



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 09:39 AM GMT

PDB ID : 3KTQ
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 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>

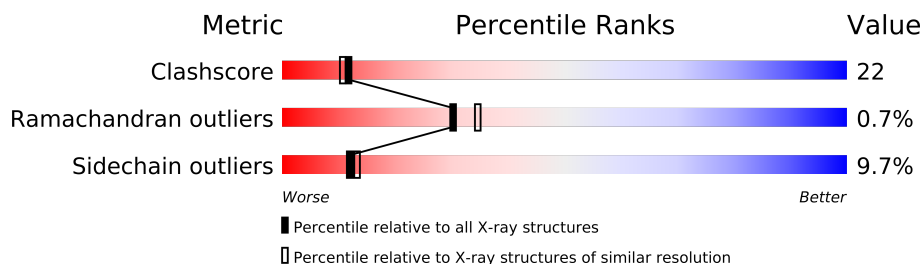
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 2.30 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	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	12	
2	C	14	
3	A	540	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4874 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 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			

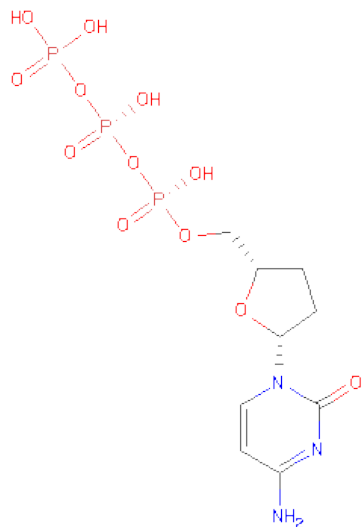
- Molecule 3 is a protein called PROTEIN (LARGE FRAGMENT OF DNA POLYMERASE I).

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE5'-TRIPHOSPHATE (three-letter code: 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	A	127	Total	O	0	0
			127	127		
6	B	10	Total	O	0	0
			10	10		
6	C	12	Total	O	0	0
			12	12		

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.

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: 



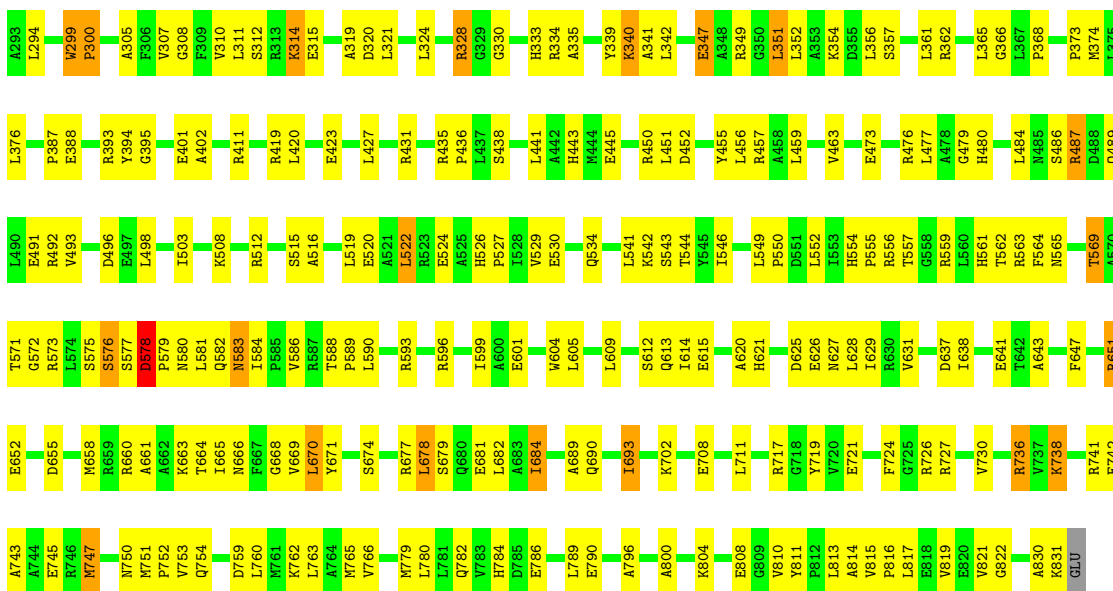
- Molecule 2: DNA (5'-D(*AP*GP*GP*GP*CP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')

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 will therefore be 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: DOC, MG, DCT

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	0.50	0/249	0.82	0/382
2	C	0.72	0/323	0.89	0/498
3	A	0.38	0/4258	0.63	1/5786 (0.0%)
All	All	0.42	0/4830	0.67	1/6666 (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
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	578	ASP	C-N-CD	6.50	142.05	128.40

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 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	B	240	0	134	6	0
2	C	288	0	158	19	0
3	A	4168	0	4160	184	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	199	1

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 22.

All (199) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:541:LEU:HD12	3:A:590:LEU:HD23	1.70	0.72
3:A:476:ARG:HH11	3:A:476:ARG:HG2	1.53	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:376:LEU:HD22	3:A:420:LEU:HD12	1.79	0.64
3:A:578:ASP:O	3:A:579:PRO:C	2.31	0.64
3:A:621:HIS:HD2	3:A:814:ALA:N	1.91	0.63
3:A:476:ARG:NH1	3:A:476:ARG:HG2	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:615:GLU:CD	5:A:113:DCT:H2"	2.21	0.60
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
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:562:THR:HG22	3:A:563:ARG:N	2.17	0.59
3:A:492:ARG:O	3:A:496:ASP:HB2	2.02	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:780:LEU:HD11	3:A:790:GLU:HB2	1.85	0.58
3:A:450:ARG:HB3	3:A:599:ILE:O	2.02	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:627:ASN:O	3:A:631:VAL:HG23	2.05	0.57
3:A:562:THR:CG2	3:A:563:ARG:N	2.68	0.57
3:A:393:ARG:HG3	3:A:393:ARG:O	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:578:ASP:O	3:A:580:ASN:N	2.40	0.55
3:A:420:LEU:HB3	3:A:427:LEU:HD21	1.88	0.55
3:A:419:ARG:NH1	3:A:419:ARG:HG2	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
3:A:498:LEU:HD23	3:A:498:LEU:N	2.23	0.54
1:B:111:DC:H2'	1:B:112:DOC:H6	1.90	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
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
3:A:613:GLN:HE22	3:A:638:ILE:H	1.57	0.52
2:C:208:DG:H4'	3:A:576:SER:O	2.10	0.52
3:A:614:ILE:HG23	3:A:615:GLU:N	2.24	0.52
3:A:443:HIS:CE1	6:A:3009:HOH:O	2.60	0.52
3:A:576:SER:HB3	3:A:580:ASN:OD1	2.10	0.51
3:A:420:LEU:HD13	3:A:427:LEU:HD23	1.92	0.51
3:A:294:LEU:HA	3:A:330:GLY:O	2.09	0.51
3:A:334:ARG:HG3	3:A:334:ARG:HH11	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:452:ASP:O	3:A:455:TYR:HB3	2.10	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: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: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: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
3:A:562:THR:OG1	3:A:581:LEU:HG	2.13	0.48
3:A:307:VAL:HG11	3:A:356:LEU:HD22	1.95	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:779:MET:HG3	3:A:789:LEU:CD2	2.44	0.48
3:A:738:LYS:O	3:A:742:GLU:HG3	2.14	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:620:ALA:HB2	3:A:628:LEU:HG	1.96	0.47
3:A:631:VAL:HG11	3:A:638:ILE:CD1	2.36	0.46
3:A:578:ASP:CB	3:A:579:PRO:CD	2.92	0.46
3:A:637:ASP:O	3:A:641:GLU:HG3	2.16	0.46
3:A:299:TRP:O	3:A:333:HIS:HB3	2.16	0.46
3:A:299:TRP:CE2	3:A:341:ALA:HB1	2.51	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:717:ARG:HG2	3:A:719:TYR:CE1	2.51	0.46
3:A:669:VAL:HG22	3:A:693:ILE:HD13	1.98	0.46
3:A:522:LEU:HB3	3:A:529:VAL:HG21	1.97	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:557:THR:OG1	3:A:561:HIS:CE1	2.58	0.45
3:A:503:ILE:CD1	3:A:522:LEU:HD13	2.45	0.45
3:A:435:ARG:HB3	3:A:436:PRO:HD3	1.96	0.45
3:A:310:VAL:HG23	3:A:402:ALA:HB2	1.97	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:455:TYR:OH	3:A:596:ARG:NH2	2.50	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
3:A:612:SER:O	3:A:613:GLN:C	2.55	0.44
2:C:204:DG:C4	3:A:668:GLY:HA2	2.52	0.44
3:A:626:GLU:O	3:A:629:ILE:HG12	2.18	0.44
2:C:203:DA:C2'	3:A:674:SER:HB3	2.45	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:562:THR:HG23	3:A:579:PRO:O	2.18	0.43
3:A:526:HIS:CE1	3:A:527:PRO:HD2	2.53	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:578:ASP:HB3	3:A:579:PRO:CD	2.50	0.42
3:A:315:GLU:CG	3:A:578:ASP:OD2	2.67	0.42
3:A:678:LEU:HD12	3:A:693:ILE:CD1	2.48	0.42
3:A:299:TRP:CZ2	3:A:341:ALA:HB1	2.55	0.42
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:738:LYS:HD3	3:A:742:GLU:CD	2.41	0.41
3:A:651:ARG:CG	3:A:651:ARG:NH1	2.83	0.41
3:A:307:VAL:CG1	3:A:308:GLY:N	2.83	0.41
3:A:609:LEU:O	3:A:786:GLU:HA	2.21	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:314:LYS:H	3:A:314:LYS:CE	2.33	0.41
3:A:736:ARG:HD2	3:A:736:ARG:HA	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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: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	Distance(Å)	Clash(Å)
6:A:3095:HOH:O	6:A:3095:HOH:O[6_555]	1.64	0.56

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
3	A	537/540 (99%)	511 (95%)	22 (4%)	4 (1%)	30 34

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 ⓘ

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%)	374 (90%)	40 (10%)	12	13

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	314	LYS
3	A	321	LEU
3	A	324	LEU
3	A	328	ARG
3	A	340	LYS
3	A	347	GLU
3	A	351	LEU
3	A	362	ARG
3	A	365	LEU
3	A	401	GLU
3	A	438	SER
3	A	457	ARG
3	A	459	LEU
3	A	484	LEU
3	A	487	ARG
3	A	508	LYS
3	A	515	SER
3	A	522	LEU
3	A	524	GLU
3	A	543	SER
3	A	552	LEU
3	A	569	THR
3	A	575	SER
3	A	576	SER
3	A	583	ASN
3	A	651	ARG
3	A	652	GLU
3	A	670	LEU
3	A	678	LEU
3	A	684	ILE
3	A	690	GLN

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Mol	Chain	Res	Type
3	A	693	ILE
3	A	711	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	613	GLN
3	A	621	HIS
3	A	633	GLN
3	A	690	GLN
3	A	754	GLN
3	A	784	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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	1,2	17,19,20	1.07	1 (5%)	20,26,29	0.87	1 (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
1	DOC	B	112	1,2	-	0/5/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	DOC	C2-N1	3.20	1.41	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	DOC	C2-N3-C4	3.07	120.01	115.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DCT	A	113	4	28,28,28	1.04	1 (3%)	40,43,43	1.50	6 (15%)

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	-	0/19/31/31	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	113	DCT	C2-N1	2.43	1.40	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	113	DCT	PB-O3B-PG	4.69	145.43	131.68
5	A	113	DCT	PB-O3A-PA	3.96	143.31	131.68
5	A	113	DCT	O3B-PB-O3A	3.49	108.77	101.66
5	A	113	DCT	C2-N3-C4	3.09	120.04	115.57
5	A	113	DCT	O2G-PG-O1G	2.84	119.73	110.44
5	A	113	DCT	O3A-PA-O5'	-2.04	94.26	103.41

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.