



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:32 am BST

PDB ID : 1KFD
Title : CRYSTAL STRUCTURES OF THE KLENOW FRAGMENT OF DNA POLYMERASE I COMPLEXED WITH DEOXYNUCLEOSIDE TRIPHOSPHATE AND PYROPHOSPHATE
Authors : Beese, L.S.; Friedman, J.M.; Steitz, T.A.
Deposited on : 1993-09-23
Resolution : 3.90 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 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)
Xtriage (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) : 2.11

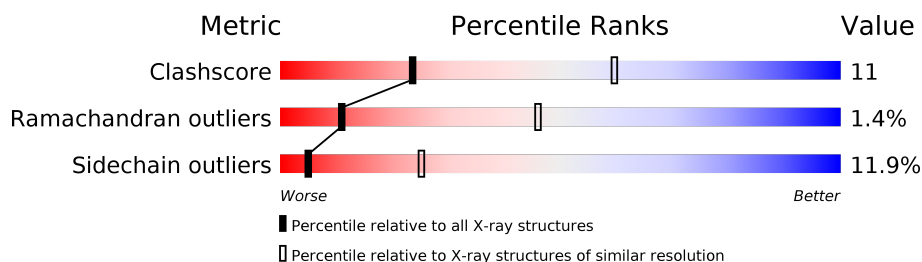
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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 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	605	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CTP	A	1	-	-	X	-

2 Entry composition [i](#)

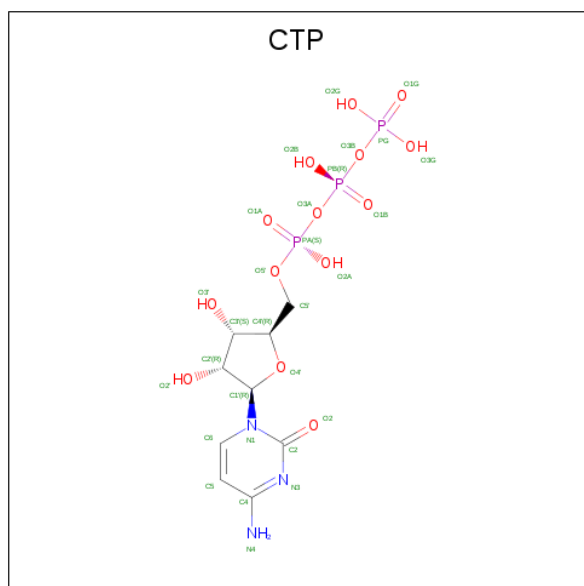
There are 2 unique types of molecules in this entry. The entry contains 4479 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA POLYMERASE I KLENOW FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4451	2817	782	837	15			

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



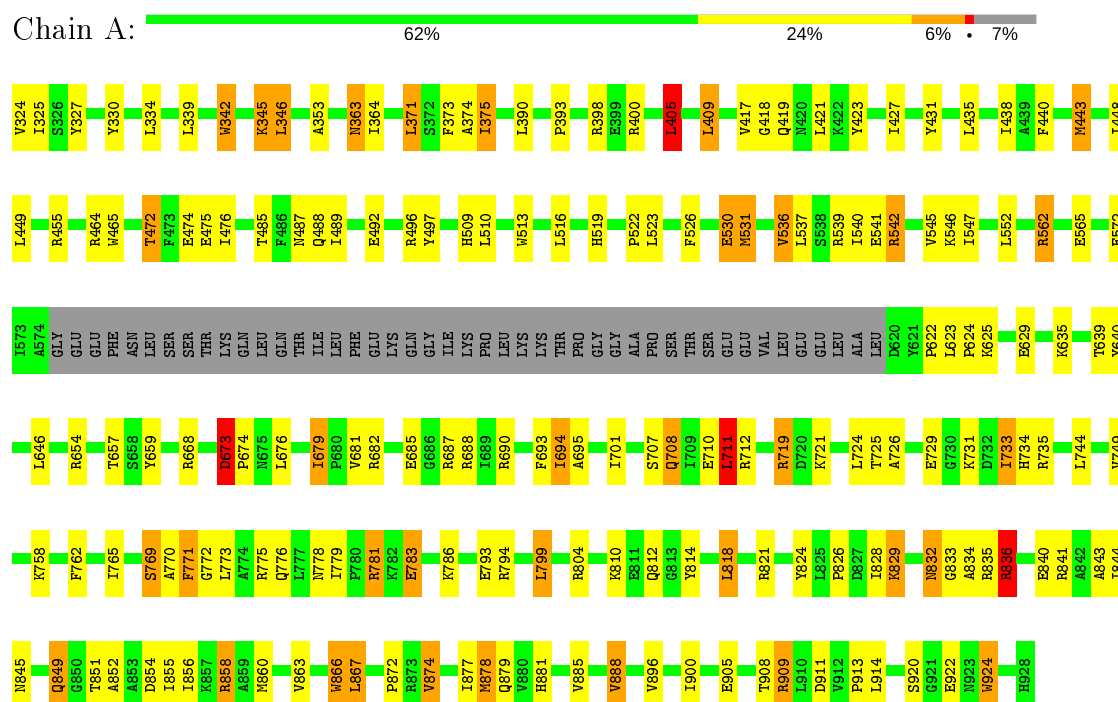
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

3 Residue-property plots [i](#)

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	104.30 Å 104.30 Å 86.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4479	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: CTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.80	0/4534	1.42	51/6137 (0.8%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	A	654	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	531	MET	CG-SD-CE	-9.42	85.12	100.20
1	A	465	TRP	CD1-CG-CD2	8.91	113.42	106.30
1	A	866	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	A	342	TRP	CD1-CG-CD2	7.93	112.65	106.30
1	A	513	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	A	513	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	562	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	924	TRP	CD1-CG-CD2	7.39	112.22	106.30
1	A	668	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	443	MET	CG-SD-CE	-7.30	88.52	100.20
1	A	465	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	539	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	513	TRP	CB-CG-CD1	-7.11	117.76	127.00
1	A	687	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	866	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	497	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	A	924	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	836	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	342	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	539	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	513	TRP	CG-CD2-CE3	6.42	139.68	133.90
1	A	719	ARG	NE-CZ-NH1	6.23	123.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	371	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	345	LYS	CA-CB-CG	6.12	126.86	113.40
1	A	542	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	878	MET	CA-CB-CG	6.02	123.54	113.30
1	A	863	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	A	799	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	542	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	465	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	A	431	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	400	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	821	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	924	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A	673	ASP	N-CA-C	-5.57	95.97	111.00
1	A	804	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	866	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	A	562	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	342	TRP	CG-CD1-NE1	-5.42	104.69	110.10
1	A	673	ASP	CA-CB-CG	-5.39	101.55	113.40
1	A	824	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	496	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	405	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	911	ASP	CA-CB-CG	5.21	124.86	113.40
1	A	794	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	464	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	711	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	474	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

There are no planarity outliers.

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	4451	0	4473	96	2
2	A	28	0	10	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4479	0	4483	100	2

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 (100) 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:A:1:CTP:C3'	2:A:1:CTP:O3'	1.64	1.41
1:A:762:PHE:CZ	2:A:1:CTP:O1A	2.27	0.87
1:A:762:PHE:HZ	2:A:1:CTP:O1A	1.58	0.85
1:A:855:ILE:HG23	1:A:908:THR:HG21	1.61	0.83
1:A:681:VAL:HB	2:A:1:CTP:HN42	1.44	0.81
1:A:421:LEU:HD23	1:A:438:ILE:HG23	1.69	0.73
1:A:858:ARG:HH21	1:A:909:ARG:HD2	1.54	0.72
1:A:418:GLY:HA3	1:A:421:LEU:HD13	1.71	0.72
1:A:485:THR:HG23	1:A:487:ASN:OD1	1.90	0.71
1:A:881:HIS:CD2	2:A:1:CTP:HN41	2.09	0.70
1:A:832:ASN:HA	1:A:836:ARG:HD3	1.74	0.70
1:A:874:VAL:HB	1:A:888:VAL:HB	1.75	0.68
1:A:325:ILE:HD11	1:A:330:TYR:HE2	1.58	0.68
2:A:1:CTP:O3'	2:A:1:CTP:C2'	2.44	0.66
1:A:623:LEU:HB3	1:A:624:PRO:HD3	1.78	0.65
2:A:1:CTP:C3'	2:A:1:CTP:HO3'	2.08	0.65
1:A:908:THR:HG22	1:A:909:ARG:H	1.61	0.64
1:A:485:THR:HG22	1:A:488:GLN:HE21	1.63	0.64
1:A:708:GLN:HG3	1:A:733:ILE:HD11	1.79	0.63
1:A:881:HIS:NE2	2:A:1:CTP:N4	2.38	0.62
1:A:836:ARG:HB2	1:A:836:ARG:HH11	1.64	0.62
1:A:417:VAL:HG13	1:A:440:PHE:HB2	1.82	0.61
1:A:690:ARG:HG2	1:A:924:TRP:CE3	2.36	0.61
1:A:881:HIS:CE1	2:A:1:CTP:N3	2.69	0.59
1:A:860:MET:HE2	1:A:879:GLN:HG3	1.84	0.59
1:A:325:ILE:HD11	1:A:330:TYR:CE2	2.37	0.59
1:A:810:LYS:HG3	1:A:828:ILE:HG13	1.83	0.59
1:A:546:LYS:HG3	1:A:694:ILE:HG22	1.85	0.59
1:A:681:VAL:CB	2:A:1:CTP:HN42	2.16	0.59
1:A:881:HIS:CD2	2:A:1:CTP:N4	2.71	0.58
1:A:485:THR:HG22	1:A:488:GLN:HG3	1.85	0.57
1:A:725:THR:O	1:A:729:GLU:HG2	2.04	0.57
1:A:363:ASN:HD22	1:A:542:ARG:HH11	1.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:LEU:HB2	1:A:909:ARG:HH21	1.72	0.54
1:A:547:ILE:HD11	1:A:693:PHE:CE2	2.41	0.54
1:A:673:ASP:HB3	1:A:674:PRO:HD3	1.88	0.53
1:A:852:ALA:O	1:A:856:ILE:HG12	2.08	0.53
1:A:472:THR:HG22	1:A:475:GLU:HG3	1.90	0.53
1:A:762:PHE:CE1	2:A:1:CTP:H4'	2.45	0.52
1:A:781:ARG:NE	1:A:781:ARG:HA	2.25	0.51
1:A:545:VAL:HG23	1:A:877:ILE:HD12	1.93	0.50
1:A:878:MET:HG2	1:A:885:VAL:HB	1.94	0.50
1:A:772:GLY:HA2	1:A:775:ARG:HG2	1.93	0.50
1:A:829:LYS:H	1:A:829:LYS:HD3	1.77	0.49
1:A:363:ASN:ND2	1:A:542:ARG:HH11	2.09	0.49
1:A:405:LEU:HB3	1:A:409:LEU:HD22	1.94	0.49
1:A:896:VAL:O	1:A:900:ILE:HG12	2.13	0.49
1:A:419:GLN:NE2	1:A:443:MET:HB2	2.28	0.49
1:A:872:PRO:HG2	1:A:874:VAL:HG13	1.95	0.48
1:A:681:VAL:HG11	2:A:1:CTP:C5	2.50	0.47
1:A:866:TRP:CE3	1:A:867:LEU:HD13	2.50	0.47
1:A:818:LEU:HD22	1:A:851:THR:HG21	1.97	0.46
1:A:845:ASN:HD21	1:A:849:GLN:NE2	2.13	0.46
1:A:353:ALA:HB3	1:A:374:ALA:HB3	1.98	0.46
1:A:729:GLU:HG3	1:A:731:LYS:HG3	1.98	0.46
1:A:519:HIS:HB2	1:A:522:PRO:HD2	1.99	0.45
1:A:735:ARG:HD2	1:A:749:VAL:CG1	2.47	0.45
1:A:476:ILE:HD12	1:A:489:ILE:HD13	1.99	0.45
1:A:324:VAL:HG13	1:A:325:ILE:H	1.80	0.45
1:A:417:VAL:HG11	1:A:509:HIS:HB2	1.99	0.45
1:A:854:ASP:HB3	1:A:909:ARG:HH12	1.82	0.44
1:A:712:ARG:HD3	1:A:913:PRO:O	2.17	0.44
1:A:327:TYR:CD1	1:A:492:GLU:HB3	2.53	0.44
1:A:353:ALA:O	1:A:373:PHE:HA	2.17	0.44
1:A:708:GLN:HG3	1:A:733:ILE:CD1	2.47	0.44
1:A:346:LEU:HD12	1:A:375:ILE:HG23	2.00	0.43
1:A:695:ALA:HB2	1:A:701:ILE:HG12	2.00	0.43
1:A:840:GLU:O	1:A:843:ALA:HB3	2.19	0.43
1:A:423:TYR:O	1:A:427:ILE:HG12	2.18	0.43
1:A:635:LYS:O	1:A:639:THR:HG22	2.18	0.43
1:A:726:ALA:HA	1:A:731:LYS:HE2	2.01	0.43
1:A:536:VAL:O	1:A:540:ILE:HG12	2.19	0.42
1:A:537:LEU:O	1:A:541:GLU:HG3	2.19	0.42
1:A:681:VAL:HB	2:A:1:CTP:N4	2.25	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:HH11	1:A:841:ARG:NH2	2.18	0.42
1:A:812:GLN:HB3	1:A:814:TYR:CE1	2.54	0.42
1:A:701:ILE:O	1:A:920:SER:HA	2.19	0.42
1:A:639:THR:HG23	1:A:640:TYR:CD2	2.55	0.41
1:A:908:THR:HG22	1:A:909:ARG:N	2.32	0.41
1:A:762:PHE:HZ	2:A:1:CTP:PA	2.40	0.41
1:A:622:PRO:O	1:A:625:LYS:HB3	2.20	0.41
1:A:769:SER:O	1:A:771:PHE:N	2.53	0.41
1:A:681:VAL:HG22	1:A:682:ARG:HG2	2.03	0.41
1:A:679:ILE:HD11	1:A:690:ARG:HE	1.85	0.41
2:A:1:CTP:C3'	2:A:1:CTP:C6	3.04	0.41
1:A:734:HIS:CD2	1:A:758:LYS:HA	2.55	0.41
1:A:448:ILE:HA	1:A:448:ILE:HD13	1.89	0.41
1:A:833:GLY:O	1:A:835:ARG:N	2.54	0.41
1:A:836:ARG:NH1	1:A:836:ARG:HB2	2.32	0.41
1:A:526:PHE:HA	1:A:530:GLU:HB2	2.03	0.41
1:A:657:THR:HG23	1:A:659:TYR:CE1	2.55	0.41
1:A:735:ARG:HD2	1:A:749:VAL:HG13	2.03	0.41
1:A:346:LEU:HD12	1:A:375:ILE:CG2	2.51	0.40
1:A:854:ASP:CB	1:A:909:ARG:HH12	2.34	0.40
1:A:342:TRP:HA	1:A:345:LYS:HG2	2.04	0.40
1:A:711:LEU:CD1	1:A:765:ILE:HD11	2.51	0.40
1:A:694:ILE:HD13	1:A:922:GLU:O	2.21	0.40
1:A:485:THR:HG22	1:A:488:GLN:NE2	2.33	0.40
1:A:783:GLU:O	1:A:786:LYS:HB3	2.22	0.40
1:A:881:HIS:CG	2:A:1:CTP:N3	2.89	0.40

All (2) 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)
1:A:572:GLU:OE1	1:A:905:GLU:OE1[2_655]	2.03	0.17
1:A:688:ARG:NH1	1:A:719:ARG:NE[2_655]	2.17	0.03

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	
1	A	556/605 (92%)	516 (93%)	32 (6%)	8 (1%)	11	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	ASP
1	A	707	SER
1	A	770	ALA
1	A	779	ILE
1	A	834	ALA
1	A	778	ASN
1	A	832	ASN
1	A	769	SER

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	471/510 (92%)	415 (88%)	56 (12%)	5	25

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	LEU
1	A	339	LEU
1	A	346	LEU
1	A	363	ASN
1	A	364	ILE
1	A	371	LEU
1	A	375	ILE
1	A	390	LEU
1	A	393	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	405	LEU
1	A	409	LEU
1	A	435	LEU
1	A	449	LEU
1	A	455	ARG
1	A	472	THR
1	A	510	LEU
1	A	516	LEU
1	A	523	LEU
1	A	530	GLU
1	A	531	MET
1	A	536	VAL
1	A	552	LEU
1	A	562	ARG
1	A	565	GLU
1	A	629	GLU
1	A	646	LEU
1	A	676	LEU
1	A	679	ILE
1	A	685	GLU
1	A	694	ILE
1	A	708	GLN
1	A	710	GLU
1	A	711	LEU
1	A	721	LYS
1	A	724	LEU
1	A	733	ILE
1	A	744	LEU
1	A	771	PHE
1	A	773	LEU
1	A	776	GLN
1	A	781	ARG
1	A	783	GLU
1	A	793	GLU
1	A	799	LEU
1	A	818	LEU
1	A	826	PRO
1	A	829	LYS
1	A	836	ARG
1	A	844	ILE
1	A	849	GLN
1	A	858	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	867	LEU
1	A	874	VAL
1	A	888	VAL
1	A	909	ARG
1	A	914	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	A	456	HIS
1	A	488	GLN
1	A	543	ASN
1	A	554	ASN
1	A	734	HIS
1	A	849	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	CTP	A	1	-	23,29,30	2.83	4 (17%)	30,45,47	2.09	7 (23%)

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	CTP	A	1	-	-	9/19/34/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CTP	O3'-C3'	10.17	1.64	1.43
2	A	1	CTP	C6-N1	6.83	1.44	1.35
2	A	1	CTP	C5-C4	2.53	1.47	1.41
2	A	1	CTP	C2-N3	-2.38	1.33	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CTP	C2-N3-C4	5.76	122.17	116.34
2	A	1	CTP	C5-C4-N3	-5.45	115.44	121.72
2	A	1	CTP	C5-C4-N4	4.05	128.17	121.14
2	A	1	CTP	O3'-C3'-C4'	3.98	125.32	110.10
2	A	1	CTP	C2'-C1'-N1	-3.10	107.13	114.27
2	A	1	CTP	C5-C6-N1	-2.87	114.27	120.68
2	A	1	CTP	O3'-C3'-C2'	-2.81	100.87	110.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CTP	C5'-O5'-PA-O1A
2	A	1	CTP	C5'-O5'-PA-O3A
2	A	1	CTP	PA-O3A-PB-O1B
2	A	1	CTP	C5'-O5'-PA-O2A
2	A	1	CTP	PB-O3B-PG-O1G
2	A	1	CTP	C4'-C5'-O5'-PA
2	A	1	CTP	PB-O3B-PG-O2G
2	A	1	CTP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

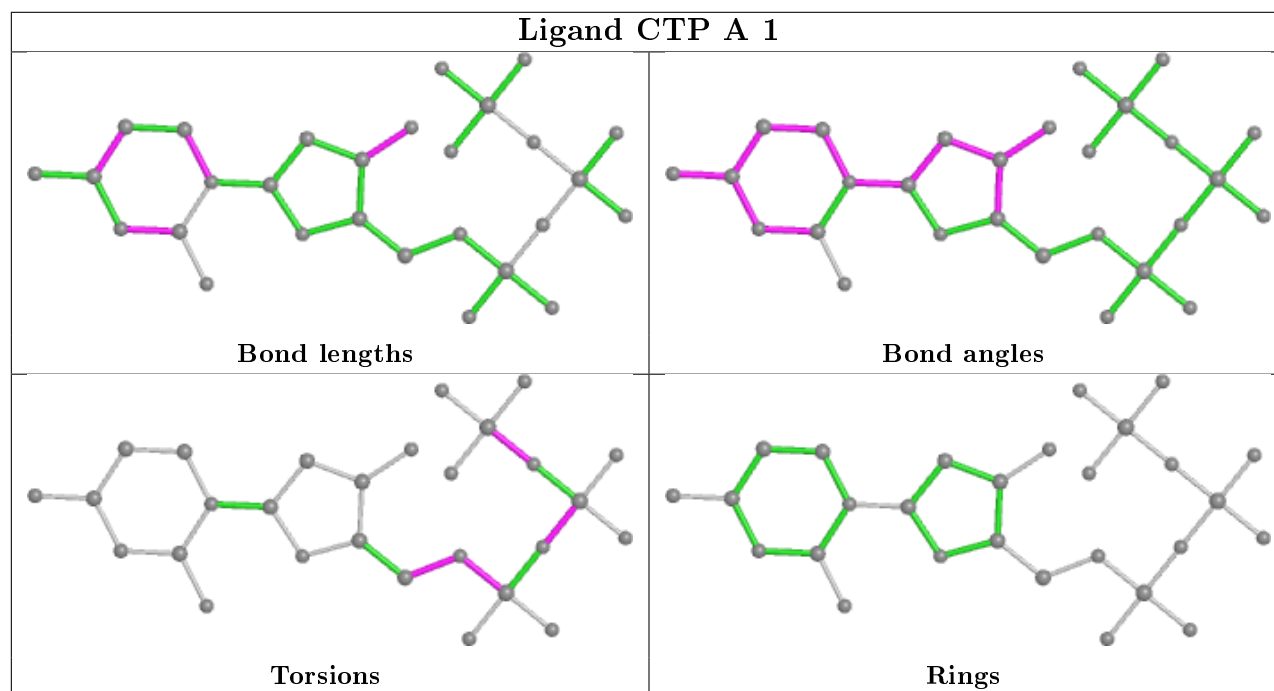
Mol	Chain	Res	Type	Atoms
2	A	1	CTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CTP	17	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.