



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:33 AM UTC

PDB ID : 5KTQ / pdb_00005ktq
Title : LARGE FRAGMENT OF TAQ DNA POLYMERASE BOUND TO DCTP
Authors : Li, Y.; Kong, Y.; Korolev, S.; Waksman, G.
Deposited on : 1998-09-22
Resolution : 2.50 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

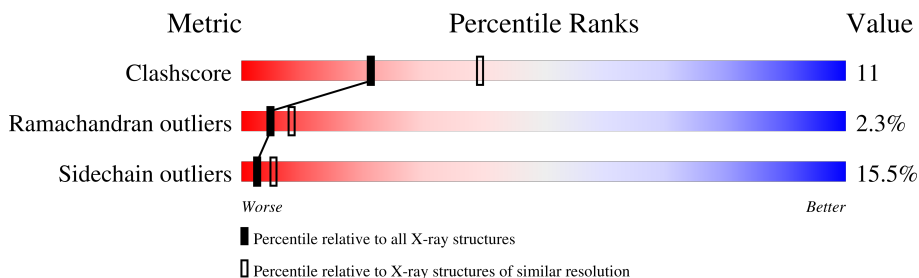
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	543	53% 34% 10% ..

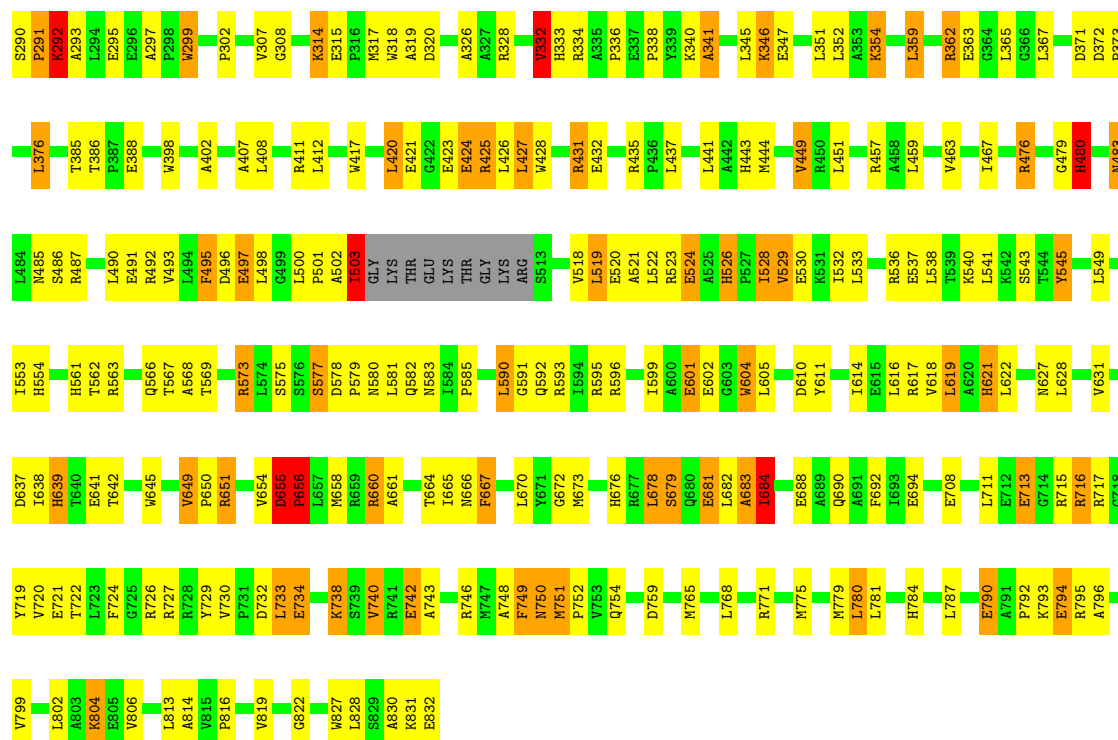
3 Residue-property plots

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: PROTEIN (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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.40 Å 137.00 Å 45.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	85.0 (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.217 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4267	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: DCP

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	1.00	12/4329 (0.3%)	1.83	96/5867 (1.6%)

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	A	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	639	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	621	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	554	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	480	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	443	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	526	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	561	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	333	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	654	VAL	CA-CB	5.90	1.62	1.54
1	A	676	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	740	VAL	CA-CB	5.37	1.61	1.54

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	LYS	N-CA-C	9.96	121.82	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	749	PHE	CA-CB-CG	9.63	123.43	113.80
1	A	796	ALA	N-CA-C	8.91	121.95	111.71
1	A	402	ALA	N-CA-C	8.59	121.72	111.33
1	A	543	SER	CA-CB-OG	8.16	127.43	111.10
1	A	292	LYS	N-CA-C	8.13	121.76	108.99
1	A	602	GLU	N-CA-C	8.02	122.64	113.01
1	A	637	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	524	GLU	N-CA-C	7.51	126.79	110.80
1	A	530	GLU	N-CA-C	-7.22	105.08	114.04
1	A	780	LEU	N-CA-C	7.21	122.14	113.12
1	A	656	PRO	N-CA-C	6.95	126.79	112.47
1	A	341	ALA	N-CA-C	6.84	118.74	111.28
1	A	326	ALA	N-CA-C	6.74	119.08	107.28
1	A	320	ASP	CA-CB-CG	6.53	119.12	112.60
1	A	372	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	804	LYS	CB-CA-C	-6.44	100.78	110.88
1	A	483	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	521	ALA	N-CA-C	6.29	118.13	111.28
1	A	684	ILE	N-CA-CB	-6.28	102.42	111.21
1	A	528	ILE	N-CA-C	6.25	116.89	110.82
1	A	577	SER	CA-C-N	-6.19	114.33	122.74
1	A	577	SER	C-N-CA	-6.19	114.33	122.74
1	A	667	PHE	CA-CB-CG	-6.12	107.68	113.80
1	A	371	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	480	HIS	CA-C-N	6.01	125.92	119.85
1	A	480	HIS	C-N-CA	6.01	125.92	119.85
1	A	367	LEU	CA-C-N	5.97	126.53	120.38
1	A	367	LEU	C-N-CA	5.97	126.53	120.38
1	A	549	LEU	N-CA-C	5.95	121.61	113.16
1	A	480	HIS	CA-CB-CG	-5.88	107.92	113.80
1	A	431	ARG	CB-CG-CD	-5.83	97.89	111.30
1	A	610	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	554	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	676	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	A	386	THR	CA-C-N	5.76	125.23	119.24
1	A	386	THR	C-N-CA	5.76	125.23	119.24
1	A	424	GLU	N-CA-C	5.73	118.47	111.82
1	A	526	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	748	ALA	CA-C-O	-5.67	114.54	120.55
1	A	642	THR	N-CA-C	-5.65	105.03	111.14
1	A	503	ILE	N-CA-CB	-5.65	101.90	111.50
1	A	654	VAL	N-CA-C	5.65	121.09	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	O-C-N	5.64	127.88	122.07
1	A	599	ILE	N-CA-C	5.64	117.30	109.29
1	A	569	THR	N-CA-C	5.60	119.10	110.42
1	A	297	ALA	O-C-N	-5.59	114.89	121.32
1	A	575	SER	CA-CB-OG	5.57	122.25	111.10
1	A	307	VAL	CA-C-N	5.54	127.06	121.35
1	A	307	VAL	C-N-CA	5.54	127.06	121.35
1	A	621	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	566	GLN	N-CA-CB	-5.53	102.98	110.67
1	A	688	GLU	CB-CG-CD	5.52	121.98	112.60
1	A	545	TYR	N-CA-C	5.49	120.09	113.17
1	A	566	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	660	ARG	N-CA-C	-5.48	106.64	113.55
1	A	561	HIS	CA-C-N	5.43	128.48	120.82
1	A	561	HIS	C-N-CA	5.43	128.48	120.82
1	A	590	LEU	N-CA-C	5.43	119.07	112.23
1	A	545	TYR	CA-C-N	-5.42	117.61	123.08
1	A	545	TYR	C-N-CA	-5.42	117.61	123.08
1	A	299	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	A	604	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	A	367	LEU	CA-C-O	-5.36	115.81	119.29
1	A	443	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	A	503	ILE	CB-CG1-CD1	5.33	124.99	113.80
1	A	354	LYS	CA-CB-CG	5.31	124.73	114.10
1	A	293	ALA	CB-CA-C	-5.30	110.48	116.63
1	A	716	ARG	N-CA-CB	-5.28	102.31	110.13
1	A	318	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	A	601	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	308	GLY	O-C-N	-5.28	118.66	123.57
1	A	476	ARG	CA-CB-CG	-5.27	103.56	114.10
1	A	573	ARG	O-C-N	-5.26	116.65	122.86
1	A	332	VAL	CB-CA-C	-5.24	104.17	110.99
1	A	679	SER	CA-CB-OG	5.21	121.53	111.10
1	A	738	LYS	N-CA-C	5.18	117.33	111.11
1	A	618	VAL	N-CA-C	-5.17	105.67	110.53
1	A	537	GLU	CA-CB-CG	-5.17	103.77	114.10
1	A	532	ILE	CB-CA-C	-5.15	105.38	111.97
1	A	681	GLU	N-CA-C	-5.14	105.57	111.07
1	A	315	GLU	CA-C-N	5.11	124.29	118.97
1	A	315	GLU	C-N-CA	5.11	124.29	118.97
1	A	407	ALA	CA-C-N	5.11	127.44	120.54
1	A	407	ALA	C-N-CA	5.11	127.44	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TRP	O-C-N	-5.09	115.93	121.53
1	A	398	TRP	N-CA-C	-5.08	100.88	108.96
1	A	708	GLU	N-CA-C	5.08	116.89	111.36
1	A	743	ALA	N-CA-C	5.06	116.48	111.07
1	A	541	LEU	N-CA-C	5.06	117.18	111.11
1	A	554	HIS	CA-C-N	5.05	124.66	119.05
1	A	554	HIS	C-N-CA	5.05	124.66	119.05
1	A	580	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	655	ASP	N-CA-C	5.05	120.97	109.81
1	A	784	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	568	ALA	N-CA-C	5.01	119.52	113.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	SER	Peptide
1	A	655	ASP	Peptide

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	A	4239	0	4273	93	0
2	A	28	0	12	1	0
All	All	4267	0	4285	93	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 11.

All (93) 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:596:ARG:HE	1:A:828:LEU:HD23	1.49	0.77
1:A:449:VAL:HG12	1:A:780:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:O	1:A:503:ILE:HB	1.89	0.71
1:A:673:MET:SD	1:A:678:LEU:HD12	2.29	0.71
1:A:722:THR:HG22	1:A:724:PHE:H	1.56	0.70
1:A:585:PRO:O	1:A:591:GLY:HA3	1.94	0.68
1:A:780:LEU:HD11	1:A:790:GLU:HG3	1.74	0.68
1:A:437:LEU:HG	1:A:441:LEU:HD13	1.76	0.67
1:A:664:THR:HG21	1:A:682:LEU:HG	1.79	0.64
1:A:420:LEU:HD23	1:A:427:LEU:HD22	1.80	0.62
1:A:768:LEU:HG	1:A:806:VAL:HG11	1.82	0.60
1:A:581:LEU:HD11	1:A:781:LEU:HD22	1.84	0.59
1:A:523:ARG:HA	1:A:529:VAL:HG23	1.85	0.59
1:A:502:ALA:C	1:A:503:ILE:HD13	2.29	0.58
1:A:545:TYR:OH	1:A:583:ASN:HB2	2.04	0.58
1:A:423:GLU:HG2	1:A:426:LEU:HD12	1.87	0.57
1:A:621:HIS:HD2	1:A:814:ALA:H	1.52	0.57
1:A:605:LEU:HG	1:A:793:LYS:HG2	1.88	0.56
1:A:299:TRP:HB2	1:A:334:ARG:O	2.06	0.56
1:A:592:GLN:HB2	1:A:828:LEU:HD13	1.88	0.56
1:A:730:VAL:HG12	1:A:733:LEU:HB2	1.88	0.55
1:A:385:THR:HG22	1:A:567:THR:O	2.08	0.54
1:A:661:ALA:O	1:A:665:ILE:HG12	2.07	0.54
1:A:495:PHE:CG	1:A:503:ILE:HG13	2.43	0.53
1:A:711:LEU:O	1:A:715:ARG:HB2	2.08	0.53
1:A:314:LYS:HB2	1:A:319:ALA:HB2	1.89	0.53
1:A:742:GLU:O	1:A:746:ARG:HG2	2.08	0.53
1:A:492:ARG:O	1:A:496:ASP:HB2	2.09	0.53
1:A:595:ARG:O	1:A:827:TRP:HB3	2.09	0.53
1:A:483:ASN:HD22	1:A:485:ASN:H	1.57	0.52
1:A:722:THR:HG21	1:A:759:ASP:OD2	2.09	0.52
1:A:376:LEU:HD12	1:A:420:LEU:HD13	1.90	0.51
1:A:528:ILE:HG23	1:A:529:VAL:HG13	1.92	0.51
1:A:750:ASN:HB3	1:A:754:GLN:HE21	1.76	0.51
1:A:751:MET:HB3	1:A:752:PRO:HD3	1.92	0.51
1:A:794:GLU:H	1:A:794:GLU:CD	2.19	0.51
1:A:487:ARG:HH22	1:A:536:ARG:NH2	2.09	0.50
1:A:621:HIS:CD2	1:A:814:ALA:H	2.28	0.50
1:A:463:VAL:HG13	1:A:538:LEU:HD22	1.93	0.50
1:A:563:ARG:HB2	1:A:577:SER:HB2	1.94	0.49
1:A:292:LYS:HB2	1:A:292:LYS:NZ	2.27	0.49
1:A:639:HIS:HE2	1:A:667:PHE:HE1	1.58	0.49
1:A:804:LYS:HA	1:A:819:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HB	1:A:651:ARG:O	2.13	0.49
1:A:775:MET:HE1	1:A:802:LEU:HD22	1.93	0.48
1:A:421:GLU:HA	1:A:427:LEU:HD23	1.95	0.48
1:A:684:ILE:HD13	1:A:692:PHE:HE1	1.78	0.47
1:A:771:ARG:HB3	1:A:802:LEU:HD21	1.97	0.46
1:A:359:LEU:O	1:A:362:ARG:HB3	2.16	0.46
1:A:463:VAL:O	1:A:467:ILE:HG13	2.15	0.46
1:A:713:GLU:O	1:A:717:ARG:HG2	2.14	0.46
1:A:617:ARG:HD3	1:A:816:PRO:O	2.15	0.46
1:A:679:SER:O	1:A:683:ALA:HA	2.15	0.46
1:A:601:GLU:HB3	1:A:604:TRP:CD1	2.51	0.46
1:A:302:PRO:HG2	1:A:328:ARG:HD3	1.98	0.46
1:A:627:ASN:O	1:A:631:VAL:HG23	2.15	0.46
1:A:822:GLY:HA3	1:A:830:ALA:O	2.17	0.45
1:A:346:LYS:HZ2	1:A:347:GLU:HG2	1.81	0.45
1:A:828:LEU:O	1:A:831:LYS:HB3	2.15	0.45
1:A:479:GLY:O	1:A:480:HIS:HD2	2.00	0.45
1:A:417:TRP:HH2	1:A:427:LEU:HD11	1.81	0.45
1:A:487:ARG:O	1:A:491:GLU:HG2	2.17	0.45
1:A:363:GLU:O	1:A:365:LEU:HD13	2.17	0.45
1:A:417:TRP:CH2	1:A:427:LEU:HD11	2.52	0.45
1:A:639:HIS:CD2	1:A:666:ASN:HD22	2.34	0.44
1:A:765:MET:HE3	1:A:787:LEU:HD21	1.98	0.44
1:A:639:HIS:HE1	2:A:901:DCP:O2B	2.01	0.44
1:A:444:MET:HG2	1:A:779:MET:O	2.18	0.44
1:A:596:ARG:NE	1:A:828:LEU:HD23	2.26	0.44
1:A:655:ASP:HA	1:A:658:MET:HE3	1.99	0.44
1:A:338:PRO:O	1:A:341:ALA:HB3	2.18	0.44
1:A:495:PHE:CE2	1:A:503:ILE:HD11	2.52	0.43
1:A:317:MET:HE3	1:A:317:MET:HB3	1.86	0.43
1:A:425:ARG:HD3	1:A:724:PHE:O	2.18	0.43
1:A:604:TRP:HA	1:A:792:PRO:HA	2.00	0.43
1:A:292:LYS:O	1:A:295:GLU:HB3	2.18	0.43
1:A:493:VAL:HA	1:A:497:GLU:HB2	2.00	0.43
1:A:619:LEU:HD13	1:A:628:LEU:HD21	2.00	0.42
1:A:719:TYR:HB3	1:A:729:TYR:CD1	2.54	0.42
1:A:351:LEU:HG	1:A:373:PRO:HG2	2.02	0.42
1:A:431:ARG:HH11	1:A:431:ARG:HD2	1.70	0.41
1:A:495:PHE:CD2	1:A:495:PHE:N	2.88	0.41
1:A:428:TRP:CE3	1:A:432:GLU:HG3	2.55	0.41
1:A:616:LEU:HD13	1:A:638:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:HD2	1:A:332:VAL:CG2	2.51	0.41
1:A:498:LEU:HD13	1:A:526:HIS:NE2	2.36	0.41
1:A:611:TYR:HB3	1:A:614:ILE:HB	2.02	0.41
1:A:732:ASP:C	1:A:734:GLU:H	2.28	0.41
1:A:451:LEU:HD12	1:A:553:ILE:HD11	2.03	0.40
1:A:661:ALA:HA	1:A:682:LEU:HD21	2.03	0.40
1:A:795:ARG:O	1:A:799:VAL:HG23	2.20	0.40
1:A:720:VAL:O	1:A:727:ARG:HA	2.21	0.40
1:A:721:GLU:HA	1:A:726:ARG: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	530/543 (98%)	474 (89%)	44 (8%)	12 (2%)	5 8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO
1	A	656	PRO
1	A	733	LEU
1	A	519	LEU
1	A	650	PRO
1	A	683	ALA
1	A	670	LEU
1	A	672	GLY
1	A	734	GLU
1	A	336	PRO
1	A	524	GLU
1	A	529	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
1	A	433/444 (98%)	366 (84%)	67 (16%)	2 5

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	A	332	VAL
1	A	340	LYS
1	A	345	LEU
1	A	346	LYS
1	A	352	LEU
1	A	354	LYS
1	A	359	LEU
1	A	376	LEU
1	A	388	GLU
1	A	408	LEU
1	A	411	ARG
1	A	412	LEU
1	A	420	LEU
1	A	424	GLU
1	A	425	ARG
1	A	427	LEU
1	A	435	ARG
1	A	449	VAL
1	A	457	ARG
1	A	459	LEU
1	A	476	ARG
1	A	480	HIS
1	A	486	SER
1	A	490	LEU
1	A	495	PHE
1	A	497	GLU
1	A	501	PRO
1	A	503	ILE
1	A	518	VAL

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Mol	Chain	Res	Type
1	A	519	LEU
1	A	520	GLU
1	A	522	LEU
1	A	533	LEU
1	A	540	LYS
1	A	562	THR
1	A	573	ARG
1	A	578	ASP
1	A	579	PRO
1	A	582	GLN
1	A	590	LEU
1	A	593	ARG
1	A	619	LEU
1	A	622	LEU
1	A	641	GLU
1	A	645	TRP
1	A	649	VAL
1	A	651	ARG
1	A	656	PRO
1	A	660	ARG
1	A	678	LEU
1	A	681	GLU
1	A	684	ILE
1	A	690	GLN
1	A	694	GLU
1	A	713	GLU
1	A	716	ARG
1	A	738	LYS
1	A	740	VAL
1	A	742	GLU
1	A	749	PHE
1	A	750	ASN
1	A	751	MET
1	A	790	GLU
1	A	794	GLU
1	A	813	LEU
1	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
1	A	333	HIS

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Mol	Chain	Res	Type
1	A	480	HIS
1	A	483	ASN
1	A	534	GLN
1	A	566	GLN
1	A	582	GLN
1	A	621	HIS
1	A	666	ASN
1	A	690	GLN
1	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
2	DCP	A	901	-	28,29,29	1.12	2 (7%)	41,45,45	1.49	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCP	A	901	-	-	12/22/34/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	DCP	PB-O3A	3.24	1.63	1.59
2	A	901	DCP	PB-O3B	2.76	1.62	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	DCP	C4'-O4'-C1'	-3.70	100.72	109.51
2	A	901	DCP	C1'-N1-C2	3.55	123.92	117.83
2	A	901	DCP	C1'-N1-C6	-2.97	115.69	121.53
2	A	901	DCP	O2-C2-N3	-2.83	117.87	122.33
2	A	901	DCP	O4'-C1'-N1	2.79	112.82	107.86
2	A	901	DCP	C2'-C1'-N1	2.58	120.26	113.81
2	A	901	DCP	O2-C2-N1	2.42	123.64	118.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

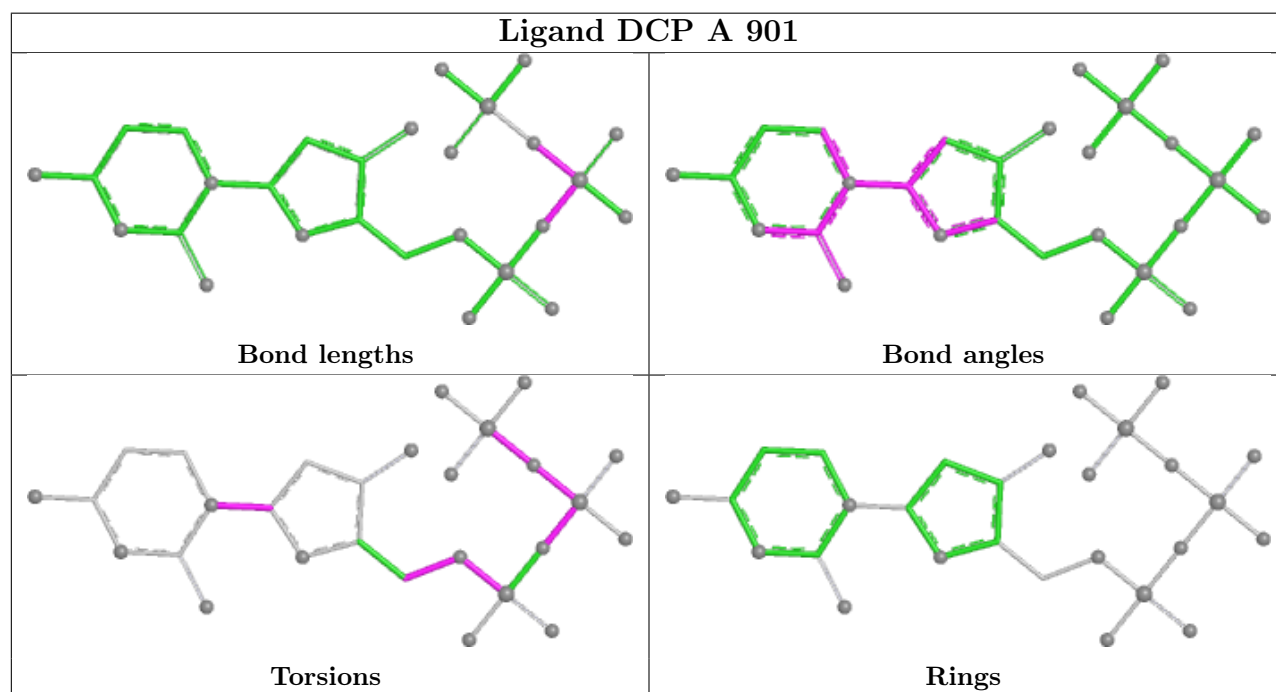
Mol	Chain	Res	Type	Atoms
2	A	901	DCP	C4'-C5'-O5'-PA
2	A	901	DCP	C5'-O5'-PA-O1A
2	A	901	DCP	PB-O3B-PG-O2G
2	A	901	DCP	C2'-C1'-N1-C2
2	A	901	DCP	C2'-C1'-N1-C6
2	A	901	DCP	C5'-O5'-PA-O3A
2	A	901	DCP	O4'-C1'-N1-C6
2	A	901	DCP	O4'-C1'-N1-C2
2	A	901	DCP	PB-O3B-PG-O1G
2	A	901	DCP	PB-O3B-PG-O3G
2	A	901	DCP	PG-O3B-PB-O1B
2	A	901	DCP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	DCP	1	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.