



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 01:07 PM EST

PDB ID : 2KTQ  
Title : OPEN TERNARY COMPLEX OF THE LARGE FRAGMENT OF DNA  
POLYMERASE I FROM THERMUS AQUATICUS  
Authors : Li, Y.; Waksman, G.  
Deposited on : 1998-07-30  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

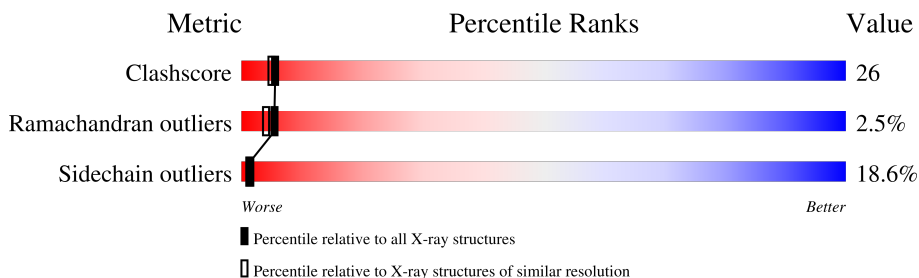
# 1 Overall quality at a glance

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	12	67% (Green), 33% (Yellow)
2	D	13	38% (Green), 62% (Yellow)
3	A	538	51% (Green), 39% (Yellow), 8% (Orange), 2% (Grey)

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4631 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 DNA chain called DNA (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*DOC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	12	240	114	48	67	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	13	267	126	51	78	12	0	0	0

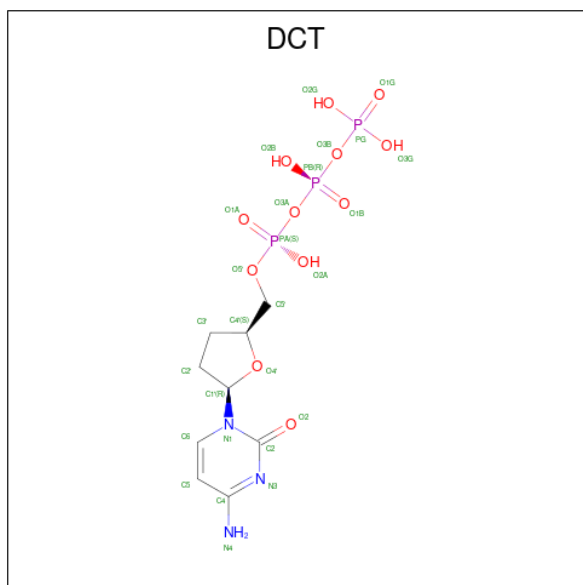
- Molecule 3 is a protein called PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	528	3948	2509	709	719	11	0	0	0

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

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

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	27	9	3	12	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	10	Total	O	0	0
			10	10		
6	D	11	Total	O	0	0
			11	11		
6	A	127	Total	O	0	0
			127	127		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

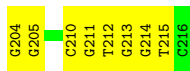
- Molecule 1: DNA (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*DOC)-3')

Chain B: 



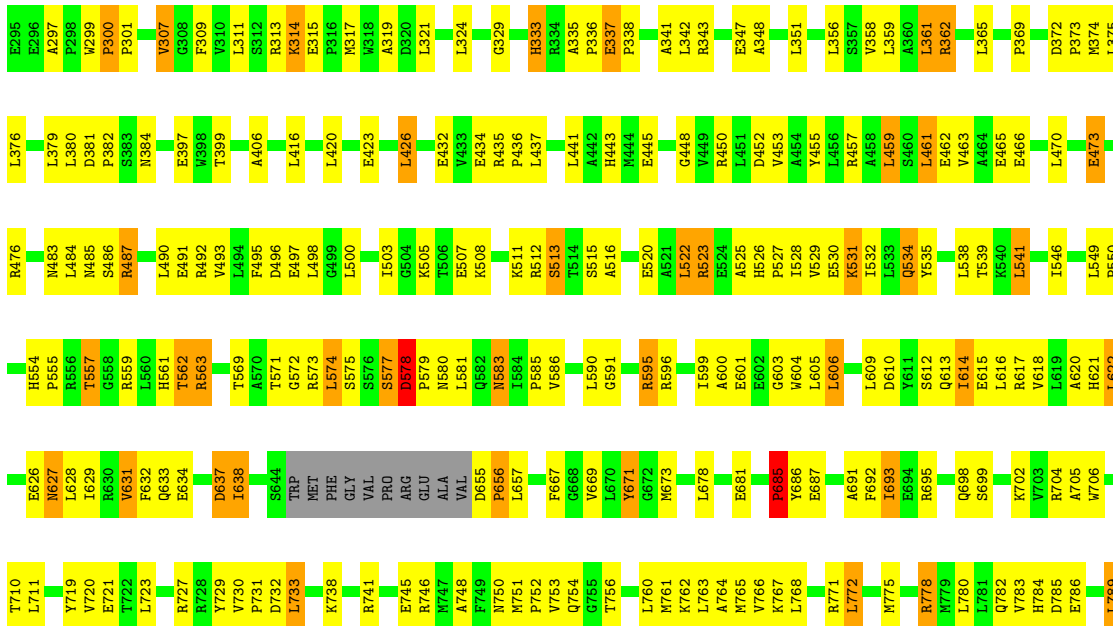
- Molecule 2: DNA (5'-D(\*GP\*GP\*GP\*CP\*GP\*CP\*CP\*GP\*TP\*GP\*GP\*TP\*C)-3')

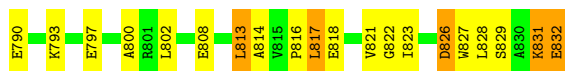
Chain D: 



- Molecule 3: PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I)

Chain A: 





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.41Å 108.41Å 89.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.6 (30.00-2.30)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	4.80	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.224 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: DCT, DOC, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.43	0/249	0.73	0/382
2	D	0.52	0/299	0.82	0/461
3	A	0.33	0/4024	0.59	4/5473 (0.1%)
All	All	0.35	0/4572	0.62	4/6316 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	578	ASP	C-N-CD	7.18	143.49	128.40
3	A	685	PRO	N-CA-CB	5.34	109.71	103.30
3	A	578	ASP	N-CA-C	-5.18	97.02	111.00
3	A	656	PRO	N-CA-CB	5.14	109.47	103.30

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	B	240	0	134	3	0
2	D	267	0	147	12	0
3	A	3948	0	3817	206	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	27	0	12	8	0
6	A	127	0	0	12	0
6	B	10	0	0	0	0
6	D	11	0	0	0	0
All	All	4631	0	4110	222	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 26.

All (222) 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)
3:A:633:GLN:C	3:A:634:GLU:CA	2.43	0.87
3:A:503:ILE:HD11	3:A:522:LEU:HD13	1.58	0.84
3:A:621:HIS:HD2	3:A:814:ALA:H	1.22	0.84
5:A:113:DCT:H6	5:A:113:DCT:O5'	1.78	0.82
3:A:563:ARG:HG2	3:A:563:ARG:HH11	1.45	0.81
3:A:621:HIS:CD2	3:A:814:ALA:H	1.98	0.81
2:D:204:DG:H2''	2:D:205:DG:OP2	1.80	0.80
3:A:613:GLN:HE21	3:A:632:PHE:HE1	1.28	0.79
3:A:563:ARG:HG2	3:A:563:ARG:NH1	2.01	0.76
3:A:609:LEU:HD23	3:A:821:VAL:HG22	1.69	0.75
3:A:600:ALA:HB2	3:A:606:LEU:HD13	1.69	0.75
3:A:466:GLU:HG3	3:A:538:LEU:HD21	1.67	0.74
3:A:768:LEU:HG	3:A:772:LEU:HD22	1.72	0.72
3:A:828:LEU:HA	3:A:832:GLU:OE1	1.90	0.71
3:A:595:ARG:HD3	3:A:832:GLU:OE2	1.91	0.71
3:A:342:LEU:HD21	3:A:356:LEU:HD11	1.74	0.70
3:A:828:LEU:HD12	3:A:832:GLU:OE1	1.92	0.69
3:A:605:LEU:HG	3:A:793:LYS:HG3	1.75	0.69
3:A:808:GLU:HG2	3:A:817:LEU:O	1.94	0.67
3:A:827:TRP:CD1	3:A:832:GLU:HB3	2.29	0.67
3:A:445:GLU:O	3:A:561:HIS:HD2	1.78	0.67
3:A:491:GLU:OE2	3:A:512:ARG:HB2	1.95	0.66
3:A:621:HIS:CD2	3:A:813:LEU:HB3	2.29	0.66
3:A:307:VAL:O	3:A:406:ALA:HA	1.96	0.65
3:A:626:GLU:HA	3:A:629:ILE:HG12	1.78	0.65
3:A:562:THR:HG22	6:A:3019:HOH:O	1.96	0.65
2:D:212:DT:H2''	2:D:213:DG:H5'	1.79	0.64
3:A:441:LEU:O	3:A:445:GLU:HG3	1.96	0.64
2:D:211:DG:H2'	2:D:212:DT:H72	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:578:ASP:O	3:A:580:ASN:N	2.32	0.63
3:A:351:LEU:HD23	3:A:374:MET:HG2	1.79	0.63
3:A:628:LEU:O	3:A:631:VAL:HG13	1.97	0.63
3:A:443:HIS:HE1	6:A:3015:HOH:O	1.81	0.63
2:D:212:DT:H2''	2:D:213:DG:C5'	2.29	0.62
3:A:750:ASN:O	3:A:753:VAL:HG22	1.99	0.62
3:A:761:MET:HE3	3:A:764:ALA:HB3	1.81	0.62
3:A:627:ASN:O	3:A:631:VAL:HG12	1.98	0.62
3:A:315:GLU:H	3:A:315:GLU:CD	2.02	0.62
3:A:615:GLU:CD	5:A:113:DCT:H2''	2.20	0.61
3:A:761:MET:HE2	3:A:765:MET:HG3	1.82	0.61
3:A:453:VAL:HG13	3:A:550:PRO:HB3	1.82	0.61
3:A:751:MET:HB3	3:A:752:PRO:HD3	1.82	0.61
3:A:333:HIS:HE1	6:A:3130:HOH:O	1.84	0.61
3:A:573:ARG:HD3	6:A:3021:HOH:O	2.01	0.60
2:D:214:DG:H1'	2:D:215:DT:H5''	1.84	0.60
3:A:578:ASP:O	3:A:579:PRO:C	2.34	0.60
3:A:493:VAL:O	3:A:498:LEU:HG	2.01	0.60
3:A:733:LEU:HD21	3:A:748:ALA:HB2	1.84	0.60
3:A:317:MET:CE	3:A:362:ARG:HB3	2.32	0.59
3:A:336:PRO:HD2	3:A:337:GLU:OE1	2.02	0.59
3:A:595:ARG:HD3	3:A:832:GLU:CD	2.23	0.59
3:A:466:GLU:HG3	3:A:538:LEU:CD2	2.33	0.59
3:A:563:ARG:HH11	3:A:563:ARG:CG	2.12	0.59
3:A:785:ASP:OD1	5:A:113:DCT:H5'	2.02	0.59
3:A:381:ASP:HB3	3:A:384:ASN:ND2	2.18	0.58
3:A:520:GLU:OE1	3:A:523:ARG:NH2	2.36	0.58
3:A:299:TRP:CZ2	3:A:341:ALA:HB1	2.39	0.58
3:A:541:LEU:HD23	3:A:590:LEU:HD23	1.87	0.57
5:A:113:DCT:H5'	5:A:113:DCT:O2B	2.03	0.57
3:A:531:LYS:N	3:A:531:LYS:HD2	2.20	0.57
3:A:531:LYS:HD2	3:A:531:LYS:H	1.70	0.56
3:A:626:GLU:HA	3:A:629:ILE:CD1	2.35	0.56
3:A:569:THR:HG22	3:A:572:GLY:H	1.70	0.56
3:A:459:LEU:HD13	3:A:546:ILE:HD13	1.87	0.56
3:A:616:LEU:HG	3:A:667:PHE:CE2	2.41	0.56
3:A:626:GLU:HA	3:A:629:ILE:CG1	2.36	0.56
3:A:706:TRP:CZ2	3:A:710:THR:HG21	2.42	0.55
3:A:829:SER:C	3:A:831:LYS:H	2.08	0.55
3:A:530:GLU:O	3:A:534:GLN:HG2	2.07	0.55
3:A:299:TRP:HB2	3:A:336:PRO:HD3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:557:THR:OG1	3:A:561:HIS:HE1	1.90	0.55
3:A:492:ARG:HA	3:A:496:ASP:HB2	1.88	0.55
3:A:615:GLU:OE1	5:A:113:DCT:H2''	2.05	0.55
2:D:215:DT:H5'	2:D:215:DT:H6	1.71	0.55
3:A:691:ALA:C	3:A:693:ILE:H	2.10	0.55
3:A:492:ARG:O	3:A:497:GLU:HG3	2.07	0.55
3:A:731:PRO:C	3:A:733:LEU:H	2.10	0.54
3:A:753:VAL:HG23	3:A:754:GLN:N	2.20	0.54
3:A:526:HIS:ND1	3:A:527:PRO:HD2	2.22	0.54
3:A:695:ARG:O	3:A:699:SER:N	2.40	0.54
3:A:351:LEU:CD2	3:A:374:MET:HG2	2.38	0.54
3:A:299:TRP:O	3:A:301:PRO:HD3	2.08	0.54
3:A:549:LEU:HB2	3:A:550:PRO:HD3	1.90	0.53
3:A:603:GLY:C	3:A:793:LYS:HD2	2.28	0.53
3:A:437:LEU:HD22	3:A:762:LYS:HD3	1.89	0.53
3:A:503:ILE:CD1	3:A:522:LEU:HD13	2.35	0.53
3:A:626:GLU:CA	3:A:629:ILE:HG12	2.39	0.53
3:A:445:GLU:O	3:A:561:HIS:CD2	2.61	0.53
3:A:562:THR:CG2	3:A:581:LEU:HD12	2.39	0.53
3:A:338:PRO:O	3:A:341:ALA:HB3	2.09	0.52
3:A:784:HIS:HD2	6:A:3012:HOH:O	1.91	0.52
3:A:655:ASP:O	3:A:657:LEU:N	2.42	0.52
3:A:730:VAL:CG1	3:A:733:LEU:HD23	2.40	0.52
3:A:311:LEU:HB3	3:A:319:ALA:HB1	1.91	0.52
3:A:614:ILE:O	3:A:614:ILE:HG13	2.08	0.51
3:A:495:PHE:HB2	3:A:512:ARG:NH1	2.25	0.51
3:A:522:LEU:O	3:A:529:VAL:HG21	2.10	0.51
3:A:535:TYR:CZ	3:A:539:THR:HG21	2.46	0.51
3:A:578:ASP:HB3	3:A:579:PRO:CD	2.40	0.51
2:D:213:DG:H2''	2:D:214:DG:O5'	2.10	0.51
3:A:780:LEU:HD11	3:A:790:GLU:HB2	1.92	0.51
3:A:450:ARG:HB3	3:A:599:ILE:O	2.11	0.51
3:A:500:LEU:HD21	3:A:526:HIS:HB2	1.92	0.51
2:D:210:DC:H2''	2:D:211:DG:C8	2.46	0.51
3:A:626:GLU:HA	3:A:629:ILE:HD11	1.93	0.51
3:A:609:LEU:HG	3:A:821:VAL:HG13	1.93	0.50
3:A:448:GLY:O	3:A:559:ARG:NH1	2.45	0.50
3:A:315:GLU:OE1	3:A:315:GLU:N	2.33	0.50
3:A:462:GLU:HG2	6:A:3138:HOH:O	2.11	0.50
3:A:828:LEU:HA	3:A:832:GLU:CD	2.32	0.49
3:A:829:SER:C	3:A:831:LYS:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:317:MET:HE3	3:A:358:VAL:HG13	1.94	0.49
3:A:523:ARG:HB3	6:A:3139:HOH:O	2.12	0.49
3:A:441:LEU:HD21	3:A:574:LEU:HD21	1.94	0.49
3:A:526:HIS:HB3	3:A:528:ILE:HG22	1.94	0.49
3:A:380:LEU:HD11	3:A:420:LEU:HD22	1.95	0.49
3:A:459:LEU:O	3:A:463:VAL:HG23	2.13	0.49
3:A:492:ARG:O	3:A:496:ASP:HB2	2.13	0.49
3:A:620:ALA:HB2	3:A:628:LEU:HG	1.95	0.49
3:A:731:PRO:O	3:A:733:LEU:N	2.46	0.49
3:A:578:ASP:HB3	3:A:579:PRO:HD3	1.95	0.48
3:A:669:VAL:HA	6:A:3110:HOH:O	2.13	0.48
3:A:297:ALA:HB3	3:A:333:HIS:CD2	2.49	0.48
3:A:461:LEU:O	3:A:465:GLU:HG3	2.13	0.48
3:A:466:GLU:CG	3:A:538:LEU:HD21	2.39	0.48
2:D:212:DT:H4'	3:A:486:SER:HA	1.95	0.47
3:A:618:VAL:HG11	3:A:756:THR:HB	1.97	0.47
3:A:831:LYS:O	3:A:832:GLU:C	2.51	0.47
3:A:577:SER:OG	3:A:578:ASP:N	2.47	0.47
3:A:753:VAL:CG2	3:A:754:GLN:N	2.77	0.47
3:A:315:GLU:CD	3:A:315:GLU:N	2.68	0.47
3:A:382:PRO:HG3	3:A:727:ARG:O	2.14	0.47
3:A:762:LYS:O	3:A:766:VAL:HG23	2.15	0.47
3:A:423:GLU:HB3	3:A:426:LEU:HB2	1.97	0.46
3:A:562:THR:HG21	3:A:581:LEU:HD12	1.97	0.46
3:A:583:ASN:HD22	3:A:583:ASN:H	1.63	0.46
3:A:437:LEU:HD11	3:A:765:MET:CE	2.46	0.46
3:A:827:TRP:NE1	3:A:832:GLU:HB3	2.30	0.46
2:D:204:DG:C2'	2:D:205:DG:OP2	2.60	0.46
3:A:678:LEU:HA	3:A:681:GLU:CB	2.46	0.46
3:A:382:PRO:HG2	6:A:3038:HOH:O	2.16	0.46
3:A:609:LEU:HD23	3:A:821:VAL:CG2	2.43	0.46
3:A:574:LEU:HD13	3:A:762:LYS:HE2	1.97	0.45
3:A:313:ARG:HG2	3:A:319:ALA:HA	1.97	0.45
3:A:359:LEU:HA	3:A:362:ARG:HG2	1.98	0.45
3:A:554:HIS:HB3	3:A:557:THR:HG1	1.82	0.45
3:A:671:TYR:O	3:A:746:ARG:HG2	2.15	0.45
3:A:453:VAL:O	3:A:457:ARG:HG2	2.16	0.45
3:A:637:ASP:O	3:A:638:ILE:C	2.54	0.45
3:A:379:LEU:HD11	3:A:434:GLU:HG3	1.98	0.45
3:A:826:ASP:OD1	3:A:828:LEU:N	2.49	0.45
3:A:719:TYR:HB3	3:A:729:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:DG:H2'	2:D:212:DT:C7	2.45	0.45
3:A:569:THR:HG21	3:A:573:ARG:H	1.81	0.45
3:A:671:TYR:O	3:A:746:ARG:CG	2.65	0.45
3:A:299:TRP:HB3	3:A:300:PRO:HD3	2.00	0.44
3:A:490:LEU:HD11	3:A:532:ILE:HD13	1.99	0.44
3:A:573:ARG:HG3	3:A:754:GLN:HE21	1.81	0.44
3:A:671:TYR:OH	5:A:113:DCT:O2	2.32	0.44
3:A:348:ALA:HB3	3:A:369:PRO:HA	1.99	0.44
3:A:397:GLU:O	3:A:399:THR:HG23	2.18	0.44
3:A:569:THR:HG22	3:A:571:THR:H	1.82	0.44
3:A:785:ASP:OD1	5:A:113:DCT:C5'	2.64	0.44
3:A:314:LYS:HG2	6:A:3020:HOH:O	2.17	0.44
3:A:335:ALA:HB1	3:A:341:ALA:HB2	1.99	0.43
3:A:618:VAL:O	3:A:622:LEU:HB2	2.18	0.43
3:A:626:GLU:H	3:A:626:GLU:CD	2.22	0.43
3:A:554:HIS:CG	3:A:555:PRO:HD2	2.53	0.43
3:A:583:ASN:HD22	3:A:583:ASN:N	2.17	0.43
3:A:617:ARG:NH1	3:A:816:PRO:O	2.51	0.43
3:A:562:THR:CG2	6:A:3019:HOH:O	2.62	0.43
3:A:554:HIS:ND1	3:A:557:THR:HG23	2.33	0.43
3:A:695:ARG:HA	3:A:698:GLN:CB	2.49	0.43
3:A:702:LYS:HA	3:A:705:ALA:HB3	2.00	0.43
3:A:459:LEU:HD13	3:A:546:ILE:CD1	2.49	0.43
3:A:466:GLU:OE2	3:A:466:GLU:HA	2.19	0.43
3:A:626:GLU:O	3:A:629:ILE:HG12	2.18	0.43
3:A:831:LYS:HA	3:A:831:LYS:HD3	1.54	0.43
3:A:821:VAL:HG12	3:A:822:GLY:N	2.33	0.42
3:A:505:LYS:HA	3:A:511:LYS:O	2.20	0.42
3:A:605:LEU:HD13	3:A:823:ILE:CG2	2.50	0.42
1:B:103:DC:H2''	1:B:104:DC:OP2	2.19	0.42
3:A:452:ASP:O	3:A:455:TYR:HB3	2.19	0.42
3:A:483:ASN:OD1	3:A:485:ASN:HB2	2.18	0.42
3:A:691:ALA:O	3:A:693:ILE:N	2.41	0.42
3:A:771:ARG:H	3:A:771:ARG:HG2	1.69	0.42
3:A:317:MET:HE1	3:A:362:ARG:HB3	2.00	0.42
3:A:569:THR:HG21	3:A:573:ARG:HB2	2.02	0.42
3:A:612:SER:O	3:A:613:GLN:C	2.58	0.42
3:A:601:GLU:OE2	3:A:604:TRP:NE1	2.53	0.42
3:A:609:LEU:HD11	3:A:789:LEU:HD22	2.00	0.42
3:A:626:GLU:OE1	3:A:626:GLU:N	2.49	0.42
3:A:299:TRP:HB2	3:A:335:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:ARG:HB3	3:A:436:PRO:HD3	2.01	0.41
3:A:606:LEU:HD12	3:A:606:LEU:HA	1.93	0.41
1:B:111:DC:H2'	1:B:112:DOC:H6	2.03	0.41
3:A:343:ARG:NE	3:A:365:LEU:HD21	2.35	0.41
3:A:361:LEU:HD12	3:A:361:LEU:HA	1.82	0.41
3:A:459:LEU:HD23	3:A:459:LEU:HA	1.88	0.41
3:A:487:ARG:HG3	6:A:3071:HOH:O	2.20	0.41
3:A:603:GLY:O	3:A:793:LYS:HD2	2.20	0.41
3:A:513:SER:HG	3:A:515:SER:HG	1.67	0.41
3:A:783:VAL:HB	3:A:786:GLU:CG	2.50	0.41
3:A:778:ARG:HD2	3:A:790:GLU:OE1	2.20	0.41
3:A:731:PRO:C	3:A:733:LEU:N	2.73	0.41
3:A:741:ARG:O	3:A:745:GLU:HG3	2.20	0.41
1:B:112:DOC:H2'	5:A:113:DCT:O4'	2.21	0.41
3:A:372:ASP:HA	3:A:373:PRO:HD2	1.94	0.41
3:A:706:TRP:CE2	3:A:710:THR:HG21	2.55	0.41
3:A:562:THR:HG22	3:A:581:LEU:HD12	2.03	0.41
3:A:585:PRO:HB2	3:A:591:GLY:CA	2.50	0.41
3:A:685:PRO:C	3:A:687:GLU:H	2.24	0.41
2:D:212:DT:H2''	2:D:213:DG:H5''	2.03	0.41
3:A:571:THR:OG1	3:A:754:GLN:NE2	2.45	0.41
3:A:800:ALA:HB1	3:A:821:VAL:HG11	2.02	0.41
3:A:627:ASN:HD22	3:A:627:ASN:HA	1.58	0.41
3:A:435:ARG:HB3	3:A:436:PRO:CD	2.51	0.40
3:A:516:ALA:O	3:A:520:GLU:HG3	2.22	0.40
3:A:309:PHE:CZ	3:A:356:LEU:HB2	2.57	0.40
3:A:730:VAL:HB	3:A:733:LEU:HD23	2.04	0.40
3:A:473:GLU:OE1	3:A:476:ARG:CZ	2.69	0.40
3:A:569:THR:CG2	3:A:571:THR:H	2.35	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
3	A	522/538 (97%)	473 (91%)	36 (7%)	13 (2%)	<b>5</b> <b>4</b>

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	525	ALA
3	A	578	ASP
3	A	656	PRO
3	A	586	VAL
3	A	693	ILE
3	A	732	ASP
3	A	329	GLY
3	A	638	ILE
3	A	685	PRO
3	A	692	PHE
3	A	637	ASP
3	A	300	PRO
3	A	686	TYR

### 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
3	A	370/440 (84%)	301 (81%)	69 (19%)	<b>1</b> <b>1</b>

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	307	VAL
3	A	314	LYS
3	A	321	LEU
3	A	324	LEU
3	A	333	HIS
3	A	337	GLU
3	A	347	GLU
3	A	361	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	A	362	ARG
3	A	375	LEU
3	A	376	LEU
3	A	416	LEU
3	A	426	LEU
3	A	432	GLU
3	A	459	LEU
3	A	461	LEU
3	A	470	LEU
3	A	473	GLU
3	A	484	LEU
3	A	487	ARG
3	A	507	GLU
3	A	508	LYS
3	A	513	SER
3	A	522	LEU
3	A	523	ARG
3	A	531	LYS
3	A	534	GLN
3	A	541	LEU
3	A	557	THR
3	A	562	THR
3	A	563	ARG
3	A	574	LEU
3	A	575	SER
3	A	577	SER
3	A	578	ASP
3	A	583	ASN
3	A	595	ARG
3	A	596	ARG
3	A	606	LEU
3	A	610	ASP
3	A	614	ILE
3	A	622	LEU
3	A	627	ASN
3	A	631	VAL
3	A	671	TYR
3	A	673	MET
3	A	704	ARG
3	A	711	LEU
3	A	720	VAL
3	A	721	GLU

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Mol	Chain	Res	Type
3	A	723	LEU
3	A	733	LEU
3	A	738	LYS
3	A	760	LEU
3	A	763	LEU
3	A	767	LYS
3	A	772	LEU
3	A	775	MET
3	A	778	ARG
3	A	782	GLN
3	A	789	LEU
3	A	797	GLU
3	A	802	LEU
3	A	813	LEU
3	A	817	LEU
3	A	818	GLU
3	A	826	ASP
3	A	831	LYS
3	A	832	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	443	HIS
3	A	561	HIS
3	A	566	GLN
3	A	582	GLN
3	A	583	ASN
3	A	613	GLN
3	A	621	HIS
3	A	627	ASN
3	A	633	GLN
3	A	754	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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
1	DOC	B	112	2,1	16,19,20	0.39	0	20,26,29	0.42	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
1	DOC	B	112	2,1	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

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
1	B	112	DOC	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
5	DCT	A	113	4	24,28,28	0.70	0	33,43,43	0.70	1 (3%)

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	DCT	A	113	4	-	2/22/31/31	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	113	DCT	O2G-PG-O1G	2.28	119.59	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	113	DCT	PB-O3B-PG-O3G
5	A	113	DCT	PB-O3B-PG-O2G

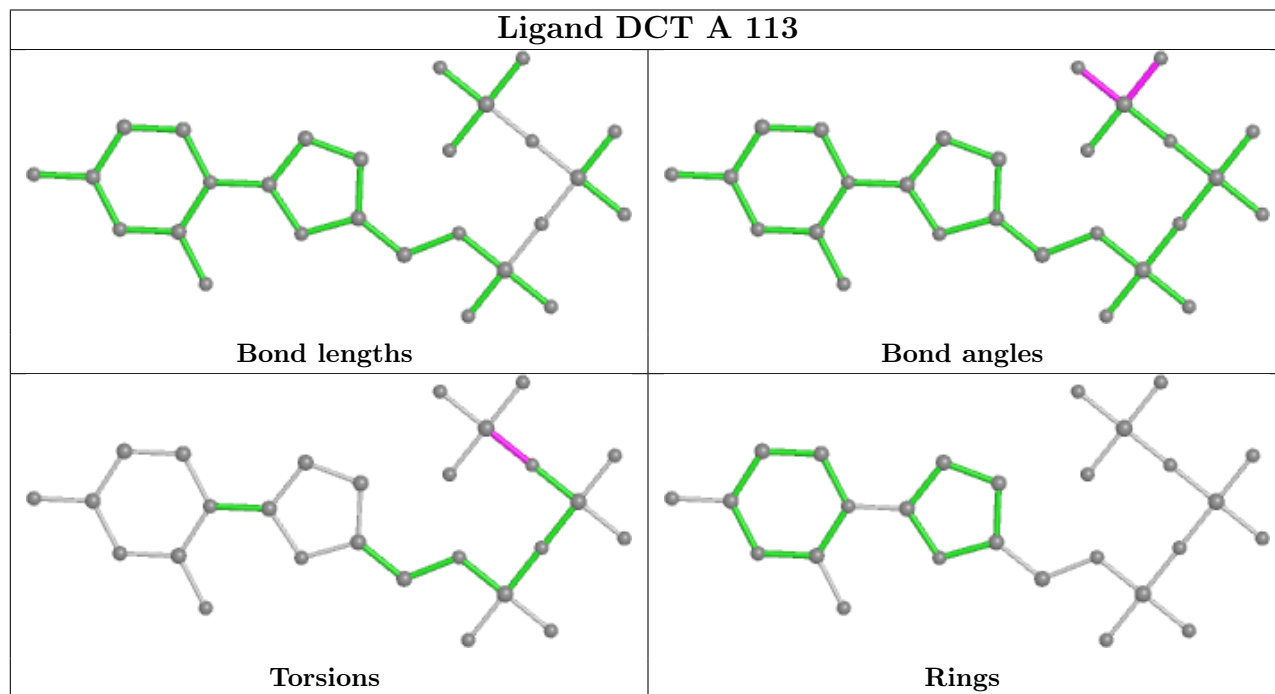
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	113	DCT	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.