



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:18 pm GMT

PDB ID : 1CY1  
Title : COMPLEX OF E.COLI DNA TOPOISOMERASE I WITH 5'PTPTPT  
Authors : Feinberg, H.; Changela, A.; Mondragon, A.  
Deposited on : 1999-08-31  
Resolution : 2.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

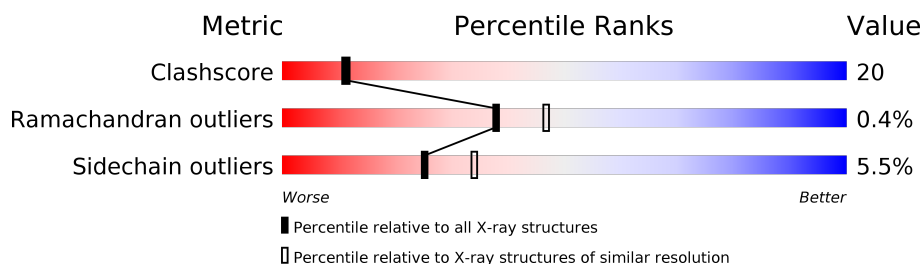
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	599	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TMP	A	600	X	-	X	-
3	TMP	A	602	X	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4642 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.

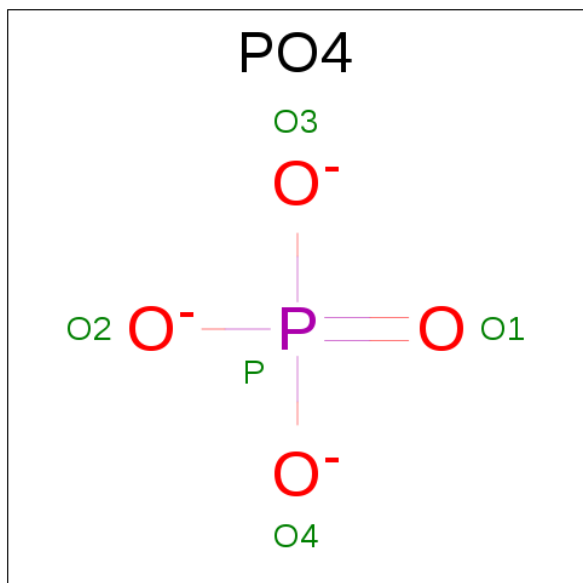
- Molecule 1 is a protein called DNA TOPOISOMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4434	2793	788	835	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

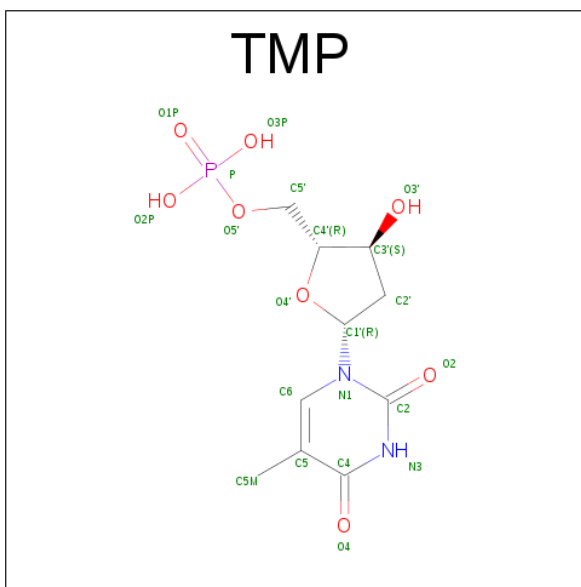
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION ARTIFACT	UNP P06612
A	0	SER	-	EXPRESSION ARTIFACT	UNP P06612

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



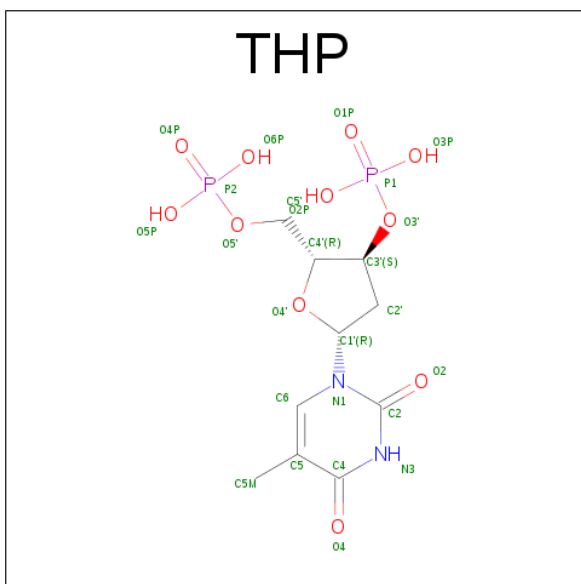
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O P		
2	A	1	5	4 1	0	0

- Molecule 3 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 4 is THYMIDINE-3',5'-DIPHOSPHATE (three-letter code: THP) (formula:  $C_{10}H_{16}N_2O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is water.

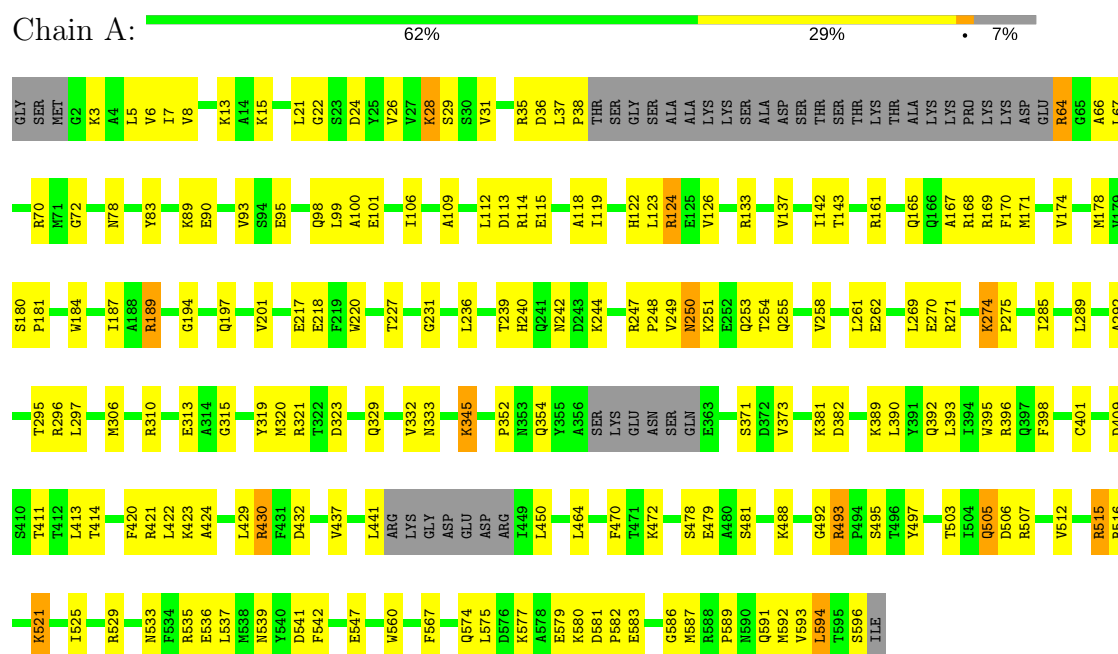
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0

### 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 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.

Note EDS was not executed.

#### • Molecule 1: DNA TOPOISOMERASE I



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.86Å 77.80Å 138.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30	Depositor
% Data completeness (in resolution range)	84.3 (19.98-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR, CNS 0.9	Depositor
R, $R_{free}$	0.242 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 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: TMP, PO4, THP

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	0.35	0/4520	0.59	0/6107

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4434	0	4415	179	0
2	A	5	0	0	1	0
3	A	42	0	24	22	0
4	A	25	0	12	2	0
5	A	136	0	0	9	0
All	All	4642	0	4451	179	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 20.

All (179) 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:295:THR:HA	3:A:602:TMP:H2'1	1.49	0.94
1:A:184:TRP:HB3	1:A:189:ARG:HG3	1.51	0.91
1:A:197:GLN:HE21	1:A:503:THR:HG21	1.36	0.89
1:A:262:GLU:HG2	1:A:464:LEU:HD12	1.54	0.87
1:A:236:LEU:HD23	1:A:424:ALA:HB2	1.56	0.87
1:A:539:ASN:HD22	1:A:542:PHE:H	1.24	0.86
1:A:250:ASN:HD21	1:A:253:GLN:HG3	1.40	0.85
1:A:396:ARG:HD3	5:A:739:HOH:O	1.77	0.84
1:A:537:LEU:H	1:A:574:GLN:HE22	1.26	0.84
1:A:187:ILE:HD11	1:A:529:ARG:HG3	1.58	0.83
1:A:250:ASN:ND2	1:A:253:GLN:H	1.78	0.81
1:A:115:GLU:H	3:A:600:TMP:H53	1.45	0.80
1:A:516:ARG:HE	3:A:602:TMP:H51	1.48	0.79
1:A:161:ARG:HH21	3:A:600:TMP:H5'2	1.48	0.77
1:A:478:SER:HB3	3:A:602:TMP:H5'2	1.65	0.77
1:A:250:ASN:HD21	1:A:253:GLN:H	1.31	0.76
1:A:321:ARG:HD3	1:A:495:SER:HB3	1.68	0.75
1:A:114:ARG:HE	3:A:600:TMP:H5'1	1.52	0.74
1:A:220:TRP:HB2	1:A:248:PRO:HG2	1.69	0.73
1:A:250:ASN:ND2	1:A:253:GLN:HG3	2.04	0.73
1:A:521:LYS:CD	1:A:521:LYS:H	2.00	0.72
1:A:591:GLN:HE21	1:A:593:VAL:HG22	1.52	0.72
1:A:168:ARG:NH1	1:A:168:ARG:HB3	2.05	0.72
1:A:594:LEU:HG	1:A:596:SER:H	1.56	0.71
1:A:28:LYS:HE2	1:A:28:LYS:HA	1.75	0.69
1:A:115:GLU:H	3:A:600:TMP:C5M	2.05	0.69
1:A:250:ASN:C	1:A:250:ASN:HD22	1.96	0.69
1:A:539:ASN:ND2	1:A:542:PHE:H	1.91	0.68
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.59	0.67
1:A:392:GLN:O	1:A:396:ARG:HG3	1.93	0.67
1:A:197:GLN:HG2	1:A:503:THR:HG22	1.75	0.66
1:A:478:SER:H	1:A:481:SER:HB3	1.60	0.65
1:A:516:ARG:NH2	3:A:602:TMP:H5'1	2.12	0.65
1:A:240:HIS:HB2	1:A:421:ARG:HB3	1.77	0.65
1:A:373:VAL:HG22	1:A:398:PHE:HE2	1.61	0.65
1:A:332:VAL:HG11	1:A:352:PRO:HB3	1.78	0.64
1:A:430:ARG:HE	1:A:430:ARG:HA	1.63	0.64
1:A:168:ARG:HH11	1:A:168:ARG:HB3	1.63	0.64
1:A:594:LEU:CD2	1:A:594:LEU:H	2.11	0.63
1:A:197:GLN:HG2	1:A:503:THR:CG2	2.28	0.63
1:A:409:ASP:OD2	1:A:430:ARG:HD2	1.98	0.63
1:A:35:ARG:HG2	1:A:83:TYR:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HH21	3:A:600:TMP:C5'	2.12	0.62
1:A:261:LEU:HD21	1:A:420:PHE:CG	2.34	0.62
1:A:594:LEU:N	1:A:594:LEU:HD23	2.14	0.62
1:A:521:LYS:HD2	1:A:521:LYS:H	1.62	0.62
1:A:591:GLN:NE2	1:A:593:VAL:HG22	2.15	0.62
1:A:13:LYS:HB2	1:A:313:GLU:HG2	1.83	0.61
1:A:113:ASP:HB2	3:A:600:TMP:H6	1.66	0.61
1:A:594:LEU:HD23	1:A:594:LEU:H	1.65	0.61
1:A:115:GLU:O	1:A:119:ILE:HG13	2.01	0.60
1:A:319:TYR:CE2	1:A:321:ARG:HB2	2.36	0.59
1:A:525:ILE:O	1:A:529:ARG:HG2	2.02	0.59
1:A:227:THR:HG23	1:A:231:GLY:HA2	1.85	0.58
1:A:533:ASN:HD21	1:A:587:MET:HA	1.68	0.58
1:A:329:GLN:HE21	1:A:333:ASN:HD21	1.52	0.58
1:A:124:ARG:CG	1:A:124:ARG:HH11	2.17	0.57
1:A:218:GLU:OE2	1:A:250:ASN:HA	2.04	0.57
1:A:254:THR:O	1:A:258:VAL:HG23	2.04	0.57
1:A:373:VAL:CG2	1:A:398:PHE:HE2	2.17	0.57
1:A:165:GLN:HA	1:A:168:ARG:HH12	1.69	0.57
1:A:516:ARG:HH22	3:A:602:TMP:H5'1	1.70	0.56
1:A:115:GLU:N	3:A:600:TMP:H53	2.17	0.56
1:A:493:ARG:HG2	3:A:600:TMP:O2	2.05	0.56
1:A:165:GLN:NE2	1:A:168:ARG:NH1	2.53	0.56
1:A:180:SER:HB2	1:A:181:PRO:HD3	1.87	0.56
1:A:581:ASP:HB3	1:A:583:GLU:CD	2.26	0.56
1:A:289:LEU:HD11	1:A:390:LEU:HD11	1.88	0.55
1:A:533:ASN:ND2	1:A:587:MET:HA	2.21	0.55
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.71	0.55
1:A:270:GLU:HG2	1:A:414:THR:HB	1.88	0.55
1:A:393:LEU:CD1	4:A:601:THP:H53	2.36	0.55
1:A:168:ARG:NH2	3:A:600:TMP:C4	2.75	0.55
1:A:515:ARG:HB3	1:A:515:ARG:NH1	2.21	0.54
1:A:285:ILE:HB	1:A:323:ASP:HA	1.89	0.54
1:A:537:LEU:HD23	1:A:537:LEU:O	2.09	0.53
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.21	0.53
1:A:112:LEU:HD12	1:A:112:LEU:C	2.28	0.53
1:A:251:LYS:O	1:A:255:GLN:HG2	2.08	0.53
1:A:36:ASP:OD1	1:A:169:ARG:NH2	2.41	0.53
1:A:168:ARG:HD3	5:A:820:HOH:O	2.10	0.52
1:A:124:ARG:NH1	1:A:124:ARG:HG2	2.24	0.52
1:A:95:GLU:O	1:A:99:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:HB2	1:A:165:GLN:HG2	1.91	0.52
1:A:15:LYS:HB2	1:A:15:LYS:NZ	2.25	0.52
1:A:170:PHE:CE2	1:A:560:TRP:HZ3	2.28	0.52
1:A:227:THR:CG2	1:A:231:GLY:HA2	2.39	0.52
1:A:296:ARG:NH1	1:A:296:ARG:HG2	2.25	0.52
1:A:422:LEU:HD12	1:A:422:LEU:N	2.24	0.52
1:A:535:ARG:HG2	1:A:535:ARG:HH11	1.75	0.51
1:A:124:ARG:HH11	1:A:124:ARG:HG2	1.74	0.51
1:A:593:VAL:HG12	1:A:594:LEU:HD23	1.92	0.51
1:A:114:ARG:NE	3:A:600:TMP:H5'1	2.23	0.51
1:A:580:LYS:O	1:A:586:GLY:HA3	2.11	0.51
1:A:165:GLN:NE2	1:A:168:ARG:HH12	2.09	0.51
1:A:64:ARG:NH1	1:A:64:ARG:HA	2.25	0.51
1:A:167:ALA:O	1:A:171:MET:HG2	2.11	0.51
1:A:395:TRP:HE3	1:A:396:ARG:HG2	1.76	0.51
1:A:594:LEU:N	1:A:594:LEU:CD2	2.73	0.51
1:A:98:GLN:O	1:A:101:GLU:HG2	2.10	0.51
1:A:539:ASN:HD21	1:A:541:ASP:HB2	1.75	0.51
1:A:516:ARG:NH2	3:A:602:TMP:H6	2.08	0.50
1:A:3:LYS:HB3	1:A:24:ASP:O	2.10	0.50
1:A:114:ARG:HG3	3:A:600:TMP:H5'2	1.94	0.50
1:A:521:LYS:CE	1:A:521:LYS:H	2.24	0.50
1:A:429:LEU:HD11	1:A:432:ASP:HA	1.93	0.50
1:A:479:GLU:HG3	5:A:713:HOH:O	2.11	0.50
1:A:89:LYS:O	1:A:93:VAL:HG23	2.11	0.50
1:A:64:ARG:CZ	1:A:64:ARG:HA	2.41	0.50
1:A:31:VAL:HG13	1:A:31:VAL:O	2.12	0.50
1:A:315:GLY:HA2	5:A:741:HOH:O	2.12	0.50
1:A:515:ARG:HB3	1:A:515:ARG:HH11	1.76	0.50
1:A:113:ASP:CG	3:A:600:TMP:H51	2.33	0.50
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.77	0.49
1:A:441:LEU:HD12	1:A:441:LEU:N	2.26	0.49
1:A:168:ARG:NH2	5:A:747:HOH:O	2.44	0.49
1:A:6:VAL:HG21	1:A:21:LEU:HD13	1.94	0.49
1:A:100:ALA:HB1	1:A:106:ILE:HD11	1.93	0.49
1:A:98:GLN:HA	1:A:101:GLU:HG2	1.94	0.49
1:A:239:THR:HG21	1:A:423:LYS:HB2	1.94	0.48
1:A:492:GLY:HA3	1:A:497:TYR:CE1	2.48	0.48
1:A:306:MET:HG2	1:A:310:ARG:HH21	1.77	0.48
1:A:292:ALA:O	1:A:296:ARG:HG3	2.14	0.48
1:A:373:VAL:HG22	1:A:398:PHE:CE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASP:HB3	1:A:583:GLU:OE2	2.14	0.47
1:A:114:ARG:HE	3:A:600:TMP:C5'	2.26	0.47
1:A:271:ARG:NH1	1:A:413:LEU:HD21	2.29	0.47
1:A:505:GLN:NE2	1:A:512:VAL:H	2.12	0.47
1:A:382:ASP:N	5:A:795:HOH:O	2.32	0.47
1:A:36:ASP:CG	1:A:37:LEU:H	2.17	0.47
1:A:582:PRO:HG2	1:A:589:PRO:HD3	1.97	0.47
1:A:274:LYS:NZ	1:A:274:LYS:HB2	2.30	0.47
1:A:577:LYS:O	1:A:586:GLY:HA2	2.16	0.46
1:A:64:ARG:HG3	1:A:66:ALA:HB3	1.98	0.46
1:A:165:GLN:HA	1:A:168:ARG:NH1	2.30	0.45
1:A:512:VAL:HA	1:A:516:ARG:O	2.16	0.45
1:A:537:LEU:H	1:A:574:GLN:NE2	2.06	0.45
1:A:36:ASP:CG	1:A:37:LEU:N	2.70	0.45
1:A:7:ILE:HG21	1:A:123:LEU:HD13	1.99	0.45
1:A:8:VAL:O	1:A:29:SER:HA	2.17	0.45
1:A:194:GLY:HA3	1:A:197:GLN:HB2	1.99	0.45
1:A:93:VAL:HG13	1:A:126:VAL:CG1	2.47	0.45
1:A:35:ARG:HH21	1:A:122:HIS:HD2	1.64	0.45
1:A:197:GLN:NE2	1:A:503:THR:HG21	2.18	0.44
1:A:217:GLU:O	1:A:470:PHE:HA	2.17	0.44
1:A:516:ARG:HH21	3:A:602:TMP:H6	1.65	0.44
1:A:507:ARG:HB3	5:A:826:HOH:O	2.16	0.44
1:A:22:GLY:HA3	5:A:727:HOH:O	2.17	0.44
1:A:250:ASN:C	1:A:250:ASN:ND2	2.68	0.44
1:A:345:LYS:HA	1:A:345:LYS:HE3	2.00	0.44
1:A:297:LEU:HD22	1:A:389:LYS:HD2	2.00	0.44
1:A:488:LYS:HB2	1:A:488:LYS:HE3	1.73	0.43
1:A:242:ASN:O	1:A:244:LYS:HG2	2.19	0.43
1:A:249:VAL:HG22	1:A:253:GLN:OE1	2.18	0.43
1:A:535:ARG:NH1	2:A:700:PO4:O1	2.52	0.43
1:A:393:LEU:HD12	4:A:601:THP:H53	2.01	0.43
1:A:174:VAL:O	1:A:178:MET:HB2	2.19	0.43
1:A:495:SER:OG	3:A:600:TMP:C5	2.72	0.43
1:A:521:LYS:H	1:A:521:LYS:HE3	1.84	0.43
1:A:478:SER:CB	3:A:602:TMP:H5'2	2.44	0.43
1:A:118:ALA:CB	1:A:165:GLN:HG2	2.48	0.42
1:A:13:LYS:HG3	1:A:142:ILE:CD1	2.49	0.42
1:A:274:LYS:HA	1:A:275:PRO:HD3	1.89	0.42
1:A:189:ARG:CG	1:A:189:ARG:NH1	2.80	0.42
1:A:35:ARG:O	1:A:36:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:O	1:A:201:VAL:HG23	2.19	0.42
1:A:575:LEU:O	1:A:579:GLU:HG3	2.20	0.42
1:A:411:THR:HB	1:A:450:LEU:HD12	2.02	0.41
1:A:5:LEU:HD12	1:A:26:VAL:O	2.20	0.41
1:A:113:ASP:HA	1:A:161:ARG:HH22	1.86	0.41
1:A:109:ALA:HA	1:A:137:VAL:HG23	2.02	0.41
1:A:143:THR:CG2	1:A:371:SER:HB3	2.51	0.41
1:A:583:GLU:H	1:A:583:GLU:CD	2.24	0.41
1:A:66:ALA:O	1:A:70:ARG:HG3	2.21	0.41
1:A:38:PRO:HD2	1:A:72:GLY:HA3	2.02	0.41
1:A:112:LEU:HD12	1:A:113:ASP:N	2.35	0.40
1:A:429:LEU:HD21	1:A:432:ASP:HB3	2.02	0.40
1:A:503:THR:HG23	1:A:507:ARG:NH2	2.37	0.40
1:A:90:GLU:HB3	5:A:799:HOH:O	2.21	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	549/599 (92%)	527 (96%)	20 (4%)	2 (0%)	38	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	LYS
1	A	594	LEU

### 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	472/507 (93%)	446 (94%)	26 (6%)	25	34

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	64	ARG
1	A	67	LEU
1	A	78	ASN
1	A	124	ARG
1	A	189	ARG
1	A	247	ARG
1	A	250	ASN
1	A	269	LEU
1	A	274	LYS
1	A	320	MET
1	A	345	LYS
1	A	354	GLN
1	A	401	CYS
1	A	430	ARG
1	A	437	VAL
1	A	472	LYS
1	A	493	ARG
1	A	505	GLN
1	A	506	ASP
1	A	515	ARG
1	A	521	LYS
1	A	536	GLU
1	A	547	GLU
1	A	567	PHE
1	A	592	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	98	GLN
1	A	122	HIS
1	A	149	GLN
1	A	165	GLN
1	A	166	GLN
1	A	237	GLN
1	A	241	GLN
1	A	242	ASN
1	A	250	ASN
1	A	333	ASN
1	A	365	HIS
1	A	454	ASN
1	A	505	GLN
1	A	533	ASN
1	A	539	ASN
1	A	545	GLN
1	A	548	ASN
1	A	573	GLN
1	A	574	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 ⓘ

4 ligands 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
3	TMP	A	600	-	17,22,22	1.69	3 (17%)	24,33,33	3.72	6 (25%)
4	THP	A	601	-	21,26,26	1.43	2 (9%)	30,40,40	3.08	7 (23%)
3	TMP	A	602	-	17,22,22	1.54	2 (11%)	24,33,33	3.76	6 (25%)
2	PO4	A	700	-	4,4,4	1.35	0	6,6,6	0.40	0

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	TMP	A	600	-	1/1/4/4	0/6/22/22	0/2/2/2
4	THP	A	601	-	-	0/11/27/27	0/2/2/2
3	TMP	A	602	-	1/1/4/4	0/6/22/22	0/2/2/2
2	PO4	A	700	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	TMP	C5M-C5	-3.06	1.45	1.51
3	A	600	TMP	P-O5'	-2.16	1.53	1.60
3	A	602	TMP	P-O2P	-2.01	1.46	1.54
4	A	601	THP	C5M-C5	2.14	1.55	1.51
4	A	601	THP	C4-N3	3.89	1.40	1.33
3	A	602	TMP	C4-N3	4.49	1.41	1.33
3	A	600	TMP	C4-N3	4.73	1.41	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	THP	C5-C4-N3	-8.54	115.82	125.24
3	A	600	TMP	C5-C4-N3	-8.16	116.25	125.24
3	A	602	TMP	C5-C4-N3	-8.07	116.35	125.24
4	A	601	THP	C5'-C4'-C3'	-2.49	108.84	114.57
4	A	601	THP	C2'-C1'-N1	-2.22	108.98	114.23
3	A	602	TMP	O2P-P-O1P	2.15	118.92	110.50
4	A	601	THP	O4'-C1'-N1	2.26	111.58	107.78
3	A	600	TMP	O2P-P-O1P	2.27	119.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	THP	O5P-P2-O4P	2.29	119.45	110.50
3	A	600	TMP	P-O5'-C5'	2.30	124.63	118.30
3	A	602	TMP	P-O5'-C5'	2.40	124.91	118.30
4	A	601	THP	O2P-P1-O1P	4.45	127.90	110.50
3	A	602	TMP	C2'-C1'-N1	6.44	129.45	114.23
3	A	600	TMP	O4'-C1'-N1	6.53	118.78	107.78
3	A	600	TMP	C2'-C1'-N1	6.94	130.63	114.23
3	A	602	TMP	O4'-C1'-N1	7.15	119.83	107.78
3	A	600	TMP	C4-N3-C2	12.39	126.00	115.16
4	A	601	THP	C4-N3-C2	12.44	126.04	115.16
3	A	602	TMP	C4-N3-C2	12.68	126.25	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	TMP	C1'
3	A	602	TMP	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	TMP	14	0
4	A	601	THP	2	0
3	A	602	TMP	8	0
2	A	700	PO4	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.