



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:24 PM UTC

PDB ID : 3KTQ / pdb_00003ktq
Title : CRYSTAL STRUCTURE OF AN ACTIVE TERNARY COMPLEX OF
THE LARGE FRAGMENT OF DNA POLYMERASE I FROM THERMUS
AQUATICUS
Authors : Li, Y.; Waksman, G.
Deposited on : 1998-07-28
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

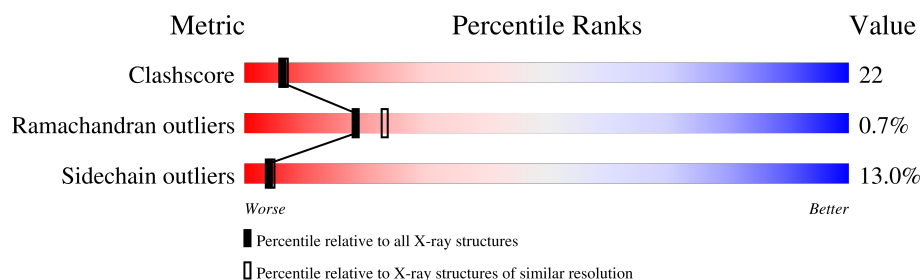
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 ≥ 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	50% 42% 8%
2	C	14	21% 64% 14%
3	A	540	55% 38% 6%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4874 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
1	B	12	Total	C	N	O	P	0	0	0
			240	114	48	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			288	136	56	83	13			

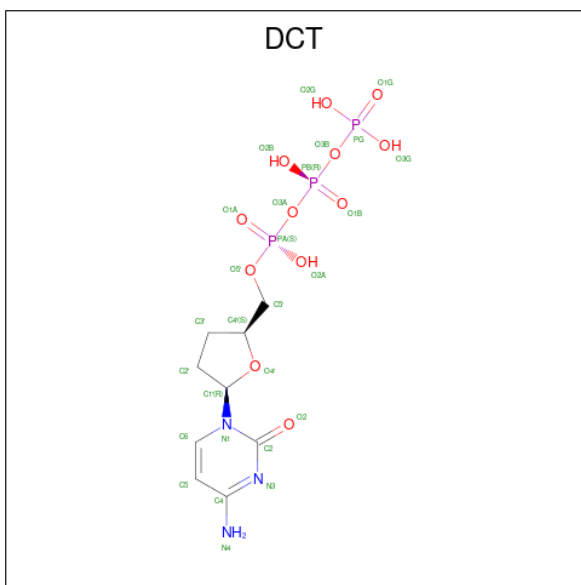
- Molecule 3 is a protein called PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	539	Total	C	N	O	S	0	0	0
			4168	2662	745	748	13			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	10	Total O 10 10	0	0
6	C	12	Total O 12 12	0	0
6	A	127	Total O 127 127	0	0

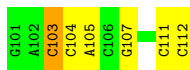
3 Residue-property plots

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.

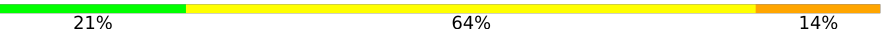
Note EDS was not executed.

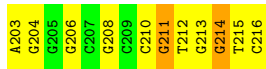
- Molecule 1: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*DOC)-3')

Chain B: 



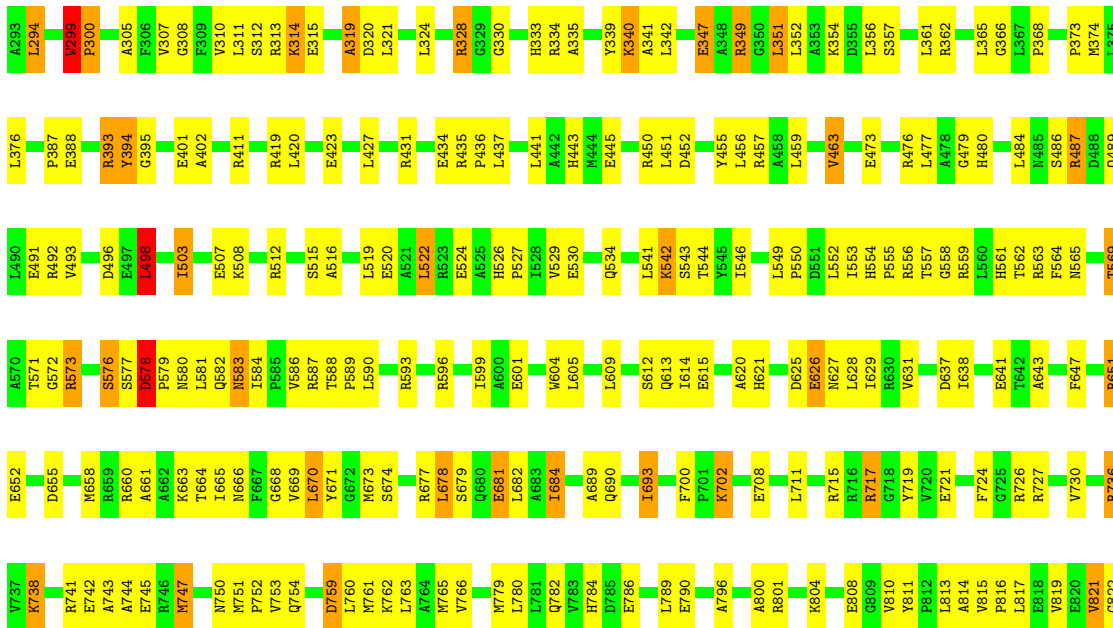
- Molecule 2: DNA (5'-D(*AP*GP*GP*GP*CP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')

Chain C: 



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

Chain A: 





4 Data and refinement statistics

Xtriage (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, α , β , γ	108.03Å 108.03Å 90.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.9 (30.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	6.00	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4874	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.35	0/249	0.73	0/382
2	C	0.46	0/323	0.88	1/498 (0.2%)
3	A	0.47	0/4258	0.98	15/5786 (0.3%)
All	All	0.46	0/4830	0.96	16/6666 (0.2%)

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
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	578	ASP	CA-C-N	-11.90	104.96	119.84
3	A	578	ASP	C-N-CA	-11.90	104.96	119.84
3	A	507	GLU	N-CA-C	10.03	121.90	110.97
3	A	700	PHE	CA-C-N	8.04	128.49	119.32
3	A	700	PHE	C-N-CA	8.04	128.49	119.32
3	A	498	LEU	N-CA-C	-7.02	101.48	110.53
3	A	587	ARG	N-CA-C	6.74	118.51	111.03
3	A	434	GLU	N-CA-C	6.35	117.89	110.97
2	C	211	DG	C5'-C4'-C3'	-6.25	105.52	114.90
3	A	319	ALA	N-CA-C	6.05	118.51	110.53
3	A	394	TYR	N-CA-C	5.69	120.96	112.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	578	ASP	N-CA-C	-5.39	97.90	109.81
3	A	744	ALA	N-CA-C	-5.35	105.36	111.14
3	A	299	TRP	N-CA-C	5.19	121.28	109.81
3	A	759	ASP	N-CA-C	-5.19	105.52	111.07
3	A	558	GLY	N-CA-C	-5.08	107.99	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	DC	Sidechain
2	C	214	DG	Sidechain

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	240	0	134	6	0
2	C	288	0	158	19	0
3	A	4168	0	4160	189	0
4	A	2	0	0	0	0
5	A	27	0	12	4	0
6	A	127	0	0	6	1
6	B	10	0	0	1	0
6	C	12	0	0	0	0
All	All	4874	0	4464	204	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 22.

All (204) 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)
2:C:215:DT:H2"	2:C:216:DC:H5"	1.29	1.14
3:A:351:LEU:HD13	3:A:373:PRO:HG2	1.33	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:DT:C2'	2:C:216:DC:H5''	1.94	0.98
3:A:621:HIS:HD2	3:A:814:ALA:H	1.10	0.97
3:A:631:VAL:HG11	3:A:638:ILE:HD11	1.53	0.91
3:A:565:ASN:HD21	3:A:577:SER:HB2	1.40	0.86
3:A:562:THR:HG21	3:A:576:SER:OG	1.80	0.81
3:A:351:LEU:HD12	3:A:374:MET:HG2	1.63	0.80
3:A:621:HIS:CD2	3:A:814:ALA:H	2.00	0.77
3:A:526:HIS:ND1	3:A:527:PRO:HD2	2.00	0.76
3:A:557:THR:OG1	3:A:561:HIS:HE1	1.67	0.76
3:A:352:LEU:HA	6:A:3074:HOH:O	1.86	0.75
3:A:554:HIS:HE1	3:A:556:ARG:HD2	1.52	0.75
3:A:463:VAL:CG2	3:A:542:LYS:HD3	2.17	0.73
3:A:542:LYS:HA	3:A:546:ILE:HB	1.71	0.73
3:A:625:ASP:O	3:A:629:ILE:HG23	1.89	0.73
3:A:351:LEU:CD1	3:A:373:PRO:HG2	2.16	0.72
3:A:476:ARG:HG2	3:A:476:ARG:HH11	1.53	0.72
3:A:541:LEU:HD12	3:A:590:LEU:HD23	1.70	0.72
2:C:214:DG:H2''	2:C:215:DT:OP2	1.88	0.71
3:A:441:LEU:O	3:A:445:GLU:HG3	1.92	0.70
3:A:708:GLU:HG3	6:A:3147:HOH:O	1.92	0.68
3:A:569:THR:HG21	3:A:573:ARG:H	1.59	0.68
3:A:578:ASP:O	3:A:579:PRO:C	2.31	0.68
3:A:516:ALA:O	3:A:520:GLU:HG2	1.93	0.68
3:A:822:GLY:HA3	3:A:830:ALA:O	1.94	0.68
3:A:651:ARG:HH11	3:A:651:ARG:HG3	1.58	0.68
3:A:815:VAL:HG13	3:A:816:PRO:HD2	1.76	0.66
3:A:682:LEU:HB2	3:A:684:ILE:HG12	1.77	0.66
6:B:3078:HOH:O	3:A:784:HIS:HE1	1.79	0.66
3:A:786:GLU:OE2	3:A:831:LYS:HE2	1.96	0.65
3:A:615:GLU:CD	5:A:113:DCT:H2''	2.21	0.65
3:A:376:LEU:HD22	3:A:420:LEU:HD12	1.79	0.64
3:A:621:HIS:HD2	3:A:814:ALA:N	1.91	0.63
3:A:476:ARG:HG2	3:A:476:ARG:NH1	2.11	0.63
3:A:625:ASP:HB2	3:A:702:LYS:HB2	1.80	0.62
3:A:638:ILE:HG22	3:A:666:ASN:ND2	2.15	0.61
3:A:813:LEU:HD12	3:A:817:LEU:HD21	1.82	0.61
3:A:678:LEU:HD12	3:A:693:ILE:HD11	1.81	0.61
3:A:810:VAL:HG13	3:A:811:TYR:H	1.65	0.61
3:A:589:PRO:O	3:A:593:ARG:HG3	2.01	0.61
3:A:569:THR:CG2	3:A:573:ARG:H	2.15	0.60
3:A:431:ARG:HG2	3:A:435:ARG:NH2	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:741:ARG:O	3:A:745:GLU:HG3	2.01	0.60
3:A:573:ARG:HD3	6:A:3064:HOH:O	2.01	0.60
3:A:315:GLU:HG3	3:A:578:ASP:OD2	2.01	0.60
3:A:492:ARG:O	3:A:496:ASP:HB2	2.02	0.59
3:A:562:THR:HG22	3:A:563:ARG:N	2.17	0.59
2:C:203:DA:H2'	3:A:674:SER:HB3	1.84	0.59
3:A:443:HIS:HE1	6:A:3009:HOH:O	1.84	0.59
3:A:583:ASN:HD22	3:A:583:ASN:H	1.51	0.59
2:C:212:DT:H2''	2:C:213:DG:H5''	1.85	0.58
3:A:450:ARG:HB3	3:A:599:ILE:O	2.02	0.58
3:A:780:LEU:HD11	3:A:790:GLU:HB2	1.85	0.58
3:A:393:ARG:HG2	3:A:394:TYR:CE2	2.39	0.58
3:A:335:ALA:HB1	3:A:341:ALA:HB2	1.85	0.58
2:C:215:DT:C3'	2:C:216:DC:H5''	2.33	0.58
3:A:810:VAL:HG13	3:A:811:TYR:N	2.18	0.58
2:C:213:DG:H2''	2:C:214:DG:O5'	2.04	0.58
3:A:366:GLY:O	3:A:368:PRO:HD3	2.04	0.58
3:A:376:LEU:HD22	3:A:420:LEU:CD1	2.34	0.57
2:C:213:DG:H2''	2:C:214:DG:C5'	2.34	0.57
2:C:211:DG:H2'	2:C:212:DT:H72	1.87	0.57
3:A:562:THR:CG2	3:A:563:ARG:N	2.68	0.57
3:A:627:ASN:O	3:A:631:VAL:HG23	2.05	0.57
3:A:393:ARG:O	3:A:393:ARG:HG3	2.06	0.56
2:C:206:DG:H4'	3:A:754:GLN:HE22	1.71	0.56
3:A:311:LEU:HB3	3:A:319:ALA:HB1	1.88	0.55
3:A:569:THR:HG21	3:A:573:ARG:N	2.21	0.55
3:A:601:GLU:O	3:A:604:TRP:HB2	2.05	0.55
3:A:615:GLU:HG2	3:A:753:VAL:HG12	1.89	0.55
3:A:420:LEU:HB3	3:A:427:LEU:HD21	1.88	0.55
3:A:578:ASP:O	3:A:580:ASN:N	2.40	0.55
3:A:419:ARG:HG2	3:A:419:ARG:NH1	2.21	0.55
1:B:107:DG:H4'	3:A:487:ARG:HD2	1.88	0.55
2:C:210:DC:H5'	3:A:544:THR:HG23	1.90	0.54
3:A:419:ARG:HG2	3:A:419:ARG:HH11	1.72	0.54
3:A:299:TRP:HB3	3:A:300:PRO:HD3	1.89	0.54
3:A:804:LYS:O	3:A:808:GLU:HG3	2.06	0.54
3:A:679:SER:HB2	3:A:684:ILE:O	2.08	0.54
1:B:111:DC:H2'	1:B:112:DOC:H6	1.90	0.54
3:A:498:LEU:N	3:A:498:LEU:HD23	2.23	0.54
3:A:347:GLU:OE2	3:A:349:ARG:HD2	2.08	0.53
3:A:609:LEU:HG	3:A:821:VAL:HG13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:DC:H2''	1:B:105:DA:C8	2.44	0.53
3:A:569:THR:HG21	3:A:573:ARG:HB2	1.91	0.53
1:B:112:DOC:OP2	3:A:660:ARG:NH1	2.42	0.52
3:A:614:ILE:HG22	5:A:113:DCT:O2B	2.09	0.52
3:A:743:ALA:O	3:A:747:MET:HG3	2.09	0.52
3:A:571:THR:HG21	3:A:754:GLN:NE2	2.25	0.52
2:C:208:DG:H4'	3:A:576:SER:O	2.10	0.52
3:A:613:GLN:HE22	3:A:638:ILE:H	1.57	0.52
3:A:443:HIS:CE1	6:A:3009:HOH:O	2.60	0.52
3:A:294:LEU:HA	3:A:330:GLY:O	2.09	0.51
3:A:420:LEU:HD13	3:A:427:LEU:HD23	1.92	0.51
3:A:576:SER:HB3	3:A:580:ASN:OD1	2.10	0.51
3:A:614:ILE:HG23	3:A:615:GLU:N	2.24	0.51
3:A:334:ARG:HH11	3:A:334:ARG:HG3	1.76	0.51
3:A:335:ALA:HB1	3:A:341:ALA:CB	2.41	0.51
3:A:549:LEU:HB2	3:A:550:PRO:HD3	1.92	0.51
3:A:678:LEU:HB3	3:A:689:ALA:HB1	1.91	0.51
3:A:452:ASP:O	3:A:455:TYR:HB3	2.10	0.50
3:A:562:THR:HG22	3:A:563:ARG:O	2.11	0.50
3:A:808:GLU:HG2	3:A:819:VAL:HG23	1.93	0.50
3:A:724:PHE:CD2	3:A:759:ASP:HB3	2.46	0.50
3:A:751:MET:HB3	3:A:752:PRO:HD3	1.93	0.50
3:A:340:LYS:HE2	3:A:341:ALA:N	2.26	0.50
3:A:583:ASN:HD22	3:A:583:ASN:N	2.09	0.50
3:A:437:LEU:HD11	3:A:765:MET:HE2	1.92	0.50
3:A:463:VAL:HG21	3:A:542:LYS:HD3	1.94	0.50
3:A:354:LYS:NZ	3:A:564:PHE:O	2.45	0.50
3:A:761:MET:HE3	3:A:761:MET:HA	1.93	0.49
3:A:486:SER:OG	3:A:489:GLN:HG3	2.11	0.49
2:C:212:DT:H4'	3:A:486:SER:HA	1.93	0.49
3:A:489:GLN:O	3:A:493:VAL:HG23	2.12	0.49
3:A:626:GLU:HA	3:A:629:ILE:HG12	1.94	0.49
1:B:103:DC:C2	1:B:104:DC:C5	3.01	0.49
3:A:554:HIS:HB3	3:A:557:THR:HG1	1.77	0.49
3:A:612:SER:O	3:A:613:GLN:C	2.55	0.49
3:A:625:ASP:CB	3:A:702:LYS:HB2	2.43	0.49
3:A:569:THR:CG2	3:A:573:ARG:N	2.75	0.49
3:A:643:ALA:O	3:A:647:PHE:HD1	1.96	0.48
2:C:213:DG:H2''	2:C:214:DG:H5'	1.94	0.48
3:A:307:VAL:HG11	3:A:356:LEU:CD2	2.44	0.48
3:A:721:GLU:HA	3:A:726:ARG:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:307:VAL:HG11	3:A:356:LEU:HD22	1.95	0.48
3:A:562:THR:OG1	3:A:581:LEU:HG	2.13	0.48
3:A:312:SER:HB3	3:A:320:ASP:HB3	1.96	0.48
3:A:621:HIS:CD2	3:A:813:LEU:HB3	2.49	0.48
3:A:738:LYS:O	3:A:742:GLU:HG3	2.14	0.48
3:A:779:MET:HG3	3:A:789:LEU:CD2	2.44	0.48
3:A:628:LEU:O	3:A:631:VAL:HB	2.14	0.48
3:A:719:TYR:CE2	3:A:727:ARG:HG2	2.50	0.47
3:A:765:MET:SD	3:A:782:GLN:HG3	2.54	0.47
3:A:800:ALA:HB1	3:A:821:VAL:HG11	1.95	0.47
3:A:677:ARG:O	3:A:681:GLU:HB2	2.15	0.47
2:C:206:DG:C4'	3:A:754:GLN:HE22	2.27	0.47
3:A:473:GLU:O	3:A:477:LEU:HD23	2.15	0.47
3:A:673:MET:HE2	3:A:677:ARG:NE	2.30	0.47
3:A:620:ALA:HB2	3:A:628:LEU:HG	1.96	0.47
3:A:578:ASP:CB	3:A:579:PRO:CD	2.92	0.46
3:A:631:VAL:HG11	3:A:638:ILE:CD1	2.36	0.46
3:A:637:ASP:O	3:A:641:GLU:HG3	2.16	0.46
3:A:299:TRP:CE2	3:A:341:ALA:HB1	2.51	0.46
3:A:299:TRP:O	3:A:333:HIS:HB3	2.16	0.46
3:A:387:PRO:HG2	3:A:388:GLU:OE1	2.15	0.46
3:A:661:ALA:O	3:A:664:THR:HG22	2.15	0.46
3:A:493:VAL:O	3:A:498:LEU:HG	2.16	0.46
3:A:554:HIS:CG	3:A:555:PRO:HD2	2.50	0.46
3:A:717:ARG:HG2	3:A:719:TYR:CE1	2.51	0.46
3:A:738:LYS:HD3	3:A:742:GLU:CD	2.41	0.46
3:A:522:LEU:HB3	3:A:529:VAL:HG21	1.97	0.46
3:A:669:VAL:HG22	3:A:693:ILE:HD13	1.98	0.46
3:A:435:ARG:N	3:A:436:PRO:HD2	2.31	0.46
3:A:451:LEU:HD21	3:A:456:LEU:HD12	1.97	0.45
3:A:581:LEU:HD23	3:A:584:ILE:HD11	1.96	0.45
3:A:503:ILE:CD1	3:A:522:LEU:HD13	2.45	0.45
3:A:557:THR:OG1	3:A:561:HIS:CE1	2.58	0.45
3:A:310:VAL:HG23	3:A:402:ALA:HB2	1.97	0.45
3:A:435:ARG:HB3	3:A:436:PRO:HD3	1.96	0.45
3:A:455:TYR:OH	3:A:596:ARG:NH2	2.50	0.45
3:A:615:GLU:OE2	5:A:113:DCT:H2"	2.16	0.45
3:A:663:LYS:HE2	5:A:113:DCT:O3G	2.16	0.45
3:A:486:SER:HG	3:A:489:GLN:HG3	1.82	0.44
3:A:588:THR:HB	3:A:589:PRO:HD2	2.00	0.44
2:C:204:DG:C4	3:A:668:GLY:HA2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:DA:C2'	3:A:674:SER:HB3	2.45	0.44
3:A:626:GLU:O	3:A:629:ILE:HG12	2.18	0.44
3:A:423:GLU:OE1	3:A:727:ARG:NH2	2.51	0.43
3:A:395:GLY:O	3:A:411:ARG:HD2	2.18	0.43
3:A:526:HIS:CE1	3:A:527:PRO:HD2	2.53	0.43
3:A:562:THR:HG23	3:A:579:PRO:O	2.18	0.43
3:A:450:ARG:HB2	3:A:559:ARG:NH1	2.34	0.42
3:A:530:GLU:O	3:A:534:GLN:HG3	2.19	0.42
3:A:519:LEU:O	3:A:529:VAL:HG11	2.19	0.42
3:A:299:TRP:O	3:A:300:PRO:C	2.62	0.42
3:A:315:GLU:CG	3:A:578:ASP:OD2	2.67	0.42
3:A:578:ASP:HB3	3:A:579:PRO:CD	2.50	0.42
3:A:299:TRP:CZ2	3:A:341:ALA:HB1	2.55	0.42
3:A:678:LEU:HD12	3:A:693:ILE:CD1	2.48	0.42
3:A:313:ARG:HH21	3:A:315:GLU:CD	2.28	0.41
3:A:762:LYS:O	3:A:766:VAL:HG23	2.19	0.41
3:A:572:GLY:O	3:A:762:LYS:HE3	2.20	0.41
3:A:305:ALA:HA	3:A:328:ARG:HG2	2.01	0.41
2:C:211:DG:H2'	2:C:212:DT:C7	2.49	0.41
3:A:307:VAL:CG1	3:A:308:GLY:N	2.83	0.41
3:A:651:ARG:NH1	3:A:651:ARG:CG	2.83	0.41
3:A:314:LYS:H	3:A:314:LYS:CE	2.33	0.41
3:A:357:SER:O	3:A:361:LEU:HG	2.21	0.41
3:A:491:GLU:OE2	3:A:512:ARG:NE	2.46	0.41
3:A:609:LEU:O	3:A:786:GLU:HA	2.21	0.41
3:A:736:ARG:HA	3:A:736:ARG:HD2	1.68	0.41
3:A:333:HIS:ND1	3:A:333:HIS:N	2.68	0.41
3:A:655:ASP:OD1	3:A:658:MET:HG3	2.21	0.41
3:A:582:GLN:NE2	6:A:3071:HOH:O	2.53	0.41
3:A:605:LEU:HD12	3:A:796:ALA:CB	2.50	0.41
3:A:638:ILE:HG22	3:A:666:ASN:HD21	1.85	0.41
3:A:665:ILE:CD1	3:A:682:LEU:HD21	2.51	0.41
3:A:670:LEU:HD13	3:A:671:TYR:CZ	2.55	0.41
3:A:479:GLY:O	3:A:480:HIS:HB3	2.20	0.40
3:A:420:LEU:HB3	3:A:427:LEU:CD2	2.52	0.40
3:A:339:TYR:O	3:A:342:LEU:HB2	2.21	0.40
1:B:103:DC:H2''	1:B:104:DC:OP2	2.21	0.40
2:C:214:DG:C2'	2:C:215:DT:OP2	2.63	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)
6:A:3095:HOH:O	6:A:3095:HOH:O[6_555]	1.64	0.56

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	537/540 (99%)	511 (95%)	22 (4%)	4 (1%)	18 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	578	ASP
3	A	299	TRP
3	A	300	PRO
3	A	586	VAL

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	414/441 (94%)	360 (87%)	54 (13%)	4 4

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	294	LEU
3	A	314	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	321	LEU
3	A	324	LEU
3	A	328	ARG
3	A	340	LYS
3	A	347	GLU
3	A	349	ARG
3	A	351	LEU
3	A	362	ARG
3	A	365	LEU
3	A	393	ARG
3	A	401	GLU
3	A	457	ARG
3	A	459	LEU
3	A	463	VAL
3	A	484	LEU
3	A	487	ARG
3	A	498	LEU
3	A	503	ILE
3	A	508	LYS
3	A	515	SER
3	A	522	LEU
3	A	524	GLU
3	A	542	LYS
3	A	543	SER
3	A	552	LEU
3	A	553	ILE
3	A	569	THR
3	A	573	ARG
3	A	576	SER
3	A	583	ASN
3	A	626	GLU
3	A	651	ARG
3	A	652	GLU
3	A	670	LEU
3	A	678	LEU
3	A	681	GLU
3	A	684	ILE
3	A	690	GLN
3	A	693	ILE
3	A	702	LYS
3	A	711	LEU
3	A	715	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	717	ARG
3	A	730	VAL
3	A	736	ARG
3	A	738	LYS
3	A	747	MET
3	A	750	ASN
3	A	760	LEU
3	A	763	LEU
3	A	801	ARG
3	A	821	VAL

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

Mol	Chain	Res	Type
3	A	443	HIS
3	A	554	HIS
3	A	561	HIS
3	A	565	ASN
3	A	566	GLN
3	A	582	GLN
3	A	583	ASN
3	A	621	HIS
3	A	633	GLN
3	A	690	GLN
3	A	754	GLN
3	A	784	HIS

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	0.37	0	20,26,29	0.50	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DCT	A	113	4	27,28,28	1.06	2 (7%)	37,43,43	0.92	2 (5%)

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	-	5/22/31/31	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	113	DCT	PB-O3A	3.07	1.62	1.59
5	A	113	DCT	PB-O3B	2.42	1.62	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	113	DCT	O3B-PB-O1B	-2.87	102.08	110.70
5	A	113	DCT	O2G-PG-O1G	2.28	119.73	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	113	DCT	PB-O3A-PA-O1A
5	A	113	DCT	PB-O3A-PA-O2A
5	A	113	DCT	PB-O3B-PG-O1G
5	A	113	DCT	PB-O3B-PG-O2G
5	A	113	DCT	PB-O3B-PG-O3G

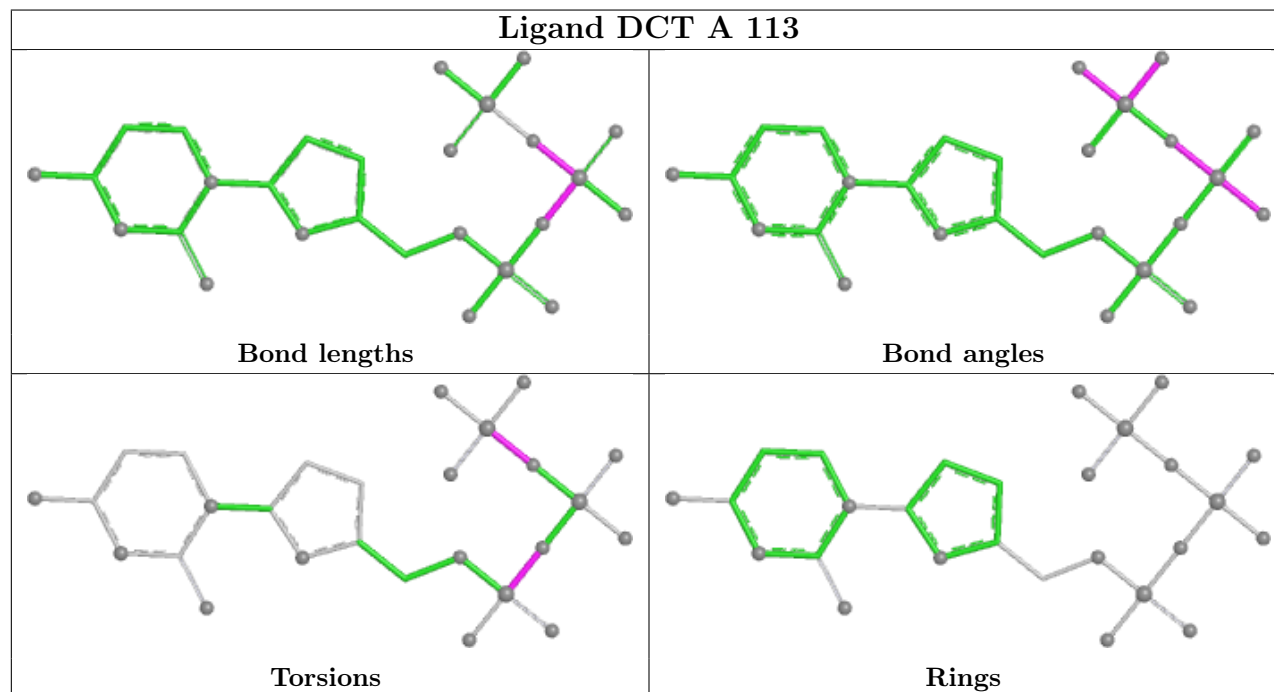
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	113	DCT	4	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

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.