



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:00 AM GMT

PDB ID : 3GV7
Title : Human DNA polymerase iota in complex with T template DNA and incoming dTTP
Authors : Kirouac, K.N.; Ling, H.
Deposited on : 2009-03-30
Resolution : 2.20 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

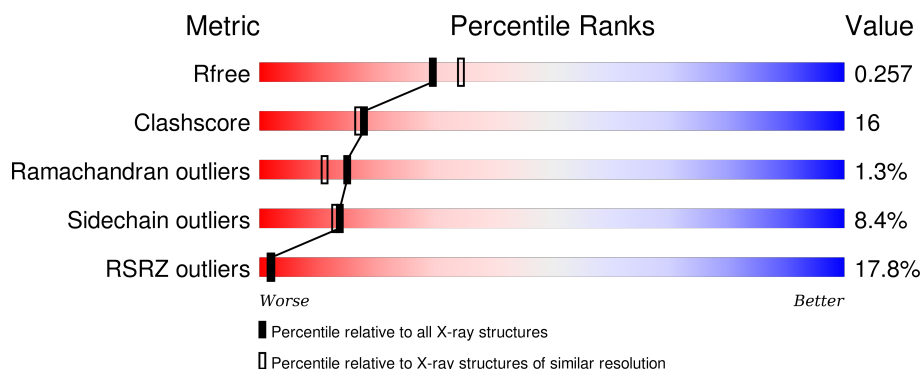
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	B	420	<div> <div>16%</div> <div>65%</div> <div>20%</div> <div>5%</div> <div>10%</div> </div>
2	T	9	<div> <div>11%</div> <div>56%</div> <div>33%</div> <div>11%</div> </div>
3	P	7	<div> <div>14%</div> <div>43%</div> <div>43%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3596 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	B	377	Total	C	N	O	S	0	0	0
			2978	1883	519	554	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			183	88	32	54	9			

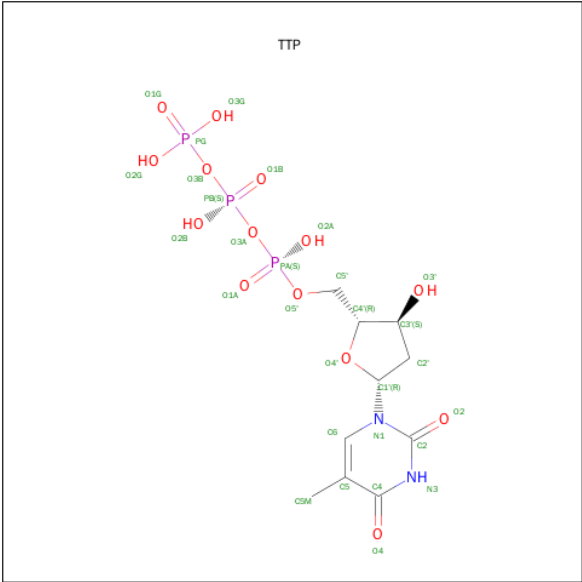
- Molecule 3 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

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

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

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



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

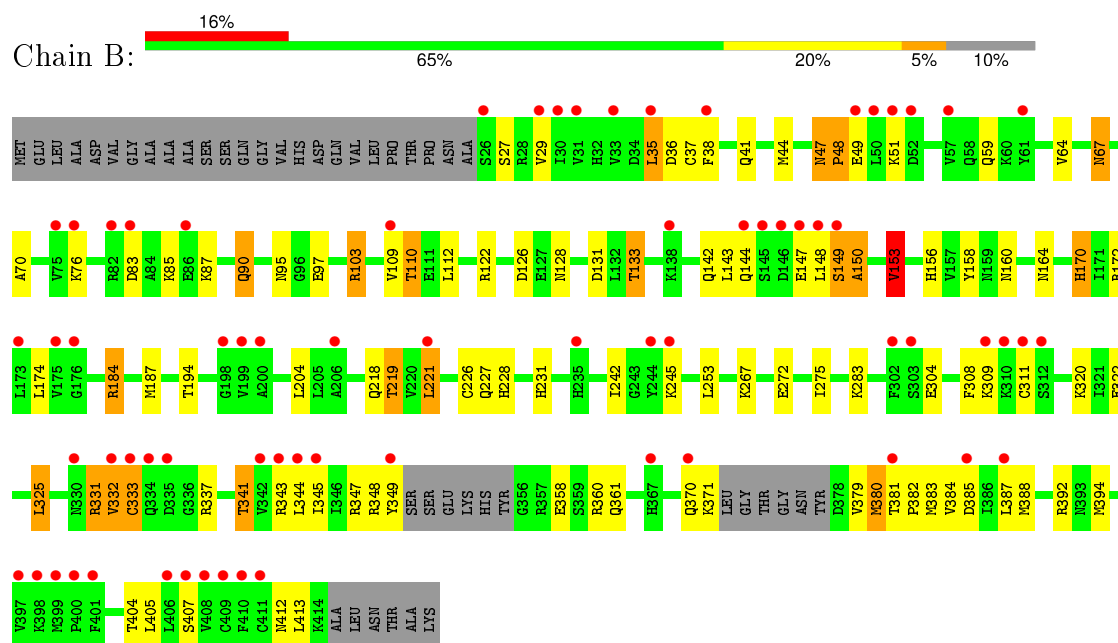
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	240	Total	O	0	0
			240	240		
6	T	16	Total	O	0	0
			16	16		
6	P	9	Total	O	0	0
			9	9		

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.

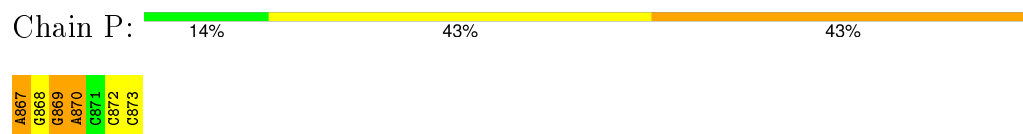
- Molecule 1: DNA polymerase iota



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



- Molecule 3: 5'-D(*AP*GP*GP*AP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.19 Å 97.19 Å 201.94 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.04 – 2.20 27.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.04-2.20) 99.8 (27.03-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.209 , 0.258 0.205 , 0.257	Depositor DCC
R_{free} test set	604 reflections (2.10%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 29366 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3596	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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: 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	B	0.59	1/3021 (0.0%)	0.74	9/4071 (0.2%)
2	T	1.18	0/204	1.74	5/313 (1.6%)
3	P	1.17	0/156	2.03	9/238 (3.8%)
All	All	0.68	1/3381 (0.0%)	0.95	23/4622 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	383	MET	CG-SD	5.75	1.96	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	867	DA	O4'-C4'-C3'	-11.69	98.99	106.00
3	P	872	DC	O4'-C4'-C3'	-8.02	101.19	106.00
1	B	184	ARG	NE-CZ-NH1	-7.52	116.54	120.30
3	P	869	DG	O4'-C1'-N9	7.23	113.06	108.00
1	B	103	ARG	NE-CZ-NH2	-6.83	116.88	120.30
3	P	870	DA	C5'-C4'-C3'	-6.38	102.61	114.10
2	T	847	DT	O4'-C1'-N1	-6.37	103.54	108.00
1	B	184	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	B	103	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	T	845	DC	O4'-C1'-N1	6.28	112.39	108.00
3	P	868	DG	O4'-C1'-C2'	-6.25	100.90	105.90
3	P	867	DA	O5'-C5'-C4'	5.86	125.64	111.00
2	T	841	DG	O4'-C1'-N9	5.78	112.04	108.00
3	P	870	DA	O4'-C1'-N9	5.72	112.00	108.00
3	P	867	DA	O4'-C1'-N9	5.65	111.95	108.00
1	B	153	VAL	CB-CA-C	-5.54	100.88	111.40
1	B	331	ARG	NE-CZ-NH2	-5.41	117.60	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	842	DG	O4'-C4'-C3'	-5.27	102.39	104.50
1	B	149	SER	C-N-CA	5.18	134.65	121.70
3	P	873	DC	O4'-C1'-N1	5.12	111.59	108.00
1	B	149	SER	N-CA-C	5.12	124.81	111.00
2	T	847	DT	N1-C1'-C2'	5.04	122.18	112.60
1	B	221	LEU	CA-CB-CG	5.04	126.89	115.30

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	B	2978	0	3073	101	0
2	T	183	0	103	0	1
3	P	139	0	77	2	1
4	B	2	0	0	0	0
5	B	29	0	13	2	0
6	B	240	0	0	15	0
6	P	9	0	0	1	0
6	T	16	0	0	0	0
All	All	3596	0	3266	104	1

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 16.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLU:HB3	1:B:394:MET:HE3	1.33	1.11
1:B:131:ASP:OD2	1:B:133:THR:HG23	1.54	1.06
1:B:226:CYS:SG	6:B:616:HOH:O	2.12	1.04
1:B:29:VAL:H	1:B:133:THR:HG22	1.16	1.03
5:B:421:TTP:O2A	6:B:496:HOH:O	1.78	1.01
1:B:153:VAL:HG13	1:B:174:LEU:HD22	1.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:OD2	1:B:194:THR:HG22	1.61	0.98
1:B:149:SER:N	1:B:150:ALA:HB3	1.80	0.95
1:B:358:GLU:HB3	1:B:394:MET:CE	2.00	0.91
1:B:41:GLN:HE22	1:B:194:THR:H	1.15	0.89
1:B:311:CYS:SG	6:B:659:HOH:O	2.31	0.88
1:B:394:MET:SD	6:B:631:HOH:O	2.31	0.87
1:B:164:ASN:H	1:B:170:HIS:HD2	1.25	0.85
1:B:36:ASP:OD2	1:B:194:THR:CG2	2.27	0.81
1:B:332:VAL:HG12	1:B:333:CYS:HB2	1.65	0.79
1:B:110:THR:CG2	1:B:122:ARG:HH11	1.96	0.79
1:B:348:ARG:O	1:B:349:TYR:HB2	1.83	0.78
1:B:90:GLN:HE21	1:B:90:GLN:H	1.29	0.78
1:B:347:ARG:HE	1:B:404:THR:HG23	1.49	0.77
1:B:325:LEU:HD21	1:B:387:LEU:HD13	1.67	0.76
1:B:110:THR:HG21	1:B:122:ARG:HH11	1.52	0.74
3:P:869:DG:H1'	6:P:197:HOH:O	1.87	0.74
1:B:332:VAL:N	1:B:333:CYS:CB	2.52	0.71
5:B:421:TTP:O1A	6:B:661:HOH:O	2.08	0.71
1:B:341:THR:HG23	1:B:412:ASN:HB3	1.72	0.70
1:B:381:THR:O	1:B:385:ASP:OD2	2.10	0.70
1:B:325:LEU:HD21	1:B:387:LEU:CD1	2.23	0.68
1:B:358:GLU:CB	1:B:394:MET:HE3	2.17	0.68
1:B:332:VAL:CA	1:B:333:CYS:HB2	2.24	0.67
1:B:358:GLU:CB	1:B:394:MET:CE	2.72	0.66
1:B:332:VAL:N	1:B:333:CYS:HB3	2.12	0.65
1:B:332:VAL:N	1:B:333:CYS:HB2	2.11	0.65
1:B:242:ILE:O	6:B:425:HOH:O	2.15	0.64
1:B:388:MET:HB3	1:B:392:ARG:NH1	2.13	0.64
1:B:156:HIS:HB2	1:B:219:THR:HB	1.79	0.64
1:B:304:GLU:OE2	6:B:486:HOH:O	2.15	0.63
1:B:29:VAL:N	1:B:133:THR:HG22	2.01	0.63
1:B:267:LYS:HE3	6:B:630:HOH:O	1.99	0.62
1:B:29:VAL:H	1:B:133:THR:CG2	2.04	0.62
1:B:345:ILE:HB	1:B:407:SER:HB3	1.83	0.61
1:B:267:LYS:HG2	6:B:471:HOH:O	2.02	0.60
1:B:332:VAL:HG12	1:B:333:CYS:CB	2.31	0.59
1:B:149:SER:N	1:B:150:ALA:CB	2.59	0.59
1:B:332:VAL:CG1	1:B:333:CYS:HB2	2.32	0.58
1:B:331:ARG:C	1:B:333:CYS:HB3	2.24	0.58
1:B:35:LEU:HD11	1:B:187:MET:CE	2.34	0.58
1:B:67:ASN:ND2	1:B:70:ALA:H	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:THR:CG2	6:B:443:HOH:O	2.51	0.58
1:B:164:ASN:H	1:B:170:HIS:CD2	2.15	0.57
1:B:90:GLN:NE2	1:B:90:GLN:H	2.00	0.57
1:B:112:LEU:C	1:B:112:LEU:HD23	2.24	0.57
1:B:322:GLU:HG2	1:B:384:VAL:HG11	1.86	0.57
1:B:103:ARG:NH2	6:B:602:HOH:O	2.38	0.56
1:B:184:ARG:HE	1:B:218:GLN:HE21	1.53	0.56
1:B:332:VAL:CA	1:B:333:CYS:CB	2.84	0.56
1:B:149:SER:H	1:B:150:ALA:HB3	1.66	0.55
1:B:347:ARG:NE	1:B:404:THR:HG23	2.22	0.55
1:B:388:MET:HB3	1:B:392:ARG:HH12	1.72	0.54
1:B:67:ASN:HD22	1:B:67:ASN:C	2.11	0.54
1:B:343:ARG:NH2	1:B:361:GLN:HE22	2.04	0.54
1:B:245:LYS:HG3	3:P:870:DA:H5'	1.90	0.52
1:B:184:ARG:HH11	1:B:218:GLN:HE21	1.57	0.52
1:B:348:ARG:O	1:B:349:TYR:CB	2.57	0.51
1:B:219:THR:HG22	6:B:443:HOH:O	2.11	0.51
1:B:35:LEU:HD11	1:B:187:MET:HE1	1.92	0.51
1:B:158:TYR:OH	1:B:228:HIS:HD2	1.94	0.50
1:B:360:ARG:HG2	1:B:394:MET:CG	2.41	0.50
1:B:344:LEU:HB2	1:B:387:LEU:HD23	1.95	0.49
1:B:144:GLN:HB2	1:B:147:GLU:HG3	1.94	0.49
1:B:35:LEU:HD23	1:B:38:PHE:CD1	2.48	0.48
1:B:110:THR:HG21	1:B:122:ARG:HG2	1.95	0.48
1:B:332:VAL:CB	1:B:333:CYS:HB2	2.43	0.48
1:B:95:ASN:HD21	1:B:97:GLU:HB2	1.79	0.48
1:B:413:LEU:N	1:B:413:LEU:HD12	2.29	0.47
1:B:44:MET:HE1	1:B:67:ASN:OD1	2.15	0.47
1:B:325:LEU:CD2	1:B:387:LEU:HD13	2.40	0.47
1:B:35:LEU:CD1	1:B:187:MET:HE1	2.45	0.47
1:B:48:PRO:O	1:B:51:LYS:HG2	2.14	0.47
1:B:231:HIS:HE1	6:B:452:HOH:O	1.97	0.47
1:B:253:LEU:HD11	1:B:272:GLU:HG2	1.95	0.47
1:B:44:MET:HE2	1:B:51:LYS:HA	1.98	0.46
1:B:110:THR:CG2	1:B:122:ARG:NH1	2.75	0.46
1:B:110:THR:HB	1:B:128:ASN:OD1	2.16	0.45
1:B:267:LYS:HA	1:B:267:LYS:HD3	1.64	0.45
1:B:35:LEU:HD21	1:B:109:VAL:HG21	1.98	0.45
1:B:83:ASP:O	1:B:87:LYS:HB2	2.16	0.45
1:B:231:HIS:HD2	6:B:439:HOH:O	2.00	0.45
1:B:227:GLN:NE2	6:B:616:HOH:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:C	1:B:150:ALA:HB3	2.36	0.44
1:B:44:MET:CE	1:B:67:ASN:OD1	2.66	0.44
1:B:380:MET:O	1:B:384:VAL:HG22	2.18	0.44
1:B:35:LEU:HD23	1:B:38:PHE:CE1	2.54	0.43
1:B:35:LEU:HD11	1:B:187:MET:HE3	2.00	0.43
1:B:41:GLN:HE22	1:B:194:THR:N	1.98	0.43
1:B:41:GLN:NE2	1:B:194:THR:H	1.98	0.42
1:B:27:SER:O	1:B:172:ARG:NH2	2.53	0.42
1:B:184:ARG:HH11	1:B:218:GLN:NE2	2.18	0.42
1:B:358:GLU:CB	1:B:394:MET:HE1	2.50	0.41
1:B:47:ASN:C	1:B:49:GLU:H	2.22	0.41
1:B:59:GLN:OE1	1:B:64:VAL:HG11	2.21	0.41
1:B:47:ASN:HD21	1:B:49:GLU:HB2	1.86	0.41
1:B:47:ASN:ND2	1:B:49:GLU:HB2	2.36	0.40
1:B:379:VAL:O	1:B:382:PRO:HG2	2.20	0.40
1:B:345:ILE:N	1:B:345:ILE:HD12	2.37	0.40

All (1) 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:T:847:DT:O3'	3:P:867:DA:O5'[12_544]	1.83	0.37

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	B	371/420 (88%)	359 (97%)	7 (2%)	5 (1%)	15 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	B	333	CYS
1	B	370	GLN
1	B	37	CYS
1	B	48	PRO

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	B	344/376 (92%)	315 (92%)	29 (8%)	14	13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	LEU
1	B	47	ASN
1	B	67	ASN
1	B	76	LYS
1	B	85	LYS
1	B	90	GLN
1	B	110	THR
1	B	126	ASP
1	B	133	THR
1	B	142	GLN
1	B	143	LEU
1	B	153	VAL
1	B	160	ASN
1	B	170	HIS
1	B	204	LEU
1	B	219	THR
1	B	221	LEU
1	B	275	ILE
1	B	283	LYS
1	B	308	PHE
1	B	309	LYS
1	B	320	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	325	LEU
1	B	332	VAL
1	B	337	ARG
1	B	341	THR
1	B	371	LYS
1	B	380	MET
1	B	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	GLN
1	B	47	ASN
1	B	58	GLN
1	B	90	GLN
1	B	95	ASN
1	B	156	HIS
1	B	170	HIS
1	B	217	GLN
1	B	218	GLN
1	B	228	HIS
1	B	231	HIS
1	B	279	GLN
1	B	319	ASN
1	B	330	ASN
1	B	361	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 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	$\# Z > 2$
5	TTP	B	421	4	21,30,30	0.58	0	31,47,47	1.59	5 (16%)

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	TTP	B	421	4	-	0/18/34/34	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	421	TTP	C5-C4-N3	-4.74	119.86	125.14
5	B	421	TTP	PB-O3B-PG	-2.45	124.44	132.67
5	B	421	TTP	PB-O3A-PA	-2.21	126.53	132.73
5	B	421	TTP	O4'-C1'-N1	3.09	113.07	107.72
5	B	421	TTP	C4-N3-C2	4.63	119.25	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
5	B	421	TTP	2	0

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, 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	B	377/420 (89%)	1.00	69 (18%)  	31, 49, 66, 72	0
2	T	9/9 (100%)	0.40	1 (11%)  	39, 42, 57, 79	0
3	P	7/7 (100%)	-0.17	0  	41, 43, 48, 52	0
All	All	393/436 (90%)	0.96	70 (17%)  	31, 48, 66, 79	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	LYS	6.1
1	B	26	SER	6.1
1	B	349	TYR	5.7
1	B	199	VAL	5.3
1	B	311	CYS	5.0
1	B	146	ASP	5.0
1	B	345	ILE	5.0
1	B	400	PRO	4.9
1	B	409	CYS	4.9
1	B	149	SER	4.8
1	B	82	ARG	4.8
1	B	399	MET	4.7
1	B	244	TYR	4.6
1	B	145	SER	4.6
1	B	401	PHE	4.4
1	B	61	TYR	4.2
1	B	33	VAL	4.2
2	T	839	DA	4.2
1	B	31	VAL	4.1
1	B	330	ASN	4.0
1	B	332	VAL	4.0
1	B	385	ASP	4.0
1	B	49	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	344	LEU	3.9
1	B	387	LEU	3.9
1	B	29	VAL	3.8
1	B	335	ASP	3.8
1	B	148	LEU	3.7
1	B	333	CYS	3.7
1	B	408	VAL	3.7
1	B	173	LEU	3.7
1	B	86	GLU	3.5
1	B	407	SER	3.4
1	B	367	HIS	3.4
1	B	334	GLN	3.3
1	B	370	GLN	3.2
1	B	342	VAL	3.0
1	B	144	GLN	3.0
1	B	397	VAL	2.9
1	B	30	ILE	2.9
1	B	175	VAL	2.9
1	B	50	LEU	2.8
1	B	221	LEU	2.7
1	B	76	LYS	2.7
1	B	200	ALA	2.7
1	B	309	LYS	2.7
1	B	75	VAL	2.7
1	B	303	SER	2.6
1	B	83	ASP	2.6
1	B	147	GLU	2.6
1	B	410	PHE	2.6
1	B	138	LYS	2.5
1	B	206	ALA	2.5
1	B	302	PHE	2.5
1	B	406	LEU	2.5
1	B	235	HIS	2.5
1	B	310	LYS	2.5
1	B	198	GLY	2.3
1	B	51	LYS	2.3
1	B	176	GLY	2.2
1	B	245	LYS	2.2
1	B	35	LEU	2.1
1	B	109	VAL	2.1
1	B	411	CYS	2.1
1	B	343	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	ASP	2.1
1	B	312	SER	2.1
1	B	38	PHE	2.0
1	B	57	VAL	2.0
1	B	381	THR	2.0

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(Å ²)	Q<0.9
5	TTP	B	421	29/29	0.97	0.11	-1.76	38,44,47,50	0
4	MG	B	871	1/1	0.96	0.03	-3.44	32,32,32,32	0
4	MG	B	422	1/1	0.75	0.28	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.