wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 12:11 PM EDT

PDB ID	:	1T3N
Title	:	Structure of the catalytic core of DNA polymerase Iota in complex with DNA and dTTP
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on	:	2004-04-27
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

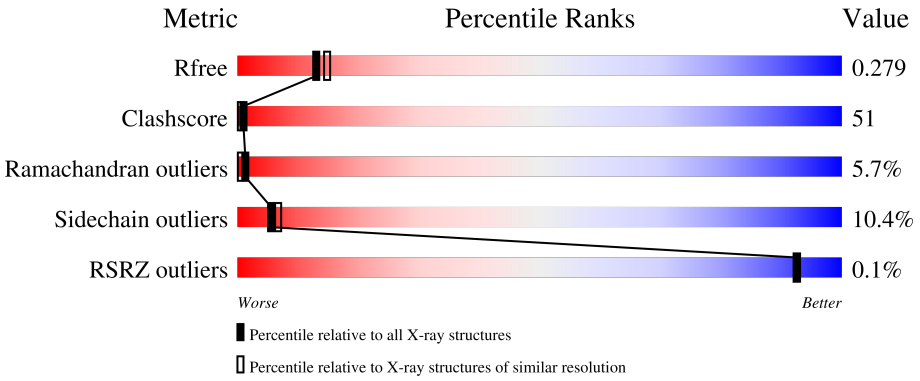
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-T	14	43% 57%
1	2-T	14	43% 57%
2	1-P	13	31% 69%
2	2-P	13	31% 69%
3	1-A	388	49% 41% 8%

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Mol	Chain	Length	Quality of chain
3	1-B	388	46% 41% 11%
3	2-A	388	48% 43% 8%
3	2-B	388	45% 41% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13538 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 Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-T	14	Total	C	N	O	P	0	0	0
			277	133	47	84	13			
1	2-T	14	Total	C	N	O	P	0	0	0
			277	133	47	84	13			

- Molecule 2 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-P	13	Total	C	N	O	P	0	0	0
			270	127	59	72	12			
2	2-P	13	Total	C	N	O	P	0	0	0
			270	127	59	72	12			

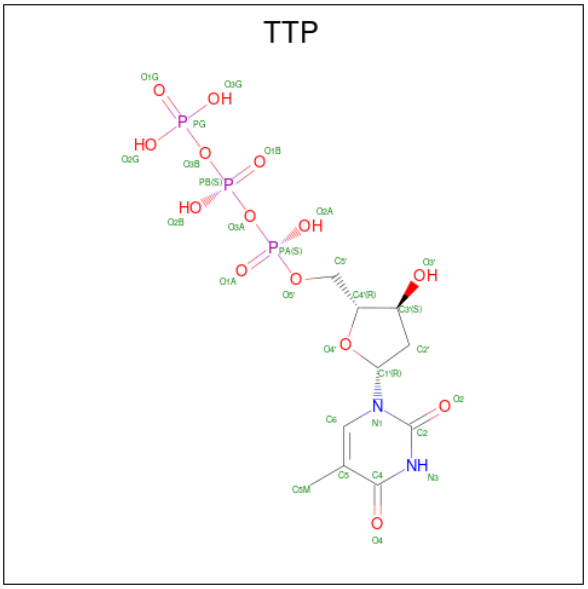
- Molecule 3 is a protein called polymerase (DNA directed) iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-A	388	Total	C	N	O	S	0	0	0
			2868	1801	502	547	18			
3	2-A	388	Total	C	N	O	S	0	0	0
			2868	1801	502	547	18			
3	1-B	388	Total	C	N	O	S	0	0	0
			2886	1812	509	547	18			
3	2-B	388	Total	C	N	O	S	0	0	0
			2886	1812	509	547	18			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	1	Total	Mg	0	0
			1	1		
4	2-B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	1-B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
5	2-B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-T	11	Total	O	0	0
			11	11		
6	2-T	209	Total	O	0	0
			209	209		
6	1-P	12	Total	O	0	0
			12	12		
6	2-P	208	Total	O	0	0
			208	208		
6	1-A	207	Total	O	0	0
			207	207		
6	2-A	11	Total	O	0	0
			11	11		
6	1-B	208	Total	O	0	0
			208	208		
6	2-B	10	Total	O	0	0
			10	10		

3 Residue-property plots (i)

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

• Molecule 1: Template DNA strand

Chain 1-T:

• Molecule 1: Template DNA strand

Chain 2-T:

• Molecule 2: Primer DNA strand

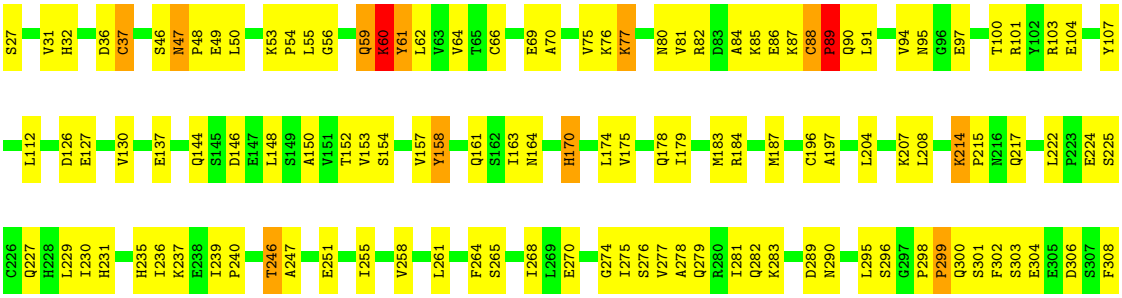
Chain 1-P:

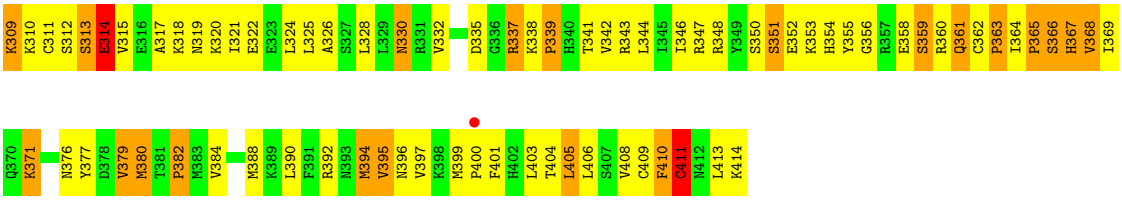
• Molecule 2: Primer DNA strand

Chain 2-P:

• Molecule 3: polymerase (DNA directed) iota

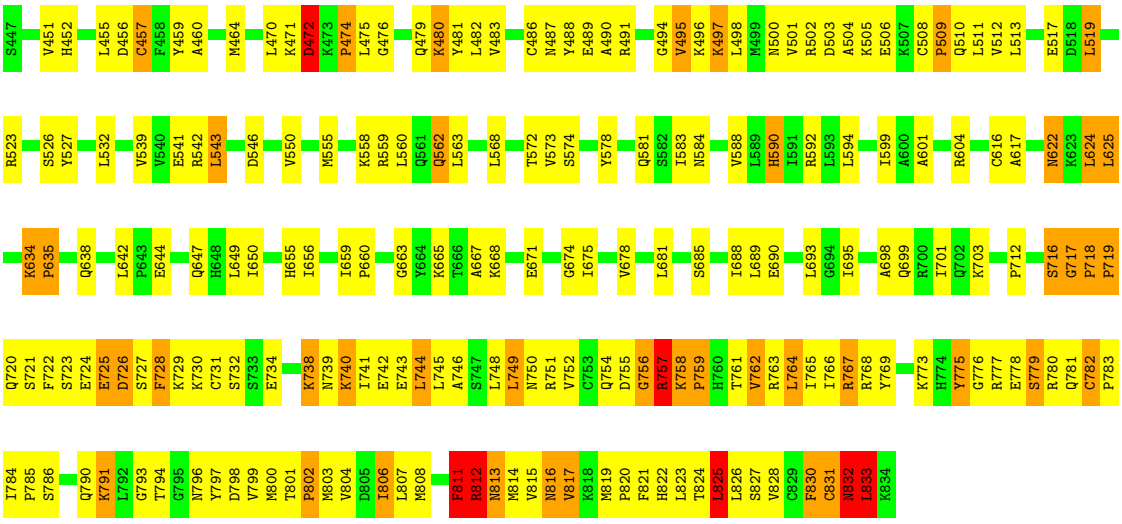
Chain 1-A:





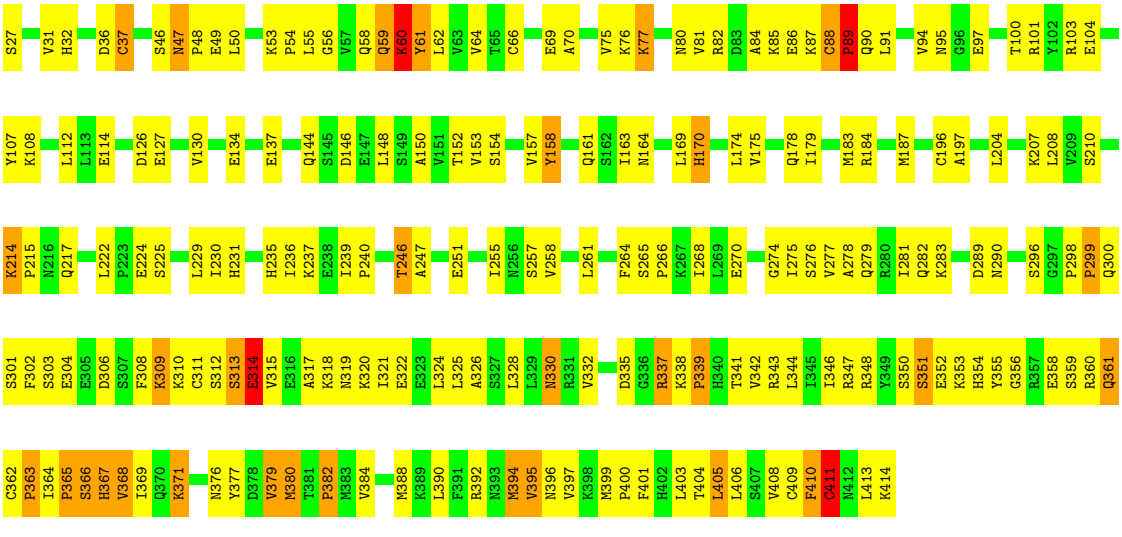
• Molecule 3: polymerase (DNA directed) iota

Chain 1-B:



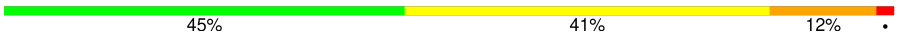
• Molecule 3: polymerase (DNA directed) iota

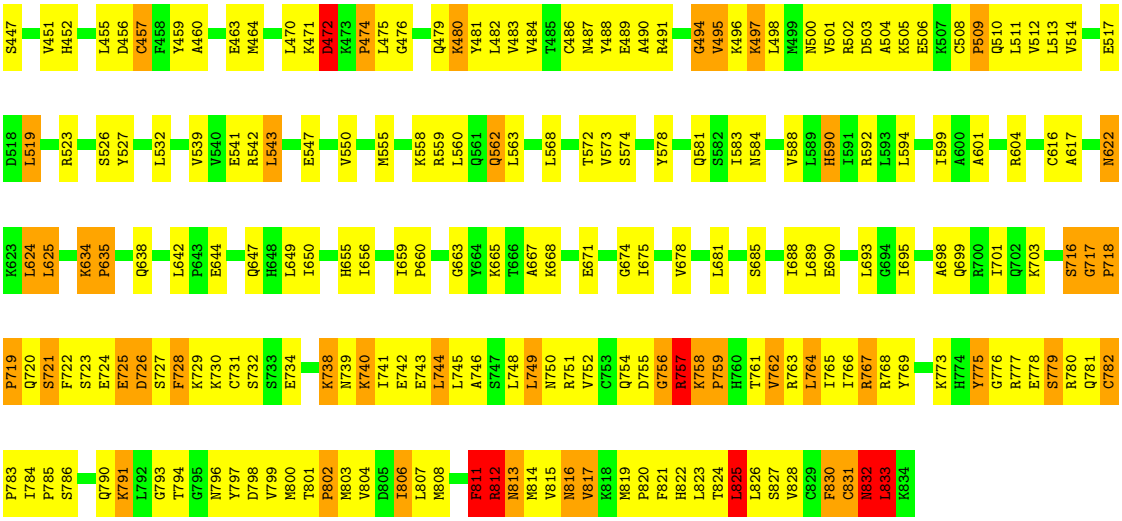
Chain 2-A:



• Molecule 3: polymerase (DNA directed) iota

Chain 2-B:




S447 V451 H452 L455 D456 C457 F458 Y459 A460 E463 M464 L470 K471 D472 K473 P474 L475 G476 Q479 K480 Y481 L482 V483 V484 T485 C486 M487 Y488 E489 A490 R491 G494 V495 K496 K497 L498 M499 N500 V501 R502 D503 A504 K505 E506 K507 C508 P509 Q510 L511 V512 L513 V514 E517
D518 L519 R523 S526 Y527 L532 V539 V540 E541 R542 L543 E547 V550 M555 K558 R559 L560 Q561 Q562 L563 L568 T572 V573 S574 Y578 Q581 S582 I583 N584 V588 L589 H590 I591 R592 L593 L594 I599 A600 A601 R604 C616 A617 N622
K623 L624 L625 K634 P635 Q638 L642 P643 E644 Q647 H648 L649 I650 H655 I656 I659 P660 G663 Y664 K665 T666 A667 K668 E671 G674 I675 V678 L681 S685 I688 L689 E690 L693 G694 I695 A698 Q699 R700 I701 Q702 K703 S716 G717 P718
P719 Q720 S721 F722 S723 E724 E725 D726 S727 F728 K729 K730 C731 S732 S733 E734 K738 N739 K740 I741 E742 E743 L744 L745 A746 S747 L748 L749 N750 R751 V752 C753 Q754 D755 G756 R757 K758 P759 H760 T761 V762 R763 L764 I765 I766 R767 R768 Y769 K773 H774 Y775 G776 R777 E778 S779 R780 Q781 C782
P783 I784 P785 S786 Q790 K791 L792 G793 T794 G795 N796 Y797 D798 V799 M800 T801 P802 M803 V804 D805 I806 L807 M808 F811 R812 M813 M814 V815 M816 V817 K818 M819 P820 F821 H822 L823 T824 L825 L826 S827 V828 C829 F830 C831 M832 L833 K834

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	98.83Å 98.83Å 202.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.30) 96.9 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.286 0.258 , 0.279	Depositor DCC
R_{free} test set	4844 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1-T	0.77	0/308	1.22	3/472 (0.6%)
1	2-T	0.76	0/308	1.22	3/472 (0.6%)
2	1-P	1.20	2/285 (0.7%)	1.55	7/440 (1.6%)
2	2-P	1.20	2/285 (0.7%)	1.54	7/440 (1.6%)
3	1-A	0.51	1/2908 (0.0%)	0.85	8/3946 (0.2%)
3	1-B	0.63	2/2928 (0.1%)	0.99	20/3975 (0.5%)
3	2-A	0.50	1/2908 (0.0%)	0.85	8/3946 (0.2%)
3	2-B	0.63	3/2928 (0.1%)	0.99	21/3975 (0.5%)
All	All	0.62	11/12858 (0.1%)	0.98	77/17666 (0.4%)

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	1-T	1	6
1	2-T	1	6
2	1-P	0	3
2	2-P	0	3
3	1-B	0	1
3	2-B	0	1
All	All	2	20

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-P	12	DC	C3'-O3'	-12.37	1.27	1.44
2	2-P	12	DC	C3'-O3'	-12.34	1.27	1.44
3	1-B	832	ASN	N-CA	7.35	1.61	1.46
3	2-B	832	ASN	N-CA	7.33	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-A	60	LYS	CB-CG	-6.49	1.35	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-A	60	LYS	CB-CG-CD	-12.63	78.75	111.60
3	2-A	60	LYS	CB-CG-CD	-12.63	78.77	111.60
3	2-B	757	ARG	CB-CG-CD	10.15	138.00	111.60
3	1-B	757	ARG	CB-CG-CD	10.15	138.00	111.60
3	1-B	831	CYS	N-CA-C	9.52	136.71	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1-T	13	DT	C3'
1	2-T	13	DT	C3'

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-T	16	DC	Sidechain
1	1-T	5	DA	Sidechain
1	1-T	6	DG	Sidechain
1	1-T	7	DG	Sidechain
1	1-T	8	DG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-T	277	0	159	59	0
1	2-T	277	0	159	55	0
2	1-P	270	0	145	46	0
2	2-P	270	0	145	39	0
3	1-A	2868	0	2764	247	0
3	1-B	2886	0	2789	306	0
3	2-A	2868	0	2764	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-B	2886	0	2789	306	0
4	1-B	1	0	0	0	0
4	2-B	1	0	0	0	0
5	1-B	29	0	10	2	0
5	2-B	29	0	10	4	0
6	1-A	207	0	0	18	0
6	1-B	208	0	0	20	0
6	1-P	12	0	0	0	0
6	1-T	11	0	0	1	0
6	2-A	11	0	0	0	0
6	2-B	10	0	0	1	0
6	2-P	208	0	0	18	0
6	2-T	209	0	0	29	0
All	All	13538	0	11734	1236	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 51.

The worst 5 of 1236 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:729:LYS:O	3:B:730:LYS:HG2	1.26	1.34
3:B:729:LYS:O	3:B:730:LYS:HG2	1.26	1.33
3:B:763:ARG:O	3:B:828:VAL:HG13	1.33	1.28
3:B:763:ARG:O	3:B:828:VAL:HG13	1.33	1.27
3:A:60:LYS:O	3:A:61:TYR:HD1	1.22	1.21

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1-A	386/388 (100%)	338 (88%)	27 (7%)	21 (5%)	1 1
3	1-B	386/388 (100%)	319 (83%)	44 (11%)	23 (6%)	1 0
3	2-A	386/388 (100%)	337 (87%)	28 (7%)	21 (5%)	1 1
3	2-B	386/388 (100%)	319 (83%)	44 (11%)	23 (6%)	1 0
All	All	1544/1552 (100%)	1313 (85%)	143 (9%)	88 (6%)	1 0

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1-A	60	LYS
3	1-A	61	TYR
3	1-A	76	LYS
3	1-A	80	ASN
3	1-A	89	PRO

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	1-A	299/353 (85%)	274 (92%)	25 (8%)	9 11
3	1-B	304/353 (86%)	266 (88%)	38 (12%)	3 4
3	2-A	299/353 (85%)	274 (92%)	25 (8%)	9 11
3	2-B	304/353 (86%)	266 (88%)	38 (12%)	3 4
All	All	1206/1412 (85%)	1080 (90%)	126 (10%)	5 7

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1-B	812	ARG
3	2-B	762	VAL
3	2-A	298	PRO
3	2-B	759	PRO
3	2-B	806	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	2-A	367	HIS
3	2-B	682	GLN
3	2-B	478	GLN
3	2-B	590	HIS
3	2-B	760	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)

2 non-standard protein/DNA/RNA residues are 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	DOC	2-P	13	2,1	16,19,20	0.78	0	20,26,29	0.78	1 (5%)
2	DOC	1-P	13	2,1	16,19,20	0.78	0	20,26,29	0.78	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
2	DOC	2-P	13	2,1	-	0/7/18/19	0/2/2/2
2	DOC	1-P	13	2,1	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-P	13	DOC	O4'-C1'-N1	2.29	111.92	107.86
2	2-P	13	DOC	O4'-C1'-N1	2.28	111.91	107.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2-P	13	DOC	2	0
2	1-P	13	DOC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TTP	1-B	902	4	29,30,30	5.38	12 (41%)	43,47,47	2.52	15 (34%)
5	TTP	2-B	902	4	29,30,30	5.40	13 (44%)	43,47,47	2.50	15 (34%)

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	TTP	1-B	902	4	-	3/22/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TTP	2-B	902	4	-	3/22/34/34	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-B	902	TTP	C5M-C5	-21.55	0.98	1.50
5	1-B	902	TTP	C5M-C5	-21.49	0.98	1.50
5	2-B	902	TTP	PA-O3A	9.73	1.70	1.59
5	1-B	902	TTP	PA-O3A	9.64	1.69	1.59
5	2-B	902	TTP	PB-O3A	8.26	1.68	1.59

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-B	902	TTP	C5-C4-N3	6.15	120.67	115.32
5	2-B	902	TTP	N3-C2-N1	6.01	122.72	114.89
5	1-B	902	TTP	N3-C2-N1	5.98	122.68	114.89
5	1-B	902	TTP	C5-C4-N3	5.74	120.31	115.32
5	1-B	902	TTP	C6-N1-C2	-5.55	115.78	121.30

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-B	902	TTP	PG-O3B-PB-O2B
5	2-B	902	TTP	PG-O3B-PB-O2B
5	1-B	902	TTP	PB-O3A-PA-O1A
5	2-B	902	TTP	PB-O3A-PA-O1A
5	1-B	902	TTP	PB-O3A-PA-O2A

There are no ring outliers.

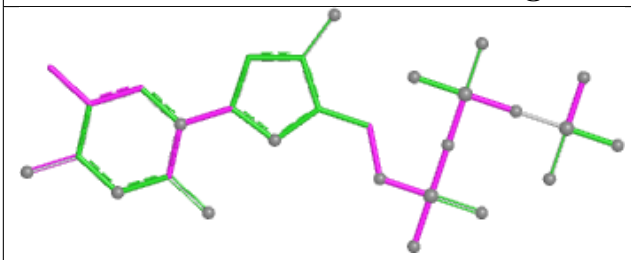
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1-B	902	TTP	2	0
5	2-B	902	TTP	4	0

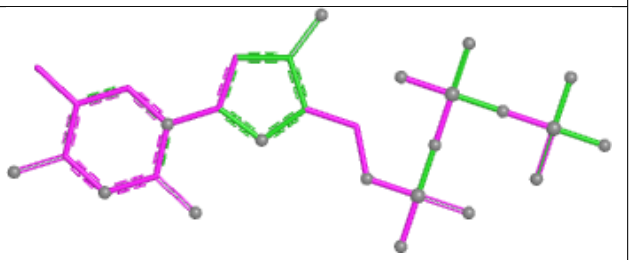
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

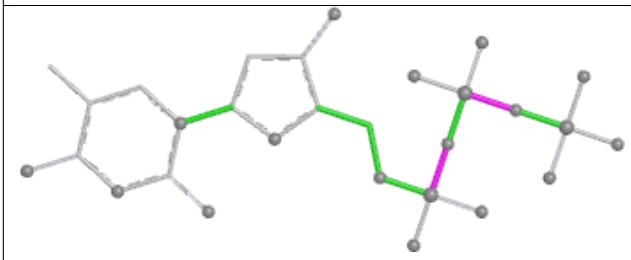
Ligand TTP B 902



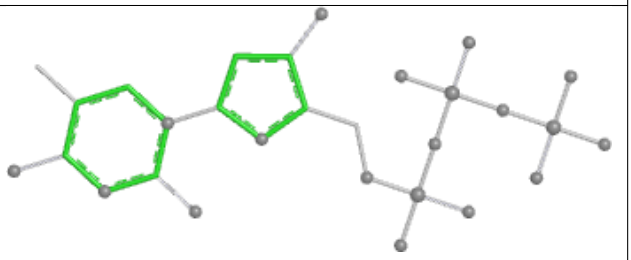
Bond lengths



Bond angles



Torsions



Rings

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1-T	14/14 (100%)	-1.55	0 100 100	21, 25, 30, 35	14 (100%)
1	2-T	0/14	-	-	-	-
2	1-P	12/13 (92%)	-1.47	0 100 100	24, 29, 35, 36	12 (100%)
2	2-P	0/13	-	-	-	-
3	1-A	388/388 (100%)	-0.98	1 (0%) 90 90	9, 25, 50, 50	388 (100%)
3	1-B	388/388 (100%)	-0.99	0 100 100	11, 25, 50, 50	388 (100%)
3	2-A	0/388	-	-	-	-
3	2-B	0/388	-	-	-	-
All	All	802/1606 (49%)	-1.00	1 (0%) 92 92	9, 25, 50, 50	802 (100%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	1-A	400	PRO	4.2

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

MODRES-RSR INFOmissingINFO

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.