:O	1:A:483:GLN:HG3	1.94	0.68
1:A:389:PRO:O	1:A:509:ARG:HD3	1.95	0.67
2:T:817:DC:C2'	2:T:818:DA:C8	2.80	0.65
2:T:815:DC:H2'	2:T:816:DA:C8	2.32	0.64
1:A:258:HIS:CB	1:A:264:VAL:HG12	2.29	0.63
1:A:9:THR:OG1	1:A:11:HIS:HE1	1.82	0.63
1:A:260:PHE:CE1	1:A:261:LYS:CE	2.82	0.62
1:A:384:ALA:O	1:A:463:LYS:HE3	1.99	0.62
3:P:912:DA:H2''	3:P:913:DOC:H5'	1.81	0.62
1:A:119:PHE:HE2	1:A:383:ARG:NH2	1.99	0.61
2:T:817:DC:H2'	2:T:818:DA:C8	2.35	0.61
1:A:126:VAL:HB	1:A:140:LEU:CD2	2.31	0.61
1:A:15:THR:HB	1:A:16:PRO:CD	2.31	0.60
1:A:260:PHE:HE1	1:A:261:LYS:CE	2.13	0.60
1:A:707:ARG:O	1:A:711:GLU:HG3	2.00	0.60
1:A:295:THR:O	1:A:299:GLU:HG3	2.02	0.59
1:A:86:HIS:HE1	1:A:109:ARG:HH11	1.50	0.59
1:A:691:PRO:HG3	1:A:724:ASN:OD1	2.03	0.59
1:A:698:ASN:C	1:A:698:ASN:OD1	2.41	0.59
2:T:817:DC:H2''	2:T:818:DA:C8	2.38	0.58
1:A:260:PHE:HE1	1:A:261:LYS:HE2	1.67	0.58
3:P:903:DG:H2''	3:P:904:DC:O5'	2.03	0.58
1:A:120:ILE:O	1:A:375:HIS:HE1	1.87	0.58
1:A:119:PHE:CE2	1:A:383:ARG:NH2	2.72	0.58
1:A:313:ARG:HH11	1:A:313:ARG:HG3	1.69	0.57
1:A:232:MET:HE2	1:A:232:MET:HA	1.87	0.57
1:A:479:GLU:OE1	1:A:482:ARG:HD3	2.05	0.55
1:A:160:THR:HG22	1:A:166:TYR:CZ	2.42	0.55
1:A:283:SER:HB2	1:A:355:ARG:HH12	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:HIS:HE1	1:A:109:ARG:NH1	2.05	0.55
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.19	0.54
1:A:258:HIS:CE1	1:A:261:LYS:HG3	2.42	0.54
1:A:782:LEU:O	1:A:783:PHE:CB	2.47	0.54
1:A:52:ARG:HG2	1:A:101:VAL:CG2	2.38	0.53
1:A:642:THR:HG23	1:A:756:GLN:NE2	2.23	0.53
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.90	0.53
1:A:298:GLN:NE2	6:A:797:HOH:O	2.36	0.53
1:A:773:ALA:O	1:A:777:THR:HG23	2.09	0.52
3:P:901:DG:C8	3:P:902:DT:H72	2.45	0.51
1:A:724:ASN:O	1:A:725:ARG:HB2	2.09	0.51
1:A:288:PHE:CE1	1:A:300:LEU:HD13	2.43	0.51
1:A:430:THR:HG21	1:A:581:LEU:HD13	1.91	0.51
1:A:311:TRP:HH2	1:A:719:PRO:HD2	1.76	0.50
1:A:125:TRP:HB2	1:A:141:LYS:HG3	1.94	0.50
1:A:424:TYR:CD2	4:A:914:TTP:H2'1	2.47	0.50
1:A:232:MET:HE2	1:A:235:LYS:HD3	1.94	0.49
1:A:264:VAL:O	1:A:264:VAL:CG1	2.60	0.49
1:A:774:THR:CG2	6:A:1449:HOH:O	2.61	0.49
1:A:775:LEU:HD12	6:A:1449:HOH:O	2.12	0.48
1:A:184:GLU:HB3	1:A:197:TYR:CE2	2.49	0.48
1:A:682:LEU:HB3	1:A:752:TYR:CZ	2.49	0.48
1:A:50:VAL:HG13	1:A:65:LEU:HD13	1.95	0.47
1:A:15:THR:HB	1:A:16:PRO:HD2	1.96	0.47
1:A:606:ILE:CG2	6:A:1389:HOH:O	2.63	0.47
1:A:235:LYS:CG	6:A:1351:HOH:O	2.43	0.47
1:A:440:GLU:HG3	1:A:463:LYS:HD3	1.97	0.47
1:A:771:ASN:OD1	1:A:773:ALA:HB3	2.15	0.47
1:A:563:ALA:O	1:A:567:ARG:HG3	2.14	0.47
1:A:294:GLU:CG	1:A:305:LYS:NZ	2.79	0.46
1:A:283:SER:CB	1:A:355:ARG:HH12	2.27	0.46
1:A:20:GLU:HG2	6:A:1078:HOH:O	2.15	0.46
1:A:774:THR:HG23	6:A:1449:HOH:O	2.16	0.46
1:A:682:LEU:HB3	1:A:752:TYR:CE1	2.51	0.46
1:A:294:GLU:HG2	1:A:305:LYS:HZ2	1.80	0.46
4:A:914:TTP:HM52	3:P:913:DOC:C5	2.45	0.46
1:A:712:GLU:HG2	1:A:742:TYR:CG	2.50	0.46
1:A:86:HIS:CE1	1:A:109:ARG:HD3	2.51	0.46
1:A:642:THR:H	1:A:756:GLN:NE2	2.13	0.45
1:A:275:ILE:HD13	1:A:364:ASP:HB3	1.98	0.45
1:A:700:PRO:HD2	1:A:703:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:O	1:A:320:ARG:HG3	2.17	0.45
1:A:313:ARG:NH1	1:A:313:ARG:HG3	2.31	0.45
1:A:405:MET:HG2	1:A:406:ASP:O	2.17	0.45
1:A:571:GLN:NE2	6:A:1485:HOH:O	2.44	0.45
1:A:294:GLU:HG3	1:A:305:LYS:HZ3	1.81	0.45
1:A:765:LEU:N	1:A:766:PRO:CD	2.80	0.45
2:T:803:DA:C2	6:T:500:HOH:O	2.52	0.44
1:A:258:HIS:CE1	1:A:261:LYS:HE3	2.52	0.44
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.66	0.44
1:A:604:PRO:HB3	6:A:1088:HOH:O	2.18	0.44
1:A:15:THR:CB	1:A:16:PRO:CD	2.94	0.44
1:A:176:ARG:NH1	1:A:192:ASP:O	2.43	0.43
1:A:554:LYS:O	1:A:557:HIS:HE1	2.01	0.43
1:A:303:GLU:OE2	1:A:334:LYS:CE	2.67	0.43
1:A:294:GLU:HG3	1:A:305:LYS:NZ	2.33	0.43
1:A:581:LEU:HD12	1:A:588:SER:CB	2.45	0.43
1:A:316:GLU:OE2	1:A:319:ARG:NH2	2.49	0.43
1:A:430:THR:CG2	1:A:581:LEU:HD13	2.48	0.42
1:A:235:LYS:HD2	6:A:1440:HOH:O	2.19	0.42
1:A:201:ARG:N	1:A:202:PRO:CD	2.82	0.42
1:A:381:MET:HE1	1:A:388:ALA:HB2	2.00	0.42
1:A:446:ASP:OD1	1:A:449:HIS:CD2	2.72	0.42
1:A:626:LYS:HE3	1:A:626:LYS:HB3	1.48	0.42
1:A:119:PHE:HE2	1:A:383:ARG:HH21	1.66	0.42
1:A:446:ASP:OD2	1:A:449:HIS:HD2	2.02	0.42
1:A:771:ASN:O	1:A:775:LEU:HD13	2.20	0.41
3:P:901:DG:N9	3:P:902:DT:H72	2.35	0.41
1:A:93:GLU:HG3	1:A:106:ALA:CB	2.49	0.41
1:A:54:GLN:NE2	6:A:1395:HOH:O	2.54	0.41
1:A:616:ARG:HD3	2:T:809:DG:H4'	2.01	0.41
1:A:699:VAL:O	1:A:704:ARG:NH2	2.53	0.41
1:A:596:THR:HG22	1:A:597:HIS:N	2.36	0.40
1:A:755:ARG:HD2	2:T:812:DA:OP2	2.20	0.40
1:A:232:MET:CE	1:A:232:MET:HA	2.51	0.40
1:A:141:LYS:HG2	6:A:1075:HOH:O	2.20	0.40
1:A:394:VAL:HA	1:A:395:PRO:HD3	1.97	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	774/786 (98%)	762 (98%)	11 (1%)	1 (0%)	56	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER

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	666/672 (99%)	651 (98%)	15 (2%)	58	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	54	GLN
1	A	66	THR
1	A	187	ASP
1	A	256	ARG
1	A	264	VAL
1	A	290	SER
1	A	298	GLN
1	A	323	GLU
1	A	500	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561	GLU
1	A	623	GLU
1	A	626	LYS
1	A	636	THR
1	A	774	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	54	GLN
1	A	86	HIS
1	A	132	ASN
1	A	298	GLN
1	A	332	ASN
1	A	375	HIS
1	A	390	ASN
1	A	449	HIS
1	A	557	HIS
1	A	713	ASN
1	A	756	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	DOC	P	913	3,2	11,19,20	0.75	0	14,26,29	1.44	2 (14%)

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	DOC	P	913	3,2	-	0/3/18/19	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	913	DOC	C2-N3-C4	3.05	119.92	115.61
3	P	913	DOC	C3'-C2'-C1'	3.21	106.29	102.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	913	DOC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are 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	TTP	A	914	5	21,30,30	2.81	5 (23%)	31,47,47	3.01	8 (25%)

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
4	TTP	A	914	5	-	0/18/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	914	TTP	PG-O1G	-2.98	1.41	1.51
4	A	914	TTP	O4-C4	-2.74	1.18	1.24
4	A	914	TTP	C4-N3	4.76	1.42	1.33
4	A	914	TTP	C6-N1	5.42	1.43	1.35
4	A	914	TTP	C5M-C5	8.96	1.68	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	914	TTP	C5-C4-N3	-4.79	119.80	125.14
4	A	914	TTP	PB-O3B-PG	-3.96	119.39	132.67
4	A	914	TTP	C2'-C1'-N1	-3.67	105.22	114.16
4	A	914	TTP	PB-O3A-PA	-3.58	122.68	132.73
4	A	914	TTP	O4'-C1'-C2'	-2.34	101.61	106.27
4	A	914	TTP	O4'-C1'-N1	2.42	111.91	107.72
4	A	914	TTP	C5M-C5-C6	4.24	127.16	118.62
4	A	914	TTP	C4-N3-C2	13.09	126.56	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	914	TTP	2	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	780/786 (99%)	0.10	35 (4%) 37 42	13, 24, 50, 68	0
2	T	17/17 (100%)	0.70	5 (29%) 1 0	21, 34, 79, 87	0
3	P	12/13 (92%)	0.46	2 (16%) 2 2	19, 50, 68, 73	0
All	All	809/816 (99%)	0.12	42 (5%) 31 36	13, 25, 53, 87	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	TRP	7.9
1	A	260	PHE	6.8
1	A	310	PRO	6.8
1	A	306	SER	5.8
1	A	259	GLY	5.2
1	A	263	GLY	5.1
1	A	305	LYS	4.8
1	A	1	MET	4.8
1	A	697	ARG	4.8
1	A	262	ASN	4.7
1	A	264	VAL	4.6
1	A	0	HIS	4.5
2	T	818	DA	4.5
1	A	304	GLY	3.6
1	A	-1	PRO	3.6
1	A	696	GLN	3.6
1	A	625	ASP	3.5
2	T	817	DC	3.4
1	A	698	ASN	3.3
1	A	258	HIS	3.3
1	A	777	THR	3.3
1	A	261	LYS	3.1
1	A	59	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	2.9
1	A	189	SER	2.8
1	A	782	LEU	2.8
2	T	816	DA	2.7
1	A	774	THR	2.7
1	A	266	PHE	2.7
1	A	265	PHE	2.6
3	P	903	DG	2.5
1	A	433	ILE	2.4
1	A	190	SER	2.4
1	A	16	PRO	2.3
1	A	214	ASN	2.3
1	A	132	ASN	2.3
3	P	901	DG	2.2
1	A	771	ASN	2.2
2	T	802	DT	2.2
1	A	294	GLU	2.1
1	A	322	ALA	2.1
2	T	803	DA	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, 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(Å ²)	Q<0.9
3	DOC	P	913	18/19	0.97	0.10	-	15,19,22,23	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. 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	TTP	A	914	29/29	0.97	0.10	-0.54	16,19,21,21	0
5	MG	A	1001	1/1	0.95	0.05	-2.39	23,23,23,23	0
5	MG	A	1002	1/1	0.98	0.08	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.