



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 06:26 AM GMT

PDB ID : 3H4B
Title : Ternary complex of human DNA polymerase iota with template U/T and incoming dATP
Authors : Jain, R.; Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on : 2009-04-18
Resolution : 2.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

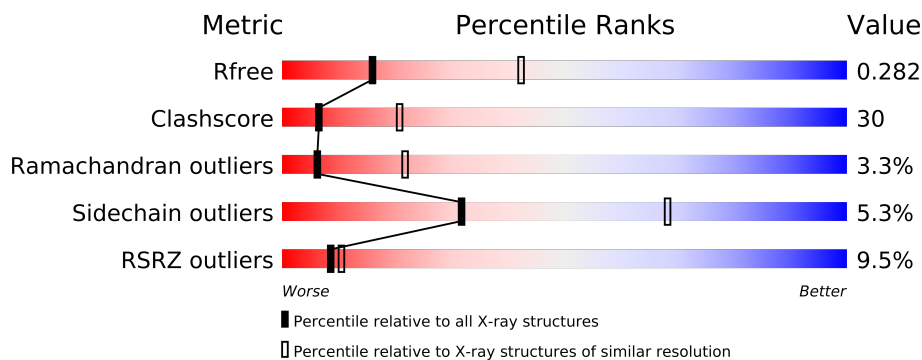
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.85 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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	390	
2	P	7	
3	T	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3404 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2877	1809	504	543	21			

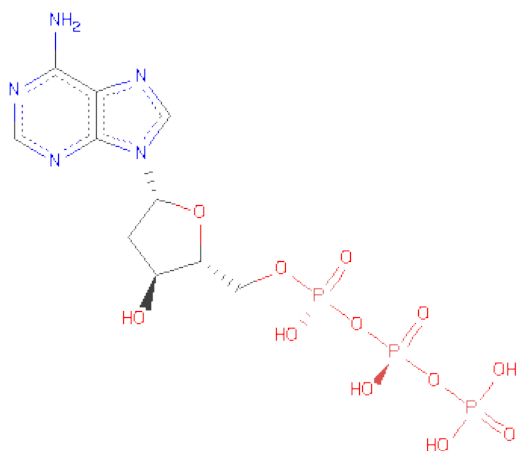
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	T	9	Total	Br	C	N	O	P	0	1	0
			201	2	96	31	63	9			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

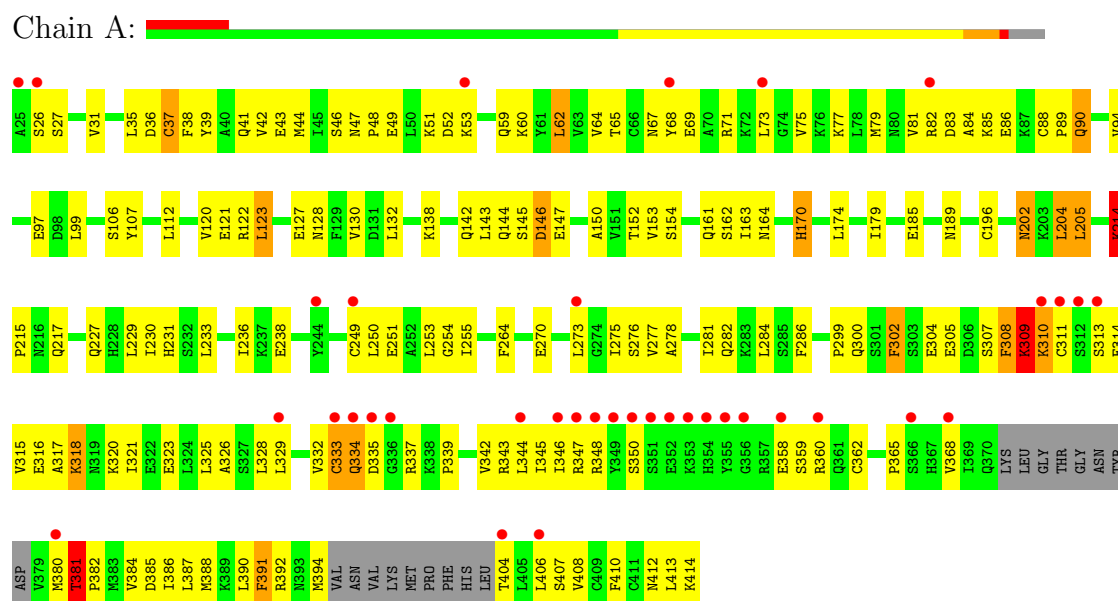
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	141	Total	O	0	0
			141	141		
6	P	7	Total	O	0	0
			7	7		
6	T	8	Total	O	0	0
			8	8		

3 Residue-property plots

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(*AP*GP*GP*AP*CP*CP*(DOC))-3'



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.00Å 98.00Å 203.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.73 – 2.85 41.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.73-2.85) 96.6 (41.54-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.91 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.281 0.240 , 0.282	Depositor DCC
R_{free} test set	1094 reflections (8.69%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14175 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3404	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, DTP, BRU

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	0.37	0/2915	0.64	1/3934 (0.0%)
2	P	0.47	0/136	0.77	0/208
3	T	0.50	0/178	0.90	0/271
All	All	0.38	0/3229	0.66	1/4413 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
3	T	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LYS	N-CA-C	6.24	127.86	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	871	DC	Sidechain
2	P	872	DC	Sidechain
3	T	842	DG	Sidechain
3	T	843	DG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2877	0	2899	163	0
2	P	139	0	79	4	0
3	T	201	0	111	29	0
4	A	30	0	10	3	0
5	A	1	0	0	0	0
6	A	141	0	0	9	0
6	P	7	0	0	1	0
6	T	8	0	0	2	0
All	All	3404	0	3099	189	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (189) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:MET:HE2	1:A:51:LYS:HA	1.41	1.01
3:T:842:DG:H2''	3:T:843:DG:H5''	1.47	0.95
1:A:77:LYS:HB2	1:A:77:LYS:NZ	1.87	0.89
1:A:344:LEU:HD11	1:A:387:LEU:HD22	1.53	0.87
3:T:842:DG:H2''	3:T:843:DG:C5'	2.06	0.85
1:A:309:LYS:H	1:A:309:LYS:HD3	1.39	0.84
1:A:365:PRO:O	1:A:368:VAL:HG22	1.77	0.84
1:A:313:SER:O	1:A:314:GLU:HB2	1.78	0.81
1:A:388:MET:O	1:A:391:PHE:HB3	1.80	0.81
3:T:839:DT:H2''	3:T:840[A]:BRU:O5'	1.82	0.79
1:A:270:GLU:HG3	1:A:275:ILE:HA	1.65	0.78
1:A:59:GLN:OE1	3:T:840[B]:BRU:H6	1.86	0.75
1:A:75:VAL:HA	1:A:79:MET:HE2	1.68	0.75
1:A:321:ILE:O	1:A:325:LEU:HD13	1.87	0.75
1:A:44:MET:CE	1:A:67:ASN:HD22	1.99	0.75
1:A:347:ARG:HD2	1:A:404:THR:OG1	1.87	0.75
1:A:309:LYS:H	1:A:309:LYS:CD	1.96	0.74
1:A:164:ASN:H	1:A:170:HIS:HD2	1.36	0.73
1:A:304:GLU:HG3	1:A:328:LEU:HG	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:T:841:DG:H2''	3:T:842:DG:H5''	1.69	0.72
1:A:384:VAL:O	1:A:388:MET:HG2	1.89	0.71
1:A:77:LYS:HB2	1:A:77:LYS:HZ2	1.54	0.70
1:A:344:LEU:HD21	1:A:387:LEU:HB3	1.71	0.70
1:A:39:TYR:HB2	1:A:65:THR:HG21	1.74	0.69
3:T:839:DT:H2'	3:T:840[A]:BRU:BR	2.48	0.68
1:A:254:GLY:O	6:A:469:HOH:O	2.12	0.68
1:A:318:LYS:HD2	1:A:388:MET:HE1	1.76	0.67
3:T:841:DG:C2'	3:T:842:DG:H5''	2.24	0.67
1:A:51:LYS:O	1:A:53:LYS:N	2.28	0.67
1:A:77:LYS:HE2	4:A:875:DTP:PB	2.34	0.67
4:A:875:DTP:O1G	6:A:526:HOH:O	2.12	0.67
1:A:310:LYS:HG3	6:A:507:HOH:O	1.94	0.67
1:A:79:MET:CE	1:A:84:ALA:HA	2.25	0.67
1:A:44:MET:HE1	1:A:67:ASN:HD22	1.59	0.66
1:A:365:PRO:HB2	1:A:368:VAL:HG13	1.78	0.66
1:A:335:ASP:OD2	1:A:337:ARG:HD3	1.96	0.66
3:T:841:DG:H1'	3:T:842:DG:H5''	1.78	0.65
1:A:71:ARG:HH22	4:A:875:DTP:PG	2.19	0.65
1:A:233:LEU:HD22	1:A:238:GLU:HB3	1.79	0.65
1:A:305:GLU:HG3	1:A:407:SER:HB3	1.78	0.65
1:A:132:LEU:HD22	1:A:179:ILE:HG21	1.79	0.64
2:P:870:DA:H1'	2:P:871:DC:H5'	1.79	0.64
1:A:325:LEU:HD11	1:A:387:LEU:CD1	2.27	0.64
1:A:320:LYS:O	1:A:323:GLU:HB2	1.97	0.64
2:P:867:DA:H1'	2:P:868:DG:H5'	1.80	0.64
1:A:315:VAL:C	1:A:317:ALA:H	2.00	0.63
1:A:381:THR:O	6:A:517:HOH:O	2.16	0.63
1:A:69:GLU:O	1:A:73:LEU:HD13	1.99	0.63
1:A:387:LEU:HA	1:A:390:LEU:HD12	1.81	0.62
1:A:381:THR:OG1	1:A:382:PRO:HD3	1.98	0.62
1:A:325:LEU:O	1:A:329:LEU:HD13	1.99	0.62
1:A:62:LEU:CD1	3:T:840[A]:BRU:H5''	2.30	0.62
1:A:88:CYS:SG	1:A:90:GLN:HG3	2.40	0.62
1:A:143:LEU:HA	1:A:147:GLU:OE2	1.98	0.62
1:A:43:GLU:HG3	1:A:94:VAL:HG21	1.81	0.61
1:A:214:LYS:HB3	1:A:215:PRO:HD3	1.83	0.61
1:A:51:LYS:C	1:A:53:LYS:H	2.04	0.60
1:A:164:ASN:H	1:A:170:HIS:CD2	2.18	0.60
1:A:202:ASN:ND2	1:A:205:LEU:H	2.00	0.59
2:P:870:DA:N3	6:P:80:HOH:O	2.32	0.58
1:A:300:GLN:NE2	6:A:491:HOH:O	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:CYS:SG	1:A:214:LYS:O	2.62	0.57
1:A:249:CYS:SG	1:A:273:LEU:HD21	2.44	0.57
1:A:107:TYR:OH	1:A:299:PRO:HG3	2.05	0.57
3:T:839:DT:H5"	6:T:170:HOH:O	2.04	0.57
1:A:62:LEU:HD11	3:T:839:DT:O2	2.05	0.57
1:A:44:MET:HE3	1:A:67:ASN:HD22	1.69	0.56
1:A:59:GLN:OE1	1:A:64:VAL:HG11	2.05	0.56
1:A:81:VAL:HG12	1:A:85:LYS:HE3	1.87	0.56
1:A:85:LYS:O	1:A:89:PRO:HG3	2.06	0.56
1:A:227:GLN:O	1:A:230:ILE:HG22	2.05	0.56
1:A:325:LEU:HD11	1:A:387:LEU:HD11	1.88	0.56
1:A:79:MET:HE3	1:A:84:ALA:HA	1.87	0.56
3:T:839:DT:H2"	3:T:840[B]:BRU:O5'	2.06	0.55
1:A:35:LEU:HD13	6:A:436:HOH:O	2.05	0.55
1:A:79:MET:HE1	1:A:84:ALA:HA	1.89	0.54
1:A:332:VAL:CG1	1:A:339:PRO:HD3	2.37	0.54
1:A:27:SER:HA	6:A:498:HOH:O	2.08	0.54
1:A:62:LEU:HD11	3:T:839:DT:C2	2.42	0.54
1:A:62:LEU:HD12	3:T:840[A]:BRU:H5"	1.89	0.54
1:A:385:ASP:HA	1:A:388:MET:HG2	1.89	0.54
1:A:163:ILE:HD13	1:A:174:LEU:HD11	1.90	0.54
1:A:339:PRO:HG3	1:A:410:PHE:HD2	1.74	0.53
1:A:250:LEU:HA	1:A:253:LEU:HD12	1.89	0.53
2:P:868:DG:H2"	2:P:869:DG:OP2	2.07	0.53
1:A:343:ARG:C	1:A:344:LEU:HD12	2.28	0.53
1:A:82:ARG:HG2	6:A:490:HOH:O	2.08	0.53
1:A:325:LEU:CD1	1:A:408:VAL:HG21	2.38	0.53
1:A:388:MET:HE3	1:A:388:MET:HA	1.89	0.53
1:A:204:LEU:HG	1:A:284:LEU:HD22	1.89	0.53
1:A:215:PRO:O	1:A:217:GLN:HG3	2.09	0.52
1:A:365:PRO:HB2	1:A:368:VAL:CG1	2.40	0.52
1:A:106:SER:OG	1:A:122:ARG:NH2	2.43	0.52
1:A:318:LYS:CD	1:A:388:MET:HE1	2.39	0.52
1:A:79:MET:HE3	1:A:84:ALA:CB	2.40	0.52
1:A:386:ILE:O	1:A:390:LEU:HG	2.10	0.51
1:A:344:LEU:O	1:A:359:SER:HA	2.11	0.51
3:T:842:DG:C2'	3:T:843:DG:H5"	2.31	0.51
1:A:270:GLU:HA	1:A:278:ALA:CB	2.41	0.51
3:T:845:DC:H2"	3:T:846:DC:OP2	2.11	0.50
1:A:161:GLN:HG2	1:A:162:SER:N	2.27	0.50
1:A:99:LEU:HD12	3:T:842:DG:H4'	1.94	0.50
1:A:347:ARG:HG2	1:A:348:ARG:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:GLU:OE2	1:A:189:ASN:ND2	2.45	0.49
1:A:309:LYS:O	1:A:310:LYS:C	2.51	0.49
1:A:343:ARG:HG2	1:A:344:LEU:N	2.26	0.49
3:T:841:DG:C1'	3:T:842:DG:H5''	2.41	0.49
1:A:309:LYS:N	1:A:309:LYS:HD3	2.18	0.49
1:A:144:GLN:O	1:A:146:ASP:N	2.37	0.49
1:A:36:ASP:O	1:A:37:CYS:C	2.50	0.49
1:A:360:ARG:HG2	1:A:394:MET:SD	2.52	0.49
1:A:144:GLN:H	1:A:147:GLU:CD	2.16	0.49
3:T:841:DG:H2''	3:T:842:DG:C5'	2.42	0.49
1:A:385:ASP:HA	1:A:388:MET:CG	2.43	0.48
1:A:82:ARG:HG3	1:A:83:ASP:H	1.77	0.48
1:A:112:LEU:HD23	1:A:112:LEU:C	2.34	0.48
1:A:153:VAL:HG22	1:A:154:SER:N	2.28	0.48
1:A:123:LEU:O	1:A:127:GLU:HB2	2.13	0.48
1:A:230:ILE:CG2	1:A:231:HIS:N	2.77	0.48
1:A:138:LYS:O	1:A:142:GLN:HG2	2.14	0.48
1:A:202:ASN:OD1	1:A:205:LEU:HD22	2.14	0.48
1:A:302:PHE:N	1:A:302:PHE:CD1	2.82	0.48
1:A:308:PHE:O	1:A:310:LYS:N	2.47	0.47
1:A:233:LEU:HD22	1:A:238:GLU:CB	2.43	0.47
1:A:85:LYS:HB2	1:A:85:LYS:NZ	2.29	0.47
1:A:79:MET:HE3	1:A:84:ALA:CA	2.45	0.47
1:A:46:SER:O	1:A:48:PRO:HD3	2.15	0.47
1:A:316:GLU:C	1:A:318:LYS:H	2.17	0.46
1:A:122:ARG:NH1	6:A:13:HOH:O	2.48	0.46
1:A:153:VAL:CB	1:A:174:LEU:HD22	2.46	0.46
1:A:236:ILE:HD12	1:A:250:LEU:HD12	1.97	0.46
1:A:144:GLN:H	1:A:147:GLU:CG	2.28	0.46
1:A:214:LYS:HB3	1:A:215:PRO:CD	2.46	0.46
1:A:412:ASN:OD1	1:A:414:LYS:HE3	2.16	0.46
1:A:31:VAL:CG1	1:A:130:VAL:HB	2.45	0.46
1:A:323:GLU:O	1:A:326:ALA:HB3	2.16	0.46
1:A:75:VAL:HA	1:A:79:MET:CE	2.42	0.45
1:A:62:LEU:CD1	3:T:840[B]:BRU:H5''	2.45	0.45
1:A:214:LYS:CB	1:A:215:PRO:HD3	2.44	0.45
1:A:47:ASN:OD1	1:A:49:GLU:HB2	2.16	0.45
1:A:315:VAL:C	1:A:317:ALA:N	2.68	0.45
3:T:846:DC:H1'	3:T:847:DT:H5''	1.99	0.45
1:A:39:TYR:HB2	1:A:65:THR:CG2	2.43	0.45
1:A:202:ASN:HD21	1:A:205:LEU:H	1.64	0.45
1:A:120:VAL:HG22	1:A:130:VAL:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:325:LEU:HD11	1:A:408:VAL:HG21	1.99	0.44
1:A:236:ILE:HD12	1:A:250:LEU:CD1	2.48	0.44
1:A:346:ILE:HG22	1:A:406:LEU:CD2	2.47	0.44
1:A:337:ARG:HB3	1:A:414:LYS:O	2.18	0.44
1:A:277:VAL:O	1:A:281:ILE:HG12	2.17	0.44
1:A:97:GLU:HG2	3:T:841:DG:OP1	2.17	0.44
1:A:345:ILE:HA	1:A:358:GLU:O	2.17	0.44
1:A:79:MET:HE3	1:A:84:ALA:HB2	2.00	0.44
3:T:847:DT:H6	3:T:847:DT:H5'	1.83	0.44
3:T:841:DG:N2	6:T:135:HOH:O	2.51	0.43
1:A:304:GLU:O	1:A:407:SER:HB2	2.18	0.43
1:A:282:GLN:O	1:A:286:PHE:HD1	2.01	0.43
1:A:381:THR:O	1:A:382:PRO:C	2.57	0.43
1:A:38:PHE:O	1:A:42:VAL:HG23	2.19	0.43
1:A:309:LYS:O	1:A:311:CYS:N	2.51	0.43
1:A:380:MET:O	1:A:381:THR:C	2.57	0.43
1:A:413:LEU:N	1:A:413:LEU:HD22	2.33	0.43
3:T:843:DG:H2'	3:T:844:DT:H72	2.01	0.43
3:T:846:DC:H2''	3:T:847:DT:H5'	2.01	0.43
1:A:153:VAL:HB	1:A:174:LEU:HD22	2.01	0.42
1:A:202:ASN:HD22	1:A:202:ASN:C	2.23	0.42
1:A:333:CYS:O	1:A:334:GLN:C	2.57	0.42
1:A:86:GLU:O	1:A:86:GLU:HG3	2.18	0.42
1:A:60:LYS:HE2	1:A:307:SER:O	2.18	0.42
1:A:82:ARG:C	1:A:84:ALA:N	2.73	0.42
1:A:313:SER:OG	1:A:315:VAL:O	2.38	0.42
3:T:842:DG:H2''	3:T:843:DG:H5'	1.94	0.42
1:A:315:VAL:O	1:A:317:ALA:N	2.47	0.42
1:A:68:TYR:OH	1:A:214:LYS:HD2	2.20	0.42
1:A:36:ASP:O	1:A:38:PHE:N	2.53	0.42
1:A:121:GLU:O	1:A:128:ASN:HA	2.20	0.42
3:T:843:DG:C8	3:T:844:DT:H72	2.55	0.42
1:A:196:CYS:HA	1:A:217:GLN:O	2.20	0.42
3:T:839:DT:C2'	3:T:840[A]:BRU:O5'	2.61	0.41
1:A:251:GLU:C	1:A:253:LEU:N	2.73	0.41
1:A:388:MET:CE	1:A:391:PHE:HD1	2.33	0.41
1:A:255:ILE:HD11	1:A:264:PHE:CG	2.56	0.41
1:A:36:ASP:O	1:A:41:GLN:NE2	2.53	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.73	0.41
1:A:150:ALA:O	1:A:152:THR:HG23	2.21	0.41
1:A:251:GLU:C	1:A:253:LEU:H	2.24	0.41
1:A:392:ARG:C	1:A:394:MET:N	2.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:LEU:N	1:A:413:LEU:CD2	2.85	0.40
1:A:380:MET:O	1:A:384:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/390 (94%)	307 (84%)	48 (13%)	12 (3%)	6	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	309	LYS
1	A	350	SER
1	A	26	SER
1	A	37	CYS
1	A	145	SER
1	A	310	LYS
1	A	334	GLN
1	A	146	ASP
1	A	276	SER
1	A	333	CYS
1	A	381	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/354 (91%)	304 (95%)	17 (5%)	32 68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	90	GLN
1	A	123	LEU
1	A	170	HIS
1	A	202	ASN
1	A	204	LEU
1	A	205	LEU
1	A	214	LYS
1	A	229	LEU
1	A	302	PHE
1	A	308	PHE
1	A	309	LYS
1	A	318	LYS
1	A	342	VAL
1	A	362	CYS
1	A	381	THR
1	A	391	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	ASN
1	A	90	GLN
1	A	170	HIS
1	A	202	ASN
1	A	235	HIS
1	A	256	ASN
1	A	262	GLN
1	A	279	GLN
1	A	334	GLN
1	A	340	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	DOC	P	873	3,2	17,19,20	0.88	1 (5%)	20,26,29	1.08	2 (10%)
3	BRU	T	840[A]	3	19,21,22	0.83	1 (5%)	22,30,33	1.58	2 (9%)
3	BRU	T	840[B]	3	19,21,22	0.98	2 (10%)	22,30,33	1.56	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	P	873	3,2	-	0/5/18/19	0/2/2/2
3	BRU	T	840[A]	3	-	0/5/21/22	0/2/2/2
3	BRU	T	840[B]	3	-	1/5/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	840[B]	BRU	C4-C5	2.56	1.44	1.39
3	T	840[A]	BRU	C4-C5	2.25	1.43	1.39
2	P	873	DOC	C2-N1	2.07	1.40	1.38
3	T	840[B]	BRU	P-OP1	2.03	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	840[A]	BRU	C6-N1-C2	-5.21	120.92	122.41
3	T	840[B]	BRU	C5-C6-N1	4.62	122.71	119.67
3	T	840[A]	BRU	C5-C6-N1	4.42	122.58	119.67
3	T	840[B]	BRU	C6-N1-C2	-4.25	121.20	122.41
2	P	873	DOC	C2-N3-C4	2.97	119.87	115.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C2'-C1'-N1	2.04	116.73	112.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	840[B]	BRU	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTP	A	875	5	32,32,32	1.25	2 (6%)	50,50,50	1.33	10 (20%)

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	DTP	A	875	5	-	0/20/34/34	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	875	DTP	C3'-C4'	4.59	1.66	1.53
4	A	875	DTP	PG-O3B	2.03	1.63	1.60

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	875	DTP	O3A-PB-O3B	3.28	108.33	101.66
4	A	875	DTP	PA-O5'-C5'	-3.13	99.54	122.03
4	A	875	DTP	O4'-C4'-C3'	-2.67	98.88	105.66
4	A	875	DTP	O2B-PB-O3A	2.63	117.62	105.14
4	A	875	DTP	O4'-C4'-C5'	-2.31	101.12	109.36
4	A	875	DTP	C8-N9-C4	-2.29	105.15	106.90
4	A	875	DTP	PB-O3B-PG	-2.28	124.99	131.68
4	A	875	DTP	C2'-C3'-C4'	-2.23	97.73	102.73
4	A	875	DTP	C5'-C4'-C3'	2.20	128.50	114.76
4	A	875	DTP	O3G-PG-O2G	2.17	116.06	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	373/390 (95%)	0.33	37 (9%) 8 10	16, 48, 99, 120	1 (0%)
2	P	7/7 (100%)	0.26	0 100 100	38, 47, 54, 56	0
3	T	9/9 (100%)	0.06	0 100 100	30, 35, 55, 77	0
All	All	389/406 (95%)	0.32	37 (9%) 8 10	16, 48, 97, 120	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	TYR	7.4
1	A	354	HIS	7.1
1	A	311	CYS	5.3
1	A	348	ARG	5.2
1	A	350	SER	4.8
1	A	25	ALA	4.7
1	A	349	TYR	4.7
1	A	310	LYS	4.6
1	A	356	GLY	4.2
1	A	313	SER	4.0
1	A	336	GLY	3.7
1	A	406	LEU	3.3
1	A	244	TYR	3.2
1	A	312	SER	3.2
1	A	73	LEU	3.2
1	A	366	SER	3.2
1	A	347	ARG	3.1
1	A	352	GLU	2.9
1	A	368	VAL	2.9
1	A	82	ARG	2.9
1	A	344	LEU	2.9
1	A	335	ASP	2.9
1	A	358	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	249	CYS	2.6
1	A	333	CYS	2.6
1	A	353	LYS	2.5
1	A	53	LYS	2.3
1	A	404	THR	2.3
1	A	351	SER	2.2
1	A	68	TYR	2.2
1	A	334	GLN	2.2
1	A	380	MET	2.1
1	A	329	LEU	2.1
1	A	360	ARG	2.1
1	A	346	ILE	2.0
1	A	273	LEU	2.0
1	A	26	SER	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DOC	P	873	18/19	0.22	1.99	35,37,43,43	0
3	BRU	T	840[B]	20/21	0.19	-0.30	50,55,65,72	20
3	BRU	T	840[A]	20/21	0.19	-0.30	42,47,68,127	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DTP	A	875	30/30	0.25	0.48	62,73,91,92	0
5	MG	A	871	1/1	0.10	-2.58	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.